



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:16 AM UTC

PDB ID : 1RYP / pdb\_00001ryp  
Title : CRYSTAL STRUCTURE OF THE 20S PROTEASOME FROM YEAST AT 2.4 ANGSTROMS RESOLUTION  
Authors : Groll, M.; Ditzel, L.; Loewe, J.; Stock, D.; Bochtler, M.; Bartunik, H.D.; Huber, R.  
Deposited on : 1997-02-26  
Resolution : 1.90 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)               | : | NOT EXECUTED                                                     |
| EDS                            | : | NOT EXECUTED                                                     |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

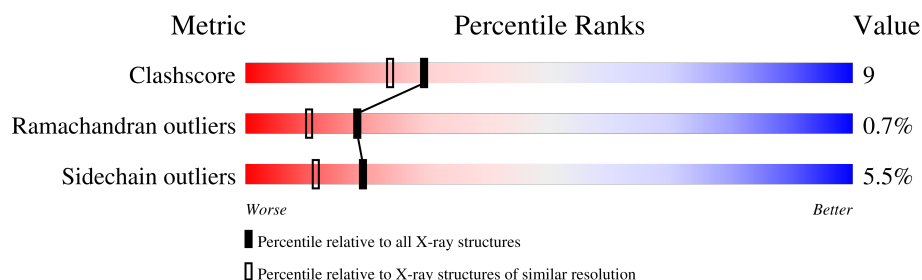
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 8410 (1.90-1.90)                                      |
| Ramachandran outliers | 187476                      | 8333 (1.90-1.90)                                      |
| Sidechain outliers    | 187428                      | 8333 (1.90-1.90)                                      |

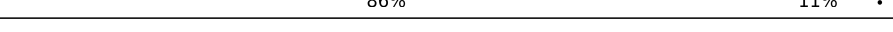
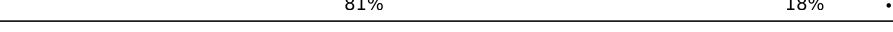
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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  $\leq 5\%$ .

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 243    | 77% 19% .        |
| 1   | O     | 243    | 73% 24% .        |
| 2   | B     | 250    | 78% 21% .        |
| 2   | P     | 250    | 78% 19% .        |
| 3   | C     | 244    | 69% 28% .        |
| 3   | Q     | 244    | 73% 25% .        |
| 4   | D     | 241    | 71% 24% 5%       |
| 4   | R     | 241    | 65% 30% 5%       |

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| Mol | Chain | Length | Quality of chain                                                                                  |
|-----|-------|--------|---------------------------------------------------------------------------------------------------|
| 5   | E     | 242    |  75% 22% .      |
| 5   | S     | 242    |  72% 25% .      |
| 6   | F     | 233    |  68% 28% .      |
| 6   | T     | 233    |  68% 27% 5% .   |
| 7   | G     | 244    |  76% 20% .      |
| 7   | U     | 244    |  71% 23% 5% .   |
| 8   | H     | 205    |  70% 28% .      |
| 8   | V     | 205    |  73% 25% .      |
| 9   | I     | 222    |  79% 19% .      |
| 9   | W     | 222    |  79% 19% .      |
| 10  | J     | 204    |  83% 14% .      |
| 10  | X     | 204    |  79% 19% .      |
| 11  | K     | 198    |  77% 18% 5% . |
| 11  | Y     | 198    |  73% 23% .    |
| 12  | L     | 212    |  84% 13% .    |
| 12  | Z     | 212    |  86% 11% .    |
| 13  | 1     | 222    |  81% 18% .    |
| 13  | M     | 222    |  78% 19% .    |
| 14  | 2     | 233    |  76% 22% .    |
| 14  | N     | 233    |  79% 19% .    |

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 52604 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 20S PROTEASOME.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 243      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1921  | 1221 | 322 | 370 | 8 |         |         |       |
| 1   | O     | 243      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1921  | 1221 | 322 | 370 | 8 |         |         |       |

- Molecule 2 is a protein called 20S PROTEASOME.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | B     | 250      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1915  | 1219 | 315 | 377 | 4 |         |         |       |
| 2   | P     | 250      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1915  | 1219 | 315 | 377 | 4 |         |         |       |

- Molecule 3 is a protein called 20S PROTEASOME.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | C     | 244      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1905  | 1201 | 321 | 380 | 3 |         |         |       |
| 3   | Q     | 244      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1905  | 1201 | 321 | 380 | 3 |         |         |       |

- Molecule 4 is a protein called 20S PROTEASOME.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | D     | 241      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1891  | 1181 | 331 | 375 | 4 |         |         |       |
| 4   | R     | 241      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1891  | 1181 | 331 | 375 | 4 |         |         |       |

- Molecule 5 is a protein called 20S PROTEASOME.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5   | E     | 242      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1862  | 1162 | 314 | 379 | 7 |         |         |       |
| 5   | S     | 242      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1862  | 1162 | 314 | 379 | 7 |         |         |       |

- Molecule 6 is a protein called 20S PROTEASOME.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 6   | F     | 233      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1795  | 1129 | 312 | 350 | 4 |         |         |       |
| 6   | T     | 233      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1795  | 1129 | 312 | 350 | 4 |         |         |       |

- Molecule 7 is a protein called 20S PROTEASOME.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 7   | G     | 244      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1897  | 1205 | 330 | 358 | 4 |         |         |       |
| 7   | U     | 244      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1897  | 1205 | 330 | 358 | 4 |         |         |       |

- Molecule 8 is a protein called 20S PROTEASOME.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | H     | 205      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1574  | 995 | 261 | 311 | 7 |         |         |       |
| 8   | V     | 205      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1574  | 995 | 261 | 311 | 7 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| H     | 1       | ALA      | THR    | conflict | UNP P38624 |
| V     | 1       | ALA      | THR    | conflict | UNP P38624 |

- Molecule 9 is a protein called 20S PROTEASOME.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 9   | I     | 222      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1685  | 1061 | 293 | 324 | 7 |         |         |       |
| 9   | W     | 222      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1685  | 1061 | 293 | 324 | 7 |         |         |       |

- Molecule 10 is a protein called 20S PROTEASOME.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 10  | J     | 204      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1581  | 1010 | 258 | 305 | 8 |         |         |       |
| 10  | X     | 204      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1581  | 1010 | 258 | 305 | 8 |         |         |       |

- Molecule 11 is a protein called 20S PROTEASOME.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 11  | K     | 198      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1585  | 1005 | 269 | 305 | 6 |         |         |       |
| 11  | Y     | 198      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1585  | 1005 | 269 | 305 | 6 |         |         |       |

- Molecule 12 is a protein called 20S PROTEASOME.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 12  | L     | 212      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1646  | 1045 | 282 | 312 | 7 |         |         |       |
| 12  | Z     | 212      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1646  | 1045 | 282 | 312 | 7 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| L     | 33      | ARG      | LYS    | conflict | UNP P30656 |
| Z     | 33      | ARG      | LYS    | conflict | UNP P30656 |

- Molecule 13 is a protein called 20S PROTEASOME.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 13  | M     | 222      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1757  | 1115 | 303 | 335 | 4 |         |         |       |
| 13  | 1     | 222      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1757  | 1115 | 303 | 335 | 4 |         |         |       |

- Molecule 14 is a protein called 20S PROTEASOME.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 14  | N     | 233      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1824  | 1154 | 312 | 351 | 7 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 14  | 2     | 233      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1824  | 1154 | 312 | 351 | 7 |         |         |       |

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 15  | A     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 15  | E     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 15  | G     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 15  | H     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 15  | I     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 15  | J     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 15  | L     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 15  | M     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 15  | O     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 15  | S     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 15  | U     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 15  | V     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 15  | W     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 15  | X     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 15  | Z     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 15  | 1     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 16 is water.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 16  | A     | 113      | Total O<br>113 113 | 0       | 0       |
| 16  | B     | 109      | Total O<br>109 109 | 0       | 0       |
| 16  | C     | 73       | Total O<br>73 73   | 0       | 0       |
| 16  | D     | 66       | Total O<br>66 66   | 0       | 0       |
| 16  | E     | 88       | Total O<br>88 88   | 0       | 0       |
| 16  | F     | 58       | Total O<br>58 58   | 0       | 0       |
| 16  | G     | 91       | Total O<br>91 91   | 0       | 0       |
| 16  | H     | 114      | Total O<br>114 114 | 0       | 0       |
| 16  | I     | 122      | Total O<br>122 122 | 0       | 0       |
| 16  | J     | 113      | Total O<br>113 113 | 0       | 0       |
| 16  | K     | 117      | Total O<br>117 117 | 0       | 0       |
| 16  | L     | 100      | Total O<br>100 100 | 0       | 0       |
| 16  | M     | 135      | Total O<br>135 135 | 0       | 0       |
| 16  | N     | 158      | Total O<br>158 158 | 0       | 0       |
| 16  | O     | 108      | Total O<br>108 108 | 0       | 0       |
| 16  | P     | 105      | Total O<br>105 105 | 0       | 0       |
| 16  | Q     | 78       | Total O<br>78 78   | 0       | 0       |
| 16  | R     | 63       | Total O<br>63 63   | 0       | 0       |
| 16  | S     | 88       | Total O<br>88 88   | 0       | 0       |
| 16  | T     | 55       | Total O<br>55 55   | 0       | 0       |
| 16  | U     | 92       | Total O<br>92 92   | 0       | 0       |
| 16  | V     | 121      | Total O<br>121 121 | 0       | 0       |

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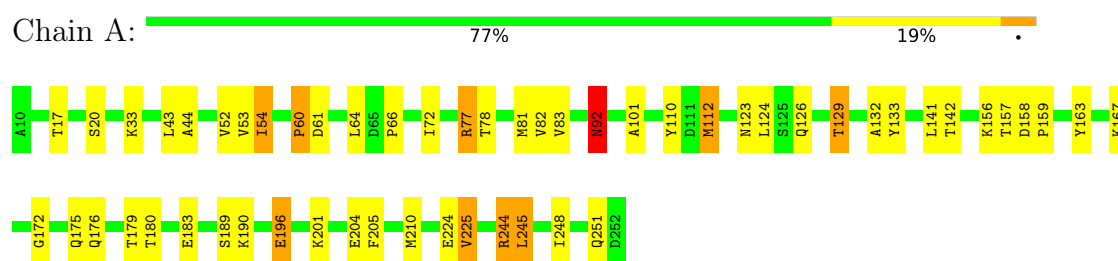
| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 16  | W     | 124      | Total<br>124 | O<br>124 | 0       | 0       |
| 16  | X     | 110      | Total<br>110 | O<br>110 | 0       | 0       |
| 16  | Y     | 115      | Total<br>115 | O<br>115 | 0       | 0       |
| 16  | Z     | 100      | Total<br>100 | O<br>100 | 0       | 0       |
| 16  | 1     | 139      | Total<br>139 | O<br>139 | 0       | 0       |
| 16  | 2     | 153      | Total<br>153 | O<br>153 | 0       | 0       |

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

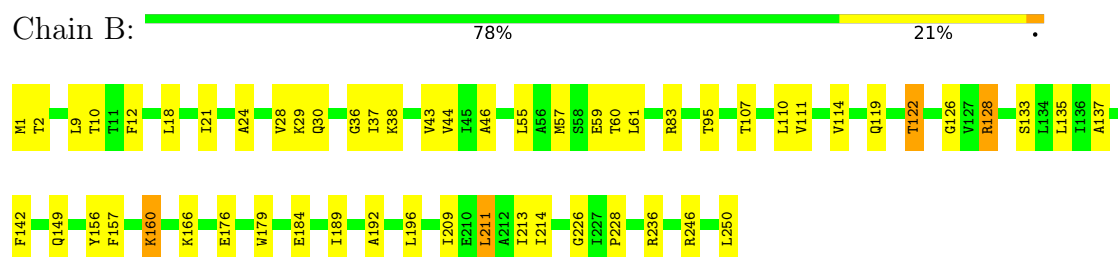
#### • Molecule 1: 20S PROTEASOME



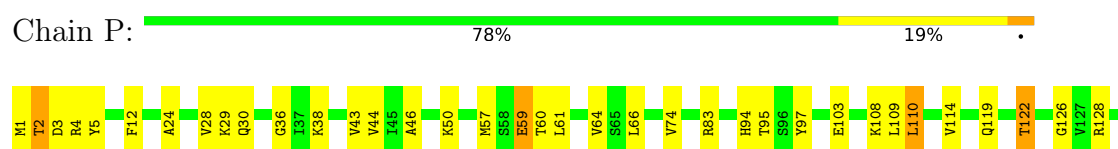
#### • Molecule 1: 20S PROTEASOME



#### • Molecule 2: 20S PROTEASOME



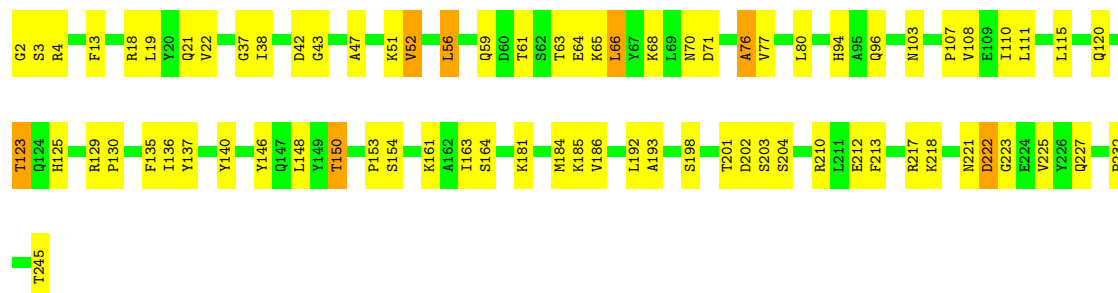
#### • Molecule 2: 20S PROTEASOME





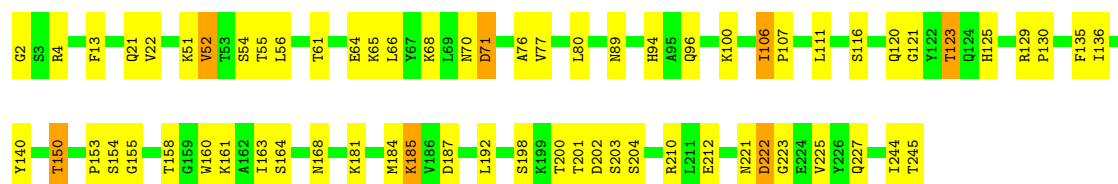
• Molecule 3: 20S PROTEASOME

Chain C: 69% 28%



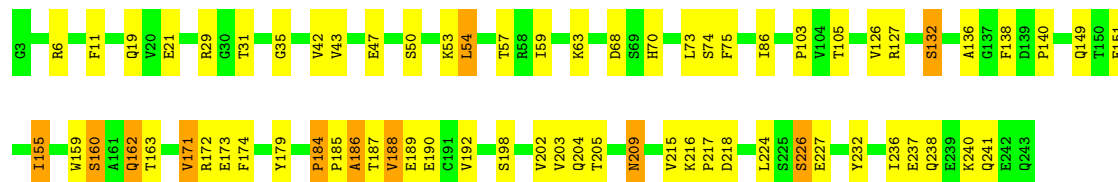
• Molecule 3: 20S PROTEASOME

Chain Q: 73% 25%



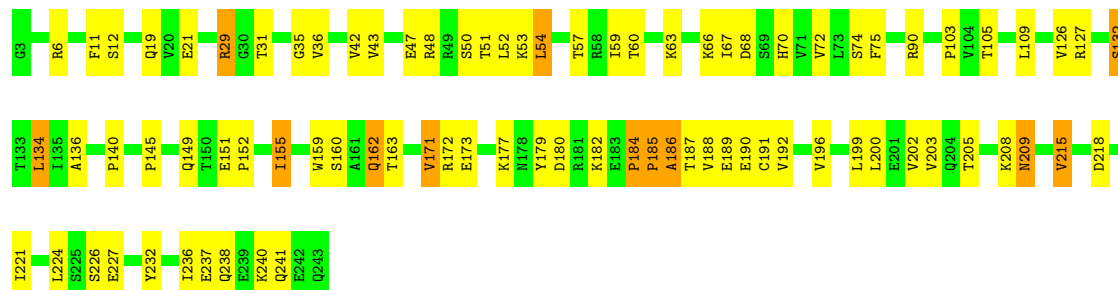
• Molecule 4: 20S PROTEASOME

Chain D: 71% 24% 5%



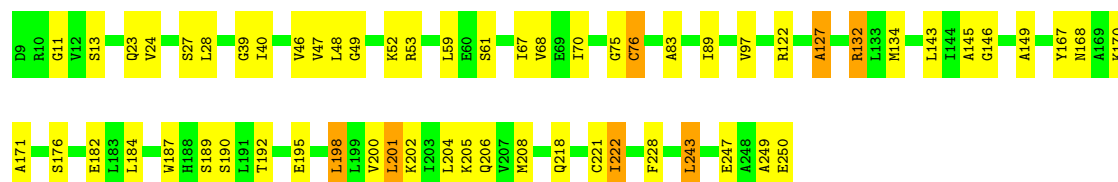
• Molecule 4: 20S PROTEASOME

Chain R: 65% 30% 5%



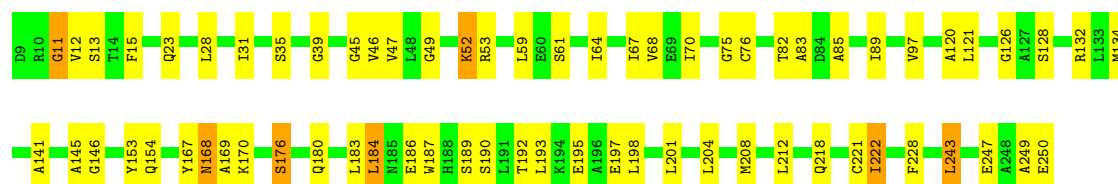
- Molecule 5: 20S PROTEASOME

Chain E:  75% 22% .



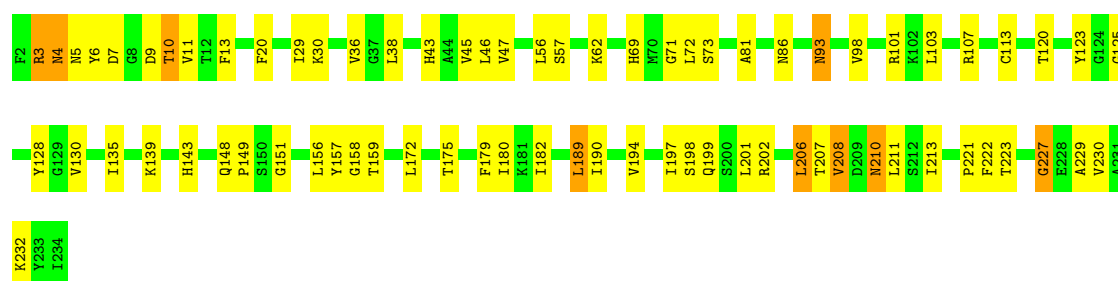
- Molecule 5: 20S PROTEASOME

Chain S:  72% 25% .



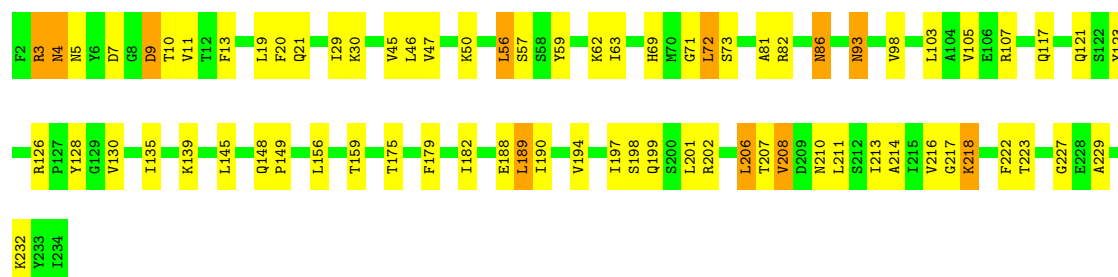
- Molecule 6: 20S PROTEASOME

Chain F:  68% 28% .



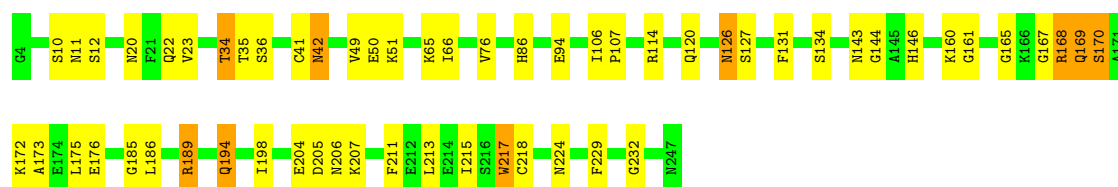
- Molecule 6: 20S PROTEASOME

Chain T:  68% 27% 5% .



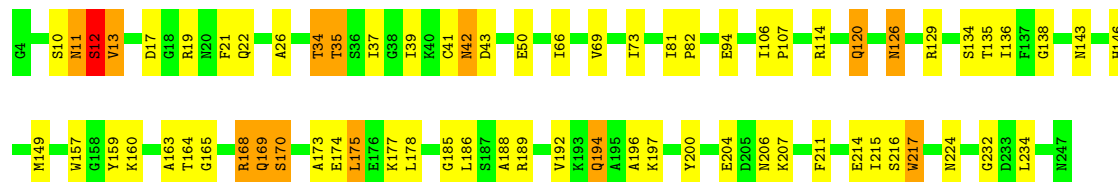
- Molecule 7: 20S PROTEASOME

Chain G:  76% 20% .



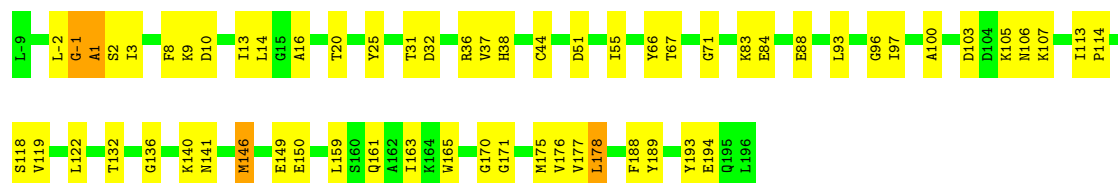
• Molecule 7: 20S PROTEASOME

Chain U: 71% 23% 5%



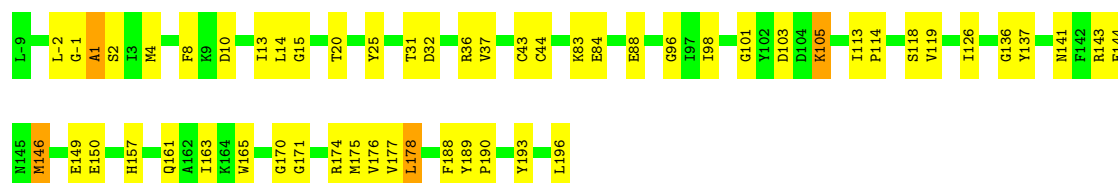
• Molecule 8: 20S PROTEASOME

Chain H: 70% 28% .



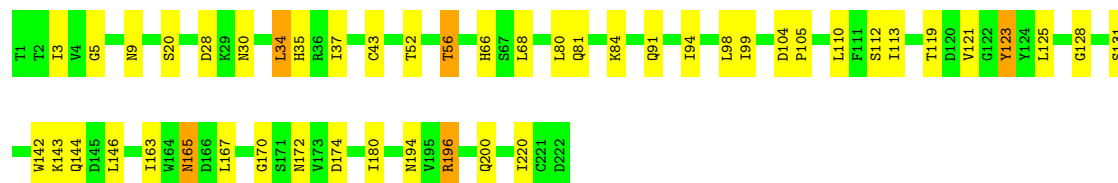
• Molecule 8: 20S PROTEASOME

Chain V: 73% 25% .



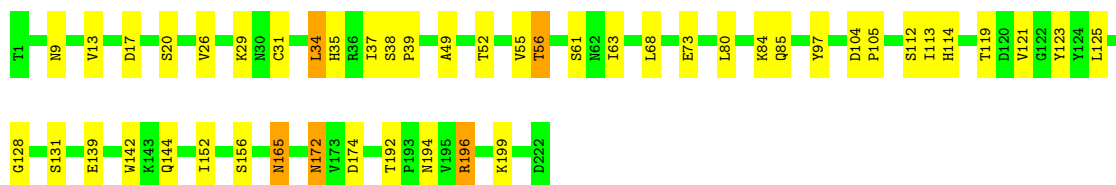
• Molecule 9: 20S PROTEASOME

Chain I: 79% 19% .



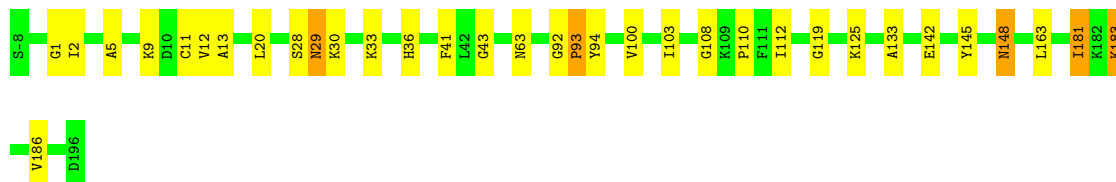
• Molecule 9: 20S PROTEASOME

Chain W: 79% 19% .



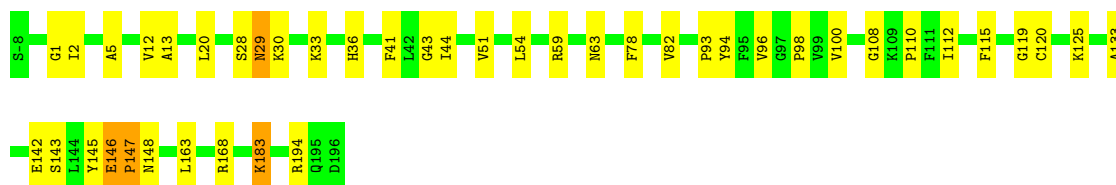
• Molecule 10: 20S PROTEASOME

Chain J: 83% 14% .



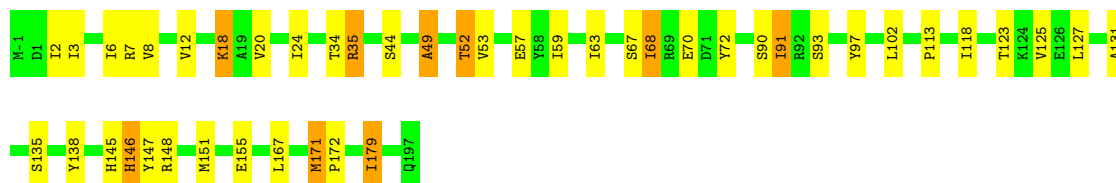
• Molecule 10: 20S PROTEASOME

Chain X: 79% 19% .



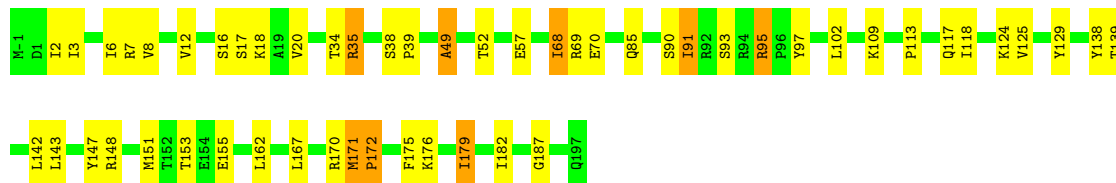
• Molecule 11: 20S PROTEASOME

Chain K: 77% 18% 5% .



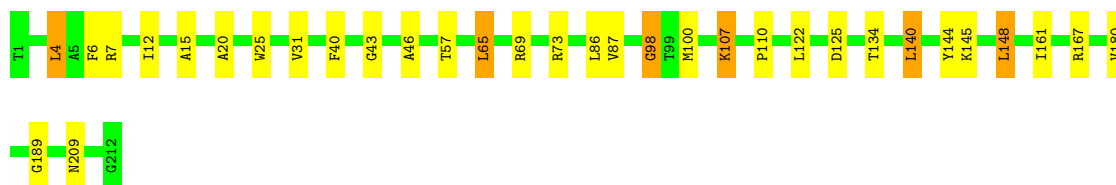
• Molecule 11: 20S PROTEASOME

Chain Y: 73% 23% .



• Molecule 12: 20S PROTEASOME

Chain L: 84% 13% .



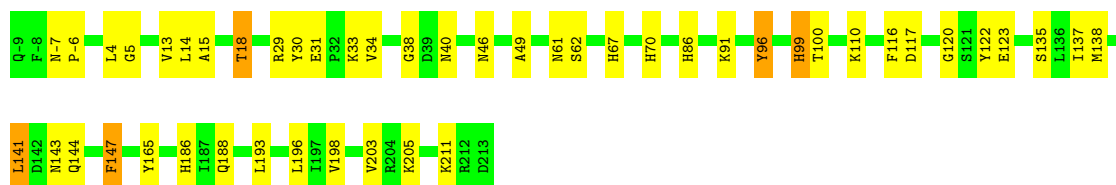
• Molecule 12: 20S PROTEASOME

Chain Z: 86% 11% .



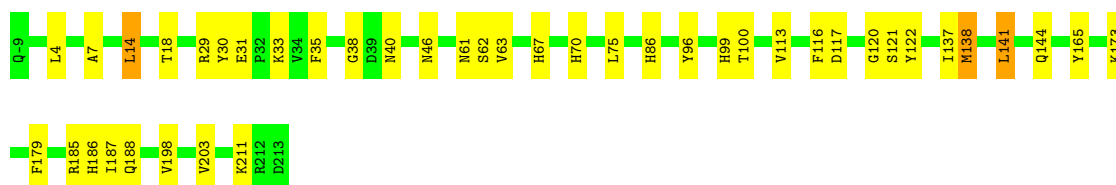
• Molecule 13: 20S PROTEASOME

Chain M: 78% 19% .



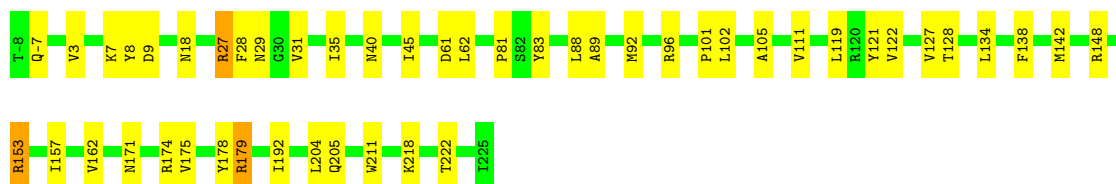
• Molecule 13: 20S PROTEASOME

Chain 1: 81% 18% .



• Molecule 14: 20S PROTEASOME

Chain N: 79% 19% .



• Molecule 14: 20S PROTEASOME

Chain 2: 76% 22% .







## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property                                                 | Value                                            | Source    |
|----------------------------------------------------------|--------------------------------------------------|-----------|
| Space group                                              | P 1 21 1                                         | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 135.49Å 300.70Å 144.42Å<br>90.00° 112.89° 90.00° | Depositor |
| Resolution (Å)                                           | 50.00 – 1.90                                     | Depositor |
| % Data completeness<br>(in resolution range)             | 90.5 (50.00-1.90)                                | Depositor |
| $R_{merge}$                                              | 0.08                                             | Depositor |
| $R_{sym}$                                                | (Not available)                                  | Depositor |
| Refinement program                                       | X-PLOR 3.1                                       | Depositor |
| R, $R_{free}$                                            | 0.286 , 0.330                                    | Depositor |
| Estimated twinning fraction                              | No twinning to report.                           | Xtriage   |
| Total number of atoms                                    | 52604                                            | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 36.0                                             | wwPDB-VP  |

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.80         | 1/1959 (0.1%)  | 1.06        | 10/2652 (0.4%)   |
| 1   | O     | 0.81         | 1/1959 (0.1%)  | 1.05        | 9/2652 (0.3%)    |
| 2   | B     | 0.72         | 0/1952         | 1.05        | 10/2642 (0.4%)   |
| 2   | P     | 0.69         | 0/1952         | 1.04        | 10/2642 (0.4%)   |
| 3   | C     | 0.69         | 0/1935         | 1.00        | 5/2618 (0.2%)    |
| 3   | Q     | 0.68         | 0/1935         | 1.04        | 9/2618 (0.3%)    |
| 4   | D     | 0.67         | 0/1920         | 1.02        | 9/2598 (0.3%)    |
| 4   | R     | 0.67         | 0/1920         | 1.03        | 8/2598 (0.3%)    |
| 5   | E     | 0.69         | 0/1887         | 1.04        | 8/2541 (0.3%)    |
| 5   | S     | 0.66         | 0/1887         | 1.03        | 8/2541 (0.3%)    |
| 6   | F     | 0.64         | 0/1823         | 1.04        | 8/2463 (0.3%)    |
| 6   | T     | 0.63         | 0/1823         | 1.01        | 6/2463 (0.2%)    |
| 7   | G     | 0.69         | 0/1937         | 1.05        | 10/2614 (0.4%)   |
| 7   | U     | 0.69         | 0/1937         | 1.08        | 11/2614 (0.4%)   |
| 8   | H     | 0.79         | 1/1603 (0.1%)  | 1.07        | 15/2168 (0.7%)   |
| 8   | V     | 0.78         | 1/1603 (0.1%)  | 1.06        | 9/2168 (0.4%)    |
| 9   | I     | 0.75         | 0/1716         | 1.02        | 7/2326 (0.3%)    |
| 9   | W     | 0.72         | 0/1716         | 1.07        | 9/2326 (0.4%)    |
| 10  | J     | 0.77         | 0/1611         | 1.06        | 7/2174 (0.3%)    |
| 10  | X     | 0.76         | 0/1611         | 1.06        | 10/2174 (0.5%)   |
| 11  | K     | 0.76         | 0/1613         | 1.06        | 11/2173 (0.5%)   |
| 11  | Y     | 0.74         | 0/1613         | 1.07        | 13/2173 (0.6%)   |
| 12  | L     | 0.73         | 0/1683         | 1.00        | 4/2277 (0.2%)    |
| 12  | Z     | 0.72         | 0/1683         | 1.01        | 6/2277 (0.3%)    |
| 13  | 1     | 0.74         | 1/1795 (0.1%)  | 1.11        | 10/2420 (0.4%)   |
| 13  | M     | 0.71         | 0/1795         | 1.09        | 9/2420 (0.4%)    |
| 14  | 2     | 0.77         | 0/1855         | 1.05        | 10/2514 (0.4%)   |
| 14  | N     | 0.75         | 0/1855         | 1.05        | 12/2514 (0.5%)   |
| All | All   | 0.72         | 5/50578 (0.0%) | 1.05        | 253/68360 (0.4%) |

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 |
|-----|-------|---------------------|---------------------|
| 9   | I     | 0                   | 1                   |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1   | A     | 112 | MET  | SD-CE | -13.28 | 1.46        | 1.79     |
| 1   | O     | 112 | MET  | SD-CE | -12.00 | 1.49        | 1.79     |
| 8   | V     | 146 | MET  | SD-CE | -5.71  | 1.65        | 1.79     |
| 13  | 1     | 138 | MET  | SD-CE | -5.48  | 1.65        | 1.79     |
| 8   | H     | 146 | MET  | SD-CE | -5.33  | 1.66        | 1.79     |

All (253) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 6   | F     | 3   | ARG  | N-CA-C | 12.18 | 124.25      | 110.97   |
| 14  | N     | 27  | ARG  | N-CA-C | 11.57 | 125.13      | 111.02   |
| 14  | 2     | 27  | ARG  | N-CA-C | 11.05 | 123.02      | 110.97   |
| 6   | T     | 3   | ARG  | N-CA-C | 10.48 | 123.80      | 111.02   |
| 12  | L     | 189 | GLY  | N-CA-C | 9.59  | 125.11      | 112.65   |
| 4   | D     | 59  | ILE  | N-CA-C | 9.49  | 120.69      | 111.67   |
| 7   | U     | 160 | LYS  | N-CA-C | -8.95 | 101.93      | 113.12   |
| 1   | A     | 251 | GLN  | N-CA-C | -8.75 | 102.73      | 113.41   |
| 7   | G     | 160 | LYS  | N-CA-C | -8.54 | 102.99      | 113.41   |
| 7   | U     | 185 | GLY  | N-CA-C | -8.43 | 101.94      | 111.63   |
| 12  | Z     | 189 | GLY  | N-CA-C | 8.28  | 125.06      | 112.81   |
| 5   | S     | 134 | MET  | N-CA-C | -8.28 | 93.17       | 110.80   |
| 14  | 2     | 102 | LEU  | N-CA-C | -8.24 | 95.14       | 108.41   |
| 5   | E     | 134 | MET  | N-CA-C | -8.07 | 93.61       | 110.80   |
| 9   | W     | 37  | ILE  | N-CA-C | -8.05 | 104.89      | 111.81   |
| 4   | R     | 105 | THR  | N-CA-C | -8.04 | 100.16      | 110.53   |
| 9   | W     | 9   | ASN  | N-CA-C | 8.00  | 121.02      | 111.33   |
| 13  | M     | 96  | TYR  | N-CA-C | -7.80 | 96.56       | 108.96   |
| 1   | A     | 20  | SER  | N-CA-C | -7.77 | 101.19      | 110.13   |
| 1   | O     | 251 | GLN  | N-CA-C | -7.72 | 102.79      | 112.90   |
| 14  | 2     | 179 | ARG  | N-CA-C | 7.67  | 122.82      | 113.38   |
| 7   | U     | 143 | ASN  | N-CA-C | 7.61  | 119.97      | 109.54   |
| 5   | E     | 149 | ALA  | N-CA-C | 7.48  | 120.31      | 111.71   |
| 2   | B     | 160 | LYS  | N-CA-C | -7.45 | 102.09      | 112.45   |
| 13  | M     | 49  | ALA  | N-CA-C | 7.45  | 120.28      | 111.71   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 14  | N     | 105 | ALA  | N-CA-C | -7.35 | 96.06       | 108.26   |
| 4   | D     | 105 | THR  | N-CA-C | -7.33 | 101.07      | 110.53   |
| 5   | E     | 70  | ILE  | N-CA-C | -7.33 | 105.51      | 111.81   |
| 14  | N     | 102 | LEU  | N-CA-C | -7.30 | 95.72       | 108.20   |
| 5   | S     | 11  | GLY  | N-CA-C | 7.29  | 120.34      | 112.33   |
| 10  | X     | 59  | ARG  | N-CA-C | -7.25 | 103.31      | 111.14   |
| 7   | G     | 143 | ASN  | N-CA-C | 7.25  | 119.47      | 109.54   |
| 5   | E     | 176 | SER  | N-CA-C | 7.20  | 119.20      | 111.36   |
| 3   | C     | 136 | ILE  | N-CA-C | -7.19 | 97.25       | 107.75   |
| 4   | R     | 132 | SER  | N-CA-C | -7.18 | 98.23       | 109.72   |
| 1   | A     | 167 | LYS  | N-CA-C | -7.18 | 102.86      | 111.69   |
| 14  | N     | 179 | ARG  | N-CA-C | 7.14  | 122.86      | 113.30   |
| 2   | B     | 214 | ILE  | N-CA-C | -6.90 | 95.66       | 107.24   |
| 11  | Y     | 170 | ARG  | N-CA-C | 6.87  | 121.75      | 113.23   |
| 1   | O     | 20  | SER  | N-CA-C | -6.86 | 101.17      | 110.36   |
| 5   | E     | 11  | GLY  | N-CA-C | 6.84  | 119.85      | 112.33   |
| 11  | K     | 171 | MET  | CA-C-N | 6.78  | 127.05      | 119.32   |
| 11  | K     | 171 | MET  | C-N-CA | 6.78  | 127.05      | 119.32   |
| 13  | 1     | 96  | TYR  | N-CA-C | -6.77 | 97.51       | 108.41   |
| 13  | M     | 120 | GLY  | N-CA-C | 6.76  | 124.74      | 115.00   |
| 8   | H     | 122 | LEU  | CA-C-N | 6.75  | 126.21      | 118.85   |
| 8   | H     | 122 | LEU  | C-N-CA | 6.75  | 126.21      | 118.85   |
| 14  | N     | 9   | ASP  | N-CA-C | 6.72  | 119.47      | 111.33   |
| 12  | L     | 167 | ARG  | N-CA-C | 6.72  | 119.95      | 111.69   |
| 14  | 2     | 105 | ALA  | N-CA-C | -6.71 | 97.41       | 108.76   |
| 12  | Z     | 57  | THR  | N-CA-C | -6.69 | 104.07      | 111.36   |
| 8   | H     | 1   | ALA  | N-CA-C | 6.68  | 125.03      | 110.80   |
| 8   | V     | 1   | ALA  | N-CA-C | 6.65  | 124.97      | 110.80   |
| 1   | O     | 167 | LYS  | N-CA-C | -6.63 | 103.54      | 111.69   |
| 6   | T     | 20  | PHE  | N-CA-C | 6.62  | 118.50      | 111.28   |
| 6   | T     | 229 | ALA  | N-CA-C | 6.62  | 121.03      | 113.15   |
| 3   | C     | 161 | LYS  | N-CA-C | -6.61 | 104.25      | 112.90   |
| 5   | S     | 70  | ILE  | N-CA-C | -6.58 | 106.15      | 111.81   |
| 2   | P     | 160 | LYS  | N-CA-C | -6.58 | 103.31      | 112.45   |
| 2   | P     | 142 | PHE  | N-CA-C | 6.56  | 121.28      | 113.28   |
| 8   | V     | 141 | ASN  | N-CA-C | 6.55  | 121.56      | 113.50   |
| 7   | U     | 13  | VAL  | N-CA-C | 6.54  | 117.48      | 109.30   |
| 4   | D     | 172 | ARG  | N-CA-C | -6.50 | 104.27      | 111.36   |
| 10  | J     | 148 | ASN  | N-CA-C | 6.48  | 120.35      | 111.54   |
| 4   | D     | 132 | SER  | N-CA-C | -6.45 | 99.32       | 109.50   |
| 10  | X     | 145 | TYR  | N-CA-C | 6.44  | 119.81      | 110.28   |
| 3   | C     | 76  | ALA  | N-CA-C | -6.43 | 99.24       | 109.59   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | B     | 142 | PHE  | N-CA-C | 6.36  | 121.04      | 113.28   |
| 14  | N     | 45  | ILE  | N-CA-C | 6.32  | 116.96      | 108.11   |
| 6   | F     | 20  | PHE  | N-CA-C | 6.31  | 118.16      | 111.28   |
| 11  | K     | 127 | LEU  | N-CA-C | 6.29  | 115.38      | 108.14   |
| 3   | Q     | 136 | ILE  | N-CA-C | -6.29 | 98.57       | 107.75   |
| 7   | U     | 232 | GLY  | N-CA-C | 6.28  | 122.70      | 111.02   |
| 8   | V     | 189 | TYR  | CA-C-N | 6.27  | 125.76      | 119.24   |
| 8   | V     | 189 | TYR  | C-N-CA | 6.27  | 125.76      | 119.24   |
| 1   | O     | 150 | LEU  | N-CA-C | 6.25  | 121.08      | 112.90   |
| 2   | P     | 214 | ILE  | N-CA-C | -6.25 | 97.35       | 107.28   |
| 14  | N     | 35  | ILE  | N-CA-C | 6.22  | 114.26      | 107.60   |
| 3   | Q     | 212 | GLU  | N-CA-C | -6.19 | 98.91       | 109.24   |
| 8   | V     | 193 | TYR  | N-CA-C | 6.18  | 118.81      | 111.71   |
| 11  | Y     | 187 | GLY  | N-CA-C | 6.16  | 117.62      | 111.21   |
| 8   | H     | 141 | ASN  | N-CA-C | 6.15  | 121.07      | 113.50   |
| 11  | K     | 146 | HIS  | N-CA-C | 6.15  | 120.79      | 113.28   |
| 11  | Y     | 139 | THR  | N-CA-C | 6.13  | 120.83      | 113.23   |
| 4   | D     | 160 | SER  | N-CA-C | -6.12 | 104.73      | 111.82   |
| 9   | W     | 172 | ASN  | N-CA-C | 6.12  | 118.76      | 109.95   |
| 9   | I     | 220 | ILE  | N-CA-C | 6.11  | 116.30      | 110.74   |
| 11  | Y     | 171 | MET  | CA-C-N | 6.08  | 125.80      | 119.05   |
| 11  | Y     | 171 | MET  | C-N-CA | 6.08  | 125.80      | 119.05   |
| 3   | Q     | 71  | ASP  | N-CA-C | -6.06 | 105.89      | 113.28   |
| 13  | M     | 31  | GLU  | CA-C-N | 6.04  | 126.40      | 119.93   |
| 13  | M     | 31  | GLU  | C-N-CA | 6.04  | 126.40      | 119.93   |
| 14  | N     | 3   | VAL  | N-CA-C | -6.04 | 98.84       | 107.77   |
| 7   | U     | 134 | SER  | N-CA-C | -6.04 | 99.35       | 109.07   |
| 6   | T     | 98  | VAL  | N-CA-C | 6.02  | 117.56      | 111.00   |
| 1   | O     | 79  | ILE  | N-CA-C | 6.02  | 116.97      | 108.36   |
| 5   | S     | 61  | SER  | N-CA-C | 6.01  | 118.61      | 111.33   |
| 4   | R     | 172 | ARG  | N-CA-C | -5.99 | 104.75      | 111.28   |
| 2   | P     | 133 | SER  | N-CA-C | -5.98 | 99.26       | 109.24   |
| 5   | S     | 53  | ARG  | N-CA-C | 5.97  | 117.90      | 110.91   |
| 9   | W     | 49  | ALA  | N-CA-C | 5.96  | 118.54      | 111.33   |
| 1   | A     | 225 | VAL  | N-CA-C | 5.94  | 116.68      | 108.12   |
| 14  | 2     | 3   | VAL  | N-CA-C | -5.94 | 98.93       | 107.78   |
| 4   | R     | 218 | ASP  | N-CA-C | 5.93  | 119.83      | 111.52   |
| 12  | L     | 98  | GLY  | N-CA-C | -5.93 | 99.13       | 113.18   |
| 2   | P     | 184 | GLU  | N-CA-C | -5.92 | 102.56      | 110.55   |
| 11  | Y     | 176 | LYS  | N-CA-C | 5.92  | 119.81      | 112.24   |
| 7   | G     | 134 | SER  | N-CA-C | -5.92 | 99.25       | 108.90   |
| 7   | G     | 144 | GLY  | N-CA-C | 5.90  | 119.25      | 111.70   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 12  | L     | 57  | THR  | N-CA-C | -5.90 | 104.98      | 111.82   |
| 6   | F     | 229 | ALA  | N-CA-C | 5.89  | 120.09      | 113.02   |
| 2   | B     | 133 | SER  | N-CA-C | -5.87 | 99.44       | 109.24   |
| 3   | C     | 108 | VAL  | N-CA-C | 5.86  | 116.51      | 110.36   |
| 8   | H     | 106 | ASN  | N-CA-C | 5.85  | 120.42      | 113.28   |
| 10  | J     | 119 | GLY  | N-CA-C | 5.84  | 122.51      | 114.92   |
| 8   | V     | 2   | SER  | N-CA-C | -5.83 | 97.71       | 107.80   |
| 8   | H     | 96  | GLY  | N-CA-C | -5.81 | 99.42       | 113.18   |
| 8   | V     | 96  | GLY  | N-CA-C | -5.81 | 99.42       | 113.18   |
| 4   | D     | 184 | PRO  | N-CA-C | -5.78 | 103.65      | 110.70   |
| 9   | W     | 165 | ASN  | N-CA-C | 5.78  | 120.49      | 113.38   |
| 7   | G     | 232 | GLY  | N-CA-C | 5.76  | 121.74      | 111.02   |
| 11  | K     | 179 | ILE  | N-CA-C | -5.76 | 100.13      | 108.36   |
| 3   | Q     | 161 | LYS  | N-CA-C | -5.75 | 105.37      | 112.90   |
| 7   | U     | 12  | SER  | N-CA-C | 5.75  | 123.05      | 110.80   |
| 1   | A     | 92  | ASN  | N-CA-C | -5.74 | 105.03      | 111.28   |
| 2   | B     | 95  | THR  | N-CA-C | 5.72  | 117.51      | 111.28   |
| 2   | B     | 126 | GLY  | N-CA-C | 5.72  | 123.13      | 114.61   |
| 3   | C     | 212 | GLU  | N-CA-C | -5.71 | 99.36       | 109.06   |
| 6   | F     | 148 | GLN  | CA-C-N | 5.71  | 126.97      | 119.84   |
| 6   | F     | 148 | GLN  | C-N-CA | 5.71  | 126.97      | 119.84   |
| 1   | A     | 172 | GLY  | CA-C-N | 5.70  | 125.38      | 119.05   |
| 1   | A     | 172 | GLY  | C-N-CA | 5.70  | 125.38      | 119.05   |
| 10  | J     | 93  | PRO  | N-CA-C | 5.70  | 120.17      | 111.34   |
| 2   | P     | 126 | GLY  | N-CA-C | 5.69  | 122.69      | 114.10   |
| 13  | 1     | 120 | GLY  | N-CA-C | 5.68  | 123.94      | 115.64   |
| 11  | K     | 49  | ALA  | N-CA-C | 5.67  | 122.88      | 110.80   |
| 10  | X     | 119 | GLY  | N-CA-C | 5.67  | 122.29      | 114.92   |
| 11  | Y     | 95  | ARG  | CA-C-N | 5.67  | 125.43      | 119.76   |
| 11  | Y     | 95  | ARG  | C-N-CA | 5.67  | 125.43      | 119.76   |
| 7   | U     | 21  | PHE  | N-CA-C | 5.65  | 118.17      | 111.33   |
| 9   | I     | 91  | GLN  | N-CA-C | 5.64  | 119.35      | 111.90   |
| 13  | 1     | 185 | ARG  | N-CA-C | 5.62  | 121.03      | 113.72   |
| 8   | H     | 2   | SER  | N-CA-C | -5.61 | 98.09       | 107.80   |
| 10  | J     | 20  | LEU  | N-CA-C | -5.61 | 98.95       | 108.26   |
| 11  | Y     | 179 | ILE  | N-CA-C | -5.61 | 100.34      | 108.36   |
| 8   | H     | 193 | TYR  | N-CA-C | 5.60  | 118.16      | 111.71   |
| 12  | Z     | 167 | ARG  | N-CA-C | 5.60  | 118.57      | 111.69   |
| 5   | S     | 168 | ASN  | N-CA-C | -5.57 | 105.60      | 112.90   |
| 5   | S     | 186 | GLU  | N-CA-C | 5.56  | 119.78      | 112.89   |
| 10  | X     | 94  | TYR  | N-CA-C | -5.55 | 100.24      | 109.46   |
| 13  | M     | 99  | HIS  | N-CA-C | -5.55 | 98.30       | 108.02   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 6   | F     | 98  | VAL  | N-CA-C | 5.51  | 117.01      | 111.00   |
| 7   | G     | 211 | PHE  | N-CA-C | 5.51  | 117.36      | 109.14   |
| 5   | S     | 176 | SER  | N-CA-C | 5.51  | 118.21      | 111.82   |
| 2   | P     | 95  | THR  | N-CA-C | 5.51  | 117.36      | 111.36   |
| 3   | Q     | 244 | ILE  | N-CA-C | -5.50 | 106.98      | 113.42   |
| 9   | I     | 172 | ASN  | N-CA-C | 5.48  | 117.84      | 109.95   |
| 1   | A     | 17  | THR  | N-CA-C | 5.47  | 118.09      | 109.39   |
| 1   | O     | 78  | THR  | N-CA-C | 5.47  | 120.09      | 113.41   |
| 7   | U     | 211 | PHE  | N-CA-C | 5.46  | 117.70      | 109.41   |
| 4   | R     | 184 | PRO  | N-CA-C | -5.45 | 104.74      | 110.58   |
| 4   | D     | 188 | VAL  | N-CA-C | -5.44 | 105.20      | 110.42   |
| 13  | 1     | 179 | PHE  | N-CA-C | 5.43  | 117.28      | 111.36   |
| 7   | G     | 185 | GLY  | N-CA-C | -5.42 | 105.40      | 111.63   |
| 9   | I     | 37  | ILE  | N-CA-C | -5.42 | 105.83      | 111.58   |
| 13  | 1     | 35  | PHE  | N-CA-C | 5.42  | 118.06      | 109.50   |
| 3   | Q     | 77  | VAL  | N-CA-C | 5.41  | 115.75      | 108.17   |
| 10  | X     | 93  | PRO  | N-CA-C | 5.40  | 119.71      | 111.34   |
| 2   | B     | 135 | LEU  | N-CA-C | -5.40 | 99.61       | 108.41   |
| 13  | M     | 38  | GLY  | N-CA-C | -5.40 | 105.80      | 112.33   |
| 14  | 2     | 203 | ASN  | N-CA-C | 5.39  | 118.87      | 111.54   |
| 2   | P     | 135 | LEU  | N-CA-C | -5.39 | 99.63       | 108.41   |
| 7   | G     | 218 | CYS  | N-CA-C | -5.38 | 99.33       | 108.26   |
| 7   | U     | 26  | ALA  | N-CA-C | -5.38 | 105.49      | 111.36   |
| 14  | N     | 29  | ASN  | N-CA-C | 5.37  | 119.53      | 112.92   |
| 8   | H     | 97  | ILE  | N-CA-C | 5.37  | 115.62      | 108.11   |
| 11  | K     | 18  | LYS  | N-CA-C | 5.37  | 119.83      | 113.28   |
| 2   | B     | 9   | LEU  | N-CA-C | -5.36 | 106.79      | 113.38   |
| 13  | 1     | 38  | GLY  | N-CA-C | -5.36 | 105.93      | 112.68   |
| 12  | Z     | 98  | GLY  | N-CA-C | -5.35 | 100.50      | 113.18   |
| 4   | R     | 134 | LEU  | N-CA-C | -5.35 | 100.18      | 108.90   |
| 11  | Y     | 172 | PRO  | N-CA-C | 5.34  | 120.95      | 113.53   |
| 9   | I     | 180 | ILE  | N-CA-C | 5.33  | 120.43      | 109.34   |
| 3   | Q     | 106 | ILE  | N-CA-C | 5.33  | 114.17      | 108.95   |
| 4   | D     | 74  | SER  | N-CA-C | -5.32 | 101.32      | 109.41   |
| 10  | J     | 145 | TYR  | N-CA-C | 5.32  | 118.16      | 110.28   |
| 2   | B     | 184 | GLU  | N-CA-C | -5.32 | 102.65      | 110.52   |
| 14  | 2     | 187 | PHE  | N-CA-C | 5.32  | 116.36      | 108.86   |
| 9   | I     | 165 | ASN  | N-CA-C | 5.31  | 119.91      | 113.38   |
| 10  | J     | 181 | ILE  | N-CA-C | 5.29  | 115.47      | 107.80   |
| 12  | Z     | 8   | PHE  | N-CA-C | 5.29  | 115.12      | 108.45   |
| 1   | A     | 132 | ALA  | N-CA-C | 5.29  | 117.79      | 111.71   |
| 5   | E     | 61  | SER  | N-CA-C | 5.29  | 118.52      | 111.75   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 10  | X     | 146 | GLU  | CA-C-N | 5.29  | 125.19      | 119.85   |
| 10  | X     | 146 | GLU  | C-N-CA | 5.29  | 125.19      | 119.85   |
| 10  | X     | 148 | ASN  | N-CA-C | 5.28  | 119.00      | 112.24   |
| 11  | Y     | 20  | VAL  | N-CA-C | -5.28 | 99.95       | 107.77   |
| 7   | G     | 161 | GLY  | N-CA-C | -5.28 | 102.74      | 110.87   |
| 8   | H     | 66  | TYR  | N-CA-C | -5.27 | 105.23      | 110.97   |
| 6   | T     | 148 | GLN  | CA-C-N | 5.27  | 126.43      | 119.84   |
| 6   | T     | 148 | GLN  | C-N-CA | 5.27  | 126.43      | 119.84   |
| 9   | I     | 9   | ASN  | N-CA-C | 5.26  | 122.02      | 110.80   |
| 6   | F     | 6   | TYR  | N-CA-C | 5.26  | 119.39      | 112.92   |
| 13  | M     | 144 | GLN  | N-CA-C | 5.24  | 119.73      | 113.23   |
| 10  | X     | 20  | LEU  | N-CA-C | -5.24 | 99.56       | 108.26   |
| 14  | 2     | 45  | ILE  | N-CA-C | 5.24  | 115.66      | 108.12   |
| 11  | Y     | 97  | TYR  | N-CA-C | -5.22 | 102.14      | 109.96   |
| 4   | D     | 218 | ASP  | N-CA-C | 5.21  | 118.43      | 111.24   |
| 1   | O     | 213 | ALA  | N-CA-C | 5.21  | 118.09      | 111.69   |
| 9   | W     | 38  | SER  | N-CA-C | -5.20 | 102.16      | 108.14   |
| 13  | 1     | 31  | GLU  | CA-C-N | 5.20  | 125.21      | 119.90   |
| 13  | 1     | 31  | GLU  | C-N-CA | 5.20  | 125.21      | 119.90   |
| 11  | Y     | 49  | ALA  | N-CA-C | 5.20  | 121.88      | 110.80   |
| 10  | J     | 94  | TYR  | N-CA-C | -5.19 | 100.84      | 109.46   |
| 8   | V     | 44  | CYS  | N-CA-C | -5.19 | 100.71      | 109.07   |
| 6   | F     | 210 | ASN  | N-CA-C | 5.19  | 119.52      | 112.04   |
| 12  | Z     | 29  | GLN  | N-CA-C | -5.19 | 105.62      | 112.94   |
| 11  | K     | 127 | LEU  | CA-C-N | 5.18  | 124.50      | 118.85   |
| 11  | K     | 127 | LEU  | C-N-CA | 5.18  | 124.50      | 118.85   |
| 11  | K     | 172 | PRO  | N-CA-C | 5.18  | 121.47      | 113.75   |
| 7   | G     | 12  | SER  | N-CA-C | 5.18  | 121.84      | 110.80   |
| 2   | P     | 181 | ASP  | N-CA-C | 5.18  | 120.25      | 113.20   |
| 8   | H     | 44  | CYS  | N-CA-C | -5.16 | 100.76      | 109.07   |
| 1   | O     | 31  | ALA  | N-CA-C | -5.16 | 105.84      | 111.82   |
| 2   | P     | 110 | LEU  | N-CA-C | -5.16 | 105.66      | 111.28   |
| 1   | O     | 92  | ASN  | N-CA-C | -5.15 | 105.57      | 111.14   |
| 14  | 2     | 2   | SER  | N-CA-C | 5.15  | 121.77      | 110.80   |
| 8   | H     | 189 | TYR  | CA-C-N | 5.14  | 124.58      | 119.24   |
| 8   | H     | 189 | TYR  | C-N-CA | 5.14  | 124.58      | 119.24   |
| 7   | U     | 136 | ILE  | N-CA-C | -5.14 | 100.97      | 108.17   |
| 13  | 1     | 144 | GLN  | N-CA-C | 5.13  | 119.60      | 113.23   |
| 9   | W     | 73  | GLU  | CA-C-N | 5.13  | 125.06      | 119.78   |
| 9   | W     | 73  | GLU  | C-N-CA | 5.13  | 125.06      | 119.78   |
| 14  | N     | -7  | GLN  | N-CA-C | 5.12  | 116.08      | 108.86   |
| 5   | E     | 53  | ARG  | N-CA-C | 5.12  | 117.42      | 111.02   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 78  | THR  | N-CA-C  | 5.12  | 120.17      | 113.88   |
| 14  | N     | 222 | THR  | N-CA-C  | 5.11  | 119.65      | 113.41   |
| 5   | E     | 206 | GLN  | N-CA-C  | 5.11  | 116.54      | 111.07   |
| 3   | Q     | 160 | TRP  | N-CA-C  | 5.09  | 116.93      | 109.24   |
| 8   | H     | 37  | VAL  | N-CA-C  | -5.08 | 107.90      | 113.43   |
| 2   | B     | 128 | ARG  | N-CA-C  | -5.08 | 102.78      | 110.50   |
| 8   | H     | 194 | GLU  | N-CA-C  | 5.05  | 117.44      | 111.33   |
| 3   | Q     | 76  | ALA  | N-CA-C  | -5.05 | 101.46      | 109.59   |
| 14  | 2     | 162 | VAL  | CB-CA-C | -5.04 | 104.35      | 112.16   |
| 13  | 1     | 121 | SER  | N-CA-C  | -5.03 | 102.25      | 110.20   |
| 4   | R     | 12  | SER  | N-CA-C  | -5.03 | 102.73      | 110.58   |
| 14  | N     | 101 | PRO  | N-CA-C  | 5.03  | 118.95      | 111.41   |
| 10  | X     | 147 | PRO  | N-CA-C  | 5.03  | 119.37      | 111.38   |
| 8   | V     | 37  | VAL  | N-CA-C  | -5.02 | 107.54      | 113.42   |
| 13  | M     | 147 | PHE  | N-CA-C  | 5.02  | 118.53      | 111.90   |
| 9   | W     | 97  | TYR  | N-CA-C  | -5.02 | 100.23      | 108.41   |
| 4   | R     | 67  | ILE  | N-CA-C  | -5.01 | 106.27      | 111.58   |
| 11  | K     | 97  | TYR  | N-CA-C  | -5.00 | 102.46      | 109.96   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 9   | I     | 123 | TYR  | Sidechain |

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1921  | 0        | 1910     | 40      | 0            |
| 1   | O     | 1921  | 0        | 1910     | 45      | 0            |
| 2   | B     | 1915  | 0        | 1929     | 31      | 0            |
| 2   | P     | 1915  | 0        | 1929     | 31      | 0            |
| 3   | C     | 1905  | 0        | 1901     | 48      | 0            |
| 3   | Q     | 1905  | 0        | 1901     | 41      | 0            |
| 4   | D     | 1891  | 0        | 1900     | 47      | 0            |
| 4   | R     | 1891  | 0        | 1900     | 59      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5   | E     | 1862  | 0        | 1836     | 35      | 0            |
| 5   | S     | 1862  | 0        | 1836     | 35      | 0            |
| 6   | F     | 1795  | 0        | 1797     | 49      | 0            |
| 6   | T     | 1795  | 0        | 1797     | 50      | 0            |
| 7   | G     | 1897  | 0        | 1886     | 29      | 0            |
| 7   | U     | 1897  | 0        | 1886     | 42      | 0            |
| 8   | H     | 1574  | 0        | 1553     | 34      | 0            |
| 8   | V     | 1574  | 0        | 1553     | 35      | 0            |
| 9   | I     | 1685  | 0        | 1688     | 27      | 0            |
| 9   | W     | 1685  | 0        | 1688     | 30      | 0            |
| 10  | J     | 1581  | 0        | 1574     | 19      | 0            |
| 10  | X     | 1581  | 0        | 1574     | 25      | 0            |
| 11  | K     | 1585  | 0        | 1590     | 30      | 0            |
| 11  | Y     | 1585  | 0        | 1590     | 32      | 0            |
| 12  | L     | 1646  | 0        | 1595     | 27      | 0            |
| 12  | Z     | 1646  | 0        | 1595     | 16      | 0            |
| 13  | 1     | 1757  | 0        | 1711     | 26      | 0            |
| 13  | M     | 1757  | 0        | 1711     | 32      | 0            |
| 14  | 2     | 1824  | 0        | 1832     | 29      | 0            |
| 14  | N     | 1824  | 0        | 1832     | 22      | 0            |
| 15  | 1     | 1     | 0        | 0        | 0       | 0            |
| 15  | A     | 2     | 0        | 0        | 0       | 0            |
| 15  | E     | 1     | 0        | 0        | 0       | 0            |
| 15  | G     | 1     | 0        | 0        | 0       | 0            |
| 15  | H     | 1     | 0        | 0        | 0       | 0            |
| 15  | I     | 1     | 0        | 0        | 0       | 0            |
| 15  | J     | 2     | 0        | 0        | 0       | 0            |
| 15  | L     | 1     | 0        | 0        | 0       | 0            |
| 15  | M     | 1     | 0        | 0        | 0       | 0            |
| 15  | O     | 2     | 0        | 0        | 0       | 0            |
| 15  | S     | 1     | 0        | 0        | 0       | 0            |
| 15  | U     | 1     | 0        | 0        | 0       | 0            |
| 15  | V     | 1     | 0        | 0        | 0       | 0            |
| 15  | W     | 1     | 0        | 0        | 0       | 0            |
| 15  | X     | 2     | 0        | 0        | 0       | 0            |
| 15  | Z     | 1     | 0        | 0        | 0       | 0            |
| 16  | 1     | 139   | 0        | 0        | 3       | 0            |
| 16  | 2     | 153   | 0        | 0        | 1       | 0            |
| 16  | A     | 113   | 0        | 0        | 0       | 0            |
| 16  | B     | 109   | 0        | 0        | 1       | 0            |
| 16  | C     | 73    | 0        | 0        | 4       | 0            |
| 16  | D     | 66    | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 16  | E     | 88    | 0        | 0        | 2       | 0            |
| 16  | F     | 58    | 0        | 0        | 1       | 0            |
| 16  | G     | 91    | 0        | 0        | 1       | 0            |
| 16  | H     | 114   | 0        | 0        | 2       | 0            |
| 16  | I     | 122   | 0        | 0        | 0       | 0            |
| 16  | J     | 113   | 0        | 0        | 0       | 0            |
| 16  | K     | 117   | 0        | 0        | 1       | 0            |
| 16  | L     | 100   | 0        | 0        | 0       | 0            |
| 16  | M     | 135   | 0        | 0        | 2       | 0            |
| 16  | N     | 158   | 0        | 0        | 0       | 0            |
| 16  | O     | 108   | 0        | 0        | 3       | 0            |
| 16  | P     | 105   | 0        | 0        | 1       | 0            |
| 16  | Q     | 78    | 0        | 0        | 3       | 0            |
| 16  | R     | 63    | 0        | 0        | 0       | 0            |
| 16  | S     | 88    | 0        | 0        | 1       | 0            |
| 16  | T     | 55    | 0        | 0        | 0       | 0            |
| 16  | U     | 92    | 0        | 0        | 1       | 0            |
| 16  | V     | 121   | 0        | 0        | 1       | 0            |
| 16  | W     | 124   | 0        | 0        | 1       | 0            |
| 16  | X     | 110   | 0        | 0        | 0       | 0            |
| 16  | Y     | 115   | 0        | 0        | 2       | 0            |
| 16  | Z     | 100   | 0        | 0        | 0       | 0            |
| All | All   | 52604 | 0        | 49404    | 850     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (850) 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:O:101:ALA:HA   | 1:O:112:MET:HE2  | 1.45                     | 0.96              |
| 3:C:125:HIS:HB3  | 4:D:126:VAL:HG12 | 1.50                     | 0.94              |
| 13:1:18:THR:CG2  | 13:1:30:TYR:HA   | 1.98                     | 0.93              |
| 1:A:101:ALA:HA   | 1:A:112:MET:HE2  | 1.51                     | 0.93              |
| 12:Z:107:LYS:H   | 12:Z:107:LYS:HD2 | 1.34                     | 0.92              |
| 13:M:33:LYS:HD2  | 13:M:46:ASN:HD22 | 1.37                     | 0.89              |
| 8:H:136:GLY:HA2  | 8:V:161:GLN:HE21 | 1.37                     | 0.88              |
| 13:1:33:LYS:HD2  | 13:1:46:ASN:HD22 | 1.40                     | 0.87              |
| 13:M:18:THR:CG2  | 13:M:30:TYR:HA   | 2.05                     | 0.87              |
| 12:L:107:LYS:H   | 12:L:107:LYS:HD2 | 1.40                     | 0.86              |
| 3:C:201:THR:HG22 | 3:C:203:SER:H    | 1.41                     | 0.86              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:2:171:ASN:HD22 | 14:2:174:ARG:HH21 | 1.15                     | 0.86              |
| 2:P:122:THR:HG22  | 3:Q:129:ARG:HH21  | 1.41                     | 0.84              |
| 9:W:35:HIS:HB3    | 9:W:56:THR:HG21   | 1.57                     | 0.84              |
| 14:N:171:ASN:HD22 | 14:N:174:ARG:HH21 | 1.26                     | 0.84              |
| 6:T:13:PHE:H      | 7:U:22:GLN:HE22   | 1.23                     | 0.82              |
| 7:G:94:GLU:HG3    | 7:G:114:ARG:HH11  | 1.44                     | 0.81              |
| 1:A:129:THR:HG22  | 2:B:128:ARG:HH21  | 1.44                     | 0.80              |
| 3:Q:201:THR:HG22  | 3:Q:203:SER:H     | 1.46                     | 0.80              |
| 4:D:11:PHE:H      | 5:E:23:GLN:HE22   | 1.27                     | 0.80              |
| 2:B:12:PHE:H      | 3:C:21:GLN:HE22   | 1.28                     | 0.80              |
| 6:F:13:PHE:H      | 7:G:22:GLN:HE22   | 1.30                     | 0.79              |
| 7:U:94:GLU:HG2    | 7:U:114:ARG:HB3   | 1.62                     | 0.79              |
| 13:1:198:VAL:HG22 | 13:1:203:VAL:HG22 | 1.65                     | 0.78              |
| 2:P:12:PHE:H      | 3:Q:21:GLN:HE22   | 1.32                     | 0.78              |
| 3:C:120:GLN:O     | 3:C:123:THR:HB    | 1.85                     | 0.77              |
| 14:2:171:ASN:HD22 | 14:2:174:ARG:NH2  | 1.85                     | 0.74              |
| 13:1:18:THR:HG22  | 13:1:29:ARG:O     | 1.88                     | 0.73              |
| 13:M:18:THR:HG23  | 13:M:30:TYR:HA    | 1.70                     | 0.73              |
| 3:Q:64:GLU:HG3    | 3:Q:65:LYS:HG3    | 1.68                     | 0.73              |
| 4:D:171:VAL:HG12  | 4:D:202:VAL:HG21  | 1.71                     | 0.73              |
| 5:E:97:VAL:HG21   | 12:L:65:LEU:HD13  | 1.71                     | 0.73              |
| 3:Q:125:HIS:HB3   | 4:R:126:VAL:HG12  | 1.71                     | 0.73              |
| 14:N:171:ASN:HD22 | 14:N:174:ARG:NH2  | 1.87                     | 0.72              |
| 3:C:123:THR:HG22  | 4:D:127:ARG:HH21  | 1.54                     | 0.72              |
| 14:2:171:ASN:ND2  | 14:2:174:ARG:HH21 | 1.87                     | 0.71              |
| 9:I:35:HIS:HB3    | 9:I:56:THR:HG21   | 1.73                     | 0.71              |
| 13:M:18:THR:HG22  | 13:M:29:ARG:O     | 1.91                     | 0.71              |
| 14:N:148:ARG:HH11 | 9:W:165:ASN:HD22  | 1.39                     | 0.71              |
| 1:A:196:GLU:HG2   | 1:A:201:LYS:CB    | 2.20                     | 0.70              |
| 8:H:136:GLY:HA2   | 8:V:161:GLN:NE2   | 2.05                     | 0.70              |
| 3:Q:96:GLN:HE22   | 10:X:63:ASN:HD22  | 1.40                     | 0.70              |
| 5:S:67:ILE:HG22   | 5:S:228:PHE:HZ    | 1.57                     | 0.70              |
| 11:K:151:MET:HE2  | 11:K:155:GLU:HB3  | 1.74                     | 0.70              |
| 4:R:151:GLU:HG2   | 4:R:155:ILE:HG22  | 1.74                     | 0.70              |
| 6:F:45:VAL:HG23   | 6:F:189:LEU:HD13  | 1.74                     | 0.69              |
| 4:D:53:LYS:HD2    | 4:D:54:LEU:N      | 2.06                     | 0.69              |
| 14:N:119:LEU:HG   | 14:N:134:LEU:HD12 | 1.73                     | 0.69              |
| 3:C:4:ARG:HG3     | 6:F:123:TYR:OH    | 1.92                     | 0.69              |
| 1:O:126:GLN:O     | 1:O:129:THR:HB    | 1.92                     | 0.69              |
| 6:T:69:HIS:HE1    | 6:T:103:LEU:O     | 1.75                     | 0.68              |
| 7:U:126:ASN:C     | 7:U:126:ASN:HD22  | 2.02                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:68:ASP:HA     | 11:K:68:ILE:CD1   | 2.23                     | 0.68              |
| 8:V:175:MET:HE3   | 8:V:188:PHE:CE2   | 2.28                     | 0.68              |
| 14:2:153:ARG:HH11 | 14:2:153:ARG:HG3  | 1.57                     | 0.68              |
| 13:M:18:THR:HG21  | 13:M:30:TYR:HD1   | 1.59                     | 0.68              |
| 14:N:171:ASN:ND2  | 14:N:174:ARG:HH21 | 1.90                     | 0.68              |
| 7:G:126:ASN:C     | 7:G:126:ASN:HD22  | 2.01                     | 0.68              |
| 1:A:157:THR:HG22  | 1:A:163:TYR:HB2   | 1.76                     | 0.67              |
| 4:D:159:TRP:CZ2   | 5:E:59:LEU:HD23   | 2.29                     | 0.67              |
| 7:U:34:THR:HG21   | 7:U:50:GLU:O      | 1.94                     | 0.67              |
| 11:Y:138:TYR:CZ   | 11:Y:171:MET:HG3  | 2.29                     | 0.67              |
| 1:A:129:THR:CG2   | 2:B:128:ARG:HH21  | 2.07                     | 0.67              |
| 1:O:129:THR:HG22  | 2:P:128:ARG:HH21  | 1.60                     | 0.67              |
| 5:E:146:GLY:HA2   | 5:E:222:ILE:HG12  | 1.76                     | 0.67              |
| 7:G:34:THR:HG21   | 7:G:50:GLU:O      | 1.95                     | 0.67              |
| 4:R:29:ARG:HG2    | 4:R:29:ARG:O      | 1.95                     | 0.66              |
| 5:E:40:ILE:HD12   | 5:E:200:VAL:HG23  | 1.77                     | 0.66              |
| 7:U:41:CYS:HB2    | 7:U:186:LEU:O     | 1.95                     | 0.66              |
| 3:Q:140:TYR:CD1   | 3:Q:225:VAL:HG21  | 2.31                     | 0.66              |
| 9:W:35:HIS:CB     | 9:W:56:THR:HG21   | 2.25                     | 0.66              |
| 13:1:18:THR:HG23  | 13:1:30:TYR:HA    | 1.77                     | 0.65              |
| 4:R:187:THR:HB    | 4:R:190:GLU:HG2   | 1.78                     | 0.65              |
| 5:S:204:LEU:O     | 5:S:208:MET:HG3   | 1.94                     | 0.65              |
| 11:K:2:ILE:HD13   | 11:K:167:LEU:HD13 | 1.78                     | 0.65              |
| 2:P:122:THR:CG2   | 3:Q:129:ARG:HH21  | 2.08                     | 0.65              |
| 6:T:190:ILE:HG23  | 6:T:213:ILE:HD13  | 1.76                     | 0.65              |
| 8:H:175:MET:HE3   | 8:H:188:PHE:CE2   | 2.32                     | 0.65              |
| 1:O:123:ASN:HD21  | 2:P:83:ARG:HE     | 1.43                     | 0.65              |
| 12:Z:12:ILE:HB    | 12:Z:180:VAL:HB   | 1.78                     | 0.65              |
| 7:U:94:GLU:HG3    | 7:U:114:ARG:HH11  | 1.60                     | 0.65              |
| 4:R:43:VAL:HG23   | 4:R:191:CYS:SG    | 2.37                     | 0.64              |
| 11:Y:151:MET:HE2  | 11:Y:155:GLU:HB3  | 1.77                     | 0.64              |
| 4:R:189:GLU:HA    | 4:R:232:TYR:OH    | 1.97                     | 0.64              |
| 12:Z:20:ALA:HB2   | 12:Z:31:VAL:HG21  | 1.80                     | 0.64              |
| 4:D:151:GLU:HG2   | 4:D:155:ILE:HG22  | 1.78                     | 0.64              |
| 7:G:168:ARG:HG3   | 7:G:172:LYS:HE3   | 1.78                     | 0.64              |
| 3:Q:13:PHE:H      | 4:R:19:GLN:HE22   | 1.46                     | 0.64              |
| 3:Q:120:GLN:O     | 3:Q:123:THR:HB    | 1.98                     | 0.64              |
| 12:L:144:TYR:O    | 12:L:145:LYS:HD2  | 1.98                     | 0.64              |
| 4:D:162:GLN:HE21  | 4:D:163:THR:H     | 1.47                     | 0.63              |
| 13:M:186:HIS:HD2  | 13:M:188:GLN:H    | 1.45                     | 0.63              |
| 11:Y:2:ILE:HD13   | 11:Y:167:LEU:HD13 | 1.80                     | 0.63              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:123:ASN:HD21 | 2:B:83:ARG:HE     | 1.47                     | 0.63              |
| 4:D:155:ILE:HD12 | 5:E:83:ALA:HB2    | 1.79                     | 0.63              |
| 10:J:2:ILE:HG21  | 10:J:133:ALA:HB3  | 1.81                     | 0.63              |
| 1:O:199:TRP:O    | 1:O:203:VAL:HG23  | 1.99                     | 0.62              |
| 2:P:1:MET:SD     | 2:P:2:THR:N       | 2.71                     | 0.62              |
| 9:W:172:ASN:HD22 | 9:W:192:THR:HA    | 1.63                     | 0.62              |
| 13:1:186:HIS:HD2 | 13:1:188:GLN:H    | 1.46                     | 0.62              |
| 8:H:38:HIS:HD2   | 16:H:276:HOH:O    | 1.82                     | 0.62              |
| 8:H:161:GLN:HE21 | 8:V:136:GLY:HA2   | 1.64                     | 0.62              |
| 4:R:53:LYS:HD2   | 4:R:54:LEU:N      | 2.14                     | 0.62              |
| 9:I:165:ASN:ND2  | 14:2:148:ARG:HH11 | 1.97                     | 0.62              |
| 2:P:196:LEU:HD23 | 2:P:209:ILE:HD12  | 1.81                     | 0.62              |
| 5:E:167:TYR:CE1  | 6:F:57:SER:HB3    | 2.35                     | 0.62              |
| 10:X:2:ILE:HG21  | 10:X:133:ALA:HB3  | 1.82                     | 0.62              |
| 1:A:179:THR:O    | 1:A:183:GLU:HG3   | 1.99                     | 0.62              |
| 7:G:169:GLN:CD   | 7:G:169:GLN:H     | 2.05                     | 0.62              |
| 12:L:7:ARG:HD2   | 12:L:110:PRO:O    | 1.99                     | 0.62              |
| 7:G:146:HIS:HD2  | 16:G:295:HOH:O    | 1.81                     | 0.61              |
| 2:B:196:LEU:HD23 | 2:B:209:ILE:HD12  | 1.82                     | 0.61              |
| 3:C:47:ALA:HB2   | 3:C:213:PHE:CE1   | 2.36                     | 0.61              |
| 4:R:53:LYS:O     | 4:R:54:LEU:HB2    | 2.00                     | 0.61              |
| 2:P:4:ARG:HH22   | 5:S:126:GLY:HA3   | 1.64                     | 0.61              |
| 4:D:53:LYS:O     | 4:D:54:LEU:HB2    | 1.99                     | 0.61              |
| 1:A:196:GLU:HG2  | 1:A:201:LYS:HB3   | 1.82                     | 0.61              |
| 10:J:28:SER:HB2  | 11:K:125:VAL:HG21 | 1.81                     | 0.60              |
| 12:L:20:ALA:HB2  | 12:L:31:VAL:HG21  | 1.82                     | 0.60              |
| 8:V:143:ARG:NH2  | 8:V:146:MET:HE3   | 2.16                     | 0.60              |
| 6:F:93:ASN:HD21  | 13:M:61:ASN:HD21  | 1.48                     | 0.60              |
| 6:F:139:LYS:HE3  | 14:N:83:TYR:OH    | 2.01                     | 0.60              |
| 8:H:8:PHE:CE2    | 8:H:10:ASP:HB2    | 2.36                     | 0.60              |
| 5:S:146:GLY:HA2  | 5:S:222:ILE:HG12  | 1.82                     | 0.60              |
| 2:B:119:GLN:O    | 2:B:122:THR:HB    | 2.02                     | 0.60              |
| 12:Z:107:LYS:H   | 12:Z:107:LYS:CD   | 2.08                     | 0.60              |
| 13:1:18:THR:HG21 | 13:1:30:TYR:HD1   | 1.66                     | 0.60              |
| 11:Y:3:ILE:HG22  | 11:Y:102:LEU:HD12 | 1.84                     | 0.60              |
| 13:1:18:THR:HG22 | 13:1:30:TYR:HA    | 1.83                     | 0.60              |
| 11:K:3:ILE:HG22  | 11:K:102:LEU:HD12 | 1.84                     | 0.60              |
| 5:S:97:VAL:HG21  | 12:Z:65:LEU:HD13  | 1.83                     | 0.60              |
| 6:T:190:ILE:CG2  | 6:T:213:ILE:HD13  | 2.31                     | 0.60              |
| 13:1:186:HIS:HE1 | 16:1:309:HOH:O    | 1.85                     | 0.60              |
| 3:C:181:LYS:O    | 3:C:184:MET:HG3   | 2.02                     | 0.60              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:123:THR:CG2  | 4:D:127:ARG:HH21  | 2.15                     | 0.59              |
| 13:M:33:LYS:HD2  | 13:M:46:ASN:ND2   | 2.12                     | 0.59              |
| 14:N:153:ARG:HG3 | 14:N:153:ARG:HH11 | 1.67                     | 0.59              |
| 7:G:94:GLU:HG2   | 7:G:114:ARG:HB3   | 1.84                     | 0.59              |
| 11:K:3:ILE:HG21  | 16:K:311:HOH:O    | 2.02                     | 0.59              |
| 14:2:89:ALA:HA   | 14:2:122:VAL:HG21 | 1.83                     | 0.59              |
| 5:E:39:GLY:HA2   | 5:E:47:VAL:O      | 2.03                     | 0.59              |
| 8:H:140:LYS:HG3  | 8:V:137:TYR:CE1   | 2.37                     | 0.59              |
| 3:C:18:ARG:HE    | 4:D:29:ARG:HH21   | 1.49                     | 0.59              |
| 4:D:163:THR:HG21 | 4:D:171:VAL:HG22  | 1.83                     | 0.59              |
| 2:P:119:GLN:O    | 2:P:122:THR:HB    | 2.02                     | 0.59              |
| 9:I:35:HIS:CB    | 9:I:56:THR:HG21   | 2.32                     | 0.59              |
| 9:I:194:ASN:HB3  | 13:1:211:LYS:HE3  | 1.83                     | 0.59              |
| 4:D:68:ASP:HA    | 11:K:68:ILE:HD13  | 1.84                     | 0.58              |
| 7:G:41:CYS:HB2   | 7:G:186:LEU:O     | 2.03                     | 0.58              |
| 3:Q:123:THR:CG2  | 4:R:127:ARG:HH21  | 2.15                     | 0.58              |
| 1:A:245:LEU:O    | 1:A:248:ILE:HG13  | 2.02                     | 0.58              |
| 3:C:96:GLN:HE22  | 10:J:63:ASN:HD22  | 1.51                     | 0.58              |
| 2:P:64:VAL:HG11  | 2:P:212:ALA:HB2   | 1.84                     | 0.58              |
| 5:S:184:LEU:HD22 | 6:T:56:LEU:HD22   | 1.85                     | 0.58              |
| 1:O:64:LEU:O     | 1:O:66:PRO:HD3    | 2.03                     | 0.58              |
| 3:Q:2:GLY:HA3    | 6:T:123:TYR:CE1   | 2.38                     | 0.58              |
| 3:Q:4:ARG:HG3    | 6:T:123:TYR:OH    | 2.04                     | 0.58              |
| 6:T:139:LYS:HE3  | 14:2:83:TYR:OH    | 2.04                     | 0.58              |
| 2:B:122:THR:CG2  | 3:C:129:ARG:HH21  | 2.16                     | 0.58              |
| 2:B:10:THR:HG22  | 2:B:18:LEU:HD22   | 1.86                     | 0.58              |
| 11:K:18:LYS:HD3  | 11:K:179:ILE:HG13 | 1.86                     | 0.58              |
| 9:W:112:SER:HB3  | 9:W:125:LEU:HD13  | 1.84                     | 0.58              |
| 11:K:148:ARG:O   | 11:K:151:MET:HG3  | 2.04                     | 0.58              |
| 12:L:43:GLY:HA2  | 12:L:100:MET:O    | 2.04                     | 0.58              |
| 1:O:212:ASP:HB3  | 16:O:1011:HOH:O   | 2.03                     | 0.57              |
| 1:O:245:LEU:O    | 1:O:248:ILE:HG13  | 2.04                     | 0.57              |
| 7:G:213:LEU:HD21 | 7:G:215:ILE:HD11  | 1.86                     | 0.57              |
| 13:M:4:LEU:HD11  | 13:M:141:LEU:HD21 | 1.84                     | 0.57              |
| 10:X:28:SER:HB2  | 11:Y:125:VAL:HG21 | 1.84                     | 0.57              |
| 4:R:103:PRO:HG2  | 4:R:140:PRO:HG3   | 1.85                     | 0.57              |
| 6:F:190:ILE:HG23 | 6:F:213:ILE:HD13  | 1.85                     | 0.57              |
| 6:T:9:ASP:HB2    | 6:T:11:VAL:HG12   | 1.86                     | 0.57              |
| 6:T:208:VAL:O    | 6:T:227:GLY:HA2   | 2.05                     | 0.57              |
| 3:C:140:TYR:CD1  | 3:C:225:VAL:HG21  | 2.40                     | 0.57              |
| 12:L:107:LYS:H   | 12:L:107:LYS:CD   | 2.13                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:126:GLN:O     | 1:A:129:THR:HB    | 2.03                     | 0.57              |
| 4:D:162:GLN:NE2   | 4:D:163:THR:H     | 2.02                     | 0.57              |
| 8:H:25:TYR:HD1    | 14:2:138:PHE:HZ   | 1.53                     | 0.57              |
| 9:W:84:LYS:HE2    | 9:W:119:THR:HG23  | 1.86                     | 0.57              |
| 6:F:198:SER:HA    | 6:F:201:LEU:HG    | 1.87                     | 0.56              |
| 1:O:72:ILE:CD1    | 1:O:224:GLU:HG2   | 2.35                     | 0.56              |
| 4:R:103:PRO:HG2   | 4:R:140:PRO:CG    | 2.35                     | 0.56              |
| 4:R:151:GLU:CG    | 4:R:155:ILE:HG22  | 2.35                     | 0.56              |
| 3:C:19:LEU:HD13   | 3:C:123:THR:HG23  | 1.87                     | 0.56              |
| 3:C:64:GLU:HG3    | 3:C:65:LYS:HG3    | 1.85                     | 0.56              |
| 12:L:145:LYS:HB2  | 12:L:148:LEU:HD13 | 1.88                     | 0.56              |
| 1:O:123:ASN:ND2   | 2:P:83:ARG:HE     | 2.03                     | 0.56              |
| 9:W:128:GLY:O     | 9:W:131:SER:HB2   | 2.04                     | 0.56              |
| 11:Y:118:ILE:HG12 | 11:Y:124:LYS:HG3  | 1.86                     | 0.56              |
| 4:D:11:PHE:N      | 5:E:23:GLN:HE22   | 2.01                     | 0.56              |
| 13:M:137:ILE:HG22 | 13:M:141:LEU:HD22 | 1.87                     | 0.56              |
| 6:T:103:LEU:HD11  | 6:T:107:ARG:HG2   | 1.86                     | 0.56              |
| 11:Y:138:TYR:CE2  | 11:Y:171:MET:HG3  | 2.40                     | 0.56              |
| 4:D:187:THR:HB    | 4:D:190:GLU:HG2   | 1.88                     | 0.56              |
| 4:D:203:VAL:HG11  | 4:D:209:ASN:HB3   | 1.88                     | 0.56              |
| 1:O:196:GLU:HG2   | 1:O:201:LYS:CB    | 2.36                     | 0.56              |
| 9:I:165:ASN:HD22  | 14:2:148:ARG:HH11 | 1.51                     | 0.56              |
| 14:N:89:ALA:HA    | 14:N:122:VAL:HG21 | 1.88                     | 0.56              |
| 11:K:3:ILE:HG22   | 11:K:102:LEU:CD1  | 2.36                     | 0.56              |
| 3:C:13:PHE:H      | 4:D:19:GLN:HE22   | 1.54                     | 0.55              |
| 7:U:37:ILE:HG22   | 7:U:163:ALA:CB    | 2.36                     | 0.55              |
| 4:D:29:ARG:O      | 4:D:29:ARG:HG2    | 2.05                     | 0.55              |
| 14:N:148:ARG:HH11 | 9:W:165:ASN:ND2   | 2.03                     | 0.55              |
| 5:S:39:GLY:HA2    | 5:S:47:VAL:O      | 2.06                     | 0.55              |
| 8:V:83:LYS:HD3    | 16:V:912:HOH:O    | 2.06                     | 0.55              |
| 11:Y:3:ILE:HG21   | 16:Y:858:HOH:O    | 2.07                     | 0.55              |
| 2:B:38:LYS:HG3    | 2:B:43:VAL:HG22   | 1.89                     | 0.55              |
| 6:F:190:ILE:CG2   | 6:F:213:ILE:HD13  | 2.37                     | 0.55              |
| 7:U:146:HIS:HD2   | 16:U:1060:HOH:O   | 1.89                     | 0.55              |
| 4:D:188:VAL:HG21  | 4:D:216:LYS:HE2   | 1.89                     | 0.55              |
| 5:E:24:VAL:O      | 5:E:27:SER:HB3    | 2.07                     | 0.55              |
| 2:P:24:ALA:O      | 2:P:28:VAL:HG23   | 2.06                     | 0.55              |
| 1:O:101:ALA:HA    | 1:O:112:MET:CE    | 2.28                     | 0.55              |
| 4:R:42:VAL:HG11   | 4:R:136:ALA:HB1   | 1.87                     | 0.55              |
| 1:A:101:ALA:HA    | 1:A:112:MET:CE    | 2.30                     | 0.55              |
| 3:C:4:ARG:HG3     | 6:F:123:TYR:HH    | 1.71                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:F:201:LEU:HD11  | 6:F:206:LEU:HD22  | 1.88                     | 0.55              |
| 4:R:11:PHE:H      | 5:S:23:GLN:HE22   | 1.54                     | 0.55              |
| 7:U:169:GLN:CD    | 7:U:169:GLN:H     | 2.15                     | 0.55              |
| 13:1:33:LYS:HD2   | 13:1:46:ASN:ND2   | 2.17                     | 0.55              |
| 6:F:227:GLY:O     | 6:F:230:VAL:HG22  | 2.07                     | 0.55              |
| 4:R:184:PRO:O     | 4:R:186:ALA:N     | 2.41                     | 0.54              |
| 7:U:165:GLY:O     | 7:U:168:ARG:HB3   | 2.07                     | 0.54              |
| 9:I:43:CYS:SG     | 9:I:98:LEU:HB3    | 2.48                     | 0.54              |
| 4:R:163:THR:HG21  | 4:R:171:VAL:HG22  | 1.89                     | 0.54              |
| 4:R:188:VAL:O     | 4:R:192:VAL:HG23  | 2.06                     | 0.54              |
| 2:P:36:GLY:HA2    | 2:P:44:VAL:O      | 2.07                     | 0.54              |
| 11:Y:148:ARG:O    | 11:Y:151:MET:HG3  | 2.07                     | 0.54              |
| 10:J:100:VAL:O    | 10:J:112:ILE:HA   | 2.07                     | 0.54              |
| 14:N:138:PHE:HZ   | 8:V:25:TYR:HD1    | 1.56                     | 0.54              |
| 12:L:46:ALA:HB3   | 12:L:98:GLY:O     | 2.07                     | 0.54              |
| 9:W:172:ASN:ND2   | 9:W:192:THR:HA    | 2.23                     | 0.54              |
| 1:O:129:THR:CG2   | 2:P:128:ARG:HH21  | 2.20                     | 0.54              |
| 4:R:192:VAL:O     | 4:R:196:VAL:HG23  | 2.07                     | 0.54              |
| 13:1:18:THR:HG21  | 13:1:30:TYR:CD1   | 2.42                     | 0.54              |
| 14:2:81:PRO:HD2   | 14:2:112:GLN:OE1  | 2.07                     | 0.54              |
| 9:I:34:LEU:HD22   | 9:I:174:ASP:HB3   | 1.90                     | 0.54              |
| 2:B:1:MET:SD      | 2:B:2:THR:N       | 2.79                     | 0.54              |
| 5:E:249:ALA:O     | 5:E:250:GLU:HG2   | 2.08                     | 0.54              |
| 9:I:128:GLY:O     | 9:I:131:SER:HB2   | 2.07                     | 0.54              |
| 1:O:60:PRO:HG2    | 1:O:61:ASP:H      | 1.73                     | 0.53              |
| 7:U:178:LEU:CD2   | 7:U:194:GLN:HG2   | 2.38                     | 0.53              |
| 3:C:68:LYS:HG3    | 3:C:227:GLN:OE1   | 2.08                     | 0.53              |
| 7:G:194:GLN:O     | 7:G:198:ILE:HG13  | 2.08                     | 0.53              |
| 8:V:163:ILE:HG23  | 8:V:170:GLY:HA2   | 1.88                     | 0.53              |
| 9:W:34:LEU:HD22   | 9:W:174:ASP:HB3   | 1.89                     | 0.53              |
| 9:W:196:ARG:NH2   | 10:X:142:GLU:HG3  | 2.23                     | 0.53              |
| 8:H:67:THR:HA     | 8:H:71:GLY:O      | 2.09                     | 0.53              |
| 9:I:196:ARG:NH2   | 10:J:142:GLU:HG3  | 2.23                     | 0.53              |
| 8:V:14:LEU:O      | 8:V:175:MET:HA    | 2.08                     | 0.53              |
| 14:2:19:LEU:HB2   | 14:2:184:SER:HB2  | 1.90                     | 0.53              |
| 1:A:82:VAL:CG1    | 1:A:142:THR:HB    | 2.38                     | 0.53              |
| 8:V:31:THR:HG22   | 8:V:32:ASP:H      | 1.74                     | 0.53              |
| 11:Y:7:ARG:O      | 11:Y:7:ARG:HG2    | 2.09                     | 0.53              |
| 3:Q:100:LYS:HZ1   | 11:Y:85:GLN:NE2   | 2.06                     | 0.53              |
| 4:D:31:THR:HB     | 4:D:47:GLU:HG3    | 1.90                     | 0.53              |
| 13:1:137:ILE:HG22 | 13:1:141:LEU:HD22 | 1.91                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:75:GLY:HA3    | 5:E:228:PHE:CD1   | 2.44                     | 0.53              |
| 8:H:114:PRO:HD2   | 8:H:118:SER:O     | 2.07                     | 0.53              |
| 9:I:112:SER:HB3   | 9:I:125:LEU:HD13  | 1.90                     | 0.53              |
| 3:C:210:ARG:HG2   | 3:C:210:ARG:HH11  | 1.72                     | 0.53              |
| 8:H:9:LYS:O       | 8:H:107:LYS:HD3   | 2.08                     | 0.53              |
| 13:M:198:VAL:HG22 | 13:M:203:VAL:HG22 | 1.90                     | 0.53              |
| 8:V:31:THR:HG22   | 8:V:32:ASP:N      | 2.23                     | 0.53              |
| 1:A:123:ASN:ND2   | 2:B:83:ARG:HE     | 2.07                     | 0.53              |
| 4:R:160:SER:HB3   | 4:R:179:TYR:CE1   | 2.44                     | 0.53              |
| 4:R:162:GLN:HA    | 4:R:162:GLN:HE21  | 1.74                     | 0.53              |
| 4:R:180:ASP:OD2   | 4:R:182:LYS:HB2   | 2.07                     | 0.53              |
| 2:B:122:THR:HG22  | 3:C:129:ARG:HH21  | 1.73                     | 0.52              |
| 8:H:-2:LEU:O      | 8:H:1:ALA:N       | 2.42                     | 0.52              |
| 2:B:37:ILE:HD12   | 2:B:192:ALA:HB2   | 1.90                     | 0.52              |
| 16:S:1049:HOH:O   | 13:1:70:HIS:HE1   | 1.91                     | 0.52              |
| 7:U:196:ALA:O     | 7:U:200:TYR:HD1   | 1.92                     | 0.52              |
| 4:R:159:TRP:CZ2   | 5:S:59:LEU:HD23   | 2.45                     | 0.52              |
| 6:F:10:THR:HG21   | 6:F:120:THR:HA    | 1.91                     | 0.52              |
| 1:O:83:VAL:HG11   | 1:O:90:ALA:CB     | 2.39                     | 0.52              |
| 4:R:68:ASP:HA     | 11:Y:68:ILE:HD13  | 1.90                     | 0.52              |
| 8:H:161:GLN:NE2   | 8:V:136:GLY:HA2   | 2.24                     | 0.52              |
| 12:L:86:LEU:HD13  | 12:L:86:LEU:C     | 2.35                     | 0.52              |
| 7:U:178:LEU:HD21  | 7:U:194:GLN:HG2   | 1.91                     | 0.52              |
| 1:A:44:ALA:HB2    | 1:A:53:VAL:HG12   | 1.91                     | 0.52              |
| 5:S:45:GLY:HA2    | 5:S:153:TYR:CE1   | 2.44                     | 0.52              |
| 5:E:67:ILE:HG22   | 5:E:228:PHE:HZ    | 1.75                     | 0.52              |
| 8:H:171:GLY:HA2   | 14:2:211:TRP:CH2  | 2.44                     | 0.52              |
| 8:V:161:GLN:HE22  | 8:V:165:TRP:HE1   | 1.56                     | 0.52              |
| 8:V:176:VAL:HG12  | 8:V:178:LEU:HD13  | 1.91                     | 0.52              |
| 6:F:3:ARG:C       | 6:F:5:ASN:H       | 2.17                     | 0.52              |
| 4:R:155:ILE:HD11  | 5:S:82:THR:OG1    | 2.10                     | 0.52              |
| 5:E:167:TYR:CD1   | 6:F:57:SER:HB3    | 2.46                     | 0.51              |
| 4:R:155:ILE:HD12  | 5:S:83:ALA:HB2    | 1.92                     | 0.51              |
| 5:S:249:ALA:O     | 5:S:250:GLU:HG2   | 2.09                     | 0.51              |
| 4:R:171:VAL:HG12  | 4:R:202:VAL:HG21  | 1.92                     | 0.51              |
| 5:E:46:VAL:HG11   | 5:E:145:ALA:HB1   | 1.93                     | 0.51              |
| 10:J:33:LYS:O     | 10:J:43:GLY:HA2   | 2.09                     | 0.51              |
| 11:K:138:TYR:CE1  | 11:K:171:MET:HG3  | 2.46                     | 0.51              |
| 14:N:8:TYR:CE2    | 14:N:162:VAL:HG22 | 2.45                     | 0.51              |
| 1:O:83:VAL:HG11   | 1:O:90:ALA:HB2    | 1.93                     | 0.51              |
| 1:A:157:THR:HG22  | 1:A:163:TYR:CB    | 2.39                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:F:208:VAL:O     | 6:F:227:GLY:HA2   | 2.10                     | 0.51              |
| 11:K:138:TYR:CZ   | 11:K:171:MET:HG3  | 2.46                     | 0.51              |
| 10:X:1:GLY:HA3    | 10:X:33:LYS:HE2   | 1.92                     | 0.51              |
| 7:U:178:LEU:HD21  | 7:U:194:GLN:CG    | 2.40                     | 0.51              |
| 1:A:82:VAL:HG12   | 1:A:142:THR:HB    | 1.92                     | 0.51              |
| 12:L:4:LEU:HD12   | 12:L:161:ILE:HD11 | 1.93                     | 0.51              |
| 9:W:104:ASP:HB2   | 9:W:105:PRO:CD    | 2.40                     | 0.51              |
| 14:2:166:GLU:O    | 14:2:170:VAL:HG23 | 2.11                     | 0.51              |
| 1:A:60:PRO:HG2    | 1:A:61:ASP:H      | 1.74                     | 0.51              |
| 7:U:34:THR:CG2    | 7:U:50:GLU:O      | 2.58                     | 0.51              |
| 11:Y:3:ILE:HG22   | 11:Y:102:LEU:CD1  | 2.41                     | 0.51              |
| 5:S:52:LYS:HG3    | 5:S:64:ILE:HG21   | 1.92                     | 0.50              |
| 8:H:84:GLU:O      | 8:H:88:GLU:HB2    | 2.11                     | 0.50              |
| 7:U:17:ASP:OD2    | 7:U:19:ARG:HD3    | 2.11                     | 0.50              |
| 7:U:94:GLU:HG2    | 7:U:114:ARG:CB    | 2.37                     | 0.50              |
| 4:R:162:GLN:HE21  | 4:R:163:THR:H     | 1.59                     | 0.50              |
| 7:U:37:ILE:HG22   | 7:U:163:ALA:HB2   | 1.93                     | 0.50              |
| 14:2:111:VAL:HG23 | 14:2:192:ILE:HG22 | 1.93                     | 0.50              |
| 4:R:68:ASP:HA     | 11:Y:68:ILE:CD1   | 2.41                     | 0.50              |
| 6:T:62:LYS:O      | 6:T:73:SER:HA     | 2.10                     | 0.50              |
| 1:A:141:LEU:O     | 1:A:156:LYS:HA    | 2.11                     | 0.50              |
| 6:F:69:HIS:HE1    | 6:F:103:LEU:O     | 1.93                     | 0.50              |
| 2:P:64:VAL:HG11   | 2:P:212:ALA:CB    | 2.41                     | 0.50              |
| 3:Q:123:THR:HG22  | 4:R:127:ARG:HH21  | 1.76                     | 0.50              |
| 14:2:40:ASN:H     | 14:2:40:ASN:HD22  | 1.59                     | 0.50              |
| 6:F:81:ALA:HB2    | 6:F:130:VAL:HG21  | 1.93                     | 0.50              |
| 9:W:52:THR:O      | 9:W:56:THR:HB     | 2.12                     | 0.50              |
| 10:X:33:LYS:O     | 10:X:43:GLY:HA2   | 2.11                     | 0.50              |
| 4:D:70:HIS:CE1    | 4:D:103:PRO:HB2   | 2.47                     | 0.50              |
| 8:H:3:ILE:HG22    | 8:H:16:ALA:CB     | 2.41                     | 0.50              |
| 3:Q:163:ILE:HG13  | 3:Q:164:SER:N     | 2.27                     | 0.50              |
| 4:R:162:GLN:NE2   | 4:R:163:THR:H     | 2.08                     | 0.50              |
| 3:C:51:LYS:HG2    | 3:C:52:VAL:HG23   | 1.94                     | 0.50              |
| 14:2:151:VAL:HG23 | 14:2:151:VAL:O    | 2.11                     | 0.50              |
| 11:Y:18:LYS:HD3   | 11:Y:179:ILE:HG13 | 1.92                     | 0.49              |
| 11:K:20:VAL:HG11  | 12:L:122:LEU:HD11 | 1.94                     | 0.49              |
| 7:U:66:ILE:HG13   | 7:U:214:GLU:OE1   | 2.13                     | 0.49              |
| 5:E:75:GLY:HA3    | 5:E:228:PHE:CE1   | 2.48                     | 0.49              |
| 14:N:175:VAL:O    | 14:N:178:TYR:HB2  | 2.13                     | 0.49              |
| 5:S:121:LEU:HD13  | 6:T:126:ARG:HH21  | 1.77                     | 0.49              |
| 8:H:83:LYS:HD3    | 16:H:337:HOH:O    | 2.11                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:K:59:ILE:O     | 11:K:63:ILE:HG12  | 2.12                     | 0.49              |
| 13:M:186:HIS:CD2  | 13:M:188:GLN:H    | 2.29                     | 0.49              |
| 5:E:243:LEU:HD22  | 5:E:247:GLU:HG3   | 1.95                     | 0.49              |
| 14:N:179:ARG:HD3  | 9:W:139:GLU:OE2   | 2.12                     | 0.49              |
| 4:R:29:ARG:CB     | 4:R:29:ARG:HH11   | 2.26                     | 0.49              |
| 10:X:5:ALA:HA     | 10:X:13:ALA:O     | 2.12                     | 0.49              |
| 1:A:72:ILE:CD1    | 1:A:224:GLU:HG2   | 2.42                     | 0.49              |
| 1:O:81:MET:HE3    | 1:O:83:VAL:CG2    | 2.42                     | 0.49              |
| 6:T:45:VAL:HG23   | 6:T:189:LEU:HD13  | 1.95                     | 0.49              |
| 12:Z:145:LYS:HB2  | 12:Z:148:LEU:HD13 | 1.94                     | 0.49              |
| 5:E:202:LYS:O     | 5:E:205:LYS:HB3   | 2.13                     | 0.49              |
| 14:N:211:TRP:CH2  | 8:V:171:GLY:HA2   | 2.48                     | 0.49              |
| 5:S:46:VAL:HG11   | 5:S:145:ALA:HB1   | 1.94                     | 0.49              |
| 5:S:75:GLY:HA3    | 5:S:228:PHE:CD1   | 2.48                     | 0.49              |
| 1:O:157:THR:HG22  | 1:O:163:TYR:HB2   | 1.95                     | 0.49              |
| 3:Q:111:LEU:C     | 3:Q:111:LEU:HD23  | 2.37                     | 0.49              |
| 3:Q:210:ARG:HG2   | 3:Q:210:ARG:HH11  | 1.78                     | 0.49              |
| 3:C:163:ILE:HG13  | 3:C:164:SER:N     | 2.27                     | 0.49              |
| 12:L:4:LEU:HD13   | 12:L:15:ALA:O     | 2.12                     | 0.48              |
| 5:S:193:LEU:O     | 5:S:197:GLU:HG3   | 2.13                     | 0.48              |
| 3:C:94:HIS:HE1    | 16:C:253:HOH:O    | 1.97                     | 0.48              |
| 7:G:167:GLY:HA2   | 7:G:205:ASP:OD2   | 2.14                     | 0.48              |
| 8:H:31:THR:HG22   | 8:H:32:ASP:N      | 2.28                     | 0.48              |
| 9:I:200:GLN:HG2   | 13:1:173:LYS:HG2  | 1.95                     | 0.48              |
| 13:M:18:THR:HG21  | 13:M:30:TYR:CD1   | 2.43                     | 0.48              |
| 1:O:123:ASN:HD22  | 2:P:83:ARG:HH21   | 1.60                     | 0.48              |
| 4:D:184:PRO:O     | 4:D:186:ALA:N     | 2.46                     | 0.48              |
| 8:H:176:VAL:HG12  | 8:H:178:LEU:HD13  | 1.95                     | 0.48              |
| 13:M:211:LYS:HE3  | 9:W:194:ASN:HB3   | 1.96                     | 0.48              |
| 13:1:86:HIS:HD2   | 16:1:343:HOH:O    | 1.96                     | 0.48              |
| 1:A:43:LEU:HD23   | 1:A:210:MET:HE3   | 1.95                     | 0.48              |
| 14:2:153:ARG:HH11 | 14:2:153:ARG:CG   | 2.25                     | 0.48              |
| 1:A:156:LYS:O     | 1:A:163:TYR:HA    | 2.14                     | 0.48              |
| 5:E:127:ALA:HA    | 6:F:125:GLY:HA2   | 1.96                     | 0.48              |
| 5:E:204:LEU:O     | 5:E:208:MET:HG3   | 2.13                     | 0.48              |
| 11:K:118:ILE:HA   | 11:K:123:THR:O    | 2.14                     | 0.48              |
| 14:N:27:ARG:HD3   | 14:N:28:PHE:CE2   | 2.49                     | 0.48              |
| 6:T:50:LYS:HB3    | 6:T:59:TYR:HB3    | 1.96                     | 0.48              |
| 6:T:194:VAL:O     | 6:T:197:ILE:HG22  | 2.14                     | 0.48              |
| 12:L:4:LEU:CD1    | 12:L:161:ILE:HD11 | 2.43                     | 0.48              |
| 4:R:42:VAL:CG2    | 4:R:145:PRO:HB2   | 2.43                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:X:108:GLY:HA2  | 10:X:183:LYS:HD3  | 1.96                     | 0.48              |
| 10:X:115:PHE:HA   | 10:X:120:CYS:O    | 2.13                     | 0.48              |
| 4:D:238:GLN:C     | 4:D:240:LYS:H     | 2.21                     | 0.48              |
| 2:P:94:HIS:HD2    | 9:W:61:SER:OG     | 1.96                     | 0.48              |
| 5:S:167:TYR:CE1   | 6:T:57:SER:HB3    | 2.49                     | 0.48              |
| 6:T:3:ARG:C       | 6:T:5:ASN:H       | 2.20                     | 0.48              |
| 2:B:57:MET:HE3    | 2:B:60:THR:HG21   | 1.95                     | 0.47              |
| 3:C:96:GLN:NE2    | 10:J:63:ASN:HD22  | 2.12                     | 0.47              |
| 7:G:165:GLY:O     | 7:G:168:ARG:HB3   | 2.14                     | 0.47              |
| 10:J:36:HIS:HB3   | 10:J:41:PHE:CD2   | 2.49                     | 0.47              |
| 13:M:34:VAL:HG12  | 13:M:196:LEU:HD22 | 1.96                     | 0.47              |
| 7:U:170:SER:O     | 7:U:173:ALA:HB3   | 2.14                     | 0.47              |
| 12:Z:4:LEU:CD1    | 12:Z:161:ILE:HD11 | 2.43                     | 0.47              |
| 1:A:204:GLU:HG3   | 1:A:244:ARG:HG3   | 1.96                     | 0.47              |
| 4:D:232:TYR:O     | 4:D:236:ILE:HG13  | 2.14                     | 0.47              |
| 6:F:3:ARG:O       | 6:F:5:ASN:N       | 2.47                     | 0.47              |
| 10:J:1:GLY:HA3    | 10:J:33:LYS:HE2   | 1.96                     | 0.47              |
| 14:N:122:VAL:HA   | 14:N:127:VAL:O    | 2.14                     | 0.47              |
| 3:Q:96:GLN:NE2    | 10:X:63:ASN:HD22  | 2.10                     | 0.47              |
| 6:T:128:TYR:O     | 6:T:149:PRO:HB3   | 2.14                     | 0.47              |
| 3:C:70:ASN:ND2    | 3:C:71:ASP:H      | 2.13                     | 0.47              |
| 7:G:51:LYS:HG2    | 7:G:65:LYS:HD2    | 1.96                     | 0.47              |
| 8:H:14:LEU:O      | 8:H:175:MET:HA    | 2.14                     | 0.47              |
| 10:J:29:ASN:HD22  | 10:J:30:LYS:HG3   | 1.78                     | 0.47              |
| 1:O:92:ASN:C      | 1:O:92:ASN:HD22   | 2.22                     | 0.47              |
| 11:Y:95:ARG:HD2   | 16:Y:861:HOH:O    | 2.14                     | 0.47              |
| 4:D:162:GLN:HE21  | 4:D:162:GLN:HA    | 1.79                     | 0.47              |
| 11:K:91:ILE:HD12  | 11:K:91:ILE:HA    | 1.78                     | 0.47              |
| 8:V:161:GLN:NE2   | 8:V:165:TRP:HE1   | 2.12                     | 0.47              |
| 2:B:107:THR:O     | 2:B:111:VAL:HG23  | 2.14                     | 0.47              |
| 6:F:103:LEU:HD11  | 6:F:107:ARG:HG2   | 1.97                     | 0.47              |
| 3:Q:70:ASN:HD22   | 3:Q:71:ASP:H      | 1.61                     | 0.47              |
| 6:T:93:ASN:HD21   | 13:1:61:ASN:HD21  | 1.61                     | 0.47              |
| 13:1:67:HIS:HD2   | 16:1:366:HOH:O    | 1.97                     | 0.47              |
| 14:2:120:ARG:HH11 | 14:2:130:SER:HB2  | 1.79                     | 0.47              |
| 4:D:159:TRP:CE2   | 5:E:59:LEU:HD23   | 2.50                     | 0.47              |
| 4:D:160:SER:HB3   | 4:D:179:TYR:CE1   | 2.50                     | 0.47              |
| 3:Q:22:VAL:HG11   | 3:Q:154:SER:HB3   | 1.95                     | 0.47              |
| 6:T:156:LEU:HD13  | 6:T:159:THR:HB    | 1.97                     | 0.47              |
| 11:Y:91:ILE:HD12  | 11:Y:91:ILE:HA    | 1.77                     | 0.47              |
| 1:A:189:SER:O     | 1:A:190:LYS:HB2   | 2.15                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:D:188:VAL:O    | 4:D:192:VAL:HG23  | 2.14                     | 0.47              |
| 2:P:38:LYS:HG3   | 2:P:43:VAL:HG22   | 1.95                     | 0.47              |
| 8:V:15:GLY:HA2   | 8:V:174:ARG:O     | 2.14                     | 0.47              |
| 8:V:146:MET:HE2  | 8:V:150:GLU:HB3   | 1.95                     | 0.47              |
| 9:W:152:ILE:O    | 9:W:156:SER:HB2   | 2.14                     | 0.47              |
| 10:X:100:VAL:O   | 10:X:112:ILE:HA   | 2.15                     | 0.47              |
| 14:2:40:ASN:HD22 | 14:2:40:ASN:N     | 2.12                     | 0.47              |
| 1:A:52:VAL:HG12  | 1:A:54:ILE:HD12   | 1.97                     | 0.47              |
| 3:C:70:ASN:HD22  | 3:C:71:ASP:H      | 1.61                     | 0.47              |
| 6:F:206:LEU:HD23 | 6:F:206:LEU:H     | 1.80                     | 0.47              |
| 7:G:126:ASN:HD22 | 7:G:127:SER:N     | 2.12                     | 0.47              |
| 1:O:135:ARG:HB3  | 7:U:12:SER:HB2    | 1.97                     | 0.47              |
| 6:T:46:LEU:HG    | 6:T:135:ILE:HD13  | 1.96                     | 0.47              |
| 7:U:81:ILE:HB    | 7:U:82:PRO:HD3    | 1.97                     | 0.47              |
| 2:B:160:LYS:HD3  | 2:B:179:TRP:CZ3   | 2.50                     | 0.47              |
| 4:D:11:PHE:H     | 5:E:23:GLN:NE2    | 2.06                     | 0.47              |
| 2:P:196:LEU:HD12 | 2:P:196:LEU:HA    | 1.80                     | 0.47              |
| 4:R:43:VAL:CG2   | 4:R:191:CYS:SG    | 3.02                     | 0.47              |
| 10:X:36:HIS:HB3  | 10:X:41:PHE:CD2   | 2.50                     | 0.47              |
| 7:G:94:GLU:HG3   | 7:G:114:ARG:NH1   | 2.22                     | 0.47              |
| 11:K:44:SER:OG   | 11:K:102:LEU:HB2  | 2.14                     | 0.47              |
| 13:M:67:HIS:HD2  | 16:M:288:HOH:O    | 1.97                     | 0.47              |
| 3:Q:135:PHE:O    | 3:Q:150:THR:HA    | 2.15                     | 0.47              |
| 4:D:103:PRO:HG2  | 4:D:140:PRO:HG3   | 1.97                     | 0.46              |
| 11:K:131:ALA:HB1 | 11:K:135:SER:HB2  | 1.98                     | 0.46              |
| 8:V:175:MET:HE3  | 8:V:188:PHE:HE2   | 1.77                     | 0.46              |
| 9:W:17:ASP:HA    | 9:W:172:ASN:O     | 2.15                     | 0.46              |
| 13:1:7:ALA:HB2   | 13:1:113:VAL:HG23 | 1.97                     | 0.46              |
| 5:E:49:GLY:HA2   | 5:E:218:GLN:O     | 2.15                     | 0.46              |
| 1:O:197:GLU:CD   | 1:O:197:GLU:H     | 2.24                     | 0.46              |
| 12:Z:25:TRP:HH2  | 13:1:138:MET:HB2  | 1.80                     | 0.46              |
| 14:2:119:LEU:HG  | 14:2:134:LEU:HD12 | 1.97                     | 0.46              |
| 1:A:196:GLU:HG2  | 1:A:201:LYS:HB2   | 1.93                     | 0.46              |
| 6:F:113:CYS:SG   | 6:F:151:GLY:O     | 2.74                     | 0.46              |
| 1:O:141:LEU:O    | 1:O:156:LYS:HA    | 2.15                     | 0.46              |
| 6:T:82:ARG:O     | 6:T:86:ASN:HB2    | 2.16                     | 0.46              |
| 1:A:244:ARG:O    | 1:A:248:ILE:HG23  | 2.16                     | 0.46              |
| 6:F:46:LEU:HG    | 6:F:135:ILE:HD13  | 1.96                     | 0.46              |
| 12:Z:145:LYS:HB2 | 12:Z:148:LEU:CD1  | 2.45                     | 0.46              |
| 5:S:192:THR:OG1  | 5:S:195:GLU:HG3   | 2.15                     | 0.46              |
| 10:J:108:GLY:HA2 | 10:J:183:LYS:HD3  | 1.97                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:F:47:VAL:CG1   | 6:F:211:LEU:HD11  | 2.45                     | 0.46              |
| 9:I:123:TYR:HB3  | 9:I:142:TRP:CZ2   | 2.51                     | 0.46              |
| 3:Q:4:ARG:CZ     | 5:S:11:GLY:HA2    | 2.46                     | 0.46              |
| 8:V:157:HIS:CD2  | 8:V:196:LEU:HD13  | 2.51                     | 0.46              |
| 7:G:42:ASN:N     | 7:G:42:ASN:HD22   | 2.14                     | 0.46              |
| 14:N:121:TYR:O   | 14:N:128:THR:HA   | 2.16                     | 0.46              |
| 4:R:35:GLY:HA2   | 4:R:43:VAL:O      | 2.16                     | 0.46              |
| 1:A:158:ASP:HB2  | 1:A:159:PRO:CD    | 2.46                     | 0.46              |
| 7:G:34:THR:CG2   | 7:G:50:GLU:O      | 2.62                     | 0.46              |
| 8:H:83:LYS:HD2   | 8:H:119:VAL:CG2   | 2.46                     | 0.46              |
| 10:J:11:CYS:HA   | 10:J:103:ILE:HD11 | 1.97                     | 0.46              |
| 11:K:12:VAL:HG23 | 11:K:113:PRO:HB2  | 1.96                     | 0.46              |
| 6:T:47:VAL:CG1   | 6:T:211:LEU:HD11  | 2.46                     | 0.46              |
| 1:A:81:MET:HE3   | 1:A:83:VAL:CG2    | 2.46                     | 0.46              |
| 8:H:175:MET:HE3  | 8:H:188:PHE:HE2   | 1.79                     | 0.46              |
| 5:S:31:ILE:HD13  | 5:S:141:ALA:HB2   | 1.98                     | 0.46              |
| 7:U:135:THR:O    | 7:U:149:MET:HA    | 2.15                     | 0.46              |
| 9:W:84:LYS:HG3   | 9:W:85:GLN:N      | 2.31                     | 0.46              |
| 12:L:4:LEU:HD11  | 12:L:15:ALA:HB3   | 1.98                     | 0.45              |
| 13:M:186:HIS:HE1 | 16:M:234:HOH:O    | 1.99                     | 0.45              |
| 14:N:7:LYS:HD2   | 14:N:157:ILE:HD13 | 1.97                     | 0.45              |
| 4:R:70:HIS:CE1   | 4:R:103:PRO:HB2   | 2.52                     | 0.45              |
| 5:S:243:LEU:HD22 | 5:S:247:GLU:HG3   | 1.98                     | 0.45              |
| 6:T:3:ARG:O      | 6:T:5:ASN:N       | 2.49                     | 0.45              |
| 8:V:84:GLU:O     | 8:V:88:GLU:HB2    | 2.16                     | 0.45              |
| 12:Z:128:CYS:HB2 | 12:Z:137:TYR:CE2  | 2.51                     | 0.45              |
| 8:V:4:MET:HB3    | 8:V:126:ILE:HG22  | 1.98                     | 0.45              |
| 2:B:43:VAL:HG11  | 2:B:137:ALA:HB1   | 1.99                     | 0.45              |
| 3:C:146:TYR:OH   | 3:C:218:LYS:HB2   | 2.16                     | 0.45              |
| 7:G:170:SER:O    | 7:G:173:ALA:HB3   | 2.16                     | 0.45              |
| 9:I:20:SER:HB3   | 9:I:28:ASP:HB3    | 1.98                     | 0.45              |
| 1:O:240:ASN:HB3  | 16:O:1085:HOH:O   | 2.16                     | 0.45              |
| 9:W:196:ARG:NH2  | 10:X:142:GLU:O    | 2.50                     | 0.45              |
| 10:X:78:PHE:O    | 10:X:82:VAL:HG23  | 2.16                     | 0.45              |
| 12:Z:5:ALA:HA    | 12:Z:13:ILE:O     | 2.17                     | 0.45              |
| 13:1:4:LEU:HD11  | 13:1:141:LEU:HD21 | 1.97                     | 0.45              |
| 7:G:106:ILE:HA   | 7:G:107:PRO:HD3   | 1.88                     | 0.45              |
| 8:H:159:LEU:O    | 8:H:163:ILE:HG13  | 2.16                     | 0.45              |
| 4:R:199:LEU:O    | 4:R:203:VAL:HG23  | 2.16                     | 0.45              |
| 8:V:83:LYS:HD2   | 8:V:119:VAL:CG2   | 2.47                     | 0.45              |
| 10:X:12:VAL:HG13 | 10:X:110:PRO:HB3  | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:37:GLY:C      | 3:C:148:LEU:HD21  | 2.42                     | 0.45              |
| 6:F:3:ARG:C       | 6:F:5:ASN:N       | 2.74                     | 0.45              |
| 11:K:24:ILE:O     | 11:K:24:ILE:HG12  | 2.16                     | 0.45              |
| 12:L:25:TRP:CH2   | 13:M:135:SER:HA   | 2.51                     | 0.45              |
| 1:O:74:CYS:O      | 1:O:98:LYS:HE2    | 2.16                     | 0.45              |
| 6:T:182:ILE:HD13  | 6:T:188:GLU:HB3   | 1.98                     | 0.45              |
| 8:V:8:PHE:CE2     | 8:V:10:ASP:HB2    | 2.52                     | 0.45              |
| 4:D:189:GLU:HA    | 4:D:232:TYR:OH    | 2.16                     | 0.45              |
| 10:J:181:ILE:HG23 | 10:J:186:VAL:HG22 | 1.97                     | 0.45              |
| 12:L:209:ASN:O    | 10:X:30:LYS:NZ    | 2.50                     | 0.45              |
| 1:O:164:VAL:HG22  | 1:O:165:GLY:N     | 2.32                     | 0.45              |
| 4:R:29:ARG:NH1    | 4:R:29:ARG:HB2    | 2.32                     | 0.45              |
| 1:A:72:ILE:HD12   | 1:A:224:GLU:HG2   | 1.98                     | 0.45              |
| 9:I:113:ILE:HG12  | 9:I:119:THR:HG22  | 1.99                     | 0.45              |
| 13:M:138:MET:HE3  | 10:X:168:ARG:NH2  | 2.32                     | 0.45              |
| 14:N:111:VAL:HG23 | 14:N:192:ILE:HG22 | 1.99                     | 0.45              |
| 3:Q:100:LYS:NZ    | 11:Y:85:GLN:NE2   | 2.64                     | 0.45              |
| 4:R:51:THR:HG22   | 4:R:52:LEU:HD22   | 1.99                     | 0.45              |
| 6:T:117:GLN:OE1   | 6:T:121:GLN:NE2   | 2.50                     | 0.45              |
| 5:E:208:MET:HE2   | 5:E:208:MET:HB3   | 1.83                     | 0.45              |
| 11:Y:90:SER:O     | 11:Y:93:SER:HB3   | 2.16                     | 0.45              |
| 4:D:42:VAL:HG11   | 4:D:136:ALA:HB1   | 1.98                     | 0.45              |
| 7:G:36:SER:HB3    | 7:G:49:VAL:HG23   | 1.99                     | 0.45              |
| 6:T:19:LEU:HD21   | 7:U:129:ARG:HD2   | 1.99                     | 0.45              |
| 6:T:175:THR:HG22  | 6:T:175:THR:O     | 2.17                     | 0.45              |
| 8:H:146:MET:CE    | 8:H:150:GLU:HB3   | 2.47                     | 0.45              |
| 9:I:52:THR:O      | 9:I:56:THR:HB     | 2.17                     | 0.45              |
| 4:R:203:VAL:HG11  | 4:R:209:ASN:HB3   | 1.98                     | 0.45              |
| 7:U:149:MET:HE2   | 7:U:159:TYR:CZ    | 2.52                     | 0.45              |
| 9:W:123:TYR:HB3   | 9:W:142:TRP:CZ2   | 2.52                     | 0.45              |
| 11:Y:17:SER:HB2   | 11:Y:175:PHE:HB2  | 1.99                     | 0.45              |
| 1:A:43:LEU:C      | 1:A:43:LEU:HD12   | 2.42                     | 0.44              |
| 2:B:12:PHE:N      | 3:C:21:GLN:HE22   | 2.07                     | 0.44              |
| 3:C:130:PRO:HG3   | 16:C:263:HOH:O    | 2.16                     | 0.44              |
| 4:D:174:PHE:CD2   | 4:D:198:SER:HB3   | 2.53                     | 0.44              |
| 6:F:93:ASN:HD21   | 13:M:61:ASN:ND2   | 2.14                     | 0.44              |
| 6:F:221:PRO:O     | 6:F:222:PHE:C     | 2.60                     | 0.44              |
| 11:K:6:ILE:HD11   | 11:K:147:TYR:CE1  | 2.52                     | 0.44              |
| 3:Q:70:ASN:ND2    | 3:Q:71:ASP:H      | 2.15                     | 0.44              |
| 5:S:176:SER:O     | 5:S:180:GLN:HB2   | 2.17                     | 0.44              |
| 9:W:114:HIS:HE1   | 16:W:340:HOH:O    | 2.00                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:I:143:LYS:O    | 9:I:146:LEU:HG   | 2.17                     | 0.44              |
| 10:J:5:ALA:HA    | 10:J:13:ALA:O    | 2.17                     | 0.44              |
| 11:K:35:ARG:NH1  | 11:K:57:GLU:OE2  | 2.51                     | 0.44              |
| 5:S:46:VAL:O     | 5:S:221:CYS:HA   | 2.18                     | 0.44              |
| 5:S:169:ALA:HB1  | 5:S:183:LEU:HD22 | 1.99                     | 0.44              |
| 9:W:84:LYS:HE2   | 9:W:119:THR:CG2  | 2.46                     | 0.44              |
| 14:2:175:VAL:O   | 14:2:178:TYR:HB2 | 2.17                     | 0.44              |
| 5:E:46:VAL:O     | 5:E:221:CYS:HA   | 2.18                     | 0.44              |
| 6:F:135:ILE:HA   | 6:F:143:HIS:O    | 2.17                     | 0.44              |
| 2:P:66:LEU:C     | 2:P:66:LEU:HD23  | 2.43                     | 0.44              |
| 3:Q:181:LYS:HG3  | 3:Q:184:MET:HG3  | 2.00                     | 0.44              |
| 8:V:-2:LEU:O     | 8:V:1:ALA:N      | 2.51                     | 0.44              |
| 2:B:110:LEU:O    | 2:B:114:VAL:HG23 | 2.17                     | 0.44              |
| 3:C:66:LEU:HD12  | 3:C:76:ALA:HA    | 1.99                     | 0.44              |
| 5:S:168:ASN:HB3  | 5:S:187:TRP:CE2  | 2.53                     | 0.44              |
| 6:T:3:ARG:C      | 6:T:5:ASN:N      | 2.76                     | 0.44              |
| 6:T:217:GLY:O    | 6:T:218:LYS:C    | 2.60                     | 0.44              |
| 6:F:43:HIS:HB2   | 6:F:189:LEU:HD12 | 2.00                     | 0.44              |
| 8:H:113:ILE:HG12 | 8:H:119:VAL:HG22 | 2.00                     | 0.44              |
| 13:M:143:ASN:O   | 13:M:147:PHE:HA  | 2.17                     | 0.44              |
| 4:R:63:LYS:HE2   | 4:R:75:PHE:CZ    | 2.52                     | 0.44              |
| 4:R:226:SER:HB2  | 4:R:227:GLU:OE2  | 2.18                     | 0.44              |
| 6:T:4:ASN:HA     | 6:T:7:ASP:OD1    | 2.18                     | 0.44              |
| 10:X:44:ILE:HB   | 10:X:51:VAL:HG13 | 1.98                     | 0.44              |
| 1:A:54:ILE:HG13  | 1:A:225:VAL:HG22 | 1.99                     | 0.44              |
| 1:A:77:ARG:HH11  | 1:A:77:ARG:HB2   | 1.82                     | 0.44              |
| 3:C:221:ASN:O    | 3:C:222:ASP:HB2  | 2.18                     | 0.44              |
| 4:D:237:GLU:O    | 4:D:241:GLN:HB2  | 2.18                     | 0.44              |
| 5:E:192:THR:OG1  | 5:E:195:GLU:HG3  | 2.17                     | 0.44              |
| 8:H:163:ILE:HG23 | 8:H:170:GLY:HA2  | 1.98                     | 0.44              |
| 11:K:52:THR:CG2  | 11:K:53:VAL:N    | 2.81                     | 0.44              |
| 1:O:92:ASN:C     | 1:O:92:ASN:ND2   | 2.75                     | 0.44              |
| 2:P:3:ASP:OD1    | 2:P:5:TYR:HB2    | 2.16                     | 0.44              |
| 3:Q:51:LYS:HG2   | 3:Q:52:VAL:HG23  | 1.99                     | 0.44              |
| 3:C:77:VAL:HG22  | 3:C:135:PHE:CE1  | 2.52                     | 0.44              |
| 12:L:4:LEU:CD1   | 12:L:15:ALA:HB3  | 2.47                     | 0.44              |
| 13:M:196:LEU:CD1 | 13:M:205:LYS:HG2 | 2.47                     | 0.44              |
| 1:O:69:VAL:HA    | 7:U:157:TRP:CZ3  | 2.53                     | 0.44              |
| 3:Q:125:HIS:CB   | 4:R:126:VAL:HG12 | 2.46                     | 0.44              |
| 8:H:20:THR:HG23  | 8:H:31:THR:OG1   | 2.17                     | 0.44              |
| 2:P:110:LEU:O    | 2:P:114:VAL:HG23 | 2.18                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:R:200:LEU:C    | 4:R:202:VAL:H     | 2.26                     | 0.44              |
| 6:T:207:THR:H    | 6:T:210:ASN:HB2   | 1.82                     | 0.44              |
| 11:Y:12:VAL:HG23 | 11:Y:113:PRO:HB2  | 2.00                     | 0.44              |
| 3:C:107:PRO:HD2  | 3:C:110:ILE:HD12  | 1.99                     | 0.44              |
| 10:J:9:LYS:HD3   | 10:J:148:ASN:HB3  | 1.99                     | 0.44              |
| 4:R:90:ARG:NH1   | 11:Y:69:ARG:HA    | 2.33                     | 0.44              |
| 7:U:11:ASN:O     | 7:U:13:VAL:N      | 2.51                     | 0.44              |
| 6:F:179:PHE:HA   | 6:F:182:ILE:HG13  | 2.00                     | 0.43              |
| 7:G:217:TRP:N    | 7:G:217:TRP:CD1   | 2.86                     | 0.43              |
| 8:V:105:LYS:O    | 8:V:105:LYS:HD3   | 2.18                     | 0.43              |
| 3:C:2:GLY:HA3    | 6:F:123:TYR:CE1   | 2.53                     | 0.43              |
| 11:K:90:SER:HA   | 11:K:93:SER:HB2   | 2.00                     | 0.43              |
| 11:Y:129:TYR:CD1 | 11:Y:143:LEU:HD13 | 2.53                     | 0.43              |
| 12:Z:144:TYR:O   | 12:Z:145:LYS:HD2  | 2.18                     | 0.43              |
| 3:C:22:VAL:HG11  | 3:C:154:SER:HB3   | 2.01                     | 0.43              |
| 9:I:200:GLN:CG   | 13:1:173:LYS:HG2  | 2.48                     | 0.43              |
| 11:K:7:ARG:O     | 11:K:7:ARG:HG2    | 2.18                     | 0.43              |
| 13:M:116:PHE:N   | 13:M:116:PHE:CD1  | 2.86                     | 0.43              |
| 1:O:17:THR:HB    | 1:O:129:THR:O     | 2.19                     | 0.43              |
| 3:Q:121:GLY:C    | 3:Q:123:THR:H     | 2.25                     | 0.43              |
| 4:D:35:GLY:HA2   | 4:D:43:VAL:O      | 2.18                     | 0.43              |
| 1:O:52:VAL:HG12  | 1:O:54:ILE:CD1    | 2.49                     | 0.43              |
| 2:P:160:LYS:HD3  | 2:P:179:TRP:CZ3   | 2.52                     | 0.43              |
| 3:Q:94:HIS:CE1   | 16:Q:1058:HOH:O   | 2.71                     | 0.43              |
| 4:R:66:LYS:HA    | 4:R:72:VAL:HG12   | 1.99                     | 0.43              |
| 7:U:42:ASN:HD22  | 7:U:43:ASP:N      | 2.16                     | 0.43              |
| 9:W:26:VAL:HG11  | 9:W:29:LYS:HG2    | 1.99                     | 0.43              |
| 14:2:144:ASN:O   | 14:2:148:ARG:HG3  | 2.19                     | 0.43              |
| 4:D:103:PRO:HG2  | 4:D:140:PRO:CG    | 2.48                     | 0.43              |
| 11:K:24:ILE:HD13 | 12:L:134:THR:HG21 | 2.01                     | 0.43              |
| 11:K:145:HIS:HD2 | 11:K:146:HIS:CE1  | 2.37                     | 0.43              |
| 1:O:14:ARG:HG2   | 1:O:26:TYR:CD2    | 2.53                     | 0.43              |
| 4:R:237:GLU:O    | 4:R:241:GLN:HB2   | 2.18                     | 0.43              |
| 6:T:81:ALA:HB2   | 6:T:130:VAL:HG21  | 1.99                     | 0.43              |
| 6:T:105:VAL:HG12 | 6:T:145:LEU:HD22  | 2.00                     | 0.43              |
| 6:T:206:LEU:HD12 | 6:T:211:LEU:HD13  | 2.01                     | 0.43              |
| 9:W:80:LEU:HD12  | 9:W:113:ILE:HD11  | 2.00                     | 0.43              |
| 9:W:196:ARG:HH21 | 10:X:142:GLU:HG3  | 1.82                     | 0.43              |
| 6:F:29:ILE:HD11  | 6:F:149:PRO:CD    | 2.48                     | 0.43              |
| 7:G:189:ARG:HG3  | 7:G:189:ARG:HH11  | 1.84                     | 0.43              |
| 11:K:6:ILE:HD11  | 11:K:147:TYR:CD1  | 2.53                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:P:57:MET:HE3   | 2:P:60:THR:HG21   | 2.01                     | 0.43              |
| 3:Q:68:LYS:HG3   | 3:Q:227:GLN:OE1   | 2.19                     | 0.43              |
| 3:Q:116:SER:HB3  | 3:Q:155:GLY:O     | 2.19                     | 0.43              |
| 4:R:238:GLN:C    | 4:R:240:LYS:H     | 2.27                     | 0.43              |
| 5:S:68:VAL:HG21  | 5:S:89:ILE:HD12   | 2.01                     | 0.43              |
| 2:B:18:LEU:HD13  | 2:B:21:ILE:HD12   | 2.01                     | 0.43              |
| 6:F:71:GLY:HA3   | 6:F:222:PHE:CZ    | 2.53                     | 0.43              |
| 8:H:14:LEU:HD11  | 8:H:100:ALA:HB3   | 2.00                     | 0.43              |
| 9:I:196:ARG:HH21 | 10:J:142:GLU:HG3  | 1.82                     | 0.43              |
| 12:L:145:LYS:HB2 | 12:L:148:LEU:CD1  | 2.49                     | 0.43              |
| 4:R:31:THR:HB    | 4:R:47:GLU:HG3    | 2.00                     | 0.43              |
| 6:T:71:GLY:HA3   | 6:T:222:PHE:CE2   | 2.53                     | 0.43              |
| 1:A:176:GLN:HE21 | 1:A:180:THR:HG23  | 1.84                     | 0.43              |
| 4:D:138:PHE:CE2  | 4:D:217:PRO:HG3   | 2.53                     | 0.43              |
| 6:F:62:LYS:O     | 6:F:73:SER:HA     | 2.19                     | 0.43              |
| 9:I:80:LEU:HD12  | 9:I:113:ILE:HD11  | 2.00                     | 0.43              |
| 3:Q:54:SER:OG    | 3:Q:55:THR:N      | 2.50                     | 0.43              |
| 7:U:126:ASN:C    | 7:U:126:ASN:ND2   | 2.70                     | 0.43              |
| 14:2:131:SER:HB3 | 14:2:133:THR:O    | 2.19                     | 0.43              |
| 1:A:64:LEU:O     | 1:A:66:PRO:HD3    | 2.19                     | 0.43              |
| 1:A:92:ASN:C     | 1:A:92:ASN:HD22   | 2.27                     | 0.43              |
| 7:G:86:HIS:HD2   | 7:G:131:PHE:CE2   | 2.37                     | 0.43              |
| 2:P:97:TYR:HD1   | 2:P:103:GLU:O     | 2.02                     | 0.43              |
| 3:Q:221:ASN:O    | 3:Q:222:ASP:HB2   | 2.19                     | 0.43              |
| 6:T:13:PHE:HB2   | 7:U:22:GLN:HE22   | 1.83                     | 0.43              |
| 4:D:63:LYS:HE2   | 4:D:75:PHE:CZ     | 2.54                     | 0.43              |
| 5:E:168:ASN:HB3  | 5:E:187:TRP:CE2   | 2.53                     | 0.43              |
| 9:I:84:LYS:HE2   | 9:I:119:THR:HG23  | 2.00                     | 0.43              |
| 1:O:88:PRO:HB2   | 7:U:120:GLN:HG3   | 1.99                     | 0.43              |
| 4:R:151:GLU:HB2  | 4:R:152:PRO:CD    | 2.49                     | 0.43              |
| 5:S:75:GLY:HA3   | 5:S:228:PHE:CE1   | 2.53                     | 0.43              |
| 7:U:194:GLN:HE21 | 7:U:197:LYS:HD3   | 1.83                     | 0.43              |
| 2:B:36:GLY:HA2   | 2:B:44:VAL:O      | 2.19                     | 0.42              |
| 6:F:45:VAL:HG12  | 6:F:46:LEU:N      | 2.34                     | 0.42              |
| 6:F:101:ARG:NH1  | 16:F:252:HOH:O    | 2.51                     | 0.42              |
| 8:H:146:MET:HE3  | 8:H:150:GLU:HB3   | 2.00                     | 0.42              |
| 12:L:12:ILE:HB   | 12:L:180:VAL:HB   | 2.02                     | 0.42              |
| 12:L:40:PHE:CD2  | 12:L:73:ARG:CZ    | 3.02                     | 0.42              |
| 2:P:46:ALA:HB2   | 2:P:211:LEU:HG    | 2.01                     | 0.42              |
| 3:Q:185:LYS:HD2  | 3:Q:187:ASP:H     | 1.83                     | 0.42              |
| 12:Z:4:LEU:HD12  | 12:Z:161:ILE:HD11 | 2.00                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 13:1:14:LEU:HD23 | 13:1:14:LEU:HA    | 1.87                     | 0.42              |
| 13:1:116:PHE:CD2 | 13:1:122:TYR:HB3  | 2.54                     | 0.42              |
| 14:2:7:LYS:HD2   | 14:2:157:ILE:HD13 | 2.01                     | 0.42              |
| 2:B:46:ALA:HB2   | 2:B:211:LEU:HG    | 2.02                     | 0.42              |
| 7:G:49:VAL:HG22  | 7:G:50:GLU:N      | 2.34                     | 0.42              |
| 9:W:113:ILE:HG12 | 9:W:119:THR:HG22  | 2.00                     | 0.42              |
| 4:D:171:VAL:HG12 | 4:D:202:VAL:CG2   | 2.46                     | 0.42              |
| 5:E:201:LEU:HD12 | 5:E:201:LEU:HA    | 1.89                     | 0.42              |
| 8:H:55:ILE:HD11  | 8:H:93:LEU:HD13   | 2.00                     | 0.42              |
| 12:L:6:PHE:HA    | 12:L:125:ASP:O    | 2.20                     | 0.42              |
| 14:N:88:LEU:O    | 14:N:92:MET:HG2   | 2.20                     | 0.42              |
| 2:P:226:GLY:O    | 2:P:228:PRO:HD3   | 2.19                     | 0.42              |
| 7:U:69:VAL:HB    | 7:U:73:ILE:HB     | 2.01                     | 0.42              |
| 6:F:206:LEU:H    | 6:F:206:LEU:CD2   | 2.32                     | 0.42              |
| 7:G:172:LYS:O    | 7:G:176:GLU:HG3   | 2.20                     | 0.42              |
| 10:J:92:GLY:N    | 10:J:93:PRO:CD    | 2.83                     | 0.42              |
| 7:U:217:TRP:CZ2  | 7:U:234:LEU:HD21  | 2.54                     | 0.42              |
| 11:Y:35:ARG:NH1  | 11:Y:57:GLU:OE2   | 2.53                     | 0.42              |
| 11:Y:171:MET:HA  | 11:Y:172:PRO:HD3  | 1.86                     | 0.42              |
| 2:B:189:ILE:HG21 | 2:B:246:ARG:HD3   | 2.01                     | 0.42              |
| 8:H:51:ASP:OD2   | 8:H:93:LEU:HA     | 2.19                     | 0.42              |
| 12:L:4:LEU:HD12  | 12:L:161:ILE:CD1  | 2.50                     | 0.42              |
| 4:R:42:VAL:HG11  | 4:R:136:ALA:CB    | 2.49                     | 0.42              |
| 8:V:114:PRO:HD2  | 8:V:118:SER:O     | 2.20                     | 0.42              |
| 6:F:194:VAL:HA   | 6:F:197:ILE:HG22  | 2.00                     | 0.42              |
| 9:I:167:LEU:HD22 | 13:1:187:ILE:O    | 2.19                     | 0.42              |
| 4:R:48:ARG:HD2   | 4:R:208:LYS:O     | 2.18                     | 0.42              |
| 6:T:29:ILE:HD11  | 6:T:149:PRO:CD    | 2.50                     | 0.42              |
| 7:U:215:ILE:HG22 | 7:U:216:SER:N     | 2.34                     | 0.42              |
| 3:C:38:ILE:HD12  | 3:C:193:ALA:HB2   | 2.02                     | 0.42              |
| 3:C:137:TYR:O    | 3:C:148:LEU:HA    | 2.19                     | 0.42              |
| 4:D:68:ASP:HA    | 11:K:68:ILE:HD11  | 2.01                     | 0.42              |
| 6:F:201:LEU:CD1  | 6:F:206:LEU:HD22  | 2.49                     | 0.42              |
| 13:M:186:HIS:CD2 | 13:M:188:GLN:HB2  | 2.54                     | 0.42              |
| 1:O:54:ILE:HD13  | 1:O:206:ALA:HB1   | 2.02                     | 0.42              |
| 2:P:59:GLU:CD    | 2:P:59:GLU:H      | 2.27                     | 0.42              |
| 6:T:135:ILE:HD12 | 6:T:216:VAL:HG12  | 2.01                     | 0.42              |
| 8:V:-2:LEU:HD23  | 8:V:20:THR:HG22   | 2.02                     | 0.42              |
| 8:V:175:MET:HE3  | 8:V:188:PHE:CD2   | 2.55                     | 0.42              |
| 3:C:42:ASP:OD1   | 3:C:42:ASP:N      | 2.53                     | 0.42              |
| 9:I:3:ILE:HG13   | 9:I:99:ILE:HD12   | 2.02                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 10:J:12:VAL:HG13  | 10:J:110:PRO:HB3 | 2.01                     | 0.42              |
| 1:O:51:THR:HG21   | 1:O:144:VAL:HB   | 2.02                     | 0.42              |
| 4:R:29:ARG:O      | 4:R:29:ARG:CG    | 2.65                     | 0.42              |
| 6:T:63:ILE:HG21   | 6:T:214:ALA:HB2  | 2.01                     | 0.42              |
| 6:T:72:LEU:HD23   | 6:T:72:LEU:C     | 2.45                     | 0.42              |
| 8:V:113:ILE:HG12  | 8:V:119:VAL:HG22 | 2.01                     | 0.42              |
| 9:W:199:LYS:HE3   | 10:X:143:SER:O   | 2.20                     | 0.42              |
| 5:E:122:ARG:C     | 5:E:132:ARG:HB2  | 2.44                     | 0.42              |
| 16:E:274:HOH:O    | 13:M:86:HIS:HD2  | 2.03                     | 0.42              |
| 6:F:175:THR:O     | 6:F:175:THR:HG22 | 2.19                     | 0.42              |
| 4:R:215:VAL:HB    | 4:R:221:ILE:HG12 | 2.01                     | 0.42              |
| 14:2:121:TYR:O    | 14:2:128:THR:HA  | 2.20                     | 0.42              |
| 1:A:110:TYR:OH    | 9:I:66:HIS:HE1   | 2.02                     | 0.42              |
| 2:B:149:GLN:O     | 2:B:156:TYR:HA   | 2.20                     | 0.42              |
| 7:G:20:ASN:ND2    | 7:G:23:VAL:HG23  | 2.35                     | 0.42              |
| 7:G:49:VAL:HB     | 7:G:76:VAL:HG21  | 2.02                     | 0.42              |
| 8:H:-2:LEU:O      | 8:H:-1:GLY:C     | 2.63                     | 0.42              |
| 9:I:5:GLY:HA3     | 9:I:110:LEU:HD11 | 2.02                     | 0.42              |
| 12:L:140:LEU:HD12 | 12:L:140:LEU:HA  | 1.88                     | 0.42              |
| 1:O:63:LEU:HA     | 1:O:63:LEU:HD23  | 1.82                     | 0.42              |
| 6:T:198:SER:HA    | 6:T:201:LEU:HG   | 2.01                     | 0.42              |
| 7:U:35:THR:HA     | 7:U:164:THR:O    | 2.20                     | 0.42              |
| 2:B:226:GLY:O     | 2:B:228:PRO:HD3  | 2.20                     | 0.41              |
| 4:D:203:VAL:HG13  | 4:D:209:ASN:OD1  | 2.20                     | 0.41              |
| 6:F:4:ASN:HA      | 6:F:7:ASP:OD1    | 2.20                     | 0.41              |
| 2:P:109:LEU:HD23  | 2:P:109:LEU:HA   | 1.89                     | 0.41              |
| 4:R:200:LEU:HA    | 4:R:200:LEU:HD23 | 1.73                     | 0.41              |
| 5:S:85:ALA:O      | 5:S:89:ILE:HG12  | 2.19                     | 0.41              |
| 7:U:106:ILE:HA    | 7:U:107:PRO:HD3  | 1.86                     | 0.41              |
| 11:Y:2:ILE:O      | 11:Y:16:SER:HA   | 2.20                     | 0.41              |
| 11:Y:38:SER:HB2   | 11:Y:39:PRO:HD2  | 2.02                     | 0.41              |
| 2:B:24:ALA:O      | 2:B:28:VAL:HG23  | 2.20                     | 0.41              |
| 3:C:115:LEU:HD23  | 3:C:115:LEU:HA   | 1.80                     | 0.41              |
| 3:C:135:PHE:O     | 3:C:150:THR:HA   | 2.20                     | 0.41              |
| 13:M:91:LYS:HD3   | 13:M:96:TYR:CE2  | 2.55                     | 0.41              |
| 5:S:52:LYS:HG3    | 5:S:64:ILE:CG2   | 2.50                     | 0.41              |
| 9:W:20:SER:HB2    | 9:W:31:CYS:SG    | 2.60                     | 0.41              |
| 10:X:29:ASN:HD22  | 10:X:30:LYS:HG3  | 1.85                     | 0.41              |
| 12:Z:40:PHE:CD2   | 12:Z:73:ARG:CZ   | 3.04                     | 0.41              |
| 9:I:104:ASP:HB2   | 9:I:105:PRO:CD   | 2.50                     | 0.41              |
| 11:K:67:SER:HA    | 11:K:72:TYR:O    | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:V:83:LYS:HD2    | 8:V:119:VAL:HG21  | 2.01                     | 0.41              |
| 9:W:104:ASP:HB2   | 9:W:105:PRO:HD2   | 2.02                     | 0.41              |
| 13:1:63:VAL:HG22  | 13:1:75:LEU:HD23  | 2.01                     | 0.41              |
| 14:2:219:GLY:HA3  | 14:2:223:GLN:HB3  | 2.03                     | 0.41              |
| 2:B:196:LEU:CD2   | 2:B:209:ILE:HD12  | 2.49                     | 0.41              |
| 5:E:170:LYS:HE3   | 5:E:171:ALA:O     | 2.21                     | 0.41              |
| 12:L:40:PHE:CD2   | 12:L:73:ARG:NH1   | 2.89                     | 0.41              |
| 13:M:15:ALA:HB1   | 13:M:193:LEU:HD11 | 2.01                     | 0.41              |
| 1:A:205:PHE:CD1   | 1:A:205:PHE:C     | 2.97                     | 0.41              |
| 5:E:68:VAL:HG21   | 5:E:89:ILE:HD12   | 2.02                     | 0.41              |
| 16:E:276:HOH:O    | 13:M:70:HIS:HE1   | 2.03                     | 0.41              |
| 14:N:138:PHE:HE2  | 14:N:142:MET:SD   | 2.43                     | 0.41              |
| 1:O:158:ASP:HB2   | 1:O:159:PRO:CD    | 2.51                     | 0.41              |
| 2:P:74:VAL:HG12   | 2:P:135:LEU:HB2   | 2.01                     | 0.41              |
| 5:S:15:PHE:HB2    | 6:T:21:GLN:OE1    | 2.20                     | 0.41              |
| 11:Y:6:ILE:HD11   | 11:Y:147:TYR:CD1  | 2.56                     | 0.41              |
| 11:Y:102:LEU:HD23 | 11:Y:117:GLN:HA   | 2.02                     | 0.41              |
| 3:C:140:TYR:CD1   | 3:C:140:TYR:C     | 2.98                     | 0.41              |
| 4:D:226:SER:HB2   | 4:D:227:GLU:OE2   | 2.21                     | 0.41              |
| 6:F:194:VAL:HG13  | 6:F:206:LEU:HD11  | 2.03                     | 0.41              |
| 7:G:66:ILE:HB     | 7:G:229:PHE:CE2   | 2.56                     | 0.41              |
| 1:O:44:ALA:HA     | 1:O:52:VAL:O      | 2.21                     | 0.41              |
| 1:O:244:ARG:O     | 1:O:248:ILE:HG23  | 2.21                     | 0.41              |
| 6:T:63:ILE:HD13   | 6:T:214:ALA:HB2   | 2.02                     | 0.41              |
| 6:T:179:PHE:HA    | 6:T:182:ILE:HG13  | 2.03                     | 0.41              |
| 6:F:157:TYR:CD1   | 6:F:180:ILE:HD13  | 2.56                     | 0.41              |
| 1:O:245:LEU:HD12  | 1:O:245:LEU:HA    | 1.88                     | 0.41              |
| 3:Q:4:ARG:HG3     | 6:T:123:TYR:HH    | 1.86                     | 0.41              |
| 4:R:232:TYR:O     | 4:R:236:ILE:HG13  | 2.20                     | 0.41              |
| 6:T:194:VAL:HG13  | 6:T:206:LEU:HD11  | 2.02                     | 0.41              |
| 2:B:55:LEU:HD23   | 2:B:55:LEU:HA     | 1.82                     | 0.41              |
| 5:E:243:LEU:HD23  | 5:E:243:LEU:HA    | 1.88                     | 0.41              |
| 8:H:161:GLN:HE22  | 8:H:165:TRP:HE1   | 1.67                     | 0.41              |
| 13:M:110:LYS:HA   | 13:M:110:LYS:HD3  | 1.89                     | 0.41              |
| 1:O:88:PRO:HG2    | 16:O:1037:HOH:O   | 2.21                     | 0.41              |
| 4:R:59:ILE:HG13   | 4:R:60:THR:N      | 2.36                     | 0.41              |
| 4:R:74:SER:OG     | 4:R:134:LEU:HB2   | 2.21                     | 0.41              |
| 10:X:28:SER:CB    | 11:Y:125:VAL:HG21 | 2.50                     | 0.41              |
| 11:Y:142:LEU:HD13 | 11:Y:162:LEU:HG   | 2.03                     | 0.41              |
| 1:A:123:ASN:HD22  | 2:B:83:ARG:HH21   | 1.68                     | 0.41              |
| 1:A:133:TYR:HD1   | 16:B:283:HOH:O    | 2.04                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:43:VAL:O      | 2:B:213:ILE:HA   | 2.21                     | 0.41              |
| 4:D:203:VAL:O     | 4:D:204:GLN:HB2  | 2.19                     | 0.41              |
| 5:E:76:CYS:HB2    | 5:E:143:LEU:O    | 2.20                     | 0.41              |
| 5:E:198:LEU:HD12  | 5:E:198:LEU:HA   | 1.81                     | 0.41              |
| 6:F:156:LEU:HD13  | 6:F:159:THR:HB   | 2.02                     | 0.41              |
| 9:I:94:ILE:HD13   | 9:I:94:ILE:HG21  | 1.84                     | 0.41              |
| 9:I:163:ILE:HG23  | 9:I:170:GLY:HA2  | 2.03                     | 0.41              |
| 10:J:29:ASN:HD22  | 10:J:29:ASN:C    | 2.29                     | 0.41              |
| 12:L:65:LEU:HD12  | 12:L:65:LEU:HA   | 1.89                     | 0.41              |
| 13:M:5:GLY:HA2    | 13:M:13:VAL:O    | 2.21                     | 0.41              |
| 1:O:52:VAL:HG12   | 1:O:54:ILE:HD12  | 2.03                     | 0.41              |
| 5:S:167:TYR:CZ    | 5:S:170:LYS:HD3  | 2.56                     | 0.41              |
| 6:T:107:ARG:HG2   | 6:T:107:ARG:HH11 | 1.86                     | 0.41              |
| 7:U:39:ILE:HG12   | 7:U:175:LEU:HD11 | 2.02                     | 0.41              |
| 7:U:174:GLU:O     | 7:U:177:LYS:HB2  | 2.21                     | 0.41              |
| 8:V:101:GLY:HA2   | 8:V:178:LEU:HD23 | 2.02                     | 0.41              |
| 12:Z:140:LEU:HD12 | 12:Z:140:LEU:HA  | 1.94                     | 0.41              |
| 3:C:63:THR:HG23   | 3:C:66:LEU:O     | 2.21                     | 0.41              |
| 3:C:71:ASP:HB2    | 16:C:294:HOH:O   | 2.21                     | 0.41              |
| 6:F:207:THR:H     | 6:F:210:ASN:HB2  | 1.86                     | 0.41              |
| 8:H:13:ILE:HG12   | 8:H:177:VAL:HG13 | 2.02                     | 0.41              |
| 13:M:-7:ASN:HD22  | 13:M:-6:PRO:HD2  | 1.86                     | 0.41              |
| 3:Q:168:ASN:ND2   | 3:Q:200:THR:O    | 2.54                     | 0.41              |
| 4:R:185:PRO:HB3   | 4:R:191:CYS:HA   | 2.03                     | 0.41              |
| 5:S:49:GLY:HA2    | 5:S:218:GLN:O    | 2.21                     | 0.41              |
| 7:U:138:GLY:HA3   | 7:U:146:HIS:O    | 2.21                     | 0.41              |
| 7:U:188:ALA:O     | 7:U:192:VAL:HG23 | 2.21                     | 0.41              |
| 12:Z:46:ALA:HB3   | 12:Z:98:GLY:O    | 2.21                     | 0.41              |
| 14:2:138:PHE:HE1  | 14:2:142:MET:SD  | 2.44                     | 0.41              |
| 6:F:38:LEU:HA     | 6:F:158:GLY:HA2  | 2.03                     | 0.40              |
| 3:Q:121:GLY:C     | 3:Q:123:THR:N    | 2.78                     | 0.40              |
| 5:S:153:TYR:C     | 5:S:154:GLN:HG3  | 2.46                     | 0.40              |
| 6:T:13:PHE:H      | 7:U:22:GLN:NE2   | 2.03                     | 0.40              |
| 14:2:35:ILE:HA    | 14:2:36:PRO:HD3  | 1.85                     | 0.40              |
| 3:C:94:HIS:CE1    | 16:C:253:HOH:O   | 2.72                     | 0.40              |
| 5:E:167:TYR:CZ    | 5:E:170:LYS:HD3  | 2.57                     | 0.40              |
| 6:F:36:VAL:HG13   | 6:F:172:LEU:HD11 | 2.04                     | 0.40              |
| 1:O:205:PHE:CD1   | 1:O:205:PHE:C    | 2.99                     | 0.40              |
| 3:Q:94:HIS:HE1    | 16:Q:1058:HOH:O  | 2.03                     | 0.40              |
| 2:B:176:GLU:HG3   | 3:C:56:LEU:HD22  | 2.03                     | 0.40              |
| 13:M:116:PHE:CD2  | 13:M:122:TYR:HB3 | 2.57                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:O:144:VAL:HA    | 1:O:153:SER:O     | 2.21                     | 0.40              |
| 3:Q:130:PRO:HG3   | 16:Q:1068:HOH:O   | 2.21                     | 0.40              |
| 6:F:128:TYR:O     | 6:F:149:PRO:HB3   | 2.20                     | 0.40              |
| 14:N:18:ASN:HA    | 14:N:31:VAL:O     | 2.21                     | 0.40              |
| 1:O:189:SER:O     | 1:O:190:LYS:HB2   | 2.20                     | 0.40              |
| 2:P:108:LYS:HG2   | 16:P:1045:HOH:O   | 2.21                     | 0.40              |
| 8:V:43:CYS:HA     | 8:V:98:ILE:O      | 2.20                     | 0.40              |
| 10:X:54:LEU:CD1   | 10:X:96:VAL:HG21  | 2.52                     | 0.40              |
| 10:X:98:PRO:HB2   | 10:X:115:PHE:CD1  | 2.56                     | 0.40              |
| 10:X:146:GLU:HA   | 10:X:147:PRO:HD3  | 1.89                     | 0.40              |
| 11:Y:153:THR:HG21 | 11:Y:182:ILE:HD13 | 2.03                     | 0.40              |
| 1:A:52:VAL:HG12   | 1:A:54:ILE:CD1    | 2.52                     | 0.40              |
| 3:C:43:GLY:HA3    | 3:C:186:VAL:HG21  | 2.04                     | 0.40              |
| 3:C:111:LEU:HD23  | 3:C:111:LEU:C     | 2.46                     | 0.40              |
| 4:D:73:LEU:HD22   | 4:D:86:ILE:HG12   | 2.04                     | 0.40              |
| 1:O:101:ALA:CA    | 1:O:112:MET:HE2   | 2.32                     | 0.40              |
| 3:Q:106:ILE:HA    | 3:Q:107:PRO:HD3   | 1.97                     | 0.40              |
| 8:V:13:ILE:HG12   | 8:V:177:VAL:HG13  | 2.03                     | 0.40              |
| 14:2:167:GLU:HG3  | 16:2:348:HOH:O    | 2.22                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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     | 241/243 (99%) | 233 (97%) | 7 (3%)  | 1 (0%)   | 30          | 22 |
| 1   | O     | 241/243 (99%) | 231 (96%) | 9 (4%)  | 1 (0%)   | 30          | 22 |
| 2   | B     | 248/250 (99%) | 238 (96%) | 9 (4%)  | 1 (0%)   | 30          | 22 |
| 2   | P     | 248/250 (99%) | 235 (95%) | 10 (4%) | 3 (1%)   | 10          | 4  |
| 3   | C     | 242/244 (99%) | 225 (93%) | 13 (5%) | 4 (2%)   | 7           | 2  |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 3   | Q     | 242/244 (99%)   | 224 (93%)  | 14 (6%)  | 4 (2%)   | 7           | 2   |
| 4   | D     | 239/241 (99%)   | 223 (93%)  | 12 (5%)  | 4 (2%)   | 7           | 2   |
| 4   | R     | 239/241 (99%)   | 222 (93%)  | 13 (5%)  | 4 (2%)   | 7           | 2   |
| 5   | E     | 240/242 (99%)   | 231 (96%)  | 7 (3%)   | 2 (1%)   | 16          | 8   |
| 5   | S     | 240/242 (99%)   | 228 (95%)  | 9 (4%)   | 3 (1%)   | 9           | 3   |
| 6   | F     | 231/233 (99%)   | 214 (93%)  | 14 (6%)  | 3 (1%)   | 9           | 3   |
| 6   | T     | 231/233 (99%)   | 209 (90%)  | 19 (8%)  | 3 (1%)   | 9           | 3   |
| 7   | G     | 242/244 (99%)   | 230 (95%)  | 10 (4%)  | 2 (1%)   | 16          | 8   |
| 7   | U     | 242/244 (99%)   | 222 (92%)  | 17 (7%)  | 3 (1%)   | 10          | 4   |
| 8   | H     | 203/205 (99%)   | 193 (95%)  | 9 (4%)   | 1 (0%)   | 24          | 16  |
| 8   | V     | 203/205 (99%)   | 192 (95%)  | 10 (5%)  | 1 (0%)   | 24          | 16  |
| 9   | I     | 220/222 (99%)   | 212 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 9   | W     | 220/222 (99%)   | 212 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 10  | J     | 202/204 (99%)   | 197 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 10  | X     | 202/204 (99%)   | 198 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 11  | K     | 196/198 (99%)   | 191 (97%)  | 3 (2%)   | 2 (1%)   | 12          | 5   |
| 11  | Y     | 196/198 (99%)   | 188 (96%)  | 6 (3%)   | 2 (1%)   | 12          | 5   |
| 12  | L     | 210/212 (99%)   | 205 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 12  | Z     | 210/212 (99%)   | 205 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 13  | 1     | 220/222 (99%)   | 212 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 13  | M     | 220/222 (99%)   | 211 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 14  | 2     | 231/233 (99%)   | 219 (95%)  | 12 (5%)  | 0        | 100         | 100 |
| 14  | N     | 231/233 (99%)   | 217 (94%)  | 14 (6%)  | 0        | 100         | 100 |
| All | All   | 6330/6386 (99%) | 6017 (95%) | 269 (4%) | 44 (1%)  | 18          | 10  |

All (44) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 222 | ASP  |
| 4   | D     | 54  | LEU  |
| 4   | D     | 185 | PRO  |
| 1   | O     | 60  | PRO  |
| 3   | Q     | 222 | ASP  |
| 4   | R     | 54  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | R     | 185 | PRO  |
| 7   | U     | 11  | ASN  |
| 3   | C     | 204 | SER  |
| 4   | D     | 205 | THR  |
| 7   | G     | 11  | ASN  |
| 11  | K     | 49  | ALA  |
| 2   | P     | 50  | LYS  |
| 3   | Q     | 204 | SER  |
| 4   | R     | 205 | THR  |
| 5   | S     | 189 | SER  |
| 6   | T     | 202 | ARG  |
| 6   | T     | 218 | LYS  |
| 7   | U     | 12  | SER  |
| 1   | A     | 60  | PRO  |
| 4   | D     | 186 | ALA  |
| 5   | E     | 127 | ALA  |
| 5   | E     | 189 | SER  |
| 6   | F     | 4   | ASN  |
| 6   | F     | 202 | ARG  |
| 3   | Q     | 52  | VAL  |
| 4   | R     | 186 | ALA  |
| 7   | U     | 207 | LYS  |
| 11  | Y     | 49  | ALA  |
| 3   | C     | 52  | VAL  |
| 8   | H     | -1  | GLY  |
| 2   | P     | 2   | THR  |
| 5   | S     | 120 | ALA  |
| 5   | S     | 128 | SER  |
| 6   | T     | 4   | ASN  |
| 2   | B     | 166 | LYS  |
| 7   | G     | 207 | LYS  |
| 2   | P     | 166 | LYS  |
| 8   | V     | -1  | GLY  |
| 11  | Y     | 8   | VAL  |
| 3   | C     | 223 | GLY  |
| 11  | K     | 8   | VAL  |
| 6   | F     | 227 | GLY  |
| 3   | Q     | 223 | GLY  |

### 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     | 207/207 (100%) | 197 (95%) | 10 (5%)  | 23          | 15 |
| 1   | O     | 207/207 (100%) | 197 (95%) | 10 (5%)  | 23          | 15 |
| 2   | B     | 209/209 (100%) | 200 (96%) | 9 (4%)   | 26          | 18 |
| 2   | P     | 209/209 (100%) | 199 (95%) | 10 (5%)  | 23          | 15 |
| 3   | C     | 203/203 (100%) | 186 (92%) | 17 (8%)  | 10          | 4  |
| 3   | Q     | 203/203 (100%) | 189 (93%) | 14 (7%)  | 14          | 7  |
| 4   | D     | 213/213 (100%) | 199 (93%) | 14 (7%)  | 15          | 8  |
| 4   | R     | 213/213 (100%) | 196 (92%) | 17 (8%)  | 11          | 5  |
| 5   | E     | 198/198 (100%) | 185 (93%) | 13 (7%)  | 15          | 8  |
| 5   | S     | 198/198 (100%) | 184 (93%) | 14 (7%)  | 13          | 7  |
| 6   | F     | 192/192 (100%) | 178 (93%) | 14 (7%)  | 13          | 6  |
| 6   | T     | 192/192 (100%) | 179 (93%) | 13 (7%)  | 14          | 7  |
| 7   | G     | 201/201 (100%) | 185 (92%) | 16 (8%)  | 11          | 5  |
| 7   | U     | 201/201 (100%) | 185 (92%) | 16 (8%)  | 11          | 5  |
| 8   | H     | 168/168 (100%) | 162 (96%) | 6 (4%)   | 31          | 23 |
| 8   | V     | 168/168 (100%) | 161 (96%) | 7 (4%)   | 26          | 19 |
| 9   | I     | 181/181 (100%) | 173 (96%) | 8 (4%)   | 25          | 17 |
| 9   | W     | 181/181 (100%) | 171 (94%) | 10 (6%)  | 19          | 11 |
| 10  | J     | 172/172 (100%) | 168 (98%) | 4 (2%)   | 44          | 40 |
| 10  | X     | 172/172 (100%) | 167 (97%) | 5 (3%)   | 37          | 31 |
| 11  | K     | 175/175 (100%) | 169 (97%) | 6 (3%)   | 32          | 25 |
| 11  | Y     | 175/175 (100%) | 168 (96%) | 7 (4%)   | 28          | 20 |
| 12  | L     | 169/169 (100%) | 162 (96%) | 7 (4%)   | 27          | 19 |
| 12  | Z     | 169/169 (100%) | 161 (95%) | 8 (5%)   | 23          | 15 |
| 13  | 1     | 185/185 (100%) | 177 (96%) | 8 (4%)   | 26          | 18 |
| 13  | M     | 185/185 (100%) | 175 (95%) | 10 (5%)  | 20          | 12 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|-------------|----|
| 14  | 2     | 199/199 (100%)   | 189 (95%)  | 10 (5%)  | 22          | 14 |
| 14  | N     | 199/199 (100%)   | 190 (96%)  | 9 (4%)   | 24          | 17 |
| All | All   | 5344/5344 (100%) | 5052 (94%) | 292 (6%) | 19          | 11 |

All (292) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 33  | LYS  |
| 1   | A     | 54  | ILE  |
| 1   | A     | 77  | ARG  |
| 1   | A     | 92  | ASN  |
| 1   | A     | 124 | LEU  |
| 1   | A     | 129 | THR  |
| 1   | A     | 175 | GLN  |
| 1   | A     | 196 | GLU  |
| 1   | A     | 244 | ARG  |
| 1   | A     | 245 | LEU  |
| 2   | B     | 29  | LYS  |
| 2   | B     | 30  | GLN  |
| 2   | B     | 59  | GLU  |
| 2   | B     | 61  | LEU  |
| 2   | B     | 122 | THR  |
| 2   | B     | 157 | PHE  |
| 2   | B     | 211 | LEU  |
| 2   | B     | 236 | ARG  |
| 2   | B     | 250 | LEU  |
| 3   | C     | 3   | SER  |
| 3   | C     | 56  | LEU  |
| 3   | C     | 59  | GLN  |
| 3   | C     | 61  | THR  |
| 3   | C     | 66  | LEU  |
| 3   | C     | 80  | LEU  |
| 3   | C     | 103 | ASN  |
| 3   | C     | 123 | THR  |
| 3   | C     | 150 | THR  |
| 3   | C     | 153 | PRO  |
| 3   | C     | 185 | LYS  |
| 3   | C     | 192 | LEU  |
| 3   | C     | 198 | SER  |
| 3   | C     | 202 | ASP  |
| 3   | C     | 217 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 232 | PRO  |
| 3   | C     | 245 | THR  |
| 4   | D     | 6   | ARG  |
| 4   | D     | 21  | GLU  |
| 4   | D     | 50  | SER  |
| 4   | D     | 57  | THR  |
| 4   | D     | 132 | SER  |
| 4   | D     | 149 | GLN  |
| 4   | D     | 155 | ILE  |
| 4   | D     | 162 | GLN  |
| 4   | D     | 171 | VAL  |
| 4   | D     | 173 | GLU  |
| 4   | D     | 209 | ASN  |
| 4   | D     | 215 | VAL  |
| 4   | D     | 224 | LEU  |
| 4   | D     | 226 | SER  |
| 5   | E     | 13  | SER  |
| 5   | E     | 28  | LEU  |
| 5   | E     | 48  | LEU  |
| 5   | E     | 52  | LYS  |
| 5   | E     | 76  | CYS  |
| 5   | E     | 132 | ARG  |
| 5   | E     | 182 | GLU  |
| 5   | E     | 184 | LEU  |
| 5   | E     | 190 | SER  |
| 5   | E     | 198 | LEU  |
| 5   | E     | 201 | LEU  |
| 5   | E     | 222 | ILE  |
| 5   | E     | 243 | LEU  |
| 6   | F     | 9   | ASP  |
| 6   | F     | 10  | THR  |
| 6   | F     | 11  | VAL  |
| 6   | F     | 30  | LYS  |
| 6   | F     | 56  | LEU  |
| 6   | F     | 72  | LEU  |
| 6   | F     | 86  | ASN  |
| 6   | F     | 93  | ASN  |
| 6   | F     | 189 | LEU  |
| 6   | F     | 199 | GLN  |
| 6   | F     | 206 | LEU  |
| 6   | F     | 208 | VAL  |
| 6   | F     | 223 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | F     | 232 | LYS  |
| 7   | G     | 10  | SER  |
| 7   | G     | 34  | THR  |
| 7   | G     | 35  | THR  |
| 7   | G     | 42  | ASN  |
| 7   | G     | 120 | GLN  |
| 7   | G     | 126 | ASN  |
| 7   | G     | 168 | ARG  |
| 7   | G     | 169 | GLN  |
| 7   | G     | 170 | SER  |
| 7   | G     | 175 | LEU  |
| 7   | G     | 189 | ARG  |
| 7   | G     | 194 | GLN  |
| 7   | G     | 204 | GLU  |
| 7   | G     | 206 | ASN  |
| 7   | G     | 217 | TRP  |
| 7   | G     | 224 | ASN  |
| 8   | H     | 36  | ARG  |
| 8   | H     | 103 | ASP  |
| 8   | H     | 105 | LYS  |
| 8   | H     | 132 | THR  |
| 8   | H     | 149 | GLU  |
| 8   | H     | 178 | LEU  |
| 9   | I     | 30  | ASN  |
| 9   | I     | 34  | LEU  |
| 9   | I     | 56  | THR  |
| 9   | I     | 68  | LEU  |
| 9   | I     | 81  | GLN  |
| 9   | I     | 121 | VAL  |
| 9   | I     | 144 | GLN  |
| 9   | I     | 196 | ARG  |
| 10  | J     | 29  | ASN  |
| 10  | J     | 125 | LYS  |
| 10  | J     | 163 | LEU  |
| 10  | J     | 183 | LYS  |
| 11  | K     | 34  | THR  |
| 11  | K     | 35  | ARG  |
| 11  | K     | 52  | THR  |
| 11  | K     | 68  | ILE  |
| 11  | K     | 70  | GLU  |
| 11  | K     | 91  | ILE  |
| 12  | L     | 4   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | L     | 65  | LEU  |
| 12  | L     | 69  | ARG  |
| 12  | L     | 87  | VAL  |
| 12  | L     | 107 | LYS  |
| 12  | L     | 140 | LEU  |
| 12  | L     | 148 | LEU  |
| 13  | M     | 14  | LEU  |
| 13  | M     | 18  | THR  |
| 13  | M     | 40  | ASN  |
| 13  | M     | 62  | SER  |
| 13  | M     | 99  | HIS  |
| 13  | M     | 100 | THR  |
| 13  | M     | 117 | ASP  |
| 13  | M     | 123 | GLU  |
| 13  | M     | 141 | LEU  |
| 13  | M     | 165 | TYR  |
| 14  | N     | 40  | ASN  |
| 14  | N     | 61  | ASP  |
| 14  | N     | 62  | LEU  |
| 14  | N     | 81  | PRO  |
| 14  | N     | 96  | ARG  |
| 14  | N     | 153 | ARG  |
| 14  | N     | 204 | LEU  |
| 14  | N     | 205 | GLN  |
| 14  | N     | 218 | LYS  |
| 1   | O     | 33  | LYS  |
| 1   | O     | 77  | ARG  |
| 1   | O     | 92  | ASN  |
| 1   | O     | 114 | CYS  |
| 1   | O     | 124 | LEU  |
| 1   | O     | 129 | THR  |
| 1   | O     | 196 | GLU  |
| 1   | O     | 230 | LYS  |
| 1   | O     | 244 | ARG  |
| 1   | O     | 245 | LEU  |
| 2   | P     | 29  | LYS  |
| 2   | P     | 30  | GLN  |
| 2   | P     | 59  | GLU  |
| 2   | P     | 61  | LEU  |
| 2   | P     | 122 | THR  |
| 2   | P     | 152 | PRO  |
| 2   | P     | 157 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | P     | 211 | LEU  |
| 2   | P     | 237 | LYS  |
| 2   | P     | 250 | LEU  |
| 3   | Q     | 56  | LEU  |
| 3   | Q     | 61  | THR  |
| 3   | Q     | 66  | LEU  |
| 3   | Q     | 80  | LEU  |
| 3   | Q     | 89  | ASN  |
| 3   | Q     | 123 | THR  |
| 3   | Q     | 150 | THR  |
| 3   | Q     | 153 | PRO  |
| 3   | Q     | 158 | THR  |
| 3   | Q     | 185 | LYS  |
| 3   | Q     | 192 | LEU  |
| 3   | Q     | 198 | SER  |
| 3   | Q     | 202 | ASP  |
| 3   | Q     | 245 | THR  |
| 4   | R     | 6   | ARG  |
| 4   | R     | 21  | GLU  |
| 4   | R     | 29  | ARG  |
| 4   | R     | 36  | VAL  |
| 4   | R     | 50  | SER  |
| 4   | R     | 57  | THR  |
| 4   | R     | 109 | LEU  |
| 4   | R     | 132 | SER  |
| 4   | R     | 149 | GLN  |
| 4   | R     | 155 | ILE  |
| 4   | R     | 162 | GLN  |
| 4   | R     | 171 | VAL  |
| 4   | R     | 173 | GLU  |
| 4   | R     | 177 | LYS  |
| 4   | R     | 209 | ASN  |
| 4   | R     | 215 | VAL  |
| 4   | R     | 224 | LEU  |
| 5   | S     | 12  | VAL  |
| 5   | S     | 13  | SER  |
| 5   | S     | 28  | LEU  |
| 5   | S     | 35  | SER  |
| 5   | S     | 52  | LYS  |
| 5   | S     | 76  | CYS  |
| 5   | S     | 132 | ARG  |
| 5   | S     | 184 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | S     | 190 | SER  |
| 5   | S     | 198 | LEU  |
| 5   | S     | 201 | LEU  |
| 5   | S     | 212 | LEU  |
| 5   | S     | 222 | ILE  |
| 5   | S     | 243 | LEU  |
| 6   | T     | 9   | ASP  |
| 6   | T     | 10  | THR  |
| 6   | T     | 30  | LYS  |
| 6   | T     | 56  | LEU  |
| 6   | T     | 72  | LEU  |
| 6   | T     | 86  | ASN  |
| 6   | T     | 93  | ASN  |
| 6   | T     | 189 | LEU  |
| 6   | T     | 199 | GLN  |
| 6   | T     | 206 | LEU  |
| 6   | T     | 208 | VAL  |
| 6   | T     | 223 | THR  |
| 6   | T     | 232 | LYS  |
| 7   | U     | 10  | SER  |
| 7   | U     | 34  | THR  |
| 7   | U     | 35  | THR  |
| 7   | U     | 42  | ASN  |
| 7   | U     | 120 | GLN  |
| 7   | U     | 126 | ASN  |
| 7   | U     | 168 | ARG  |
| 7   | U     | 169 | GLN  |
| 7   | U     | 170 | SER  |
| 7   | U     | 175 | LEU  |
| 7   | U     | 189 | ARG  |
| 7   | U     | 194 | GLN  |
| 7   | U     | 204 | GLU  |
| 7   | U     | 206 | ASN  |
| 7   | U     | 217 | TRP  |
| 7   | U     | 224 | ASN  |
| 8   | V     | 36  | ARG  |
| 8   | V     | 103 | ASP  |
| 8   | V     | 105 | LYS  |
| 8   | V     | 144 | GLU  |
| 8   | V     | 149 | GLU  |
| 8   | V     | 178 | LEU  |
| 8   | V     | 190 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | W     | 13  | VAL  |
| 9   | W     | 34  | LEU  |
| 9   | W     | 39  | PRO  |
| 9   | W     | 55  | VAL  |
| 9   | W     | 56  | THR  |
| 9   | W     | 63  | ILE  |
| 9   | W     | 68  | LEU  |
| 9   | W     | 121 | VAL  |
| 9   | W     | 144 | GLN  |
| 9   | W     | 196 | ARG  |
| 10  | X     | 29  | ASN  |
| 10  | X     | 125 | LYS  |
| 10  | X     | 163 | LEU  |
| 10  | X     | 183 | LYS  |
| 10  | X     | 194 | ARG  |
| 11  | Y     | 34  | THR  |
| 11  | Y     | 35  | ARG  |
| 11  | Y     | 52  | THR  |
| 11  | Y     | 68  | ILE  |
| 11  | Y     | 70  | GLU  |
| 11  | Y     | 91  | ILE  |
| 11  | Y     | 109 | LYS  |
| 12  | Z     | 4   | LEU  |
| 12  | Z     | 9   | GLN  |
| 12  | Z     | 65  | LEU  |
| 12  | Z     | 69  | ARG  |
| 12  | Z     | 87  | VAL  |
| 12  | Z     | 107 | LYS  |
| 12  | Z     | 140 | LEU  |
| 12  | Z     | 148 | LEU  |
| 13  | 1     | 14  | LEU  |
| 13  | 1     | 40  | ASN  |
| 13  | 1     | 62  | SER  |
| 13  | 1     | 99  | HIS  |
| 13  | 1     | 100 | THR  |
| 13  | 1     | 117 | ASP  |
| 13  | 1     | 141 | LEU  |
| 13  | 1     | 165 | TYR  |
| 14  | 2     | 40  | ASN  |
| 14  | 2     | 61  | ASP  |
| 14  | 2     | 62  | LEU  |
| 14  | 2     | 74  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | 2     | 96  | ARG  |
| 14  | 2     | 153 | ARG  |
| 14  | 2     | 162 | VAL  |
| 14  | 2     | 204 | LEU  |
| 14  | 2     | 205 | GLN  |
| 14  | 2     | 218 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (188) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 92  | ASN  |
| 1   | A     | 123 | ASN  |
| 1   | A     | 126 | GLN  |
| 1   | A     | 130 | GLN  |
| 1   | A     | 175 | GLN  |
| 1   | A     | 176 | GLN  |
| 1   | A     | 184 | ASN  |
| 1   | A     | 193 | HIS  |
| 1   | A     | 195 | ASN  |
| 1   | A     | 251 | GLN  |
| 2   | B     | 94  | HIS  |
| 3   | C     | 21  | GLN  |
| 3   | C     | 70  | ASN  |
| 3   | C     | 94  | HIS  |
| 3   | C     | 96  | GLN  |
| 3   | C     | 120 | GLN  |
| 3   | C     | 124 | GLN  |
| 3   | C     | 156 | ASN  |
| 3   | C     | 177 | GLN  |
| 3   | C     | 233 | GLN  |
| 4   | D     | 19  | GLN  |
| 4   | D     | 79  | ASN  |
| 4   | D     | 118 | GLN  |
| 4   | D     | 122 | GLN  |
| 4   | D     | 149 | GLN  |
| 4   | D     | 162 | GLN  |
| 4   | D     | 167 | ASN  |
| 5   | E     | 23  | GLN  |
| 5   | E     | 108 | ASN  |
| 5   | E     | 154 | GLN  |
| 5   | E     | 168 | ASN  |
| 5   | E     | 206 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | E     | 233 | ASN  |
| 6   | F     | 5   | ASN  |
| 6   | F     | 69  | HIS  |
| 6   | F     | 86  | ASN  |
| 6   | F     | 100 | ASN  |
| 6   | F     | 117 | GLN  |
| 6   | F     | 121 | GLN  |
| 6   | F     | 152 | ASN  |
| 6   | F     | 185 | ASN  |
| 7   | G     | 22  | GLN  |
| 7   | G     | 42  | ASN  |
| 7   | G     | 89  | ASN  |
| 7   | G     | 120 | GLN  |
| 7   | G     | 126 | ASN  |
| 7   | G     | 146 | HIS  |
| 7   | G     | 206 | ASN  |
| 7   | G     | 247 | ASN  |
| 8   | H     | 38  | HIS  |
| 8   | H     | 141 | ASN  |
| 8   | H     | 157 | HIS  |
| 8   | H     | 161 | GLN  |
| 9   | I     | 30  | ASN  |
| 9   | I     | 66  | HIS  |
| 9   | I     | 91  | GLN  |
| 9   | I     | 109 | HIS  |
| 9   | I     | 114 | HIS  |
| 9   | I     | 144 | GLN  |
| 9   | I     | 165 | ASN  |
| 9   | I     | 172 | ASN  |
| 9   | I     | 189 | ASN  |
| 10  | J     | 29  | ASN  |
| 10  | J     | 55  | ASN  |
| 11  | K     | 36  | GLN  |
| 11  | K     | 54  | GLN  |
| 11  | K     | 62  | ASN  |
| 11  | K     | 85  | GLN  |
| 11  | K     | 111 | ASN  |
| 11  | K     | 117 | GLN  |
| 11  | K     | 145 | HIS  |
| 11  | K     | 190 | GLN  |
| 12  | L     | 9   | GLN  |
| 12  | L     | 24  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | L     | 62  | GLN  |
| 12  | L     | 85  | ASN  |
| 12  | L     | 176 | ASN  |
| 13  | M     | -7  | ASN  |
| 13  | M     | 27  | ASN  |
| 13  | M     | 40  | ASN  |
| 13  | M     | 46  | ASN  |
| 13  | M     | 61  | ASN  |
| 13  | M     | 67  | HIS  |
| 13  | M     | 70  | HIS  |
| 13  | M     | 71  | ASN  |
| 13  | M     | 126 | GLN  |
| 13  | M     | 144 | GLN  |
| 13  | M     | 156 | ASN  |
| 13  | M     | 186 | HIS  |
| 14  | N     | 10  | ASN  |
| 14  | N     | 40  | ASN  |
| 14  | N     | 94  | GLN  |
| 14  | N     | 163 | GLN  |
| 14  | N     | 171 | ASN  |
| 14  | N     | 186 | ASN  |
| 14  | N     | 205 | GLN  |
| 1   | O     | 39  | ASN  |
| 1   | O     | 92  | ASN  |
| 1   | O     | 123 | ASN  |
| 1   | O     | 126 | GLN  |
| 1   | O     | 130 | GLN  |
| 1   | O     | 175 | GLN  |
| 1   | O     | 184 | ASN  |
| 1   | O     | 193 | HIS  |
| 1   | O     | 195 | ASN  |
| 1   | O     | 251 | GLN  |
| 2   | P     | 94  | HIS  |
| 2   | P     | 190 | HIS  |
| 3   | Q     | 21  | GLN  |
| 3   | Q     | 70  | ASN  |
| 3   | Q     | 89  | ASN  |
| 3   | Q     | 94  | HIS  |
| 3   | Q     | 96  | GLN  |
| 3   | Q     | 120 | GLN  |
| 3   | Q     | 124 | GLN  |
| 3   | Q     | 177 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Q     | 233 | GLN  |
| 4   | R     | 19  | GLN  |
| 4   | R     | 79  | ASN  |
| 4   | R     | 118 | GLN  |
| 4   | R     | 122 | GLN  |
| 4   | R     | 149 | GLN  |
| 4   | R     | 162 | GLN  |
| 4   | R     | 167 | ASN  |
| 5   | S     | 23  | GLN  |
| 5   | S     | 108 | ASN  |
| 5   | S     | 114 | GLN  |
| 5   | S     | 168 | ASN  |
| 5   | S     | 206 | GLN  |
| 5   | S     | 233 | ASN  |
| 6   | T     | 31  | GLN  |
| 6   | T     | 69  | HIS  |
| 6   | T     | 91  | GLN  |
| 6   | T     | 117 | GLN  |
| 6   | T     | 121 | GLN  |
| 6   | T     | 148 | GLN  |
| 6   | T     | 199 | GLN  |
| 7   | U     | 22  | GLN  |
| 7   | U     | 42  | ASN  |
| 7   | U     | 86  | HIS  |
| 7   | U     | 89  | ASN  |
| 7   | U     | 120 | GLN  |
| 7   | U     | 126 | ASN  |
| 7   | U     | 146 | HIS  |
| 7   | U     | 206 | ASN  |
| 7   | U     | 247 | ASN  |
| 8   | V     | 38  | HIS  |
| 8   | V     | 141 | ASN  |
| 8   | V     | 157 | HIS  |
| 8   | V     | 161 | GLN  |
| 9   | W     | 30  | ASN  |
| 9   | W     | 66  | HIS  |
| 9   | W     | 91  | GLN  |
| 9   | W     | 114 | HIS  |
| 9   | W     | 141 | HIS  |
| 9   | W     | 144 | GLN  |
| 9   | W     | 165 | ASN  |
| 9   | W     | 172 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | W     | 189 | ASN  |
| 10  | X     | 29  | ASN  |
| 10  | X     | 55  | ASN  |
| 10  | X     | 80  | GLN  |
| 10  | X     | 148 | ASN  |
| 10  | X     | 164 | ASN  |
| 11  | Y     | 54  | GLN  |
| 11  | Y     | 62  | ASN  |
| 11  | Y     | 85  | GLN  |
| 11  | Y     | 117 | GLN  |
| 11  | Y     | 190 | GLN  |
| 12  | Z     | 9   | GLN  |
| 12  | Z     | 85  | ASN  |
| 12  | Z     | 143 | ASN  |
| 12  | Z     | 176 | ASN  |
| 13  | 1     | -7  | ASN  |
| 13  | 1     | 40  | ASN  |
| 13  | 1     | 46  | ASN  |
| 13  | 1     | 61  | ASN  |
| 13  | 1     | 71  | ASN  |
| 13  | 1     | 86  | HIS  |
| 13  | 1     | 99  | HIS  |
| 13  | 1     | 144 | GLN  |
| 13  | 1     | 150 | GLN  |
| 13  | 1     | 156 | ASN  |
| 13  | 1     | 186 | HIS  |
| 14  | 2     | 18  | ASN  |
| 14  | 2     | 40  | ASN  |
| 14  | 2     | 100 | ASN  |
| 14  | 2     | 171 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 20 ligands modelled in this entry, 20 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.