



## Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 08:47 AM UTC

PDB ID : 5IYC / pdb\_00005iyc  
EMDB ID : EMD-8137  
Title : Human core-PIC in the initial transcribing state  
Authors : He, Y.; Yan, C.; Fang, J.; Inouye, C.; Tjian, R.; Ivanov, I.; Nogales, E.  
Deposited on : 2016-03-24  
Resolution : 3.90 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

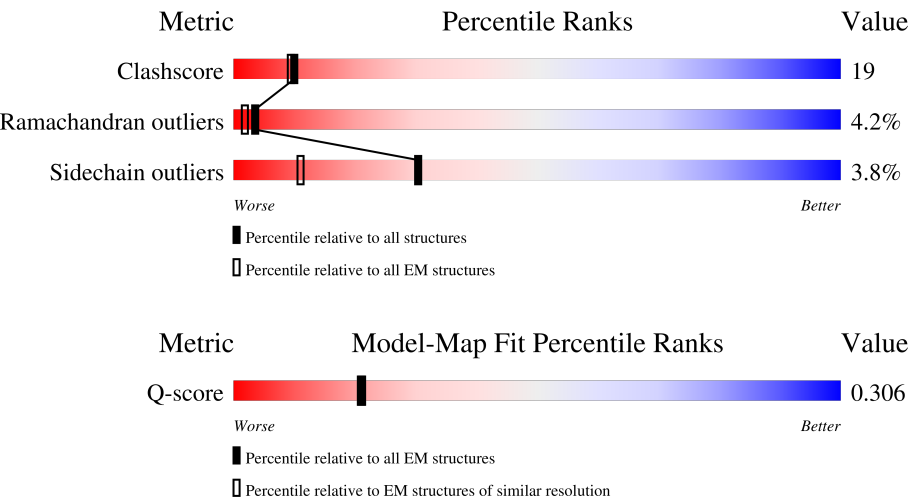
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.90 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.



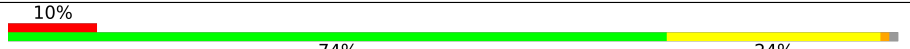
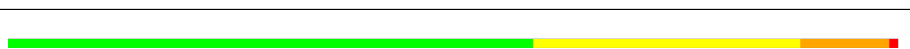
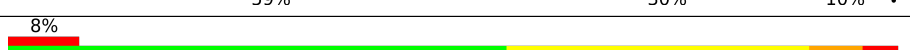
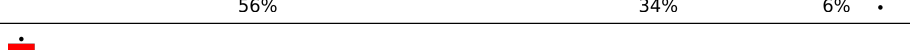
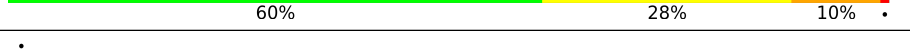
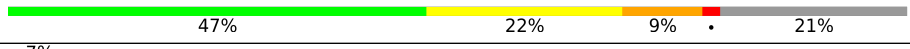
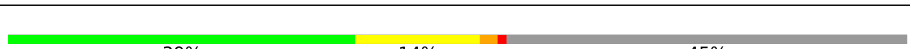
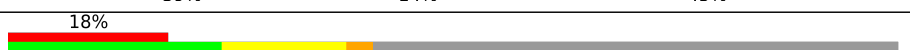
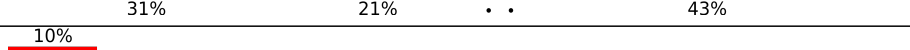
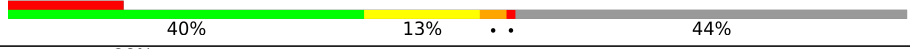
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 8855 ( 3.40 - 4.40 )                                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                    |
|-----|-------|--------|---------------------------------------------------------------------|
| 1   | A     | 1970   | <div><div>47%</div><div>22%</div><div>• •</div><div>26%</div></div> |
| 2   | B     | 1174   | <div><div>59%</div><div>33%</div><div>6%</div><div>• •</div></div>  |
| 3   | C     | 275    | <div><div>69%</div><div>26%</div><div>• •</div></div>               |
| 4   | D     | 142    | <div><div>8%</div><div>81%</div><div>10%</div><div>9%</div></div>   |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 5   | E     | 210    |    |
| 6   | F     | 127    |    |
| 7   | G     | 172    |    |
| 8   | H     | 150    |    |
| 9   | I     | 125    |    |
| 10  | J     | 67     |    |
| 11  | K     | 117    |    |
| 12  | L     | 58     |    |
| 13  | M     | 316    |    |
| 14  | N     | 376    |    |
| 15  | O     | 109    |    |
| 16  | P     | 339    |    |
| 17  | Q     | 439    |   |
| 18  | R     | 291    |  |
| 19  | S     | 517    |  |
| 20  | T     | 249    |  |
| 21  | U     | 301    |  |
| 22  | X     | 80     |  |
| 23  | Y     | 80     |  |

## 2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 47927 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1   | A     | 1454     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 11515 | 7234 | 2058 | 2150 | 73 |         |       |

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 2   | B     | 1165     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 9317  | 5878 | 1637 | 1738 | 64 |         |       |

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | C     | 275      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2213  | 1386 | 380 | 440 | 7 |         |       |

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | D     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1062  | 665 | 179 | 214 | 4 |         |       |

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB5.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5   | E     | 210      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1723  | 1088 | 301 | 325 | 9 |         |       |

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | F     | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 689   | 437 | 120 | 127 | 5 |         |       |

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | G     | 171      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1351  | 875 | 219 | 249 | 8 |         |       |

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | H     | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1205  | 764 | 196 | 239 | 6 |         |       |

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 9   | I     | 125      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1013  | 626 | 177 | 198 | 12 |         |       |

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB10.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 10  | J     | 67       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 533   | 345 | 90 | 92 | 6 |         |       |

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | K     | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 937   | 604 | 154 | 177 | 2 |         |       |

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB12.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 12  | L     | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 388   | 241 | 75 | 66 | 6 |         |       |

- Molecule 13 is a protein called Transcription initiation factor IIB.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 13  | M     | 310      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2391  | 1490 | 426 | 457 | 18 |         |       |

- Molecule 14 is a protein called Transcription initiation factor IIA subunit 1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | N     | 113      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 930   | 585 | 152 | 189 | 4 |         |       |

- Molecule 15 is a protein called Transcription initiation factor IIA subunit 2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | O     | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 806   | 510 | 142 | 151 | 3 |         |       |

- Molecule 16 is a protein called TATA-box-binding protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | P     | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1462  | 946 | 257 | 252 | 7 |         |       |

- Molecule 17 is a protein called General transcription factor IIE subunit 1.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 17  | Q     | 180      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1484  | 938 | 262 | 273 | 11 |         |       |

- Molecule 18 is a protein called Transcription initiation factor IIE subunit beta.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | R     | 165      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1357  | 865 | 235 | 253 | 4 |         |       |

- Molecule 19 is a protein called General transcription factor IIF subunit 1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | S     | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1138  | 719 | 208 | 208 | 3 |         |       |

- Molecule 20 is a protein called General transcription factor IIF subunit 2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 20  | T     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1788  | 1127 | 320 | 338 | 3 |         |       |

- Molecule 21 is a protein called Transcription elongation factor A protein 1.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 21  | U     | 170      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1343  | 818 | 247 | 263 | 15 |         |       |

- Molecule 22 is a DNA chain called SCP-X.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 22  | X     | 80       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1645  | 785 | 292 | 489 | 79 |         |       |

- Molecule 23 is a DNA chain called SCP-Y.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 23  | Y     | 80       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1624  | 771 | 291 | 483 | 79 |         |       |

- Molecule 24 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 24  | A     | 2        | Total | Mg | 0       |
|     |       |          | 2     | 2  |         |

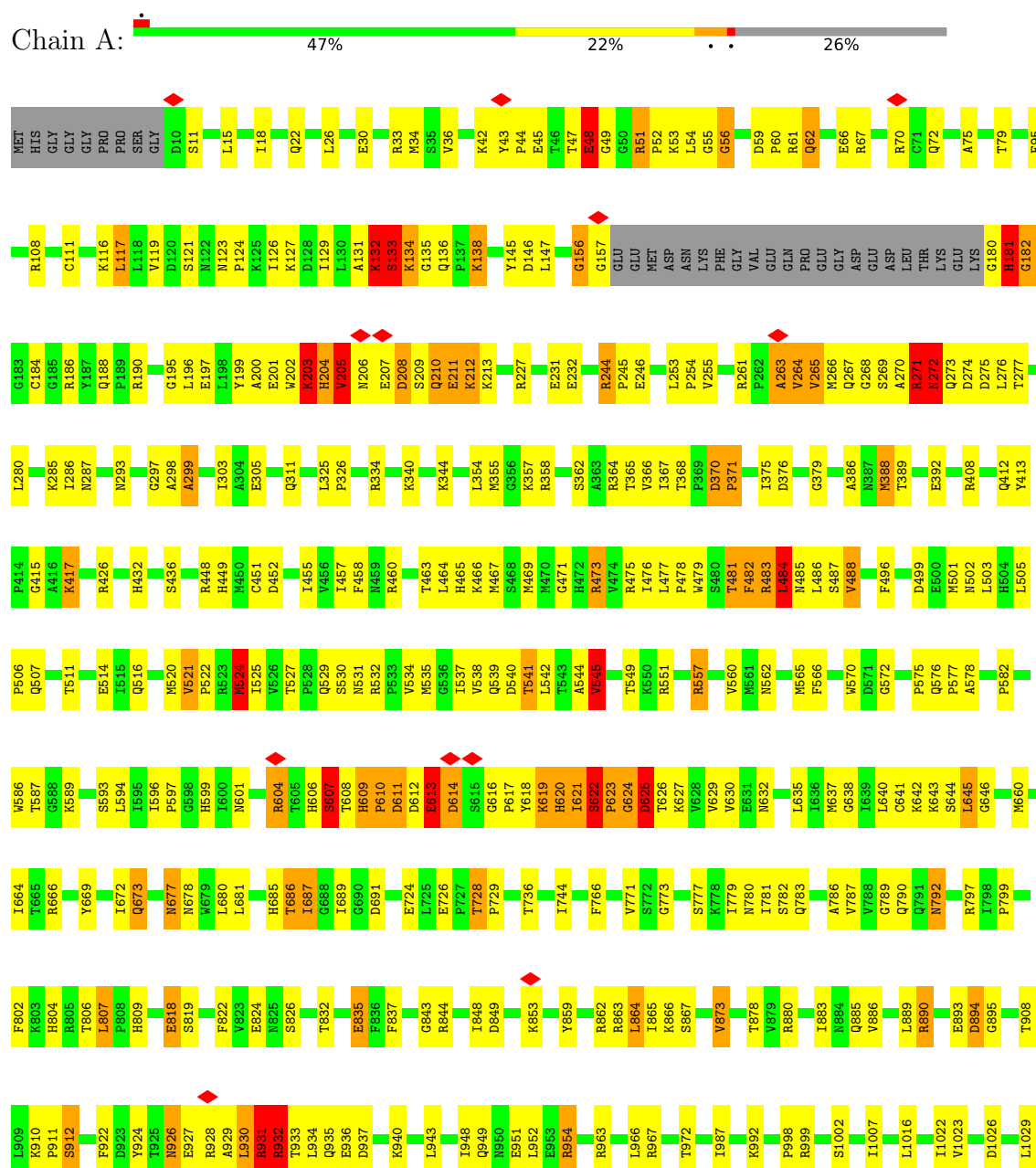
- Molecule 25 is ZINC ION (CCD ID: ZN) (formula: Zn).

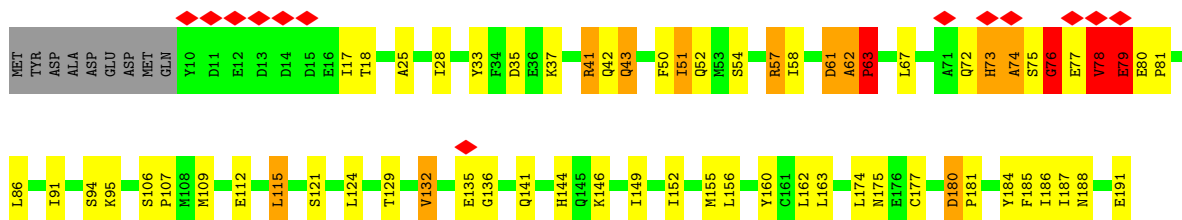
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 25  | A     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 25  | B     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 25  | C     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 25  | I     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 25  | J     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 25  | L     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 25  | M     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 25  | Q     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 25  | U     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

### 3 Residue-property plots

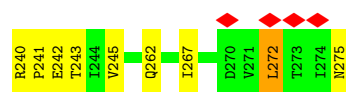
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

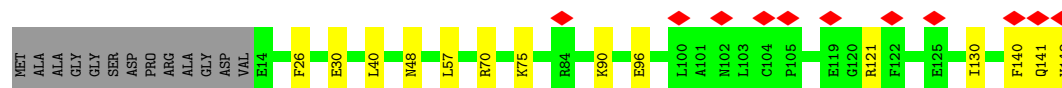
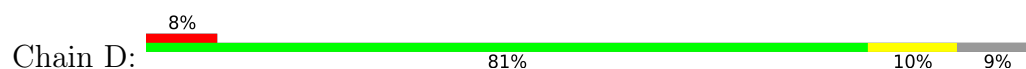




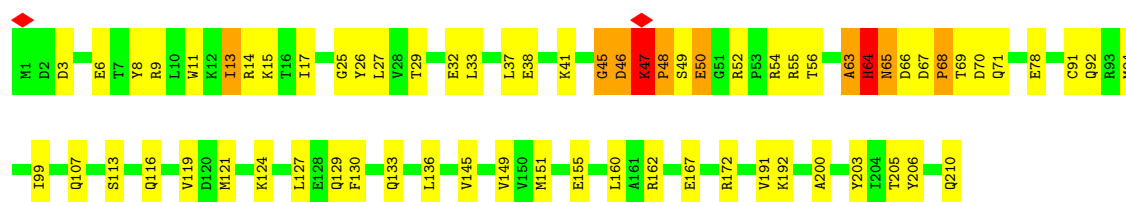




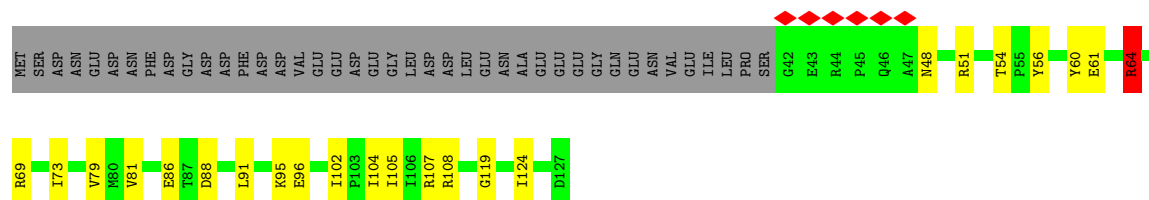
- Molecule 4: DNA-directed RNA polymerase II subunit RPB4



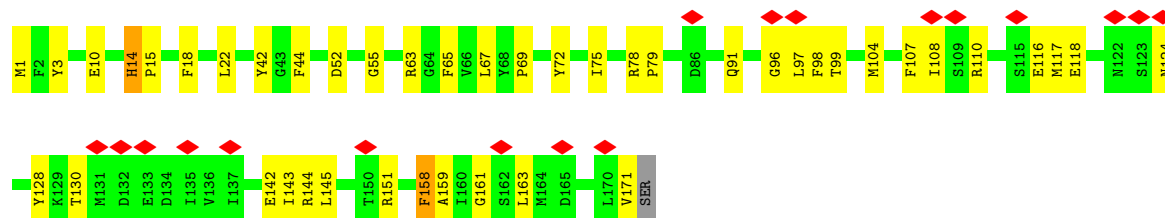
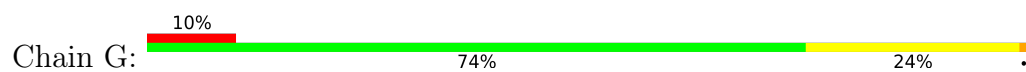
- Molecule 5: DNA-directed RNA polymerase II subunit RPB5



- Molecule 6: DNA-directed RNA polymerase II subunit RPB6



- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

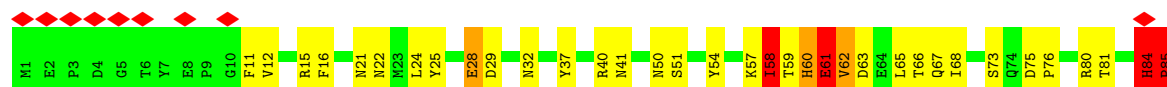


- Molecule 8: DNA-directed RNA polymerase II subunit RPB8

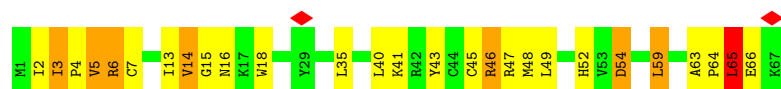




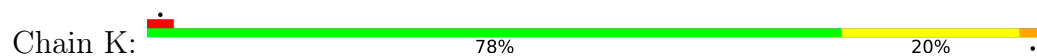
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9



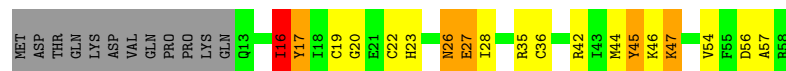
• Molecule 10: DNA-directed RNA polymerase II subunit RPB10



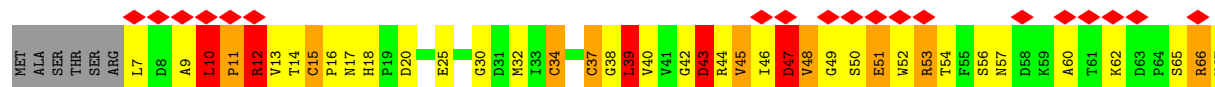
• Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a



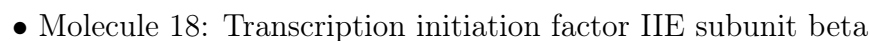
• Molecule 12: DNA-directed RNA polymerase II subunit RPB12

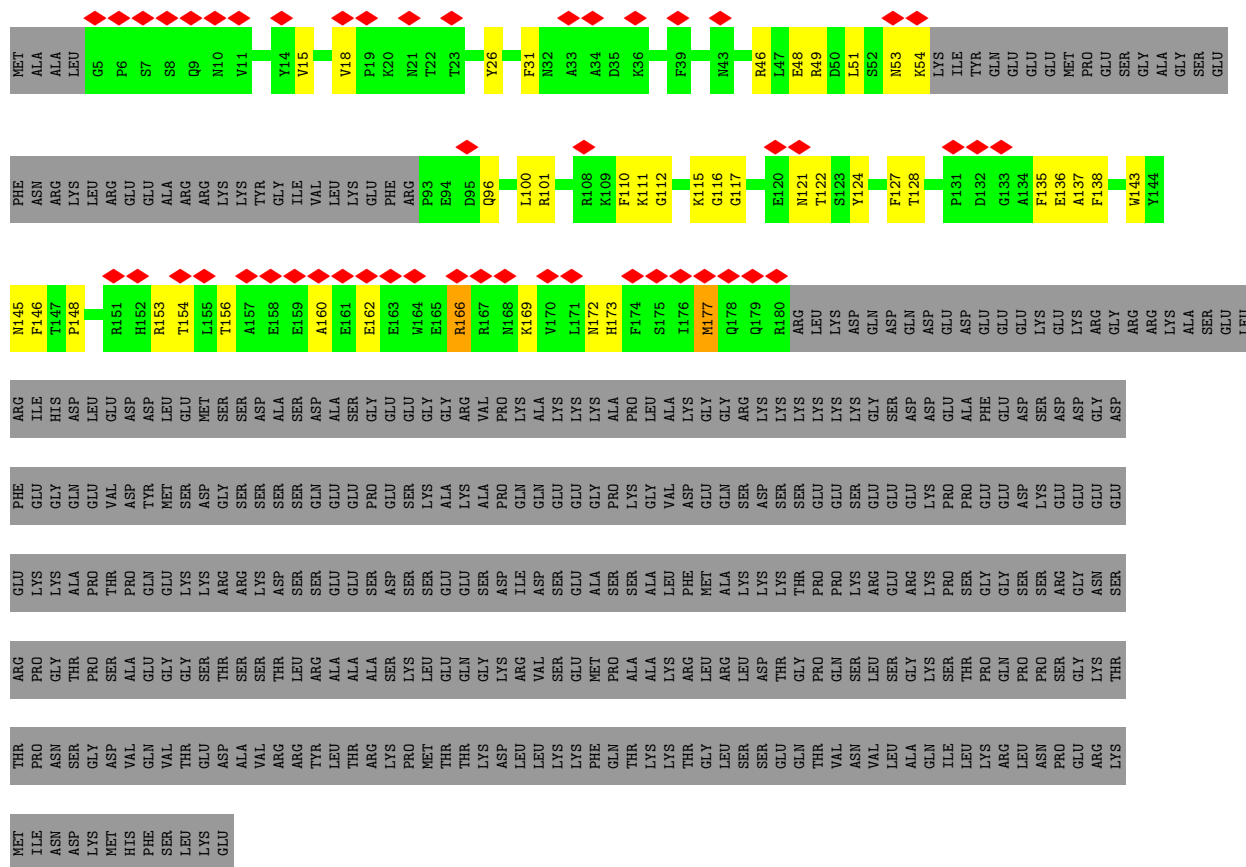


• Molecule 13: Transcription initiation factor IIB

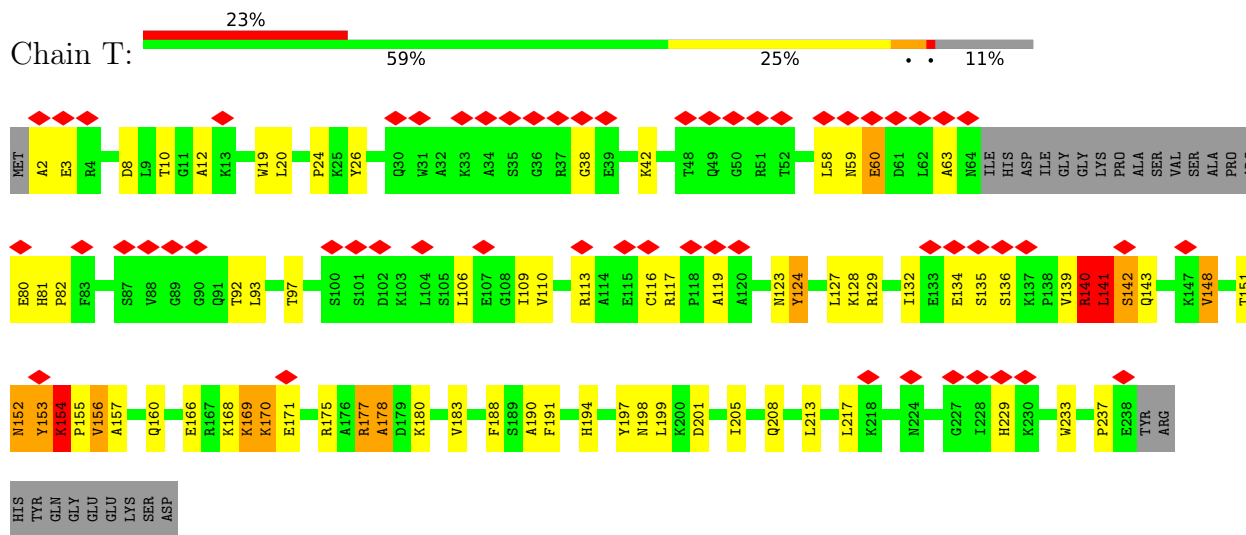




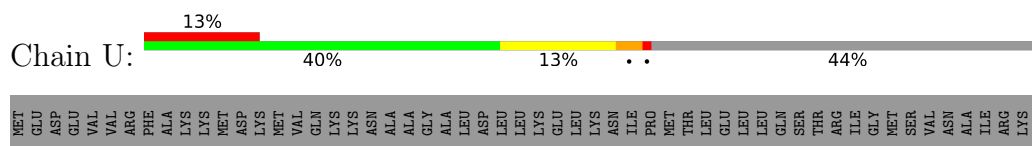


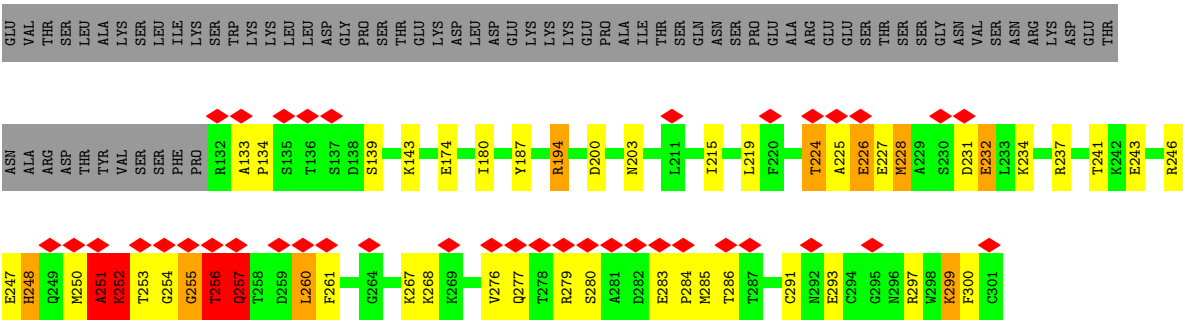


• Molecule 20: General transcription factor IIF subunit 2

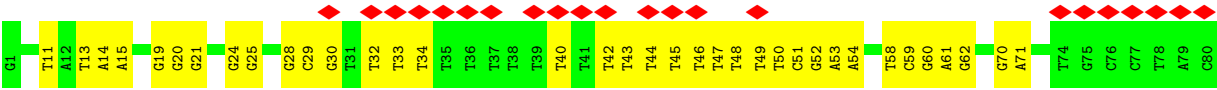


• Molecule 21: Transcription elongation factor A protein 1

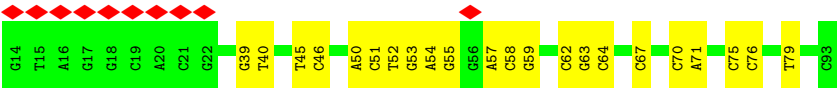




• Molecule 22: SCP-X



• Molecule 23: SCP-Y



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 90590                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 42                                      | Depositor |
| Minimum defocus (nm)                 | 2000                                    | Depositor |
| Maximum defocus (nm)                 | 4000                                    | Depositor |
| Magnification                        | 27500                                   | Depositor |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 0.164                                   | Depositor |
| Minimum map value                    | -0.103                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.002                                   | Depositor |
| Recommended contour level            | 0.01                                    | Depositor |
| Map size (Å)                         | 503.03998, 503.03998, 503.03998         | wwPDB     |
| Map dimensions                       | 384, 384, 384                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.31, 1.31, 1.31                        | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.82         | 14/11727 (0.1%) | 1.26        | 97/15833 (0.6%)  |
| 2   | B     | 0.94         | 10/9503 (0.1%)  | 1.31        | 92/12831 (0.7%)  |
| 3   | C     | 0.76         | 0/2259          | 1.14        | 17/3073 (0.6%)   |
| 4   | D     | 0.30         | 0/1077          | 0.81        | 0/1446           |
| 5   | E     | 0.57         | 0/1753          | 1.13        | 9/2368 (0.4%)    |
| 6   | F     | 0.83         | 0/700           | 1.07        | 1/946 (0.1%)     |
| 7   | G     | 0.39         | 0/1382          | 0.93        | 6/1874 (0.3%)    |
| 8   | H     | 0.54         | 0/1227          | 1.12        | 5/1654 (0.3%)    |
| 9   | I     | 0.44         | 0/1038          | 1.20        | 8/1407 (0.6%)    |
| 10  | J     | 0.86         | 0/542           | 1.52        | 7/730 (1.0%)     |
| 11  | K     | 0.65         | 0/956           | 1.10        | 6/1294 (0.5%)    |
| 12  | L     | 0.66         | 0/394           | 1.08        | 2/524 (0.4%)     |
| 13  | M     | 0.54         | 0/2429          | 1.25        | 30/3281 (0.9%)   |
| 14  | N     | 0.34         | 0/945           | 1.04        | 7/1274 (0.5%)    |
| 15  | O     | 0.31         | 0/816           | 0.83        | 2/1105 (0.2%)    |
| 16  | P     | 0.40         | 0/1489          | 0.97        | 6/2005 (0.3%)    |
| 17  | Q     | 0.44         | 0/1507          | 1.14        | 3/2023 (0.1%)    |
| 18  | R     | 0.69         | 3/1380 (0.2%)   | 1.35        | 13/1854 (0.7%)   |
| 19  | S     | 0.31         | 0/1167          | 0.81        | 0/1576           |
| 20  | T     | 0.45         | 0/1817          | 1.08        | 13/2445 (0.5%)   |
| 21  | U     | 0.40         | 0/1358          | 1.07        | 9/1820 (0.5%)    |
| 22  | X     | 0.27         | 0/1843          | 0.49        | 0/2847           |
| 23  | Y     | 0.25         | 0/1817          | 0.45        | 0/2800           |
| All | All   | 0.69         | 27/49126 (0.1%) | 1.15        | 333/67010 (0.5%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 2                   |
| 2   | B     | 0                   | 3                   |
| 7   | G     | 0                   | 1                   |
| 13  | M     | 0                   | 1                   |
| 14  | N     | 0                   | 2                   |
| 16  | P     | 0                   | 1                   |
| 17  | Q     | 0                   | 1                   |
| 18  | R     | 0                   | 1                   |
| 19  | S     | 0                   | 1                   |
| 20  | T     | 0                   | 2                   |
| All | All   | 0                   | 15                  |

All (27) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 18  | R     | 204  | ASN  | CA-C   | 7.67  | 1.61        | 1.52     |
| 1   | A     | 521  | VAL  | CA-CB  | 7.50  | 1.57        | 1.54     |
| 18  | R     | 204  | ASN  | N-CA   | 7.17  | 1.54        | 1.46     |
| 1   | A     | 1159 | CYS  | CA-CB  | 6.95  | 1.64        | 1.53     |
| 1   | A     | 482  | PHE  | C-O    | -6.85 | 1.15        | 1.24     |
| 18  | R     | 203  | PHE  | CA-C   | 6.78  | 1.61        | 1.53     |
| 2   | B     | 923  | VAL  | C-O    | -6.70 | 1.16        | 1.24     |
| 1   | A     | 481  | THR  | C-O    | -6.43 | 1.15        | 1.23     |
| 1   | A     | 502  | ASN  | CA-C   | -6.02 | 1.45        | 1.52     |
| 2   | B     | 186  | ILE  | C-O    | -5.93 | 1.17        | 1.24     |
| 1   | A     | 890  | ARG  | CA-C   | -5.93 | 1.45        | 1.52     |
| 1   | A     | 835  | GLU  | CA-C   | -5.84 | 1.45        | 1.52     |
| 2   | B     | 939  | HIS  | CA-C   | -5.80 | 1.45        | 1.52     |
| 2   | B     | 43   | GLN  | CA-C   | -5.79 | 1.45        | 1.52     |
| 1   | A     | 1159 | CYS  | N-CA   | -5.78 | 1.39        | 1.46     |
| 2   | B     | 478  | THR  | CA-CB  | -5.67 | 1.44        | 1.53     |
| 2   | B     | 1048 | TYR  | CA-C   | -5.47 | 1.46        | 1.52     |
| 1   | A     | 673  | GLN  | C-O    | -5.46 | 1.17        | 1.24     |
| 2   | B     | 469  | VAL  | CA-C   | -5.43 | 1.46        | 1.52     |
| 1   | A     | 488  | VAL  | CA-CB  | -5.32 | 1.47        | 1.54     |
| 1   | A     | 1160 | ARG  | CD-NE  | -5.19 | 1.39        | 1.46     |
| 2   | B     | 924  | ARG  | CZ-NH1 | 5.16  | 1.40        | 1.32     |
| 2   | B     | 481  | HIS  | C-O    | -5.13 | 1.18        | 1.24     |
| 1   | A     | 835  | GLU  | C-O    | -5.07 | 1.18        | 1.24     |
| 1   | A     | 457  | ILE  | CA-CB  | -5.06 | 1.48        | 1.54     |
| 2   | B     | 785  | TYR  | CA-C   | 5.01  | 1.57        | 1.53     |
| 1   | A     | 368  | THR  | CA-C   | -5.00 | 1.47        | 1.52     |

All (333) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 17  | Q     | 102 | VAL  | N-CA-C  | -26.24 | 88.29       | 112.43   |
| 10  | J     | 65  | LEU  | N-CA-C  | -18.91 | 89.71       | 113.16   |
| 9   | I     | 84  | HIS  | C-N-CD  | -16.57 | 57.05       | 125.00   |
| 21  | U     | 231 | ASP  | N-CA-C  | -15.62 | 94.28       | 113.50   |
| 2   | B     | 882 | SER  | N-CA-C  | -15.12 | 90.04       | 111.81   |
| 8   | H     | 74  | GLU  | N-CA-C  | -14.96 | 87.87       | 109.11   |
| 13  | M     | 42  | GLY  | N-CA-C  | 14.79  | 137.18      | 111.15   |
| 18  | R     | 194 | ARG  | C-N-CD  | -14.31 | 66.35       | 125.00   |
| 9   | I     | 61  | GLU  | N-CA-C  | -14.23 | 90.91       | 110.68   |
| 9   | I     | 103 | ARG  | N-CA-C  | -13.95 | 81.08       | 110.80   |
| 1   | A     | 182 | GLY  | N-CA-C  | 13.50  | 127.55      | 111.35   |
| 13  | M     | 10  | LEU  | C-N-CD  | -13.29 | 70.51       | 125.00   |
| 2   | B     | 880 | LEU  | N-CA-C  | 12.11  | 127.35      | 112.58   |
| 3   | C     | 6   | GLN  | C-N-CD  | -11.98 | 75.89       | 125.00   |
| 1   | A     | 521 | VAL  | CB-CA-C | -11.91 | 102.39      | 113.70   |
| 13  | M     | 39  | LEU  | N-CA-C  | 11.60  | 135.51      | 110.80   |
| 3   | C     | 137 | ASN  | N-CA-C  | -11.39 | 92.54       | 109.62   |
| 1   | A     | 370 | ASP  | CA-C-N  | 11.18  | 133.81      | 119.84   |
| 1   | A     | 370 | ASP  | C-N-CA  | 11.18  | 133.81      | 119.84   |
| 11  | K     | 62  | LYS  | CA-C-N  | -10.65 | 115.36      | 122.60   |
| 11  | K     | 62  | LYS  | C-N-CA  | -10.65 | 115.36      | 122.60   |
| 1   | A     | 271 | ARG  | N-CA-C  | -10.43 | 91.95       | 108.63   |
| 18  | R     | 195 | PRO  | N-CA-C  | -10.37 | 91.11       | 112.47   |
| 13  | M     | 51  | GLU  | N-CA-C  | 10.34  | 122.13      | 111.07   |
| 18  | R     | 214 | GLU  | N-CA-C  | -10.23 | 99.95       | 111.71   |
| 13  | M     | 94  | ASP  | N-CA-C  | -10.09 | 89.32       | 110.80   |
| 12  | L     | 26  | ASN  | N-CA-C  | -10.00 | 98.55       | 112.45   |
| 13  | M     | 91  | ALA  | N-CA-C  | -9.92  | 89.66       | 110.80   |
| 1   | A     | 483 | ARG  | N-CA-C  | -9.85  | 93.21       | 109.07   |
| 2   | B     | 249 | LYS  | N-CA-C  | -9.85  | 89.82       | 110.80   |
| 18  | R     | 204 | ASN  | N-CA-C  | 9.77   | 122.86      | 108.60   |
| 2   | B     | 719 | SER  | CA-C-N  | -9.30  | 110.17      | 119.56   |
| 2   | B     | 719 | SER  | C-N-CA  | -9.30  | 110.17      | 119.56   |
| 2   | B     | 699 | HIS  | CA-C-N  | 9.26   | 129.33      | 119.05   |
| 2   | B     | 699 | HIS  | C-N-CA  | 9.26   | 129.33      | 119.05   |
| 20  | T     | 60  | GLU  | N-CA-C  | -9.21  | 100.36      | 111.69   |
| 2   | B     | 62  | ALA  | CA-C-N  | -9.15  | 110.96      | 120.38   |
| 2   | B     | 62  | ALA  | C-N-CA  | -9.15  | 110.96      | 120.38   |
| 1   | A     | 205 | VAL  | N-CA-C  | 9.01   | 128.07      | 109.34   |
| 2   | B     | 294 | ASP  | CA-C-N  | 8.84   | 129.01      | 119.28   |
| 2   | B     | 294 | ASP  | C-N-CA  | 8.84   | 129.01      | 119.28   |
| 3   | C     | 211 | LEU  | N-CA-C  | -8.83  | 92.00       | 110.80   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 5   | E     | 47   | LYS  | CA-C-N | -8.80 | 108.84      | 119.84   |
| 5   | E     | 47   | LYS  | C-N-CA | -8.80 | 108.84      | 119.84   |
| 18  | R     | 194  | ARG  | CA-C-N | 8.70  | 130.71      | 119.84   |
| 18  | R     | 194  | ARG  | C-N-CA | 8.70  | 130.71      | 119.84   |
| 21  | U     | 255  | GLY  | N-CA-C | 8.58  | 133.52      | 113.18   |
| 18  | R     | 163  | LEU  | N-CA-C | 8.35  | 128.58      | 110.80   |
| 8   | H     | 85   | ALA  | N-CA-C | -8.34 | 97.11       | 109.62   |
| 14  | N     | 326  | GLN  | N-CA-C | 8.33  | 124.87      | 113.37   |
| 1   | A     | 524  | MET  | CA-C-N | -8.27 | 114.73      | 123.08   |
| 1   | A     | 524  | MET  | C-N-CA | -8.27 | 114.73      | 123.08   |
| 1   | A     | 545  | VAL  | N-CA-C | 8.21  | 119.00      | 110.62   |
| 1   | A     | 677  | ASN  | N-CA-C | 8.14  | 120.16      | 111.28   |
| 2   | B     | 1044 | GLY  | CA-C-N | -8.04 | 112.43      | 120.31   |
| 2   | B     | 1044 | GLY  | C-N-CA | -8.04 | 112.43      | 120.31   |
| 1   | A     | 673  | GLN  | N-CA-C | 7.99  | 120.07      | 111.36   |
| 20  | T     | 141  | LEU  | N-CA-C | -7.96 | 93.85       | 110.80   |
| 2   | B     | 492  | ASP  | N-CA-C | 7.90  | 122.41      | 111.74   |
| 1   | A     | 1314 | THR  | N-CA-C | -7.84 | 104.88      | 114.75   |
| 9   | I     | 58   | ILE  | N-CA-C | -7.76 | 93.19       | 109.34   |
| 13  | M     | 87   | GLY  | CA-C-N | -7.76 | 108.33      | 122.38   |
| 13  | M     | 87   | GLY  | C-N-CA | -7.76 | 108.33      | 122.38   |
| 2   | B     | 748  | ALA  | N-CA-C | 7.75  | 121.16      | 108.99   |
| 10  | J     | 46   | ARG  | N-CA-C | 7.73  | 119.49      | 111.14   |
| 1   | A     | 565  | MET  | N-CA-C | 7.71  | 119.68      | 111.28   |
| 10  | J     | 45   | CYS  | N-CA-C | -7.71 | 102.88      | 111.82   |
| 2   | B     | 224  | CYS  | N-CA-C | 7.69  | 121.66      | 111.28   |
| 18  | R     | 203  | PHE  | N-CA-C | 7.68  | 118.82      | 108.23   |
| 13  | M     | 89   | GLY  | N-CA-C | -7.56 | 95.26       | 113.18   |
| 1   | A     | 777  | SER  | N-CA-C | 7.55  | 118.21      | 108.24   |
| 1   | A     | 133  | SER  | N-CA-C | 7.54  | 126.85      | 110.80   |
| 1   | A     | 1057 | GLU  | N-CA-C | 7.52  | 119.26      | 111.14   |
| 8   | H     | 73   | GLY  | N-CA-C | 7.50  | 130.94      | 113.18   |
| 1   | A     | 1425 | GLY  | CA-C-N | 7.48  | 127.36      | 119.05   |
| 1   | A     | 1425 | GLY  | C-N-CA | 7.48  | 127.36      | 119.05   |
| 18  | R     | 205  | ASP  | N-CA-C | 7.46  | 126.68      | 110.80   |
| 13  | M     | 130  | LEU  | CA-C-N | 7.43  | 127.39      | 120.03   |
| 13  | M     | 130  | LEU  | C-N-CA | 7.43  | 127.39      | 120.03   |
| 2   | B     | 473  | LEU  | N-CA-C | 7.42  | 119.36      | 111.28   |
| 1   | A     | 611  | ASP  | N-CA-C | 7.40  | 120.59      | 108.08   |
| 1   | A     | 1371 | ILE  | N-CA-C | 7.33  | 118.12      | 110.72   |
| 13  | M     | 49   | GLY  | N-CA-C | 7.31  | 123.34      | 113.99   |
| 11  | K     | 3    | ALA  | CA-C-N | 7.29  | 124.91      | 119.66   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 11  | K     | 3    | ALA  | C-N-CA     | 7.29  | 124.91      | 119.66   |
| 3   | C     | 135  | ARG  | N-CA-C     | -7.20 | 101.57      | 110.65   |
| 2   | B     | 798  | ARG  | N-CA-C     | 7.12  | 119.05      | 111.28   |
| 2   | B     | 180  | ASP  | CA-C-N     | 7.12  | 128.73      | 119.84   |
| 2   | B     | 180  | ASP  | C-N-CA     | 7.12  | 128.73      | 119.84   |
| 2   | B     | 58   | ILE  | N-CA-C     | 7.11  | 117.90      | 110.72   |
| 2   | B     | 785  | TYR  | CB-CA-C    | -7.11 | 108.38      | 116.63   |
| 1   | A     | 1116 | ASN  | N-CA-C     | 7.10  | 121.15      | 110.64   |
| 2   | B     | 1055 | VAL  | N-CA-C     | 7.10  | 117.86      | 110.62   |
| 8   | H     | 84   | ARG  | N-CA-C     | 7.09  | 120.24      | 110.24   |
| 13  | M     | 43   | ASP  | N-CA-C     | -7.05 | 94.64       | 107.75   |
| 1   | A     | 539  | GLN  | CB-CA-C    | -7.02 | 108.48      | 116.63   |
| 1   | A     | 539  | GLN  | N-CA-C     | 6.96  | 119.85      | 108.08   |
| 2   | B     | 77   | GLU  | N-CA-C     | 6.96  | 125.63      | 110.80   |
| 13  | M     | 86   | LYS  | N-CA-C     | 6.95  | 119.27      | 110.24   |
| 20  | T     | 154  | LYS  | N-CA-C     | 6.94  | 125.14      | 109.81   |
| 13  | M     | 38   | GLY  | N-CA-C     | -6.89 | 96.86       | 113.18   |
| 13  | M     | 15   | CYS  | CA-C-N     | 6.87  | 126.12      | 118.97   |
| 13  | M     | 15   | CYS  | C-N-CA     | 6.87  | 126.12      | 118.97   |
| 1   | A     | 244  | ARG  | CA-C-N     | 6.87  | 127.15      | 119.32   |
| 1   | A     | 244  | ARG  | C-N-CA     | 6.87  | 127.15      | 119.32   |
| 13  | M     | 37   | CYS  | CA-C-N     | -6.87 | 107.95      | 121.41   |
| 13  | M     | 37   | CYS  | C-N-CA     | -6.87 | 107.95      | 121.41   |
| 1   | A     | 1117 | VAL  | N-CA-C     | -6.83 | 95.12       | 109.34   |
| 1   | A     | 843  | GLY  | N-CA-C     | 6.81  | 120.90      | 112.73   |
| 2   | B     | 79   | GLU  | CA-C-N     | -6.76 | 105.31      | 121.80   |
| 2   | B     | 79   | GLU  | C-N-CA     | -6.76 | 105.31      | 121.80   |
| 21  | U     | 251  | ALA  | N-CA-C     | -6.75 | 96.42       | 110.80   |
| 2   | B     | 162  | LEU  | N-CA-C     | 6.75  | 120.39      | 111.75   |
| 1   | A     | 417  | LYS  | N-CA-C     | 6.74  | 119.62      | 111.40   |
| 5   | E     | 13   | ILE  | N-CA-C     | 6.73  | 117.52      | 110.72   |
| 9   | I     | 84   | HIS  | N-CA-C     | 6.72  | 124.66      | 109.81   |
| 2   | B     | 924  | ARG  | NE-CZ-NH1  | -6.70 | 114.80      | 121.50   |
| 1   | A     | 483  | ARG  | NH1-CZ-NH2 | -6.67 | 110.63      | 119.30   |
| 1   | A     | 521  | VAL  | N-CA-CB    | 6.65  | 114.98      | 110.52   |
| 2   | B     | 938  | ARG  | N-CA-C     | 6.61  | 121.05      | 113.19   |
| 18  | R     | 169  | GLU  | N-CA-C     | 6.57  | 118.44      | 111.28   |
| 5   | E     | 63   | ALA  | N-CA-C     | 6.54  | 120.51      | 107.62   |
| 1   | A     | 566  | PHE  | N-CA-C     | 6.54  | 120.52      | 112.54   |
| 3   | C     | 136  | ASP  | N-CA-C     | 6.54  | 120.25      | 107.57   |
| 1   | A     | 476  | ILE  | N-CA-C     | 6.53  | 117.46      | 109.30   |
| 2   | B     | 186  | ILE  | CA-C-N     | -6.51 | 114.61      | 123.14   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | B     | 186  | ILE  | C-N-CA  | -6.51 | 114.61      | 123.14   |
| 1   | A     | 844  | ARG  | N-CA-C  | 6.51  | 118.37      | 111.28   |
| 1   | A     | 1121 | VAL  | CB-CA-C | -6.50 | 107.52      | 113.70   |
| 3   | C     | 199  | LYS  | CA-C-N  | 6.50  | 126.19      | 119.56   |
| 3   | C     | 199  | LYS  | C-N-CA  | 6.50  | 126.19      | 119.56   |
| 16  | P     | 292  | ILE  | N-CA-C  | 6.48  | 117.17      | 107.51   |
| 14  | N     | 356  | GLY  | N-CA-C  | 6.46  | 128.48      | 113.18   |
| 1   | A     | 1481 | LYS  | N-CA-C  | 6.43  | 118.29      | 111.28   |
| 2   | B     | 713  | PHE  | CB-CA-C | -6.37 | 104.72      | 110.71   |
| 20  | T     | 109  | ILE  | N-CA-C  | 6.34  | 117.04      | 108.17   |
| 2   | B     | 86   | LEU  | N-CA-C  | 6.33  | 119.22      | 108.90   |
| 6   | F     | 64   | ARG  | N-CA-C  | 6.33  | 117.84      | 111.07   |
| 7   | G     | 124  | ASN  | CA-C-N  | -6.30 | 113.89      | 120.38   |
| 7   | G     | 124  | ASN  | C-N-CA  | -6.30 | 113.89      | 120.38   |
| 13  | M     | 72   | ASN  | CA-C-N  | 6.30  | 126.01      | 119.64   |
| 13  | M     | 72   | ASN  | C-N-CA  | 6.30  | 126.01      | 119.64   |
| 9   | I     | 86   | CYS  | N-CA-C  | -6.30 | 100.33      | 109.59   |
| 1   | A     | 596  | ILE  | CA-C-N  | 6.29  | 126.50      | 119.90   |
| 1   | A     | 596  | ILE  | C-N-CA  | 6.29  | 126.50      | 119.90   |
| 9   | I     | 120  | GLY  | N-CA-C  | -6.28 | 105.23      | 114.90   |
| 1   | A     | 1376 | LYS  | N-CA-C  | 6.28  | 117.92      | 111.14   |
| 1   | A     | 611  | ASP  | CB-CA-C | -6.27 | 109.35      | 116.63   |
| 20  | T     | 134  | GLU  | N-CA-C  | 6.26  | 118.10      | 111.28   |
| 2   | B     | 982  | ILE  | N-CA-C  | 6.25  | 117.00      | 110.62   |
| 21  | U     | 224  | THR  | N-CA-C  | -6.22 | 104.19      | 110.97   |
| 3   | C     | 71   | ILE  | CB-CA-C | -6.18 | 104.95      | 111.00   |
| 2   | B     | 63   | PRO  | CA-C-N  | -6.18 | 113.41      | 119.90   |
| 2   | B     | 63   | PRO  | C-N-CA  | -6.18 | 113.41      | 119.90   |
| 2   | B     | 598  | VAL  | N-CA-C  | 6.17  | 116.36      | 110.74   |
| 1   | A     | 1071 | GLU  | N-CA-C  | 6.15  | 118.07      | 111.36   |
| 2   | B     | 507  | GLY  | N-CA-C  | -6.15 | 107.28      | 115.40   |
| 1   | A     | 620  | HIS  | N-CA-C  | 6.13  | 123.04      | 113.72   |
| 5   | E     | 45   | GLY  | O-C-N   | 6.13  | 127.48      | 122.51   |
| 14  | N     | 310  | GLU  | N-CA-C  | -6.12 | 104.43      | 113.61   |
| 2   | B     | 944  | THR  | CA-C-N  | 6.12  | 131.21      | 121.66   |
| 2   | B     | 944  | THR  | C-N-CA  | 6.12  | 131.21      | 121.66   |
| 1   | A     | 867  | SER  | N-CA-C  | 6.12  | 117.82      | 111.03   |
| 21  | U     | 283  | GLU  | CA-C-N  | 6.09  | 126.10      | 119.89   |
| 21  | U     | 283  | GLU  | C-N-CA  | 6.09  | 126.10      | 119.89   |
| 16  | P     | 153  | THR  | CA-C-N  | 6.09  | 127.45      | 119.84   |
| 16  | P     | 153  | THR  | C-N-CA  | 6.09  | 127.45      | 119.84   |
| 8   | H     | 60   | ILE  | N-CA-C  | 6.07  | 116.86      | 108.12   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | A     | 744  | ILE  | N-CA-C   | 6.06  | 116.80      | 110.62   |
| 1   | A     | 527  | THR  | CA-C-N   | 6.05  | 126.84      | 120.12   |
| 1   | A     | 527  | THR  | C-N-CA   | 6.05  | 126.84      | 120.12   |
| 2   | B     | 446  | TYR  | N-CA-C   | 6.03  | 117.52      | 111.07   |
| 21  | U     | 232  | GLU  | N-CA-C   | 6.03  | 123.64      | 110.80   |
| 11  | K     | 82   | SER  | CA-C-N   | 6.01  | 125.89      | 119.28   |
| 11  | K     | 82   | SER  | C-N-CA   | 6.01  | 125.89      | 119.28   |
| 3   | C     | 35   | ARG  | CG-CD-NE | -6.00 | 98.79       | 112.00   |
| 10  | J     | 59   | LEU  | N-CA-C   | 6.00  | 117.82      | 111.28   |
| 2   | B     | 706  | VAL  | N-CA-C   | -5.99 | 105.98      | 111.67   |
| 1   | A     | 609  | HIS  | O-C-N    | 5.94  | 126.19      | 120.55   |
| 2   | B     | 144  | HIS  | N-CA-C   | 5.92  | 119.47      | 109.76   |
| 2   | B     | 1058 | LYS  | N-CA-C   | 5.92  | 120.23      | 112.89   |
| 1   | A     | 203  | LYS  | N-CA-C   | 5.90  | 117.81      | 108.67   |
| 3   | C     | 49   | TRP  | CA-CB-CG | 5.89  | 124.79      | 113.60   |
| 18  | R     | 169  | GLU  | CB-CA-C  | -5.89 | 101.01      | 110.79   |
| 2   | B     | 959  | GLU  | N-CA-C   | -5.88 | 105.21      | 112.38   |
| 7   | G     | 96   | GLY  | N-CA-C   | 5.87  | 118.78      | 110.74   |
| 1   | A     | 368  | THR  | CA-C-N   | -5.84 | 113.95      | 120.14   |
| 1   | A     | 368  | THR  | C-N-CA   | -5.84 | 113.95      | 120.14   |
| 14  | N     | 325  | GLY  | N-CA-C   | 5.82  | 126.98      | 113.18   |
| 1   | A     | 622  | SER  | C-N-CD   | -5.81 | 101.17      | 125.00   |
| 1   | A     | 123  | ASN  | CA-C-N   | 5.81  | 125.94      | 119.32   |
| 1   | A     | 123  | ASN  | C-N-CA   | 5.81  | 125.94      | 119.32   |
| 14  | N     | 21   | VAL  | N-CA-C   | 5.80  | 115.99      | 110.42   |
| 1   | A     | 502  | ASN  | N-CA-CB  | -5.80 | 101.35      | 110.69   |
| 2   | B     | 956  | PHE  | N-CA-C   | 5.80  | 117.78      | 109.14   |
| 2   | B     | 1103 | LEU  | N-CA-C   | 5.79  | 117.27      | 111.07   |
| 18  | R     | 229  | ASP  | N-CA-C   | -5.79 | 103.66      | 111.54   |
| 3   | C     | 159  | LEU  | N-CA-C   | 5.78  | 117.81      | 107.80   |
| 7   | G     | 14   | HIS  | CA-C-N   | 5.78  | 125.91      | 119.32   |
| 7   | G     | 14   | HIS  | C-N-CA   | 5.78  | 125.91      | 119.32   |
| 2   | B     | 945  | CYS  | CA-CB-SG | 5.78  | 127.69      | 114.40   |
| 2   | B     | 785  | TYR  | N-CA-C   | 5.78  | 117.84      | 108.08   |
| 1   | A     | 728  | THR  | CA-C-N   | 5.77  | 126.11      | 119.93   |
| 1   | A     | 728  | THR  | C-N-CA   | 5.77  | 126.11      | 119.93   |
| 20  | T     | 142  | SER  | N-CA-C   | 5.76  | 123.07      | 110.80   |
| 2   | B     | 941  | GLN  | CA-CB-CG | -5.75 | 102.61      | 114.10   |
| 2   | B     | 1093 | CYS  | N-CA-C   | 5.75  | 117.54      | 111.28   |
| 1   | A     | 388  | MET  | N-CA-C   | 5.74  | 118.60      | 109.24   |
| 13  | M     | 34   | CYS  | CA-C-N   | 5.74  | 127.02      | 119.84   |
| 13  | M     | 34   | CYS  | C-N-CA   | 5.74  | 127.02      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 5   | E     | 64   | HIS  | N-CA-C     | 5.73  | 123.01      | 110.80   |
| 5   | E     | 92   | GLN  | N-CA-C     | -5.73 | 105.04      | 111.28   |
| 13  | M     | 216  | SER  | N-CA-C     | 5.71  | 117.19      | 110.97   |
| 1   | A     | 1396 | ARG  | CA-C-N     | 5.70  | 128.19      | 120.44   |
| 1   | A     | 1396 | ARG  | C-N-CA     | 5.70  | 128.19      | 120.44   |
| 1   | A     | 645  | LEU  | N-CA-C     | 5.68  | 120.20      | 113.28   |
| 17  | Q     | 103  | VAL  | N-CA-C     | 5.67  | 117.17      | 111.00   |
| 13  | M     | 10   | LEU  | N-CA-C     | 5.65  | 122.29      | 109.81   |
| 16  | P     | 186  | ARG  | N-CA-C     | 5.62  | 117.21      | 111.14   |
| 2   | B     | 972  | ILE  | CA-C-N     | 5.62  | 125.08      | 119.24   |
| 2   | B     | 972  | ILE  | C-N-CA     | 5.62  | 125.08      | 119.24   |
| 21  | U     | 256  | THR  | N-CA-C     | -5.62 | 98.84       | 110.80   |
| 1   | A     | 932  | ARG  | CA-C-N     | -5.61 | 113.42      | 122.23   |
| 1   | A     | 932  | ARG  | C-N-CA     | -5.61 | 113.42      | 122.23   |
| 2   | B     | 497  | LYS  | CA-C-N     | -5.57 | 111.30      | 120.88   |
| 2   | B     | 497  | LYS  | C-N-CA     | -5.57 | 111.30      | 120.88   |
| 1   | A     | 848  | ILE  | CB-CA-C    | -5.57 | 104.53      | 112.22   |
| 2   | B     | 51   | ILE  | N-CA-C     | 5.56  | 116.34      | 110.72   |
| 2   | B     | 1054 | MET  | CB-CG-SD   | 5.55  | 129.35      | 112.70   |
| 1   | A     | 1371 | ILE  | CB-CA-C    | -5.55 | 104.56      | 112.22   |
| 9   | I     | 85   | PRO  | N-CA-C     | 5.54  | 123.89      | 112.47   |
| 2   | B     | 874  | PRO  | N-CA-C     | -5.54 | 105.83      | 113.53   |
| 2   | B     | 925  | SER  | CA-C-N     | -5.53 | 115.75      | 123.10   |
| 2   | B     | 925  | SER  | C-N-CA     | -5.53 | 115.75      | 123.10   |
| 1   | A     | 484  | LEU  | N-CA-C     | 5.52  | 117.79      | 109.23   |
| 17  | Q     | 101  | ASN  | N-CA-C     | 5.52  | 119.25      | 110.70   |
| 2   | B     | 923  | VAL  | O-C-N      | -5.51 | 117.39      | 123.18   |
| 13  | M     | 87   | GLY  | N-CA-C     | 5.50  | 126.23      | 113.18   |
| 3   | C     | 68   | LEU  | N-CA-C     | 5.49  | 117.34      | 111.36   |
| 1   | A     | 466  | LYS  | N-CA-C     | 5.47  | 118.75      | 111.75   |
| 3   | C     | 66   | HIS  | N-CA-C     | 5.47  | 116.92      | 111.07   |
| 16  | P     | 293  | TYR  | N-CA-C     | 5.47  | 117.64      | 108.73   |
| 1   | A     | 1385 | VAL  | N-CA-C     | 5.46  | 116.18      | 110.62   |
| 14  | N     | 319  | ASP  | N-CA-C     | 5.45  | 119.75      | 113.38   |
| 2   | B     | 1155 | CYS  | N-CA-C     | 5.44  | 117.29      | 111.36   |
| 20  | T     | 170  | LYS  | CA-C-N     | 5.43  | 131.92      | 121.54   |
| 20  | T     | 170  | LYS  | C-N-CA     | 5.43  | 131.92      | 121.54   |
| 1   | A     | 138  | LYS  | N-CA-C     | 5.41  | 116.86      | 111.07   |
| 2   | B     | 924  | ARG  | NH1-CZ-NH2 | 5.40  | 126.33      | 119.30   |
| 2   | B     | 63   | PRO  | N-CA-C     | 5.39  | 117.28      | 110.70   |
| 1   | A     | 502  | ASN  | N-CA-C     | 5.39  | 118.26      | 109.59   |
| 14  | N     | 360  | LEU  | N-CA-C     | 5.36  | 117.15      | 108.41   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 20  | T     | 205  | ILE  | N-CA-C   | 5.35  | 117.78      | 111.09   |
| 20  | T     | 152  | ASN  | N-CA-C   | 5.35  | 119.09      | 112.24   |
| 1   | A     | 503  | LEU  | CA-CB-CG | 5.34  | 134.98      | 116.30   |
| 1   | A     | 458  | PHE  | N-CA-CB  | -5.33 | 102.10      | 110.69   |
| 2   | B     | 723  | THR  | CB-CA-C  | -5.33 | 101.79      | 110.85   |
| 2   | B     | 115  | LEU  | N-CA-C   | 5.32  | 117.16      | 111.36   |
| 20  | T     | 140  | ARG  | N-CA-C   | 5.31  | 117.88      | 107.57   |
| 2   | B     | 296  | GLU  | N-CA-C   | 5.30  | 116.75      | 111.07   |
| 2   | B     | 1168 | ALA  | CA-C-N   | 5.30  | 125.06      | 119.76   |
| 2   | B     | 1168 | ALA  | C-N-CA   | 5.30  | 125.06      | 119.76   |
| 1   | A     | 181  | HIS  | N-CA-C   | -5.28 | 102.52      | 110.70   |
| 2   | B     | 156  | LEU  | N-CA-C   | 5.27  | 118.08      | 110.28   |
| 1   | A     | 432  | HIS  | CA-C-N   | 5.26  | 125.57      | 119.47   |
| 1   | A     | 432  | HIS  | C-N-CA   | 5.26  | 125.57      | 119.47   |
| 1   | A     | 622  | SER  | N-CA-C   | -5.26 | 98.19       | 109.81   |
| 1   | A     | 807  | LEU  | CA-C-N   | -5.26 | 114.28      | 120.12   |
| 1   | A     | 807  | LEU  | C-N-CA   | -5.26 | 114.28      | 120.12   |
| 1   | A     | 211  | GLU  | N-CA-C   | 5.26  | 122.00      | 110.80   |
| 2   | B     | 508  | MET  | N-CA-C   | 5.25  | 119.67      | 112.68   |
| 2   | B     | 529  | MET  | CB-CG-SD | 5.25  | 128.46      | 112.70   |
| 20  | T     | 135  | SER  | N-CA-C   | 5.25  | 117.08      | 111.36   |
| 2   | B     | 1001 | PRO  | CA-C-N   | -5.25 | 115.39      | 122.95   |
| 2   | B     | 1001 | PRO  | C-N-CA   | -5.25 | 115.39      | 122.95   |
| 13  | M     | 42   | GLY  | CA-C-O   | 5.25  | 125.72      | 120.89   |
| 18  | R     | 162  | GLY  | N-CA-C   | 5.24  | 125.60      | 113.18   |
| 21  | U     | 252  | LYS  | N-CA-C   | -5.23 | 99.67       | 110.80   |
| 13  | M     | 126  | ASP  | N-CA-C   | 5.23  | 117.88      | 111.82   |
| 1   | A     | 771  | VAL  | N-CA-C   | 5.21  | 115.99      | 110.72   |
| 1   | A     | 593  | SER  | N-CA-C   | 5.21  | 118.73      | 112.38   |
| 7   | G     | 159  | ALA  | N-CA-C   | 5.21  | 117.59      | 109.52   |
| 10  | J     | 65   | LEU  | CA-C-N   | -5.20 | 112.38      | 122.06   |
| 10  | J     | 65   | LEU  | C-N-CA   | -5.20 | 112.38      | 122.06   |
| 1   | A     | 609  | HIS  | CA-C-N   | 5.19  | 126.32      | 119.84   |
| 1   | A     | 609  | HIS  | C-N-CA   | 5.19  | 126.32      | 119.84   |
| 2   | B     | 1050 | ARG  | N-CA-C   | -5.19 | 101.25      | 109.76   |
| 3   | C     | 240  | ARG  | CA-C-N   | 5.19  | 124.64      | 119.24   |
| 3   | C     | 240  | ARG  | C-N-CA   | 5.19  | 124.64      | 119.24   |
| 2   | B     | 753  | TYR  | CA-C-N   | -5.18 | 115.23      | 120.31   |
| 2   | B     | 753  | TYR  | C-N-CA   | -5.18 | 115.23      | 120.31   |
| 1   | A     | 473  | ARG  | CG-CD-NE | -5.17 | 100.62      | 112.00   |
| 1   | A     | 1311 | LEU  | N-CA-C   | 5.17  | 118.53      | 109.48   |
| 1   | A     | 1035 | GLU  | N-CA-C   | 5.17  | 116.60      | 111.07   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2   | B     | 256  | ILE  | N-CA-C   | 5.17  | 115.90      | 108.93   |
| 5   | E     | 70   | ASP  | CB-CA-C  | -5.16 | 110.22      | 117.23   |
| 3   | C     | 71   | ILE  | N-CA-C   | 5.15  | 113.81      | 109.02   |
| 1   | A     | 541  | THR  | CA-C-N   | -5.15 | 113.38      | 120.28   |
| 1   | A     | 541  | THR  | C-N-CA   | -5.15 | 113.38      | 120.28   |
| 1   | A     | 1405 | MET  | N-CA-C   | 5.15  | 116.89      | 111.28   |
| 1   | A     | 545  | VAL  | CB-CA-C  | -5.14 | 105.20      | 112.14   |
| 16  | P     | 325  | PHE  | N-CA-C   | 5.14  | 116.96      | 111.36   |
| 20  | T     | 136  | SER  | N-CA-C   | 5.13  | 119.64      | 113.17   |
| 13  | M     | 179  | GLU  | N-CA-C   | 5.13  | 116.95      | 111.36   |
| 2   | B     | 728  | MET  | N-CA-C   | 5.13  | 117.77      | 111.82   |
| 1   | A     | 773  | GLY  | N-CA-C   | -5.12 | 107.73      | 115.32   |
| 2   | B     | 896  | LEU  | N-CA-C   | 5.11  | 117.57      | 109.96   |
| 12  | L     | 47   | LYS  | N-CA-C   | 5.11  | 117.12      | 110.43   |
| 13  | M     | 140  | ASN  | N-CA-C   | 5.10  | 116.53      | 111.07   |
| 2   | B     | 747  | LEU  | CA-CB-CG | -5.09 | 98.47       | 116.30   |
| 1   | A     | 211  | GLU  | CA-C-N   | 5.09  | 128.78      | 121.71   |
| 1   | A     | 211  | GLU  | C-N-CA   | 5.09  | 128.78      | 121.71   |
| 2   | B     | 933  | ASP  | N-CA-C   | -5.08 | 101.42      | 109.96   |
| 10  | J     | 48   | MET  | N-CA-C   | -5.08 | 105.43      | 110.97   |
| 2   | B     | 1134 | THR  | CB-CA-C  | -5.07 | 108.06      | 114.40   |
| 1   | A     | 864  | LEU  | CA-C-N   | 5.07  | 126.95      | 120.56   |
| 1   | A     | 864  | LEU  | C-N-CA   | 5.07  | 126.95      | 120.56   |
| 2   | B     | 982  | ILE  | CB-CA-C  | -5.07 | 105.30      | 112.14   |
| 1   | A     | 686  | THR  | N-CA-C   | 5.06  | 115.02      | 107.88   |
| 2   | B     | 735  | VAL  | N-CA-C   | 5.06  | 116.03      | 108.54   |
| 2   | B     | 603  | MET  | N-CA-C   | 5.05  | 116.65      | 108.26   |
| 2   | B     | 735  | VAL  | CB-CA-C  | -5.04 | 105.18      | 111.08   |
| 1   | A     | 951  | GLU  | N-CA-C   | 5.02  | 116.83      | 111.36   |
| 2   | B     | 76   | GLY  | N-CA-C   | 5.02  | 125.08      | 113.18   |
| 15  | O     | 29   | THR  | CA-C-N   | 5.02  | 125.04      | 119.32   |
| 15  | O     | 29   | THR  | C-N-CA   | 5.02  | 125.04      | 119.32   |
| 1   | A     | 604  | ARG  | CB-CA-C  | -5.01 | 110.42      | 117.23   |
| 2   | B     | 915  | GLY  | N-CA-C   | -5.01 | 108.33      | 115.64   |
| 2   | B     | 990  | SER  | N-CA-C   | 5.01  | 116.43      | 111.07   |
| 3   | C     | 61   | ASP  | N-CA-C   | 5.01  | 116.43      | 111.07   |
| 2   | B     | 163  | LEU  | N-CA-C   | 5.00  | 118.48      | 112.38   |
| 2   | B     | 643  | LEU  | N-CA-C   | 5.00  | 116.73      | 111.28   |
| 5   | E     | 145  | VAL  | N-CA-C   | 5.00  | 112.81      | 107.76   |

There are no chirality outliers.

All (15) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | A     | 1086 | MET  | Peptide   |
| 1   | A     | 1308 | TYR  | Peptide   |
| 2   | B     | 416  | ARG  | Sidechain |
| 2   | B     | 525  | ASN  | Peptide   |
| 2   | B     | 873  | LEU  | Mainchain |
| 7   | G     | 151  | ARG  | Sidechain |
| 13  | M     | 45   | VAL  | Mainchain |
| 14  | N     | 355  | ASP  | Peptide   |
| 14  | N     | 371  | ILE  | Peptide   |
| 16  | P     | 158  | SER  | Peptide   |
| 17  | Q     | 125  | ALA  | Peptide   |
| 18  | R     | 215  | GLU  | Mainchain |
| 19  | S     | 148  | PRO  | Peptide   |
| 20  | T     | 123  | ASN  | Peptide   |
| 20  | T     | 177  | ARG  | Peptide   |

## 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     | 11515 | 0        | 11607    | 540     | 0            |
| 2   | B     | 9317  | 0        | 9308     | 380     | 0            |
| 3   | C     | 2213  | 0        | 2153     | 93      | 0            |
| 4   | D     | 1062  | 0        | 1042     | 11      | 0            |
| 5   | E     | 1723  | 0        | 1745     | 63      | 0            |
| 6   | F     | 689   | 0        | 715      | 19      | 0            |
| 7   | G     | 1351  | 0        | 1358     | 25      | 0            |
| 8   | H     | 1205  | 0        | 1168     | 49      | 0            |
| 9   | I     | 1013  | 0        | 932      | 61      | 0            |
| 10  | J     | 533   | 0        | 553      | 35      | 0            |
| 11  | K     | 937   | 0        | 959      | 32      | 0            |
| 12  | L     | 388   | 0        | 393      | 28      | 0            |
| 13  | M     | 2391  | 0        | 2410     | 131     | 0            |
| 14  | N     | 930   | 0        | 888      | 25      | 0            |
| 15  | O     | 806   | 0        | 818      | 16      | 0            |
| 16  | P     | 1462  | 0        | 1549     | 57      | 0            |
| 17  | Q     | 1484  | 0        | 1494     | 147     | 0            |
| 18  | R     | 1357  | 0        | 1379     | 207     | 0            |
| 19  | S     | 1138  | 0        | 1103     | 34      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 20  | T     | 1788  | 0        | 1819     | 101     | 0            |
| 21  | U     | 1343  | 0        | 1338     | 45      | 0            |
| 22  | X     | 1645  | 0        | 908      | 34      | 0            |
| 23  | Y     | 1624  | 0        | 899      | 27      | 0            |
| 24  | A     | 2     | 0        | 0        | 0       | 0            |
| 25  | A     | 2     | 0        | 0        | 0       | 0            |
| 25  | B     | 1     | 0        | 0        | 0       | 0            |
| 25  | C     | 1     | 0        | 0        | 0       | 0            |
| 25  | I     | 2     | 0        | 0        | 0       | 0            |
| 25  | J     | 1     | 0        | 0        | 0       | 0            |
| 25  | L     | 1     | 0        | 0        | 0       | 0            |
| 25  | M     | 1     | 0        | 0        | 0       | 0            |
| 25  | Q     | 1     | 0        | 0        | 0       | 0            |
| 25  | U     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 47927 | 0        | 46538    | 1803    | 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 19.

All (1803) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:932:ARG:CG    | 1:A:943:LEU:CD1   | 1.74                     | 1.56              |
| 18:R:195:PRO:CG   | 18:R:199:LYS:CB   | 1.86                     | 1.52              |
| 5:E:64:HIS:CE1    | 5:E:68:PRO:HG3    | 1.44                     | 1.52              |
| 13:M:37:CYS:SG    | 13:M:39:LEU:HD22  | 1.46                     | 1.52              |
| 1:A:932:ARG:CD    | 1:A:943:LEU:HD21  | 1.38                     | 1.50              |
| 17:Q:54:PHE:CD1   | 18:R:194:ARG:CD   | 1.94                     | 1.50              |
| 18:R:195:PRO:HG2  | 18:R:199:LYS:CB   | 1.01                     | 1.46              |
| 17:Q:54:PHE:CD1   | 18:R:194:ARG:HD2  | 1.51                     | 1.45              |
| 16:P:206:GLU:CG   | 16:P:236:LYS:NZ   | 1.77                     | 1.44              |
| 13:M:9:ALA:C      | 13:M:10:LEU:HD13  | 1.44                     | 1.43              |
| 1:A:932:ARG:HG3   | 1:A:943:LEU:CD1   | 1.33                     | 1.42              |
| 17:Q:113:ARG:NH2  | 18:R:218:LYS:HE3  | 1.34                     | 1.41              |
| 1:A:932:ARG:CG    | 1:A:943:LEU:HD11  | 0.91                     | 1.38              |
| 16:P:206:GLU:HG3  | 16:P:236:LYS:NZ   | 1.33                     | 1.37              |
| 17:Q:112:ARG:CD   | 18:R:237:LEU:HD11 | 1.54                     | 1.36              |
| 16:P:297:LYS:HB3  | 16:P:298:PRO:CD   | 1.44                     | 1.36              |
| 17:Q:20:TYR:CE2   | 18:R:210:PHE:CB   | 1.93                     | 1.36              |
| 18:R:154:LEU:HD23 | 18:R:163:LEU:CD2  | 1.54                     | 1.35              |
| 17:Q:20:TYR:CE2   | 18:R:210:PHE:HB3  | 1.08                     | 1.34              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:133:ARG:HA    | 3:C:136:ASP:OD2   | 1.23                     | 1.34              |
| 1:A:133:SER:OG    | 1:A:136:GLN:HB2   | 1.21                     | 1.33              |
| 17:Q:112:ARG:NE   | 18:R:237:LEU:HD11 | 1.45                     | 1.32              |
| 1:A:551:ARG:HD3   | 1:A:625:ASP:OD2   | 1.31                     | 1.30              |
| 18:R:195:PRO:CG   | 18:R:199:LYS:HB3  | 1.50                     | 1.30              |
| 1:A:199:TYR:OH    | 13:M:93:PHE:CE2   | 1.80                     | 1.29              |
| 17:Q:113:ARG:NH2  | 18:R:218:LYS:CE   | 1.93                     | 1.29              |
| 1:A:1163:HIS:H    | 1:A:1305:SER:C    | 1.26                     | 1.28              |
| 1:A:263:ALA:O     | 1:A:264:VAL:CG1   | 1.80                     | 1.28              |
| 17:Q:54:PHE:CE1   | 18:R:194:ARG:HD2  | 1.66                     | 1.27              |
| 1:A:1163:HIS:O    | 1:A:1305:SER:CB   | 1.82                     | 1.27              |
| 16:P:298:PRO:O    | 16:P:300:ILE:HG12 | 1.14                     | 1.26              |
| 5:E:26:TYR:HA     | 5:E:64:HIS:O      | 1.11                     | 1.26              |
| 1:A:201:GLU:HA    | 1:A:212:LYS:O     | 1.17                     | 1.25              |
| 18:R:195:PRO:CG   | 18:R:199:LYS:HB2  | 1.54                     | 1.24              |
| 3:C:6:GLN:HB2     | 11:K:100:LEU:CD2  | 1.67                     | 1.23              |
| 17:Q:187:ILE:HD13 | 18:R:210:PHE:O    | 1.37                     | 1.23              |
| 18:R:151:LEU:HD12 | 18:R:163:LEU:CD1  | 1.67                     | 1.22              |
| 1:A:608:THR:C     | 1:A:610:PRO:HD2   | 1.64                     | 1.22              |
| 1:A:932:ARG:HG3   | 1:A:943:LEU:CG    | 1.70                     | 1.21              |
| 3:C:6:GLN:CB      | 11:K:100:LEU:HD23 | 1.70                     | 1.21              |
| 13:M:94:ASP:OD2   | 13:M:97:GLY:O     | 1.55                     | 1.20              |
| 5:E:46:ASP:O      | 5:E:48:PRO:HD3    | 1.42                     | 1.19              |
| 1:A:199:TYR:OH    | 13:M:93:PHE:CZ    | 1.96                     | 1.19              |
| 17:Q:180:PHE:CZ   | 18:R:213:ASP:CA   | 2.26                     | 1.18              |
| 1:A:622:SER:O     | 1:A:624:GLY:N     | 1.73                     | 1.18              |
| 1:A:932:ARG:HG2   | 1:A:943:LEU:CD1   | 1.49                     | 1.18              |
| 13:M:15:CYS:SG    | 13:M:39:LEU:HD21  | 1.83                     | 1.18              |
| 17:Q:105:TYR:CE1  | 18:R:234:GLU:CD   | 2.22                     | 1.17              |
| 17:Q:180:PHE:CZ   | 18:R:213:ASP:HA   | 1.79                     | 1.17              |
| 8:H:74:GLU:O      | 8:H:76:ASN:N      | 1.75                     | 1.17              |
| 3:C:6:GLN:HG3     | 11:K:100:LEU:HD21 | 1.23                     | 1.17              |
| 21:U:227:GLU:O    | 21:U:228:MET:HE2  | 1.45                     | 1.17              |
| 5:E:25:GLY:O      | 5:E:65:ASN:HA     | 1.44                     | 1.16              |
| 12:L:16:ILE:O     | 12:L:17:TYR:HB2   | 1.46                     | 1.16              |
| 16:P:298:PRO:O    | 16:P:300:ILE:CG1  | 1.93                     | 1.16              |
| 2:B:52:GLN:HA     | 20:T:141:LEU:CD1  | 1.75                     | 1.15              |
| 1:A:1163:HIS:N    | 1:A:1305:SER:C    | 1.98                     | 1.15              |
| 1:A:132:LYS:O     | 1:A:133:SER:HB2   | 1.46                     | 1.14              |
| 5:E:64:HIS:HE1    | 5:E:68:PRO:CG     | 1.60                     | 1.14              |
| 18:R:164:GLY:CA   | 18:R:203:PHE:CZ   | 2.30                     | 1.14              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:P:297:LYS:HB3  | 16:P:298:PRO:HD3  | 1.22                     | 1.13              |
| 2:B:880:LEU:O     | 2:B:881:GLU:HB2   | 1.40                     | 1.13              |
| 18:R:164:GLY:HA2  | 18:R:203:PHE:CZ   | 1.84                     | 1.12              |
| 1:A:932:ARG:CD    | 1:A:943:LEU:CD2   | 2.29                     | 1.11              |
| 1:A:932:ARG:CB    | 1:A:943:LEU:HD11  | 1.80                     | 1.11              |
| 2:B:225:LEU:C     | 2:B:227:ASN:H     | 1.52                     | 1.11              |
| 17:Q:54:PHE:CD1   | 18:R:194:ARG:HD3  | 1.66                     | 1.11              |
| 1:A:263:ALA:O     | 1:A:264:VAL:HG13  | 0.96                     | 1.11              |
| 5:E:63:ALA:O      | 5:E:64:HIS:HB2    | 1.32                     | 1.10              |
| 21:U:227:GLU:O    | 21:U:228:MET:HB3  | 1.50                     | 1.09              |
| 16:P:206:GLU:HB3  | 16:P:207:PRO:CD   | 1.82                     | 1.09              |
| 17:Q:112:ARG:NE   | 18:R:237:LEU:CD1  | 2.15                     | 1.08              |
| 18:R:225:VAL:HG12 | 18:R:227:SER:HB2  | 1.17                     | 1.08              |
| 16:P:206:GLU:CB   | 16:P:207:PRO:CD   | 2.32                     | 1.08              |
| 16:P:297:LYS:HB3  | 16:P:298:PRO:HD2  | 1.33                     | 1.08              |
| 16:P:206:GLU:HB3  | 16:P:207:PRO:HD3  | 1.34                     | 1.07              |
| 2:B:52:GLN:HA     | 20:T:141:LEU:HD12 | 1.33                     | 1.07              |
| 13:M:9:ALA:O      | 13:M:10:LEU:HD13  | 1.52                     | 1.07              |
| 13:M:46:ILE:O     | 13:M:47:ASP:HB2   | 1.42                     | 1.06              |
| 17:Q:23:ARG:NH2   | 18:R:206:LYS:CA   | 2.18                     | 1.06              |
| 18:R:195:PRO:HG2  | 18:R:199:LYS:CA   | 1.86                     | 1.06              |
| 1:A:1163:HIS:C    | 1:A:1305:SER:HB2  | 1.79                     | 1.06              |
| 2:B:132:VAL:HG21  | 2:B:141:GLN:HG2   | 1.35                     | 1.06              |
| 18:R:162:GLY:O    | 18:R:163:LEU:CG   | 2.04                     | 1.06              |
| 2:B:132:VAL:HG23  | 2:B:141:GLN:HB3   | 1.36                     | 1.05              |
| 16:P:206:GLU:CG   | 16:P:236:LYS:HZ3  | 1.51                     | 1.05              |
| 17:Q:112:ARG:HD3  | 18:R:237:LEU:HD11 | 1.35                     | 1.05              |
| 17:Q:180:PHE:CE1  | 18:R:212:VAL:O    | 2.10                     | 1.05              |
| 17:Q:54:PHE:HD1   | 18:R:194:ARG:HD3  | 0.95                     | 1.05              |
| 17:Q:180:PHE:CZ   | 18:R:212:VAL:O    | 2.10                     | 1.05              |
| 1:A:1163:HIS:H    | 1:A:1306:LYS:N    | 1.53                     | 1.05              |
| 1:A:264:VAL:HG23  | 1:A:272:ASN:CG    | 1.81                     | 1.04              |
| 16:P:206:GLU:HG2  | 16:P:236:LYS:HZ3  | 0.93                     | 1.04              |
| 21:U:251:ALA:O    | 21:U:252:LYS:HB2  | 1.51                     | 1.04              |
| 1:A:1162:GLU:HB3  | 1:A:1306:LYS:CB   | 1.87                     | 1.04              |
| 1:A:1163:HIS:O    | 1:A:1305:SER:HB2  | 0.86                     | 1.04              |
| 2:B:51:ILE:O      | 20:T:141:LEU:HD12 | 1.57                     | 1.04              |
| 1:A:264:VAL:HG23  | 1:A:272:ASN:OD1   | 1.57                     | 1.03              |
| 1:A:1116:ASN:ND2  | 1:A:1339:ASP:OD1  | 1.91                     | 1.03              |
| 13:M:10:LEU:O     | 13:M:13:VAL:HG22  | 1.56                     | 1.03              |
| 17:Q:23:ARG:NH2   | 18:R:206:LYS:CB   | 2.21                     | 1.03              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:Q:54:PHE:HD1   | 18:R:194:ARG:CD   | 1.44                     | 1.03              |
| 5:E:64:HIS:CE1    | 5:E:68:PRO:CG     | 2.39                     | 1.03              |
| 5:E:63:ALA:O      | 5:E:64:HIS:CB     | 2.06                     | 1.02              |
| 16:P:206:GLU:CG   | 16:P:236:LYS:HZ2  | 1.50                     | 1.02              |
| 3:C:6:GLN:HG2     | 11:K:104:ARG:HH12 | 1.20                     | 1.02              |
| 2:B:51:ILE:HG22   | 20:T:141:LEU:CD1  | 1.88                     | 1.02              |
| 18:R:162:GLY:O    | 18:R:163:LEU:CD2  | 2.09                     | 1.01              |
| 1:A:1306:LYS:O    | 1:A:1308:TYR:HD1  | 1.40                     | 1.01              |
| 18:R:154:LEU:HD23 | 18:R:163:LEU:HD22 | 1.02                     | 1.01              |
| 1:A:522:PRO:HA    | 1:A:666:ARG:HE    | 1.25                     | 1.01              |
| 1:A:1162:GLU:HB3  | 1:A:1306:LYS:HB3  | 1.04                     | 1.01              |
| 18:R:164:GLY:HA3  | 18:R:203:PHE:HZ   | 1.23                     | 1.01              |
| 1:A:932:ARG:HG2   | 1:A:943:LEU:HD11  | 1.05                     | 1.01              |
| 16:P:297:LYS:CB   | 16:P:298:PRO:CD   | 2.35                     | 1.00              |
| 1:A:1162:GLU:CB   | 1:A:1306:LYS:HB3  | 1.92                     | 1.00              |
| 2:B:51:ILE:CG2    | 20:T:141:LEU:HD11 | 1.90                     | 1.00              |
| 10:J:63:ALA:HB3   | 10:J:64:PRO:HD3   | 1.40                     | 1.00              |
| 18:R:164:GLY:HA3  | 18:R:203:PHE:CZ   | 1.95                     | 1.00              |
| 1:A:1306:LYS:O    | 1:A:1308:TYR:CD1  | 2.15                     | 1.00              |
| 17:Q:23:ARG:NH2   | 18:R:206:LYS:HB3  | 1.76                     | 1.00              |
| 20:T:139:VAL:CG1  | 20:T:142:SER:CB   | 2.39                     | 1.00              |
| 5:E:26:TYR:CA     | 5:E:64:HIS:O      | 2.08                     | 0.99              |
| 1:A:201:GLU:CA    | 1:A:212:LYS:O     | 2.10                     | 0.99              |
| 1:A:609:HIS:N     | 1:A:610:PRO:CD    | 2.24                     | 0.99              |
| 17:Q:23:ARG:HH22  | 18:R:206:LYS:HB3  | 1.26                     | 0.99              |
| 1:A:932:ARG:HD2   | 1:A:943:LEU:CD2   | 1.91                     | 0.99              |
| 18:R:162:GLY:O    | 18:R:163:LEU:HD23 | 1.61                     | 0.99              |
| 16:P:206:GLU:HB2  | 16:P:207:PRO:HD2  | 1.44                     | 0.98              |
| 17:Q:105:TYR:CD1  | 18:R:234:GLU:OE1  | 2.16                     | 0.98              |
| 18:R:151:LEU:HD13 | 18:R:163:LEU:HD22 | 1.44                     | 0.98              |
| 16:P:206:GLU:HG2  | 16:P:236:LYS:NZ   | 1.53                     | 0.98              |
| 1:A:1307:VAL:O    | 1:A:1308:TYR:O    | 1.78                     | 0.98              |
| 1:A:932:ARG:HG2   | 1:A:943:LEU:HD13  | 1.46                     | 0.97              |
| 1:A:132:LYS:O     | 1:A:133:SER:CB    | 2.13                     | 0.97              |
| 1:A:535:MET:O     | 1:A:669:TYR:OH    | 1.80                     | 0.97              |
| 18:R:195:PRO:HG2  | 18:R:199:LYS:HB3  | 1.07                     | 0.97              |
| 1:A:932:ARG:HD2   | 1:A:943:LEU:HD21  | 0.97                     | 0.96              |
| 17:Q:105:TYR:CE1  | 18:R:234:GLU:OE2  | 2.17                     | 0.96              |
| 18:R:154:LEU:CD2  | 18:R:163:LEU:HD22 | 1.95                     | 0.96              |
| 17:Q:20:TYR:HE2   | 18:R:210:PHE:CB   | 1.70                     | 0.96              |
| 1:A:133:SER:OG    | 1:A:136:GLN:CB    | 2.13                     | 0.96              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:Q:23:ARG:HH22  | 18:R:206:LYS:CB   | 1.78                     | 0.96              |
| 18:R:162:GLY:O    | 18:R:163:LEU:HG   | 1.63                     | 0.96              |
| 3:C:6:GLN:HG3     | 11:K:100:LEU:CD2  | 1.96                     | 0.96              |
| 1:A:45:GLU:OE1    | 1:A:48:GLU:HG3    | 1.65                     | 0.96              |
| 18:R:195:PRO:CB   | 18:R:199:LYS:CB   | 2.42                     | 0.95              |
| 2:B:52:GLN:CA     | 20:T:141:LEU:HD12 | 1.95                     | 0.95              |
| 3:C:6:GLN:CG      | 11:K:104:ARG:NH1  | 2.29                     | 0.95              |
| 17:Q:23:ARG:NH2   | 18:R:206:LYS:C    | 2.04                     | 0.95              |
| 1:A:1224:ARG:NH2  | 1:A:1306:LYS:HD3  | 1.82                     | 0.95              |
| 2:B:225:LEU:O     | 2:B:227:ASN:N     | 2.00                     | 0.95              |
| 3:C:6:GLN:CG      | 11:K:104:ARG:HH12 | 1.79                     | 0.95              |
| 18:R:151:LEU:HD12 | 18:R:163:LEU:HD13 | 1.46                     | 0.94              |
| 1:A:609:HIS:N     | 1:A:610:PRO:HD2   | 1.83                     | 0.94              |
| 18:R:151:LEU:CD1  | 18:R:163:LEU:HD13 | 1.97                     | 0.94              |
| 17:Q:184:ILE:HD13 | 18:R:218:LYS:HZ1  | 1.31                     | 0.94              |
| 2:B:645:GLU:OE1   | 2:B:649:ASN:ND2   | 2.01                     | 0.94              |
| 17:Q:105:TYR:CD1  | 18:R:234:GLU:CD   | 2.45                     | 0.94              |
| 2:B:958:CYS:SG    | 2:B:959:GLU:N     | 2.37                     | 0.94              |
| 3:C:6:GLN:HG2     | 11:K:104:ARG:NH1  | 1.83                     | 0.94              |
| 1:A:263:ALA:C     | 1:A:264:VAL:HG13  | 1.93                     | 0.93              |
| 13:M:9:ALA:C      | 13:M:10:LEU:CD1   | 2.39                     | 0.93              |
| 18:R:195:PRO:CB   | 18:R:199:LYS:HB3  | 1.99                     | 0.93              |
| 17:Q:23:ARG:HH22  | 18:R:206:LYS:CA   | 1.79                     | 0.93              |
| 13:M:182:ALA:HB1  | 20:T:152:ASN:OD1  | 1.68                     | 0.93              |
| 17:Q:105:TYR:HE1  | 18:R:234:GLU:OE2  | 1.49                     | 0.93              |
| 16:P:206:GLU:CB   | 16:P:207:PRO:HD2  | 1.99                     | 0.92              |
| 17:Q:113:ARG:HH21 | 18:R:218:LYS:HE3  | 1.09                     | 0.92              |
| 13:M:94:ASP:O     | 13:M:96:PHE:N     | 2.01                     | 0.92              |
| 5:E:45:GLY:O      | 5:E:46:ASP:O      | 1.85                     | 0.92              |
| 3:C:133:ARG:CA    | 3:C:136:ASP:OD2   | 2.17                     | 0.92              |
| 1:A:1116:ASN:O    | 1:A:1117:VAL:HG23 | 1.70                     | 0.92              |
| 18:R:151:LEU:HD12 | 18:R:163:LEU:CD2  | 2.00                     | 0.92              |
| 1:A:355:MET:SD    | 2:B:1091:ARG:NH1  | 2.43                     | 0.92              |
| 18:R:154:LEU:HD23 | 18:R:163:LEU:HD23 | 1.50                     | 0.92              |
| 2:B:933:ASP:OD2   | 2:B:1050:ARG:NH2  | 2.02                     | 0.91              |
| 18:R:151:LEU:CD1  | 18:R:163:LEU:HD22 | 1.99                     | 0.91              |
| 1:A:157:GLY:N     | 1:A:181:HIS:NE2   | 2.19                     | 0.91              |
| 1:A:197:GLU:OE1   | 13:M:93:PHE:CD2   | 2.23                     | 0.91              |
| 2:B:874:PRO:O     | 2:B:875:GLU:HB2   | 1.68                     | 0.91              |
| 3:C:6:GLN:CG      | 11:K:100:LEU:HD21 | 2.01                     | 0.91              |
| 16:P:205:ARG:O    | 16:P:206:GLU:O    | 1.87                     | 0.91              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:65:ASN:OD1    | 5:E:66:ASP:N      | 2.03                     | 0.91              |
| 2:B:132:VAL:HG21  | 2:B:141:GLN:CG    | 2.00                     | 0.91              |
| 1:A:544:ALA:HB2   | 1:A:680:LEU:HD22  | 1.54                     | 0.90              |
| 17:Q:112:ARG:CD   | 18:R:237:LEU:CD1  | 2.48                     | 0.90              |
| 1:A:932:ARG:CG    | 1:A:943:LEU:HD21  | 2.01                     | 0.90              |
| 2:B:51:ILE:C      | 20:T:141:LEU:HD12 | 1.96                     | 0.90              |
| 13:M:34:CYS:HB3   | 13:M:39:LEU:CB    | 2.01                     | 0.90              |
| 2:B:224:CYS:O     | 2:B:226:GLU:N     | 2.06                     | 0.89              |
| 1:A:932:ARG:CG    | 1:A:943:LEU:CD2   | 2.50                     | 0.89              |
| 1:A:201:GLU:OE2   | 1:A:203:LYS:NZ    | 2.04                     | 0.89              |
| 1:A:516:GLN:HA    | 1:A:520:MET:HE2   | 1.52                     | 0.89              |
| 21:U:227:GLU:O    | 21:U:228:MET:CB   | 2.19                     | 0.89              |
| 21:U:227:GLU:O    | 21:U:228:MET:CE   | 2.19                     | 0.89              |
| 1:A:264:VAL:CG2   | 1:A:272:ASN:CG    | 2.44                     | 0.89              |
| 1:A:199:TYR:HH    | 13:M:93:PHE:HE2   | 0.92                     | 0.89              |
| 13:M:92:SER:O     | 13:M:93:PHE:O     | 1.91                     | 0.89              |
| 17:Q:180:PHE:CE1  | 18:R:213:ASP:HA   | 2.07                     | 0.88              |
| 1:A:932:ARG:CG    | 1:A:943:LEU:CG    | 2.40                     | 0.88              |
| 1:A:197:GLU:OE1   | 13:M:93:PHE:CE2   | 2.26                     | 0.88              |
| 1:A:932:ARG:NE    | 1:A:943:LEU:HD21  | 1.88                     | 0.88              |
| 2:B:52:GLN:CA     | 20:T:141:LEU:CD1  | 2.52                     | 0.88              |
| 3:C:275:ASN:ND2   | 11:K:31:CYS:SG    | 2.47                     | 0.88              |
| 2:B:225:LEU:C     | 2:B:227:ASN:N     | 2.27                     | 0.88              |
| 2:B:52:GLN:HA     | 20:T:141:LEU:HD13 | 1.56                     | 0.88              |
| 17:Q:113:ARG:HH22 | 18:R:218:LYS:HE3  | 1.25                     | 0.87              |
| 20:T:139:VAL:HG13 | 20:T:142:SER:CB   | 2.04                     | 0.87              |
| 17:Q:113:ARG:HH21 | 18:R:218:LYS:CE   | 1.70                     | 0.87              |
| 18:R:151:LEU:CD1  | 18:R:163:LEU:CD2  | 2.52                     | 0.87              |
| 13:M:178:LYS:C    | 20:T:154:LYS:HE3  | 1.98                     | 0.87              |
| 18:R:151:LEU:CD1  | 18:R:163:LEU:CD1  | 2.51                     | 0.87              |
| 18:R:195:PRO:HG2  | 18:R:199:LYS:HB2  | 0.88                     | 0.87              |
| 18:R:151:LEU:HD12 | 18:R:163:LEU:HD11 | 1.55                     | 0.87              |
| 1:A:265:VAL:HA    | 1:A:272:ASN:HB2   | 1.57                     | 0.87              |
| 1:A:264:VAL:CG2   | 1:A:272:ASN:ND2   | 2.34                     | 0.86              |
| 3:C:6:GLN:CB      | 11:K:100:LEU:CD2  | 2.42                     | 0.86              |
| 9:I:61:GLU:O      | 9:I:63:ASP:N      | 2.07                     | 0.86              |
| 18:R:164:GLY:HA2  | 18:R:203:PHE:CE2  | 2.10                     | 0.86              |
| 18:R:154:LEU:CD2  | 18:R:163:LEU:CD2  | 2.49                     | 0.86              |
| 1:A:1457:ASN:OD1  | 1:A:1462:GLN:NE2  | 2.09                     | 0.85              |
| 13:M:46:ILE:O     | 13:M:47:ASP:CB    | 2.24                     | 0.85              |
| 2:B:132:VAL:CG2   | 2:B:141:GLN:HB3   | 2.06                     | 0.85              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:M:89:GLY:O     | 13:M:90:ALA:CB    | 2.25                     | 0.85              |
| 9:I:89:CYS:HB3    | 9:I:119:CYS:SG    | 2.17                     | 0.85              |
| 1:A:273:GLN:NE2   | 13:M:79:ASP:OD2   | 2.10                     | 0.85              |
| 2:B:492:ASP:O     | 23:Y:45:DT:C2'    | 2.24                     | 0.85              |
| 1:A:1163:HIS:ND1  | 1:A:1302:GLU:O    | 2.09                     | 0.85              |
| 2:B:132:VAL:CG2   | 2:B:141:GLN:CG    | 2.55                     | 0.85              |
| 8:H:65:TYR:HE2    | 8:H:70:LEU:HB2    | 1.42                     | 0.85              |
| 5:E:49:SER:O      | 5:E:50:GLU:O      | 1.96                     | 0.84              |
| 17:Q:24:GLY:HA3   | 18:R:210:PHE:CE2  | 2.13                     | 0.84              |
| 17:Q:105:TYR:HE1  | 18:R:234:GLU:CD   | 1.78                     | 0.84              |
| 3:C:6:GLN:CG      | 11:K:100:LEU:CD2  | 2.55                     | 0.84              |
| 1:A:79:THR:HG21   | 13:M:43:ASP:OD1   | 1.77                     | 0.83              |
| 1:A:551:ARG:CD    | 1:A:625:ASP:OD2   | 2.23                     | 0.83              |
| 12:L:16:ILE:O     | 12:L:17:TYR:CB    | 2.25                     | 0.83              |
| 18:R:164:GLY:CA   | 18:R:203:PHE:CE2  | 2.61                     | 0.83              |
| 1:A:1112:VAL:O    | 21:U:252:LYS:HB3  | 1.78                     | 0.83              |
| 8:H:65:TYR:CE2    | 8:H:70:LEU:HB2    | 2.13                     | 0.83              |
| 17:Q:52:LEU:HB3   | 17:Q:54:PHE:HD2   | 1.43                     | 0.83              |
| 20:T:139:VAL:CG1  | 20:T:142:SER:HB3  | 2.07                     | 0.82              |
| 1:A:375:ILE:HG21  | 1:A:666:ARG:CZ    | 2.08                     | 0.82              |
| 17:Q:184:ILE:HD13 | 18:R:218:LYS:NZ   | 1.94                     | 0.82              |
| 8:H:65:TYR:CD2    | 8:H:70:LEU:HD22   | 2.15                     | 0.82              |
| 5:E:46:ASP:O      | 5:E:48:PRO:CD     | 2.27                     | 0.82              |
| 17:Q:20:TYR:CE2   | 18:R:210:PHE:HB2  | 2.10                     | 0.81              |
| 17:Q:113:ARG:HH22 | 18:R:218:LYS:CD   | 1.93                     | 0.81              |
| 2:B:761:THR:H     | 2:B:764:MET:HE3   | 1.44                     | 0.81              |
| 16:P:297:LYS:CB   | 16:P:298:PRO:HD2  | 2.06                     | 0.81              |
| 17:Q:113:ARG:NH1  | 18:R:218:LYS:HG3  | 1.96                     | 0.81              |
| 17:Q:69:ASP:HA    | 18:R:226:ASP:OD1  | 1.80                     | 0.81              |
| 17:Q:113:ARG:NH2  | 18:R:218:LYS:CD   | 2.43                     | 0.81              |
| 2:B:226:GLU:OE2   | 2:B:617:ASP:HB2   | 1.81                     | 0.81              |
| 21:U:256:THR:O    | 21:U:257:GLN:HB2  | 1.81                     | 0.81              |
| 3:C:6:GLN:HB2     | 11:K:100:LEU:HD23 | 0.85                     | 0.80              |
| 13:M:9:ALA:O      | 13:M:10:LEU:CD1   | 2.27                     | 0.80              |
| 1:A:1312:PRO:HB3  | 1:A:1334:TRP:CZ3  | 2.16                     | 0.80              |
| 3:C:209:SER:O     | 3:C:212:ASP:OD1   | 1.97                     | 0.80              |
| 5:E:41:LYS:HG3    | 5:E:46:ASP:OD2    | 1.82                     | 0.80              |
| 16:P:298:PRO:O    | 16:P:300:ILE:CD1  | 2.30                     | 0.80              |
| 2:B:51:ILE:O      | 20:T:141:LEU:CD1  | 2.30                     | 0.80              |
| 1:A:133:SER:O     | 1:A:134:LYS:C     | 2.22                     | 0.80              |
| 17:Q:68:GLY:O     | 18:R:226:ASP:HB3  | 1.82                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:206:ASN:O     | 1:A:207:GLU:HB2   | 1.80                     | 0.80              |
| 2:B:51:ILE:C      | 20:T:141:LEU:CD1  | 2.55                     | 0.79              |
| 1:A:932:ARG:HG3   | 1:A:943:LEU:HD11  | 0.83                     | 0.79              |
| 16:P:206:GLU:HG3  | 16:P:236:LYS:HZ2  | 0.67                     | 0.79              |
| 18:R:205:ASP:O    | 18:R:206:LYS:HD2  | 1.82                     | 0.79              |
| 1:A:79:THR:HG21   | 13:M:43:ASP:CG    | 2.08                     | 0.79              |
| 4:D:48:ASN:HD22   | 4:D:57:LEU:HG     | 1.48                     | 0.79              |
| 1:A:199:TYR:OH    | 13:M:93:PHE:HE2   | 1.36                     | 0.78              |
| 2:B:566:LYS:HD3   | 2:B:573:TRP:HE1   | 1.47                     | 0.78              |
| 5:E:55:ARG:NH1    | 5:E:107:GLN:OE1   | 2.17                     | 0.78              |
| 17:Q:184:ILE:CD1  | 18:R:218:LYS:NZ   | 2.47                     | 0.78              |
| 17:Q:23:ARG:HH22  | 18:R:206:LYS:C    | 1.59                     | 0.78              |
| 1:A:621:ILE:O     | 1:A:623:PRO:N     | 2.16                     | 0.78              |
| 3:C:157:GLN:CG    | 10:J:65:LEU:HB3   | 2.13                     | 0.78              |
| 2:B:492:ASP:O     | 23:Y:45:DT:H2'    | 1.83                     | 0.78              |
| 2:B:51:ILE:HG22   | 20:T:141:LEU:HD11 | 0.93                     | 0.78              |
| 3:C:6:GLN:HG3     | 11:K:104:ARG:NH1  | 1.97                     | 0.78              |
| 1:A:485:ASN:OD1   | 1:A:486:LEU:N     | 2.16                     | 0.77              |
| 17:Q:112:ARG:CZ   | 18:R:237:LEU:HD11 | 2.14                     | 0.77              |
| 2:B:897:ARG:O     | 2:B:900:GLU:CG    | 2.32                     | 0.77              |
| 2:B:73:HIS:C      | 2:B:75:SER:H      | 1.93                     | 0.77              |
| 13:M:182:ALA:HB1  | 20:T:152:ASN:CG   | 2.10                     | 0.77              |
| 2:B:490:GLY:O     | 2:B:491:ARG:HB2   | 1.83                     | 0.77              |
| 19:S:49:ARG:NH1   | 19:S:96:GLN:O     | 2.18                     | 0.77              |
| 20:T:155:PRO:O    | 20:T:157:ALA:N    | 2.17                     | 0.76              |
| 2:B:591:ARG:NH1   | 2:B:663:GLU:OE2   | 2.18                     | 0.76              |
| 17:Q:180:PHE:CE1  | 18:R:212:VAL:C    | 2.62                     | 0.76              |
| 1:A:930:LEU:HB3   | 1:A:934:LEU:HB2   | 1.67                     | 0.76              |
| 2:B:132:VAL:HG23  | 2:B:141:GLN:CB    | 2.16                     | 0.76              |
| 2:B:897:ARG:O     | 2:B:900:GLU:HG3   | 1.86                     | 0.76              |
| 1:A:890:ARG:HH21  | 1:A:1023:VAL:HG13 | 1.51                     | 0.75              |
| 23:Y:63:DG:H3'    | 23:Y:64:DC:H2'    | 1.67                     | 0.75              |
| 2:B:73:HIS:O      | 2:B:75:SER:N      | 2.19                     | 0.75              |
| 13:M:34:CYS:HB3   | 13:M:39:LEU:HB2   | 1.68                     | 0.75              |
| 13:M:178:LYS:HB3  | 20:T:154:LYS:HD3  | 1.68                     | 0.75              |
| 20:T:139:VAL:HG13 | 20:T:142:SER:HB2  | 1.68                     | 0.75              |
| 20:T:139:VAL:HG12 | 20:T:142:SER:HB3  | 1.67                     | 0.75              |
| 1:A:608:THR:C     | 1:A:610:PRO:CD    | 2.50                     | 0.75              |
| 1:A:265:VAL:HA    | 1:A:272:ASN:CB    | 2.14                     | 0.75              |
| 1:A:298:ALA:HB1   | 1:A:303:ILE:HD11  | 1.68                     | 0.74              |
| 1:A:930:LEU:O     | 1:A:931:ARG:O     | 2.05                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:Q:113:ARG:HH22 | 18:R:218:LYS:CE   | 1.79                     | 0.74              |
| 18:R:195:PRO:HG2  | 18:R:199:LYS:C    | 2.12                     | 0.74              |
| 18:R:204:ASN:ND2  | 18:R:205:ASP:N    | 2.36                     | 0.74              |
| 20:T:152:ASN:O    | 20:T:154:LYS:N    | 2.20                     | 0.74              |
| 1:A:199:TYR:OH    | 13:M:93:PHE:HZ    | 1.69                     | 0.74              |
| 14:N:347:ASN:ND2  | 14:N:375:GLU:OE2  | 2.21                     | 0.74              |
| 17:Q:188:TYR:HA   | 17:Q:191:LEU:HD13 | 1.70                     | 0.74              |
| 21:U:256:THR:OG1  | 21:U:257:GLN:N    | 2.13                     | 0.74              |
| 1:A:263:ALA:O     | 1:A:264:VAL:CB    | 2.36                     | 0.74              |
| 13:M:94:ASP:HB2   | 13:M:99:SER:H     | 1.53                     | 0.73              |
| 17:Q:112:ARG:CZ   | 18:R:237:LEU:CD1  | 2.66                     | 0.73              |
| 1:A:1116:ASN:O    | 1:A:1117:VAL:CG2  | 2.37                     | 0.73              |
| 17:Q:42:CYS:HB3   | 17:Q:95:ASN:HD21  | 1.54                     | 0.73              |
| 18:R:222:SER:O    | 18:R:224:THR:N    | 2.21                     | 0.73              |
| 1:A:156:GLY:HA2   | 1:A:181:HIS:ND1   | 2.03                     | 0.72              |
| 1:A:79:THR:CG2    | 13:M:43:ASP:OD1   | 2.38                     | 0.72              |
| 2:B:492:ASP:O     | 23:Y:45:DT:H2"    | 1.88                     | 0.72              |
| 17:Q:184:ILE:HD11 | 18:R:218:LYS:HZ2  | 1.54                     | 0.72              |
| 2:B:838:GLN:HB3   | 2:B:890:ARG:HA    | 1.70                     | 0.72              |
| 1:A:608:THR:CB    | 1:A:610:PRO:HD2   | 2.19                     | 0.72              |
| 16:P:206:GLU:C    | 16:P:208:ARG:H    | 1.98                     | 0.72              |
| 17:Q:68:GLY:O     | 18:R:226:ASP:CG   | 2.31                     | 0.72              |
| 2:B:490:GLY:O     | 2:B:491:ARG:CB    | 2.36                     | 0.72              |
| 2:B:873:LEU:HB3   | 2:B:874:PRO:HD3   | 1.69                     | 0.72              |
| 17:Q:20:TYR:HE2   | 18:R:210:PHE:HB2  | 1.50                     | 0.72              |
| 1:A:932:ARG:NE    | 1:A:943:LEU:CD2   | 2.49                     | 0.72              |
| 1:A:1211:LEU:HD11 | 1:A:1258:ARG:HG3  | 1.72                     | 0.72              |
| 2:B:793:SER:HA    | 2:B:944:THR:O     | 1.89                     | 0.72              |
| 17:Q:68:GLY:O     | 18:R:226:ASP:CB   | 2.38                     | 0.72              |
| 2:B:429:PHE:H     | 20:T:160:GLN:HG2  | 1.55                     | 0.72              |
| 17:Q:54:PHE:CE1   | 18:R:194:ARG:CD   | 2.49                     | 0.72              |
| 1:A:269:SER:O     | 1:A:270:ALA:HB3   | 1.89                     | 0.72              |
| 4:D:96:GLU:OE1    | 4:D:121:ARG:NH1   | 2.23                     | 0.72              |
| 12:L:19:CYS:SG    | 12:L:20:GLY:N     | 2.62                     | 0.71              |
| 15:O:79:VAL:HG21  | 15:O:93:VAL:HG12  | 1.72                     | 0.71              |
| 2:B:132:VAL:CG2   | 2:B:141:GLN:CB    | 2.68                     | 0.71              |
| 5:E:3:ASP:HB2     | 5:E:50:GLU:OE1    | 1.90                     | 0.71              |
| 8:H:66:GLU:O      | 8:H:67:ASP:HB2    | 1.90                     | 0.71              |
| 17:Q:19:LYS:O     | 17:Q:22:ILE:HG13  | 1.88                     | 0.71              |
| 1:A:643:LYS:NZ    | 21:U:299:LYS:O    | 2.22                     | 0.71              |
| 14:N:320:VAL:HB   | 16:P:236:LYS:HE3  | 1.71                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1006:VAL:HG23 | 2:B:1010:LYS:HB2  | 1.72                     | 0.71              |
| 3:C:136:ASP:N     | 3:C:136:ASP:OD1   | 2.22                     | 0.71              |
| 18:R:151:LEU:HD12 | 18:R:163:LEU:CG   | 2.20                     | 0.71              |
| 18:R:195:PRO:CB   | 18:R:199:LYS:HB2  | 2.14                     | 0.71              |
| 1:A:926:ASN:HA    | 1:A:931:ARG:HG3   | 1.73                     | 0.70              |
| 2:B:285:LEU:HD21  | 2:B:298:MET:HE3   | 1.73                     | 0.70              |
| 17:Q:187:ILE:CD1  | 18:R:210:PHE:O    | 2.29                     | 0.70              |
| 18:R:193:ASN:ND2  | 18:R:197:LYS:O    | 2.22                     | 0.70              |
| 20:T:8:ASP:OD2    | 20:T:10:THR:OG1   | 2.08                     | 0.70              |
| 3:C:56:SER:HG     | 3:C:158:GLU:H     | 1.39                     | 0.70              |
| 14:N:32:ASP:HB3   | 14:N:34:VAL:HG23  | 1.73                     | 0.70              |
| 14:N:317:GLU:HG3  | 16:P:235:ARG:HG2  | 1.71                     | 0.70              |
| 1:A:18:ILE:HB     | 1:A:1460:LEU:HD21 | 1.70                     | 0.70              |
| 5:E:25:GLY:O      | 5:E:65:ASN:CA     | 2.34                     | 0.70              |
| 8:H:65:TYR:CZ     | 8:H:70:LEU:HD13   | 2.25                     | 0.70              |
| 2:B:721:ARG:HG3   | 2:B:939:HIS:O     | 1.91                     | 0.70              |
| 2:B:812:ARG:HD3   | 2:B:814:TYR:OH    | 1.92                     | 0.70              |
| 3:C:24:GLU:HG2    | 3:C:228:ARG:HG3   | 1.73                     | 0.70              |
| 1:A:505:LEU:O     | 2:B:1106:ARG:NH2  | 2.24                     | 0.70              |
| 1:A:298:ALA:O     | 17:Q:60:ARG:NE    | 2.24                     | 0.70              |
| 18:R:195:PRO:HB2  | 18:R:199:LYS:CB   | 2.21                     | 0.70              |
| 1:A:932:ARG:HB3   | 1:A:940:LYS:CB    | 2.22                     | 0.70              |
| 11:K:111:ASP:O    | 11:K:113:GLN:N    | 2.19                     | 0.70              |
| 1:A:79:THR:CG2    | 13:M:43:ASP:CG    | 2.65                     | 0.70              |
| 1:A:609:HIS:N     | 1:A:610:PRO:HD3   | 2.07                     | 0.70              |
| 21:U:180:ILE:HG21 | 21:U:187:TYR:HB2  | 1.73                     | 0.70              |
| 2:B:939:HIS:NE2   | 2:B:983:GLU:OE1   | 2.24                     | 0.69              |
| 18:R:202:PHE:C    | 18:R:203:PHE:CD1  | 2.70                     | 0.69              |
| 19:S:115:LYS:HB2  | 19:S:143:TRP:HB3  | 1.73                     | 0.69              |
| 1:A:926:ASN:CB    | 1:A:931:ARG:HG3   | 2.22                     | 0.69              |
| 2:B:881:GLU:C     | 2:B:883:THR:H     | 2.00                     | 0.69              |
| 17:Q:184:ILE:HG12 | 18:R:211:SER:HB2  | 1.74                     | 0.69              |
| 18:R:201:LEU:HB3  | 18:R:203:PHE:HE1  | 1.57                     | 0.69              |
| 2:B:274:ARG:NH1   | 2:B:281:ASP:OD1   | 2.25                     | 0.69              |
| 9:I:84:HIS:H      | 9:I:84:HIS:CD2    | 2.10                     | 0.69              |
| 17:Q:180:PHE:CZ   | 18:R:212:VAL:C    | 2.71                     | 0.69              |
| 18:R:222:SER:C    | 18:R:224:THR:H    | 1.99                     | 0.69              |
| 1:A:1162:GLU:HG2  | 1:A:1306:LYS:HB2  | 1.74                     | 0.69              |
| 1:A:1309:MET:HB2  | 21:U:252:LYS:HE2  | 1.74                     | 0.69              |
| 2:B:905:ASP:OD2   | 2:B:922:ARG:NH2   | 2.22                     | 0.69              |
| 1:A:471:GLY:O     | 1:A:521:VAL:HG23  | 1.93                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:M:238:LYS:HD2  | 13:M:299:LEU:HA   | 1.74                     | 0.69              |
| 16:P:267:PRO:HB2  | 16:P:337:LYS:HD2  | 1.73                     | 0.69              |
| 1:A:1162:GLU:HG2  | 1:A:1306:LYS:CB   | 2.23                     | 0.69              |
| 3:C:272:LEU:HD21  | 11:K:84:GLN:HG2   | 1.74                     | 0.69              |
| 1:A:608:THR:OG1   | 1:A:610:PRO:HG2   | 1.92                     | 0.68              |
| 8:H:65:TYR:CE2    | 8:H:70:LEU:CB     | 2.76                     | 0.68              |
| 1:A:932:ARG:HG3   | 1:A:943:LEU:HG    | 1.74                     | 0.68              |
| 13:M:34:CYS:HB3   | 13:M:39:LEU:HB3   | 1.73                     | 0.68              |
| 1:A:1319:LYS:HE2  | 1:A:1333:GLU:OE2  | 1.93                     | 0.68              |
| 1:A:60:PRO:HD2    | 1:A:62:GLN:HG2    | 1.75                     | 0.68              |
| 16:P:206:GLU:OE2  | 16:P:206:GLU:HA   | 1.91                     | 0.68              |
| 18:R:202:PHE:O    | 18:R:203:PHE:CD1  | 2.47                     | 0.68              |
| 1:A:138:LYS:NZ    | 1:A:1441:GLU:OE2  | 2.25                     | 0.68              |
| 1:A:729:PRO:HG2   | 21:U:250:MET:HB2  | 1.76                     | 0.68              |
| 2:B:1062:ARG:HH21 | 2:B:1065:GLY:H    | 1.41                     | 0.68              |
| 18:R:127:ASN:HD21 | 18:R:140:LYS:HD3  | 1.57                     | 0.68              |
| 1:A:1306:LYS:O    | 1:A:1308:TYR:N    | 2.27                     | 0.68              |
| 17:Q:113:ARG:NH2  | 18:R:218:LYS:CG   | 2.57                     | 0.68              |
| 20:T:177:ARG:N    | 20:T:178:ALA:O    | 2.27                     | 0.68              |
| 13:M:10:LEU:HD13  | 13:M:10:LEU:N     | 2.04                     | 0.67              |
| 18:R:205:ASP:O    | 18:R:206:LYS:CD   | 2.42                     | 0.67              |
| 1:A:1052:ARG:NH1  | 1:A:1056:GLU:OE1  | 2.28                     | 0.67              |
| 1:A:1162:GLU:CB   | 1:A:1306:LYS:CB   | 2.62                     | 0.67              |
| 12:L:35:ARG:HH12  | 12:L:42:ARG:HH21  | 1.39                     | 0.67              |
| 2:B:198:GLU:OE1   | 2:B:388:TYR:OH    | 2.07                     | 0.67              |
| 1:A:199:TYR:CE2   | 13:M:93:PHE:HZ    | 2.13                     | 0.67              |
| 3:C:157:GLN:CD    | 10:J:65:LEU:HD22  | 2.19                     | 0.67              |
| 13:M:34:CYS:CB    | 13:M:39:LEU:HB3   | 2.23                     | 0.67              |
| 17:Q:184:ILE:HG12 | 18:R:211:SER:CB   | 2.25                     | 0.67              |
| 13:M:89:GLY:O     | 13:M:90:ALA:HB2   | 1.93                     | 0.67              |
| 17:Q:109:HIS:CE1  | 18:R:233:ILE:HG21 | 2.30                     | 0.67              |
| 17:Q:113:ARG:HH12 | 18:R:218:LYS:HG3  | 1.60                     | 0.67              |
| 1:A:1154:ALA:HB1  | 1:A:1310:HIS:HE1  | 1.59                     | 0.67              |
| 5:E:65:ASN:CG     | 5:E:66:ASP:H      | 2.00                     | 0.67              |
| 1:A:926:ASN:CA    | 1:A:931:ARG:HG3   | 2.25                     | 0.67              |
| 2:B:57:ARG:NH1    | 2:B:537:GLN:OE1   | 2.27                     | 0.67              |
| 1:A:67:ARG:NH2    | 13:M:45:VAL:O     | 2.28                     | 0.67              |
| 1:A:1022:ILE:HG23 | 1:A:1023:VAL:HG23 | 1.77                     | 0.66              |
| 9:I:84:HIS:CG     | 9:I:85:PRO:CD     | 2.65                     | 0.66              |
| 11:K:82:SER:OG    | 11:K:84:GLN:OE1   | 2.12                     | 0.66              |
| 21:U:226:GLU:HA   | 21:U:226:GLU:OE2  | 1.93                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:455:ILE:HD13 | 1:A:520:MET:HE1  | 1.76                     | 0.66              |
| 1:A:931:ARG:O    | 1:A:933:THR:N    | 2.28                     | 0.66              |
| 1:A:1162:GLU:CG  | 1:A:1306:LYS:CB  | 2.74                     | 0.66              |
| 16:P:297:LYS:O   | 16:P:299:ARG:N   | 2.26                     | 0.66              |
| 1:A:156:GLY:HA2  | 1:A:181:HIS:CG   | 2.29                     | 0.66              |
| 1:A:181:HIS:H    | 1:A:181:HIS:CD2  | 2.13                     | 0.66              |
| 21:U:284:PRO:O   | 21:U:286:THR:N   | 2.28                     | 0.66              |
| 3:C:148:ILE:HG13 | 10:J:5:VAL:HG22  | 1.77                     | 0.66              |
| 5:E:29:THR:HB    | 5:E:32:GLU:HG3   | 1.77                     | 0.66              |
| 18:R:195:PRO:HG3 | 18:R:199:LYS:HB3 | 1.72                     | 0.66              |
| 1:A:1471:PHE:CE1 | 6:F:64:ARG:HD3   | 2.30                     | 0.66              |
| 3:C:134:ASN:N    | 3:C:136:ASP:OD1  | 2.28                     | 0.66              |
| 20:T:139:VAL:CG1 | 20:T:142:SER:HB2 | 2.26                     | 0.66              |
| 1:A:487:SER:HB2  | 1:A:673:GLN:HE22 | 1.59                     | 0.66              |
| 1:A:912:SER:H    | 1:A:1327:GLU:HB3 | 1.61                     | 0.66              |
| 2:B:873:LEU:HB3  | 2:B:874:PRO:CD   | 2.25                     | 0.66              |
| 22:X:14:DA:H2"   | 22:X:15:DA:C8    | 2.30                     | 0.66              |
| 1:A:1196:TYR:OH  | 1:A:1247:PHE:O   | 2.12                     | 0.66              |
| 3:C:56:SER:OG    | 3:C:158:GLU:N    | 2.21                     | 0.66              |
| 4:D:26:PHE:HZ    | 7:G:42:TYR:HA    | 1.60                     | 0.66              |
| 10:J:64:PRO:C    | 10:J:66:GLU:H    | 2.02                     | 0.66              |
| 17:Q:141:ALA:HB1 | 17:Q:152:PHE:HE2 | 1.60                     | 0.66              |
| 9:I:65:LEU:O     | 9:I:122:ARG:NH2  | 2.29                     | 0.66              |
| 10:J:63:ALA:CB   | 10:J:64:PRO:HD3  | 2.13                     | 0.66              |
| 18:R:195:PRO:CD  | 18:R:199:LYS:HB2 | 2.25                     | 0.66              |
| 1:A:202:TRP:H    | 1:A:212:LYS:HA   | 1.60                     | 0.66              |
| 1:A:1319:LYS:HG2 | 1:A:1333:GLU:OE2 | 1.96                     | 0.66              |
| 12:L:35:ARG:HH12 | 12:L:42:ARG:HE   | 1.44                     | 0.65              |
| 1:A:541:THR:O    | 1:A:545:VAL:HG23 | 1.96                     | 0.65              |
| 1:A:1177:TYR:OH  | 9:I:28:GLU:OE2   | 2.14                     | 0.65              |
| 1:A:1307:VAL:O   | 1:A:1308:TYR:C   | 2.40                     | 0.65              |
| 2:B:754:PRO:HB2  | 2:B:773:PRO:HG2  | 1.78                     | 0.65              |
| 2:B:881:GLU:C    | 2:B:883:THR:N    | 2.51                     | 0.65              |
| 5:E:46:ASP:C     | 5:E:48:PRO:HD3   | 2.20                     | 0.65              |
| 7:G:10:GLU:HB3   | 7:G:67:LEU:HD11  | 1.77                     | 0.65              |
| 1:A:157:GLY:N    | 1:A:181:HIS:CE1  | 2.65                     | 0.65              |
| 1:A:274:ASP:O    | 1:A:277:THR:N    | 2.29                     | 0.65              |
| 8:H:17:PRO:O     | 8:H:19:GLY:N     | 2.28                     | 0.65              |
| 17:Q:105:TYR:CE1 | 18:R:234:GLU:OE1 | 2.40                     | 0.65              |
| 3:C:157:GLN:CD   | 10:J:65:LEU:HB3  | 2.22                     | 0.65              |
| 17:Q:23:ARG:HH21 | 18:R:206:LYS:CB  | 2.10                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:R:195:PRO:O    | 18:R:196:ASP:HB3  | 1.95                     | 0.65              |
| 2:B:685:LYS:HD2   | 2:B:691:SER:HA    | 1.76                     | 0.65              |
| 12:L:35:ARG:NH1   | 12:L:42:ARG:HE    | 1.94                     | 0.65              |
| 18:R:195:PRO:CG   | 18:R:199:LYS:C    | 2.69                     | 0.65              |
| 21:U:255:GLY:O    | 21:U:256:THR:OG1  | 2.09                     | 0.65              |
| 1:A:133:SER:HG    | 1:A:136:GLN:HB2   | 1.58                     | 0.65              |
| 1:A:623:PRO:C     | 1:A:625:ASP:H     | 2.05                     | 0.65              |
| 1:A:932:ARG:HB3   | 1:A:940:LYS:HB2   | 1.79                     | 0.65              |
| 9:I:84:HIS:CG     | 9:I:85:PRO:HD3    | 1.89                     | 0.65              |
| 1:A:42:LYS:HE3    | 1:A:56:GLY:HA3    | 1.79                     | 0.65              |
| 1:A:640:LEU:HD23  | 1:A:645:LEU:HD11  | 1.79                     | 0.65              |
| 1:A:367:ILE:HG13  | 1:A:496:PHE:HD1   | 1.62                     | 0.64              |
| 2:B:1137:CYS:HB3  | 2:B:1142:ASN:HB3  | 1.78                     | 0.64              |
| 6:F:48:ASN:ND2    | 6:F:51:ARG:O      | 2.26                     | 0.64              |
| 1:A:190:ARG:NH2   | 22:X:58:DT:OP2    | 2.29                     | 0.64              |
| 1:A:358:ARG:HH21  | 2:B:1076:GLU:HA   | 1.62                     | 0.64              |
| 2:B:333:GLU:OE1   | 19:S:53:ASN:ND2   | 2.27                     | 0.64              |
| 1:A:549:THR:O     | 1:A:589:LYS:NZ    | 2.27                     | 0.64              |
| 1:A:608:THR:HB    | 1:A:610:PRO:CD    | 2.27                     | 0.64              |
| 1:A:1162:GLU:HA   | 1:A:1305:SER:O    | 1.97                     | 0.64              |
| 5:E:41:LYS:HG3    | 5:E:46:ASP:CG     | 2.23                     | 0.64              |
| 7:G:78:ARG:NH1    | 7:G:79:PRO:O      | 2.31                     | 0.64              |
| 3:C:37:VAL:HG13   | 3:C:41:GLU:HB2    | 1.79                     | 0.64              |
| 20:T:20:LEU:HD23  | 20:T:113:ARG:HG2  | 1.79                     | 0.64              |
| 19:S:166:ARG:HH11 | 19:S:166:ARG:HG3  | 1.63                     | 0.64              |
| 13:M:90:ALA:HB2   | 13:M:100:LYS:HE3  | 1.80                     | 0.64              |
| 1:A:1116:ASN:OD1  | 1:A:1136:THR:HB   | 1.97                     | 0.64              |
| 2:B:501:LEU:HD12  | 2:B:505:LEU:HD12  | 1.79                     | 0.64              |
| 1:A:156:GLY:HA2   | 1:A:181:HIS:CE1   | 2.33                     | 0.64              |
| 1:A:180:GLY:C     | 1:A:182:GLY:H     | 2.04                     | 0.64              |
| 2:B:823:PHE:HA    | 13:M:140:ASN:HD21 | 1.63                     | 0.64              |
| 2:B:906:GLN:HG2   | 12:L:45:TYR:OH    | 1.98                     | 0.64              |
| 17:Q:184:ILE:CD1  | 18:R:218:LYS:HZ2  | 2.08                     | 0.64              |
| 1:A:673:GLN:O     | 1:A:677:ASN:HB2   | 1.98                     | 0.64              |
| 3:C:157:GLN:OE1   | 10:J:65:LEU:HD22  | 1.98                     | 0.64              |
| 9:I:61:GLU:C      | 9:I:63:ASP:N      | 2.52                     | 0.64              |
| 17:Q:25:PHE:O     | 18:R:219:LEU:HD21 | 1.98                     | 0.64              |
| 1:A:285:LYS:HE3   | 13:M:80:LEU:HD23  | 1.80                     | 0.63              |
| 9:I:63:ASP:OD1    | 9:I:66:THR:OG1    | 2.16                     | 0.63              |
| 15:O:75:VAL:HG22  | 15:O:94:LYS:HG2   | 1.81                     | 0.63              |
| 2:B:52:GLN:N      | 20:T:141:LEU:HD12 | 2.14                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:247:ALA:O     | 19:S:169:LYS:NZ   | 2.25                     | 0.63              |
| 2:B:785:TYR:CZ    | 2:B:955:PRO:HD3   | 2.32                     | 0.63              |
| 2:B:1062:ARG:HH12 | 2:B:1075:MET:H    | 1.45                     | 0.63              |
| 18:R:195:PRO:HB2  | 18:R:199:LYS:HB3  | 1.77                     | 0.63              |
| 1:A:1319:LYS:HB3  | 1:A:1331:LEU:HB3  | 1.81                     | 0.63              |
| 2:B:761:THR:H     | 2:B:764:MET:CE    | 2.11                     | 0.63              |
| 8:H:85:ALA:HB1    | 8:H:88:PHE:CE2    | 2.33                     | 0.63              |
| 1:A:133:SER:O     | 1:A:135:GLY:N     | 2.31                     | 0.63              |
| 5:E:26:TYR:HA     | 5:E:64:HIS:C      | 2.14                     | 0.63              |
| 1:A:199:TYR:CZ    | 13:M:93:PHE:CZ    | 2.87                     | 0.63              |
| 18:R:181:ALA:HA   | 18:R:184:ALA:HB3  | 1.80                     | 0.63              |
| 1:A:108:ARG:NH1   | 1:A:145:TYR:OH    | 2.32                     | 0.63              |
| 2:B:76:GLY:O      | 2:B:78:VAL:HG22   | 1.98                     | 0.63              |
| 2:B:588:ARG:NH1   | 2:B:669:GLU:OE2   | 2.31                     | 0.63              |
| 2:B:747:LEU:HD11  | 2:B:810:PHE:CZ    | 2.34                     | 0.63              |
| 19:S:100:LEU:HD23 | 19:S:110:PHE:HD2  | 1.64                     | 0.63              |
| 1:A:264:VAL:HG23  | 1:A:272:ASN:ND2   | 1.95                     | 0.63              |
| 2:B:998:ASP:OD1   | 2:B:999:ALA:N     | 2.32                     | 0.63              |
| 1:A:1246:ILE:HD11 | 1:A:1258:ARG:HD2  | 1.81                     | 0.62              |
| 13:M:86:LYS:NZ    | 22:X:40:DT:C4     | 2.66                     | 0.62              |
| 18:R:212:VAL:O    | 18:R:213:ASP:CG   | 2.41                     | 0.62              |
| 1:A:924:TYR:O     | 1:A:926:ASN:ND2   | 2.32                     | 0.62              |
| 1:A:1158:LEU:HD13 | 1:A:1336:LEU:HD22 | 1.81                     | 0.62              |
| 17:Q:60:ARG:O     | 17:Q:64:ASN:ND2   | 2.28                     | 0.62              |
| 1:A:157:GLY:H     | 1:A:181:HIS:CE1   | 2.16                     | 0.62              |
| 8:H:108:ALA:O     | 8:H:110:THR:N     | 2.32                     | 0.62              |
| 18:R:204:ASN:CG   | 18:R:205:ASP:H    | 2.06                     | 0.62              |
| 1:A:95:PHE:N      | 1:A:311:GLN:OE1   | 2.31                     | 0.62              |
| 16:P:205:ARG:O    | 16:P:206:GLU:C    | 2.42                     | 0.62              |
| 1:A:201:GLU:HG3   | 1:A:212:LYS:HB3   | 1.81                     | 0.62              |
| 1:A:1312:PRO:HB3  | 1:A:1334:TRP:HZ3  | 1.65                     | 0.62              |
| 1:A:1316:ASN:ND2  | 1:A:1318:LYS:HE3  | 2.14                     | 0.62              |
| 1:A:51:ARG:H      | 1:A:52:PRO:HD2    | 1.65                     | 0.62              |
| 2:B:898:THR:O     | 2:B:900:GLU:HG3   | 2.00                     | 0.62              |
| 16:P:165:LEU:HD23 | 16:P:168:ILE:HD11 | 1.80                     | 0.62              |
| 17:Q:109:HIS:HE1  | 18:R:233:ILE:HG21 | 1.63                     | 0.62              |
| 17:Q:113:ARG:CZ   | 18:R:218:LYS:HG3  | 2.29                     | 0.62              |
| 18:R:205:ASP:O    | 18:R:206:LYS:HB2  | 1.98                     | 0.62              |
| 1:A:455:ILE:HG21  | 1:A:520:MET:HE1   | 1.81                     | 0.62              |
| 2:B:1144:THR:O    | 2:B:1146:ILE:N    | 2.33                     | 0.62              |
| 10:J:64:PRO:C     | 10:J:66:GLU:N     | 2.56                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:T:141:LEU:O    | 20:T:142:SER:HB3  | 1.99                     | 0.62              |
| 20:T:139:VAL:HG12 | 20:T:142:SER:CB   | 2.25                     | 0.62              |
| 1:A:157:GLY:CA    | 1:A:181:HIS:NE2   | 2.62                     | 0.61              |
| 1:A:786:ALA:O     | 1:A:826:SER:HB3   | 2.00                     | 0.61              |
| 2:B:749:HIS:CD2   | 2:B:810:PHE:CD1   | 2.88                     | 0.61              |
| 18:R:151:LEU:HD11 | 18:R:163:LEU:HD13 | 1.82                     | 0.61              |
| 1:A:263:ALA:HB1   | 1:A:272:ASN:HB3   | 1.82                     | 0.61              |
| 1:A:1162:GLU:HA   | 1:A:1306:LYS:HA   | 1.82                     | 0.61              |
| 8:H:137:VAL:HG22  | 8:H:138:ASP:H     | 1.63                     | 0.61              |
| 9:I:104:ALA:C     | 9:I:106:ASP:H     | 2.08                     | 0.61              |
| 21:U:243:GLU:CD   | 21:U:246:ARG:HH12 | 2.08                     | 0.61              |
| 1:A:344:LYS:HA    | 1:A:1435:THR:HG21 | 1.82                     | 0.61              |
| 1:A:379:GLY:HA2   | 1:A:475:ARG:O     | 2.01                     | 0.61              |
| 16:P:153:THR:N    | 16:P:326:GLU:OE2  | 2.34                     | 0.61              |
| 2:B:1040:GLN:H    | 2:B:1040:GLN:CD   | 2.08                     | 0.61              |
| 2:B:529:MET:SD    | 2:B:623:ARG:HB2   | 2.41                     | 0.61              |
| 2:B:968:ASN:OD1   | 2:B:969:PRO:HD2   | 2.00                     | 0.61              |
| 15:O:84:VAL:HG23  | 15:O:85:THR:HG23  | 1.81                     | 0.61              |
| 18:R:204:ASN:CG   | 18:R:205:ASP:N    | 2.59                     | 0.61              |
| 19:S:48:GLU:OE1   | 19:S:101:ARG:NH2  | 2.33                     | 0.61              |
| 5:E:46:ASP:C      | 5:E:48:PRO:CD     | 2.73                     | 0.61              |
| 7:G:52:ASP:H      | 7:G:72:TYR:HA     | 1.64                     | 0.61              |
| 9:I:105:GLU:O     | 9:I:106:ASP:CB    | 2.49                     | 0.61              |
| 14:N:319:ASP:C    | 14:N:321:SER:H    | 2.08                     | 0.61              |
| 1:A:883:ILE:HG13  | 1:A:885:GLN:HG3   | 1.83                     | 0.61              |
| 1:A:157:GLY:C     | 1:A:181:HIS:NE2   | 2.59                     | 0.60              |
| 1:A:1309:MET:CB   | 21:U:252:LYS:HE2  | 2.31                     | 0.60              |
| 2:B:880:LEU:O     | 2:B:881:GLU:CB    | 2.24                     | 0.60              |
| 13:M:178:LYS:HZ2  | 20:T:156:VAL:HG11 | 1.65                     | 0.60              |
| 22:X:49:DT:H3'    | 22:X:50:DT:H5''   | 1.83                     | 0.60              |
| 17:Q:70:LYS:O     | 17:Q:102:VAL:HG11 | 2.01                     | 0.60              |
| 2:B:676:ALA:HB2   | 2:B:693:TYR:CD1   | 2.36                     | 0.60              |
| 9:I:105:GLU:O     | 9:I:106:ASP:HB3   | 2.02                     | 0.60              |
| 1:A:199:TYR:CZ    | 13:M:93:PHE:HZ    | 2.19                     | 0.60              |
| 8:H:66:GLU:HA     | 8:H:66:GLU:OE2    | 2.00                     | 0.60              |
| 13:M:50:SER:O     | 13:M:53:ARG:HB2   | 2.01                     | 0.60              |
| 13:M:90:ALA:HB2   | 13:M:100:LYS:CE   | 2.31                     | 0.60              |
| 13:M:91:ALA:O     | 13:M:93:PHE:N     | 2.34                     | 0.60              |
| 1:A:685:HIS:HB3   | 2:B:784:SER:OG    | 2.01                     | 0.60              |
| 2:B:380:ARG:NE    | 2:B:609:GLU:OE2   | 2.34                     | 0.60              |
| 3:C:134:ASN:H     | 3:C:136:ASP:CG    | 2.10                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:513:GLU:CD    | 2:B:707:CYS:HB2   | 2.26                     | 0.60              |
| 2:B:841:ARG:NH2   | 2:B:893:SER:O     | 2.35                     | 0.60              |
| 16:P:297:LYS:CB   | 16:P:298:PRO:HD3  | 2.15                     | 0.60              |
| 18:R:205:ASP:O    | 18:R:206:LYS:CB   | 2.48                     | 0.60              |
| 22:X:32:DT:H4'    | 22:X:33:DT:H5'    | 1.82                     | 0.60              |
| 17:Q:112:ARG:HD3  | 18:R:237:LEU:CD1  | 2.22                     | 0.60              |
| 18:R:118:TRP:NE1  | 18:R:122:GLU:OE1  | 2.34                     | 0.60              |
| 1:A:376:ASP:HB3   | 1:A:522:PRO:HD3   | 1.84                     | 0.60              |
| 2:B:898:THR:O     | 2:B:900:GLU:N     | 2.35                     | 0.60              |
| 14:N:21:VAL:HG21  | 15:O:40:PHE:HD1   | 1.67                     | 0.60              |
| 17:Q:25:PHE:CD1   | 18:R:210:PHE:CZ   | 2.90                     | 0.60              |
| 1:A:622:SER:C     | 1:A:624:GLY:N     | 2.56                     | 0.60              |
| 1:A:930:LEU:O     | 1:A:931:ARG:C     | 2.44                     | 0.60              |
| 1:A:1016:LEU:HD22 | 1:A:1069:LEU:HD22 | 1.83                     | 0.60              |
| 2:B:52:GLN:CA     | 20:T:141:LEU:HD13 | 2.28                     | 0.60              |
| 2:B:819:SER:HB3   | 2:B:821:LYS:HG3   | 1.84                     | 0.60              |
| 2:B:823:PHE:HA    | 13:M:140:ASN:ND2  | 2.16                     | 0.60              |
| 6:F:88:ASP:OD2    | 6:F:91:LEU:N      | 2.35                     | 0.60              |
| 1:A:540:ASP:CB    | 2:B:790:GLN:HE21  | 2.15                     | 0.59              |
| 1:A:1116:ASN:O    | 1:A:1117:VAL:CB   | 2.49                     | 0.59              |
| 7:G:145:LEU:HD13  | 7:G:161:GLY:HA3   | 1.84                     | 0.59              |
| 9:I:65:LEU:HD22   | 9:I:122:ARG:HG2   | 1.82                     | 0.59              |
| 20:T:129:ARG:HA   | 20:T:132:ILE:HD12 | 1.84                     | 0.59              |
| 1:A:608:THR:CA    | 1:A:610:PRO:HD2   | 2.30                     | 0.59              |
| 1:A:1306:LYS:C    | 1:A:1308:TYR:N    | 2.57                     | 0.59              |
| 17:Q:52:LEU:HB3   | 17:Q:54:PHE:CD2   | 2.33                     | 0.59              |
| 1:A:386:ALA:O     | 1:A:449:HIS:ND1   | 2.35                     | 0.59              |
| 1:A:540:ASP:HB2   | 2:B:790:GLN:HE21  | 1.66                     | 0.59              |
| 13:M:218:PHE:HD1  | 13:M:277:ILE:HG22 | 1.67                     | 0.59              |
| 1:A:354:LEU:O     | 1:A:357:LYS:HE2   | 2.02                     | 0.59              |
| 2:B:216:ALA:HB2   | 2:B:241:ALA:HB2   | 1.84                     | 0.59              |
| 1:A:415:GLY:C     | 1:A:449:HIS:HD2   | 2.11                     | 0.59              |
| 1:A:621:ILE:O     | 1:A:621:ILE:HG22  | 2.02                     | 0.59              |
| 1:A:1102:MET:HG2  | 21:U:277:GLN:HB2  | 1.85                     | 0.59              |
| 2:B:254:GLN:HG3   | 2:B:303:PRO:HG2   | 1.85                     | 0.59              |
| 7:G:110:ARG:NH2   | 7:G:118:GLU:OE2   | 2.36                     | 0.59              |
| 9:I:80:ARG:HD3    | 9:I:95:VAL:HG12   | 1.83                     | 0.59              |
| 1:A:271:ARG:O     | 1:A:272:ASN:CB    | 2.48                     | 0.59              |
| 2:B:160:TYR:OH    | 20:T:141:LEU:HD13 | 2.02                     | 0.59              |
| 2:B:489:ILE:HG21  | 2:B:522:LEU:HD13  | 1.83                     | 0.59              |
| 5:E:52:ARG:HG3    | 5:E:54:ARG:HG3    | 1.85                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:N:318:ASP:OD1  | 16:P:239:ARG:NH2  | 2.36                     | 0.59              |
| 16:P:298:PRO:O    | 16:P:299:ARG:C    | 2.43                     | 0.59              |
| 17:Q:98:THR:HG22  | 17:Q:100:VAL:H    | 1.67                     | 0.59              |
| 1:A:932:ARG:HG3   | 1:A:940:LYS:HA    | 1.84                     | 0.59              |
| 1:A:998:PRO:HA    | 1:A:1059:ARG:HG2  | 1.85                     | 0.59              |
| 1:A:1431:SER:CB   | 1:A:1459:MET:HE1  | 2.32                     | 0.59              |
| 17:Q:180:PHE:CE1  | 18:R:213:ASP:CA   | 2.75                     | 0.59              |
| 1:A:26:LEU:HD23   | 2:B:1168:ALA:HB2  | 1.84                     | 0.59              |
| 1:A:575:PRO:HG2   | 1:A:594:LEU:HD11  | 1.83                     | 0.59              |
| 5:E:133:GLN:N     | 5:E:133:GLN:OE1   | 2.36                     | 0.59              |
| 18:R:214:GLU:OE1  | 18:R:217:GLN:NE2  | 2.31                     | 0.59              |
| 1:A:865:ILE:HG13  | 1:A:866:LYS:N     | 2.17                     | 0.59              |
| 2:B:42:GLN:HG2    | 2:B:43:GLN:N      | 2.15                     | 0.59              |
| 2:B:249:LYS:O     | 2:B:250:SER:HB2   | 2.02                     | 0.59              |
| 8:H:146:LYS:O     | 8:H:148:LEU:N     | 2.29                     | 0.59              |
| 13:M:17:ASN:OD1   | 13:M:18:HIS:ND1   | 2.36                     | 0.59              |
| 17:Q:112:ARG:NE   | 18:R:237:LEU:HD12 | 2.13                     | 0.59              |
| 1:A:1191:GLU:O    | 1:A:1195:VAL:HG23 | 2.04                     | 0.58              |
| 2:B:690:CYS:SG    | 2:B:691:SER:N     | 2.76                     | 0.58              |
| 12:L:26:ASN:O     | 12:L:27:GLU:HB3   | 2.02                     | 0.58              |
| 3:C:59:LEU:HD22   | 3:C:151:VAL:HG23  | 1.84                     | 0.58              |
| 1:A:261:ARG:C     | 1:A:263:ALA:H     | 2.11                     | 0.58              |
| 1:A:622:SER:C     | 1:A:624:GLY:H     | 2.01                     | 0.58              |
| 17:Q:180:PHE:HE1  | 18:R:212:VAL:C    | 2.12                     | 0.58              |
| 19:S:115:LYS:NZ   | 19:S:117:GLY:O    | 2.28                     | 0.58              |
| 1:A:910:LYS:HD2   | 1:A:911:PRO:HD2   | 1.86                     | 0.58              |
| 2:B:790:GLN:HA    | 2:B:968:ASN:HD22  | 1.67                     | 0.58              |
| 3:C:60:HIS:NE2    | 3:C:63:PHE:HB2    | 2.18                     | 0.58              |
| 1:A:601:ASN:HD21  | 1:A:632:ASN:H     | 1.52                     | 0.58              |
| 1:A:832:THR:N     | 1:A:835:GLU:OE1   | 2.25                     | 0.58              |
| 2:B:73:HIS:C      | 2:B:75:SER:N      | 2.61                     | 0.58              |
| 3:C:6:GLN:CG      | 11:K:100:LEU:HD23 | 2.29                     | 0.58              |
| 8:H:74:GLU:C      | 8:H:76:ASN:N      | 2.57                     | 0.58              |
| 16:P:171:THR:HG22 | 16:P:220:VAL:HG13 | 1.85                     | 0.58              |
| 17:Q:24:GLY:HA2   | 18:R:209:GLN:HG2  | 1.84                     | 0.58              |
| 2:B:718:GLN:HG2   | 2:B:720:PRO:HD2   | 1.84                     | 0.58              |
| 2:B:857:GLY:HA2   | 2:B:903:ILE:HD11  | 1.86                     | 0.58              |
| 13:M:10:LEU:N     | 13:M:10:LEU:HD22  | 2.19                     | 0.58              |
| 1:A:624:GLY:O     | 1:A:626:THR:N     | 2.35                     | 0.58              |
| 2:B:438:ARG:NE    | 2:B:442:ASP:OD2   | 2.31                     | 0.58              |
| 11:K:39:ASP:OD1   | 11:K:39:ASP:N     | 2.37                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:290:TYR:CE2   | 2:B:562:ALA:HA    | 2.39                     | 0.58              |
| 2:B:1090:GLU:OE1  | 2:B:1090:GLU:N    | 2.37                     | 0.58              |
| 3:C:85:SER:HB2    | 3:C:166:LYS:HE3   | 1.86                     | 0.58              |
| 11:K:63:VAL:HB    | 11:K:71:ILE:HG22  | 1.86                     | 0.58              |
| 21:U:224:THR:O    | 21:U:226:GLU:N    | 2.36                     | 0.58              |
| 1:A:121:SER:HA    | 1:A:126:ILE:HG21  | 1.86                     | 0.58              |
| 2:B:1062:ARG:NH1  | 2:B:1074:PRO:HB3  | 2.19                     | 0.58              |
| 8:H:65:TYR:CE2    | 8:H:70:LEU:HD13   | 2.39                     | 0.58              |
| 1:A:264:VAL:O     | 1:A:266:MET:N     | 2.36                     | 0.57              |
| 1:A:271:ARG:O     | 1:A:272:ASN:HB2   | 2.04                     | 0.57              |
| 1:A:641:CYS:SG    | 1:A:643:LYS:N     | 2.77                     | 0.57              |
| 1:A:1431:SER:HB2  | 1:A:1459:MET:HE1  | 1.86                     | 0.57              |
| 2:B:1104:ARG:O    | 2:B:1108:PHE:HB3  | 2.04                     | 0.57              |
| 1:A:1127:LEU:HD21 | 1:A:1381:GLU:HB3  | 1.84                     | 0.57              |
| 2:B:1029:TYR:CE1  | 2:B:1036:LYS:HG2  | 2.39                     | 0.57              |
| 17:Q:25:PHE:CD1   | 18:R:210:PHE:HZ   | 2.23                     | 0.57              |
| 1:A:1303:GLN:O    | 1:A:1304:ILE:HG23 | 2.04                     | 0.57              |
| 2:B:839:GLY:HA3   | 2:B:891:ASP:HB3   | 1.86                     | 0.57              |
| 2:B:921:ILE:HG13  | 2:B:921:ILE:O     | 2.03                     | 0.57              |
| 2:B:1040:GLN:HG2  | 3:C:203:TRP:CZ2   | 2.38                     | 0.57              |
| 1:A:200:ALA:O     | 1:A:213:LYS:HA    | 2.03                     | 0.57              |
| 1:A:244:ARG:HD2   | 1:A:245:PRO:HD2   | 1.85                     | 0.57              |
| 1:A:1112:VAL:O    | 21:U:252:LYS:CB   | 2.49                     | 0.57              |
| 1:A:926:ASN:HB3   | 1:A:931:ARG:CB    | 2.34                     | 0.57              |
| 1:A:927:GLU:O     | 1:A:929:ALA:N     | 2.37                     | 0.57              |
| 2:B:230:ARG:HD2   | 2:B:405:ARG:HH12  | 1.69                     | 0.57              |
| 9:I:104:ALA:O     | 9:I:106:ASP:N     | 2.37                     | 0.57              |
| 17:Q:68:GLY:C     | 18:R:226:ASP:CG   | 2.73                     | 0.57              |
| 1:A:1319:LYS:CG   | 1:A:1333:GLU:CD   | 2.77                     | 0.57              |
| 13:M:89:GLY:O     | 13:M:90:ALA:HB3   | 2.01                     | 0.57              |
| 13:M:178:LYS:HB3  | 20:T:154:LYS:CD   | 2.35                     | 0.57              |
| 18:R:154:LEU:CD2  | 18:R:163:LEU:HD23 | 2.23                     | 0.57              |
| 1:A:305:GLU:OE1   | 13:M:102:GLN:NE2  | 2.38                     | 0.57              |
| 2:B:798:ARG:HD3   | 2:B:950:ARG:HG2   | 1.86                     | 0.57              |
| 5:E:15:LYS:NZ     | 5:E:33:LEU:O      | 2.31                     | 0.57              |
| 12:L:35:ARG:HH12  | 12:L:42:ARG:NH2   | 2.02                     | 0.57              |
| 20:T:58:LEU:HD23  | 20:T:63:ALA:HB2   | 1.87                     | 0.57              |
| 14:N:359:ASN:ND2  | 14:N:364:ASP:OD1  | 2.38                     | 0.57              |
| 1:A:47:THR:HG23   | 1:A:53:LYS:HG2    | 1.86                     | 0.56              |
| 1:A:606:HIS:CG    | 1:A:607:SER:N     | 2.72                     | 0.56              |
| 1:A:1029:LEU:H    | 5:E:162:ARG:NH1   | 2.02                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:812:ARG:HH22  | 23:Y:52:DT:P      | 2.26                     | 0.56              |
| 6:F:88:ASP:CG     | 6:F:91:LEU:H      | 2.12                     | 0.56              |
| 23:Y:39:DG:H2'    | 23:Y:40:DT:C6     | 2.40                     | 0.56              |
| 2:B:52:GLN:N      | 20:T:141:LEU:CD1  | 2.67                     | 0.56              |
| 13:M:179:GLU:HG3  | 20:T:154:LYS:HE2  | 1.87                     | 0.56              |
| 18:R:142:LYS:HD3  | 18:R:145:VAL:HG23 | 1.87                     | 0.56              |
| 1:A:537:ILE:HG13  | 1:A:672:ILE:HD13  | 1.86                     | 0.56              |
| 1:A:789:GLY:HA2   | 1:A:822:PHE:CE1   | 2.40                     | 0.56              |
| 1:A:1443:ALA:HB2  | 2:B:1167:ILE:HG23 | 1.86                     | 0.56              |
| 2:B:223:SER:OG    | 2:B:232:THR:O     | 2.23                     | 0.56              |
| 2:B:881:GLU:OE1   | 2:B:883:THR:OG1   | 2.23                     | 0.56              |
| 9:I:61:GLU:O      | 9:I:62:VAL:C      | 2.46                     | 0.56              |
| 17:Q:105:TYR:CD1  | 18:R:234:GLU:HB2  | 2.40                     | 0.56              |
| 22:X:53:DA:H2'    | 22:X:54:DA:C8     | 2.40                     | 0.56              |
| 1:A:1117:VAL:O    | 1:A:1117:VAL:HG12 | 2.04                     | 0.56              |
| 1:A:1128:ILE:HG23 | 1:A:1414:ILE:HD11 | 1.87                     | 0.56              |
| 13:M:60:ALA:HB1   | 23:Y:54:DA:H2     | 1.70                     | 0.56              |
| 1:A:207:GLU:O     | 1:A:209:SER:N     | 2.39                     | 0.56              |
| 1:A:926:ASN:HB3   | 1:A:931:ARG:CG    | 2.36                     | 0.56              |
| 2:B:1069:ILE:HD11 | 13:M:45:VAL:HG22  | 1.87                     | 0.56              |
| 11:K:16:GLU:OE1   | 11:K:36:ASN:ND2   | 2.39                     | 0.56              |
| 1:A:608:THR:CB    | 1:A:610:PRO:CD    | 2.82                     | 0.56              |
| 1:A:1316:ASN:CG   | 1:A:1318:LYS:HE2  | 2.31                     | 0.56              |
| 22:X:47:DT:H3'    | 22:X:48:DT:H5''   | 1.88                     | 0.56              |
| 1:A:205:VAL:O     | 1:A:206:ASN:HB2   | 2.06                     | 0.56              |
| 17:Q:113:ARG:CZ   | 18:R:218:LYS:CG   | 2.84                     | 0.56              |
| 18:R:204:ASN:ND2  | 18:R:205:ASP:H    | 2.03                     | 0.56              |
| 9:I:61:GLU:C      | 9:I:63:ASP:H      | 2.13                     | 0.56              |
| 13:M:183:VAL:HG12 | 20:T:152:ASN:HD21 | 1.71                     | 0.56              |
| 2:B:499:ARG:NH2   | 2:B:522:LEU:HD11  | 2.20                     | 0.56              |
| 2:B:1094:GLN:NE2  | 2:B:1102:PHE:HD2  | 2.04                     | 0.56              |
| 5:E:94:MET:HB2    | 5:E:99:ILE:HD11   | 1.88                     | 0.56              |
| 16:P:167:ASN:ND2  | 23:Y:79:DT:O2     | 2.34                     | 0.56              |
| 1:A:623:PRO:O     | 1:A:625:ASP:N     | 2.39                     | 0.55              |
| 2:B:255:ARG:NE    | 2:B:307:GLU:OE2   | 2.38                     | 0.55              |
| 2:B:1076:GLU:HB2  | 13:M:54:THR:OG1   | 2.06                     | 0.55              |
| 3:C:154:ARG:HB3   | 10:J:65:LEU:HD21  | 1.88                     | 0.55              |
| 1:A:1143:LEU:HD11 | 1:A:1336:LEU:HG   | 1.88                     | 0.55              |
| 2:B:873:LEU:CB    | 2:B:874:PRO:CD    | 2.85                     | 0.55              |
| 8:H:64:LEU:H      | 8:H:70:LEU:HD21   | 1.71                     | 0.55              |
| 8:H:106:THR:O     | 8:H:108:ALA:N     | 2.37                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:L:35:ARG:NH1   | 12:L:42:ARG:HH21  | 2.04                     | 0.55              |
| 16:P:239:ARG:NH1  | 16:P:242:GLN:OE1  | 2.40                     | 0.55              |
| 20:T:82:PRO:HG2   | 20:T:117:ARG:HB2  | 1.89                     | 0.55              |
| 1:A:293:ASN:OD1   | 1:A:298:ALA:HA    | 2.06                     | 0.55              |
| 1:A:522:PRO:HB3   | 1:A:666:ARG:CG    | 2.36                     | 0.55              |
| 2:B:91:ILE:HD11   | 2:B:124:LEU:HD21  | 1.89                     | 0.55              |
| 1:A:625:ASP:O     | 1:A:638:GLY:HA2   | 2.06                     | 0.55              |
| 17:Q:113:ARG:HH21 | 18:R:218:LYS:HE2  | 1.67                     | 0.55              |
| 1:A:1223:ASP:OD1  | 1:A:1224:ARG:NH1  | 2.39                     | 0.55              |
| 2:B:1040:GLN:CD   | 2:B:1040:GLN:N    | 2.63                     | 0.55              |
| 19:S:46:ARG:NH2   | 20:T:2:ALA:O      | 2.39                     | 0.55              |
| 1:A:522:PRO:HB3   | 1:A:666:ARG:HG3   | 1.89                     | 0.55              |
| 13:M:34:CYS:CB    | 13:M:39:LEU:CB    | 2.79                     | 0.55              |
| 1:A:632:ASN:CA    | 1:A:992:LYS:HD2   | 2.36                     | 0.55              |
| 4:D:90:LYS:HE3    | 4:D:130:ILE:HD11  | 1.88                     | 0.55              |
| 19:S:46:ARG:HB2   | 19:S:101:ARG:HB2  | 1.89                     | 0.55              |
| 21:U:291:CYS:SG   | 21:U:293:GLU:HB2  | 2.46                     | 0.55              |
| 1:A:116:LYS:HE2   | 1:A:181:HIS:CB    | 2.36                     | 0.55              |
| 1:A:1109:TYR:HE2  | 1:A:1113:SER:H    | 1.55                     | 0.55              |
| 13:M:179:GLU:N    | 20:T:154:LYS:HE3  | 2.22                     | 0.55              |
| 20:T:140:ARG:O    | 20:T:141:LEU:CB   | 2.55                     | 0.55              |
| 8:H:108:ALA:O     | 8:H:109:ALA:C     | 2.47                     | 0.54              |
| 1:A:181:HIS:CD2   | 1:A:181:HIS:N     | 2.74                     | 0.54              |
| 2:B:248:LYS:HA    | 19:S:169:LYS:HG2  | 1.89                     | 0.54              |
| 13:M:90:ALA:CB    | 13:M:100:LYS:HE3  | 2.37                     | 0.54              |
| 1:A:61:ARG:HB3    | 1:A:72:GLN:HE21   | 1.72                     | 0.54              |
| 1:A:1222:THR:HB   | 21:U:241:THR:HG21 | 1.88                     | 0.54              |
| 19:S:31:PHE:HB2   | 20:T:92:THR:HB    | 1.89                     | 0.54              |
| 19:S:172:ASN:OD1  | 19:S:173:HIS:N    | 2.37                     | 0.54              |
| 1:A:930:LEU:C     | 1:A:931:ARG:O     | 2.49                     | 0.54              |
| 2:B:360:LYS:HG3   | 2:B:553:LEU:HD23  | 1.88                     | 0.54              |
| 5:E:67:ASP:O      | 5:E:69:THR:N      | 2.41                     | 0.54              |
| 13:M:52:TRP:CD1   | 13:M:52:TRP:O     | 2.60                     | 0.54              |
| 16:P:294:ARG:NH1  | 22:X:14:DA:OP1    | 2.28                     | 0.54              |
| 1:A:621:ILE:C     | 1:A:623:PRO:N     | 2.62                     | 0.54              |
| 1:A:1281:ASP:O    | 1:A:1285:LEU:N    | 2.35                     | 0.54              |
| 6:F:102:ILE:HG22  | 6:F:104:ILE:HG12  | 1.89                     | 0.54              |
| 20:T:139:VAL:CG1  | 20:T:142:SER:OG   | 2.55                     | 0.54              |
| 1:A:936:GLU:HA    | 1:A:1002:SER:HB2  | 1.89                     | 0.54              |
| 2:B:733:MET:HE1   | 2:B:1054:MET:SD   | 2.47                     | 0.54              |
| 5:E:91:CYS:HA     | 5:E:94:MET:HE3    | 1.90                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:M:103:ASN:HB3  | 13:M:105:ARG:HH22 | 1.72                     | 0.54              |
| 17:Q:153:ARG:HH11 | 17:Q:158:HIS:HB3  | 1.71                     | 0.54              |
| 1:A:1163:HIS:N    | 1:A:1306:LYS:N    | 2.37                     | 0.54              |
| 2:B:992:ASN:ND2   | 2:B:1018:TYR:CD2  | 2.74                     | 0.54              |
| 2:B:1078:ARG:NH1  | 23:Y:50:DA:O3'    | 2.41                     | 0.54              |
| 1:A:926:ASN:HB3   | 1:A:931:ARG:HG3   | 1.89                     | 0.54              |
| 1:A:1306:LYS:O    | 1:A:1307:VAL:C    | 2.49                     | 0.54              |
| 1:A:802:PHE:CE1   | 2:B:504:THR:HG22  | 2.43                     | 0.54              |
| 1:A:894:ASP:OD1   | 1:A:895:GLY:N     | 2.41                     | 0.54              |
| 2:B:529:MET:HE2   | 2:B:624:PRO:HD2   | 1.88                     | 0.54              |
| 19:S:51:LEU:HD21  | 19:S:54:LYS:HD3   | 1.90                     | 0.54              |
| 1:A:34:MET:SD     | 2:B:1124:ILE:HG21 | 2.48                     | 0.54              |
| 3:C:30:VAL:HG22   | 11:K:45:ILE:HD11  | 1.90                     | 0.54              |
| 8:H:115:TYR:CE1   | 8:H:124:ARG:HG3   | 2.43                     | 0.54              |
| 13:M:193:ARG:NH1  | 23:Y:75:DC:OP1    | 2.41                     | 0.54              |
| 1:A:522:PRO:HA    | 1:A:666:ARG:NE    | 2.09                     | 0.53              |
| 1:A:1097:GLU:O    | 1:A:1100:THR:OG1  | 2.23                     | 0.53              |
| 2:B:529:MET:HG2   | 2:B:530:ALA:N     | 2.22                     | 0.53              |
| 1:A:253:LEU:HD12  | 1:A:254:PRO:HD2   | 1.90                     | 0.53              |
| 2:B:109:MET:HG3   | 2:B:174:LEU:HD11  | 1.89                     | 0.53              |
| 2:B:529:MET:HG3   | 2:B:624:PRO:HD2   | 1.90                     | 0.53              |
| 5:E:6:GLU:OE2     | 5:E:9:ARG:NH1     | 2.39                     | 0.53              |
| 9:I:103:ARG:O     | 9:I:105:GLU:HG2   | 2.09                     | 0.53              |
| 3:C:47:ILE:H      | 3:C:47:ILE:HD12   | 1.73                     | 0.53              |
| 3:C:154:ARG:HB3   | 10:J:65:LEU:CD2   | 2.38                     | 0.53              |
| 12:L:35:ARG:HH12  | 12:L:42:ARG:NE    | 2.07                     | 0.53              |
| 14:N:15:ARG:HA    | 14:N:18:ILE:HD12  | 1.90                     | 0.53              |
| 18:R:151:LEU:HB2  | 18:R:163:LEU:HD21 | 1.90                     | 0.53              |
| 1:A:484:LEU:HD12  | 1:A:484:LEU:O     | 2.08                     | 0.53              |
| 5:E:14:ARG:O      | 5:E:17:ILE:HG13   | 2.09                     | 0.53              |
| 14:N:314:LEU:HD21 | 16:P:250:PHE:HB2  | 1.90                     | 0.53              |
| 14:N:332:GLU:HB2  | 15:O:92:LYS:O     | 2.09                     | 0.53              |
| 18:R:162:GLY:O    | 18:R:163:LEU:CB   | 2.56                     | 0.53              |
| 1:A:269:SER:O     | 1:A:270:ALA:CB    | 2.55                     | 0.53              |
| 1:A:629:VAL:HG21  | 1:A:637:MET:HE3   | 1.89                     | 0.53              |
| 2:B:598:VAL:C     | 2:B:600:GLU:H     | 2.16                     | 0.53              |
| 3:C:70:LEU:HD23   | 10:J:5:VAL:O      | 2.07                     | 0.53              |
| 3:C:82:LEU:HD23   | 3:C:167:LYS:HB2   | 1.90                     | 0.53              |
| 6:F:86:GLU:OE2    | 6:F:95:LYS:NZ     | 2.42                     | 0.53              |
| 6:F:56:TYR:CE1    | 6:F:124:ILE:HB    | 2.43                     | 0.53              |
| 13:M:13:VAL:HG12  | 13:M:20:ASP:HB3   | 1.90                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:M:45:VAL:C     | 13:M:47:ASP:H     | 2.15                     | 0.53              |
| 18:R:195:PRO:HB2  | 18:R:199:LYS:CG   | 2.38                     | 0.53              |
| 1:A:299:ALA:HA    | 17:Q:60:ARG:NH2   | 2.23                     | 0.53              |
| 1:A:1304:ILE:HG22 | 1:A:1340:GLY:HA3  | 1.91                     | 0.53              |
| 3:C:147:ASP:O     | 10:J:16:ASN:HB3   | 2.08                     | 0.53              |
| 2:B:250:SER:O     | 2:B:251:ALA:C     | 2.52                     | 0.53              |
| 1:A:270:ALA:O     | 1:A:272:ASN:N     | 2.42                     | 0.53              |
| 2:B:386:ASP:OD2   | 2:B:502:HIS:HB2   | 2.09                     | 0.53              |
| 8:H:60:ILE:HD11   | 8:H:123:MET:HE1   | 1.90                     | 0.53              |
| 1:A:30:GLU:CD     | 1:A:33:ARG:HH21   | 2.16                     | 0.53              |
| 1:A:297:GLY:HA3   | 17:Q:57:LYS:HB3   | 1.90                     | 0.53              |
| 2:B:675:LEU:HD11  | 2:B:697:GLU:OE2   | 2.09                     | 0.53              |
| 17:Q:125:ALA:HB1  | 17:Q:138:ASP:HB3  | 1.91                     | 0.53              |
| 21:U:248:HIS:O    | 21:U:252:LYS:NZ   | 2.37                     | 0.53              |
| 1:A:263:ALA:O     | 1:A:264:VAL:CG2   | 2.57                     | 0.52              |
| 1:A:542:LEU:HD21  | 1:A:642:LYS:HB2   | 1.91                     | 0.52              |
| 9:I:24:LEU:HB3    | 9:I:37:TYR:HB3    | 1.92                     | 0.52              |
| 17:Q:69:ASP:HA    | 18:R:226:ASP:CG   | 2.34                     | 0.52              |
| 1:A:521:VAL:HB    | 1:A:522:PRO:HD3   | 1.90                     | 0.52              |
| 18:R:80:LYS:HD3   | 20:T:188:PHE:HE2  | 1.74                     | 0.52              |
| 20:T:12:ALA:HB2   | 20:T:106:LEU:HD13 | 1.90                     | 0.52              |
| 1:A:1316:ASN:ND2  | 1:A:1318:LYS:CE   | 2.72                     | 0.52              |
| 2:B:1163:MET:HA   | 2:B:1168:ALA:H    | 1.73                     | 0.52              |
| 6:F:79:VAL:HG12   | 6:F:81:VAL:H      | 1.74                     | 0.52              |
| 13:M:25:GLU:OE1   | 13:M:44:ARG:NH2   | 2.36                     | 0.52              |
| 17:Q:25:PHE:HA    | 18:R:219:LEU:HD13 | 1.90                     | 0.52              |
| 17:Q:180:PHE:CZ   | 18:R:213:ASP:N    | 2.76                     | 0.52              |
| 19:S:26:TYR:CD2   | 19:S:138:PHE:HB3  | 2.43                     | 0.52              |
| 20:T:208:GLN:HE21 | 20:T:213:LEU:HB2  | 1.74                     | 0.52              |
| 21:U:279:ARG:NH1  | 21:U:280:SER:O    | 2.43                     | 0.52              |
| 1:A:389:THR:HG21  | 1:A:417:LYS:HD2   | 1.90                     | 0.52              |
| 1:A:582:PRO:HD2   | 8:H:47:ILE:HD12   | 1.91                     | 0.52              |
| 18:R:151:LEU:HD12 | 18:R:163:LEU:HD21 | 1.89                     | 0.52              |
| 2:B:1022:LEU:HD11 | 2:B:1023:ARG:NH1  | 2.24                     | 0.52              |
| 6:F:73:ILE:HD11   | 6:F:96:GLU:OE2    | 2.08                     | 0.52              |
| 17:Q:25:PHE:HD1   | 18:R:210:PHE:CZ   | 2.27                     | 0.52              |
| 1:A:116:LYS:HE2   | 1:A:181:HIS:HB2   | 1.92                     | 0.52              |
| 1:A:364:ARG:HB2   | 2:B:1084:LEU:HD11 | 1.91                     | 0.52              |
| 1:A:729:PRO:CG    | 21:U:250:MET:HB2  | 2.38                     | 0.52              |
| 6:F:69:ARG:HG3    | 6:F:102:ILE:HD12  | 1.91                     | 0.52              |
| 7:G:91:GLN:HB3    | 7:G:98:PHE:HD2    | 1.75                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:J:52:HIS:HE1   | 10:J:54:ASP:HA    | 1.75                     | 0.52              |
| 1:A:1212:LEU:HB2  | 1:A:1285:LEU:HD21 | 1.92                     | 0.52              |
| 1:A:1319:LYS:HG2  | 1:A:1333:GLU:CD   | 2.33                     | 0.52              |
| 2:B:483:ARG:NH1   | 2:B:527:ALA:O     | 2.43                     | 0.52              |
| 2:B:906:GLN:HB3   | 12:L:45:TYR:HE1   | 1.75                     | 0.52              |
| 2:B:976:MET:O     | 2:B:978:ILE:N     | 2.41                     | 0.52              |
| 17:Q:75:ARG:HH21  | 17:Q:95:ASN:HD22  | 1.57                     | 0.52              |
| 20:T:177:ARG:N    | 20:T:178:ALA:HB3  | 2.24                     | 0.52              |
| 22:X:44:DT:H3'    | 22:X:45:DT:H5''   | 1.91                     | 0.52              |
| 1:A:358:ARG:NH2   | 2:B:1076:GLU:HA   | 2.25                     | 0.52              |
| 1:A:790:GLN:CD    | 1:A:797:ARG:HG2   | 2.34                     | 0.52              |
| 17:Q:23:ARG:CZ    | 18:R:207:SER:O    | 2.48                     | 0.52              |
| 1:A:180:GLY:C     | 1:A:182:GLY:N     | 2.67                     | 0.52              |
| 1:A:263:ALA:O     | 1:A:264:VAL:HG22  | 2.10                     | 0.52              |
| 1:A:467:MET:SD    | 1:A:524:MET:HB3   | 2.49                     | 0.52              |
| 2:B:834:ARG:HB3   | 2:B:840:MET:HE2   | 1.91                     | 0.52              |
| 3:C:60:HIS:CD2    | 3:C:63:PHE:HB2    | 2.45                     | 0.52              |
| 17:Q:105:TYR:HD1  | 18:R:234:GLU:HB2  | 1.75                     | 0.52              |
| 23:Y:45:DT:H5''   | 23:Y:46:DC:H5''   | 1.92                     | 0.52              |
| 13:M:245:VAL:HG12 | 13:M:291:LEU:HD23 | 1.92                     | 0.52              |
| 1:A:608:THR:HB    | 1:A:610:PRO:HD2   | 1.92                     | 0.51              |
| 2:B:931:ILE:HD11  | 2:B:947:ILE:HA    | 1.92                     | 0.51              |
| 9:I:119:CYS:HB3   | 9:I:121:HIS:HB2   | 1.90                     | 0.51              |
| 13:M:178:LYS:HB3  | 20:T:154:LYS:CE   | 2.40                     | 0.51              |
| 20:T:191:PHE:HZ   | 20:T:237:PRO:HG3  | 1.74                     | 0.51              |
| 2:B:62:ALA:N      | 2:B:63:PRO:HD3    | 2.25                     | 0.51              |
| 2:B:552:ASN:OD1   | 2:B:553:LEU:N     | 2.43                     | 0.51              |
| 16:P:256:GLN:O    | 16:P:316:LYS:NZ   | 2.32                     | 0.51              |
| 17:Q:44:LYS:HG3   | 17:Q:47:ASP:H     | 1.76                     | 0.51              |
| 1:A:790:GLN:NE2   | 1:A:797:ARG:HG2   | 2.25                     | 0.51              |
| 2:B:490:GLY:O     | 2:B:491:ARG:CG    | 2.59                     | 0.51              |
| 3:C:157:GLN:CG    | 10:J:65:LEU:CB    | 2.85                     | 0.51              |
| 5:E:151:MET:HE2   | 5:E:155:GLU:HB3   | 1.91                     | 0.51              |
| 5:E:172:ARG:HD3   | 5:E:210:GLN:HG2   | 1.92                     | 0.51              |
| 13:M:128:ILE:HG23 | 13:M:183:VAL:HG11 | 1.93                     | 0.51              |
| 18:R:212:VAL:O    | 18:R:213:ASP:OD1  | 2.28                     | 0.51              |
| 1:A:255:VAL:HG13  | 1:A:280:LEU:HD21  | 1.91                     | 0.51              |
| 1:A:972:THR:HA    | 1:A:1320:ILE:HG21 | 1.91                     | 0.51              |
| 2:B:50:PHE:O      | 2:B:54:SER:HB2    | 2.11                     | 0.51              |
| 2:B:363:TYR:CD2   | 2:B:553:LEU:HD21  | 2.45                     | 0.51              |
| 3:C:267:ILE:HG13  | 3:C:272:LEU:HB3   | 1.92                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:Q:109:HIS:CE1  | 18:R:233:ILE:CG2  | 2.93                     | 0.51              |
| 1:A:1158:LEU:HD11 | 1:A:1308:TYR:HD2  | 1.76                     | 0.51              |
| 9:I:61:GLU:O      | 9:I:63:ASP:HB2    | 2.10                     | 0.51              |
| 17:Q:25:PHE:CD2   | 18:R:219:LEU:CD1  | 2.94                     | 0.51              |
| 1:A:334:ARG:NH2   | 13:M:66:ARG:O     | 2.44                     | 0.51              |
| 1:A:623:PRO:C     | 1:A:625:ASP:N     | 2.68                     | 0.51              |
| 2:B:749:HIS:CD2   | 2:B:810:PHE:HD1   | 2.27                     | 0.51              |
| 5:E:52:ARG:NH2    | 5:E:54:ARG:HD3    | 2.26                     | 0.51              |
| 5:E:149:VAL:HG23  | 5:E:192:LYS:HB3   | 1.92                     | 0.51              |
| 13:M:94:ASP:O     | 13:M:97:GLY:N     | 2.42                     | 0.51              |
| 1:A:426:ARG:HB3   | 13:M:40:VAL:HG21  | 1.93                     | 0.51              |
| 1:A:818:GLU:H     | 1:A:818:GLU:CD    | 2.19                     | 0.51              |
| 2:B:224:CYS:O     | 2:B:225:LEU:C     | 2.54                     | 0.51              |
| 2:B:309:PHE:CZ    | 9:I:40:ARG:HB2    | 2.46                     | 0.51              |
| 9:I:65:LEU:CA     | 9:I:122:ARG:HE    | 2.24                     | 0.51              |
| 14:N:366:ILE:O    | 15:O:54:ASN:ND2   | 2.44                     | 0.51              |
| 1:A:362:SER:OG    | 2:B:1084:LEU:HB2  | 2.11                     | 0.51              |
| 1:A:859:TYR:OH    | 1:A:863:ARG:NH2   | 2.41                     | 0.51              |
| 1:A:1162:GLU:HB3  | 1:A:1306:LYS:CA   | 2.40                     | 0.51              |
| 5:E:63:ALA:O      | 5:E:64:HIS:CG     | 2.64                     | 0.51              |
| 8:H:95:LYS:HB2    | 8:H:139:SER:HA    | 1.92                     | 0.51              |
| 9:I:103:ARG:O     | 9:I:105:GLU:N     | 2.44                     | 0.51              |
| 10:J:66:GLU:HG3   | 12:L:23:HIS:CG    | 2.46                     | 0.51              |
| 22:X:42:DT:H2"    | 22:X:43:DT:H5"    | 1.92                     | 0.51              |
| 1:A:469:MET:HE3   | 2:B:1094:GLN:OE1  | 2.11                     | 0.51              |
| 1:A:604:ARG:HG3   | 1:A:606:HIS:HE1   | 1.76                     | 0.51              |
| 13:M:178:LYS:HG2  | 20:T:156:VAL:HG12 | 1.91                     | 0.51              |
| 17:Q:141:ALA:HB1  | 17:Q:152:PHE:CE2  | 2.44                     | 0.51              |
| 1:A:261:ARG:HD2   | 1:A:277:THR:OG1   | 2.11                     | 0.51              |
| 1:A:678:ASN:O     | 1:A:681:LEU:HB3   | 2.10                     | 0.51              |
| 2:B:914:GLU:OE1   | 2:B:914:GLU:N     | 2.40                     | 0.51              |
| 9:I:58:ILE:C      | 9:I:60:HIS:H      | 2.18                     | 0.51              |
| 11:K:7:PHE:HA     | 11:K:10:PHE:CE2   | 2.46                     | 0.51              |
| 11:K:111:ASP:C    | 11:K:113:GLN:H    | 2.15                     | 0.51              |
| 12:L:26:ASN:HD21  | 12:L:28:ILE:HD12  | 1.76                     | 0.51              |
| 20:T:93:LEU:HB2   | 20:T:110:VAL:HB   | 1.91                     | 0.51              |
| 1:A:11:SER:O      | 2:B:1135:TYR:OH   | 2.27                     | 0.50              |
| 2:B:553:LEU:HB2   | 2:B:573:TRP:HZ3   | 1.75                     | 0.50              |
| 2:B:796:MET:HE1   | 2:B:935:PHE:CE2   | 2.46                     | 0.50              |
| 2:B:939:HIS:NE2   | 2:B:980:HIS:HA    | 2.26                     | 0.50              |
| 3:C:49:TRP:CZ3    | 12:L:54:VAL:HG21  | 2.46                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:O:64:THR:HG22  | 15:O:75:VAL:HB    | 1.92                     | 0.50              |
| 19:S:26:TYR:CD1   | 20:T:97:THR:HG22  | 2.46                     | 0.50              |
| 22:X:52:DG:H2''   | 22:X:53:DA:O4'    | 2.11                     | 0.50              |
| 1:A:201:GLU:CG    | 1:A:212:LYS:HB3   | 2.40                     | 0.50              |
| 2:B:499:ARG:CZ    | 2:B:522:LEU:HD11  | 2.41                     | 0.50              |
| 17:Q:17:LEU:HD21  | 17:Q:191:LEU:HB3  | 1.93                     | 0.50              |
| 2:B:716:HIS:CE1   | 2:B:1007:ASN:HD21 | 2.29                     | 0.50              |
| 2:B:867:ILE:O     | 2:B:893:SER:HB2   | 2.11                     | 0.50              |
| 2:B:1060:HIS:HB2  | 2:B:1078:ARG:HE   | 1.75                     | 0.50              |
| 1:A:126:ILE:HD13  | 1:A:129:ILE:HD12  | 1.92                     | 0.50              |
| 1:A:604:ARG:HG3   | 1:A:606:HIS:CE1   | 2.45                     | 0.50              |
| 2:B:380:ARG:HE    | 2:B:609:GLU:CD    | 2.19                     | 0.50              |
| 2:B:1072:ARG:HG3  | 2:B:1072:ARG:O    | 2.10                     | 0.50              |
| 8:H:74:GLU:C      | 8:H:76:ASN:H      | 2.13                     | 0.50              |
| 2:B:240:LEU:O     | 2:B:253:GLY:HA2   | 2.11                     | 0.50              |
| 2:B:513:GLU:HG3   | 2:B:726:SER:HB3   | 1.94                     | 0.50              |
| 2:B:891:ASP:OD1   | 2:B:892:CYS:N     | 2.44                     | 0.50              |
| 7:G:158:PHE:N     | 7:G:158:PHE:CD1   | 2.80                     | 0.50              |
| 21:U:286:THR:HG21 | 21:U:299:LYS:HD2  | 1.93                     | 0.50              |
| 2:B:72:GLN:HB3    | 2:B:76:GLY:HA3    | 1.92                     | 0.50              |
| 2:B:1101:GLN:HE22 | 6:F:64:ARG:HG2    | 1.76                     | 0.50              |
| 22:X:19:DG:N2     | 23:Y:76:DC:O2     | 2.44                     | 0.50              |
| 1:A:366:VAL:O     | 1:A:481:THR:HB    | 2.12                     | 0.50              |
| 2:B:483:ARG:HG3   | 2:B:526:LEU:HB3   | 1.94                     | 0.50              |
| 2:B:855:ALA:HB2   | 12:L:46:LYS:HE2   | 1.93                     | 0.50              |
| 2:B:907:VAL:HG13  | 2:B:921:ILE:HG22  | 1.93                     | 0.50              |
| 17:Q:25:PHE:O     | 18:R:219:LEU:CD2  | 2.59                     | 0.50              |
| 1:A:931:ARG:C     | 1:A:933:THR:H     | 2.20                     | 0.50              |
| 1:A:1319:LYS:HG3  | 1:A:1333:GLU:CD   | 2.36                     | 0.50              |
| 1:A:1407:CYS:SG   | 1:A:1408:ARG:N    | 2.84                     | 0.50              |
| 2:B:957:THR:O     | 2:B:960:GLY:N     | 2.36                     | 0.50              |
| 2:B:1132:THR:HG23 | 2:B:1133:HIS:ND1  | 2.27                     | 0.50              |
| 3:C:49:TRP:O      | 3:C:163:ALA:HA    | 2.12                     | 0.50              |
| 13:M:94:ASP:C     | 13:M:96:PHE:N     | 2.70                     | 0.50              |
| 17:Q:113:ARG:NH2  | 18:R:218:LYS:HE2  | 2.11                     | 0.50              |
| 20:T:166:GLU:HA   | 20:T:169:LYS:HE3  | 1.92                     | 0.50              |
| 1:A:274:ASP:OD2   | 1:A:276:LEU:HB3   | 2.12                     | 0.50              |
| 1:A:618:TYR:C     | 1:A:620:HIS:H     | 2.20                     | 0.50              |
| 1:A:673:GLN:O     | 1:A:677:ASN:CB    | 2.60                     | 0.50              |
| 1:A:1276:VAL:HG12 | 1:A:1279:MET:HB2  | 1.93                     | 0.50              |
| 2:B:326:ALA:HB2   | 2:B:338:TYR:HE2   | 1.76                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:333:GLU:CD    | 19:S:53:ASN:HD21  | 2.17                     | 0.50              |
| 3:C:212:ASP:O     | 3:C:213:GLU:C     | 2.53                     | 0.50              |
| 14:N:312:GLU:C    | 14:N:314:LEU:H    | 2.20                     | 0.50              |
| 17:Q:188:TYR:HD1  | 17:Q:191:LEU:HD22 | 1.77                     | 0.50              |
| 18:R:227:SER:O    | 18:R:228:MET:O    | 2.30                     | 0.50              |
| 1:A:197:GLU:CD    | 13:M:93:PHE:CE2   | 2.89                     | 0.49              |
| 1:A:263:ALA:C     | 1:A:264:VAL:HG22  | 2.37                     | 0.49              |
| 2:B:489:ILE:HG13  | 2:B:490:GLY:H     | 1.77                     | 0.49              |
| 19:S:26:TYR:HD1   | 20:T:97:THR:HG22  | 1.76                     | 0.49              |
| 22:X:13:DT:H2''   | 22:X:14:DA:H8     | 1.77                     | 0.49              |
| 22:X:45:DT:H4'    | 22:X:45:DT:OP1    | 2.12                     | 0.49              |
| 23:Y:62:DC:H1'    | 23:Y:63:DG:H4'    | 1.93                     | 0.49              |
| 1:A:267:GLN:O     | 1:A:268:GLY:C     | 2.55                     | 0.49              |
| 1:A:1158:LEU:HD11 | 1:A:1308:TYR:CD2  | 2.47                     | 0.49              |
| 1:A:1471:PHE:HE1  | 6:F:64:ARG:HD3    | 1.77                     | 0.49              |
| 13:M:7:LEU:HG     | 13:M:10:LEU:HD11  | 1.94                     | 0.49              |
| 17:Q:164:ASP:O    | 17:Q:166:SER:N    | 2.45                     | 0.49              |
| 20:T:217:LEU:HB3  | 20:T:233:TRP:CE3  | 2.46                     | 0.49              |
| 1:A:893:GLU:HG2   | 5:E:203:TYR:CD1   | 2.46                     | 0.49              |
| 2:B:728:MET:HE2   | 2:B:942:LYS:HG2   | 1.93                     | 0.49              |
| 1:A:375:ILE:HG21  | 1:A:666:ARG:NH1   | 2.26                     | 0.49              |
| 2:B:626:LEU:HG    | 2:B:698:ILE:HG22  | 1.95                     | 0.49              |
| 7:G:63:ARG:C      | 7:G:65:PHE:H      | 2.21                     | 0.49              |
| 7:G:97:LEU:HB3    | 7:G:108:ILE:HB    | 1.93                     | 0.49              |
| 12:L:19:CYS:HB3   | 12:L:22:CYS:SG    | 2.53                     | 0.49              |
| 13:M:276:ASP:HA   | 20:T:153:TYR:CE1  | 2.47                     | 0.49              |
| 17:Q:95:ASN:OD1   | 17:Q:96:TYR:N     | 2.45                     | 0.49              |
| 18:R:80:LYS:HB2   | 20:T:188:PHE:CE2  | 2.47                     | 0.49              |
| 19:S:15:VAL:HA    | 20:T:42:LYS:HG2   | 1.93                     | 0.49              |
| 1:A:890:ARG:NH2   | 1:A:1023:VAL:HG13 | 2.23                     | 0.49              |
| 2:B:935:PHE:CE1   | 2:B:1050:ARG:HG3  | 2.48                     | 0.49              |
| 2:B:1028:LEU:C    | 2:B:1029:TYR:HD1  | 2.21                     | 0.49              |
| 2:B:1060:HIS:CE1  | 2:B:1078:ARG:HG3  | 2.47                     | 0.49              |
| 3:C:116:THR:HB    | 3:C:146:ASP:HB2   | 1.93                     | 0.49              |
| 12:L:56:ASP:OD1   | 12:L:56:ASP:N     | 2.46                     | 0.49              |
| 20:T:140:ARG:O    | 20:T:141:LEU:HB2  | 2.13                     | 0.49              |
| 20:T:175:ARG:HE   | 22:X:21:DG:P      | 2.36                     | 0.49              |
| 1:A:624:GLY:C     | 1:A:626:THR:H     | 2.20                     | 0.49              |
| 1:A:862:ARG:HG3   | 2:B:1089:MET:HE2  | 1.95                     | 0.49              |
| 12:L:36:CYS:HB2   | 12:L:44:MET:HE1   | 1.93                     | 0.49              |
| 13:M:178:LYS:HB3  | 20:T:154:LYS:HE3  | 1.93                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:P:297:LYS:C    | 16:P:299:ARG:N    | 2.71                     | 0.49              |
| 2:B:555:GLU:OE1   | 19:S:124:TYR:OH   | 2.18                     | 0.49              |
| 3:C:262:GLN:HG3   | 11:K:18:LYS:HG2   | 1.94                     | 0.49              |
| 5:E:48:PRO:O      | 5:E:52:ARG:NH1    | 2.45                     | 0.49              |
| 9:I:57:LYS:O      | 9:I:58:ILE:HG12   | 2.13                     | 0.49              |
| 2:B:1092:ASP:HA   | 2:B:1095:ILE:HD12 | 1.94                     | 0.49              |
| 10:J:5:VAL:HG12   | 10:J:6:ARG:HG3    | 1.94                     | 0.49              |
| 17:Q:23:ARG:HD3   | 18:R:207:SER:O    | 2.12                     | 0.49              |
| 21:U:255:GLY:C    | 21:U:256:THR:HG23 | 2.37                     | 0.49              |
| 1:A:426:ARG:HB3   | 13:M:40:VAL:CG2   | 2.43                     | 0.49              |
| 1:A:522:PRO:CA    | 1:A:666:ARG:HE    | 2.10                     | 0.49              |
| 1:A:1167:ARG:HA   | 1:A:1293:LEU:HD22 | 1.93                     | 0.49              |
| 2:B:177:CYS:HB3   | 2:B:180:ASP:HB2   | 1.95                     | 0.49              |
| 2:B:324:ARG:NH1   | 19:S:162:GLU:OE2  | 2.46                     | 0.49              |
| 14:N:323:GLU:HG2  | 14:N:325:GLY:HA3  | 1.94                     | 0.49              |
| 20:T:177:ARG:H    | 20:T:178:ALA:HB3  | 1.76                     | 0.49              |
| 1:A:53:LYS:HE3    | 1:A:59:ASP:HB3    | 1.95                     | 0.49              |
| 1:A:560:VAL:HG21  | 1:A:586:TRP:CE3   | 2.48                     | 0.49              |
| 2:B:677:MET:HG3   | 2:B:678:THR:HG23  | 1.95                     | 0.49              |
| 2:B:871:VAL:HG13  | 2:B:890:ARG:HB2   | 1.95                     | 0.49              |
| 3:C:134:ASN:C     | 3:C:136:ASP:OD1   | 2.56                     | 0.49              |
| 17:Q:112:ARG:CG   | 18:R:237:LEU:HD11 | 2.37                     | 0.49              |
| 1:A:932:ARG:HE    | 1:A:943:LEU:HD22  | 1.78                     | 0.48              |
| 3:C:169:PHE:HE1   | 3:C:171:LYS:HB3   | 1.78                     | 0.48              |
| 3:C:169:PHE:CE1   | 3:C:171:LYS:HB3   | 2.47                     | 0.48              |
| 7:G:1:MET:N       | 7:G:78:ARG:O      | 2.45                     | 0.48              |
| 8:H:85:ALA:HB1    | 8:H:88:PHE:CD2    | 2.47                     | 0.48              |
| 10:J:43:TYR:HA    | 10:J:46:ARG:HB2   | 1.95                     | 0.48              |
| 19:S:124:TYR:HB3  | 20:T:20:LEU:HD11  | 1.95                     | 0.48              |
| 2:B:418:TYR:CD1   | 2:B:434:ALA:HB2   | 2.48                     | 0.48              |
| 3:C:75:SER:HB3    | 3:C:79:VAL:HB     | 1.95                     | 0.48              |
| 22:X:29:DC:H2''   | 22:X:30:DG:H5'    | 1.94                     | 0.48              |
| 1:A:1065:PHE:CE2  | 1:A:1069:LEU:HD11 | 2.49                     | 0.48              |
| 3:C:7:PRO:O       | 3:C:8:THR:OG1     | 2.29                     | 0.48              |
| 13:M:300:PHE:HD2  | 13:M:306:PHE:HE1  | 1.62                     | 0.48              |
| 17:Q:188:TYR:CE1  | 18:R:210:PHE:HB2  | 2.48                     | 0.48              |
| 20:T:139:VAL:HG13 | 20:T:142:SER:OG   | 2.12                     | 0.48              |
| 1:A:1162:GLU:CG   | 1:A:1306:LYS:HB2  | 2.38                     | 0.48              |
| 2:B:422:PHE:HD1   | 2:B:428:ASP:H     | 1.62                     | 0.48              |
| 2:B:810:PHE:CD2   | 2:B:927:ARG:NH2   | 2.81                     | 0.48              |
| 2:B:1101:GLN:NE2  | 6:F:64:ARG:CG     | 2.77                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:Q:184:ILE:HD11 | 18:R:213:ASP:OD2  | 2.14                     | 0.48              |
| 20:T:190:ALA:O    | 20:T:197:TYR:OH   | 2.24                     | 0.48              |
| 22:X:46:DT:H2'    | 22:X:47:DT:C5     | 2.48                     | 0.48              |
| 2:B:295:PRO:HB2   | 9:I:11:PHE:HD2    | 1.77                     | 0.48              |
| 2:B:798:ARG:O     | 2:B:801:VAL:HG22  | 2.14                     | 0.48              |
| 2:B:852:GLY:O     | 2:B:868:GLY:N     | 2.30                     | 0.48              |
| 10:J:6:ARG:HA     | 10:J:13:ILE:HA    | 1.96                     | 0.48              |
| 2:B:464:ALA:HB1   | 13:M:62:LYS:NZ    | 2.28                     | 0.48              |
| 3:C:69:GLY:HA3    | 12:L:57:ALA:HB1   | 1.95                     | 0.48              |
| 5:E:13:ILE:HG22   | 5:E:136:LEU:HA    | 1.94                     | 0.48              |
| 5:E:64:HIS:HE1    | 5:E:68:PRO:CB     | 2.21                     | 0.48              |
| 8:H:93:TYR:HE1    | 8:H:140:ARG:HA    | 1.79                     | 0.48              |
| 1:A:1130:ILE:HD13 | 1:A:1411:LEU:HD22 | 1.96                     | 0.48              |
| 5:E:71:GLN:HE21   | 5:E:99:ILE:HG22   | 1.79                     | 0.48              |
| 1:A:265:VAL:HG23  | 1:A:266:MET:H     | 1.79                     | 0.48              |
| 1:A:1162:GLU:CB   | 1:A:1306:LYS:CA   | 2.91                     | 0.48              |
| 2:B:474:THR:HG23  | 2:B:732:ALA:O     | 2.13                     | 0.48              |
| 3:C:148:ILE:HG12  | 3:C:149:LEU:N     | 2.28                     | 0.48              |
| 5:E:45:GLY:C      | 5:E:46:ASP:O      | 2.54                     | 0.48              |
| 11:K:47:LYS:HD2   | 11:K:61:TYR:HD1   | 1.78                     | 0.48              |
| 17:Q:113:ARG:NH2  | 18:R:218:LYS:HG3  | 2.29                     | 0.48              |
| 22:X:50:DT:H4'    | 22:X:50:DT:OP1    | 2.13                     | 0.48              |
| 1:A:686:THR:OG1   | 1:A:687:ILE:N     | 2.46                     | 0.48              |
| 2:B:356:PHE:O     | 19:S:116:GLY:HA2  | 2.13                     | 0.48              |
| 2:B:726:SER:O     | 2:B:730:LYS:HE2   | 2.14                     | 0.48              |
| 2:B:929:PRO:HB3   | 2:B:935:PHE:HZ    | 1.78                     | 0.48              |
| 2:B:964:ASP:OD1   | 2:B:964:ASP:N     | 2.47                     | 0.48              |
| 9:I:41:ASN:HA     | 19:S:177:MET:HE1  | 1.95                     | 0.48              |
| 1:A:117:LEU:HB2   | 1:A:232:GLU:HG2   | 1.96                     | 0.48              |
| 1:A:612:ASP:O     | 1:A:613:GLU:C     | 2.57                     | 0.48              |
| 1:A:621:ILE:O     | 1:A:623:PRO:CD    | 2.61                     | 0.48              |
| 2:B:422:PHE:CD1   | 2:B:422:PHE:C     | 2.91                     | 0.48              |
| 2:B:728:MET:HE1   | 2:B:940:GLY:C     | 2.39                     | 0.48              |
| 13:M:91:ALA:O     | 13:M:92:SER:C     | 2.55                     | 0.48              |
| 16:P:156:SER:O    | 16:P:158:SER:N    | 2.47                     | 0.48              |
| 18:R:195:PRO:HB2  | 18:R:199:LYS:HG3  | 1.95                     | 0.48              |
| 1:A:807:LEU:HB3   | 1:A:809:HIS:HD2   | 1.78                     | 0.47              |
| 1:A:1306:LYS:C    | 1:A:1308:TYR:H    | 2.20                     | 0.47              |
| 2:B:964:ASP:O     | 2:B:965:ILE:HG13  | 2.14                     | 0.47              |
| 3:C:157:GLN:HG3   | 10:J:65:LEU:CB    | 2.44                     | 0.47              |
| 13:M:74:LEU:O     | 13:M:143:LYS:NZ   | 2.47                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:M:86:LYS:NZ    | 22:X:40:DT:N3     | 2.61                     | 0.47              |
| 16:P:293:TYR:HD2  | 16:P:302:LEU:HD13 | 1.78                     | 0.47              |
| 17:Q:105:TYR:CD1  | 18:R:234:GLU:CB   | 2.97                     | 0.47              |
| 18:R:167:LEU:HD22 | 18:R:200:ILE:HB   | 1.96                     | 0.47              |
| 20:T:81:HIS:HB3   | 20:T:116:CYS:SG   | 2.54                     | 0.47              |
| 23:Y:52:DT:H2"    | 23:Y:53:DG:O4'    | 2.13                     | 0.47              |
| 1:A:264:VAL:HG22  | 1:A:272:ASN:CG    | 2.35                     | 0.47              |
| 2:B:470:LEU:HD11  | 2:B:478:THR:HG23  | 1.96                     | 0.47              |
| 2:B:812:ARG:NH2   | 23:Y:52:DT:OP1    | 2.38                     | 0.47              |
| 2:B:1000:THR:HG23 | 2:B:1001:PRO:HD2  | 1.96                     | 0.47              |
| 5:E:129:GLN:OE1   | 5:E:130:PHE:N     | 2.47                     | 0.47              |
| 13:M:214:PHE:HB3  | 13:M:218:PHE:CE2  | 2.49                     | 0.47              |
| 20:T:168:LYS:C    | 20:T:170:LYS:H    | 2.22                     | 0.47              |
| 2:B:94:SER:OG     | 2:B:95:LYS:N      | 2.47                     | 0.47              |
| 2:B:455:ASP:O     | 2:B:457:LYS:N     | 2.40                     | 0.47              |
| 4:D:30:GLU:O      | 7:G:3:TYR:HA      | 2.13                     | 0.47              |
| 18:R:119:LEU:HA   | 18:R:123:ALA:HB3  | 1.95                     | 0.47              |
| 1:A:632:ASN:HA    | 1:A:992:LYS:HD2   | 1.95                     | 0.47              |
| 2:B:79:GLU:C      | 2:B:80:GLU:HG2    | 2.39                     | 0.47              |
| 2:B:184:TYR:HE2   | 2:B:191:GLU:HG2   | 1.79                     | 0.47              |
| 2:B:628:VAL:HG21  | 2:B:682:LEU:HD11  | 1.97                     | 0.47              |
| 3:C:184:PHE:HD1   | 3:C:231:TYR:CE1   | 2.33                     | 0.47              |
| 13:M:75:LEU:HD22  | 13:M:139:ASN:OD1  | 2.14                     | 0.47              |
| 17:Q:153:ARG:HD3  | 17:Q:158:HIS:HB3  | 1.94                     | 0.47              |
| 1:A:275:ASP:OD1   | 1:A:276:LEU:N     | 2.47                     | 0.47              |
| 2:B:676:ALA:HB2   | 2:B:693:TYR:CG    | 2.50                     | 0.47              |
| 7:G:55:GLY:HA3    | 7:G:69:PRO:HG2    | 1.97                     | 0.47              |
| 13:M:9:ALA:CA     | 13:M:10:LEU:HD13  | 2.37                     | 0.47              |
| 13:M:32:MET:O     | 13:M:40:VAL:HA    | 2.15                     | 0.47              |
| 1:A:889:LEU:HD21  | 5:E:206:TYR:HE1   | 1.80                     | 0.47              |
| 2:B:124:LEU:HD23  | 2:B:149:ILE:HD11  | 1.95                     | 0.47              |
| 2:B:947:ILE:HG12  | 2:B:948:GLN:N     | 2.29                     | 0.47              |
| 2:B:1124:ILE:HG22 | 2:B:1126:ALA:H    | 1.78                     | 0.47              |
| 3:C:86:ARG:HH22   | 11:K:10:PHE:HE1   | 1.62                     | 0.47              |
| 8:H:90:TYR:HB3    | 8:H:145:MET:HB3   | 1.96                     | 0.47              |
| 9:I:98:GLN:O      | 9:I:100:HIS:N     | 2.48                     | 0.47              |
| 17:Q:173:ALA:O    | 17:Q:177:LEU:HD23 | 2.15                     | 0.47              |
| 18:R:195:PRO:O    | 18:R:196:ASP:CB   | 2.59                     | 0.47              |
| 1:A:197:GLU:CD    | 13:M:93:PHE:CD2   | 2.92                     | 0.47              |
| 1:A:265:VAL:C     | 1:A:272:ASN:CG    | 2.77                     | 0.47              |
| 1:A:557:ARG:HB3   | 1:A:557:ARG:HH11  | 1.79                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:616:GLY:O     | 1:A:619:LYS:HB2   | 2.15                     | 0.47              |
| 1:A:880:ARG:HG2   | 1:A:886:VAL:HA    | 1.97                     | 0.47              |
| 1:A:1263:ASN:HB2  | 1:A:1268:LYS:HD2  | 1.96                     | 0.47              |
| 1:A:1320:ILE:HD12 | 1:A:1329:LYS:O    | 2.14                     | 0.47              |
| 2:B:718:GLN:HB2   | 2:B:976:MET:HE3   | 1.97                     | 0.47              |
| 2:B:960:GLY:O     | 2:B:962:THR:N     | 2.48                     | 0.47              |
| 13:M:196:LYS:NZ   | 22:X:13:DT:OP1    | 2.41                     | 0.47              |
| 20:T:141:LEU:HB3  | 20:T:142:SER:H    | 1.50                     | 0.47              |
| 1:A:119:VAL:HG21  | 1:A:147:LEU:HD21  | 1.97                     | 0.47              |
| 1:A:1307:VAL:C    | 1:A:1308:TYR:O    | 2.50                     | 0.47              |
| 1:A:1319:LYS:HA   | 1:A:1319:LYS:HD3  | 1.69                     | 0.47              |
| 2:B:1091:ARG:O    | 2:B:1095:ILE:HG13 | 2.14                     | 0.47              |
| 13:M:30:GLY:HA2   | 13:M:44:ARG:HG2   | 1.96                     | 0.47              |
| 14:N:319:ASP:C    | 14:N:321:SER:N    | 2.72                     | 0.47              |
| 1:A:1171:ALA:O    | 9:I:59:THR:HG23   | 2.15                     | 0.47              |
| 2:B:796:MET:O     | 2:B:948:GLN:HA    | 2.14                     | 0.47              |
| 2:B:954:MET:HE2   | 2:B:963:PRO:O     | 2.15                     | 0.47              |
| 2:B:1066:PRO:HB2  | 2:B:1075:MET:HG3  | 1.97                     | 0.47              |
| 9:I:73:SER:HA     | 9:I:95:VAL:HG21   | 1.97                     | 0.47              |
| 17:Q:101:ASN:ND2  | 17:Q:202:GLU:OE2  | 2.40                     | 0.47              |
| 20:T:80:GLU:O     | 20:T:119:ALA:HB2  | 2.14                     | 0.47              |
| 1:A:264:VAL:CG2   | 1:A:272:ASN:OD1   | 2.44                     | 0.47              |
| 1:A:1189:ASP:O    | 1:A:1192:TRP:N    | 2.48                     | 0.47              |
| 2:B:239:MET:HE2   | 2:B:372:LEU:HD21  | 1.97                     | 0.47              |
| 9:I:60:HIS:C      | 9:I:62:VAL:N      | 2.71                     | 0.47              |
| 10:J:40:LEU:HD11  | 10:J:49:LEU:HD13  | 1.97                     | 0.47              |
| 18:R:164:GLY:CA   | 18:R:203:PHE:HZ   | 1.88                     | 0.47              |
| 21:U:215:ILE:HG23 | 21:U:219:LEU:HD23 | 1.97                     | 0.47              |
| 1:A:365:THR:HG22  | 2:B:1059:ILE:HG22 | 1.98                     | 0.46              |
| 1:A:576:GLN:HG3   | 1:A:577:PRO:HD2   | 1.97                     | 0.46              |
| 3:C:35:ARG:HG2    | 3:C:36:ARG:N      | 2.30                     | 0.46              |
| 3:C:76:ASP:OD1    | 3:C:243:THR:HG21  | 2.15                     | 0.46              |
| 9:I:84:HIS:ND1    | 9:I:85:PRO:HD3    | 2.28                     | 0.46              |
| 10:J:63:ALA:N     | 10:J:64:PRO:CD    | 2.77                     | 0.46              |
| 15:O:77:ASN:OD1   | 15:O:78:ASP:N     | 2.48                     | 0.46              |
| 18:R:222:SER:C    | 18:R:224:THR:N    | 2.64                     | 0.46              |
| 20:T:198:ASN:OD1  | 20:T:199:LEU:N    | 2.49                     | 0.46              |
| 1:A:578:ALA:HB3   | 1:A:587:THR:HG23  | 1.96                     | 0.46              |
| 1:A:1116:ASN:O    | 1:A:1117:VAL:HB   | 2.14                     | 0.46              |
| 2:B:213:SER:HA    | 2:B:242:ARG:HD2   | 1.96                     | 0.46              |
| 2:B:282:ARG:HD2   | 9:I:21:ASN:HD21   | 1.81                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:R:224:THR:OG1  | 18:R:225:VAL:N    | 2.48                     | 0.46              |
| 20:T:3:GLU:H      | 20:T:3:GLU:CD     | 2.24                     | 0.46              |
| 1:A:367:ILE:HA    | 1:A:482:PHE:O     | 2.15                     | 0.46              |
| 1:A:804:HIS:NE2   | 9:I:100:HIS:HA    | 2.31                     | 0.46              |
| 1:A:966:LEU:HD13  | 1:A:1043:ILE:HD11 | 1.96                     | 0.46              |
| 2:B:348:LEU:HD13  | 2:B:364:PHE:HD2   | 1.79                     | 0.46              |
| 8:H:65:TYR:CE2    | 8:H:70:LEU:HD22   | 2.50                     | 0.46              |
| 8:H:65:TYR:CG     | 8:H:70:LEU:HD22   | 2.50                     | 0.46              |
| 19:S:122:THR:HA   | 20:T:24:PRO:HA    | 1.97                     | 0.46              |
| 1:A:206:ASN:C     | 1:A:208:ASP:H     | 2.23                     | 0.46              |
| 1:A:455:ILE:HD13  | 1:A:520:MET:CE    | 2.43                     | 0.46              |
| 1:A:511:THR:HG21  | 2:B:1105:GLU:OE2  | 2.16                     | 0.46              |
| 1:A:525:ILE:HG12  | 1:A:666:ARG:NH2   | 2.30                     | 0.46              |
| 1:A:837:PHE:HB2   | 2:B:506:TRP:HZ3   | 1.79                     | 0.46              |
| 1:A:1224:ARG:HH22 | 1:A:1306:LYS:HD3  | 1.72                     | 0.46              |
| 1:A:1319:LYS:O    | 1:A:1321:ILE:HG23 | 2.15                     | 0.46              |
| 1:A:1472:ASP:HB2  | 6:F:107:ARG:HB3   | 1.97                     | 0.46              |
| 2:B:950:ARG:HB2   | 2:B:952:GLU:OE1   | 2.15                     | 0.46              |
| 2:B:1101:GLN:HE22 | 6:F:64:ARG:CG     | 2.29                     | 0.46              |
| 3:C:6:GLN:O       | 11:K:104:ARG:NH1  | 2.49                     | 0.46              |
| 3:C:157:GLN:NE2   | 10:J:65:LEU:HB3   | 2.31                     | 0.46              |
| 17:Q:180:PHE:CE1  | 18:R:213:ASP:N    | 2.84                     | 0.46              |
| 18:R:163:LEU:HD12 | 18:R:163:LEU:O    | 2.15                     | 0.46              |
| 1:A:1117:VAL:O    | 1:A:1118:THR:C    | 2.57                     | 0.46              |
| 2:B:526:LEU:HD12  | 2:B:526:LEU:HA    | 1.48                     | 0.46              |
| 20:T:155:PRO:C    | 20:T:157:ALA:N    | 2.73                     | 0.46              |
| 1:A:42:LYS:NZ     | 1:A:43:TYR:O      | 2.49                     | 0.46              |
| 1:A:79:THR:HG23   | 13:M:43:ASP:CG    | 2.40                     | 0.46              |
| 1:A:1158:LEU:O    | 1:A:1162:GLU:HG3  | 2.15                     | 0.46              |
| 1:A:1162:GLU:CB   | 1:A:1306:LYS:HA   | 2.45                     | 0.46              |
| 1:A:1185:VAL:HG21 | 9:I:51:SER:OG     | 2.16                     | 0.46              |
| 5:E:65:ASN:OD1    | 5:E:67:ASP:N      | 2.42                     | 0.46              |
| 1:A:196:LEU:HG    | 1:A:325:LEU:HD21  | 1.98                     | 0.46              |
| 1:A:1128:ILE:HD12 | 1:A:1414:ILE:HD11 | 1.98                     | 0.46              |
| 1:A:1162:GLU:CA   | 1:A:1306:LYS:HA   | 2.46                     | 0.46              |
| 1:A:1318:LYS:HE2  | 1:A:1318:LYS:HB2  | 1.70                     | 0.46              |
| 1:A:1408:ARG:O    | 1:A:1410:HIS:N    | 2.48                     | 0.46              |
| 2:B:802:ASP:C     | 2:B:804:GLY:H     | 2.24                     | 0.46              |
| 17:Q:188:TYR:CE1  | 18:R:210:PHE:CG   | 3.04                     | 0.46              |
| 19:S:128:THR:HG22 | 19:S:136:GLU:HB3  | 1.98                     | 0.46              |
| 23:Y:54:DA:H3'    | 23:Y:55:DG:H5''   | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:116:LYS:HE2   | 1:A:181:HIS:HB3   | 1.98                     | 0.46              |
| 1:A:608:THR:CB    | 1:A:610:PRO:HG2   | 2.45                     | 0.46              |
| 1:A:1431:SER:HB3  | 1:A:1459:MET:HE1  | 1.97                     | 0.46              |
| 13:M:183:VAL:HG12 | 20:T:152:ASN:ND2  | 2.31                     | 0.46              |
| 17:Q:104:LYS:HE3  | 17:Q:105:TYR:CZ   | 2.50                     | 0.46              |
| 18:R:80:LYS:HG2   | 18:R:108:HIS:HE1  | 1.81                     | 0.46              |
| 18:R:151:LEU:HB3  | 18:R:154:LEU:HB3  | 1.97                     | 0.46              |
| 2:B:248:LYS:O     | 2:B:249:LYS:HB2   | 2.16                     | 0.46              |
| 2:B:422:PHE:CD1   | 2:B:427:LYS:HA    | 2.50                     | 0.46              |
| 9:I:84:HIS:HB2    | 9:I:85:PRO:HD3    | 0.94                     | 0.46              |
| 10:J:3:ILE:HD13   | 10:J:18:TRP:CD2   | 2.50                     | 0.46              |
| 10:J:66:GLU:HG3   | 12:L:23:HIS:CE1   | 2.49                     | 0.46              |
| 14:N:313:PRO:HD2  | 16:P:250:PHE:HB3  | 1.98                     | 0.46              |
| 17:Q:185:GLU:HB3  | 17:Q:186:PRO:HD3  | 1.97                     | 0.46              |
| 20:T:229:HIS:CD2  | 22:X:28:DG:H21    | 2.33                     | 0.46              |
| 22:X:59:DC:H2''   | 22:X:60:DG:O5'    | 2.16                     | 0.46              |
| 1:A:133:SER:C     | 1:A:135:GLY:N     | 2.74                     | 0.46              |
| 12:L:16:ILE:HG21  | 12:L:47:LYS:HD2   | 1.98                     | 0.46              |
| 18:R:116:LYS:HA   | 18:R:119:LEU:HD12 | 1.98                     | 0.46              |
| 19:S:18:VAL:HG22  | 19:S:137:ALA:HB3  | 1.98                     | 0.46              |
| 21:U:243:GLU:O    | 21:U:247:GLU:N    | 2.46                     | 0.46              |
| 23:Y:58:DC:H1'    | 23:Y:59:DG:C4     | 2.51                     | 0.46              |
| 2:B:972:ILE:O     | 2:B:976:MET:N     | 2.48                     | 0.45              |
| 2:B:1062:ARG:HH12 | 2:B:1075:MET:N    | 2.11                     | 0.45              |
| 5:E:41:LYS:HG3    | 5:E:46:ASP:HB2    | 1.97                     | 0.45              |
| 5:E:91:CYS:HA     | 5:E:94:MET:HG2    | 1.98                     | 0.45              |
| 9:I:11:PHE:HE1    | 9:I:54:TYR:HA     | 1.81                     | 0.45              |
| 9:I:103:ARG:C     | 9:I:105:GLU:N     | 2.72                     | 0.45              |
| 14:N:333:ASN:HB3  | 14:N:359:ASN:O    | 2.16                     | 0.45              |
| 1:A:460:ARG:HB3   | 1:A:501:MET:HE3   | 1.98                     | 0.45              |
| 1:A:1138:SER:OG   | 1:A:1139:LEU:N    | 2.46                     | 0.45              |
| 1:A:1199:MET:SD   | 1:A:1200:PRO:HD2  | 2.56                     | 0.45              |
| 8:H:108:ALA:C     | 8:H:110:THR:N     | 2.72                     | 0.45              |
| 17:Q:128:LYS:HG3  | 17:Q:129:CYS:N    | 2.31                     | 0.45              |
| 19:S:166:ARG:HH11 | 19:S:166:ARG:CG   | 2.28                     | 0.45              |
| 1:A:117:LEU:H     | 1:A:232:GLU:CD    | 2.24                     | 0.45              |
| 1:A:340:LYS:HG3   | 1:A:1436:VAL:HG21 | 1.99                     | 0.45              |
| 2:B:529:MET:HE2   | 2:B:624:PRO:CD    | 2.46                     | 0.45              |
| 2:B:934:LYS:HE2   | 2:B:942:LYS:HD2   | 1.99                     | 0.45              |
| 3:C:31:ALA:HB1    | 3:C:184:PHE:HE1   | 1.80                     | 0.45              |
| 3:C:68:LEU:HA     | 3:C:68:LEU:HD12   | 1.66                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 7:G:107:PHE:CZ    | 17:Q:127:PHE:HZ  | 2.34                     | 0.45              |
| 8:H:88:PHE:CE1    | 8:H:146:LYS:HD2  | 2.51                     | 0.45              |
| 10:J:3:ILE:HG13   | 10:J:52:HIS:CD2  | 2.51                     | 0.45              |
| 17:Q:112:ARG:NH2  | 18:R:237:LEU:O   | 2.50                     | 0.45              |
| 1:A:26:LEU:O      | 1:A:26:LEU:HD12  | 2.17                     | 0.45              |
| 1:A:375:ILE:HA    | 1:A:375:ILE:HD13 | 1.69                     | 0.45              |
| 1:A:672:ILE:HD13  | 1:A:672:ILE:HG21 | 1.74                     | 0.45              |
| 1:A:787:VAL:HG23  | 1:A:824:GLU:C    | 2.42                     | 0.45              |
| 1:A:878:THR:HG1   | 1:A:880:ARG:HE   | 1.64                     | 0.45              |
| 1:A:963:ARG:O     | 1:A:967:ARG:HG3  | 2.16                     | 0.45              |
| 1:A:1128:ILE:HD13 | 1:A:1128:ILE:HA  | 1.80                     | 0.45              |
| 1:A:1158:LEU:HD21 | 1:A:1308:TYR:CD2 | 2.51                     | 0.45              |
| 2:B:81:PRO:HD2    | 2:B:135:GLU:HG3  | 1.97                     | 0.45              |
| 2:B:226:GLU:OE2   | 2:B:617:ASP:CB   | 2.57                     | 0.45              |
| 2:B:1001:PRO:HB2  | 2:B:1002:PHE:CE1 | 2.51                     | 0.45              |
| 8:H:8:ASP:HB3     | 8:H:10:PHE:CE1   | 2.52                     | 0.45              |
| 13:M:92:SER:O     | 13:M:93:PHE:C    | 2.59                     | 0.45              |
| 16:P:263:ASP:OD1  | 16:P:264:VAL:N   | 2.49                     | 0.45              |
| 1:A:43:TYR:O      | 1:A:45:GLU:N     | 2.49                     | 0.45              |
| 1:A:111:CYS:SG    | 1:A:188:GLN:NE2  | 2.90                     | 0.45              |
| 3:C:133:ARG:HA    | 3:C:136:ASP:CG   | 2.23                     | 0.45              |
| 4:D:140:PHE:CZ    | 4:D:142:TYR:HB3  | 2.52                     | 0.45              |
| 5:E:116:GLN:O     | 5:E:119:VAL:HB   | 2.16                     | 0.45              |
| 9:I:41:ASN:HB2    | 19:S:153:ARG:HD2 | 1.99                     | 0.45              |
| 13:M:157:ASP:OD2  | 13:M:185:ARG:NH2 | 2.49                     | 0.45              |
| 16:P:298:PRO:O    | 16:P:300:ILE:N   | 2.49                     | 0.45              |
| 19:S:127:PHE:HB2  | 20:T:19:TRP:HB2  | 1.98                     | 0.45              |
| 1:A:208:ASP:OD1   | 1:A:209:SER:N    | 2.38                     | 0.45              |
| 1:A:392:GLU:OE1   | 1:A:448:ARG:NE   | 2.45                     | 0.45              |
| 4:D:40:LEU:HD13   | 7:G:75:ILE:HD11  | 1.97                     | 0.45              |
| 9:I:25:TYR:HD2    | 9:I:40:ARG:HG3   | 1.82                     | 0.45              |
| 13:M:130:LEU:HA   | 13:M:131:PRO:HD3 | 1.82                     | 0.45              |
| 17:Q:184:ILE:HD11 | 18:R:218:LYS:NZ  | 2.19                     | 0.45              |
| 18:R:171:ILE:HG12 | 18:R:177:ASN:H   | 1.81                     | 0.45              |
| 18:R:205:ASP:O    | 18:R:206:LYS:HE3 | 2.16                     | 0.45              |
| 1:A:201:GLU:HG3   | 1:A:212:LYS:C    | 2.42                     | 0.45              |
| 1:A:873:VAL:HG22  | 1:A:1083:PRO:HA  | 1.99                     | 0.45              |
| 13:M:17:ASN:CG    | 13:M:18:HIS:HD1  | 2.23                     | 0.45              |
| 13:M:70:SER:C     | 13:M:72:ASN:H    | 2.25                     | 0.45              |
| 18:R:123:ALA:O    | 18:R:127:ASN:HB2 | 2.16                     | 0.45              |
| 1:A:375:ILE:HD12  | 1:A:375:ILE:HG23 | 1.54                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:451:CYS:SG    | 1:A:452:ASP:N     | 2.88                     | 0.45              |
| 1:A:524:MET:N     | 1:A:524:MET:SD    | 2.82                     | 0.45              |
| 1:A:865:ILE:HD12  | 2:B:1092:ASP:OD1  | 2.17                     | 0.45              |
| 1:A:1026:ASP:O    | 1:A:1031:ARG:NH2  | 2.49                     | 0.45              |
| 1:A:1119:LEU:HD13 | 1:A:1388:PHE:CG   | 2.52                     | 0.45              |
| 1:A:1130:ILE:HG21 | 1:A:1411:LEU:HD13 | 1.98                     | 0.45              |
| 1:A:1162:GLU:HG2  | 1:A:1306:LYS:CA   | 2.47                     | 0.45              |
| 1:A:1408:ARG:HH22 | 1:A:1421:ARG:HB2  | 1.81                     | 0.45              |
| 1:A:1451:MET:CE   | 1:A:1456:GLU:HB3  | 2.47                     | 0.45              |
| 3:C:85:SER:CB     | 3:C:166:LYS:HE3   | 2.47                     | 0.45              |
| 3:C:149:LEU:HD21  | 3:C:152:LYS:HG3   | 1.98                     | 0.45              |
| 13:M:178:LYS:NZ   | 20:T:156:VAL:HG11 | 2.31                     | 0.45              |
| 17:Q:36:ILE:HG23  | 17:Q:39:ARG:NH2   | 2.32                     | 0.45              |
| 1:A:529:GLN:HG3   | 1:A:1094:SER:HB3  | 1.98                     | 0.45              |
| 1:A:610:PRO:HB3   | 1:A:626:THR:CG2   | 2.47                     | 0.45              |
| 2:B:79:GLU:O      | 2:B:80:GLU:HG2    | 2.17                     | 0.45              |
| 2:B:180:ASP:OD1   | 2:B:181:PRO:HD2   | 2.16                     | 0.45              |
| 2:B:508:MET:HE2   | 2:B:670:GLU:OE1   | 2.16                     | 0.45              |
| 2:B:531:TYR:CD2   | 2:B:532:ILE:N     | 2.85                     | 0.45              |
| 6:F:61:GLU:CD     | 6:F:108:ARG:HH21  | 2.25                     | 0.45              |
| 7:G:116:GLU:O     | 7:G:130:THR:HA    | 2.16                     | 0.45              |
| 9:I:92:LYS:HG3    | 9:I:93:GLU:HG2    | 1.99                     | 0.45              |
| 13:M:52:TRP:CD1   | 13:M:52:TRP:C     | 2.92                     | 0.45              |
| 17:Q:25:PHE:CE1   | 18:R:210:PHE:CZ   | 3.05                     | 0.45              |
| 17:Q:187:ILE:HG21 | 18:R:210:PHE:O    | 2.16                     | 0.45              |
| 1:A:599:HIS:O     | 1:A:992:LYS:NZ    | 2.50                     | 0.45              |
| 1:A:1103:THR:HG23 | 1:A:1106:THR:OG1  | 2.17                     | 0.45              |
| 2:B:91:ILE:HD11   | 2:B:124:LEU:HD11  | 1.98                     | 0.45              |
| 2:B:109:MET:O     | 2:B:112:GLU:N     | 2.50                     | 0.45              |
| 2:B:496:ALA:HB3   | 2:B:498:PRO:HD2   | 1.99                     | 0.45              |
| 2:B:765:GLU:OE1   | 2:B:770:ARG:NE    | 2.49                     | 0.45              |
| 5:E:47:LYS:HA     | 5:E:47:LYS:HD3    | 1.63                     | 0.45              |
| 9:I:104:ALA:C     | 9:I:106:ASP:N     | 2.75                     | 0.45              |
| 11:K:5:PRO:HB2    | 11:K:7:PHE:CE2    | 2.52                     | 0.45              |
| 1:A:205:VAL:O     | 1:A:206:ASN:CB    | 2.66                     | 0.44              |
| 1:A:1429:LYS:HB2  | 1:A:1438:VAL:HG21 | 2.00                     | 0.44              |
| 2:B:74:ALA:HB2    | 20:T:201:ASP:CG   | 2.42                     | 0.44              |
| 2:B:936:ALA:O     | 2:B:1049:GLN:N    | 2.42                     | 0.44              |
| 2:B:1062:ARG:HH21 | 2:B:1065:GLY:N    | 2.10                     | 0.44              |
| 5:E:11:TRP:CE3    | 5:E:37:LEU:HD13   | 2.51                     | 0.44              |
| 10:J:3:ILE:HG22   | 10:J:15:GLY:HA2   | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:M:179:GLU:HA   | 20:T:154:LYS:HZ1  | 1.81                     | 0.44              |
| 17:Q:188:TYR:CE2  | 18:R:211:SER:HB3  | 2.52                     | 0.44              |
| 22:X:48:DT:OP1    | 22:X:48:DT:H4'    | 2.16                     | 0.44              |
| 1:A:932:ARG:NE    | 1:A:943:LEU:HD22  | 2.30                     | 0.44              |
| 1:A:1468:THR:HA   | 6:F:60:TYR:HB3    | 1.98                     | 0.44              |
| 2:B:573:TRP:O     | 2:B:573:TRP:HE3   | 2.00                     | 0.44              |
| 2:B:836:THR:C     | 2:B:886:ARG:HA    | 2.42                     | 0.44              |
| 3:C:275:ASN:ND2   | 11:K:23:LYS:HA    | 2.31                     | 0.44              |
| 5:E:52:ARG:NH2    | 5:E:54:ARG:HH11   | 2.15                     | 0.44              |
| 14:N:25:VAL:HG11  | 15:O:36:VAL:HG13  | 1.97                     | 0.44              |
| 1:A:186:ARG:HH11  | 1:A:208:ASP:HB2   | 1.82                     | 0.44              |
| 1:A:465:HIS:CE1   | 1:A:467:MET:HB2   | 2.52                     | 0.44              |
| 2:B:322:GLY:O     | 2:B:326:ALA:N     | 2.34                     | 0.44              |
| 14:N:376:TRP:HD1  | 15:O:62:LEU:O     | 2.01                     | 0.44              |
| 20:T:194:HIS:N    | 20:T:197:TYR:OH   | 2.50                     | 0.44              |
| 21:U:134:PRO:HG2  | 21:U:174:GLU:HG2  | 1.99                     | 0.44              |
| 2:B:747:LEU:HD11  | 2:B:810:PHE:HZ    | 1.79                     | 0.44              |
| 2:B:899:SER:O     | 2:B:901:THR:N     | 2.51                     | 0.44              |
| 2:B:975:ARG:C     | 2:B:976:MET:HG3   | 2.42                     | 0.44              |
| 7:G:18:PHE:HA     | 7:G:22:LEU:HD13   | 2.00                     | 0.44              |
| 8:H:71:ASP:OD1    | 8:H:71:ASP:N      | 2.48                     | 0.44              |
| 1:A:729:PRO:O     | 21:U:252:LYS:O    | 2.36                     | 0.44              |
| 1:A:893:GLU:O     | 5:E:200:ALA:HB2   | 2.17                     | 0.44              |
| 1:A:931:ARG:C     | 1:A:933:THR:N     | 2.76                     | 0.44              |
| 1:A:1103:THR:HG21 | 1:A:1119:LEU:HG   | 1.99                     | 0.44              |
| 1:A:1112:VAL:HG12 | 21:U:254:GLY:HA2  | 2.00                     | 0.44              |
| 2:B:41:ARG:HD2    | 2:B:41:ARG:HA     | 1.36                     | 0.44              |
| 2:B:271:ILE:HD12  | 2:B:311:ILE:HD11  | 2.00                     | 0.44              |
| 6:F:105:ILE:HG22  | 6:F:119:GLY:HA2   | 2.00                     | 0.44              |
| 13:M:34:CYS:HB2   | 13:M:39:LEU:HB3   | 1.99                     | 0.44              |
| 15:O:7:ARG:HB3    | 15:O:16:GLN:NE2   | 2.32                     | 0.44              |
| 1:A:131:ALA:C     | 1:A:133:SER:H     | 2.26                     | 0.44              |
| 1:A:948:ILE:HG23  | 1:A:1007:ILE:HD11 | 1.99                     | 0.44              |
| 2:B:809:VAL:HG23  | 2:B:924:ARG:HG3   | 1.99                     | 0.44              |
| 2:B:1055:VAL:HG13 | 2:B:1056:ASP:N    | 2.33                     | 0.44              |
| 2:B:1078:ARG:C    | 2:B:1080:ARG:H    | 2.24                     | 0.44              |
| 2:B:1162:LEU:O    | 2:B:1167:ILE:HB   | 2.18                     | 0.44              |
| 13:M:52:TRP:O     | 13:M:54:THR:N     | 2.45                     | 0.44              |
| 17:Q:126:SER:O    | 17:Q:164:ASP:HB2  | 2.18                     | 0.44              |
| 18:R:88:ARG:NH1   | 18:R:97:LEU:HD11  | 2.33                     | 0.44              |
| 1:A:263:ALA:CB    | 1:A:272:ASN:HB3   | 2.46                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1139:LEU:HB3  | 1:A:1338:THR:OG1  | 2.17                     | 0.44              |
| 1:A:1407:CYS:SG   | 1:A:1408:ARG:HG2  | 2.58                     | 0.44              |
| 2:B:289:ILE:HG12  | 2:B:291:ASP:H     | 1.82                     | 0.44              |
| 4:D:70:ARG:NE     | 7:G:142:GLU:OE2   | 2.42                     | 0.44              |
| 8:H:146:LYS:C     | 8:H:148:LEU:H     | 2.21                     | 0.44              |
| 9:I:84:HIS:CD2    | 9:I:84:HIS:N      | 2.81                     | 0.44              |
| 9:I:86:CYS:C      | 9:I:88:LYS:H      | 2.25                     | 0.44              |
| 15:O:80:GLU:HG3   | 15:O:89:LYS:HG2   | 1.98                     | 0.44              |
| 1:A:614:ASP:OD2   | 21:U:267:LYS:HG3  | 2.17                     | 0.44              |
| 2:B:17:ILE:HG23   | 2:B:18:THR:HG23   | 2.00                     | 0.44              |
| 2:B:783:ALA:HB2   | 2:B:1041:ILE:CG2  | 2.48                     | 0.44              |
| 3:C:24:GLU:HG2    | 3:C:228:ARG:CG    | 2.46                     | 0.44              |
| 4:D:26:PHE:CE2    | 7:G:78:ARG:HG2    | 2.53                     | 0.44              |
| 18:R:157:GLN:HG3  | 18:R:159:ASP:H    | 1.82                     | 0.44              |
| 1:A:932:ARG:HB3   | 1:A:940:LYS:HA    | 2.00                     | 0.44              |
| 1:A:987:ILE:HD13  | 1:A:1058:PHE:CD2  | 2.53                     | 0.44              |
| 2:B:758:LEU:HD23  | 2:B:758:LEU:HA    | 1.68                     | 0.44              |
| 3:C:45:ILE:HD11   | 3:C:82:LEU:HD22   | 2.00                     | 0.44              |
| 9:I:103:ARG:C     | 9:I:105:GLU:H     | 2.26                     | 0.44              |
| 10:J:4:PRO:O      | 10:J:14:VAL:HG12  | 2.18                     | 0.44              |
| 13:M:60:ALA:HB1   | 23:Y:54:DA:C2     | 2.51                     | 0.44              |
| 16:P:317:VAL:HG12 | 16:P:319:ALA:H    | 1.83                     | 0.44              |
| 20:T:155:PRO:C    | 20:T:157:ALA:H    | 2.14                     | 0.44              |
| 1:A:231:GLU:OE1   | 1:A:231:GLU:N     | 2.41                     | 0.43              |
| 1:A:415:GLY:O     | 1:A:449:HIS:HD2   | 2.00                     | 0.43              |
| 1:A:514:GLU:OE1   | 2:B:1099:ALA:HB1  | 2.18                     | 0.43              |
| 2:B:461:GLN:H     | 2:B:461:GLN:CD    | 2.26                     | 0.43              |
| 2:B:1068:GLN:HB3  | 13:M:51:GLU:HB3   | 1.99                     | 0.43              |
| 9:I:65:LEU:HA     | 9:I:122:ARG:HE    | 1.83                     | 0.43              |
| 13:M:214:PHE:HB3  | 13:M:218:PHE:HE2  | 1.83                     | 0.43              |
| 16:P:204:ILE:HD12 | 16:P:206:GLU:HB2  | 1.98                     | 0.43              |
| 17:Q:100:VAL:O    | 17:Q:103:VAL:HG23 | 2.18                     | 0.43              |
| 2:B:294:ASP:HA    | 2:B:295:PRO:HD2   | 1.79                     | 0.43              |
| 5:E:3:ASP:O       | 5:E:6:GLU:HB2     | 2.18                     | 0.43              |
| 10:J:46:ARG:HH11  | 10:J:46:ARG:HD3   | 1.59                     | 0.43              |
| 13:M:57:ASN:HA    | 23:Y:51:DC:N4     | 2.33                     | 0.43              |
| 1:A:376:ASP:HB3   | 1:A:521:VAL:HB    | 2.00                     | 0.43              |
| 1:A:522:PRO:HG3   | 1:A:666:ARG:HG3   | 1.99                     | 0.43              |
| 1:A:894:ASP:OD1   | 1:A:894:ASP:C     | 2.62                     | 0.43              |
| 1:A:1371:ILE:HD13 | 1:A:1409:GLY:O    | 2.17                     | 0.43              |
| 2:B:759:VAL:CG1   | 2:B:999:ALA:HB2   | 2.48                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:926:VAL:HG23  | 2:B:926:VAL:O     | 2.17                     | 0.43              |
| 3:C:71:ILE:CG2    | 3:C:148:ILE:HG21  | 2.48                     | 0.43              |
| 4:D:48:ASN:ND2    | 4:D:57:LEU:HG     | 2.24                     | 0.43              |
| 7:G:44:PHE:HE2    | 7:G:104:MET:HB2   | 1.83                     | 0.43              |
| 8:H:96:VAL:HG22   | 8:H:116:VAL:HG13  | 2.00                     | 0.43              |
| 16:P:178:LEU:HB3  | 16:P:183:ILE:HD11 | 2.00                     | 0.43              |
| 21:U:256:THR:O    | 21:U:257:GLN:CB   | 2.59                     | 0.43              |
| 1:A:133:SER:O     | 1:A:136:GLN:N     | 2.37                     | 0.43              |
| 2:B:52:GLN:HB2    | 2:B:160:TYR:OH    | 2.19                     | 0.43              |
| 2:B:967:ILE:HD12  | 2:B:968:ASN:H     | 1.83                     | 0.43              |
| 13:M:94:ASP:CG    | 13:M:97:GLY:O     | 2.49                     | 0.43              |
| 16:P:329:TYR:N    | 16:P:330:PRO:HD2  | 2.33                     | 0.43              |
| 21:U:251:ALA:O    | 21:U:252:LYS:CB   | 2.36                     | 0.43              |
| 1:A:505:LEU:HD23  | 1:A:507:GLN:HE22  | 1.84                     | 0.43              |
| 1:A:1316:ASN:CG   | 1:A:1318:LYS:CE   | 2.91                     | 0.43              |
| 2:B:290:TYR:HE2   | 2:B:562:ALA:HA    | 1.83                     | 0.43              |
| 2:B:952:GLU:CD    | 2:B:952:GLU:H     | 2.26                     | 0.43              |
| 5:E:41:LYS:HG3    | 5:E:46:ASP:CB     | 2.48                     | 0.43              |
| 9:I:50:ASN:OD1    | 9:I:51:SER:N      | 2.51                     | 0.43              |
| 11:K:53:ASP:OD1   | 11:K:54:PRO:HD2   | 2.18                     | 0.43              |
| 14:N:42:LEU:HB2   | 15:O:22:LEU:HD11  | 1.99                     | 0.43              |
| 18:R:148:LYS:HD3  | 18:R:174:ALA:HB2  | 2.00                     | 0.43              |
| 18:R:212:VAL:C    | 18:R:213:ASP:CG   | 2.86                     | 0.43              |
| 1:A:156:GLY:CA    | 1:A:181:HIS:CE1   | 3.02                     | 0.43              |
| 1:A:264:VAL:HB    | 13:M:52:TRP:CE3   | 2.53                     | 0.43              |
| 1:A:866:LYS:HG2   | 1:A:1432:PHE:CD1  | 2.54                     | 0.43              |
| 1:A:1307:VAL:CG1  | 1:A:1339:ASP:H    | 2.32                     | 0.43              |
| 2:B:76:GLY:O      | 2:B:78:VAL:CG2    | 2.66                     | 0.43              |
| 2:B:761:THR:N     | 2:B:764:MET:HE3   | 2.22                     | 0.43              |
| 10:J:66:GLU:HG3   | 12:L:23:HIS:ND1   | 2.34                     | 0.43              |
| 13:M:178:LYS:HG2  | 20:T:156:VAL:CG1  | 2.48                     | 0.43              |
| 13:M:184:SER:OG   | 13:M:185:ARG:N    | 2.52                     | 0.43              |
| 17:Q:137:THR:OG1  | 17:Q:139:LEU:HG   | 2.18                     | 0.43              |
| 2:B:1072:ARG:HD3  | 2:B:1153:TYR:CD2  | 2.53                     | 0.43              |
| 3:C:74:ILE:O      | 3:C:128:ILE:HG13  | 2.19                     | 0.43              |
| 5:E:121:MET:HG2   | 5:E:127:LEU:HD13  | 2.00                     | 0.43              |
| 12:L:26:ASN:O     | 12:L:27:GLU:CB    | 2.62                     | 0.43              |
| 2:B:1124:ILE:HD11 | 2:B:1170:ARG:HD3  | 2.00                     | 0.43              |
| 8:H:10:PHE:CE2    | 8:H:39:LEU:HD13   | 2.54                     | 0.43              |
| 1:A:477:LEU:HD23  | 1:A:477:LEU:HA    | 1.82                     | 0.43              |
| 1:A:505:LEU:HA    | 1:A:506:PRO:HD2   | 1.93                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:540:ASP:CB    | 2:B:790:GLN:NE2  | 2.79                     | 0.43              |
| 1:A:779:ILE:O     | 1:A:783:GLN:HG3  | 2.19                     | 0.43              |
| 1:A:922:PHE:HA    | 1:A:1052:ARG:HD3 | 2.01                     | 0.43              |
| 1:A:924:TYR:CE2   | 1:A:949:GLN:HG2  | 2.54                     | 0.43              |
| 1:A:932:ARG:O     | 1:A:940:LYS:HB3  | 2.18                     | 0.43              |
| 2:B:281:ASP:CG    | 9:I:22:ASN:HD22  | 2.27                     | 0.43              |
| 2:B:598:VAL:O     | 2:B:600:GLU:N    | 2.49                     | 0.43              |
| 3:C:125:PRO:C     | 3:C:127:VAL:H    | 2.27                     | 0.43              |
| 8:H:11:ASP:HB2    | 8:H:55:LYS:HG2   | 2.00                     | 0.43              |
| 14:N:360:LEU:C    | 14:N:362:GLY:N   | 2.75                     | 0.43              |
| 20:T:82:PRO:HD2   | 20:T:117:ARG:O   | 2.19                     | 0.43              |
| 20:T:124:TYR:O    | 20:T:127:LEU:HB3 | 2.19                     | 0.43              |
| 21:U:133:ALA:HA   | 21:U:134:PRO:HD3 | 1.89                     | 0.43              |
| 21:U:139:SER:O    | 21:U:143:LYS:HG2 | 2.19                     | 0.43              |
| 1:A:1162:GLU:HG2  | 1:A:1306:LYS:HA  | 2.01                     | 0.43              |
| 1:A:1218:ARG:HG2  | 21:U:237:ARG:NH2 | 2.34                     | 0.43              |
| 2:B:285:LEU:HD22  | 9:I:16:PHE:HZ    | 1.84                     | 0.43              |
| 3:C:60:HIS:CE1    | 3:C:63:PHE:HB2   | 2.54                     | 0.43              |
| 3:C:212:ASP:C     | 3:C:214:ASP:N    | 2.76                     | 0.43              |
| 8:H:34:SER:O      | 8:H:36:LYS:HG3   | 2.19                     | 0.43              |
| 13:M:178:LYS:HD3  | 20:T:154:LYS:HD3 | 2.01                     | 0.43              |
| 14:N:354:LYS:C    | 14:N:355:ASP:O   | 2.62                     | 0.43              |
| 17:Q:170:LYS:O    | 17:Q:174:ARG:N   | 2.47                     | 0.43              |
| 20:T:59:ASN:OD1   | 20:T:60:GLU:N    | 2.52                     | 0.43              |
| 1:A:326:PRO:HD3   | 13:M:92:SER:OG   | 2.18                     | 0.42              |
| 1:A:370:ASP:HA    | 1:A:371:PRO:HD2  | 1.91                     | 0.42              |
| 1:A:609:HIS:O     | 1:A:610:PRO:O    | 2.36                     | 0.42              |
| 1:A:766:PHE:CD1   | 1:A:781:ILE:HD11 | 2.54                     | 0.42              |
| 1:A:1301:ILE:HG13 | 1:A:1302:GLU:HG2 | 2.01                     | 0.42              |
| 2:B:510:CYS:SG    | 2:B:511:PRO:HD2  | 2.60                     | 0.42              |
| 2:B:613:ARG:HD3   | 2:B:615:TYR:OH   | 2.19                     | 0.42              |
| 2:B:978:ILE:HD12  | 2:B:978:ILE:HG23 | 1.83                     | 0.42              |
| 2:B:1071:ASN:O    | 2:B:1072:ARG:HG2 | 2.19                     | 0.42              |
| 3:C:71:ILE:HG22   | 3:C:148:ILE:HG21 | 2.00                     | 0.42              |
| 16:P:288:PHE:CD1  | 16:P:289:PRO:HD2 | 2.53                     | 0.42              |
| 20:T:229:HIS:HD2  | 22:X:28:DG:H21   | 1.65                     | 0.42              |
| 22:X:33:DT:H2"    | 22:X:34:DT:C5    | 2.54                     | 0.42              |
| 1:A:617:PRO:O     | 1:A:621:ILE:HG12 | 2.18                     | 0.42              |
| 1:A:937:ASP:O     | 1:A:940:LYS:HD2  | 2.19                     | 0.42              |
| 3:C:225:LYS:O     | 3:C:227:GLU:HG2  | 2.19                     | 0.42              |
| 5:E:56:THR:N      | 5:E:78:GLU:OE2   | 2.52                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:H:74:GLU:O     | 8:H:75:TYR:C      | 2.53                     | 0.42              |
| 20:T:93:LEU:HD11 | 20:T:113:ARG:HD2  | 2.01                     | 0.42              |
| 22:X:51:DC:H2'   | 22:X:52:DG:C4     | 2.53                     | 0.42              |
| 1:A:15:LEU:HD12  | 2:B:1148:LEU:O    | 2.19                     | 0.42              |
| 1:A:156:GLY:O    | 1:A:180:GLY:HA2   | 2.19                     | 0.42              |
| 1:A:478:PRO:O    | 1:A:479:TRP:HB2   | 2.19                     | 0.42              |
| 1:A:483:ARG:HH12 | 2:B:788:TYR:HE2   | 1.68                     | 0.42              |
| 1:A:799:PRO:O    | 1:A:806:THR:HG22  | 2.19                     | 0.42              |
| 2:B:1029:TYR:CD1 | 2:B:1036:LYS:HG2  | 2.54                     | 0.42              |
| 1:A:924:TYR:OH   | 1:A:952:LEU:HD12  | 2.19                     | 0.42              |
| 2:B:566:LYS:HD3  | 2:B:573:TRP:NE1   | 2.23                     | 0.42              |
| 3:C:67:ARG:NH1   | 3:C:150:ILE:HA    | 2.35                     | 0.42              |
| 7:G:117:MET:HG2  | 7:G:128:TYR:HB3   | 2.00                     | 0.42              |
| 9:I:29:ASP:OD2   | 9:I:32:ASN:ND2    | 2.37                     | 0.42              |
| 1:A:22:GLN:OE1   | 1:A:1448:SER:OG   | 2.32                     | 0.42              |
| 2:B:79:GLU:O     | 2:B:80:GLU:CG     | 2.67                     | 0.42              |
| 2:B:106:SER:HB2  | 2:B:107:PRO:HD2   | 2.00                     | 0.42              |
| 17:Q:163:GLU:HB3 | 17:Q:164:ASP:H    | 1.62                     | 0.42              |
| 1:A:954:ARG:HD3  | 1:A:954:ARG:HA    | 1.84                     | 0.42              |
| 1:A:1251:ASN:HB3 | 21:U:234:LYS:HE2  | 2.01                     | 0.42              |
| 2:B:187:ILE:HG22 | 2:B:188:ASN:OD1   | 2.20                     | 0.42              |
| 2:B:202:THR:OG1  | 2:B:226:GLU:OE1   | 2.38                     | 0.42              |
| 2:B:235:ILE:CD1  | 2:B:261:PRO:HD3   | 2.50                     | 0.42              |
| 3:C:134:ASN:N    | 3:C:136:ASP:CG    | 2.75                     | 0.42              |
| 9:I:66:THR:O     | 9:I:68:ILE:HG22   | 2.20                     | 0.42              |
| 13:M:263:GLN:HA  | 13:M:268:LYS:HG2  | 2.01                     | 0.42              |
| 18:R:77:VAL:HG21 | 18:R:111:ILE:HD11 | 2.01                     | 0.42              |
| 18:R:113:LEU:HA  | 18:R:116:LYS:HE3  | 2.01                     | 0.42              |
| 21:U:194:ARG:HD3 | 21:U:194:ARG:HA   | 1.61                     | 0.42              |
| 21:U:200:ASP:OD2 | 21:U:203:ASN:N    | 2.52                     | 0.42              |
| 22:X:45:DT:H6    | 22:X:45:DT:H2'    | 1.73                     | 0.42              |
| 23:Y:70:DC:H2''  | 23:Y:71:DA:C8     | 2.54                     | 0.42              |
| 1:A:611:ASP:HB3  | 1:A:612:ASP:H     | 1.31                     | 0.42              |
| 1:A:1319:LYS:HG3 | 1:A:1333:GLU:OE1  | 2.20                     | 0.42              |
| 2:B:629:GLU:O    | 2:B:631:GLN:N     | 2.53                     | 0.42              |
| 2:B:800:ALA:O    | 2:B:805:PHE:HB2   | 2.20                     | 0.42              |
| 2:B:899:SER:C    | 2:B:901:THR:H     | 2.27                     | 0.42              |
| 2:B:1115:GLN:HB2 | 2:B:1148:LEU:HD11 | 2.00                     | 0.42              |
| 3:C:6:GLN:HG2    | 3:C:6:GLN:O       | 2.17                     | 0.42              |
| 3:C:73:LEU:O     | 3:C:238:SER:HB3   | 2.20                     | 0.42              |
| 10:J:35:LEU:HD13 | 10:J:46:ARG:HG2   | 2.00                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:L:17:TYR:HE1   | 12:L:46:LYS:HG3   | 1.84                     | 0.42              |
| 13:M:218:PHE:CD1  | 13:M:277:ILE:HG22 | 2.51                     | 0.42              |
| 13:M:245:VAL:HB   | 13:M:248:ARG:HB2  | 2.01                     | 0.42              |
| 19:S:51:LEU:HG    | 19:S:54:LYS:HB2   | 2.00                     | 0.42              |
| 21:U:268:LYS:NZ   | 21:U:293:GLU:OE1  | 2.35                     | 0.42              |
| 22:X:70:DG:H2''   | 22:X:71:DA:C8     | 2.54                     | 0.42              |
| 1:A:36:VAL:HG11   | 1:A:72:GLN:HE22   | 1.85                     | 0.42              |
| 2:B:155:MET:HB2   | 2:B:185:PHE:CE1   | 2.54                     | 0.42              |
| 2:B:793:SER:CA    | 2:B:944:THR:O     | 2.65                     | 0.42              |
| 8:H:69:THR:HG22   | 8:H:140:ARG:NH1   | 2.35                     | 0.42              |
| 9:I:81:THR:HG22   | 9:I:94:ALA:O      | 2.19                     | 0.42              |
| 13:M:15:CYS:HA    | 13:M:16:PRO:HD3   | 1.75                     | 0.42              |
| 13:M:45:VAL:HG12  | 13:M:47:ASP:H     | 1.84                     | 0.42              |
| 17:Q:184:ILE:HG12 | 18:R:211:SER:HB3  | 2.02                     | 0.42              |
| 20:T:128:LYS:O    | 20:T:132:ILE:N    | 2.44                     | 0.42              |
| 1:A:932:ARG:CG    | 1:A:940:LYS:HA    | 2.49                     | 0.42              |
| 1:A:1376:LYS:HA   | 1:A:1376:LYS:HD2  | 1.80                     | 0.42              |
| 2:B:343:LEU:O     | 2:B:347:MET:HB3   | 2.20                     | 0.42              |
| 3:C:19:VAL:HB     | 3:C:241:PRO:HB2   | 2.02                     | 0.42              |
| 3:C:47:ILE:HD12   | 3:C:47:ILE:N      | 2.34                     | 0.42              |
| 8:H:65:TYR:CD1    | 8:H:65:TYR:N      | 2.88                     | 0.42              |
| 20:T:26:TYR:CE2   | 20:T:127:LEU:HD21 | 2.54                     | 0.42              |
| 21:U:226:GLU:HB3  | 21:U:227:GLU:H    | 1.56                     | 0.42              |
| 23:Y:70:DC:H2''   | 23:Y:71:DA:H8     | 1.85                     | 0.42              |
| 23:Y:79:DT:H6     | 23:Y:79:DT:H2'    | 1.69                     | 0.42              |
| 1:A:244:ARG:HA    | 1:A:245:PRO:HD3   | 1.87                     | 0.42              |
| 1:A:460:ARG:NH2   | 1:A:499:ASP:HB3   | 2.35                     | 0.42              |
| 1:A:779:ILE:O     | 1:A:782:SER:HB2   | 2.20                     | 0.42              |
| 2:B:146:LYS:HB2   | 2:B:146:LYS:HE2   | 1.83                     | 0.42              |
| 2:B:198:GLU:HA    | 2:B:393:LEU:HD23  | 2.02                     | 0.42              |
| 2:B:203:ASN:O     | 2:B:571:GLY:HA3   | 2.20                     | 0.42              |
| 2:B:838:GLN:OE1   | 2:B:886:ARG:NH1   | 2.53                     | 0.42              |
| 2:B:1027:VAL:HG12 | 2:B:1029:TYR:HE1  | 1.84                     | 0.42              |
| 8:H:81:ARG:HA     | 8:H:82:PRO:HD3    | 1.83                     | 0.42              |
| 9:I:75:ASP:HA     | 9:I:76:PRO:HD3    | 1.87                     | 0.42              |
| 17:Q:25:PHE:HA    | 18:R:219:LEU:CD1  | 2.50                     | 0.42              |
| 17:Q:28:ILE:HA    | 17:Q:31:ALA:HB3   | 2.02                     | 0.42              |
| 22:X:61:DA:H2''   | 22:X:62:DG:C8     | 2.54                     | 0.42              |
| 1:A:482:PHE:HE2   | 1:A:501:MET:O     | 2.03                     | 0.41              |
| 1:A:641:CYS:SG    | 1:A:642:LYS:N     | 2.93                     | 0.41              |
| 1:A:672:ILE:HG23  | 1:A:673:GLN:N     | 2.35                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1389:ASP:O    | 21:U:297:ARG:NH2  | 2.53                     | 0.41              |
| 2:B:198:GLU:OE2   | 2:B:391:LYS:HD3   | 2.20                     | 0.41              |
| 2:B:598:VAL:C     | 2:B:600:GLU:N     | 2.78                     | 0.41              |
| 2:B:628:VAL:HG23  | 2:B:632:LYS:C     | 2.45                     | 0.41              |
| 2:B:1008:VAL:HG13 | 2:B:1009:GLN:N    | 2.35                     | 0.41              |
| 6:F:102:ILE:CG2   | 6:F:104:ILE:HG12  | 2.49                     | 0.41              |
| 10:J:6:ARG:HG2    | 10:J:13:ILE:HG22  | 2.02                     | 0.41              |
| 13:M:65:SER:O     | 13:M:67:VAL:N     | 2.53                     | 0.41              |
| 1:A:124:PRO:HA    | 1:A:127:LYS:HE3   | 2.02                     | 0.41              |
| 1:A:455:ILE:HG12  | 1:A:473:ARG:HG2   | 2.02                     | 0.41              |
| 1:A:792:ASN:OD1   | 1:A:792:ASN:N     | 2.53                     | 0.41              |
| 2:B:623:ARG:NH2   | 2:B:675:LEU:HD21  | 2.35                     | 0.41              |
| 2:B:721:ARG:HA    | 2:B:721:ARG:NE    | 2.34                     | 0.41              |
| 3:C:6:GLN:HG3     | 11:K:104:ARG:CZ   | 2.50                     | 0.41              |
| 3:C:157:GLN:HG2   | 10:J:65:LEU:HB3   | 1.95                     | 0.41              |
| 5:E:50:GLU:C      | 5:E:52:ARG:N      | 2.77                     | 0.41              |
| 13:M:10:LEU:H     | 13:M:11:PRO:HD3   | 1.60                     | 0.41              |
| 18:R:166:ILE:HG22 | 18:R:168:LEU:H    | 1.84                     | 0.41              |
| 1:A:261:ARG:HB2   | 1:A:274:ASP:CB    | 2.50                     | 0.41              |
| 1:A:597:PRO:HB2   | 1:A:660:MET:HG3   | 2.01                     | 0.41              |
| 1:A:666:ARG:HD3   | 1:A:666:ARG:HA    | 1.79                     | 0.41              |
| 1:A:999:ARG:CZ    | 8:H:99:ILE:HG21   | 2.49                     | 0.41              |
| 1:A:1191:GLU:HA   | 1:A:1194:ASN:ND2  | 2.35                     | 0.41              |
| 2:B:193:VAL:HG21  | 2:B:482:LEU:HD23  | 2.03                     | 0.41              |
| 2:B:278:PHE:HZ    | 2:B:359:THR:HG22  | 1.86                     | 0.41              |
| 2:B:588:ARG:NH2   | 2:B:663:GLU:OE1   | 2.51                     | 0.41              |
| 2:B:1001:PRO:HB2  | 2:B:1002:PHE:CD1  | 2.56                     | 0.41              |
| 16:P:206:GLU:O    | 16:P:208:ARG:N    | 2.53                     | 0.41              |
| 20:T:229:HIS:CD2  | 23:Y:67:DC:H1'    | 2.55                     | 0.41              |
| 1:A:199:TYR:CE2   | 13:M:93:PHE:CZ    | 3.02                     | 0.41              |
| 1:A:570:TRP:CZ3   | 1:A:572:GLY:HA2   | 2.56                     | 0.41              |
| 1:A:890:ARG:HD3   | 1:A:890:ARG:HA    | 1.87                     | 0.41              |
| 1:A:932:ARG:HD3   | 1:A:932:ARG:HA    | 1.38                     | 0.41              |
| 1:A:1113:SER:HB3  | 1:A:1114:ALA:H    | 1.69                     | 0.41              |
| 1:A:1116:ASN:C    | 1:A:1117:VAL:HG23 | 2.42                     | 0.41              |
| 2:B:33:TYR:CE1    | 2:B:37:LYS:HG3    | 2.55                     | 0.41              |
| 2:B:1029:TYR:CD1  | 2:B:1029:TYR:N    | 2.85                     | 0.41              |
| 2:B:1142:ASN:ND2  | 2:B:1145:GLN:HG2  | 2.36                     | 0.41              |
| 13:M:10:LEU:C     | 13:M:12:ARG:N     | 2.76                     | 0.41              |
| 20:T:143:GLN:OE1  | 20:T:143:GLN:N    | 2.53                     | 0.41              |
| 21:U:260:LEU:HB3  | 21:U:261:PHE:H    | 1.61                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:209:SER:O     | 1:A:210:GLN:HG2   | 2.21                     | 0.41              |
| 1:A:244:ARG:HG3   | 1:A:246:GLU:CD    | 2.45                     | 0.41              |
| 1:A:612:ASP:O     | 1:A:613:GLU:O     | 2.38                     | 0.41              |
| 2:B:1060:HIS:CD2  | 2:B:1078:ARG:HD2  | 2.56                     | 0.41              |
| 7:G:108:ILE:HG21  | 7:G:163:LEU:HG    | 2.02                     | 0.41              |
| 8:H:92:MET:CE     | 8:H:143:LEU:HD23  | 2.51                     | 0.41              |
| 9:I:29:ASP:CG     | 9:I:32:ASN:HD22   | 2.27                     | 0.41              |
| 9:I:86:CYS:C      | 9:I:88:LYS:N      | 2.78                     | 0.41              |
| 14:N:347:ASN:HB3  | 16:P:208:ARG:HH11 | 1.84                     | 0.41              |
| 20:T:140:ARG:HH11 | 20:T:140:ARG:CG   | 2.32                     | 0.41              |
| 22:X:43:DT:H2'    | 22:X:44:DT:C6     | 2.55                     | 0.41              |
| 1:A:818:GLU:HG2   | 1:A:819:SER:N     | 2.36                     | 0.41              |
| 1:A:865:ILE:HD12  | 2:B:1092:ASP:CG   | 2.45                     | 0.41              |
| 1:A:1175:ILE:HG23 | 1:A:1285:LEU:HD23 | 2.01                     | 0.41              |
| 2:B:35:ASP:OD2    | 2:B:646:ARG:NH2   | 2.50                     | 0.41              |
| 2:B:192:LYS:HE2   | 2:B:449:ALA:O     | 2.20                     | 0.41              |
| 2:B:230:ARG:HB2   | 2:B:405:ARG:CZ    | 2.50                     | 0.41              |
| 2:B:520:VAL:O     | 2:B:520:VAL:HG13  | 2.20                     | 0.41              |
| 9:I:65:LEU:HD22   | 9:I:122:ARG:O     | 2.21                     | 0.41              |
| 9:I:65:LEU:CB     | 9:I:122:ARG:HE    | 2.33                     | 0.41              |
| 15:O:66:ARG:N     | 15:O:73:THR:O     | 2.54                     | 0.41              |
| 18:R:88:ARG:HH21  | 18:R:95:HIS:HB3   | 1.85                     | 0.41              |
| 19:S:111:LYS:O    | 19:S:146:PHE:HA   | 2.20                     | 0.41              |
| 22:X:11:DT:H6     | 22:X:11:DT:H2'    | 1.71                     | 0.41              |
| 1:A:630:VAL:HG12  | 1:A:635:LEU:CD1   | 2.51                     | 0.41              |
| 1:A:926:ASN:HA    | 1:A:931:ARG:CG    | 2.48                     | 0.41              |
| 1:A:1411:LEU:HD23 | 1:A:1411:LEU:HA   | 1.92                     | 0.41              |
| 2:B:78:VAL:HB     | 2:B:79:GLU:H      | 1.62                     | 0.41              |
| 3:C:242:GLU:OE1   | 3:C:242:GLU:N     | 2.54                     | 0.41              |
| 5:E:45:GLY:O      | 5:E:48:PRO:HD3    | 2.21                     | 0.41              |
| 14:N:360:LEU:HD21 | 15:O:81:PHE:HE2   | 1.84                     | 0.41              |
| 20:T:166:GLU:HA   | 20:T:169:LYS:CE   | 2.50                     | 0.41              |
| 22:X:20:DG:N2     | 23:Y:75:DC:O2     | 2.54                     | 0.41              |
| 1:A:261:ARG:C     | 1:A:263:ALA:N     | 2.78                     | 0.41              |
| 1:A:413:TYR:C     | 1:A:415:GLY:H     | 2.28                     | 0.41              |
| 1:A:413:TYR:OH    | 1:A:451:CYS:HA    | 2.21                     | 0.41              |
| 1:A:522:PRO:O     | 1:A:525:ILE:HG13  | 2.21                     | 0.41              |
| 2:B:25:ALA:HA     | 2:B:28:ILE:HD12   | 2.01                     | 0.41              |
| 2:B:51:ILE:HB     | 2:B:160:TYR:CE2   | 2.56                     | 0.41              |
| 2:B:470:LEU:HD23  | 2:B:472:ARG:HH11  | 1.85                     | 0.41              |
| 2:B:759:VAL:HG13  | 2:B:999:ALA:HB2   | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:783:ALA:HB2   | 2:B:1041:ILE:HG21 | 2.01                     | 0.41              |
| 2:B:928:ILE:HG21  | 2:B:928:ILE:HD13  | 1.83                     | 0.41              |
| 7:G:14:HIS:HA     | 7:G:15:PRO:HD3    | 1.93                     | 0.41              |
| 8:H:1:MET:HE1     | 8:H:85:ALA:HB2    | 2.02                     | 0.41              |
| 13:M:45:VAL:C     | 13:M:47:ASP:N     | 2.77                     | 0.41              |
| 17:Q:30:HIS:O     | 17:Q:34:LEU:HB2   | 2.20                     | 0.41              |
| 18:R:181:ALA:O    | 18:R:185:LEU:N    | 2.52                     | 0.41              |
| 1:A:530:SER:O     | 1:A:532:ARG:N     | 2.54                     | 0.41              |
| 1:A:626:THR:OG1   | 1:A:627:LYS:N     | 2.54                     | 0.41              |
| 1:A:660:MET:HE3   | 1:A:664:ILE:HD13  | 2.03                     | 0.41              |
| 1:A:880:ARG:HH11  | 1:A:880:ARG:HD3   | 1.76                     | 0.41              |
| 1:A:1029:LEU:H    | 5:E:162:ARG:HH12  | 1.66                     | 0.41              |
| 2:B:115:LEU:HA    | 2:B:115:LEU:HD23  | 1.93                     | 0.41              |
| 2:B:175:ASN:HD21  | 10:J:64:PRO:HG2   | 1.86                     | 0.41              |
| 2:B:197:GLN:NE2   | 2:B:466:VAL:HG22  | 2.36                     | 0.41              |
| 2:B:778:SER:O     | 2:B:1045:PRO:HA   | 2.21                     | 0.41              |
| 2:B:1022:LEU:HD11 | 2:B:1023:ARG:CZ   | 2.51                     | 0.41              |
| 3:C:59:LEU:HA     | 3:C:59:LEU:HD12   | 1.73                     | 0.41              |
| 8:H:34:SER:HB3    | 8:H:36:LYS:NZ     | 2.36                     | 0.41              |
| 8:H:84:ARG:HB3    | 8:H:86:ASP:HB2    | 2.03                     | 0.41              |
| 9:I:58:ILE:C      | 9:I:60:HIS:N      | 2.79                     | 0.41              |
| 12:L:35:ARG:HH12  | 12:L:42:ARG:CZ    | 2.34                     | 0.41              |
| 13:M:195:PHE:CZ   | 13:M:199:LEU:HD11 | 2.56                     | 0.41              |
| 19:S:15:VAL:HG22  | 20:T:42:LYS:HE2   | 2.03                     | 0.41              |
| 20:T:8:ASP:CG     | 20:T:10:THR:HG1   | 2.25                     | 0.41              |
| 20:T:175:ARG:HB3  | 20:T:208:GLN:HA   | 2.02                     | 0.41              |
| 23:Y:50:DA:H2''   | 23:Y:51:DC:O5'    | 2.20                     | 0.41              |
| 1:A:408:ARG:HG2   | 1:A:412:GLN:OE1   | 2.22                     | 0.41              |
| 1:A:522:PRO:CG    | 1:A:666:ARG:HG3   | 2.50                     | 0.41              |
| 1:A:728:THR:HG23  | 1:A:736:THR:HG23  | 2.02                     | 0.41              |
| 1:A:790:GLN:HA    | 1:A:822:PHE:HA    | 2.03                     | 0.41              |
| 1:A:893:GLU:HG2   | 5:E:203:TYR:CE1   | 2.56                     | 0.41              |
| 1:A:1194:ASN:O    | 1:A:1197:TYR:HD2  | 2.04                     | 0.41              |
| 2:B:254:GLN:HG3   | 2:B:303:PRO:CG    | 2.50                     | 0.41              |
| 2:B:363:TYR:CG    | 2:B:553:LEU:HD21  | 2.56                     | 0.41              |
| 2:B:699:HIS:CE1   | 2:B:701:SER:OG    | 2.74                     | 0.41              |
| 2:B:749:HIS:HD2   | 2:B:810:PHE:HD1   | 1.66                     | 0.41              |
| 2:B:906:GLN:HB3   | 12:L:45:TYR:CE1   | 2.54                     | 0.41              |
| 4:D:75:LYS:HE2    | 4:D:141:GLN:HB3   | 2.03                     | 0.41              |
| 5:E:160:LEU:HD11  | 5:E:167:GLU:HG2   | 2.03                     | 0.41              |
| 8:H:13:LYS:HE2    | 8:H:31:GLU:HB2    | 2.02                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:H:81:ARG:C     | 8:H:83:SER:H      | 2.28                     | 0.41              |
| 8:H:139:SER:HB3  | 8:H:140:ARG:H     | 1.60                     | 0.41              |
| 15:O:80:GLU:OE2  | 15:O:82:ARG:NE    | 2.44                     | 0.41              |
| 16:P:246:PHE:HA  | 16:P:247:PRO:HD3  | 1.95                     | 0.41              |
| 17:Q:28:ILE:HD12 | 18:R:192:VAL:HG12 | 2.03                     | 0.41              |
| 17:Q:45:GLU:OE2  | 17:Q:56:ARG:NH1   | 2.52                     | 0.41              |
| 17:Q:138:ASP:OD1 | 17:Q:138:ASP:N    | 2.54                     | 0.41              |
| 18:R:129:LYS:HE2 | 18:R:140:LYS:O    | 2.21                     | 0.41              |
| 23:Y:57:DA:H5''  | 23:Y:58:DC:H2'    | 2.02                     | 0.41              |
| 1:A:286:ILE:HG13 | 1:A:287:ASN:N     | 2.36                     | 0.40              |
| 1:A:464:LEU:HA   | 1:A:464:LEU:HD23  | 1.87                     | 0.40              |
| 1:A:931:ARG:HD3  | 1:A:931:ARG:HA    | 1.43                     | 0.40              |
| 2:B:121:SER:HB2  | 2:B:152:ILE:O     | 2.21                     | 0.40              |
| 2:B:430:ASN:CG   | 2:B:433:LEU:HG    | 2.45                     | 0.40              |
| 2:B:544:PHE:HD1  | 2:B:544:PHE:HA    | 1.78                     | 0.40              |
| 2:B:602:SER:OG   | 2:B:620:ARG:NH1   | 2.54                     | 0.40              |
| 2:B:1022:LEU:CD1 | 2:B:1023:ARG:HG3  | 2.50                     | 0.40              |
| 7:G:99:THR:HG21  | 7:G:143:ILE:HD11  | 2.03                     | 0.40              |
| 12:L:27:GLU:O    | 12:L:28:ILE:C     | 2.60                     | 0.40              |
| 13:M:57:ASN:OD1  | 13:M:57:ASN:N     | 2.54                     | 0.40              |
| 13:M:107:MET:HG3 | 13:M:108:SER:H    | 1.87                     | 0.40              |
| 14:N:337:CYS:HB2 | 14:N:355:ASP:O    | 2.22                     | 0.40              |
| 16:P:283:TYR:CZ  | 16:P:285:PRO:HB3  | 2.56                     | 0.40              |
| 1:A:375:ILE:HG13 | 1:A:666:ARG:NH1   | 2.36                     | 0.40              |
| 1:A:607:SER:HB2  | 1:A:643:LYS:CD    | 2.52                     | 0.40              |
| 2:B:51:ILE:HA    | 2:B:51:ILE:HD13   | 1.75                     | 0.40              |
| 2:B:347:MET:CE   | 2:B:365:LEU:HD13  | 2.51                     | 0.40              |
| 2:B:797:ASN:OD1  | 2:B:797:ASN:C     | 2.62                     | 0.40              |
| 2:B:958:CYS:C    | 2:B:960:GLY:N     | 2.78                     | 0.40              |
| 2:B:966:ILE:HG21 | 2:B:966:ILE:HD13  | 1.83                     | 0.40              |
| 3:C:38:PHE:HE1   | 3:C:245:VAL:HA    | 1.86                     | 0.40              |
| 16:P:199:ALA:HB2 | 16:P:214:PHE:CE1  | 2.56                     | 0.40              |
| 22:X:24:DG:H2'   | 22:X:25:DG:C8     | 2.56                     | 0.40              |
| 1:A:540:ASP:HB2  | 2:B:790:GLN:NE2   | 2.33                     | 0.40              |
| 1:A:689:ILE:HD11 | 2:B:982:ILE:HD13  | 2.03                     | 0.40              |
| 1:A:1350:LYS:HE2 | 5:E:8:TYR:CG      | 2.57                     | 0.40              |
| 13:M:12:ARG:O    | 13:M:12:ARG:CG    | 2.69                     | 0.40              |
| 16:P:162:VAL:HA  | 16:P:163:PRO:HD2  | 1.79                     | 0.40              |
| 18:R:205:ASP:O   | 18:R:206:LYS:CE   | 2.69                     | 0.40              |
| 1:A:388:MET:HE2  | 1:A:388:MET:HB3   | 1.82                     | 0.40              |
| 1:A:642:LYS:O    | 1:A:646:GLY:N     | 2.49                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:837:PHE:HB2   | 2:B:506:TRP:CZ3   | 2.56                     | 0.40              |
| 1:A:1320:ILE:HD11 | 1:A:1328:PHE:HB3  | 2.03                     | 0.40              |
| 3:C:189:ASP:N     | 3:C:189:ASP:OD1   | 2.53                     | 0.40              |
| 3:C:267:ILE:HG13  | 3:C:272:LEU:CB    | 2.51                     | 0.40              |
| 7:G:144:ARG:HE    | 7:G:171:VAL:HG11  | 1.86                     | 0.40              |
| 10:J:5:VAL:O      | 10:J:6:ARG:HB2    | 2.22                     | 0.40              |
| 16:P:203:ARG:NH2  | 23:Y:79:DT:OP1    | 2.45                     | 0.40              |
| 18:R:97:LEU:C     | 18:R:136:LYS:HD2  | 2.46                     | 0.40              |
| 1:A:780:ASN:ND2   | 2:B:976:MET:SD    | 2.94                     | 0.40              |
| 1:A:1295:ASP:O    | 1:A:1297:THR:HG23 | 2.21                     | 0.40              |
| 2:B:232:THR:OG1   | 2:B:233:SER:N     | 2.38                     | 0.40              |
| 2:B:269:ILE:HD13  | 2:B:269:ILE:HA    | 1.82                     | 0.40              |
| 2:B:552:ASN:O     | 2:B:555:GLU:HG2   | 2.20                     | 0.40              |
| 2:B:1043:ILE:HD13 | 2:B:1043:ILE:HG21 | 1.86                     | 0.40              |
| 3:C:25:ASN:HA     | 3:C:227:GLU:OE1   | 2.21                     | 0.40              |
| 9:I:12:VAL:HG11   | 9:I:15:ARG:HH21   | 1.85                     | 0.40              |
| 9:I:99:SER:OG     | 9:I:100:HIS:N     | 2.52                     | 0.40              |
| 17:Q:128:LYS:HE3  | 17:Q:133:SER:HA   | 2.03                     | 0.40              |
| 19:S:112:GLY:HA2  | 19:S:145:ASN:O    | 2.21                     | 0.40              |
| 20:T:177:ARG:H    | 20:T:178:ALA:C    | 2.25                     | 0.40              |
| 22:X:24:DG:H2''   | 22:X:25:DG:H5'    | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 1   | A     | 1450/1970 (74%) | 1270 (88%) | 118 (8%)  | 62 (4%)  | 2           | 20  |
| 2   | B     | 1163/1174 (99%) | 1001 (86%) | 110 (10%) | 52 (4%)  | 2           | 19  |
| 3   | C     | 273/275 (99%)   | 242 (89%)  | 24 (9%)   | 7 (3%)   | 4           | 28  |
| 4   | D     | 127/142 (89%)   | 120 (94%)  | 7 (6%)    | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 5   | E     | 208/210 (99%)   | 191 (92%)  | 8 (4%)   | 9 (4%)   | 2           | 20  |
| 6   | F     | 84/127 (66%)    | 80 (95%)   | 4 (5%)   | 0        | 100         | 100 |
| 7   | G     | 169/172 (98%)   | 161 (95%)  | 8 (5%)   | 0        | 100         | 100 |
| 8   | H     | 148/150 (99%)   | 117 (79%)  | 14 (10%) | 17 (12%) | 0           | 5   |
| 9   | I     | 123/125 (98%)   | 90 (73%)   | 22 (18%) | 11 (9%)  | 0           | 10  |
| 10  | J     | 65/67 (97%)     | 56 (86%)   | 5 (8%)   | 4 (6%)   | 1           | 15  |
| 11  | K     | 115/117 (98%)   | 106 (92%)  | 8 (7%)   | 1 (1%)   | 14          | 47  |
| 12  | L     | 44/58 (76%)     | 32 (73%)   | 9 (20%)  | 3 (7%)   | 1           | 14  |
| 13  | M     | 308/316 (98%)   | 262 (85%)  | 28 (9%)  | 18 (6%)  | 1           | 16  |
| 14  | N     | 109/376 (29%)   | 95 (87%)   | 11 (10%) | 3 (3%)   | 4           | 27  |
| 15  | O     | 97/109 (89%)    | 96 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 16  | P     | 183/339 (54%)   | 170 (93%)  | 7 (4%)   | 6 (3%)   | 3           | 24  |
| 17  | Q     | 176/439 (40%)   | 160 (91%)  | 8 (4%)   | 8 (4%)   | 2           | 19  |
| 18  | R     | 163/291 (56%)   | 142 (87%)  | 15 (9%)  | 6 (4%)   | 2           | 22  |
| 19  | S     | 134/517 (26%)   | 119 (89%)  | 11 (8%)  | 4 (3%)   | 3           | 26  |
| 20  | T     | 218/249 (88%)   | 190 (87%)  | 16 (7%)  | 12 (6%)  | 1           | 17  |
| 21  | U     | 168/301 (56%)   | 142 (84%)  | 18 (11%) | 8 (5%)   | 2           | 18  |
| All | All   | 5525/7524 (73%) | 4842 (88%) | 452 (8%) | 231 (4%) | 3           | 20  |

All (231) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 51  | ARG  |
| 1   | A     | 70  | ARG  |
| 1   | A     | 133 | SER  |
| 1   | A     | 205 | VAL  |
| 1   | A     | 208 | ASP  |
| 1   | A     | 264 | VAL  |
| 1   | A     | 265 | VAL  |
| 1   | A     | 272 | ASN  |
| 1   | A     | 531 | ASN  |
| 1   | A     | 607 | SER  |
| 1   | A     | 610 | PRO  |
| 1   | A     | 622 | SER  |
| 1   | A     | 623 | PRO  |
| 1   | A     | 931 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 932  | ARG  |
| 1   | A     | 1087 | VAL  |
| 1   | A     | 1117 | VAL  |
| 1   | A     | 1200 | PRO  |
| 1   | A     | 1304 | ILE  |
| 1   | A     | 1308 | TYR  |
| 2   | B     | 74   | ALA  |
| 2   | B     | 78   | VAL  |
| 2   | B     | 225  | LEU  |
| 2   | B     | 226  | GLU  |
| 2   | B     | 231  | PRO  |
| 2   | B     | 249  | LYS  |
| 2   | B     | 251  | ALA  |
| 2   | B     | 452  | ASN  |
| 2   | B     | 460  | HIS  |
| 2   | B     | 491  | ARG  |
| 2   | B     | 513  | GLU  |
| 2   | B     | 526  | LEU  |
| 2   | B     | 879  | GLU  |
| 2   | B     | 898  | THR  |
| 2   | B     | 1108 | PHE  |
| 3   | C     | 6    | GLN  |
| 3   | C     | 7    | PRO  |
| 5   | E     | 46   | ASP  |
| 5   | E     | 47   | LYS  |
| 5   | E     | 50   | GLU  |
| 5   | E     | 64   | HIS  |
| 5   | E     | 65   | ASN  |
| 5   | E     | 68   | PRO  |
| 8   | H     | 18   | GLU  |
| 8   | H     | 67   | ASP  |
| 8   | H     | 75   | TYR  |
| 9   | I     | 85   | PRO  |
| 9   | I     | 99   | SER  |
| 9   | I     | 103  | ARG  |
| 10  | J     | 2    | ILE  |
| 11  | K     | 112  | LYS  |
| 12  | L     | 17   | TYR  |
| 13  | M     | 11   | PRO  |
| 13  | M     | 90   | ALA  |
| 13  | M     | 92   | SER  |
| 13  | M     | 93   | PHE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 13  | M     | 94   | ASP  |
| 13  | M     | 95   | GLU  |
| 14  | N     | 355  | ASP  |
| 16  | P     | 206  | GLU  |
| 16  | P     | 297  | LYS  |
| 16  | P     | 299  | ARG  |
| 17  | Q     | 126  | SER  |
| 18  | R     | 163  | LEU  |
| 18  | R     | 195  | PRO  |
| 18  | R     | 206  | LYS  |
| 18  | R     | 223  | VAL  |
| 18  | R     | 226  | ASP  |
| 18  | R     | 228  | MET  |
| 19  | S     | 160  | ALA  |
| 20  | T     | 124  | TYR  |
| 20  | T     | 151  | THR  |
| 20  | T     | 153  | TYR  |
| 20  | T     | 156  | VAL  |
| 20  | T     | 180  | LYS  |
| 21  | U     | 228  | MET  |
| 21  | U     | 285  | MET  |
| 21  | U     | 300  | PHE  |
| 1   | A     | 48   | GLU  |
| 1   | A     | 66   | GLU  |
| 1   | A     | 204  | HIS  |
| 1   | A     | 263  | ALA  |
| 1   | A     | 613  | GLU  |
| 1   | A     | 624  | GLY  |
| 1   | A     | 625  | ASP  |
| 1   | A     | 912  | SER  |
| 1   | A     | 926  | ASN  |
| 1   | A     | 928  | ARG  |
| 1   | A     | 935  | GLN  |
| 1   | A     | 1307 | VAL  |
| 1   | A     | 1409 | GLY  |
| 2   | B     | 76   | GLY  |
| 2   | B     | 456  | GLN  |
| 2   | B     | 599  | SER  |
| 2   | B     | 705  | GLY  |
| 2   | B     | 873  | LEU  |
| 2   | B     | 881  | GLU  |
| 2   | B     | 899  | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 1145 | GLN  |
| 3   | C     | 143  | VAL  |
| 3   | C     | 211  | LEU  |
| 3   | C     | 272  | LEU  |
| 5   | E     | 124  | LYS  |
| 8   | H     | 35   | PHE  |
| 8   | H     | 73   | GLY  |
| 8   | H     | 109  | ALA  |
| 8   | H     | 111  | ARG  |
| 8   | H     | 139  | SER  |
| 9   | I     | 62   | VAL  |
| 9   | I     | 105  | GLU  |
| 10  | J     | 41   | LYS  |
| 12  | L     | 16   | ILE  |
| 13  | M     | 10   | LEU  |
| 13  | M     | 47   | ASP  |
| 13  | M     | 48   | VAL  |
| 13  | M     | 53   | ARG  |
| 13  | M     | 66   | ARG  |
| 13  | M     | 91   | ALA  |
| 13  | M     | 110  | SER  |
| 14  | N     | 320  | VAL  |
| 16  | P     | 157  | GLU  |
| 16  | P     | 208  | ARG  |
| 17  | Q     | 125  | ALA  |
| 17  | Q     | 158  | HIS  |
| 20  | T     | 169  | LYS  |
| 20  | T     | 178  | ALA  |
| 21  | U     | 225  | ALA  |
| 21  | U     | 252  | LYS  |
| 21  | U     | 256  | THR  |
| 1   | A     | 49   | GLY  |
| 1   | A     | 54   | LEU  |
| 1   | A     | 134  | LYS  |
| 1   | A     | 156  | GLY  |
| 1   | A     | 195  | GLY  |
| 1   | A     | 614  | ASP  |
| 1   | A     | 724  | GLU  |
| 1   | A     | 1085 | GLU  |
| 1   | A     | 1265 | ASP  |
| 1   | A     | 1274 | GLU  |
| 1   | A     | 1299 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1316 | ASN  |
| 2   | B     | 63   | PRO  |
| 2   | B     | 242  | ARG  |
| 2   | B     | 250  | SER  |
| 2   | B     | 548  | TRP  |
| 2   | B     | 630  | LYS  |
| 2   | B     | 691  | SER  |
| 2   | B     | 839  | GLY  |
| 2   | B     | 892  | CYS  |
| 2   | B     | 1136 | GLU  |
| 8   | H     | 21   | LYS  |
| 8   | H     | 66   | GLU  |
| 8   | H     | 70   | LEU  |
| 8   | H     | 138  | ASP  |
| 8   | H     | 140  | ARG  |
| 8   | H     | 148  | LEU  |
| 9   | I     | 106  | ASP  |
| 9   | I     | 118  | HIS  |
| 13  | M     | 12   | ARG  |
| 13  | M     | 14   | THR  |
| 13  | M     | 101  | TYR  |
| 14  | N     | 325  | GLY  |
| 17  | Q     | 40   | ASN  |
| 17  | Q     | 164  | ASP  |
| 17  | Q     | 165  | GLU  |
| 19  | S     | 156  | THR  |
| 20  | T     | 141  | LEU  |
| 21  | U     | 251  | ALA  |
| 1   | A     | 44   | PRO  |
| 1   | A     | 62   | GLN  |
| 1   | A     | 75   | ALA  |
| 1   | A     | 132  | LYS  |
| 1   | A     | 184  | CYS  |
| 1   | A     | 726  | GLU  |
| 1   | A     | 894  | ASP  |
| 1   | A     | 1103 | THR  |
| 2   | B     | 427  | LYS  |
| 2   | B     | 527  | ALA  |
| 2   | B     | 823  | PHE  |
| 3   | C     | 217  | GLN  |
| 5   | E     | 27   | LEU  |
| 8   | H     | 22   | PHE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | H     | 149  | ALA  |
| 9   | I     | 104  | ALA  |
| 12  | L     | 45   | TYR  |
| 13  | M     | 56   | SER  |
| 13  | M     | 71   | GLN  |
| 17  | Q     | 25   | PHE  |
| 17  | Q     | 100  | VAL  |
| 19  | S     | 154  | THR  |
| 20  | T     | 154  | LYS  |
| 1   | A     | 56   | GLY  |
| 1   | A     | 210  | GLN  |
| 1   | A     | 1271 | GLU  |
| 2   | B     | 232  | THR  |
| 2   | B     | 511  | PRO  |
| 2   | B     | 631  | GLN  |
| 2   | B     | 803  | ARG  |
| 2   | B     | 875  | GLU  |
| 2   | B     | 876  | ASN  |
| 2   | B     | 886  | ARG  |
| 2   | B     | 900  | GLU  |
| 9   | I     | 67   | GLN  |
| 10  | J     | 5    | VAL  |
| 16  | P     | 162  | VAL  |
| 20  | T     | 148  | VAL  |
| 21  | U     | 257  | GLN  |
| 1   | A     | 299  | ALA  |
| 1   | A     | 1414 | ILE  |
| 2   | B     | 61   | ASP  |
| 2   | B     | 685  | LYS  |
| 2   | B     | 884  | ASN  |
| 2   | B     | 1069 | ILE  |
| 9   | I     | 58   | ILE  |
| 10  | J     | 6    | ARG  |
| 19  | S     | 121  | ASN  |
| 20  | T     | 171  | GLU  |
| 1   | A     | 1275 | VAL  |
| 9   | I     | 117  | PRO  |
| 2   | B     | 136  | GLY  |
| 2   | B     | 330  | VAL  |
| 2   | B     | 561  | ILE  |
| 1   | A     | 1312 | PRO  |
| 2   | B     | 253  | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | E     | 48  | PRO  |
| 8   | H     | 82  | PRO  |
| 2   | B     | 931 | ILE  |
| 3   | C     | 151 | VAL  |
| 20  | T     | 38  | GLY  |
| 1   | A     | 55  | GLY  |
| 1   | A     | 371 | PRO  |

### 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 PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 1   | A     | 1279/1748 (73%) | 1222 (96%) | 57 (4%)  | 24          | 49  |
| 2   | B     | 1020/1028 (99%) | 978 (96%)  | 42 (4%)  | 27          | 51  |
| 3   | C     | 252/252 (100%)  | 244 (97%)  | 8 (3%)   | 34          | 56  |
| 4   | D     | 119/126 (94%)   | 119 (100%) | 0        | 100         | 100 |
| 5   | E     | 192/192 (100%)  | 186 (97%)  | 6 (3%)   | 35          | 57  |
| 6   | F     | 74/111 (67%)    | 72 (97%)   | 2 (3%)   | 39          | 60  |
| 7   | G     | 152/153 (99%)   | 151 (99%)  | 1 (1%)   | 76          | 78  |
| 8   | H     | 131/131 (100%)  | 125 (95%)  | 6 (5%)   | 24          | 48  |
| 9   | I     | 112/112 (100%)  | 108 (96%)  | 4 (4%)   | 31          | 54  |
| 10  | J     | 56/56 (100%)    | 49 (88%)   | 7 (12%)  | 4           | 20  |
| 11  | K     | 106/106 (100%)  | 103 (97%)  | 3 (3%)   | 38          | 59  |
| 12  | L     | 43/55 (78%)     | 41 (95%)   | 2 (5%)   | 23          | 48  |
| 13  | M     | 263/268 (98%)   | 253 (96%)  | 10 (4%)  | 29          | 52  |
| 14  | N     | 105/324 (32%)   | 103 (98%)  | 2 (2%)   | 50          | 66  |
| 15  | O     | 90/98 (92%)     | 89 (99%)   | 1 (1%)   | 65          | 74  |
| 16  | P     | 159/293 (54%)   | 156 (98%)  | 3 (2%)   | 50          | 66  |
| 17  | Q     | 164/373 (44%)   | 153 (93%)  | 11 (7%)  | 15          | 41  |
| 18  | R     | 150/261 (58%)   | 144 (96%)  | 6 (4%)   | 28          | 51  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 19  | S     | 121/448 (27%)   | 118 (98%)  | 3 (2%)   | 42          | 62 |
| 20  | T     | 196/218 (90%)   | 191 (97%)  | 5 (3%)   | 40          | 60 |
| 21  | U     | 148/266 (56%)   | 138 (93%)  | 10 (7%)  | 14          | 41 |
| All | All   | 4932/6619 (74%) | 4743 (96%) | 189 (4%) | 30          | 52 |

All (189) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 48  | GLU  |
| 1   | A     | 117 | LEU  |
| 1   | A     | 132 | LYS  |
| 1   | A     | 146 | ASP  |
| 1   | A     | 181 | HIS  |
| 1   | A     | 203 | LYS  |
| 1   | A     | 204 | HIS  |
| 1   | A     | 205 | VAL  |
| 1   | A     | 211 | GLU  |
| 1   | A     | 212 | LYS  |
| 1   | A     | 227 | ARG  |
| 1   | A     | 271 | ARG  |
| 1   | A     | 272 | ASN  |
| 1   | A     | 436 | SER  |
| 1   | A     | 463 | THR  |
| 1   | A     | 484 | LEU  |
| 1   | A     | 488 | VAL  |
| 1   | A     | 524 | MET  |
| 1   | A     | 534 | VAL  |
| 1   | A     | 538 | VAL  |
| 1   | A     | 545 | VAL  |
| 1   | A     | 557 | ARG  |
| 1   | A     | 562 | ASN  |
| 1   | A     | 607 | SER  |
| 1   | A     | 613 | GLU  |
| 1   | A     | 619 | LYS  |
| 1   | A     | 621 | ILE  |
| 1   | A     | 625 | ASP  |
| 1   | A     | 644 | SER  |
| 1   | A     | 687 | ILE  |
| 1   | A     | 691 | ASP  |
| 1   | A     | 792 | ASN  |
| 1   | A     | 818 | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 849  | ASP  |
| 1   | A     | 853  | LYS  |
| 1   | A     | 864  | LEU  |
| 1   | A     | 873  | VAL  |
| 1   | A     | 908  | THR  |
| 1   | A     | 930  | LEU  |
| 1   | A     | 931  | ARG  |
| 1   | A     | 932  | ARG  |
| 1   | A     | 954  | ARG  |
| 1   | A     | 1036 | ASN  |
| 1   | A     | 1128 | ILE  |
| 1   | A     | 1160 | ARG  |
| 1   | A     | 1165 | THR  |
| 1   | A     | 1203 | ASP  |
| 1   | A     | 1282 | ASP  |
| 1   | A     | 1298 | LEU  |
| 1   | A     | 1304 | ILE  |
| 1   | A     | 1306 | LYS  |
| 1   | A     | 1308 | TYR  |
| 1   | A     | 1309 | MET  |
| 1   | A     | 1311 | LEU  |
| 1   | A     | 1318 | LYS  |
| 1   | A     | 1341 | VAL  |
| 1   | A     | 1485 | GLU  |
| 2   | B     | 41   | ARG  |
| 2   | B     | 57   | ARG  |
| 2   | B     | 61   | ASP  |
| 2   | B     | 67   | LEU  |
| 2   | B     | 73   | HIS  |
| 2   | B     | 78   | VAL  |
| 2   | B     | 79   | GLU  |
| 2   | B     | 129  | THR  |
| 2   | B     | 132  | VAL  |
| 2   | B     | 225  | LEU  |
| 2   | B     | 226  | GLU  |
| 2   | B     | 250  | SER  |
| 2   | B     | 269  | ILE  |
| 2   | B     | 302  | LYS  |
| 2   | B     | 330  | VAL  |
| 2   | B     | 371  | ARG  |
| 2   | B     | 388  | TYR  |
| 2   | B     | 416  | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 422  | PHE  |
| 2   | B     | 448  | LEU  |
| 2   | B     | 485  | LEU  |
| 2   | B     | 604  | ILE  |
| 2   | B     | 621  | ILE  |
| 2   | B     | 628  | VAL  |
| 2   | B     | 655  | ASP  |
| 2   | B     | 667  | THR  |
| 2   | B     | 711  | ILE  |
| 2   | B     | 733  | MET  |
| 2   | B     | 735  | VAL  |
| 2   | B     | 737  | ILE  |
| 2   | B     | 747  | LEU  |
| 2   | B     | 784  | SER  |
| 2   | B     | 853  | LEU  |
| 2   | B     | 879  | GLU  |
| 2   | B     | 880  | LEU  |
| 2   | B     | 921  | ILE  |
| 2   | B     | 958  | CYS  |
| 2   | B     | 961  | ILE  |
| 2   | B     | 1022 | LEU  |
| 2   | B     | 1035 | ARG  |
| 2   | B     | 1071 | ASN  |
| 2   | B     | 1092 | ASP  |
| 3   | C     | 6    | GLN  |
| 3   | C     | 35   | ARG  |
| 3   | C     | 58   | VAL  |
| 3   | C     | 70   | LEU  |
| 3   | C     | 135  | ARG  |
| 3   | C     | 136  | ASP  |
| 3   | C     | 137  | ASN  |
| 3   | C     | 148  | ILE  |
| 5   | E     | 38   | GLU  |
| 5   | E     | 47   | LYS  |
| 5   | E     | 64   | HIS  |
| 5   | E     | 113  | SER  |
| 5   | E     | 191  | VAL  |
| 5   | E     | 205  | THR  |
| 6   | F     | 54   | THR  |
| 6   | F     | 64   | ARG  |
| 7   | G     | 158  | PHE  |
| 8   | H     | 65   | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | H     | 66  | GLU  |
| 8   | H     | 74  | GLU  |
| 8   | H     | 107 | GLU  |
| 8   | H     | 116 | VAL  |
| 8   | H     | 144 | LEU  |
| 9   | I     | 28  | GLU  |
| 9   | I     | 60  | HIS  |
| 9   | I     | 61  | GLU  |
| 9   | I     | 84  | HIS  |
| 10  | J     | 3   | ILE  |
| 10  | J     | 7   | CYS  |
| 10  | J     | 14  | VAL  |
| 10  | J     | 47  | ARG  |
| 10  | J     | 54  | ASP  |
| 10  | J     | 59  | LEU  |
| 10  | J     | 65  | LEU  |
| 11  | K     | 39  | ASP  |
| 11  | K     | 48  | SER  |
| 11  | K     | 63  | VAL  |
| 12  | L     | 16  | ILE  |
| 12  | L     | 27  | GLU  |
| 13  | M     | 10  | LEU  |
| 13  | M     | 12  | ARG  |
| 13  | M     | 39  | LEU  |
| 13  | M     | 43  | ASP  |
| 13  | M     | 47  | ASP  |
| 13  | M     | 48  | VAL  |
| 13  | M     | 110 | SER  |
| 13  | M     | 111 | ASP  |
| 13  | M     | 133 | ASN  |
| 13  | M     | 282 | ASP  |
| 14  | N     | 20  | ASP  |
| 14  | N     | 360 | LEU  |
| 15  | O     | 88  | ILE  |
| 16  | P     | 180 | LEU  |
| 16  | P     | 206 | GLU  |
| 16  | P     | 297 | LYS  |
| 17  | Q     | 17  | LEU  |
| 17  | Q     | 72  | ILE  |
| 17  | Q     | 76  | MET  |
| 17  | Q     | 135 | THR  |
| 17  | Q     | 138 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | Q     | 151 | THR  |
| 17  | Q     | 159 | THR  |
| 17  | Q     | 171 | LYS  |
| 17  | Q     | 177 | LEU  |
| 17  | Q     | 184 | ILE  |
| 17  | Q     | 191 | LEU  |
| 18  | R     | 163 | LEU  |
| 18  | R     | 169 | GLU  |
| 18  | R     | 206 | LYS  |
| 18  | R     | 209 | GLN  |
| 18  | R     | 223 | VAL  |
| 18  | R     | 235 | GLU  |
| 19  | S     | 135 | PHE  |
| 19  | S     | 166 | ARG  |
| 19  | S     | 177 | MET  |
| 20  | T     | 140 | ARG  |
| 20  | T     | 141 | LEU  |
| 20  | T     | 148 | VAL  |
| 20  | T     | 154 | LYS  |
| 20  | T     | 183 | VAL  |
| 21  | U     | 194 | ARG  |
| 21  | U     | 226 | GLU  |
| 21  | U     | 232 | GLU  |
| 21  | U     | 248 | HIS  |
| 21  | U     | 252 | LYS  |
| 21  | U     | 253 | THR  |
| 21  | U     | 257 | GLN  |
| 21  | U     | 260 | LEU  |
| 21  | U     | 276 | VAL  |
| 21  | U     | 299 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 72  | GLN  |
| 1   | A     | 122 | ASN  |
| 1   | A     | 136 | GLN  |
| 1   | A     | 222 | HIS  |
| 1   | A     | 273 | GLN  |
| 1   | A     | 296 | ASN  |
| 1   | A     | 504 | HIS  |
| 1   | A     | 507 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 529  | GLN  |
| 1   | A     | 609  | HIS  |
| 1   | A     | 632  | ASN  |
| 1   | A     | 673  | GLN  |
| 1   | A     | 746  | ASN  |
| 1   | A     | 757  | GLN  |
| 1   | A     | 783  | GLN  |
| 1   | A     | 989  | ASN  |
| 1   | A     | 1101 | GLN  |
| 1   | A     | 1445 | HIS  |
| 2   | B     | 98   | HIS  |
| 2   | B     | 175  | ASN  |
| 2   | B     | 790  | GLN  |
| 2   | B     | 817  | GLN  |
| 2   | B     | 842  | HIS  |
| 2   | B     | 941  | GLN  |
| 2   | B     | 1101 | GLN  |
| 3   | C     | 6    | GLN  |
| 3   | C     | 25   | ASN  |
| 3   | C     | 275  | ASN  |
| 4   | D     | 48   | ASN  |
| 5   | E     | 64   | HIS  |
| 6   | F     | 46   | GLN  |
| 7   | G     | 24   | ASN  |
| 9   | I     | 21   | ASN  |
| 9   | I     | 22   | ASN  |
| 9   | I     | 41   | ASN  |
| 9   | I     | 45   | GLN  |
| 9   | I     | 84   | HIS  |
| 10  | J     | 52   | HIS  |
| 11  | K     | 29   | ASN  |
| 11  | K     | 89   | ASN  |
| 12  | L     | 26   | ASN  |
| 13  | M     | 71   | GLN  |
| 13  | M     | 102  | GLN  |
| 13  | M     | 116  | ASN  |
| 13  | M     | 144  | GLN  |
| 13  | M     | 227  | GLN  |
| 14  | N     | 333  | ASN  |
| 16  | P     | 189  | ASN  |
| 17  | Q     | 109  | HIS  |
| 18  | R     | 204  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | T     | 30  | GLN  |
| 20  | T     | 81  | HIS  |
| 21  | U     | 203 | ASN  |
| 21  | U     | 248 | HIS  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 13 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.

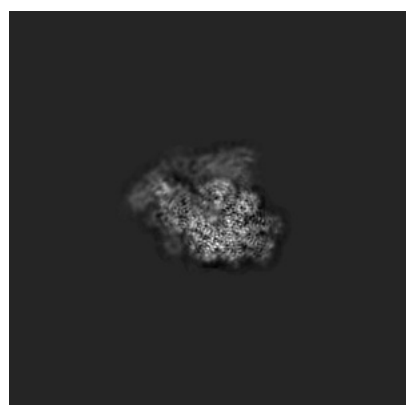
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8137. These allow visual inspection of the internal detail of the map and identification of artifacts.

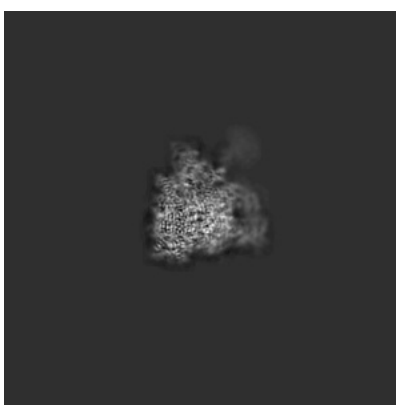
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

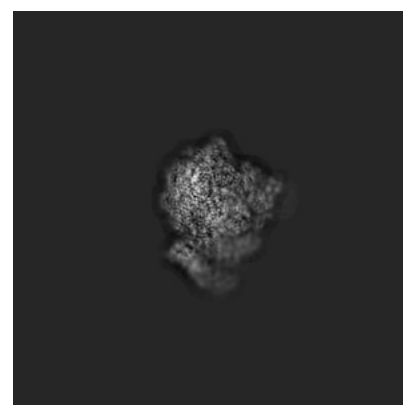
#### 6.1.1 Primary map



X



Y

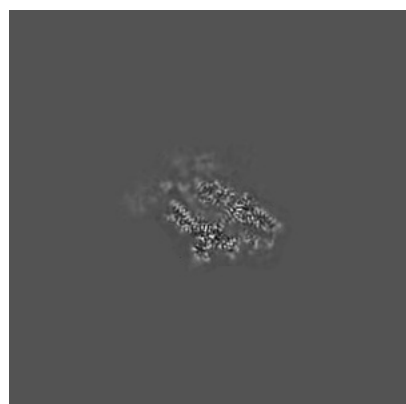


Z

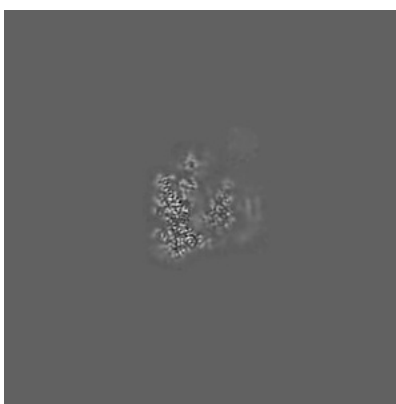
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

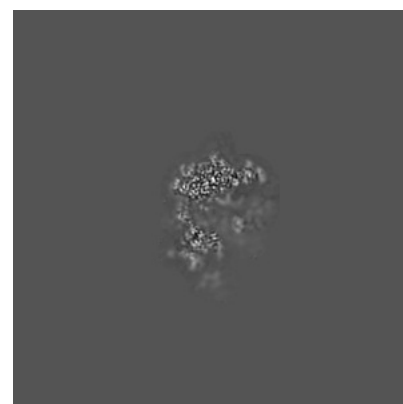
#### 6.2.1 Primary map



X Index: 192



Y Index: 192

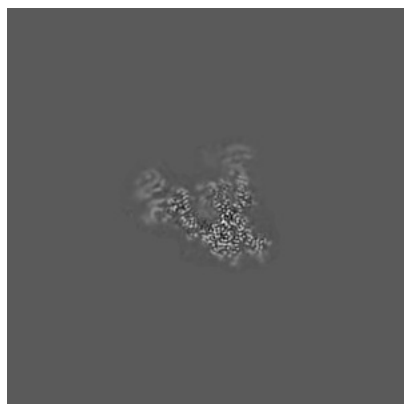


Z Index: 192

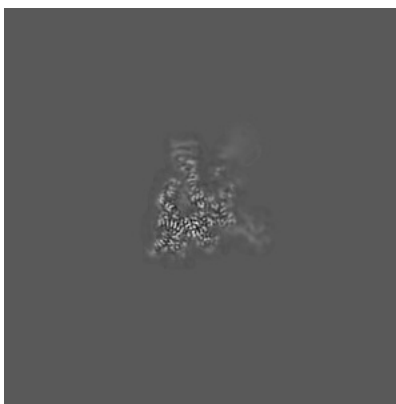
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

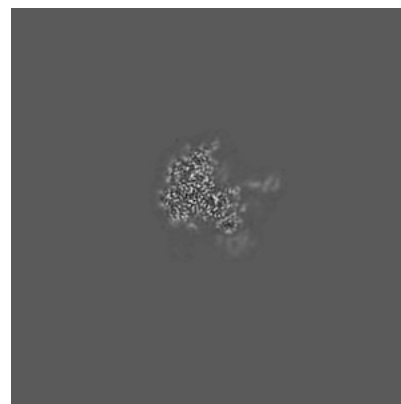
### 6.3.1 Primary map



X Index: 175



Y Index: 210

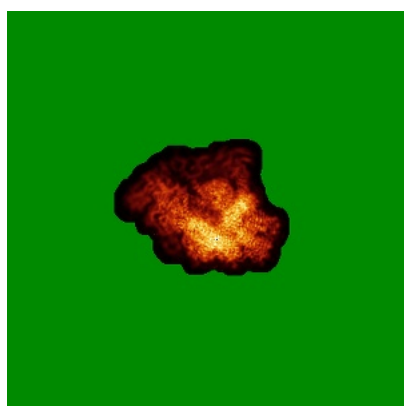


Z Index: 163

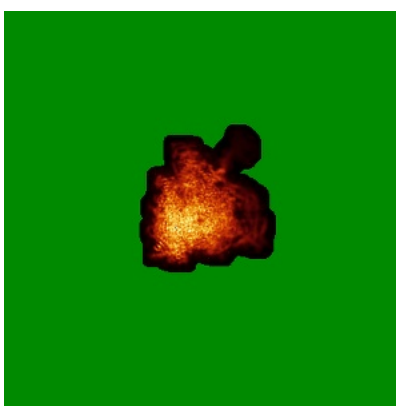
The images above show the largest variance slices of the map in three orthogonal directions.

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

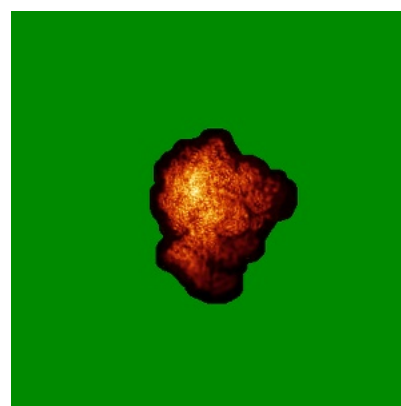
### 6.4.1 Primary map



X



Y

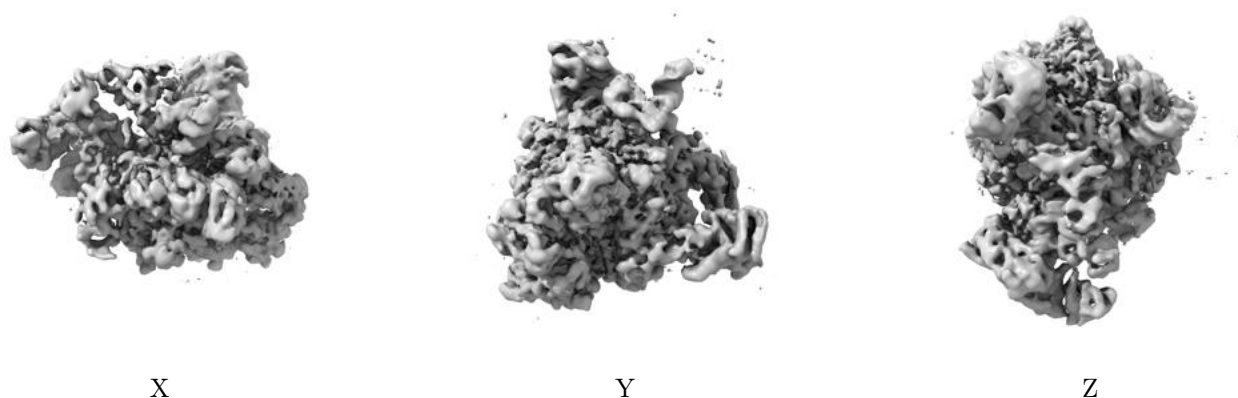


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

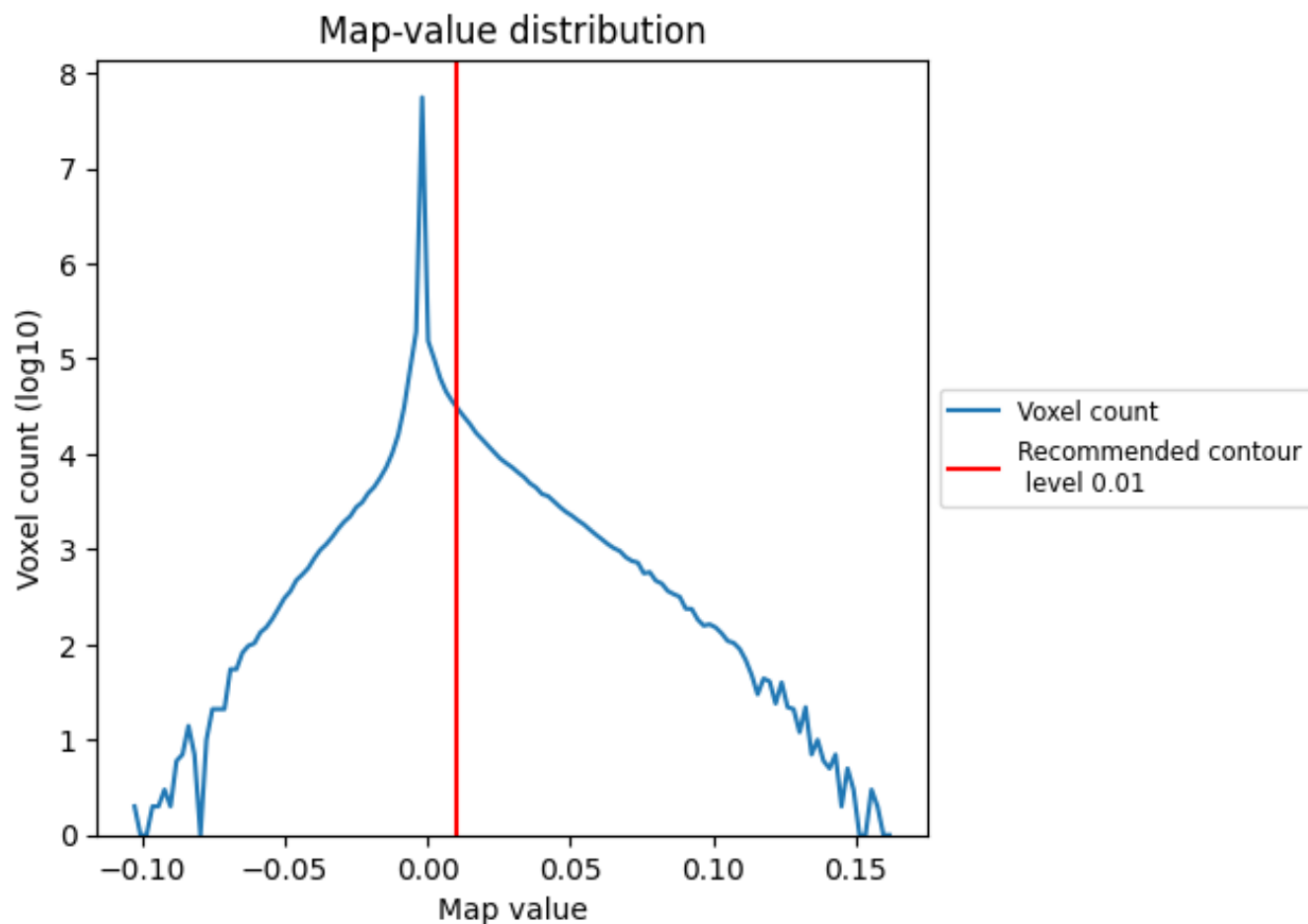
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

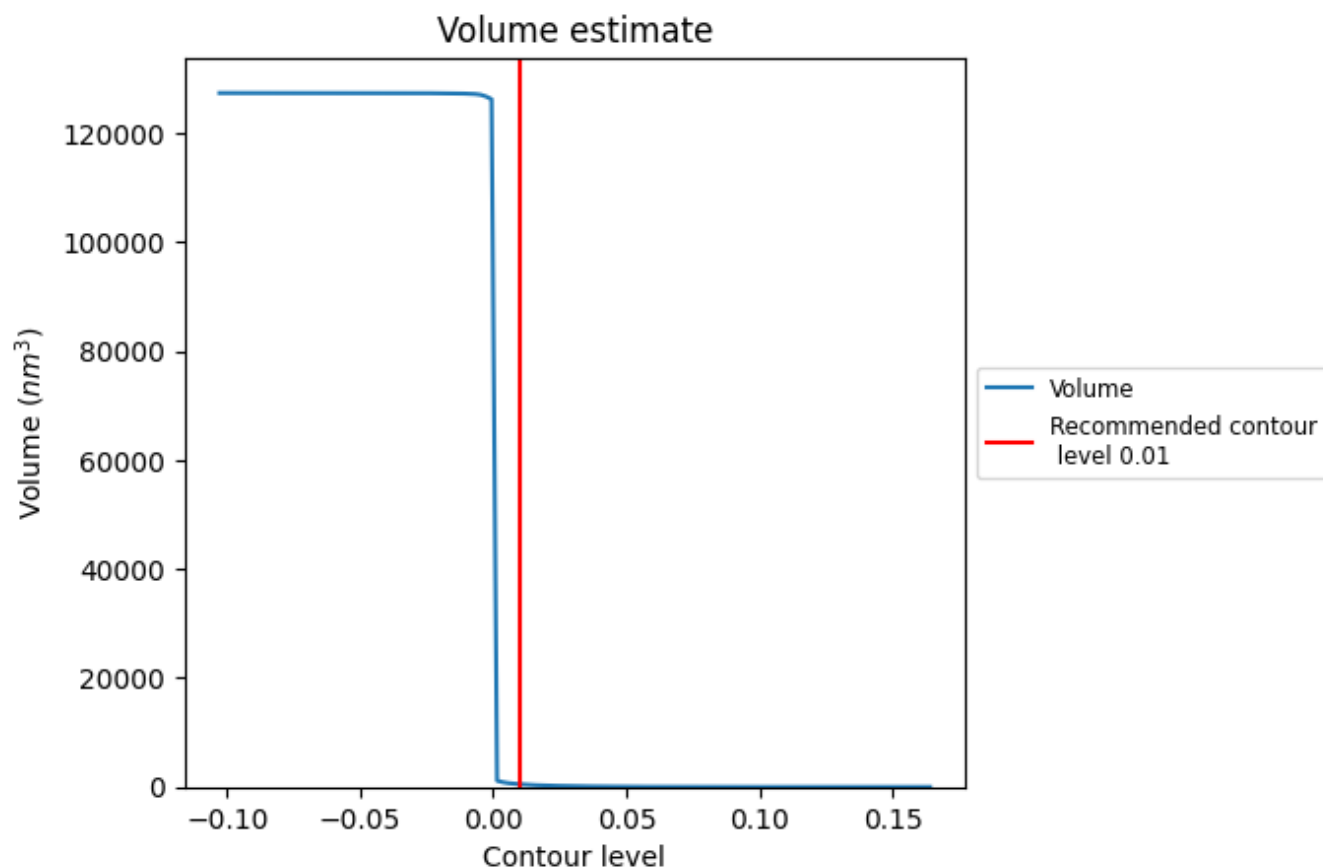
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

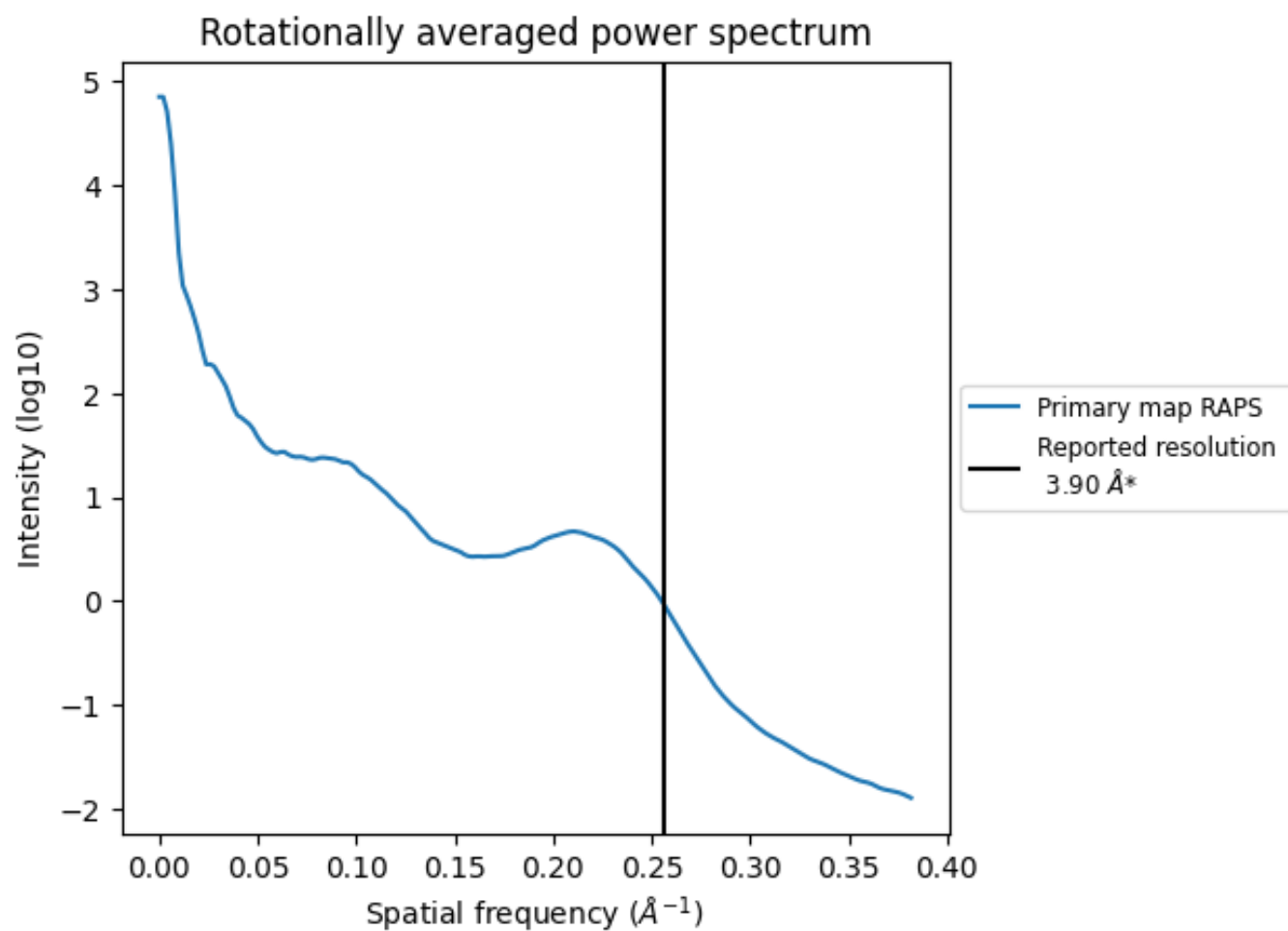
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 500 nm<sup>3</sup>; this corresponds to an approximate mass of 451 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)

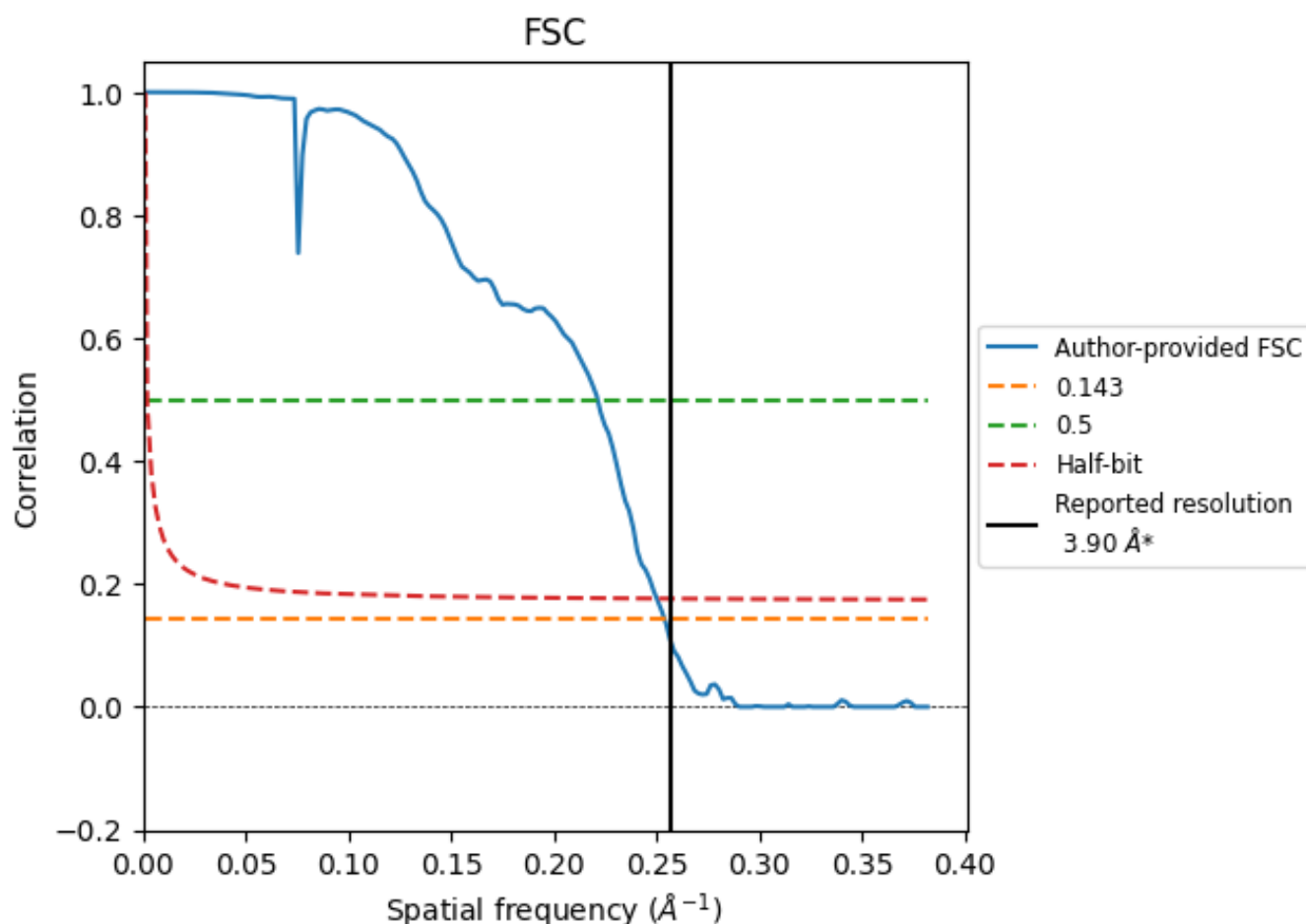


\*Reported resolution corresponds to spatial frequency of 0.256  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.256 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

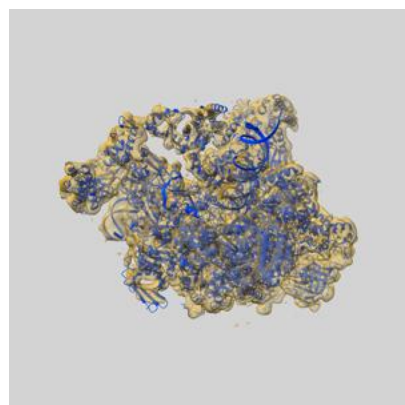
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.90                               | -    | -        |
| Author-provided FSC curve | 3.94                               | 4.52 | 4.00     |
| Unmasked-calculated*      | -                                  | -    | -        |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

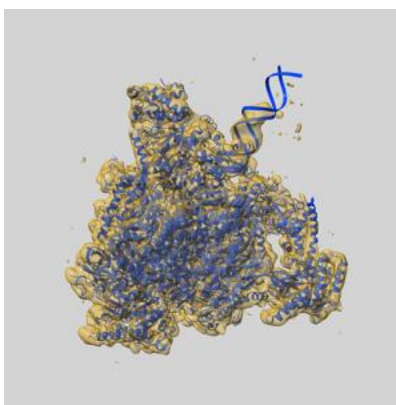
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8137 and PDB model 5IYC. Per-residue inclusion information can be found in section [3](#) on page [8](#).

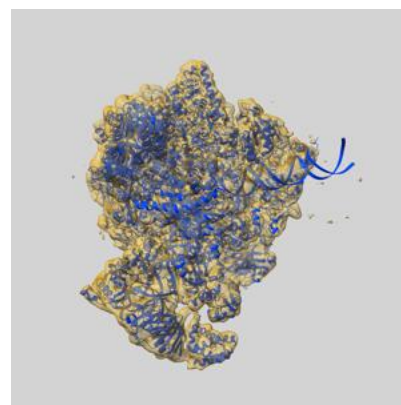
### 9.1 Map-model overlay [i](#)



X



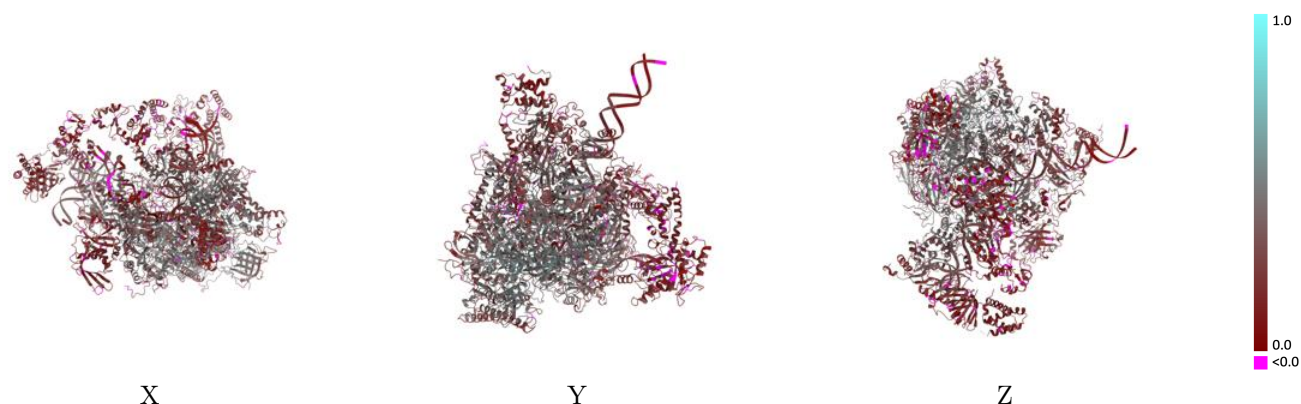
Y



Z

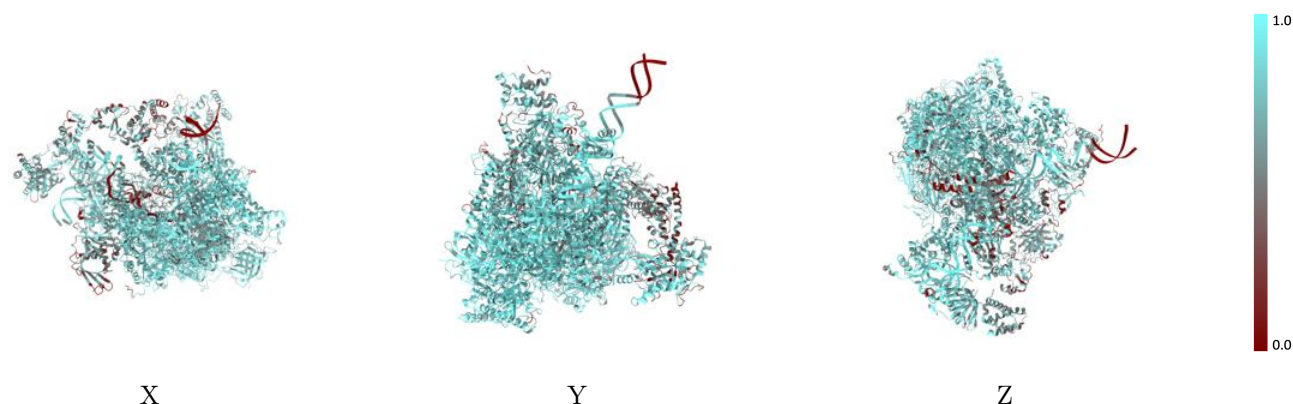
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



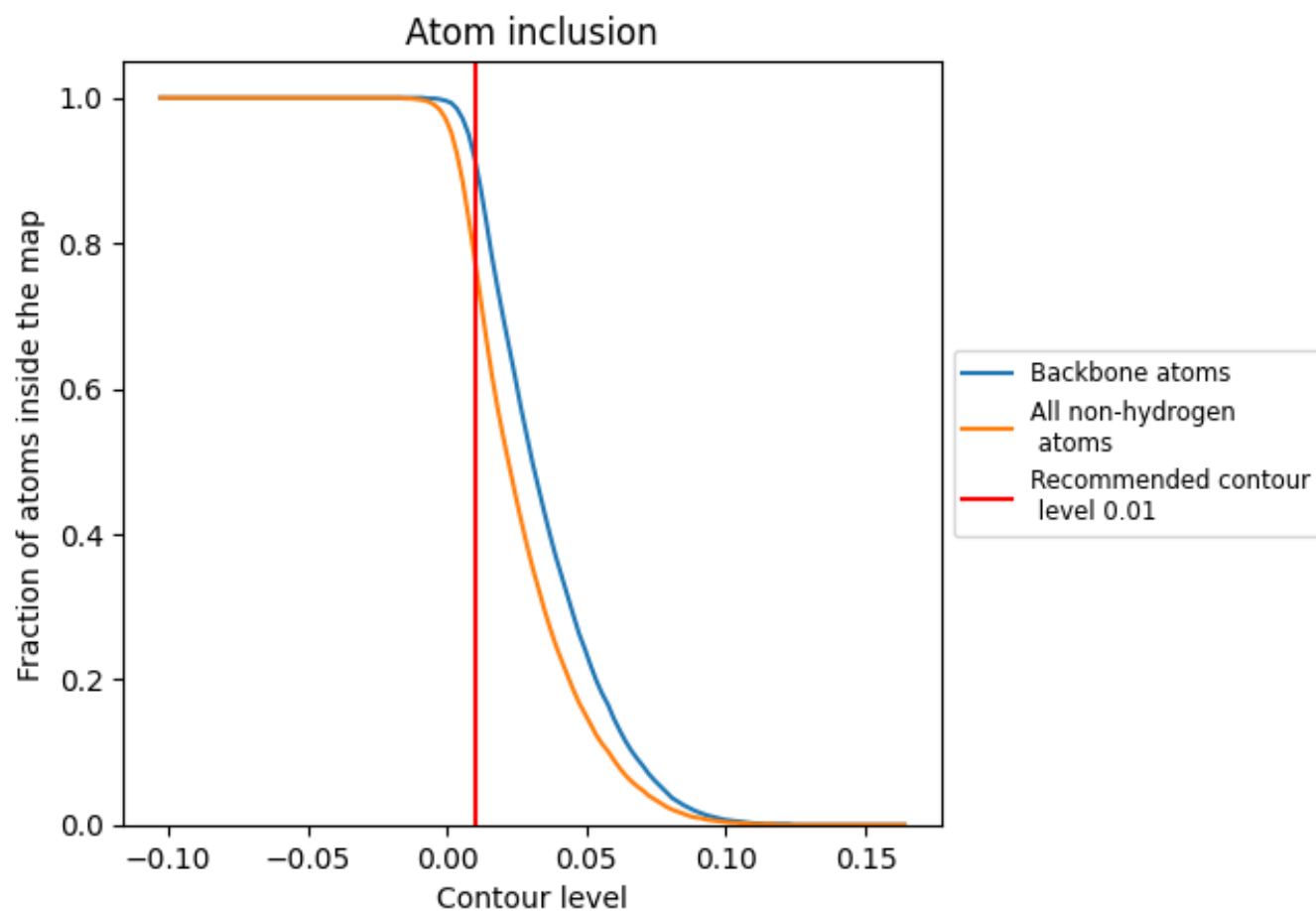
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7760   |  0.3060   |
| A     |  0.8490   |  0.3730   |
| B     |  0.8490   |  0.3980   |
| C     |  0.8750   |  0.3840   |
| D     |  0.7110   |  0.1630   |
| E     |  0.8390   |  0.3450   |
| F     |  0.8310   |  0.3900   |
| G     |  0.7450   |  0.2050   |
| H     |  0.8440   |  0.3320   |
| I     |  0.7830   |  0.2840   |
| J     |  0.8770   |  0.3930   |
| K     |  0.8750   |  0.3840   |
| L     |  0.8820   |  0.3710   |
| M     |  0.7870   |  0.3020   |
| N     |  0.6690  |  0.1670  |
| O     |  0.6880 |  0.1690 |
| P     |  0.8190 |  0.2500 |
| Q     |  0.4570 |  0.1260 |
| R     |  0.4910 |  0.1260 |
| S     |  0.4990 |  0.1530 |
| T     |  0.5520 |  0.1590 |
| U     |  0.5860 |  0.1460 |
| X     |  0.6790 |  0.2090 |
| Y     |  0.7800 |  0.2350 |

