



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:13 PM UTC

PDB ID : 7MKQ / pdb\_00007mkq  
EMDB ID : EMD-23903  
Title : Escherichia coli RNA polymerase and RapA binary complex  
Authors : Qayyum, M.Z.; Murakami, K.S.  
Deposited on : 2021-04-26  
Resolution : 4.80 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:

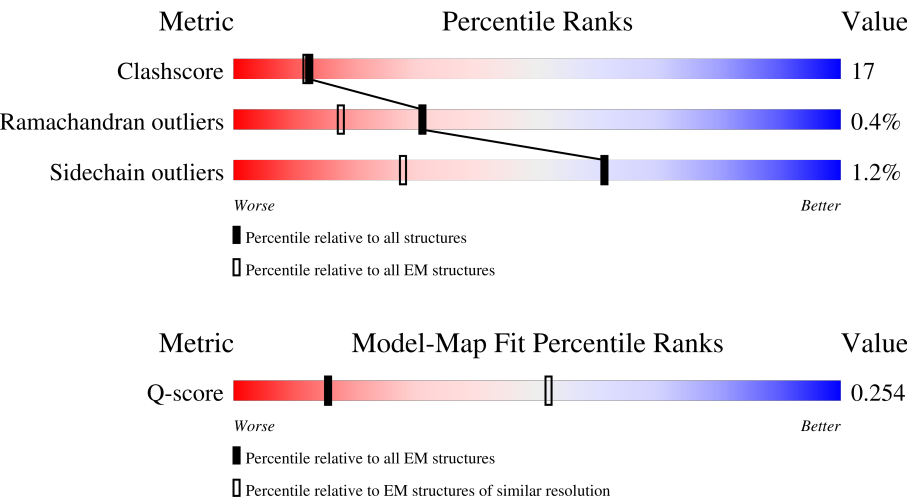
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : 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 4.80 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                       | 1575 ( 4.30 - 5.30 )                                     |

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     | 237    | <div><div></div><div>62%</div><div>35%</div><div>.</div></div>   |
| 1   | B     | 237    | <div><div></div><div>54%</div><div>42%</div><div>..</div></div>  |
| 2   | C     | 1340   | <div><div>8%</div><div>62%</div><div>37%</div><div>.</div></div> |
| 3   | D     | 1363   | <div><div>6%</div><div>60%</div><div>38%</div><div>.</div></div> |

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| Mol | Chain | Length | Quality of chain                                                               |
|-----|-------|--------|--------------------------------------------------------------------------------|
| 4   | E     | 91     | <div><div></div><div>18%</div><div>49%</div><div>34%</div><div>16%</div></div> |
| 5   | L     | 968    | <div><div></div><div>67%</div><div>33%</div></div>                             |

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 32822 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 subunit alpha.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | A     | 231      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1794  | 1117 | 318 | 353 | 6 |         |       |
| 1   | B     | 230      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1786  | 1112 | 317 | 351 | 6 |         |       |

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

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 2   | C     | 1340     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10570 | 6631 | 1841 | 2055 | 43 |         |       |

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 3   | D     | 1338     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10368 | 6514 | 1847 | 1958 | 49 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | E     | 76       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 605   | 368 | 115 | 121 | 1 |         |       |

- Molecule 5 is a protein called RNA polymerase-associated protein RapA.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 5   | L     | 967      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 7696  | 4820 | 1378 | 1470 | 28 |         |       |

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 6   | D     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

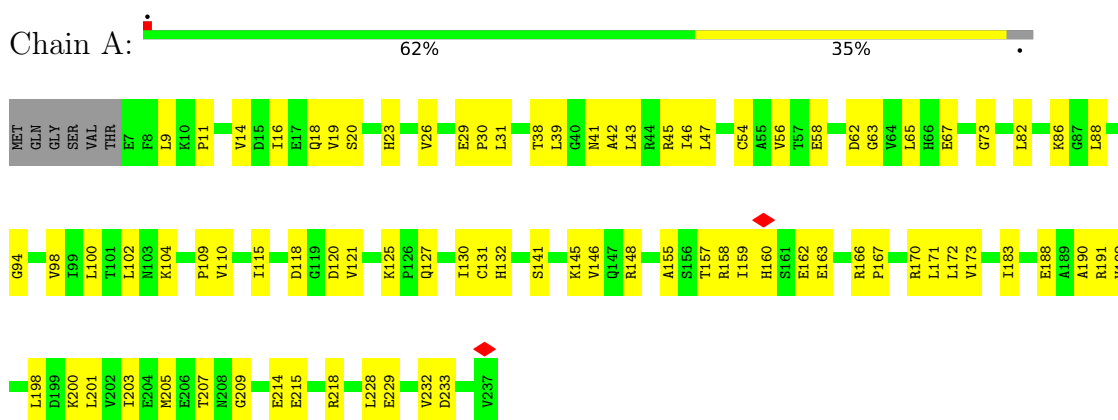
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 7   | D     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |

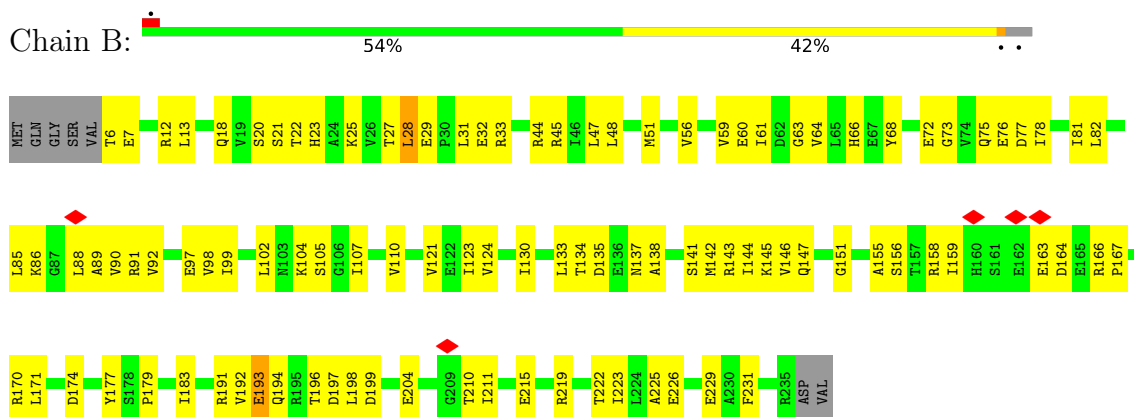
### 3 Residue-property plots

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.

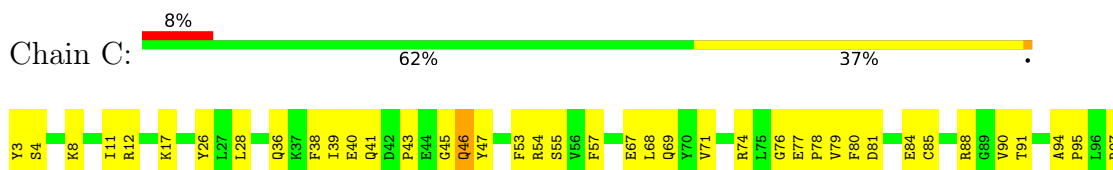
- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha



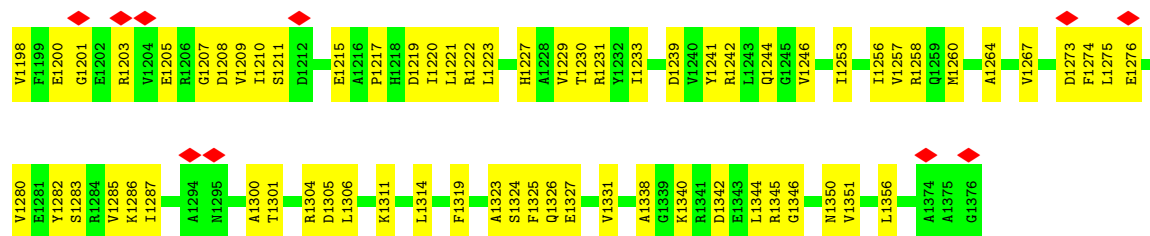
- Molecule 2: DNA-directed RNA polymerase subunit beta



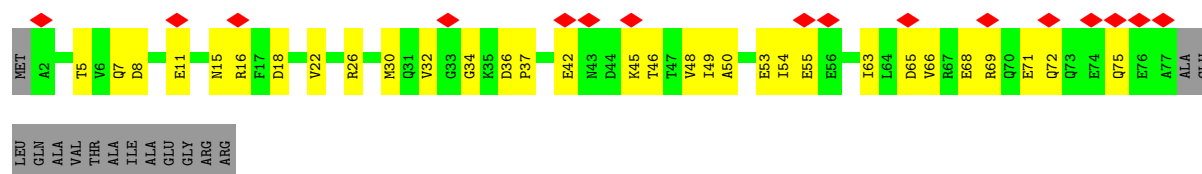


Chain D: 6% 60% 38%

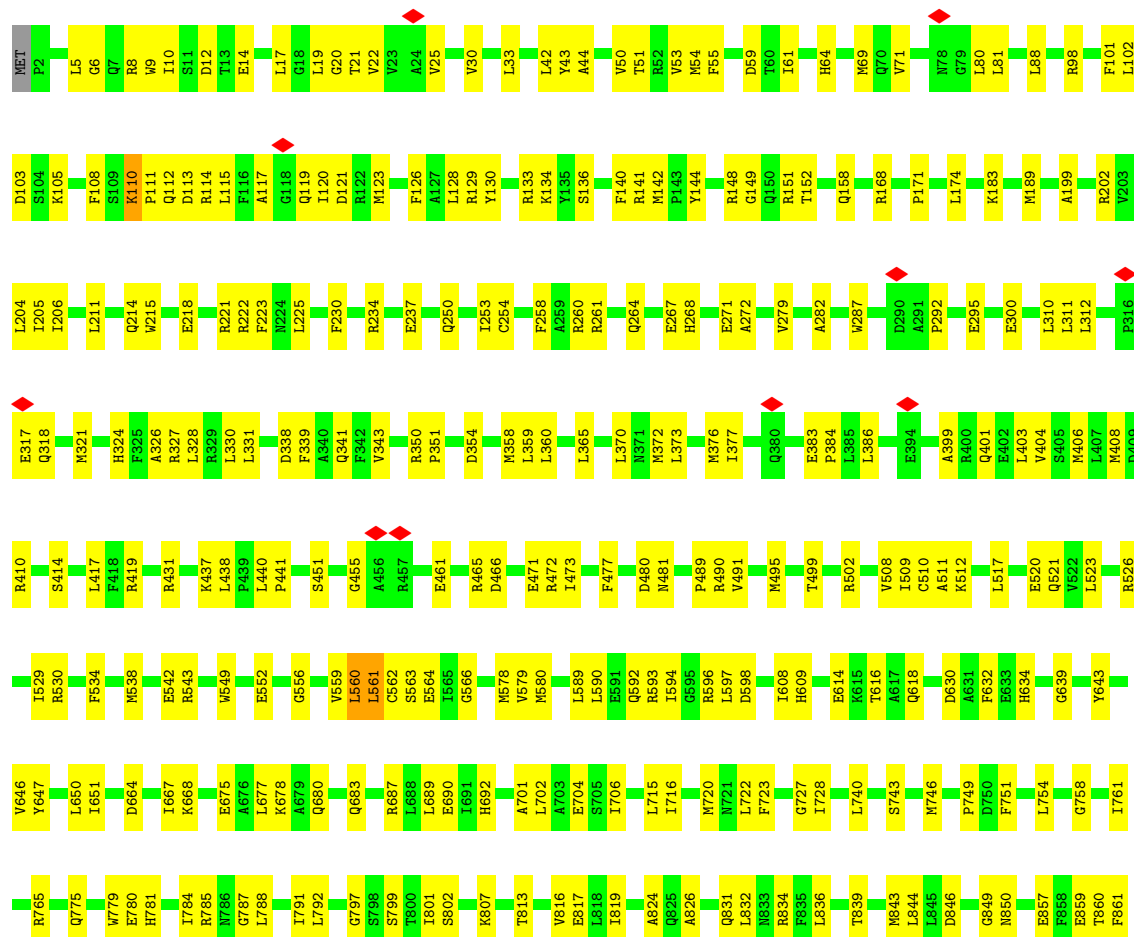
The visualization displays a hierarchical tree structure representing Chain D. The nodes are color-coded based on their segment: green (6%), yellow (60%), and orange (38%). The tree structure is complex, with many nodes having multiple children, and the overall structure is highly branched. The nodes are arranged in a way that shows the flow of information or data from the root node (T14) down to the leaf nodes (e.g., T1104, T1105, etc.). The bar chart at the top provides a visual summary of the distribution of the nodes across the three segments.



• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 5: RNA polymerase-associated protein RapA





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 88511                                   | 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 ( $e^-/\text{\AA}^2$ ) | 45                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 0.021                                   | Depositor |
| Minimum map value                    | -0.010                                  | Depositor |
| Average map value                    | -0.000                                  | Depositor |
| Map value standard deviation         | 0.001                                   | Depositor |
| Recommended contour level            | 0.004                                   | Depositor |
| Map size (Å)                         | 388.80002, 388.80002, 388.80002         | wwPDB     |
| Map dimensions                       | 360, 360, 360                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.08, 1.08, 1.08                        | 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     | 0.16         | 0/1816      | 0.49        | 0/2461         |
| 1   | B     | 0.25         | 0/1808      | 0.60        | 0/2450         |
| 2   | C     | 0.21         | 0/10739     | 0.53        | 1/14489 (0.0%) |
| 3   | D     | 0.20         | 0/10525     | 0.55        | 2/14214 (0.0%) |
| 4   | E     | 0.13         | 0/607       | 0.40        | 0/817          |
| 5   | L     | 0.16         | 0/7840      | 0.48        | 1/10622 (0.0%) |
| All | All   | 0.20         | 0/33335     | 0.52        | 4/45053 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | C     | 0                   | 2                   |
| 3   | D     | 0                   | 3                   |
| 5   | L     | 0                   | 3                   |
| All | All   | 0                   | 8                   |

There are no bond length outliers.

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | D     | 758 | PRO  | CA-N-CD  | -7.70 | 101.22      | 112.00   |
| 2   | C     | 46  | GLN  | CA-CB-CG | 5.60  | 125.29      | 114.10   |
| 5   | L     | 912 | GLU  | N-CA-CB  | 5.58  | 118.07      | 109.98   |
| 3   | D     | 77  | ARG  | CB-CG-CD | -5.42 | 98.84       | 111.30   |

There are no chirality outliers.

All (8) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 2   | C     | 236  | LYS  | Peptide |
| 2   | C     | 595  | THR  | Peptide |
| 3   | D     | 1184 | ASP  | Peptide |
| 3   | D     | 860  | ARG  | Peptide |
| 3   | D     | 901  | ARG  | Peptide |
| 5   | L     | 110  | LYS  | Peptide |
| 5   | L     | 560  | LEU  | Peptide |
| 5   | L     | 564  | GLU  | 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     | 1794  | 0        | 1819     | 57      | 0            |
| 1   | B     | 1786  | 0        | 1813     | 74      | 0            |
| 2   | C     | 10570 | 0        | 10582    | 364     | 0            |
| 3   | D     | 10368 | 0        | 10556    | 411     | 0            |
| 4   | E     | 605   | 0        | 612      | 22      | 0            |
| 5   | L     | 7696  | 0        | 7542     | 225     | 0            |
| 6   | D     | 1     | 0        | 0        | 0       | 0            |
| 7   | D     | 2     | 0        | 0        | 0       | 0            |
| All | All   | 32822 | 0        | 32924    | 1111    | 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 17.

All (1111) 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) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:1061:VAL:HB  | 3:D:1105:ALA:HB3 | 1.50                     | 0.92              |
| 5:L:414:SER:HG   | 5:L:692:HIS:HD1  | 1.18                     | 0.88              |
| 3:D:141:PHE:HA   | 3:D:180:MET:HE2  | 1.57                     | 0.86              |
| 3:D:1344:LEU:O   | 3:D:1346:GLY:N   | 2.08                     | 0.85              |
| 5:L:579:VAL:HG12 | 5:L:609:HIS:HB2  | 1.57                     | 0.84              |
| 3:D:1346:GLY:O   | 3:D:1350:ASN:ND2 | 2.12                     | 0.83              |
| 2:C:211:ARG:NH2  | 2:C:217:THR:OG1  | 2.12                     | 0.82              |
| 3:D:1075:ARG:NH2 | 3:D:1169:THR:OG1 | 2.11                     | 0.82              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:L:260:ARG:NH1   | 5:L:295:GLU:OE1   | 2.11                     | 0.82              |
| 3:D:77:ARG:NH2    | 5:L:749:PRO:O     | 2.14                     | 0.81              |
| 1:B:134:THR:HG22  | 1:B:135:ASP:H     | 1.47                     | 0.80              |
| 1:B:133:LEU:HD12  | 1:B:138:ALA:HA    | 1.63                     | 0.79              |
| 1:B:66:HIS:HE1    | 1:B:68:TYR:HD2    | 1.27                     | 0.79              |
| 2:C:1136:GLN:HB2  | 2:C:1140:LYS:HE2  | 1.64                     | 0.78              |
| 3:D:816:THR:OG1   | 3:D:818:GLU:OE1   | 2.01                     | 0.78              |
| 3:D:205:LEU:O     | 3:D:214:ARG:NH1   | 2.15                     | 0.78              |
| 2:C:131:THR:HG22  | 2:C:135:THR:H     | 1.50                     | 0.77              |
| 2:C:1298:VAL:HG12 | 2:C:1301:ARG:HH21 | 1.50                     | 0.77              |
| 1:A:38:THR:OG1    | 1:B:45:ARG:NH1    | 2.18                     | 0.77              |
| 2:C:161:LYS:HB3   | 2:C:170:VAL:HG23  | 1.66                     | 0.76              |
| 3:D:972:LYS:HE3   | 3:D:1002:VAL:HA   | 1.67                     | 0.76              |
| 3:D:1062:LEU:HB3  | 3:D:1066:GLU:HG3  | 1.67                     | 0.76              |
| 3:D:126:LEU:O     | 3:D:220:ARG:NH1   | 2.19                     | 0.76              |
| 5:L:438:LEU:HD23  | 5:L:489:PRO:HB2   | 1.68                     | 0.76              |
| 1:B:155:ALA:HA    | 1:B:158:ARG:HH21  | 1.50                     | 0.75              |
| 3:D:955:LYS:HE3   | 3:D:1010:GLN:HG3  | 1.66                     | 0.75              |
| 5:L:410:ARG:NH2   | 5:L:927:VAL:O     | 2.19                     | 0.75              |
| 2:C:1132:LEU:HD11 | 2:C:1170:MET:HE1  | 1.68                     | 0.75              |
| 5:L:149:GLY:N     | 5:L:780:GLU:OE2   | 2.20                     | 0.75              |
| 2:C:1176:LEU:HD23 | 2:C:1180:MET:HG3  | 1.68                     | 0.74              |
| 2:C:551:HIS:CD2   | 2:C:552:PRO:HD2   | 2.22                     | 0.74              |
| 1:B:91:ARG:HE     | 1:B:210:THR:HG21  | 1.52                     | 0.74              |
| 2:C:1142:ARG:NH1  | 2:C:1165:SER:O    | 2.21                     | 0.74              |
| 3:D:133:ARG:NH1   | 3:D:136:GLU:OE1   | 2.17                     | 0.74              |
| 3:D:849:LEU:HD12  | 3:D:855:ASP:H     | 1.53                     | 0.74              |
| 2:C:194:LEU:HD22  | 2:C:429:MET:HE3   | 1.68                     | 0.73              |
| 2:C:398:SER:HB2   | 2:C:401:GLY:H     | 1.51                     | 0.73              |
| 2:C:538:LEU:HD13  | 2:C:543:ALA:HB2   | 1.69                     | 0.73              |
| 2:C:387:ASN:HA    | 2:C:391:SER:HB3   | 1.69                     | 0.73              |
| 1:B:61:ILE:HG22   | 1:B:63:GLY:H      | 1.54                     | 0.73              |
| 1:B:25:LYS:HG2    | 1:B:204:GLU:HG2   | 1.71                     | 0.73              |
| 5:L:495:MET:SD    | 5:L:526:ARG:NH2   | 2.62                     | 0.73              |
| 3:D:836:ARG:HG3   | 3:D:869:CYS:HB3   | 1.70                     | 0.72              |
| 2:C:808:ASN:H     | 3:D:633:ALA:HB2   | 1.53                     | 0.72              |
| 3:D:749:LYS:HG2   | 3:D:750:PRO:HD2   | 1.70                     | 0.72              |
| 5:L:912:GLU:HG2   | 5:L:913:LYS:HD2   | 1.71                     | 0.72              |
| 3:D:1061:VAL:HG13 | 3:D:1076:PRO:HG2  | 1.71                     | 0.71              |
| 1:A:191:ARG:NH1   | 1:A:192:VAL:O     | 2.23                     | 0.71              |
| 3:D:1221:LEU:HD12 | 3:D:1229:VAL:HG11 | 1.71                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:L:152:THR:HG22  | 5:L:222:ARG:HH21  | 1.55                     | 0.71              |
| 5:L:141:ARG:NH2   | 5:L:839:THR:OG1   | 2.24                     | 0.70              |
| 5:L:509:ILE:HA    | 5:L:561:LEU:HD22  | 1.73                     | 0.70              |
| 2:C:1290:MET:SD   | 2:C:1294:LYS:NZ   | 2.65                     | 0.70              |
| 2:C:842:ASP:HB2   | 2:C:1047:LEU:HD21 | 1.74                     | 0.70              |
| 2:C:213:LEU:HD12  | 2:C:422:LYS:HE2   | 1.73                     | 0.70              |
| 3:D:1239:ASP:OD1  | 3:D:1242:ARG:NH1  | 2.24                     | 0.70              |
| 2:C:957:LYS:HD3   | 2:C:1029:LEU:HD11 | 1.73                     | 0.69              |
| 3:D:205:LEU:HD21  | 3:D:217:LEU:HB3   | 1.74                     | 0.69              |
| 2:C:1072:ASN:HD21 | 2:C:1230:MET:HE1  | 1.58                     | 0.69              |
| 1:B:66:HIS:CE1    | 1:B:68:TYR:HD2    | 2.10                     | 0.69              |
| 5:L:471:GLU:OE2   | 5:L:490:ARG:NH2   | 2.21                     | 0.69              |
| 5:L:119:GLN:NE2   | 5:L:120:ILE:O     | 2.26                     | 0.69              |
| 1:A:100:LEU:HD23  | 1:A:115:ILE:HG21  | 1.75                     | 0.69              |
| 2:C:301:TYR:OH    | 2:C:334:GLU:OE1   | 2.11                     | 0.69              |
| 3:D:773:PHE:O     | 3:D:776:THR:OG1   | 2.11                     | 0.69              |
| 3:D:426:ALA:HB3   | 3:D:427:PRO:HD3   | 1.74                     | 0.69              |
| 3:D:672:LEU:HD12  | 3:D:673:VAL:HG13  | 1.76                     | 0.68              |
| 2:C:1138:VAL:HG12 | 2:C:1142:ARG:HD2  | 1.76                     | 0.68              |
| 1:A:218:ARG:NH1   | 1:B:231:PHE:O     | 2.27                     | 0.68              |
| 2:C:714:VAL:HB    | 2:C:787:PRO:HD2   | 1.75                     | 0.68              |
| 3:D:481:ARG:HA    | 3:D:485:MET:HE2   | 1.74                     | 0.68              |
| 1:B:166:ARG:HB3   | 1:B:170:ARG:HG3   | 1.74                     | 0.68              |
| 3:D:982:LEU:HD23  | 3:D:997:VAL:HB    | 1.76                     | 0.68              |
| 3:D:1038:THR:HG21 | 3:D:1079:LYS:HD3  | 1.74                     | 0.68              |
| 1:B:18:GLN:NE2    | 1:B:23:HIS:O      | 2.27                     | 0.68              |
| 3:D:874:GLU:OE1   | 3:D:875:ASN:ND2   | 2.26                     | 0.68              |
| 2:C:1024:GLU:HA   | 2:C:1027:LYS:HE2  | 1.73                     | 0.68              |
| 3:D:120:LEU:HB3   | 3:D:121:PRO:HD3   | 1.75                     | 0.68              |
| 2:C:138:ILE:HG21  | 2:C:143:ARG:HD2   | 1.76                     | 0.68              |
| 3:D:848:VAL:HG22  | 3:D:858:VAL:HG22  | 1.75                     | 0.68              |
| 1:A:157:THR:O     | 1:A:160:HIS:ND1   | 2.27                     | 0.67              |
| 3:D:1065:ALA:HB2  | 3:D:1192:LYS:HB3  | 1.77                     | 0.67              |
| 2:C:214:ASN:OD1   | 2:C:359:ARG:NE    | 2.23                     | 0.67              |
| 3:D:317:THR:HB    | 3:D:324:LEU:HB3   | 1.75                     | 0.67              |
| 5:L:831:GLN:OE1   | 5:L:834:ARG:NH1   | 2.28                     | 0.67              |
| 2:C:731:ARG:HE    | 2:C:750:ILE:HD11  | 1.60                     | 0.67              |
| 1:B:99:ILE:HD11   | 1:B:143:ARG:HD2   | 1.76                     | 0.67              |
| 2:C:692:THR:HG22  | 2:C:693:LEU:H     | 1.57                     | 0.67              |
| 3:D:1061:VAL:HG11 | 3:D:1101:LEU:HB2  | 1.77                     | 0.67              |
| 3:D:1205:GLU:HG3  | 3:D:1208:ASP:HB2  | 1.77                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:759:ILE:HA    | 3:D:771:GLN:HE21  | 1.60                     | 0.67              |
| 2:C:264:GLU:HG2   | 2:C:267:ARG:HH12  | 1.60                     | 0.66              |
| 2:C:525:THR:HG21  | 2:C:687:ARG:HD2   | 1.77                     | 0.66              |
| 2:C:841:ARG:N     | 2:C:848:GLU:OE2   | 2.27                     | 0.66              |
| 2:C:594:VAL:HG11  | 2:C:650:VAL:HG23  | 1.77                     | 0.66              |
| 2:C:893:THR:HG21  | 2:C:910:ALA:HB1   | 1.78                     | 0.66              |
| 3:D:821:MET:O     | 3:D:1231:ARG:NH2  | 2.28                     | 0.66              |
| 3:D:826:ILE:HG22  | 3:D:831:VAL:HG12  | 1.77                     | 0.66              |
| 3:D:147:ILE:HD11  | 3:D:179:LYS:HE3   | 1.76                     | 0.66              |
| 3:D:1162:ILE:HD11 | 3:D:1201:GLY:HA2  | 1.76                     | 0.66              |
| 1:B:72:GLU:OE1    | 1:B:137:ASN:ND2   | 2.28                     | 0.66              |
| 2:C:189:ASP:OD1   | 2:C:193:ASN:N     | 2.24                     | 0.66              |
| 3:D:697:MET:HE1   | 3:D:738:ARG:HA    | 1.77                     | 0.66              |
| 5:L:918:LEU:HD21  | 5:L:940:GLU:HG2   | 1.78                     | 0.66              |
| 2:C:68:LEU:HD21   | 2:C:100:LEU:HD23  | 1.79                     | 0.65              |
| 1:A:11:PRO:HA     | 1:A:30:PRO:HG2    | 1.78                     | 0.65              |
| 1:A:18:GLN:NE2    | 1:A:20:SER:O      | 2.30                     | 0.65              |
| 3:D:208:THR:O     | 3:D:214:ARG:NH1   | 2.26                     | 0.65              |
| 3:D:819:GLY:O     | 3:D:881:LYS:NZ    | 2.23                     | 0.65              |
| 5:L:860:THR:HA    | 5:L:863:ARG:HE    | 1.61                     | 0.65              |
| 2:C:1291:LEU:HD11 | 3:D:1351:VAL:HG13 | 1.78                     | 0.65              |
| 1:B:13:LEU:HD11   | 1:B:29:GLU:HB3    | 1.78                     | 0.65              |
| 2:C:199:ASP:O     | 2:C:200:ARG:NE    | 2.26                     | 0.65              |
| 2:C:303:ASP:HB2   | 2:C:310:ILE:HD11  | 1.77                     | 0.65              |
| 2:C:1137:GLU:O    | 2:C:1140:LYS:HG3  | 1.97                     | 0.65              |
| 2:C:169:LYS:O     | 2:C:171:LEU:HD12  | 1.97                     | 0.65              |
| 3:D:133:ARG:O     | 3:D:137:ARG:HG2   | 1.96                     | 0.65              |
| 3:D:482:ALA:O     | 3:D:488:ASN:ND2   | 2.27                     | 0.65              |
| 5:L:129:ARG:HH22  | 5:L:133:ARG:HH21  | 1.45                     | 0.65              |
| 2:C:80:PHE:HE2    | 2:C:88:ARG:HD2    | 1.62                     | 0.64              |
| 1:A:82:LEU:HD23   | 1:A:173:VAL:HG22  | 1.79                     | 0.64              |
| 3:D:665:GLN:OE1   | 3:D:669:GLN:NE2   | 2.30                     | 0.64              |
| 1:B:215:GLU:OE1   | 1:B:219:ARG:NH1   | 2.30                     | 0.64              |
| 2:C:39:ILE:HG13   | 2:C:40:GLU:H      | 1.62                     | 0.64              |
| 1:A:39:LEU:O      | 1:A:43:LEU:HG     | 1.96                     | 0.64              |
| 2:C:1018:TYR:HE1  | 2:C:1022:LYS:HZ2  | 1.43                     | 0.64              |
| 5:L:761:ILE:HG22  | 5:L:775:GLN:HB2   | 1.79                     | 0.64              |
| 2:C:185:ASP:OD2   | 2:C:200:ARG:NH2   | 2.30                     | 0.64              |
| 5:L:174:LEU:HD21  | 5:L:324:HIS:HD1   | 1.63                     | 0.63              |
| 1:A:131:CYS:SG    | 1:A:132:HIS:N     | 2.71                     | 0.63              |
| 5:L:128:LEU:HD11  | 5:L:722:LEU:HA    | 1.81                     | 0.63              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:222:THR:O    | 1:B:226:GLU:HG2   | 1.99                     | 0.63              |
| 2:C:403:MET:HG2  | 2:C:414:ILE:HD12  | 1.80                     | 0.62              |
| 2:C:1313:HIS:O   | 2:C:1314:GLN:NE2  | 2.32                     | 0.62              |
| 5:L:911:ASP:OD1  | 5:L:912:GLU:N     | 2.31                     | 0.62              |
| 1:A:16:ILE:HG23  | 1:A:26:VAL:HG22   | 1.80                     | 0.62              |
| 5:L:664:ASP:O    | 5:L:667:ILE:HG22  | 2.00                     | 0.62              |
| 2:C:12:ARG:NH1   | 2:C:1182:ILE:O    | 2.33                     | 0.62              |
| 3:D:749:LYS:CG   | 3:D:750:PRO:HD2   | 2.28                     | 0.62              |
| 1:A:67:GLU:HG3   | 1:A:171:LEU:HD22  | 1.81                     | 0.62              |
| 2:C:254:ASP:HB2  | 2:C:265:LYS:HB2   | 1.82                     | 0.62              |
| 3:D:949:SER:HB2  | 3:D:1016:THR:HG23 | 1.81                     | 0.62              |
| 5:L:943:ARG:O    | 5:L:947:MET:HG2   | 1.99                     | 0.62              |
| 3:D:1110:GLU:HG2 | 3:D:1111:ASP:H    | 1.65                     | 0.62              |
| 5:L:461:GLU:O    | 5:L:465:ARG:HG2   | 2.00                     | 0.62              |
| 5:L:807:LYS:HD3  | 5:L:967:HIS:HD2   | 1.64                     | 0.62              |
| 2:C:755:LYS:NZ   | 2:C:767:GLN:O     | 2.32                     | 0.62              |
| 3:D:338:PHE:HA   | 3:D:342:LEU:HB2   | 1.82                     | 0.62              |
| 2:C:142:GLU:HB3  | 2:C:515:MET:HE3   | 1.82                     | 0.62              |
| 5:L:110:LYS:HB2  | 5:L:112:GLN:HE22  | 1.64                     | 0.62              |
| 2:C:79:VAL:HG13  | 2:C:80:PHE:HD1    | 1.65                     | 0.62              |
| 5:L:664:ASP:O    | 5:L:668:LYS:HG2   | 2.00                     | 0.62              |
| 2:C:629:PHE:HB2  | 2:C:647:ARG:HG2   | 1.82                     | 0.61              |
| 2:C:677:ASN:OD1  | 2:C:678:ARG:N     | 2.33                     | 0.61              |
| 3:D:1208:ASP:OD1 | 3:D:1209:VAL:N    | 2.33                     | 0.61              |
| 5:L:130:TYR:CZ   | 5:L:134:LYS:HD2   | 2.35                     | 0.61              |
| 5:L:431:ARG:NH2  | 5:L:632:PHE:O     | 2.30                     | 0.61              |
| 1:A:188:GLU:OE2  | 1:A:200:LYS:NZ    | 2.28                     | 0.61              |
| 1:A:104:LYS:HD2  | 1:A:110:VAL:HG22  | 1.82                     | 0.61              |
| 1:B:88:LEU:HD21  | 1:B:130:ILE:HD11  | 1.83                     | 0.61              |
| 3:D:216:LYS:O    | 3:D:219:LYS:HG2   | 2.00                     | 0.61              |
| 2:C:67:GLU:OE1   | 2:C:69:GLN:HG3    | 2.00                     | 0.61              |
| 2:C:558:VAL:HG11 | 2:C:573:ASN:HB3   | 1.83                     | 0.61              |
| 2:C:1243:MET:HE1 | 3:D:371:LYS:HD2   | 1.83                     | 0.61              |
| 2:C:1168:GLU:OE1 | 2:C:1171:ARG:NH2  | 2.34                     | 0.61              |
| 5:L:534:PHE:HE1  | 5:L:543:ARG:HB3   | 1.65                     | 0.60              |
| 3:D:1219:ASP:OD1 | 3:D:1220:ILE:N    | 2.34                     | 0.60              |
| 2:C:131:THR:HG23 | 2:C:133:ASN:H     | 1.65                     | 0.60              |
| 2:C:231:GLU:N    | 2:C:238:GLN:O     | 2.33                     | 0.60              |
| 2:C:231:GLU:O    | 2:C:238:GLN:N     | 2.33                     | 0.60              |
| 2:C:718:ALA:HB2  | 2:C:783:LEU:HD11  | 1.84                     | 0.60              |
| 5:L:110:LYS:HD3  | 5:L:957:LEU:HB2   | 1.84                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:L:534:PHE:CE1   | 5:L:543:ARG:HB3   | 2.36                     | 0.60              |
| 5:L:801:ILE:HG22  | 5:L:962:LEU:HB2   | 1.83                     | 0.60              |
| 1:B:104:LYS:HG2   | 1:B:110:VAL:HG22  | 1.83                     | 0.60              |
| 2:C:633:LEU:HG    | 2:C:644:LEU:HB3   | 1.83                     | 0.60              |
| 3:D:160:LEU:HD12  | 3:D:164:GLN:HB3   | 1.84                     | 0.60              |
| 3:D:357:VAL:HG23  | 3:D:358:GLY:H     | 1.66                     | 0.60              |
| 5:L:64:HIS:ND1    | 5:L:101:PHE:HB3   | 2.17                     | 0.60              |
| 1:B:191:ARG:HH11  | 1:B:193:GLU:HA    | 1.66                     | 0.60              |
| 3:D:1040:MET:HE1  | 3:D:1046:ILE:HG21 | 1.84                     | 0.60              |
| 3:D:1151:LYS:HG3  | 3:D:1152:GLU:OE1  | 2.01                     | 0.60              |
| 1:A:42:ALA:O      | 1:A:46:ILE:HG12   | 2.02                     | 0.59              |
| 2:C:458:GLU:O     | 2:C:462:ASN:ND2   | 2.35                     | 0.59              |
| 3:D:755:ILE:HD12  | 3:D:755:ILE:H     | 1.66                     | 0.59              |
| 3:D:1089:LEU:HD12 | 3:D:1094:ASP:HA   | 1.84                     | 0.59              |
| 2:C:464:PHE:O     | 2:C:468:LEU:HD23  | 2.02                     | 0.59              |
| 3:D:1002:VAL:HB   | 3:D:1019:ASN:HB2  | 1.84                     | 0.59              |
| 5:L:578:MET:HE1   | 5:L:580:MET:HG2   | 1.84                     | 0.59              |
| 1:A:58:GLU:HG3    | 1:A:170:ARG:HD2   | 1.85                     | 0.59              |
| 1:B:82:LEU:HD11   | 1:B:171:LEU:HD21  | 1.83                     | 0.59              |
| 2:C:358:ASP:OD1   | 2:C:359:ARG:N     | 2.36                     | 0.59              |
| 3:D:337:ARG:O     | 3:D:340:GLN:N     | 2.34                     | 0.59              |
| 3:D:973:LEU:HB3   | 3:D:1003:LEU:HD22 | 1.83                     | 0.59              |
| 1:A:229:GLU:O     | 1:A:232:VAL:HG22  | 2.03                     | 0.59              |
| 2:C:1013:GLN:O    | 2:C:1016:GLU:HG2  | 2.03                     | 0.59              |
| 5:L:530:ARG:HD2   | 5:L:549:TRP:HZ2   | 1.68                     | 0.59              |
| 2:C:206:ALA:O     | 2:C:209:ILE:HG22  | 2.02                     | 0.59              |
| 2:C:582:ASN:HD22  | 2:C:586:PHE:HB2   | 1.67                     | 0.59              |
| 3:D:1172:LYS:HE3  | 3:D:1189:MET:HB3  | 1.84                     | 0.59              |
| 5:L:151:ARG:NH2   | 5:L:221:ARG:O     | 2.36                     | 0.59              |
| 5:L:370:LEU:HB3   | 5:L:386:LEU:HD21  | 1.85                     | 0.59              |
| 2:C:85:CYS:SG     | 2:C:90:VAL:HG13   | 2.42                     | 0.59              |
| 2:C:1060:ILE:HD13 | 2:C:1234:LYS:HD2  | 1.84                     | 0.59              |
| 2:C:470:ARG:O     | 2:C:473:ARG:HG2   | 2.02                     | 0.59              |
| 3:D:782:GLY:O     | 3:D:786:THR:HG23  | 2.03                     | 0.59              |
| 5:L:936:LEU:O     | 5:L:940:GLU:HG3   | 2.02                     | 0.59              |
| 1:B:124:VAL:HG11  | 1:B:210:THR:HG22  | 1.85                     | 0.58              |
| 3:D:79:LYS:O      | 3:D:81:ARG:NH1    | 2.36                     | 0.58              |
| 3:D:968:ASN:ND2   | 3:D:1117:SER:O    | 2.36                     | 0.58              |
| 5:L:508:VAL:HG23  | 5:L:579:VAL:HG23  | 1.84                     | 0.58              |
| 1:B:12:ARG:HG2    | 1:B:13:LEU:N      | 2.17                     | 0.58              |
| 2:C:17:LYS:N      | 2:C:1188:ASP:OD2  | 2.35                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:423:ASP:HA    | 2:C:426:ILE:HG12  | 1.85                     | 0.58              |
| 3:D:515:ARG:HH21  | 3:D:717:VAL:HG13  | 1.68                     | 0.58              |
| 5:L:12:ASP:OD1    | 5:L:51:THR:OG1    | 2.21                     | 0.58              |
| 2:C:560:PRO:O     | 3:D:780:ARG:NH2   | 2.36                     | 0.58              |
| 3:D:818:GLU:OE1   | 3:D:818:GLU:N     | 2.37                     | 0.58              |
| 3:D:964:LYS:O     | 3:D:976:THR:OG1   | 2.21                     | 0.58              |
| 3:D:143:SER:OG    | 3:D:160:LEU:O     | 2.18                     | 0.58              |
| 3:D:146:VAL:HG12  | 3:D:178:ALA:HB2   | 1.86                     | 0.58              |
| 3:D:646:ILE:HD11  | 3:D:762:ASN:HD21  | 1.69                     | 0.58              |
| 3:D:1048:ARG:HG2  | 3:D:1059:LEU:HD21 | 1.84                     | 0.58              |
| 2:C:888:THR:HB    | 2:C:914:LYS:HD3   | 1.85                     | 0.58              |
| 2:C:1128:ILE:HA   | 2:C:1131:MET:HG2  | 1.85                     | 0.58              |
| 2:C:1274:GLU:HG3  | 3:D:428:THR:HG21  | 1.84                     | 0.58              |
| 5:L:129:ARG:NH2   | 5:L:958:ASP:OD1   | 2.36                     | 0.58              |
| 3:D:1162:ILE:HD13 | 3:D:1203:ARG:HH22 | 1.68                     | 0.58              |
| 5:L:114:ARG:HD2   | 5:L:117:ALA:HB3   | 1.85                     | 0.58              |
| 3:D:306:LEU:O     | 3:D:326:SER:OG    | 2.21                     | 0.58              |
| 3:D:66:LYS:HD3    | 3:D:69:GLU:HG2    | 1.84                     | 0.58              |
| 3:D:905:ARG:NH2   | 3:D:907:HIS:HB2   | 2.17                     | 0.58              |
| 3:D:1075:ARG:HH21 | 3:D:1168:GLU:HB3  | 1.68                     | 0.58              |
| 5:L:98:ARG:HG3    | 5:L:98:ARG:HH11   | 1.69                     | 0.58              |
| 2:C:1290:MET:HA   | 2:C:1294:LYS:HG3  | 1.85                     | 0.58              |
| 3:D:532:GLU:HA    | 3:D:535:ARG:HD3   | 1.84                     | 0.58              |
| 2:C:575:LEU:HD21  | 2:C:579:ALA:HB3   | 1.86                     | 0.58              |
| 3:D:417:ARG:HB3   | 3:D:418:GLU:OE1   | 2.04                     | 0.58              |
| 2:C:1142:ARG:HH22 | 2:C:1165:SER:HA   | 1.68                     | 0.57              |
| 3:D:660:GLU:O     | 3:D:663:GLU:HG3   | 2.04                     | 0.57              |
| 2:C:314:ASN:ND2   | 2:C:352:ARG:HE    | 2.01                     | 0.57              |
| 3:D:528:THR:N     | 3:D:532:GLU:OE2   | 2.28                     | 0.57              |
| 3:D:1067:ARG:HH21 | 3:D:1076:PRO:HD2  | 1.67                     | 0.57              |
| 1:B:73:GLY:O      | 1:B:134:THR:OG1   | 2.12                     | 0.57              |
| 2:C:231:GLU:OE2   | 2:C:233:ARG:NH1   | 2.38                     | 0.57              |
| 4:E:32:VAL:O      | 4:E:34:GLY:N      | 2.33                     | 0.57              |
| 5:L:826:ALA:HB3   | 5:L:832:LEU:HD13  | 1.86                     | 0.57              |
| 1:B:91:ARG:HH22   | 1:B:179:PRO:HB3   | 1.69                     | 0.57              |
| 1:B:225:ALA:O     | 1:B:229:GLU:HG3   | 2.03                     | 0.57              |
| 3:D:413:ASP:OD1   | 3:D:417:ARG:NH1   | 2.37                     | 0.57              |
| 5:L:108:PHE:HE1   | 5:L:114:ARG:HD3   | 1.69                     | 0.57              |
| 1:B:33:ARG:NH1    | 2:C:1081:PRO:HG3  | 2.20                     | 0.57              |
| 1:B:92:VAL:HB     | 1:B:121:VAL:HG12  | 1.85                     | 0.57              |
| 2:C:1062:PRO:HA   | 2:C:1076:ILE:HG23 | 1.85                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:860:ARG:HG3   | 3:D:861:ASN:H     | 1.70                     | 0.57              |
| 3:D:424:ASN:OD1   | 3:D:425:ARG:N     | 2.38                     | 0.57              |
| 2:C:81:ASP:OD1    | 2:C:84:GLU:HB3    | 2.05                     | 0.57              |
| 5:L:813:THR:HG22  | 5:L:965:VAL:HB    | 1.87                     | 0.57              |
| 2:C:402:ARG:NH2   | 2:C:417:SER:O     | 2.28                     | 0.57              |
| 3:D:961:SER:OG    | 3:D:981:GLU:HB3   | 2.05                     | 0.57              |
| 3:D:45:ASN:C      | 3:D:47:ARG:H      | 2.13                     | 0.57              |
| 3:D:980:THR:OG1   | 3:D:997:VAL:O     | 2.21                     | 0.57              |
| 5:L:785:ARG:HH11  | 5:L:785:ARG:HG2   | 1.70                     | 0.57              |
| 5:L:359:LEU:HB2   | 5:L:365:LEU:HD11  | 1.86                     | 0.56              |
| 5:L:523:LEU:HD22  | 5:L:529:ILE:HD12  | 1.86                     | 0.56              |
| 1:B:90:VAL:HG12   | 1:B:123:ILE:HG22  | 1.87                     | 0.56              |
| 2:C:153:PRO:HA    | 2:C:177:ILE:HG13  | 1.86                     | 0.56              |
| 3:D:418:GLU:HG2   | 4:E:48:VAL:HG21   | 1.87                     | 0.56              |
| 3:D:473:THR:HG23  | 3:D:476:ALA:H     | 1.70                     | 0.56              |
| 3:D:1264:ALA:HB2  | 3:D:1280:VAL:HG22 | 1.87                     | 0.56              |
| 1:A:45:ARG:HE     | 2:C:1083:GLU:HG3  | 1.71                     | 0.56              |
| 1:A:162:GLU:OE1   | 1:A:162:GLU:N     | 2.39                     | 0.56              |
| 2:C:802:VAL:HG12  | 2:C:1096:ILE:HB   | 1.86                     | 0.56              |
| 3:D:1045:THR:OG1  | 3:D:1071:GLY:HA3  | 2.06                     | 0.56              |
| 1:B:91:ARG:NH2    | 1:B:210:THR:OG1   | 2.38                     | 0.56              |
| 4:E:72:GLN:HA     | 4:E:75:GLN:HE21   | 1.69                     | 0.56              |
| 2:C:1291:LEU:O    | 3:D:345:LYS:NZ    | 2.38                     | 0.56              |
| 3:D:1163:VAL:HG23 | 3:D:1177:ILE:HD13 | 1.88                     | 0.56              |
| 2:C:987:GLU:HG3   | 2:C:988:LYS:H     | 1.70                     | 0.56              |
| 3:D:491:LEU:HB2   | 3:D:904:ALA:HA    | 1.87                     | 0.56              |
| 5:L:727:GLY:O     | 5:L:743:SER:OG    | 2.17                     | 0.56              |
| 3:D:399:LYS:O     | 3:D:403:ARG:HG3   | 2.05                     | 0.56              |
| 3:D:821:MET:HA    | 3:D:881:LYS:HA    | 1.88                     | 0.56              |
| 5:L:578:MET:HG2   | 5:L:597:LEU:HD21  | 1.88                     | 0.56              |
| 3:D:1157:ALA:O    | 3:D:1207:GLY:N    | 2.33                     | 0.55              |
| 2:C:12:ARG:HD3    | 2:C:1183:ALA:HB2  | 1.88                     | 0.55              |
| 3:D:370:LYS:HA    | 3:D:441:LEU:HD12  | 1.88                     | 0.55              |
| 3:D:607:THR:HA    | 3:D:610:ARG:HG2   | 1.88                     | 0.55              |
| 5:L:561:LEU:HD23  | 5:L:562:CYS:N     | 2.21                     | 0.55              |
| 5:L:873:GLY:O     | 5:L:877:VAL:HG23  | 2.06                     | 0.55              |
| 3:D:742:GLY:O     | 3:D:762:ASN:HB3   | 2.06                     | 0.55              |
| 5:L:566:GLY:HA3   | 5:L:596:ARG:HE    | 1.71                     | 0.55              |
| 1:A:82:LEU:O      | 1:A:86:LYS:HG3    | 2.06                     | 0.55              |
| 1:B:219:ARG:O     | 1:B:223:ILE:HG13  | 2.07                     | 0.55              |
| 3:D:1037:PHE:HB3  | 3:D:1040:MET:HB3  | 1.87                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:82:GLY:O      | 5:L:43:TYR:HA     | 2.07                     | 0.55              |
| 5:L:110:LYS:O     | 5:L:112:GLN:N     | 2.40                     | 0.55              |
| 5:L:817:GLU:HG3   | 5:L:844:LEU:HD13  | 1.87                     | 0.55              |
| 2:C:960:LEU:O     | 2:C:963:GLU:HG3   | 2.06                     | 0.55              |
| 3:D:1344:LEU:C    | 3:D:1346:GLY:H    | 2.13                     | 0.55              |
| 5:L:317:GLU:O     | 5:L:318:GLN:HG2   | 2.06                     | 0.55              |
| 3:D:1173:ARG:N    | 3:D:1192:LYS:HZ1  | 2.04                     | 0.55              |
| 3:D:131:PRO:HG2   | 3:D:134:ASP:OD2   | 2.07                     | 0.55              |
| 3:D:282:LEU:HD12  | 3:D:295:GLU:HG3   | 1.88                     | 0.55              |
| 3:D:1082:ASP:HB2  | 3:D:1088:VAL:HG23 | 1.88                     | 0.55              |
| 5:L:647:TYR:O     | 5:L:651:ILE:HG12  | 2.07                     | 0.55              |
| 1:B:163:GLU:N     | 1:B:163:GLU:OE1   | 2.40                     | 0.55              |
| 3:D:218:THR:HA    | 3:D:221:ILE:HG22  | 1.89                     | 0.55              |
| 3:D:267:ASP:OD1   | 3:D:270:ARG:NH2   | 2.40                     | 0.55              |
| 3:D:1061:VAL:HG21 | 3:D:1101:LEU:HD12 | 1.88                     | 0.55              |
| 5:L:630:ASP:OD2   | 5:L:634:HIS:ND1   | 2.34                     | 0.55              |
| 2:C:241:LEU:HD21  | 2:C:246:LEU:HD21  | 1.88                     | 0.54              |
| 2:C:1030:GLU:OE2  | 2:C:1034:ARG:NH1  | 2.40                     | 0.54              |
| 5:L:675:GLU:HA    | 5:L:678:LYS:HG2   | 1.89                     | 0.54              |
| 1:B:105:SER:HA    | 1:B:138:ALA:O     | 2.07                     | 0.54              |
| 3:D:1189:MET:O    | 3:D:1190:ILE:HD13 | 2.07                     | 0.54              |
| 5:L:324:HIS:CE1   | 5:L:327:ARG:HH21  | 2.26                     | 0.54              |
| 2:C:1244:HIS:NE2  | 2:C:1265:PHE:O    | 2.40                     | 0.54              |
| 5:L:21:THR:N      | 5:L:33:LEU:O      | 2.39                     | 0.54              |
| 5:L:282:ALA:HB2   | 5:L:311:LEU:HD12  | 1.88                     | 0.54              |
| 2:C:11:ILE:HG21   | 2:C:1159:VAL:HG11 | 1.89                     | 0.54              |
| 2:C:683:ALA:O     | 2:C:687:ARG:HG3   | 2.07                     | 0.54              |
| 2:C:1142:ARG:NH2  | 2:C:1165:SER:HA   | 2.23                     | 0.54              |
| 3:D:450:HIS:NE2   | 3:D:625:MET:HE1   | 2.22                     | 0.54              |
| 3:D:1052:GLU:OE1  | 3:D:1052:GLU:N    | 2.35                     | 0.54              |
| 2:C:393:ASP:OD1   | 2:C:394:ARG:N     | 2.41                     | 0.54              |
| 2:C:368:ARG:HH11  | 2:C:373:GLY:H     | 1.56                     | 0.54              |
| 3:D:515:ARG:NH2   | 3:D:718:SER:O     | 2.31                     | 0.54              |
| 5:L:5:LEU:HA      | 5:L:22:VAL:HG12   | 1.89                     | 0.54              |
| 1:A:56:VAL:HG12   | 1:A:146:VAL:HG22  | 1.89                     | 0.54              |
| 1:A:88:LEU:HD11   | 1:A:130:ILE:HD11  | 1.90                     | 0.54              |
| 3:D:128:LEU:HB3   | 3:D:130:MET:HE2   | 1.88                     | 0.54              |
| 5:L:321:MET:O     | 5:L:324:HIS:HB2   | 2.08                     | 0.54              |
| 2:C:3:TYR:O       | 2:C:8:LYS:NZ      | 2.41                     | 0.54              |
| 2:C:149:LEU:HD23  | 2:C:451:ARG:HH21  | 1.73                     | 0.54              |
| 2:C:469:VAL:O     | 2:C:472:GLU:HG3   | 2.08                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:363:LEU:HA   | 3:D:450:HIS:CD2   | 2.44                     | 0.53              |
| 1:B:99:ILE:HD11  | 1:B:143:ARG:CD    | 2.38                     | 0.53              |
| 1:B:145:LYS:NZ   | 1:B:147:GLN:OE1   | 2.40                     | 0.53              |
| 3:D:1033:GLY:HA3 | 3:D:1082:ASP:HA   | 1.90                     | 0.53              |
| 5:L:287:TRP:CD1  | 5:L:292:PRO:HB3   | 2.43                     | 0.53              |
| 2:C:187:GLU:O    | 2:C:195:PHE:N     | 2.31                     | 0.53              |
| 2:C:211:ARG:NE   | 2:C:357:ASN:O     | 2.42                     | 0.53              |
| 2:C:813:GLU:HB2  | 3:D:461:PHE:HD2   | 1.74                     | 0.53              |
| 3:D:572:THR:HG21 | 3:D:589:TYR:CE2   | 2.44                     | 0.53              |
| 5:L:19:LEU:HD12  | 5:L:103:ASP:O     | 2.08                     | 0.53              |
| 5:L:935:GLU:O    | 5:L:939:ILE:HD12  | 2.09                     | 0.53              |
| 3:D:111:THR:HG21 | 3:D:303:VAL:HG11  | 1.90                     | 0.53              |
| 1:A:73:GLY:N     | 2:C:728:ASP:OD1   | 2.42                     | 0.53              |
| 2:C:88:ARG:NH2   | 2:C:1036:ILE:O    | 2.42                     | 0.53              |
| 3:D:161:THR:HG22 | 3:D:164:GLN:HB2   | 1.91                     | 0.53              |
| 3:D:952:VAL:O    | 3:D:1014:GLY:N    | 2.28                     | 0.53              |
| 5:L:105:LYS:HD3  | 5:L:105:LYS:N     | 2.23                     | 0.53              |
| 5:L:440:LEU:HD12 | 5:L:441:PRO:HD2   | 1.89                     | 0.53              |
| 5:L:517:LEU:HA   | 5:L:520:GLU:HG2   | 1.91                     | 0.53              |
| 3:D:1219:ASP:O   | 3:D:1223:LEU:HG   | 2.09                     | 0.53              |
| 5:L:338:ASP:O    | 5:L:341:GLN:HG2   | 2.08                     | 0.53              |
| 1:A:109:PRO:HB3  | 1:A:132:HIS:CE1   | 2.44                     | 0.53              |
| 1:B:6:THR:OG1    | 1:B:7:GLU:N       | 2.39                     | 0.53              |
| 2:C:224:PHE:HB2  | 2:C:347:ILE:HD13  | 1.90                     | 0.53              |
| 2:C:1023:HIS:O   | 2:C:1026:GLU:HG3  | 2.08                     | 0.53              |
| 3:D:77:ARG:NH2   | 5:L:746:MET:HE3   | 2.24                     | 0.53              |
| 1:A:228:LEU:O    | 1:A:232:VAL:HG13  | 2.10                     | 0.52              |
| 3:D:294:ASN:OD1  | 3:D:297:ARG:NH2   | 2.42                     | 0.52              |
| 3:D:1005:LYS:HD3 | 3:D:1011:VAL:HG22 | 1.90                     | 0.52              |
| 5:L:360:LEU:HB3  | 5:L:687:ARG:HH21  | 1.73                     | 0.52              |
| 5:L:889:GLN:HA   | 5:L:892:GLU:HG3   | 1.92                     | 0.52              |
| 2:C:348:SER:O    | 2:C:352:ARG:HG2   | 2.10                     | 0.52              |
| 2:C:468:LEU:HA   | 2:C:471:VAL:HG12  | 1.90                     | 0.52              |
| 2:C:1275:VAL:O   | 2:C:1279:GLU:HG3  | 2.10                     | 0.52              |
| 3:D:747:MET:HE2  | 3:D:759:ILE:HD12  | 1.92                     | 0.52              |
| 3:D:901:ARG:HD2  | 3:D:906:GLY:O     | 2.08                     | 0.52              |
| 2:C:624:ASP:O    | 2:C:626:GLU:N     | 2.40                     | 0.52              |
| 2:C:696:ASP:OD1  | 2:C:697:LYS:N     | 2.36                     | 0.52              |
| 1:B:90:VAL:O     | 1:B:91:ARG:HD3    | 2.10                     | 0.52              |
| 2:C:895:LEU:HB2  | 2:C:900:LYS:HG3   | 1.90                     | 0.52              |
| 2:C:1017:GLN:O   | 2:C:1021:LEU:HD23 | 2.08                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1259:LEU:O    | 2:C:1266:GLY:HA2  | 2.10                     | 0.52              |
| 3:D:820:ILE:HG12  | 3:D:1227:HIS:ND1  | 2.24                     | 0.52              |
| 1:B:20:SER:O      | 1:B:22:THR:N      | 2.43                     | 0.52              |
| 2:C:275:ARG:O     | 2:C:279:LYS:HG2   | 2.10                     | 0.52              |
| 2:C:600:THR:OG1   | 2:C:602:GLU:OE1   | 2.23                     | 0.52              |
| 2:C:947:GLU:O     | 2:C:950:GLU:HG3   | 2.10                     | 0.52              |
| 3:D:974:VAL:HG11  | 3:D:1028:ILE:HG21 | 1.92                     | 0.52              |
| 2:C:249:GLU:O     | 2:C:269:ILE:HG22  | 2.09                     | 0.52              |
| 3:D:824:PRO:HD3   | 3:D:835:LEU:HD13  | 1.90                     | 0.52              |
| 3:D:1048:ARG:HG2  | 3:D:1048:ARG:HH11 | 1.75                     | 0.52              |
| 2:C:719:LYS:O     | 2:C:779:ARG:NH1   | 2.42                     | 0.52              |
| 3:D:526:VAL:HG12  | 3:D:549:LYS:HB2   | 1.91                     | 0.52              |
| 3:D:1024:THR:O    | 3:D:1025:MET:HE2  | 2.10                     | 0.52              |
| 3:D:952:VAL:HG13  | 3:D:984:LEU:HD22  | 1.92                     | 0.52              |
| 3:D:972:LYS:NZ    | 3:D:974:VAL:HA    | 2.25                     | 0.52              |
| 3:D:1002:VAL:N    | 3:D:1019:ASN:O    | 2.43                     | 0.52              |
| 1:B:76:GLU:HG3    | 1:B:81:ILE:HD11   | 1.92                     | 0.52              |
| 2:C:672:GLU:HG3   | 2:C:673:HIS:CD2   | 2.45                     | 0.52              |
| 2:C:1298:VAL:HG23 | 2:C:1299:ASN:H    | 1.75                     | 0.52              |
| 1:B:75:GLN:HG2    | 1:B:76:GLU:N      | 2.25                     | 0.51              |
| 1:B:192:VAL:O     | 1:B:194:GLN:N     | 2.39                     | 0.51              |
| 2:C:1070:HIS:NE2  | 2:C:1114:GLU:OE1  | 2.43                     | 0.51              |
| 3:D:1305:ASP:OD1  | 3:D:1306:LEU:N    | 2.43                     | 0.51              |
| 1:A:19:VAL:HG21   | 1:A:23:HIS:HD2    | 1.75                     | 0.51              |
| 2:C:4:SER:C       | 2:C:8:LYS:HZ3     | 2.18                     | 0.51              |
| 2:C:699:LEU:HG    | 2:C:799:ASN:ND2   | 2.25                     | 0.51              |
| 3:D:518:VAL:HG12  | 3:D:707:ILE:HD11  | 1.93                     | 0.51              |
| 5:L:230:PHE:CD1   | 5:L:234:ARG:HG2   | 2.44                     | 0.51              |
| 5:L:350:ARG:HB3   | 5:L:351:PRO:HD3   | 1.93                     | 0.51              |
| 1:A:215:GLU:OE1   | 1:A:215:GLU:N     | 2.40                     | 0.51              |
| 2:C:812:PHE:O     | 2:C:1099:ASN:ND2  | 2.44                     | 0.51              |
| 2:C:1103:VAL:HG22 | 2:C:1111:GLN:HE21 | 1.75                     | 0.51              |
| 3:D:959:LYS:HA    | 3:D:959:LYS:HE2   | 1.92                     | 0.51              |
| 3:D:978:ARG:HD3   | 3:D:999:TYR:HB2   | 1.91                     | 0.51              |
| 3:D:1280:VAL:HG11 | 3:D:1304:ARG:HH21 | 1.75                     | 0.51              |
| 5:L:300:GLU:HA    | 5:L:330:LEU:HD11  | 1.93                     | 0.51              |
| 3:D:212:THR:O     | 3:D:215:LYS:HG2   | 2.11                     | 0.51              |
| 3:D:615:LYS:NZ    | 4:E:5:THR:HB      | 2.26                     | 0.51              |
| 3:D:850:LYS:HE2   | 3:D:851:PRO:HD2   | 1.92                     | 0.51              |
| 3:D:1067:ARG:HE   | 3:D:1076:PRO:HD2  | 1.75                     | 0.51              |
| 3:D:1221:LEU:HD13 | 3:D:1306:LEU:HB2  | 1.93                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:L:215:TRP:O    | 5:L:218:GLU:HG3   | 2.10                     | 0.51              |
| 2:C:788:SER:OG   | 2:C:795:ALA:O     | 2.27                     | 0.51              |
| 3:D:163:GLU:HA   | 3:D:166:LEU:HD12  | 1.93                     | 0.51              |
| 3:D:1170:LYS:HB3 | 3:D:1174:ARG:HH12 | 1.76                     | 0.51              |
| 2:C:819:SER:HB3  | 2:C:1085:MET:HE2  | 1.93                     | 0.51              |
| 2:C:987:GLU:HG3  | 2:C:988:LYS:N     | 2.25                     | 0.51              |
| 3:D:863:LEU:HD11 | 3:D:901:ARG:HB3   | 1.91                     | 0.51              |
| 3:D:1273:ASP:H   | 3:D:1276:GLU:CD   | 2.19                     | 0.51              |
| 5:L:538:MET:HB3  | 5:L:542:GLU:HG3   | 1.92                     | 0.51              |
| 3:D:337:ARG:HG3  | 3:D:338:PHE:H     | 1.76                     | 0.51              |
| 3:D:1164:SER:HA  | 3:D:1200:GLU:HG2  | 1.93                     | 0.51              |
| 5:L:54:MET:HG3   | 5:L:81:LEU:HD13   | 1.93                     | 0.51              |
| 1:A:183:ILE:HD13 | 1:A:205:MET:HG3   | 1.93                     | 0.51              |
| 3:D:139:LEU:HD21 | 3:D:300:GLN:HG2   | 1.93                     | 0.51              |
| 3:D:545:HIS:CE1  | 3:D:719:PHE:HE2   | 2.28                     | 0.51              |
| 5:L:924:LEU:O    | 5:L:928:ASN:N     | 2.43                     | 0.51              |
| 2:C:106:GLU:HB3  | 2:C:109:ALA:HB3   | 1.93                     | 0.51              |
| 2:C:1033:ARG:HA  | 2:C:1036:ILE:HG22 | 1.93                     | 0.51              |
| 2:C:1269:ARG:NH2 | 3:D:340:GLN:HA    | 2.25                     | 0.51              |
| 3:D:1075:ARG:HB3 | 3:D:1100:PHE:HE2  | 1.76                     | 0.51              |
| 5:L:9:TRP:CE3    | 5:L:50:VAL:HG12   | 2.45                     | 0.51              |
| 2:C:466:VAL:O    | 2:C:469:VAL:HG22  | 2.12                     | 0.50              |
| 3:D:661:VAL:HG22 | 3:D:685:ILE:HD11  | 1.92                     | 0.50              |
| 3:D:514:THR:HG21 | 3:D:596:LEU:HD12  | 1.93                     | 0.50              |
| 3:D:1323:ALA:HA  | 3:D:1331:VAL:HG11 | 1.92                     | 0.50              |
| 5:L:64:HIS:HA    | 5:L:103:ASP:OD1   | 2.11                     | 0.50              |
| 1:B:77:ASP:OD1   | 1:B:78:ILE:N      | 2.39                     | 0.50              |
| 1:B:156:SER:HA   | 1:B:159:ILE:HG22  | 1.94                     | 0.50              |
| 2:C:551:HIS:HD2  | 2:C:552:PRO:HD2   | 1.73                     | 0.50              |
| 3:D:197:GLU:N    | 3:D:197:GLU:OE1   | 2.44                     | 0.50              |
| 2:C:230:PHE:HE2  | 2:C:335:THR:HG21  | 1.75                     | 0.50              |
| 3:D:984:LEU:O    | 3:D:991:THR:HA    | 2.12                     | 0.50              |
| 5:L:404:VAL:O    | 5:L:408:MET:HG3   | 2.12                     | 0.50              |
| 2:C:469:VAL:HA   | 2:C:472:GLU:HG3   | 1.93                     | 0.50              |
| 3:D:327:LEU:HA   | 3:D:330:MET:HE2   | 1.94                     | 0.50              |
| 3:D:527:LEU:HD22 | 3:D:532:GLU:HG3   | 1.92                     | 0.50              |
| 3:D:1075:ARG:NH2 | 3:D:1168:GLU:HB3  | 2.26                     | 0.50              |
| 3:D:1311:LYS:HZ2 | 3:D:1314:LEU:HD13 | 1.76                     | 0.50              |
| 5:L:466:ASP:HB3  | 5:L:473:ILE:HD11  | 1.93                     | 0.50              |
| 1:B:44:ARG:HA    | 1:B:183:ILE:HD13  | 1.94                     | 0.50              |
| 2:C:1122:LYS:HG2 | 2:C:1229:TYR:CE1  | 2.47                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:18:ASP:N      | 3:D:18:ASP:OD1    | 2.45                     | 0.50              |
| 3:D:357:VAL:HG23  | 3:D:358:GLY:N     | 2.26                     | 0.50              |
| 3:D:861:ASN:ND2   | 3:D:861:ASN:O     | 2.45                     | 0.50              |
| 5:L:10:ILE:HG23   | 5:L:19:LEU:HD23   | 1.94                     | 0.50              |
| 1:B:137:ASN:OD1   | 1:B:138:ALA:N     | 2.36                     | 0.50              |
| 2:C:808:ASN:OD1   | 2:C:1216:ARG:NH2  | 2.45                     | 0.50              |
| 2:C:985:GLU:OE2   | 2:C:988:LYS:N     | 2.45                     | 0.50              |
| 2:C:1082:ILE:H    | 2:C:1082:ILE:HD12 | 1.76                     | 0.50              |
| 3:D:41:PRO:HG3    | 3:D:274:ASN:OD1   | 2.11                     | 0.50              |
| 2:C:829:THR:HG22  | 2:C:1059:ARG:HA   | 1.94                     | 0.50              |
| 3:D:137:ARG:HA    | 3:D:142:GLU:OE2   | 2.11                     | 0.50              |
| 3:D:1155:ILE:HD12 | 3:D:1211:SER:HB3  | 1.94                     | 0.50              |
| 5:L:934:ASP:OD1   | 5:L:935:GLU:N     | 2.44                     | 0.50              |
| 1:A:201:LEU:HG    | 1:A:203:ILE:HD11  | 1.94                     | 0.50              |
| 2:C:595:THR:O     | 2:C:597:GLY:N     | 2.45                     | 0.50              |
| 3:D:356:THR:HG22  | 3:D:357:VAL:H     | 1.75                     | 0.50              |
| 3:D:981:GLU:OE2   | 3:D:994:SER:OG    | 2.20                     | 0.50              |
| 3:D:1215:GLU:OE1  | 3:D:1215:GLU:N    | 2.38                     | 0.50              |
| 5:L:279:VAL:HB    | 5:L:311:LEU:HD13  | 1.93                     | 0.50              |
| 2:C:102:LEU:HD12  | 2:C:489:PRO:HG3   | 1.94                     | 0.49              |
| 3:D:188:LEU:O     | 3:D:192:MET:HG2   | 2.12                     | 0.49              |
| 2:C:582:ASN:HD21  | 2:C:607:SER:HB3   | 1.77                     | 0.49              |
| 2:C:590:PRO:HB2   | 2:C:655:VAL:HG21  | 1.94                     | 0.49              |
| 2:C:1269:ARG:HH21 | 3:D:340:GLN:HA    | 1.75                     | 0.49              |
| 3:D:275:ARG:NH1   | 3:D:298:MET:HB3   | 2.27                     | 0.49              |
| 3:D:512:TYR:HD1   | 3:D:724:MET:HE1   | 1.77                     | 0.49              |
| 5:L:639:GLY:O     | 5:L:643:TYR:HB2   | 2.11                     | 0.49              |
| 5:L:646:VAL:HG12  | 5:L:650:LEU:HB2   | 1.94                     | 0.49              |
| 1:A:158:ARG:HH21  | 1:A:172:LEU:HD22  | 1.78                     | 0.49              |
| 2:C:81:ASP:O      | 2:C:85:CYS:HB2    | 2.12                     | 0.49              |
| 2:C:1033:ARG:HH12 | 2:C:1037:THR:HG21 | 1.77                     | 0.49              |
| 3:D:407:VAL:O     | 3:D:411:ILE:HG12  | 2.13                     | 0.49              |
| 2:C:120:GLN:H     | 2:C:120:GLN:CD    | 2.20                     | 0.49              |
| 3:D:215:LYS:HA    | 3:D:218:THR:HG22  | 1.95                     | 0.49              |
| 3:D:418:GLU:HB2   | 4:E:45:LYS:HE2    | 1.94                     | 0.49              |
| 3:D:1227:HIS:HA   | 3:D:1230:THR:HG22 | 1.94                     | 0.49              |
| 1:B:98:VAL:HG21   | 1:B:121:VAL:HG11  | 1.95                     | 0.49              |
| 1:B:102:LEU:O     | 1:B:141:SER:HA    | 2.13                     | 0.49              |
| 2:C:46:GLN:NE2    | 2:C:47:TYR:HB2    | 2.28                     | 0.49              |
| 4:E:18:ASP:O      | 4:E:22:VAL:HG12   | 2.12                     | 0.49              |
| 5:L:589:LEU:HA    | 5:L:592:GLN:HG2   | 1.94                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:94:ALA:HB2   | 2:C:129:LEU:HD11  | 1.94                     | 0.49              |
| 2:C:1087:TYR:CE1 | 2:C:1215:GLY:HA2  | 2.48                     | 0.49              |
| 3:D:535:ARG:HG2  | 3:D:535:ARG:HH11  | 1.76                     | 0.49              |
| 2:C:685:MET:HE1  | 2:C:1073:LYS:HG2  | 1.94                     | 0.49              |
| 2:C:1284:ALA:HB1 | 3:D:1356:LEU:HD22 | 1.93                     | 0.49              |
| 3:D:1197:ASN:OD1 | 3:D:1198:VAL:HG13 | 2.13                     | 0.49              |
| 3:D:1327:GLU:CD  | 3:D:1327:GLU:H    | 2.21                     | 0.49              |
| 4:E:7:GLN:O      | 4:E:11:GLU:HG3    | 2.12                     | 0.49              |
| 2:C:371:ARG:HA   | 2:C:371:ARG:HH11  | 1.78                     | 0.49              |
| 2:C:1312:ASN:OD1 | 2:C:1313:HIS:N    | 2.46                     | 0.49              |
| 3:D:196:GLN:O    | 3:D:199:GLU:HG3   | 2.13                     | 0.49              |
| 3:D:555:TYR:HB2  | 3:D:585:LYS:HB3   | 1.94                     | 0.49              |
| 3:D:733:SER:N    | 3:D:736:GLN:OE1   | 2.41                     | 0.49              |
| 3:D:925:GLU:HG3  | 3:D:926:PRO:HD3   | 1.95                     | 0.49              |
| 2:C:675:ASP:OD1  | 2:C:676:ALA:N     | 2.45                     | 0.49              |
| 2:C:750:ILE:HD13 | 2:C:959:ASP:OD2   | 2.12                     | 0.49              |
| 3:D:84:ILE:HG12  | 3:D:91:GLU:HB2    | 1.93                     | 0.49              |
| 3:D:553:THR:HG22 | 3:D:567:THR:HB    | 1.95                     | 0.49              |
| 3:D:886:VAL:HA   | 3:D:1258:ARG:HG3  | 1.95                     | 0.49              |
| 3:D:1021:ASP:HB3 | 3:D:1024:THR:HB   | 1.93                     | 0.49              |
| 3:D:1110:GLU:HG2 | 3:D:1111:ASP:N    | 2.27                     | 0.49              |
| 5:L:715:LEU:HD13 | 5:L:779:TRP:CE2   | 2.48                     | 0.49              |
| 1:A:41:ASN:O     | 1:A:45:ARG:HG2    | 2.13                     | 0.49              |
| 3:D:796:LEU:HA   | 3:D:799:ARG:HH21  | 1.78                     | 0.49              |
| 3:D:975:ILE:HG23 | 3:D:980:THR:HG21  | 1.95                     | 0.49              |
| 5:L:9:TRP:HE3    | 5:L:50:VAL:HG12   | 1.77                     | 0.49              |
| 2:C:77:GLU:OE1   | 2:C:78:PRO:HD2    | 2.13                     | 0.48              |
| 2:C:1285:TYR:HB2 | 3:D:479:GLU:OE2   | 2.13                     | 0.48              |
| 4:E:30:MET:HE3   | 4:E:46:THR:HG23   | 1.94                     | 0.48              |
| 1:B:123:ILE:O    | 1:B:123:ILE:HG13  | 2.13                     | 0.48              |
| 2:C:405:PHE:CE2  | 2:C:424:ASP:HB3   | 2.48                     | 0.48              |
| 2:C:557:ARG:HD3  | 2:C:587:LEU:HB3   | 1.95                     | 0.48              |
| 3:D:1194:ARG:HA  | 3:D:1194:ARG:NE   | 2.28                     | 0.48              |
| 5:L:723:PHE:HD1  | 5:L:728:ILE:HD12  | 1.78                     | 0.48              |
| 5:L:781:HIS:O    | 5:L:784:ILE:HG22  | 2.13                     | 0.48              |
| 2:C:848:GLU:HG3  | 2:C:886:LYS:HD2   | 1.95                     | 0.48              |
| 2:C:912:ASP:O    | 2:C:913:VAL:HG22  | 2.14                     | 0.48              |
| 3:D:507:VAL:HG23 | 3:D:601:ILE:HD12  | 1.95                     | 0.48              |
| 3:D:744:ARG:NH2  | 3:D:747:MET:HE1   | 2.28                     | 0.48              |
| 3:D:865:HIS:CE1  | 3:D:867:GLN:HB3   | 2.48                     | 0.48              |
| 5:L:399:ALA:O    | 5:L:403:LEU:HD23  | 2.12                     | 0.48              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:1158:GLU:HG3  | 3:D:1186:TYR:CZ  | 2.48                     | 0.48              |
| 5:L:716:ILE:O     | 5:L:720:MET:HG3  | 2.14                     | 0.48              |
| 2:C:57:PHE:HE1    | 2:C:68:LEU:HD22  | 1.78                     | 0.48              |
| 2:C:192:ASP:HB3   | 2:C:346:TYR:CE1  | 2.49                     | 0.48              |
| 3:D:77:ARG:HG3    | 3:D:79:LYS:H     | 1.78                     | 0.48              |
| 3:D:201:LEU:O     | 3:D:205:LEU:HD23 | 2.14                     | 0.48              |
| 2:C:693:LEU:HG    | 2:C:829:THR:O    | 2.13                     | 0.48              |
| 2:C:826:ASP:OD1   | 2:C:829:THR:OG1  | 2.27                     | 0.48              |
| 2:C:1246:ARG:HD2  | 2:C:1266:GLY:C   | 2.38                     | 0.48              |
| 4:E:26:ARG:NE     | 4:E:53:GLU:OE1   | 2.47                     | 0.48              |
| 2:C:232:ILE:HG12  | 2:C:331:LYS:HA   | 1.95                     | 0.48              |
| 3:D:423:LEU:HD23  | 3:D:466:MET:HE1  | 1.94                     | 0.48              |
| 5:L:264:GLN:O     | 5:L:268:HIS:ND1  | 2.47                     | 0.48              |
| 2:C:716:ALA:HB3   | 2:C:784:ALA:HB3  | 1.96                     | 0.48              |
| 3:D:156:ARG:HG2   | 3:D:157:GLN:OE1  | 2.13                     | 0.48              |
| 3:D:1219:ASP:HA   | 3:D:1222:ARG:NH1 | 2.28                     | 0.48              |
| 5:L:451:SER:O     | 5:L:455:GLY:N    | 2.47                     | 0.48              |
| 5:L:909:GLU:HA    | 5:L:912:GLU:OE2  | 2.13                     | 0.48              |
| 1:A:98:VAL:HG11   | 1:A:121:VAL:HG11 | 1.96                     | 0.48              |
| 2:C:257:ALA:HB3   | 2:C:262:TYR:CE2  | 2.49                     | 0.48              |
| 2:C:1247:SER:HB3  | 3:D:375:GLU:O    | 2.13                     | 0.48              |
| 3:D:709:ARG:HG3   | 3:D:710:ASP:H    | 1.78                     | 0.48              |
| 3:D:1046:ILE:HD11 | 3:D:1076:PRO:HG3 | 1.94                     | 0.48              |
| 5:L:130:TYR:CE2   | 5:L:134:LYS:HD2  | 2.49                     | 0.48              |
| 1:B:61:ILE:HG21   | 1:B:64:VAL:HG22  | 1.95                     | 0.48              |
| 2:C:97:ARG:HB3    | 2:C:121:GLU:HG3  | 1.95                     | 0.48              |
| 2:C:120:GLN:OE1   | 2:C:120:GLN:N    | 2.39                     | 0.48              |
| 2:C:589:THR:HG23  | 2:C:591:TYR:CE2  | 2.49                     | 0.48              |
| 3:D:885:VAL:HG23  | 3:D:894:VAL:HG11 | 1.96                     | 0.48              |
| 3:D:1319:PHE:CE2  | 3:D:1342:ASP:HB2 | 2.49                     | 0.48              |
| 2:C:53:PHE:HD1    | 2:C:57:PHE:HE2   | 1.62                     | 0.47              |
| 2:C:720:ARG:NH1   | 2:C:736:VAL:HG11 | 2.29                     | 0.47              |
| 3:D:1044:GLN:N    | 3:D:1044:GLN:OE1 | 2.46                     | 0.47              |
| 5:L:354:ASP:O     | 5:L:358:MET:HG2  | 2.14                     | 0.47              |
| 1:B:47:LEU:O      | 1:B:51:MET:HG3   | 2.14                     | 0.47              |
| 1:B:60:GLU:HB2    | 1:B:143:ARG:HG2  | 1.96                     | 0.47              |
| 2:C:1246:ARG:HD2  | 2:C:1266:GLY:O   | 2.15                     | 0.47              |
| 3:D:44:ILE:HG23   | 3:D:50:LYS:O     | 2.14                     | 0.47              |
| 3:D:146:VAL:CG2   | 3:D:158:GLN:HB3  | 2.44                     | 0.47              |
| 5:L:258:PHE:HA    | 5:L:261:ARG:HH12 | 1.80                     | 0.47              |
| 5:L:473:ILE:HG23  | 5:L:477:PHE:HE1  | 1.78                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:101:ARG:HD3  | 2:C:118:LYS:HD3  | 1.95                     | 0.47              |
| 2:C:271:ALA:HA   | 2:C:274:ILE:HD12 | 1.96                     | 0.47              |
| 2:C:472:GLU:HA   | 2:C:475:VAL:HG12 | 1.96                     | 0.47              |
| 3:D:756:GLU:O    | 3:D:758:PRO:HD2  | 2.14                     | 0.47              |
| 5:L:126:PHE:HA   | 5:L:797:GLY:O    | 2.14                     | 0.47              |
| 5:L:495:MET:HE2  | 5:L:523:LEU:HA   | 1.94                     | 0.47              |
| 5:L:751:PHE:HB3  | 5:L:754:LEU:HB2  | 1.96                     | 0.47              |
| 1:A:190:ALA:N    | 1:A:198:LEU:O    | 2.32                     | 0.47              |
| 3:D:759:ILE:HA   | 3:D:771:GLN:NE2  | 2.28                     | 0.47              |
| 3:D:954:ASN:HD21 | 3:D:992:LYS:HG3  | 1.80                     | 0.47              |
| 4:E:68:GLU:OE2   | 4:E:69:ARG:HG3   | 2.15                     | 0.47              |
| 5:L:843:MET:HE1  | 5:L:895:ILE:HA   | 1.97                     | 0.47              |
| 1:B:164:ASP:N    | 1:B:164:ASP:OD1  | 2.47                     | 0.47              |
| 2:C:378:ARG:NH1  | 2:C:379:GLU:HG2  | 2.29                     | 0.47              |
| 2:C:692:THR:HG22 | 2:C:693:LEU:N    | 2.27                     | 0.47              |
| 3:D:311:ARG:O    | 3:D:312:ARG:HD3  | 2.14                     | 0.47              |
| 3:D:644:MET:HG3  | 3:D:764:ARG:HD2  | 1.95                     | 0.47              |
| 2:C:172:TYR:CE2  | 2:C:436:ARG:HA   | 2.49                     | 0.47              |
| 2:C:488:MET:HE3  | 2:C:489:PRO:HD2  | 1.97                     | 0.47              |
| 3:D:572:THR:HG21 | 3:D:589:TYR:HE2  | 1.78                     | 0.47              |
| 5:L:8:ARG:HA     | 5:L:20:GLY:O     | 2.14                     | 0.47              |
| 2:C:55:SER:OG    | 2:C:465:ARG:NH1  | 2.48                     | 0.47              |
| 2:C:305:SER:OG   | 2:C:306:THR:N    | 2.48                     | 0.47              |
| 2:C:524:ILE:O    | 2:C:528:ARG:HG2  | 2.15                     | 0.47              |
| 2:C:678:ARG:NH2  | 2:C:681:MET:SD   | 2.88                     | 0.47              |
| 2:C:705:GLU:HB3  | 2:C:794:LEU:H    | 1.80                     | 0.47              |
| 2:C:864:LYS:HE2  | 2:C:881:ASP:HB3  | 1.97                     | 0.47              |
| 3:D:77:ARG:HH22  | 5:L:746:MET:HE3  | 1.78                     | 0.47              |
| 3:D:557:LYS:HA   | 3:D:562:GLU:O    | 2.15                     | 0.47              |
| 5:L:98:ARG:HG3   | 5:L:98:ARG:NH1   | 2.29                     | 0.47              |
| 5:L:234:ARG:HA   | 5:L:237:GLU:HG2  | 1.95                     | 0.47              |
| 5:L:523:LEU:HB3  | 5:L:529:ILE:HB   | 1.95                     | 0.47              |
| 1:A:118:ASP:HB2  | 1:A:121:VAL:HG22 | 1.96                     | 0.47              |
| 2:C:36:GLN:O     | 2:C:40:GLU:HB2   | 2.15                     | 0.47              |
| 2:C:131:THR:HG23 | 2:C:133:ASN:N    | 2.30                     | 0.47              |
| 2:C:1023:HIS:CD2 | 2:C:1027:LYS:NZ  | 2.83                     | 0.47              |
| 3:D:1055:GLY:O   | 3:D:1108:GLN:NE2 | 2.48                     | 0.47              |
| 4:E:36:ASP:OD1   | 4:E:37:PRO:HD2   | 2.14                     | 0.47              |
| 5:L:6:GLY:N      | 5:L:22:VAL:O     | 2.43                     | 0.47              |
| 5:L:932:ARG:HA   | 5:L:932:ARG:NE   | 2.30                     | 0.47              |
| 2:C:801:ARG:HD2  | 2:C:1229:TYR:OH  | 2.15                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:996:ARG:C     | 2:C:997:TRP:HD1   | 2.22                     | 0.47              |
| 2:C:1167:GLU:HG3  | 2:C:1168:GLU:N    | 2.30                     | 0.47              |
| 3:D:930:LEU:HD11  | 3:D:1241:TYR:HE1  | 1.80                     | 0.47              |
| 3:D:1174:ARG:HG2  | 3:D:1187:GLU:CD   | 2.40                     | 0.47              |
| 1:A:14:VAL:HG21   | 1:A:29:GLU:HG2    | 1.97                     | 0.47              |
| 1:B:56:VAL:HA     | 1:B:146:VAL:HG12  | 1.96                     | 0.47              |
| 3:D:77:ARG:HA     | 3:D:77:ARG:HD3    | 1.61                     | 0.47              |
| 3:D:822:MET:HE2   | 3:D:838:ARG:NE    | 2.29                     | 0.47              |
| 3:D:1045:THR:O    | 3:D:1046:ILE:HD13 | 2.14                     | 0.47              |
| 5:L:846:ASP:OD1   | 5:L:850:ASN:N     | 2.28                     | 0.47              |
| 1:A:9:LEU:HD11    | 1:A:30:PRO:HB2    | 1.97                     | 0.46              |
| 2:C:499:SER:HA    | 2:C:502:VAL:HG12  | 1.97                     | 0.46              |
| 2:C:1307:ASN:OD1  | 2:C:1312:ASN:HB3  | 2.15                     | 0.46              |
| 3:D:1196:LEU:HD22 | 3:D:1210:ILE:HG22 | 1.96                     | 0.46              |
| 5:L:148:ARG:HH12  | 5:L:779:TRP:HD1   | 1.62                     | 0.46              |
| 5:L:559:VAL:HG12  | 5:L:560:LEU:N     | 2.30                     | 0.46              |
| 5:L:908:ASN:O     | 5:L:912:GLU:OE1   | 2.33                     | 0.46              |
| 2:C:76:GLY:N      | 2:C:95:PRO:O      | 2.39                     | 0.46              |
| 2:C:277:LEU:HD22  | 2:C:282:VAL:HG11  | 1.97                     | 0.46              |
| 2:C:423:ASP:OD1   | 2:C:424:ASP:N     | 2.48                     | 0.46              |
| 2:C:559:CYS:HB2   | 2:C:662:SER:HB2   | 1.97                     | 0.46              |
| 3:D:19:ALA:HA     | 3:D:1342:ASP:O    | 2.16                     | 0.46              |
| 3:D:1034:PHE:N    | 3:D:1081:VAL:O    | 2.49                     | 0.46              |
| 4:E:42:GLU:OE1    | 4:E:42:GLU:N      | 2.47                     | 0.46              |
| 2:C:636:CYS:O     | 2:C:642:SER:HA    | 2.15                     | 0.46              |
| 3:D:450:HIS:CE1   | 3:D:452:LEU:HB2   | 2.50                     | 0.46              |
| 3:D:910:ASN:ND2   | 4:E:15:ASN:O      | 2.49                     | 0.46              |
| 1:B:28:LEU:HD13   | 1:B:28:LEU:HA     | 1.72                     | 0.46              |
| 2:C:564:PRO:HG2   | 2:C:572:ILE:HG13  | 1.98                     | 0.46              |
| 5:L:526:ARG:HG2   | 5:L:526:ARG:O     | 2.15                     | 0.46              |
| 5:L:846:ASP:OD1   | 5:L:849:GLY:N     | 2.47                     | 0.46              |
| 2:C:130:MET:SD    | 2:C:134:GLY:HA2   | 2.56                     | 0.46              |
| 3:D:146:VAL:HG22  | 3:D:158:GLN:HB3   | 1.97                     | 0.46              |
| 1:B:86:LYS:NZ     | 1:B:174:ASP:HB2   | 2.29                     | 0.46              |
| 2:C:74:ARG:NH2    | 2:C:97:ARG:HG3    | 2.31                     | 0.46              |
| 2:C:551:HIS:H     | 2:C:554:HIS:CE1   | 2.34                     | 0.46              |
| 2:C:881:ASP:O     | 2:C:920:VAL:HG23  | 2.16                     | 0.46              |
| 2:C:1072:ASN:OD1  | 2:C:1072:ASN:N    | 2.49                     | 0.46              |
| 3:D:1282:TYR:HA   | 3:D:1285:VAL:HG22 | 1.96                     | 0.46              |
| 5:L:271:GLU:O     | 5:L:271:GLU:HG2   | 2.16                     | 0.46              |
| 2:C:122:VAL:HG21  | 2:C:493:ILE:HG21  | 1.98                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:45:ASN:O      | 3:D:47:ARG:N      | 2.48                     | 0.46              |
| 3:D:831:VAL:HG23  | 3:D:831:VAL:O     | 2.15                     | 0.46              |
| 3:D:848:VAL:HG11  | 3:D:880:VAL:HG13  | 1.97                     | 0.46              |
| 5:L:530:ARG:NH2   | 5:L:556:GLY:O     | 2.46                     | 0.46              |
| 1:A:155:ALA:O     | 1:A:159:ILE:HG12  | 2.16                     | 0.46              |
| 1:B:192:VAL:C     | 1:B:194:GLN:H     | 2.23                     | 0.46              |
| 2:C:960:LEU:HB3   | 2:C:1025:PHE:CE1  | 2.50                     | 0.46              |
| 3:D:141:PHE:HA    | 3:D:180:MET:CE    | 2.39                     | 0.46              |
| 3:D:834:PRO:HD2   | 3:D:837:ASP:OD2   | 2.16                     | 0.46              |
| 5:L:677:LEU:O     | 5:L:680:GLN:HG2   | 2.15                     | 0.46              |
| 2:C:135:THR:HG21  | 2:C:515:MET:HE2   | 1.97                     | 0.46              |
| 2:C:1140:LYS:HD2  | 2:C:1141:LEU:N    | 2.31                     | 0.46              |
| 3:D:611:ILE:HG22  | 3:D:612:LEU:HD12  | 1.98                     | 0.46              |
| 3:D:615:LYS:HZ1   | 4:E:5:THR:HB      | 1.81                     | 0.46              |
| 3:D:1217:PRO:HA   | 3:D:1220:ILE:HG12 | 1.97                     | 0.46              |
| 5:L:112:GLN:O     | 5:L:115:LEU:HD22  | 2.16                     | 0.46              |
| 5:L:480:ASP:OD1   | 5:L:481:ASN:N     | 2.49                     | 0.46              |
| 1:A:58:GLU:OE2    | 1:A:145:LYS:HD3   | 2.15                     | 0.46              |
| 1:B:97:GLU:HG2    | 1:B:147:GLN:HG2   | 1.98                     | 0.46              |
| 2:C:994:ARG:HA    | 2:C:997:TRP:NE1   | 2.31                     | 0.46              |
| 2:C:1122:LYS:HG2  | 2:C:1229:TYR:CZ   | 2.51                     | 0.46              |
| 3:D:579:LEU:O     | 3:D:582:ILE:HG12  | 2.16                     | 0.46              |
| 3:D:857:LEU:HD22  | 3:D:871:LEU:HD21  | 1.98                     | 0.46              |
| 1:A:58:GLU:HB3    | 1:A:172:LEU:HD23  | 1.98                     | 0.45              |
| 2:C:1298:VAL:HG23 | 2:C:1299:ASN:N    | 2.31                     | 0.45              |
| 2:C:1246:ARG:NH1  | 3:D:348:ASP:OD1   | 2.48                     | 0.45              |
| 3:D:710:ASP:OD1   | 3:D:711:GLY:N     | 2.49                     | 0.45              |
| 5:L:205:ILE:HB    | 5:L:253:ILE:HD13  | 1.98                     | 0.45              |
| 1:A:207:THR:HG23  | 1:A:209:GLY:H     | 1.81                     | 0.45              |
| 2:C:1073:LYS:HE3  | 3:D:462:ASP:HB2   | 1.98                     | 0.45              |
| 3:D:297:ARG:NH2   | 3:D:298:MET:HE3   | 2.32                     | 0.45              |
| 3:D:646:ILE:CD1   | 3:D:762:ASN:HD21  | 2.30                     | 0.45              |
| 3:D:772:TYR:O     | 3:D:776:THR:HG23  | 2.16                     | 0.45              |
| 3:D:914:ALA:O     | 3:D:918:ILE:HG13  | 2.16                     | 0.45              |
| 5:L:205:ILE:HB    | 5:L:253:ILE:CD1   | 2.46                     | 0.45              |
| 5:L:206:ILE:HA    | 5:L:254:CYS:O     | 2.16                     | 0.45              |
| 5:L:401:GLN:HA    | 5:L:404:VAL:HG22  | 1.98                     | 0.45              |
| 2:C:213:LEU:HD12  | 2:C:422:LYS:HB3   | 1.98                     | 0.45              |
| 2:C:1033:ARG:O    | 2:C:1036:ILE:HG22 | 2.17                     | 0.45              |
| 3:D:91:GLU:OE1    | 5:L:44:ALA:HB2    | 2.16                     | 0.45              |
| 3:D:662:ALA:O     | 3:D:665:GLN:HG3   | 2.17                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:986:ASP:OD1   | 3:D:987:GLU:N     | 2.47                     | 0.45              |
| 3:D:1040:MET:CE   | 3:D:1046:ILE:HG13 | 2.45                     | 0.45              |
| 3:D:1342:ASP:OD2  | 3:D:1344:LEU:HD23 | 2.17                     | 0.45              |
| 5:L:687:ARG:O     | 5:L:690:GLU:HG2   | 2.16                     | 0.45              |
| 5:L:860:THR:HA    | 5:L:863:ARG:NE    | 2.29                     | 0.45              |
| 2:C:77:GLU:CD     | 2:C:78:PRO:HD2    | 2.42                     | 0.45              |
| 2:C:102:LEU:CD1   | 2:C:489:PRO:HG3   | 2.46                     | 0.45              |
| 2:C:742:TYR:O     | 2:C:746:ALA:HB2   | 2.16                     | 0.45              |
| 3:D:245:LEU:O     | 3:D:250:ARG:NE    | 2.47                     | 0.45              |
| 5:L:914:LEU:HD13  | 5:L:917:GLU:OE2   | 2.16                     | 0.45              |
| 2:C:469:VAL:HA    | 2:C:472:GLU:CG    | 2.47                     | 0.45              |
| 2:C:607:SER:OG    | 2:C:610:GLU:OE2   | 2.29                     | 0.45              |
| 2:C:726:TYR:HB3   | 2:C:733:VAL:HB    | 1.97                     | 0.45              |
| 3:D:79:LYS:HE2    | 5:L:749:PRO:HD3   | 1.97                     | 0.45              |
| 3:D:134:ASP:OD1   | 3:D:159:ILE:HG13  | 2.16                     | 0.45              |
| 5:L:136:SER:O     | 5:L:140:PHE:HD1   | 1.99                     | 0.45              |
| 5:L:807:LYS:HA    | 5:L:967:HIS:CD2   | 2.52                     | 0.45              |
| 1:A:190:ALA:HB2   | 1:A:200:LYS:HB3   | 1.99                     | 0.45              |
| 2:C:88:ARG:HD3    | 2:C:1040:ASP:OD2  | 2.17                     | 0.45              |
| 2:C:256:GLU:HA    | 2:C:261:VAL:HA    | 1.99                     | 0.45              |
| 2:C:521:LEU:HA    | 2:C:524:ILE:HG22  | 1.99                     | 0.45              |
| 2:C:849:GLU:HG2   | 2:C:851:THR:H     | 1.82                     | 0.45              |
| 3:D:554:GLU:HG3   | 3:D:566:LYS:HG3   | 1.99                     | 0.45              |
| 3:D:1256:ILE:O    | 3:D:1260:MET:HG3  | 2.17                     | 0.45              |
| 3:D:1280:VAL:HG11 | 3:D:1304:ARG:NH2  | 2.31                     | 0.45              |
| 5:L:264:GLN:HA    | 5:L:267:GLU:HG3   | 1.98                     | 0.45              |
| 5:L:339:PHE:O     | 5:L:343:VAL:HG23  | 2.17                     | 0.45              |
| 5:L:740:LEU:O     | 5:L:758:GLY:HA2   | 2.17                     | 0.45              |
| 5:L:743:SER:O     | 5:L:746:MET:HG2   | 2.17                     | 0.45              |
| 3:D:1075:ARG:HB3  | 3:D:1100:PHE:CE2  | 2.51                     | 0.45              |
| 4:E:65:ASP:O      | 4:E:68:GLU:HG3    | 2.16                     | 0.45              |
| 5:L:54:MET:HG2    | 5:L:55:PHE:N      | 2.32                     | 0.45              |
| 2:C:147:SER:HB2   | 2:C:530:ILE:HD13  | 1.98                     | 0.45              |
| 2:C:726:TYR:CE2   | 2:C:728:ASP:HB2   | 2.52                     | 0.45              |
| 2:C:813:GLU:HB2   | 3:D:461:PHE:CD2   | 2.52                     | 0.45              |
| 2:C:1136:GLN:HB2  | 2:C:1140:LYS:HG2  | 1.99                     | 0.45              |
| 3:D:304:ASP:OD1   | 3:D:305:ALA:N     | 2.49                     | 0.45              |
| 4:E:26:ARG:HG3    | 4:E:30:MET:HE2    | 1.98                     | 0.45              |
| 5:L:510:CYS:SG    | 5:L:511:ALA:N     | 2.90                     | 0.45              |
| 5:L:801:ILE:HG21  | 5:L:877:VAL:HG22  | 1.97                     | 0.45              |
| 2:C:26:TYR:CE2    | 2:C:28:LEU:HB2    | 2.51                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:979:LEU:HD22 | 2:C:989:LEU:HD22  | 1.99                     | 0.45              |
| 2:C:232:ILE:HG22 | 2:C:237:LEU:HD23  | 1.99                     | 0.44              |
| 2:C:591:TYR:CE1  | 2:C:616:ILE:HG21  | 2.51                     | 0.44              |
| 2:C:662:SER:OG   | 2:C:663:VAL:N     | 2.50                     | 0.44              |
| 2:C:1121:ALA:O   | 2:C:1124:ILE:HG12 | 2.16                     | 0.44              |
| 3:D:28:ASP:OD1   | 3:D:29:MET:N      | 2.50                     | 0.44              |
| 3:D:97:VAL:C     | 3:D:99:ARG:H      | 2.24                     | 0.44              |
| 5:L:204:LEU:HD11 | 5:L:254:CYS:SG    | 2.57                     | 0.44              |
| 1:A:54:CYS:HB3   | 1:A:148:ARG:HG2   | 2.00                     | 0.44              |
| 1:A:205:MET:HE3  | 1:A:207:THR:HB    | 2.00                     | 0.44              |
| 2:C:271:ALA:O    | 2:C:275:ARG:HG2   | 2.18                     | 0.44              |
| 3:D:36:GLY:HA3   | 3:D:61:ILE:HG12   | 1.98                     | 0.44              |
| 3:D:69:GLU:HB2   | 3:D:76:LYS:HG2    | 1.99                     | 0.44              |
| 3:D:369:PRO:HB3  | 3:D:444:GLY:O     | 2.18                     | 0.44              |
| 3:D:850:LYS:C    | 3:D:852:GLY:H     | 2.25                     | 0.44              |
| 3:D:1267:VAL:O   | 3:D:1274:PHE:HE1  | 2.01                     | 0.44              |
| 4:E:71:GLU:O     | 4:E:75:GLN:HG3    | 2.16                     | 0.44              |
| 5:L:199:ALA:HB2  | 5:L:831:GLN:NE2   | 2.32                     | 0.44              |
| 5:L:520:GLU:HG3  | 5:L:521:GLN:N     | 2.32                     | 0.44              |
| 5:L:592:GLN:HG3  | 5:L:596:ARG:NH1   | 2.32                     | 0.44              |
| 1:B:56:VAL:HG22  | 1:B:146:VAL:HG12  | 1.99                     | 0.44              |
| 1:B:191:ARG:NH1  | 1:B:193:GLU:HA    | 2.32                     | 0.44              |
| 1:B:193:GLU:HG2  | 1:B:194:GLN:HG2   | 1.99                     | 0.44              |
| 3:D:267:ASP:HA   | 3:D:270:ARG:CZ    | 2.47                     | 0.44              |
| 5:L:372:MET:O    | 5:L:376:MET:HG2   | 2.17                     | 0.44              |
| 5:L:578:MET:SD   | 5:L:608:ILE:HG23  | 2.58                     | 0.44              |
| 1:A:167:PRO:HG2  | 1:A:170:ARG:NH2   | 2.32                     | 0.44              |
| 2:C:17:LYS:H     | 2:C:1188:ASP:CG   | 2.26                     | 0.44              |
| 2:C:387:ASN:O    | 2:C:394:ARG:HD2   | 2.17                     | 0.44              |
| 2:C:397:LEU:O    | 2:C:398:SER:OG    | 2.28                     | 0.44              |
| 2:C:1119:MET:HE2 | 2:C:1227:VAL:HG23 | 1.98                     | 0.44              |
| 5:L:310:LEU:HD23 | 5:L:310:LEU:HA    | 1.87                     | 0.44              |
| 3:D:252:LEU:O    | 3:D:252:LEU:HD23  | 2.18                     | 0.44              |
| 3:D:269:TYR:O    | 3:D:273:ILE:HG13  | 2.17                     | 0.44              |
| 3:D:847:ASP:HB2  | 3:D:856:ILE:HG23  | 1.99                     | 0.44              |
| 5:L:133:ARG:HG2  | 5:L:792:LEU:HD22  | 1.99                     | 0.44              |
| 5:L:211:LEU:HD23 | 5:L:215:TRP:HE1   | 1.82                     | 0.44              |
| 2:C:241:LEU:HD11 | 2:C:246:LEU:CD2   | 2.48                     | 0.44              |
| 2:C:409:LEU:HB2  | 2:C:411:ARG:NE    | 2.33                     | 0.44              |
| 3:D:210:SER:O    | 3:D:214:ARG:HG3   | 2.18                     | 0.44              |
| 3:D:638:SER:OG   | 3:D:639:VAL:N     | 2.51                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:59:VAL:HG23   | 1:B:144:ILE:HG22  | 2.00                     | 0.44              |
| 2:C:300:ASP:OD1   | 2:C:312:ALA:HA    | 2.17                     | 0.44              |
| 2:C:855:PRO:HG2   | 2:C:915:ASP:OD1   | 2.18                     | 0.44              |
| 3:D:198:CYS:SG    | 3:D:202:ARG:NH2   | 2.90                     | 0.44              |
| 3:D:225:GLU:HA    | 3:D:228:VAL:HG12  | 2.00                     | 0.44              |
| 3:D:278:ARG:HA    | 3:D:281:ARG:HG2   | 2.00                     | 0.44              |
| 3:D:557:LYS:HB3   | 3:D:563:LEU:HD23  | 1.99                     | 0.44              |
| 4:E:50:ALA:O      | 4:E:54:ILE:HG12   | 2.17                     | 0.44              |
| 5:L:552:GLU:HB2   | 5:L:556:GLY:HA3   | 2.00                     | 0.44              |
| 2:C:155:VAL:HA    | 2:C:175:ARG:O     | 2.17                     | 0.44              |
| 2:C:519:ASN:HB3   | 2:C:522:SER:OG    | 2.18                     | 0.44              |
| 3:D:155:GLU:OE2   | 3:D:158:GLN:HB2   | 2.18                     | 0.44              |
| 3:D:697:MET:SD    | 3:D:741:ALA:HB3   | 2.58                     | 0.44              |
| 3:D:1219:ASP:HA   | 3:D:1222:ARG:HH12 | 1.83                     | 0.44              |
| 1:A:166:ARG:HD3   | 1:A:166:ARG:N     | 2.32                     | 0.44              |
| 2:C:227:LYS:HE3   | 2:C:227:LYS:HA    | 2.00                     | 0.44              |
| 5:L:905:ALA:O     | 5:L:909:GLU:HG2   | 2.18                     | 0.44              |
| 1:A:125:LYS:HG3   | 1:A:127:GLN:OE1   | 2.18                     | 0.43              |
| 2:C:632:ASP:HA    | 2:C:647:ARG:HD3   | 1.99                     | 0.43              |
| 2:C:1319:MET:HE3  | 2:C:1324:ASN:HD21 | 1.82                     | 0.43              |
| 3:D:1287:ILE:HD11 | 3:D:1300:ALA:HB3  | 1.99                     | 0.43              |
| 3:D:1338:ALA:HB3  | 3:D:1340:LYS:HG2  | 1.99                     | 0.43              |
| 5:L:419:ARG:HB3   | 5:L:689:LEU:HD23  | 2.00                     | 0.43              |
| 5:L:884:VAL:HA    | 5:L:887:ILE:HD12  | 2.00                     | 0.43              |
| 1:A:233:ASP:OD1   | 1:A:233:ASP:N     | 2.51                     | 0.43              |
| 2:C:251:ALA:H     | 2:C:268:ARG:HA    | 1.83                     | 0.43              |
| 3:D:657:ALA:O     | 3:D:661:VAL:HG23  | 2.18                     | 0.43              |
| 5:L:42:LEU:H      | 5:L:42:LEU:HD23   | 1.83                     | 0.43              |
| 2:C:91:THR:HB     | 2:C:138:ILE:O     | 2.17                     | 0.43              |
| 2:C:257:ALA:HB2   | 2:C:285:ILE:HG22  | 2.00                     | 0.43              |
| 2:C:624:ASP:C     | 2:C:626:GLU:H     | 2.25                     | 0.43              |
| 2:C:850:ILE:HG22  | 2:C:850:ILE:O     | 2.19                     | 0.43              |
| 2:C:854:ILE:O     | 2:C:857:VAL:HG22  | 2.18                     | 0.43              |
| 2:C:1283:ALA:HA   | 3:D:479:GLU:OE1   | 2.18                     | 0.43              |
| 5:L:59:ASP:O      | 5:L:71:VAL:HG22   | 2.18                     | 0.43              |
| 5:L:111:PRO:C     | 5:L:113:ASP:H     | 2.26                     | 0.43              |
| 5:L:616:THR:HG23  | 5:L:618:GLN:H     | 1.83                     | 0.43              |
| 2:C:813:GLU:C     | 2:C:815:SER:H     | 2.26                     | 0.43              |
| 2:C:964:LEU:HD22  | 2:C:1025:PHE:CG   | 2.53                     | 0.43              |
| 2:C:1125:GLY:O    | 2:C:1128:ILE:HG22 | 2.18                     | 0.43              |
| 3:D:85:CYS:HB3    | 3:D:88:CYS:O      | 2.18                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:167:ASP:OD1   | 3:D:168:ALA:N    | 2.52                     | 0.43              |
| 3:D:1036:ARG:HH21 | 3:D:1038:THR:CG2 | 2.31                     | 0.43              |
| 5:L:873:GLY:HA2   | 5:L:876:LEU:HB3  | 2.00                     | 0.43              |
| 3:D:160:LEU:CD1   | 3:D:164:GLN:HB3  | 2.47                     | 0.43              |
| 3:D:210:SER:H     | 3:D:214:ARG:HG3  | 1.83                     | 0.43              |
| 3:D:297:ARG:O     | 3:D:301:GLU:OE1  | 2.35                     | 0.43              |
| 3:D:814:CYS:SG    | 3:D:816:THR:HG22 | 2.59                     | 0.43              |
| 3:D:955:LYS:HD2   | 3:D:1011:VAL:O   | 2.18                     | 0.43              |
| 1:B:85:LEU:HD21   | 1:B:142:MET:HE1  | 2.01                     | 0.43              |
| 2:C:218:GLU:HG3   | 2:C:219:GLN:N    | 2.33                     | 0.43              |
| 2:C:840:SER:OG    | 2:C:1048:LYS:HG2 | 2.19                     | 0.43              |
| 3:D:48:THR:HG23   | 3:D:50:LYS:HG2   | 2.00                     | 0.43              |
| 3:D:552:ILE:O     | 3:D:567:THR:HA   | 2.18                     | 0.43              |
| 3:D:826:ILE:HG13  | 3:D:826:ILE:O    | 2.18                     | 0.43              |
| 2:C:210:LEU:HB3   | 2:C:220:ILE:HD11 | 1.99                     | 0.43              |
| 2:C:733:VAL:HG22  | 2:C:750:ILE:HG13 | 2.01                     | 0.43              |
| 2:C:797:GLY:N     | 2:C:1231:TYR:OH  | 2.41                     | 0.43              |
| 3:D:514:THR:OG1   | 3:D:595:ALA:O    | 2.32                     | 0.43              |
| 2:C:551:HIS:CD2   | 2:C:552:PRO:CD   | 3.00                     | 0.43              |
| 3:D:167:ASP:O     | 3:D:171:GLU:HG3  | 2.17                     | 0.43              |
| 3:D:371:LYS:HG3   | 3:D:372:MET:N    | 2.34                     | 0.43              |
| 3:D:528:THR:HG22  | 3:D:532:GLU:CD   | 2.44                     | 0.43              |
| 3:D:586:GLY:HA3   | 3:D:612:LEU:HD11 | 1.99                     | 0.43              |
| 3:D:1325:PHE:CZ   | 3:D:1326:GLN:HG3 | 2.54                     | 0.43              |
| 4:E:63:ILE:HA     | 4:E:66:VAL:HG22  | 2.01                     | 0.43              |
| 5:L:701:ALA:O     | 5:L:704:GLU:HG3  | 2.19                     | 0.43              |
| 2:C:38:PHE:HE1    | 2:C:461:GLU:HB2  | 1.84                     | 0.43              |
| 2:C:500:ALA:O     | 2:C:504:GLU:HG3  | 2.17                     | 0.43              |
| 2:C:1023:HIS:HA   | 2:C:1026:GLU:HG3 | 1.99                     | 0.43              |
| 2:C:1319:MET:HE3  | 2:C:1324:ASN:ND2 | 2.33                     | 0.43              |
| 3:D:198:CYS:SG    | 3:D:221:ILE:HD11 | 2.59                     | 0.43              |
| 3:D:582:ILE:HG13  | 3:D:583:VAL:N    | 2.34                     | 0.43              |
| 3:D:605:LEU:HD23  | 3:D:605:LEU:HA   | 1.90                     | 0.43              |
| 5:L:183:LYS:HE2   | 5:L:312:LEU:HD23 | 2.01                     | 0.43              |
| 1:B:89:ALA:O      | 1:B:124:VAL:HG22 | 2.18                     | 0.43              |
| 1:B:166:ARG:NE    | 1:B:167:PRO:HD2  | 2.34                     | 0.43              |
| 2:C:107:ARG:HD2   | 2:C:107:ARG:HA   | 1.34                     | 0.43              |
| 2:C:182:SER:HB2   | 2:C:389:PHE:HE1  | 1.84                     | 0.43              |
| 2:C:1124:ILE:CD1  | 2:C:1180:MET:HE2 | 2.49                     | 0.43              |
| 3:D:572:THR:HG22  | 3:D:593:ASN:OD1  | 2.18                     | 0.43              |
| 5:L:202:ARG:HA    | 5:L:250:GLN:O    | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:L:223:PHE:O     | 5:L:225:LEU:HG    | 2.19                     | 0.43              |
| 5:L:370:LEU:HD23  | 5:L:373:LEU:HD21  | 2.01                     | 0.43              |
| 5:L:508:VAL:O     | 5:L:561:LEU:HD22  | 2.19                     | 0.43              |
| 5:L:716:ILE:H     | 5:L:716:ILE:HD12  | 1.84                     | 0.43              |
| 1:A:94:GLY:H      | 1:A:120:ASP:CG    | 2.27                     | 0.42              |
| 2:C:975:ILE:HA    | 2:C:978:VAL:HG12  | 2.01                     | 0.42              |
| 3:D:216:LYS:HA    | 3:D:219:LYS:CD    | 2.49                     | 0.42              |
| 3:D:218:THR:O     | 3:D:221:ILE:HG22  | 2.19                     | 0.42              |
| 3:D:221:ILE:O     | 3:D:225:GLU:HG3   | 2.19                     | 0.42              |
| 3:D:587:LEU:HD11  | 3:D:608:CYS:HB2   | 2.01                     | 0.42              |
| 5:L:148:ARG:O     | 5:L:765:ARG:NH2   | 2.50                     | 0.42              |
| 5:L:857:GLU:OE1   | 5:L:860:THR:HG23  | 2.19                     | 0.42              |
| 2:C:192:ASP:HB3   | 2:C:346:TYR:CD1   | 2.53                     | 0.42              |
| 2:C:576:SER:OG    | 2:C:577:VAL:N     | 2.53                     | 0.42              |
| 2:C:590:PRO:HB3   | 2:C:605:TYR:CE1   | 2.54                     | 0.42              |
| 2:C:696:ASP:O     | 2:C:697:LYS:HB3   | 2.18                     | 0.42              |
| 5:L:787:GLY:O     | 5:L:791:ILE:HG22  | 2.18                     | 0.42              |
| 1:B:48:LEU:HD11   | 3:D:535:ARG:HA    | 1.99                     | 0.42              |
| 1:B:107:ILE:HD12  | 1:B:134:THR:C     | 2.44                     | 0.42              |
| 2:C:164:THR:OG1   | 2:C:168:GLY:O     | 2.36                     | 0.42              |
| 2:C:213:LEU:O     | 2:C:214:ASN:HB2   | 2.18                     | 0.42              |
| 2:C:297:VAL:HG12  | 2:C:315:MET:O     | 2.19                     | 0.42              |
| 2:C:522:SER:OG    | 2:C:687:ARG:O     | 2.33                     | 0.42              |
| 2:C:843:THR:OG1   | 2:C:846:GLY:O     | 2.36                     | 0.42              |
| 2:C:1186:VAL:HG23 | 2:C:1187:PHE:H    | 1.84                     | 0.42              |
| 3:D:29:MET:HG3    | 3:D:33:TRP:CE2    | 2.54                     | 0.42              |
| 3:D:71:LEU:H      | 3:D:90:VAL:HG11   | 1.84                     | 0.42              |
| 3:D:553:THR:HG22  | 3:D:567:THR:CB    | 2.50                     | 0.42              |
| 3:D:1253:ILE:O    | 3:D:1257:VAL:HG23 | 2.19                     | 0.42              |
| 5:L:120:ILE:HG22  | 5:L:799:SER:O     | 2.20                     | 0.42              |
| 5:L:328:LEU:HD21  | 5:L:417:LEU:HD11  | 2.01                     | 0.42              |
| 5:L:816:VAL:HG21  | 5:L:887:ILE:HG21  | 2.02                     | 0.42              |
| 5:L:861:PHE:O     | 5:L:865:LEU:HD13  | 2.19                     | 0.42              |
| 2:C:688:GLN:HB2   | 2:C:1235:LEU:HD22 | 2.00                     | 0.42              |
| 3:D:814:CYS:HB2   | 3:D:889:ASP:HB3   | 2.00                     | 0.42              |
| 3:D:868:TRP:O     | 3:D:872:LEU:HG    | 2.19                     | 0.42              |
| 3:D:1024:THR:OG1  | 3:D:1123:ARG:NH2  | 2.50                     | 0.42              |
| 5:L:538:MET:HE2   | 5:L:542:GLU:HG3   | 2.00                     | 0.42              |
| 1:A:162:GLU:HG2   | 1:A:163:GLU:N     | 2.35                     | 0.42              |
| 2:C:1156:ARG:HH22 | 2:C:1185:PRO:HG2  | 1.83                     | 0.42              |
| 3:D:213:LYS:O     | 3:D:217:LEU:HD23  | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:394:ILE:O     | 3:D:398:LYS:HG3   | 2.19                     | 0.42              |
| 5:L:123:MET:SD    | 5:L:802:SER:HB2   | 2.59                     | 0.42              |
| 5:L:142:MET:SD    | 5:L:144:TYR:N     | 2.82                     | 0.42              |
| 5:L:214:GLN:OE1   | 5:L:214:GLN:N     | 2.51                     | 0.42              |
| 5:L:702:LEU:O     | 5:L:706:ILE:HG12  | 2.19                     | 0.42              |
| 1:B:76:GLU:CG     | 1:B:81:ILE:HD11   | 2.49                     | 0.42              |
| 1:B:91:ARG:NH2    | 1:B:179:PRO:HB3   | 2.33                     | 0.42              |
| 1:B:151:GLY:O     | 1:B:177:TYR:HB2   | 2.19                     | 0.42              |
| 2:C:211:ARG:HH12  | 2:C:217:THR:N     | 2.18                     | 0.42              |
| 5:L:120:ILE:HG22  | 5:L:121:ASP:H     | 1.83                     | 0.42              |
| 5:L:123:MET:HE1   | 5:L:865:LEU:HB3   | 2.01                     | 0.42              |
| 5:L:168:ARG:HB2   | 5:L:171:PRO:HG3   | 2.02                     | 0.42              |
| 2:C:41:GLN:HA     | 2:C:41:GLN:OE1    | 2.19                     | 0.42              |
| 2:C:232:ILE:O     | 2:C:232:ILE:HG13  | 2.18                     | 0.42              |
| 3:D:1026:PRO:HA   | 3:D:1120:THR:HG23 | 2.01                     | 0.42              |
| 3:D:1046:ILE:HG23 | 3:D:1060:VAL:O    | 2.19                     | 0.42              |
| 4:E:8:ASP:HB2     | 4:E:55:GLU:OE2    | 2.19                     | 0.42              |
| 5:L:158:GLN:HB3   | 5:L:189:MET:HE1   | 2.02                     | 0.42              |
| 5:L:597:LEU:HD12  | 5:L:598:ASP:N     | 2.34                     | 0.42              |
| 2:C:179:TYR:HB2   | 2:C:397:LEU:O     | 2.20                     | 0.42              |
| 2:C:519:ASN:OD1   | 2:C:521:LEU:N     | 2.47                     | 0.42              |
| 2:C:1172:LEU:HG   | 2:C:1176:LEU:HD13 | 2.02                     | 0.42              |
| 2:C:1298:VAL:HG12 | 2:C:1301:ARG:NH2  | 2.28                     | 0.42              |
| 3:D:650:LYS:O     | 3:D:654:ILE:HG12  | 2.19                     | 0.42              |
| 5:L:19:LEU:HD21   | 5:L:53:VAL:HG11   | 2.00                     | 0.42              |
| 1:B:199:ASP:OD1   | 1:B:199:ASP:N     | 2.52                     | 0.42              |
| 2:C:936:ARG:HG3   | 2:C:1042:LEU:HB2  | 2.01                     | 0.42              |
| 3:D:399:LYS:HD2   | 3:D:399:LYS:HA    | 1.92                     | 0.42              |
| 3:D:1274:PHE:O    | 3:D:1274:PHE:CD1  | 2.73                     | 0.42              |
| 4:E:46:THR:HA     | 4:E:49:ILE:HD12   | 2.01                     | 0.42              |
| 5:L:261:ARG:NH1   | 5:L:261:ARG:HB2   | 2.35                     | 0.42              |
| 1:A:31:LEU:HA     | 1:A:31:LEU:HD23   | 1.81                     | 0.42              |
| 2:C:734:ILE:HD11  | 2:C:783:LEU:HD21  | 2.02                     | 0.42              |
| 2:C:1232:MET:C    | 2:C:1233:LEU:HD12 | 2.44                     | 0.42              |
| 3:D:218:THR:O     | 3:D:222:LYS:HG2   | 2.20                     | 0.42              |
| 3:D:316:ILE:HG22  | 3:D:317:THR:N     | 2.34                     | 0.42              |
| 5:L:174:LEU:HB2   | 5:L:331:LEU:HD11  | 2.02                     | 0.42              |
| 5:L:437:LYS:NZ    | 5:L:614:GLU:HA    | 2.34                     | 0.42              |
| 1:A:62:ASP:OD1    | 1:A:63:GLY:N      | 2.45                     | 0.41              |
| 2:C:941:LYS:HD3   | 2:C:941:LYS:HA    | 1.54                     | 0.41              |
| 3:D:267:ASP:O     | 3:D:271:ARG:HG2   | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:L:215:TRP:HA    | 5:L:218:GLU:HG3   | 2.01                     | 0.41              |
| 5:L:358:MET:HB2   | 5:L:365:LEU:HD21  | 2.02                     | 0.41              |
| 5:L:590:LEU:O     | 5:L:594:ILE:HG13  | 2.20                     | 0.41              |
| 5:L:593:ARG:HA    | 5:L:596:ARG:HH11  | 1.85                     | 0.41              |
| 5:L:859:GLU:O     | 5:L:863:ARG:HG3   | 2.20                     | 0.41              |
| 1:B:210:THR:OG1   | 1:B:211:ILE:N     | 2.53                     | 0.41              |
| 2:C:1268:GLN:OE1  | 3:D:352:ARG:HD2   | 2.20                     | 0.41              |
| 3:D:515:ARG:NH2   | 3:D:717:VAL:O     | 2.53                     | 0.41              |
| 3:D:666:GLU:HA    | 3:D:669:GLN:NE2   | 2.35                     | 0.41              |
| 2:C:71:VAL:HB     | 2:C:99:LYS:HB3    | 2.01                     | 0.41              |
| 2:C:154:GLY:O     | 2:C:176:ILE:HA    | 2.21                     | 0.41              |
| 2:C:194:LEU:HD11  | 2:C:432:LEU:HD23  | 2.01                     | 0.41              |
| 2:C:1291:LEU:HD23 | 2:C:1291:LEU:HA   | 1.86                     | 0.41              |
| 3:D:288:PRO:HD2   | 3:D:291:ILE:HD12  | 2.03                     | 0.41              |
| 3:D:741:ALA:C     | 3:D:762:ASN:HD22  | 2.28                     | 0.41              |
| 3:D:955:LYS:HD2   | 3:D:1012:ALA:HA   | 2.02                     | 0.41              |
| 3:D:1079:LYS:HG2  | 3:D:1098:GLN:HG2  | 2.02                     | 0.41              |
| 3:D:1155:ILE:C    | 3:D:1156:LEU:HD12 | 2.45                     | 0.41              |
| 3:D:1174:ARG:HG2  | 3:D:1187:GLU:OE2  | 2.21                     | 0.41              |
| 5:L:69:MET:HA     | 5:L:88:LEU:HG     | 2.01                     | 0.41              |
| 5:L:383:GLU:HB3   | 5:L:384:PRO:HD3   | 2.02                     | 0.41              |
| 5:L:675:GLU:O     | 5:L:678:LYS:HG2   | 2.20                     | 0.41              |
| 2:C:609:ILE:HG13  | 2:C:610:GLU:H     | 1.86                     | 0.41              |
| 2:C:989:LEU:O     | 2:C:992:LEU:HG    | 2.20                     | 0.41              |
| 2:C:1004:ASP:O    | 2:C:1005:GLU:HG3  | 2.21                     | 0.41              |
| 3:D:357:VAL:HG12  | 3:D:461:PHE:CE2   | 2.56                     | 0.41              |
| 3:D:533:ALA:HB1   | 3:D:574:VAL:HG13  | 2.02                     | 0.41              |
| 3:D:649:LYS:HE2   | 3:D:649:LYS:HB2   | 1.89                     | 0.41              |
| 3:D:709:ARG:CG    | 3:D:710:ASP:H     | 2.33                     | 0.41              |
| 3:D:1048:ARG:HG2  | 3:D:1048:ARG:NH1  | 2.34                     | 0.41              |
| 3:D:1229:VAL:O    | 3:D:1233:ILE:HG22 | 2.21                     | 0.41              |
| 3:D:1283:SER:O    | 3:D:1287:ILE:HG12 | 2.20                     | 0.41              |
| 5:L:788:LEU:O     | 5:L:792:LEU:HG    | 2.20                     | 0.41              |
| 2:C:45:GLY:HA3    | 2:C:54:ARG:HH21   | 1.85                     | 0.41              |
| 2:C:685:MET:HE1   | 2:C:1073:LYS:CG   | 2.51                     | 0.41              |
| 2:C:801:ARG:HD2   | 2:C:1229:TYR:CZ   | 2.56                     | 0.41              |
| 2:C:886:LYS:HE3   | 2:C:916:SER:HB2   | 2.02                     | 0.41              |
| 2:C:1223:ARG:HH21 | 3:D:721:SER:HB3   | 1.86                     | 0.41              |
| 3:D:211:GLU:HG2   | 3:D:215:LYS:HZ1   | 1.85                     | 0.41              |
| 3:D:429:LEU:HD23  | 3:D:429:LEU:HA    | 1.91                     | 0.41              |
| 3:D:452:LEU:HD23  | 3:D:452:LEU:HA    | 1.84                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:233:ARG:O     | 2:C:238:GLN:NE2   | 2.49                     | 0.41              |
| 2:C:241:LEU:HD12  | 2:C:242:VAL:N     | 2.35                     | 0.41              |
| 2:C:595:THR:O     | 2:C:598:VAL:N     | 2.53                     | 0.41              |
| 2:C:634:VAL:HG13  | 2:C:636:CYS:SG    | 2.60                     | 0.41              |
| 3:D:615:LYS:O     | 3:D:619:ILE:HG23  | 2.21                     | 0.41              |
| 3:D:620:PHE:CZ    | 3:D:624:ILE:HD11  | 2.56                     | 0.41              |
| 3:D:744:ARG:HG3   | 3:D:759:ILE:HB    | 2.02                     | 0.41              |
| 3:D:825:VAL:HG22  | 3:D:827:GLU:HG3   | 2.02                     | 0.41              |
| 3:D:963:VAL:HB    | 3:D:980:THR:HG22  | 2.01                     | 0.41              |
| 3:D:1274:PHE:C    | 3:D:1275:LEU:HD12 | 2.45                     | 0.41              |
| 5:L:114:ARG:HD2   | 5:L:117:ALA:CB    | 2.50                     | 0.41              |
| 5:L:530:ARG:HD2   | 5:L:549:TRP:CZ2   | 2.53                     | 0.41              |
| 5:L:680:GLN:O     | 5:L:683:GLN:HG2   | 2.20                     | 0.41              |
| 1:A:45:ARG:HD2    | 2:C:1083:GLU:HB2  | 2.01                     | 0.41              |
| 1:A:214:GLU:O     | 1:A:218:ARG:HG3   | 2.21                     | 0.41              |
| 2:C:223:LEU:HD21  | 2:C:426:ILE:HD12  | 2.01                     | 0.41              |
| 2:C:689:ALA:HB2   | 2:C:1233:LEU:HD23 | 2.02                     | 0.41              |
| 3:D:528:THR:HG22  | 3:D:532:GLU:OE2   | 2.20                     | 0.41              |
| 3:D:641:ILE:O     | 3:D:764:ARG:NH1   | 2.53                     | 0.41              |
| 3:D:1282:TYR:O    | 3:D:1286:LYS:HG2  | 2.20                     | 0.41              |
| 5:L:61:ILE:HD12   | 5:L:102:LEU:HD21  | 2.03                     | 0.41              |
| 5:L:377:ILE:HD12  | 5:L:406:MET:SD    | 2.61                     | 0.41              |
| 1:A:166:ARG:HD3   | 1:A:166:ARG:H     | 1.84                     | 0.41              |
| 2:C:195:PHE:CD2   | 2:C:203:LYS:HD2   | 2.56                     | 0.41              |
| 2:C:285:ILE:O     | 2:C:285:ILE:HG13  | 2.21                     | 0.41              |
| 2:C:685:MET:HE1   | 2:C:1073:LYS:HD3  | 2.03                     | 0.41              |
| 2:C:865:LEU:HD22  | 2:C:869:GLY:C     | 2.46                     | 0.41              |
| 3:D:152:THR:OG1   | 3:D:153:ASN:N     | 2.53                     | 0.41              |
| 3:D:662:ALA:HA    | 3:D:665:GLN:HG3   | 2.03                     | 0.41              |
| 5:L:962:LEU:O     | 5:L:963:ILE:HD13  | 2.20                     | 0.41              |
| 1:B:44:ARG:HG3    | 1:B:183:ILE:HG23  | 2.03                     | 0.41              |
| 1:B:197:ASP:O     | 1:B:198:LEU:HD12  | 2.21                     | 0.41              |
| 2:C:465:ARG:HH11  | 2:C:465:ARG:HG3   | 1.86                     | 0.41              |
| 2:C:591:TYR:CZ    | 2:C:616:ILE:HD13  | 2.56                     | 0.41              |
| 2:C:614:TYR:N     | 2:C:614:TYR:CD1   | 2.88                     | 0.41              |
| 2:C:629:PHE:CE2   | 2:C:634:VAL:HG11  | 2.56                     | 0.41              |
| 2:C:976:ARG:HB2   | 2:C:997:TRP:HZ3   | 1.86                     | 0.41              |
| 2:C:1101:LEU:HD12 | 3:D:505:ASP:OD1   | 2.21                     | 0.41              |
| 2:C:1159:VAL:O    | 2:C:1160:ASP:HB2  | 2.20                     | 0.41              |
| 2:C:1180:MET:HA   | 2:C:1181:PRO:HD3  | 1.92                     | 0.41              |
| 2:C:1276:TRP:CD2  | 3:D:801:VAL:HG11  | 2.55                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1336:ASN:N    | 3:D:23:ALA:O      | 2.53                     | 0.41              |
| 3:D:51:PRO:HD2    | 3:D:71:LEU:HD11   | 2.03                     | 0.41              |
| 3:D:216:LYS:HA    | 3:D:219:LYS:HD3   | 2.02                     | 0.41              |
| 3:D:268:LEU:HD21  | 3:D:324:LEU:HD11  | 2.02                     | 0.41              |
| 3:D:510:LEU:HD23  | 3:D:510:LEU:HA    | 1.89                     | 0.41              |
| 5:L:111:PRO:C     | 5:L:113:ASP:N     | 2.79                     | 0.41              |
| 5:L:119:GLN:HG3   | 5:L:870:ARG:HD3   | 2.03                     | 0.41              |
| 5:L:261:ARG:HB2   | 5:L:261:ARG:HH11  | 1.86                     | 0.41              |
| 2:C:149:LEU:HB2   | 2:C:530:ILE:HG22  | 2.01                     | 0.41              |
| 2:C:492:MET:SD    | 2:C:493:ILE:HB    | 2.60                     | 0.41              |
| 2:C:624:ASP:O     | 2:C:625:GLU:HG3   | 2.21                     | 0.41              |
| 2:C:1172:LEU:O    | 2:C:1176:LEU:HD13 | 2.21                     | 0.41              |
| 3:D:413:ASP:O     | 3:D:416:ILE:HG22  | 2.20                     | 0.41              |
| 3:D:960:LEU:HB3   | 3:D:963:VAL:HG11  | 2.02                     | 0.41              |
| 5:L:14:GLU:HG3    | 5:L:17:LEU:HD12   | 2.02                     | 0.41              |
| 5:L:499:THR:HG23  | 5:L:502:ARG:HH21  | 1.86                     | 0.41              |
| 1:A:102:LEU:O     | 1:A:141:SER:HA    | 2.21                     | 0.40              |
| 2:C:755:LYS:O     | 2:C:757:THR:HG23  | 2.20                     | 0.40              |
| 2:C:1130:ALA:O    | 2:C:1133:LYS:HG2  | 2.21                     | 0.40              |
| 3:D:905:ARG:HD2   | 4:E:16:ARG:HH11   | 1.85                     | 0.40              |
| 3:D:1078:LEU:HB2  | 3:D:1101:LEU:HD11 | 2.03                     | 0.40              |
| 5:L:25:VAL:HG12   | 5:L:30:VAL:HG23   | 2.04                     | 0.40              |
| 1:A:47:LEU:HD13   | 1:A:183:ILE:HD12  | 2.02                     | 0.40              |
| 2:C:229:ILE:HB    | 2:C:240:GLU:HB3   | 2.03                     | 0.40              |
| 2:C:464:PHE:CZ    | 2:C:468:LEU:HD21  | 2.57                     | 0.40              |
| 2:C:706:ARG:HG3   | 2:C:793:GLU:HG2   | 2.03                     | 0.40              |
| 2:C:798:GLN:OE1   | 2:C:827:ARG:HB2   | 2.21                     | 0.40              |
| 2:C:878:THR:HG22  | 2:C:879:GLY:N     | 2.36                     | 0.40              |
| 2:C:1124:ILE:HD11 | 2:C:1180:MET:HB3  | 2.03                     | 0.40              |
| 2:C:1186:VAL:HG23 | 2:C:1187:PHE:N    | 2.36                     | 0.40              |
| 2:C:1329:GLU:CD   | 3:D:337:ARG:HH12  | 2.30                     | 0.40              |
| 3:D:69:GLU:HA     | 3:D:76:LYS:HA     | 2.02                     | 0.40              |
| 3:D:246:PRO:HA    | 3:D:247:PRO:HD3   | 1.94                     | 0.40              |
| 3:D:814:CYS:HB3   | 3:D:890:THR:OG1   | 2.21                     | 0.40              |
| 3:D:850:LYS:C     | 3:D:852:GLY:N     | 2.78                     | 0.40              |
| 3:D:972:LYS:HZ2   | 3:D:974:VAL:HA    | 1.85                     | 0.40              |
| 5:L:5:LEU:O       | 5:L:80:LEU:HD21   | 2.21                     | 0.40              |
| 1:B:191:ARG:HB3   | 1:B:196:THR:HA    | 2.03                     | 0.40              |
| 2:C:90:VAL:HG22   | 2:C:91:THR:N      | 2.37                     | 0.40              |
| 2:C:324:LYS:HB2   | 2:C:324:LYS:HE3   | 1.86                     | 0.40              |
| 2:C:685:MET:HG3   | 2:C:686:GLN:N     | 2.37                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:124:ILE:O     | 3:D:128:LEU:HD23  | 2.21                     | 0.40              |
| 3:D:135:ILE:H     | 3:D:135:ILE:HG13  | 1.70                     | 0.40              |
| 3:D:149:GLY:O     | 3:D:152:THR:HG22  | 2.22                     | 0.40              |
| 3:D:205:LEU:CD2   | 3:D:217:LEU:HB3   | 2.48                     | 0.40              |
| 3:D:338:PHE:CD2   | 3:D:1324:SER:HA   | 2.56                     | 0.40              |
| 3:D:530:PRO:HB2   | 3:D:581:MET:SD    | 2.62                     | 0.40              |
| 3:D:663:GLU:O     | 3:D:666:GLU:HG2   | 2.20                     | 0.40              |
| 3:D:865:HIS:HE1   | 3:D:867:GLN:HB3   | 1.87                     | 0.40              |
| 3:D:983:LYS:HB2   | 3:D:991:THR:HG23  | 2.04                     | 0.40              |
| 5:L:174:LEU:HB3   | 5:L:417:LEU:CD2   | 2.52                     | 0.40              |
| 5:L:472:ARG:HD2   | 5:L:512:LYS:HE3   | 2.02                     | 0.40              |
| 5:L:491:VAL:O     | 5:L:495:MET:HG3   | 2.21                     | 0.40              |
| 5:L:728:ILE:HD13  | 5:L:754:LEU:HD11  | 2.04                     | 0.40              |
| 5:L:807:LYS:HA    | 5:L:967:HIS:HD2   | 1.86                     | 0.40              |
| 5:L:819:ILE:HD13  | 5:L:959:ALA:HB3   | 2.02                     | 0.40              |
| 5:L:824:ALA:HB2   | 5:L:836:LEU:HD23  | 2.04                     | 0.40              |
| 2:C:565:GLU:CD    | 2:C:681:MET:HG2   | 2.47                     | 0.40              |
| 2:C:624:ASP:C     | 2:C:625:GLU:HG3   | 2.47                     | 0.40              |
| 2:C:895:LEU:H     | 2:C:895:LEU:HG    | 1.73                     | 0.40              |
| 2:C:1002:LEU:HD23 | 2:C:1003:THR:N    | 2.36                     | 0.40              |
| 3:D:167:ASP:O     | 3:D:170:GLU:HG2   | 2.22                     | 0.40              |
| 3:D:351:GLY:O     | 3:D:467:ALA:HA    | 2.22                     | 0.40              |
| 3:D:682:VAL:HA    | 3:D:685:ILE:HG12  | 2.04                     | 0.40              |
| 3:D:926:PRO:HB2   | 3:D:1246:VAL:HG21 | 2.03                     | 0.40              |
| 3:D:1036:ARG:HH21 | 3:D:1038:THR:HG22 | 1.85                     | 0.40              |
| 5:L:287:TRP:HB3   | 5:L:326:ALA:HB1   | 2.04                     | 0.40              |
| 1:A:65:LEU:HD13   | 2:C:873:ILE:O     | 2.20                     | 0.40              |
| 2:C:587:LEU:HD23  | 2:C:587:LEU:HA    | 1.91                     | 0.40              |
| 3:D:212:THR:HA    | 3:D:215:LYS:NZ    | 2.37                     | 0.40              |
| 3:D:213:LYS:HA    | 3:D:216:LYS:HG2   | 2.02                     | 0.40              |
| 3:D:337:ARG:O     | 3:D:339:ARG:N     | 2.54                     | 0.40              |
| 3:D:422:LEU:HD23  | 3:D:422:LEU:HA    | 1.91                     | 0.40              |
| 3:D:822:MET:CE    | 3:D:838:ARG:HB3   | 2.50                     | 0.40              |
| 3:D:930:LEU:HD23  | 3:D:1244:GLN:HG3  | 2.04                     | 0.40              |
| 3:D:956:GLY:HA3   | 3:D:984:LEU:HD11  | 2.04                     | 0.40              |
| 3:D:966:VAL:HG11  | 3:D:1030:GLU:OE1  | 2.21                     | 0.40              |
| 5:L:202:ARG:HH21  | 5:L:272:ALA:HB1   | 1.86                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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     | 229/237 (97%)    | 213 (93%)  | 16 (7%)  | 0        | 100         | 100 |
| 1   | B     | 228/237 (96%)    | 206 (90%)  | 20 (9%)  | 2 (1%)   | 14          | 49  |
| 2   | C     | 1338/1340 (100%) | 1225 (92%) | 104 (8%) | 9 (1%)   | 18          | 55  |
| 3   | D     | 1332/1363 (98%)  | 1216 (91%) | 111 (8%) | 5 (0%)   | 30          | 67  |
| 4   | E     | 74/91 (81%)      | 69 (93%)   | 5 (7%)   | 0        | 100         | 100 |
| 5   | L     | 965/968 (100%)   | 928 (96%)  | 35 (4%)  | 2 (0%)   | 43          | 78  |
| All | All   | 4166/4236 (98%)  | 3857 (93%) | 291 (7%) | 18 (0%)  | 31          | 67  |

All (18) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 21   | SER  |
| 2   | C     | 199  | ASP  |
| 2   | C     | 913  | VAL  |
| 2   | C     | 938  | GLY  |
| 2   | C     | 1041 | ASP  |
| 3   | D     | 338  | PHE  |
| 3   | D     | 1345 | ARG  |
| 5   | L     | 561  | LEU  |
| 5   | L     | 563  | SER  |
| 2   | C     | 398  | SER  |
| 1   | B     | 193  | GLU  |
| 2   | C     | 625  | GLU  |
| 2   | C     | 1160 | ASP  |
| 3   | D     | 860  | ARG  |
| 2   | C     | 43   | PRO  |
| 3   | D     | 46   | TYR  |
| 3   | D     | 1151 | LYS  |
| 2   | C     | 1223 | ARG  |

### 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     | 199/204 (98%)    | 199 (100%)  | 0        | 100         | 100 |
| 1   | B     | 198/204 (97%)    | 194 (98%)   | 4 (2%)   | 48          | 66  |
| 2   | C     | 1155/1155 (100%) | 1123 (97%)  | 32 (3%)  | 38          | 59  |
| 3   | D     | 1111/1136 (98%)  | 1106 (100%) | 5 (0%)   | 81          | 82  |
| 4   | E     | 65/75 (87%)      | 65 (100%)   | 0        | 100         | 100 |
| 5   | L     | 820/829 (99%)    | 820 (100%)  | 0        | 100         | 100 |
| All | All   | 3548/3603 (98%)  | 3507 (99%)  | 41 (1%)  | 61          | 73  |

All (41) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 27  | THR  |
| 1   | B     | 28  | LEU  |
| 1   | B     | 31  | LEU  |
| 1   | B     | 32  | GLU  |
| 2   | C     | 107 | ARG  |
| 2   | C     | 882 | ILE  |
| 2   | C     | 883 | LEU  |
| 2   | C     | 884 | VAL  |
| 2   | C     | 887 | VAL  |
| 2   | C     | 888 | THR  |
| 2   | C     | 890 | LYS  |
| 2   | C     | 895 | LEU  |
| 2   | C     | 896 | THR  |
| 2   | C     | 898 | GLU  |
| 2   | C     | 901 | LEU  |
| 2   | C     | 902 | LEU  |
| 2   | C     | 905 | ILE  |
| 2   | C     | 908 | GLU  |
| 2   | C     | 909 | LYS  |
| 2   | C     | 913 | VAL  |
| 2   | C     | 914 | LYS  |
| 2   | C     | 915 | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 916  | SER  |
| 2   | C     | 917  | SER  |
| 2   | C     | 935  | THR  |
| 2   | C     | 936  | ARG  |
| 2   | C     | 937  | ASP  |
| 2   | C     | 939  | VAL  |
| 2   | C     | 940  | GLU  |
| 2   | C     | 941  | LYS  |
| 2   | C     | 942  | ASP  |
| 2   | C     | 943  | LYS  |
| 2   | C     | 1159 | VAL  |
| 2   | C     | 1161 | LEU  |
| 2   | C     | 1162 | SER  |
| 2   | C     | 1163 | THR  |
| 3   | D     | 52   | GLU  |
| 3   | D     | 54   | ASP  |
| 3   | D     | 56   | LEU  |
| 3   | D     | 861  | ASN  |
| 3   | D     | 1301 | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 23   | HIS  |
| 1   | A     | 84   | ASN  |
| 1   | A     | 132  | HIS  |
| 1   | B     | 93   | GLN  |
| 2   | C     | 20   | GLN  |
| 2   | C     | 46   | GLN  |
| 2   | C     | 582  | ASN  |
| 2   | C     | 622  | ASN  |
| 2   | C     | 659  | GLN  |
| 2   | C     | 688  | GLN  |
| 2   | C     | 932  | GLN  |
| 2   | C     | 955  | GLN  |
| 2   | C     | 1010 | GLN  |
| 2   | C     | 1023 | HIS  |
| 2   | C     | 1111 | GLN  |
| 2   | C     | 1237 | HIS  |
| 3   | D     | 186  | GLN  |
| 3   | D     | 667  | GLN  |
| 3   | D     | 762  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 771  | GLN  |
| 3   | D     | 897  | HIS  |
| 3   | D     | 1279 | GLN  |
| 5   | L     | 119  | GLN  |
| 5   | L     | 250  | GLN  |
| 5   | L     | 297  | GLN  |
| 5   | L     | 301  | GLN  |
| 5   | L     | 609  | HIS  |
| 5   | L     | 626  | 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 3 ligands modelled in this entry, 3 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 ⓘ

There are no chain breaks in this entry.

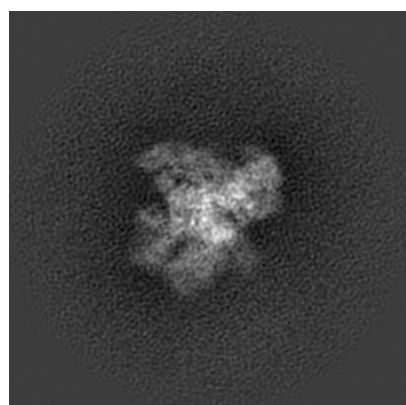
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23903. These allow visual inspection of the internal detail of the map and identification of artifacts.

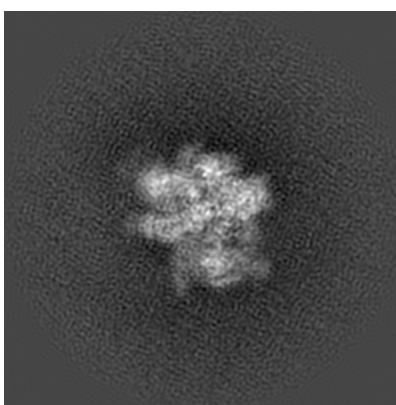
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

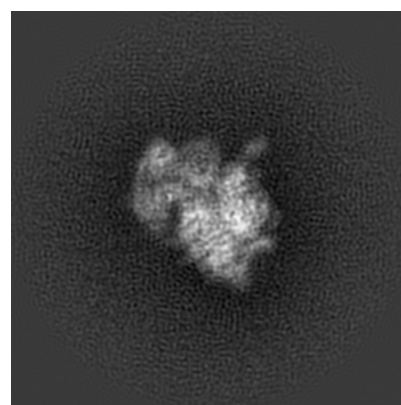
#### 6.1.1 Primary map



X



Y

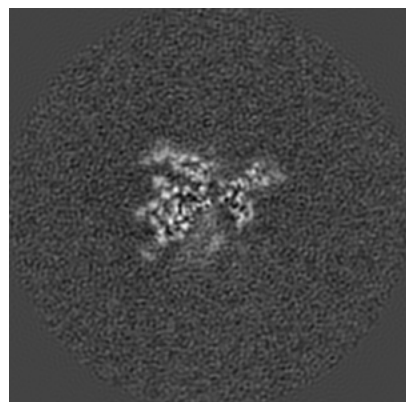


Z

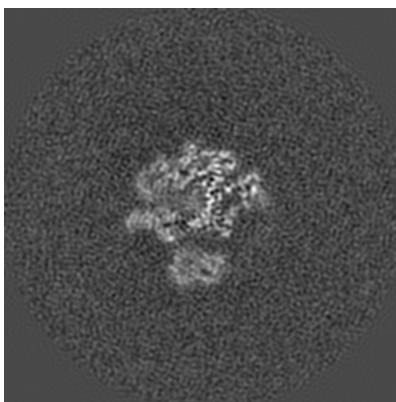
The images above show the map projected in three orthogonal directions.

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

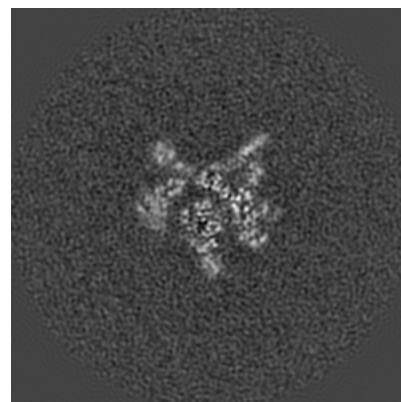
#### 6.2.1 Primary map



X Index: 180



Y Index: 180

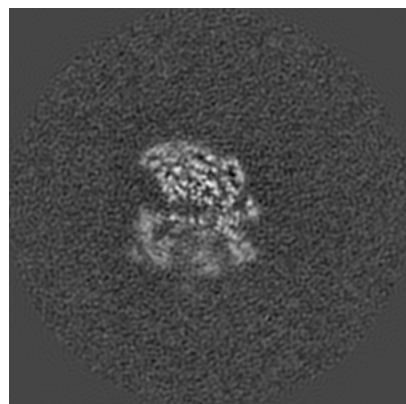


Z Index: 180

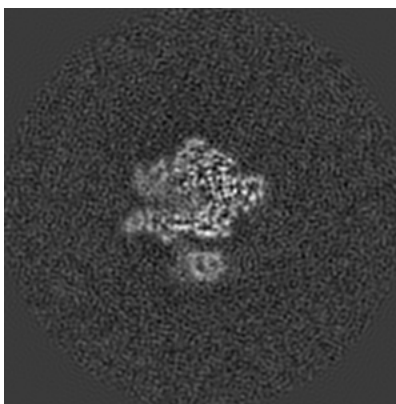
The images above show central slices of the map in three orthogonal directions.

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

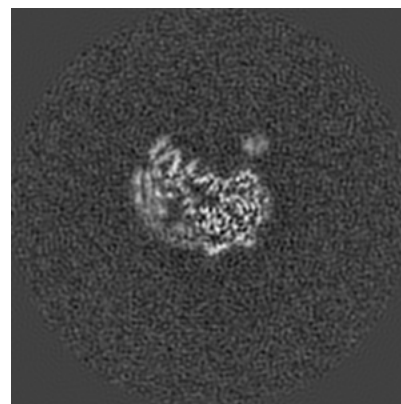
### 6.3.1 Primary map



X Index: 196



Y Index: 175

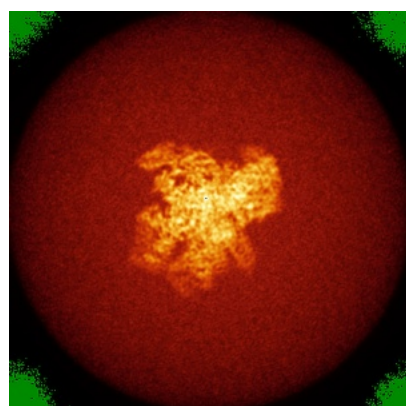


Z Index: 192

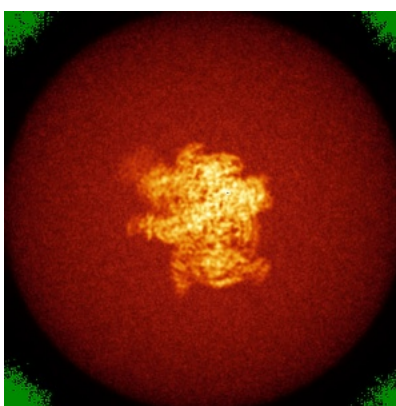
The images above show the largest variance slices of the map in three orthogonal directions.

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

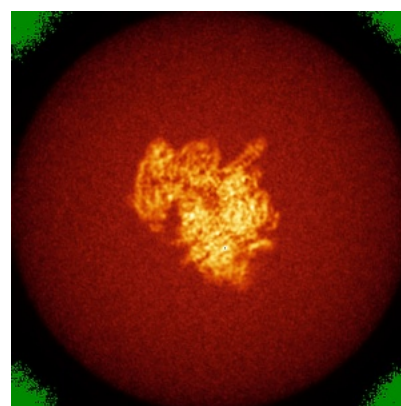
### 6.4.1 Primary map



X



Y

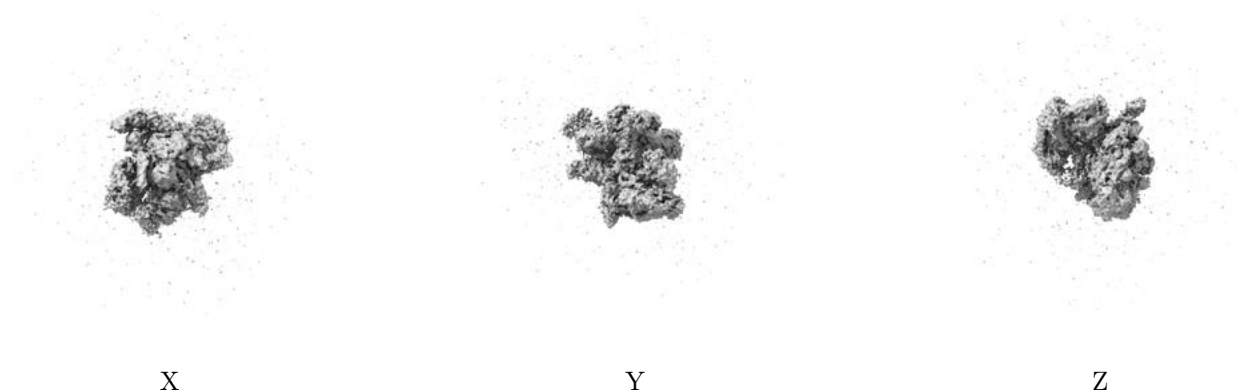


Z

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 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

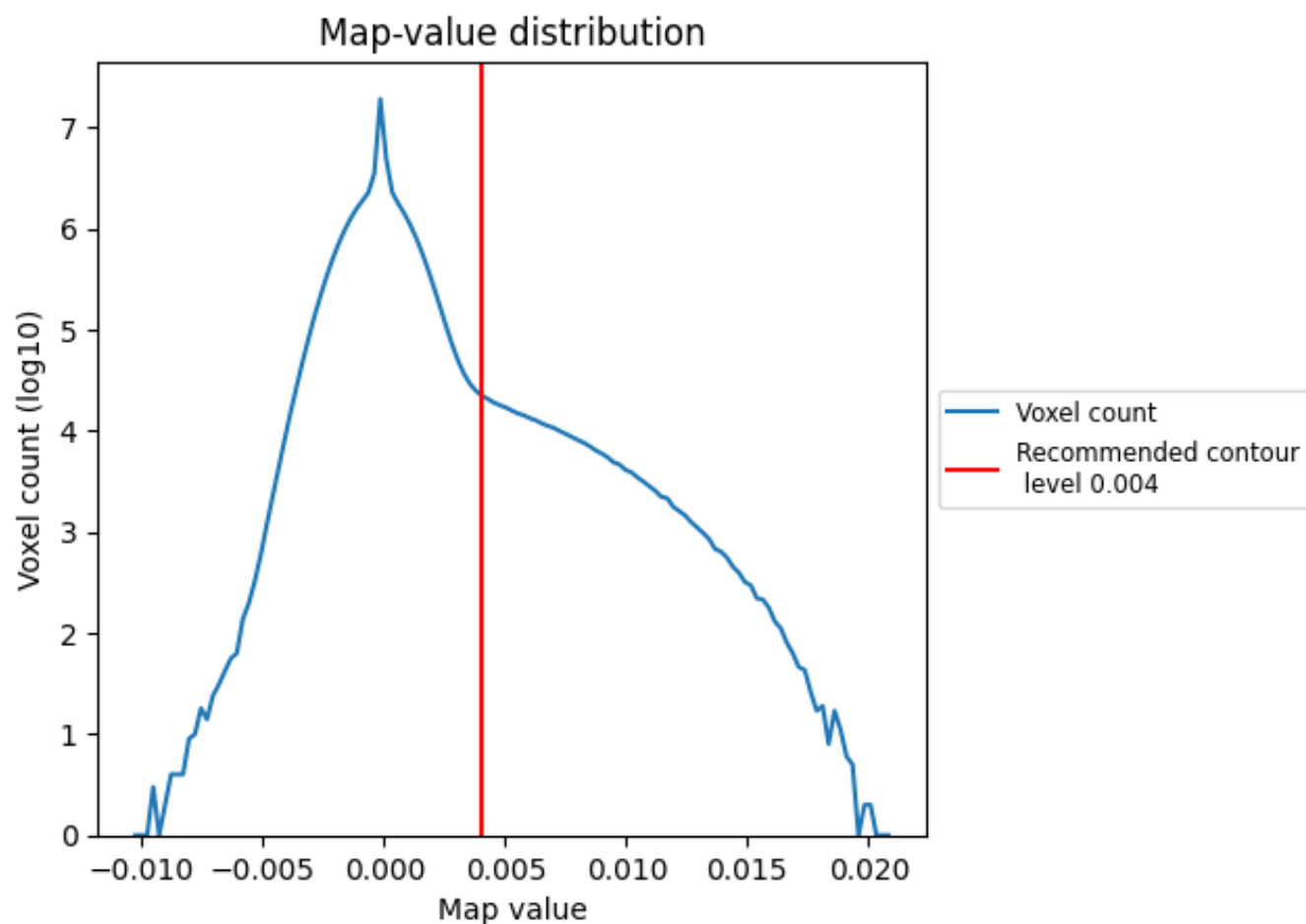
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

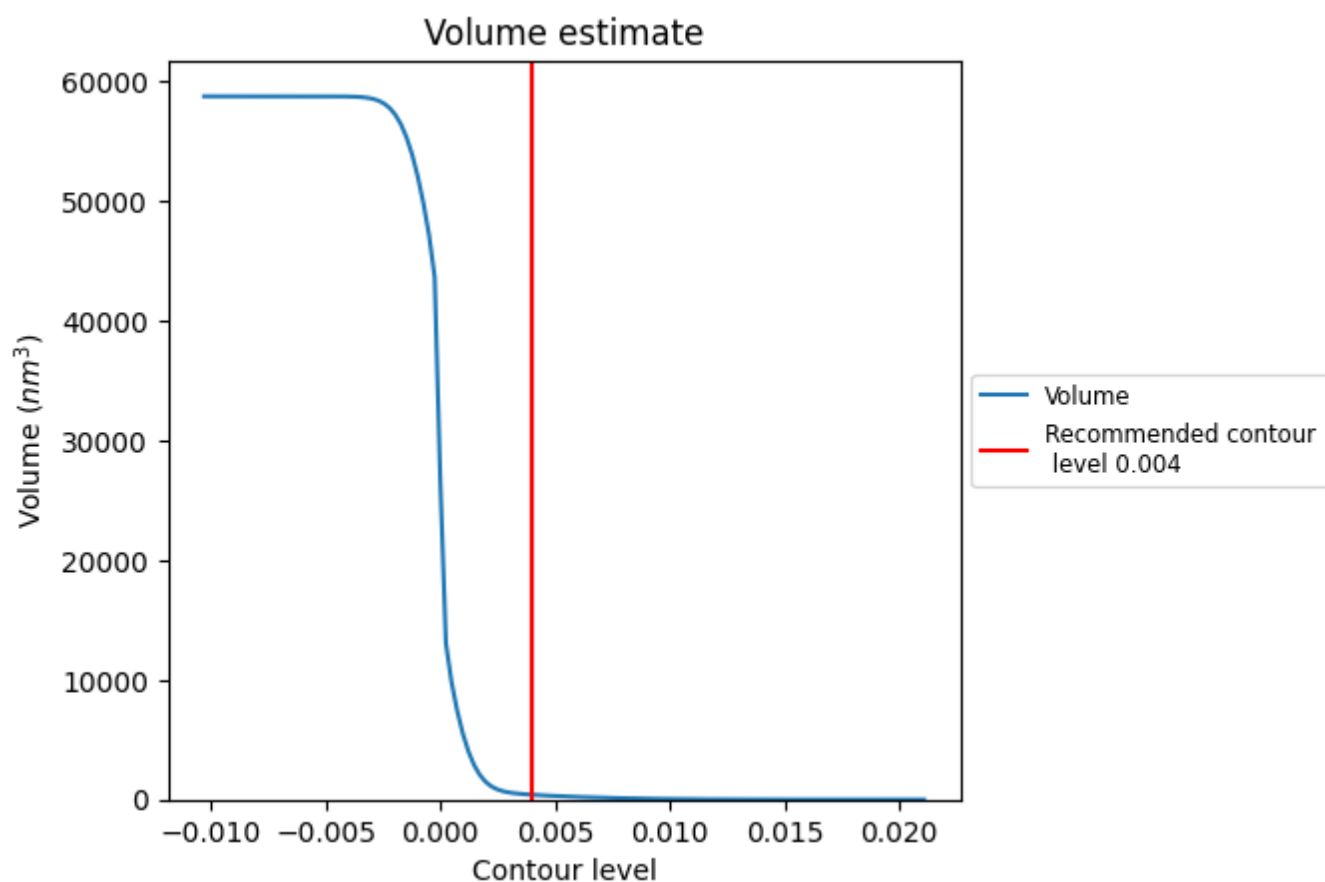
This section contains the results of statistical analysis of the map.

### 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.

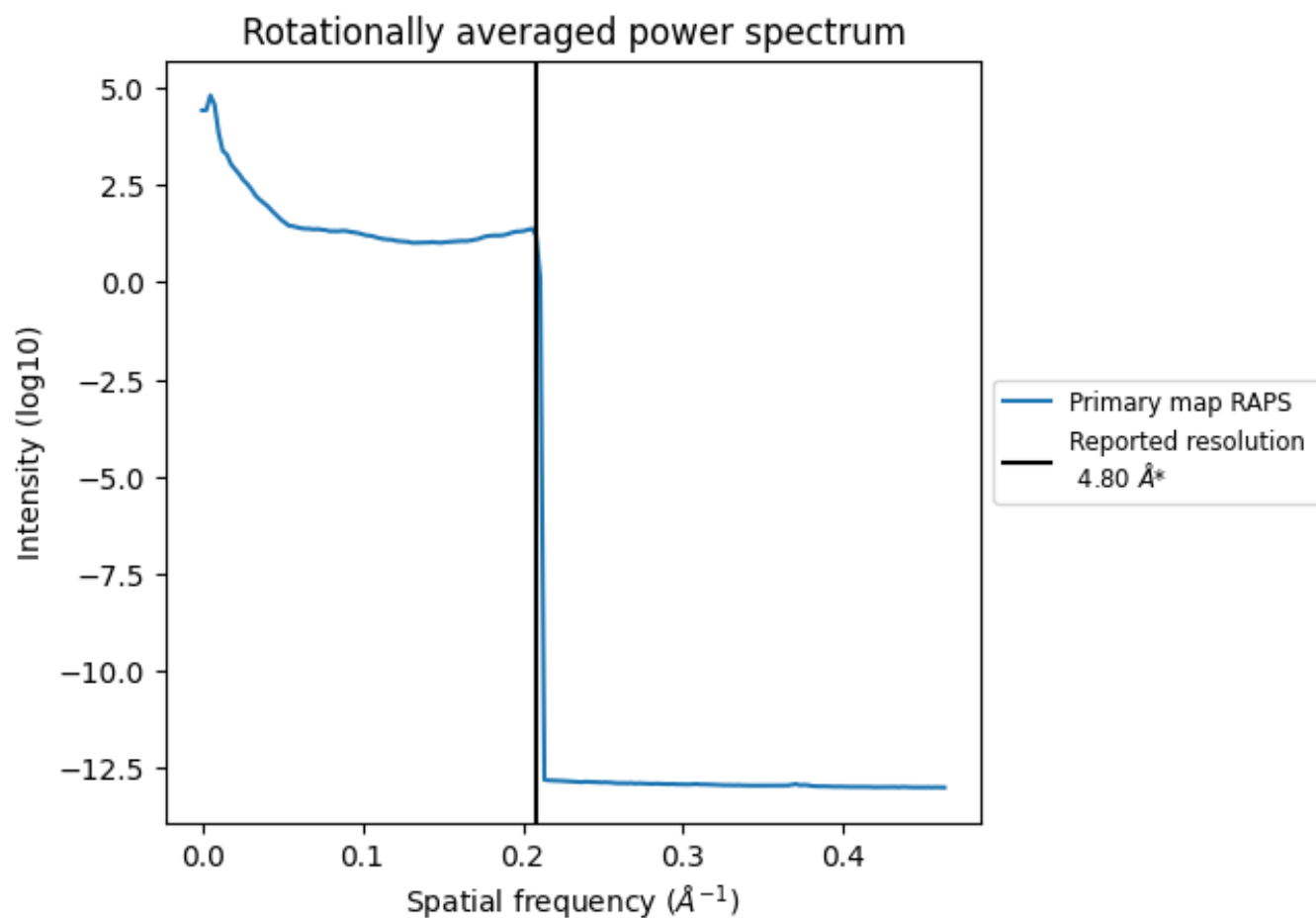
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 404 nm<sup>3</sup>; this corresponds to an approximate mass of 365 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 ⓘ



\*Reported resolution corresponds to spatial frequency of 0.208 Å<sup>-1</sup>

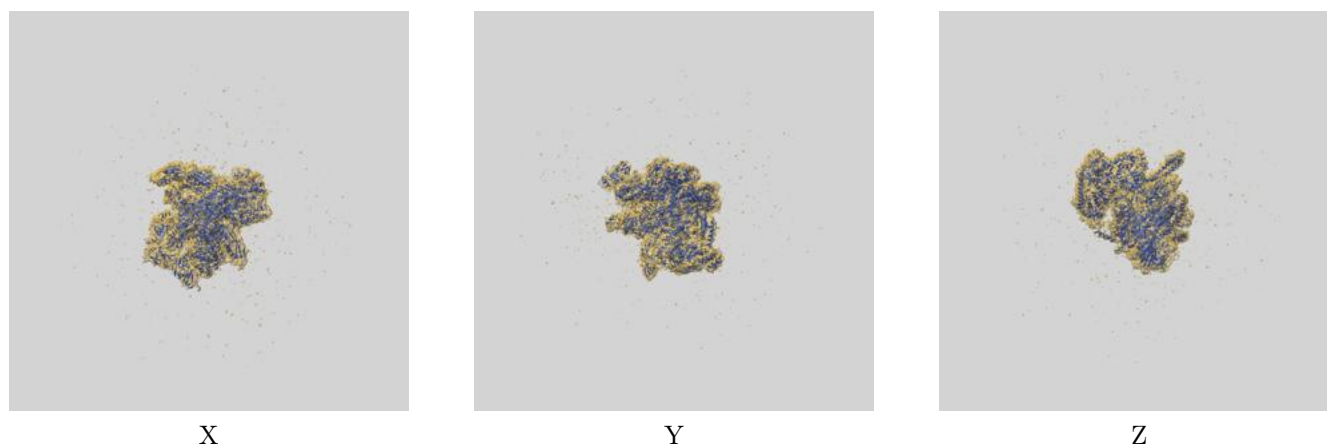
## 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

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

This section contains information regarding the fit between EMDB map EMD-23903 and PDB model 7MKQ. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

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



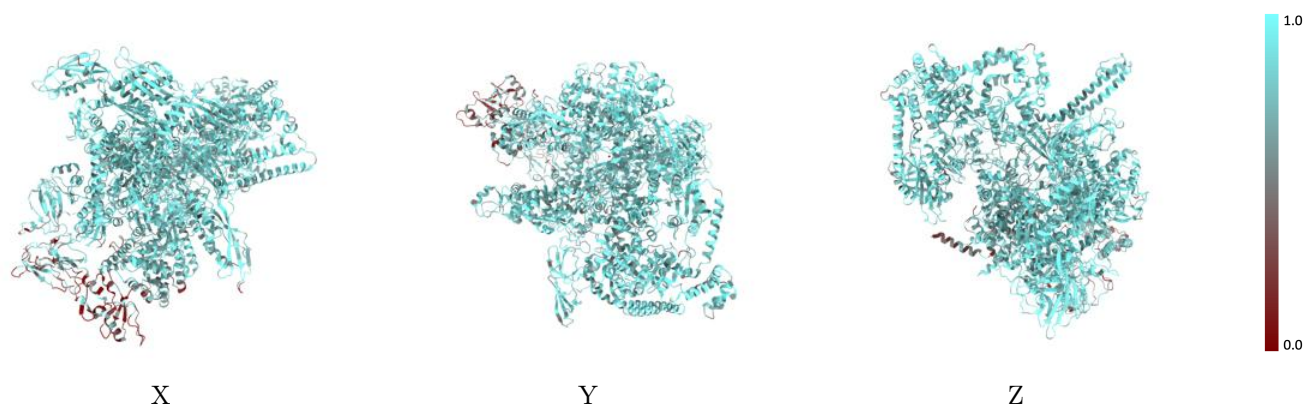
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



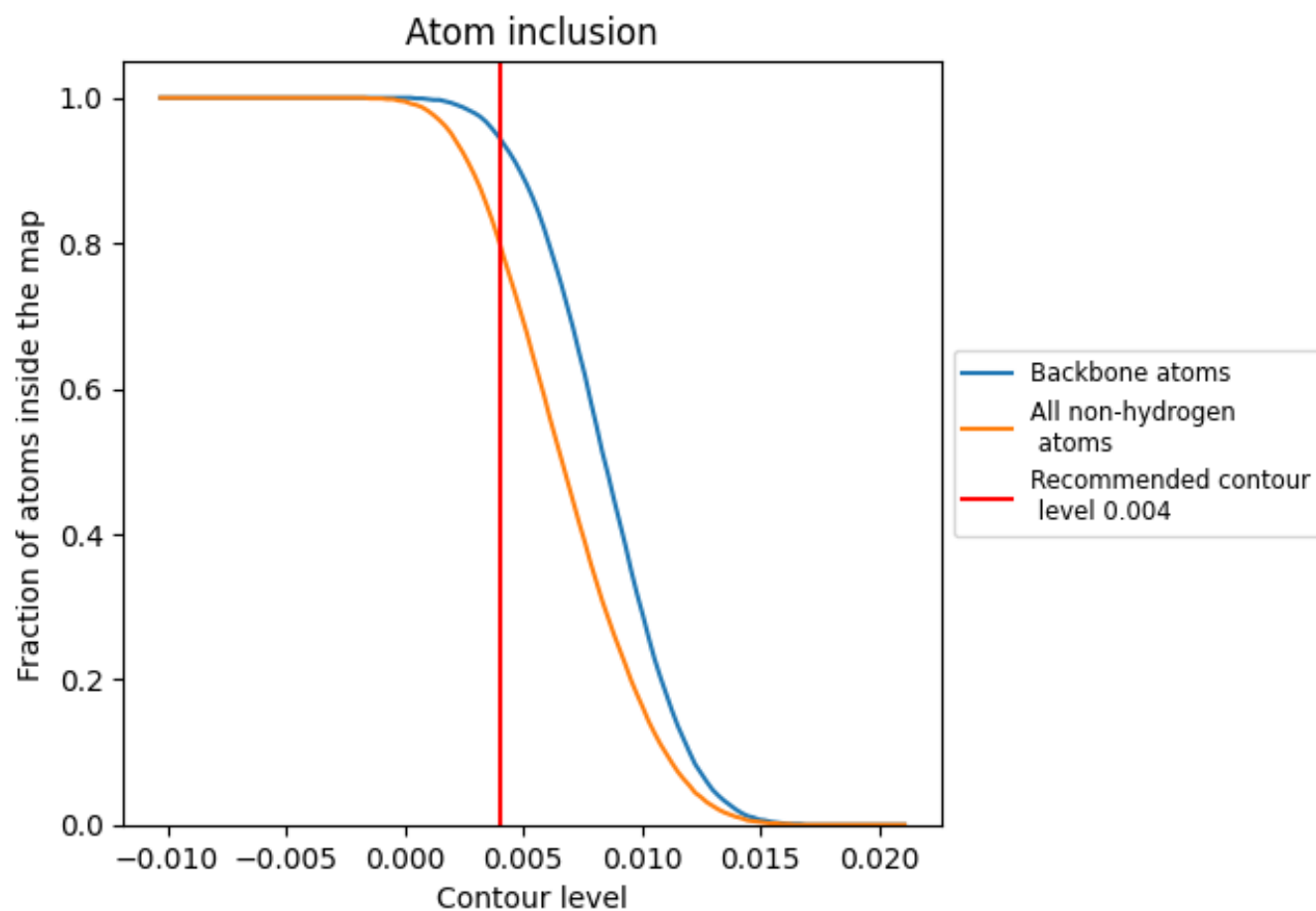
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.004).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 80% 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 (0.004) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion               | Q-score                      |
|-------|------------------------------|------------------------------|
| All   | <div><div></div>0.8010</div> | <div><div></div>0.2540</div> |
| A     | <div><div></div>0.8540</div> | <div><div></div>0.3050</div> |
| B     | <div><div></div>0.8480</div> | <div><div></div>0.2620</div> |
| C     | <div><div></div>0.7730</div> | <div><div></div>0.2610</div> |
| D     | <div><div></div>0.8020</div> | <div><div></div>0.2520</div> |
| E     | <div><div></div>0.6040</div> | <div><div></div>0.2230</div> |
| L     | <div><div></div>0.8290</div> | <div><div></div>0.2350</div> |

1.0

0.0

<0.0