



## Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:54 AM UTC

PDB ID : 7E8H / pdb\_00007e8h  
EMDB ID : EMD-31019  
Title : CryoEM structure of human Kv4.2-DPP6S-KChIP1 complex  
Authors : Kise, Y.; Nureki, O.  
Deposited on : 2021-03-01  
Resolution : 4.50 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

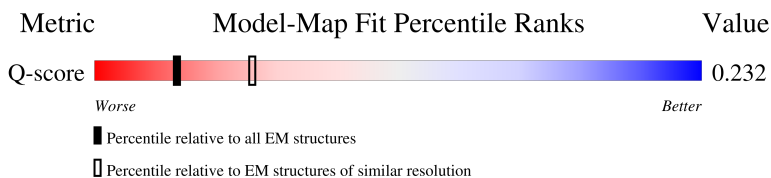
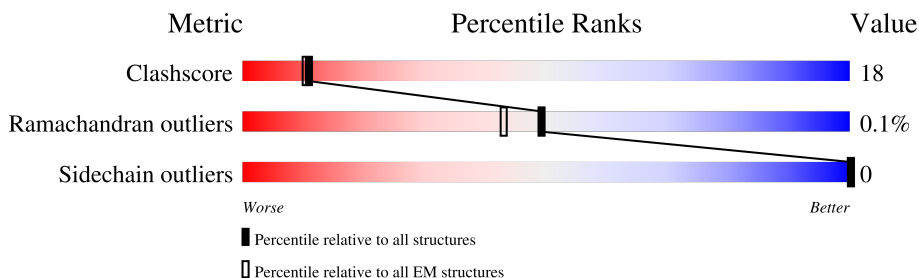
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.50 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                       | 2937 ( 4.00 - 5.00 )                                     |

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   | J     | 757    |                  |
| 1   | L     | 757    |                  |
| 2   | I     | 760    |                  |
| 2   | K     | 760    |                  |

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| Mol | Chain | Length | Quality of chain      |
|-----|-------|--------|-----------------------|
| 3   | F     | 180    | <p>66% 32% •</p>      |
| 3   | H     | 180    | <p>66% 32% •</p>      |
| 4   | A     | 494    | <p>15% 58% 35% 7%</p> |
| 4   | B     | 494    | <p>15% 55% 37% 7%</p> |
| 4   | C     | 494    | <p>15% 59% 34% 7%</p> |
| 4   | D     | 494    | <p>15% 55% 38% 7%</p> |
| 5   | E     | 181    | <p>78% 60% 38% •</p>  |
| 5   | G     | 181    | <p>79% 62% 36% •</p>  |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 44894 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 Dipeptidyl aminopeptidase-like protein 6.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1   | J     | 756      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6071  | 3872 | 1025 | 1149 | 25 |         |       |
| 1   | L     | 756      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6071  | 3872 | 1025 | 1149 | 25 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| J     | 31      | ALA      | -      | expression tag | UNP P42658 |
| L     | 31      | ALA      | -      | expression tag | UNP P42658 |

- Molecule 2 is a protein called Dipeptidyl aminopeptidase-like protein 6.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 2   | I     | 760      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6093  | 3886 | 1029 | 1153 | 25 |         |       |
| 2   | K     | 760      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6093  | 3886 | 1029 | 1153 | 25 |         |       |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| I     | 28      | ALA      | -      | expression tag | UNP P42658 |
| I     | 29      | ALA      | -      | expression tag | UNP P42658 |
| I     | 30      | ALA      | -      | expression tag | UNP P42658 |
| I     | 31      | ALA      | -      | expression tag | UNP P42658 |
| K     | 28      | ALA      | -      | expression tag | UNP P42658 |
| K     | 29      | ALA      | -      | expression tag | UNP P42658 |
| K     | 30      | ALA      | -      | expression tag | UNP P42658 |
| K     | 31      | ALA      | -      | expression tag | UNP P42658 |

- Molecule 3 is a protein called Kv channel-interacting protein 1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3   | F     | 176      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1459  | 932 | 237 | 281 | 9 |         |       |
| 3   | H     | 176      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1459  | 932 | 237 | 281 | 9 |         |       |

- Molecule 4 is a protein called Potassium voltage-gated channel subfamily D member 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | B     | 459      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3675  | 2365 | 638 | 652 | 20 |         |       |
| 4   | A     | 460      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3683  | 2371 | 639 | 653 | 20 |         |       |
| 4   | D     | 459      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3675  | 2365 | 638 | 652 | 20 |         |       |
| 4   | C     | 460      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3683  | 2371 | 639 | 653 | 20 |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| B     | 450     | SER      | ASN    | conflict | UNP Q9NZV8 |
| A     | 450     | SER      | ASN    | conflict | UNP Q9NZV8 |
| D     | 450     | SER      | ASN    | conflict | UNP Q9NZV8 |
| C     | 450     | SER      | ASN    | conflict | UNP Q9NZV8 |

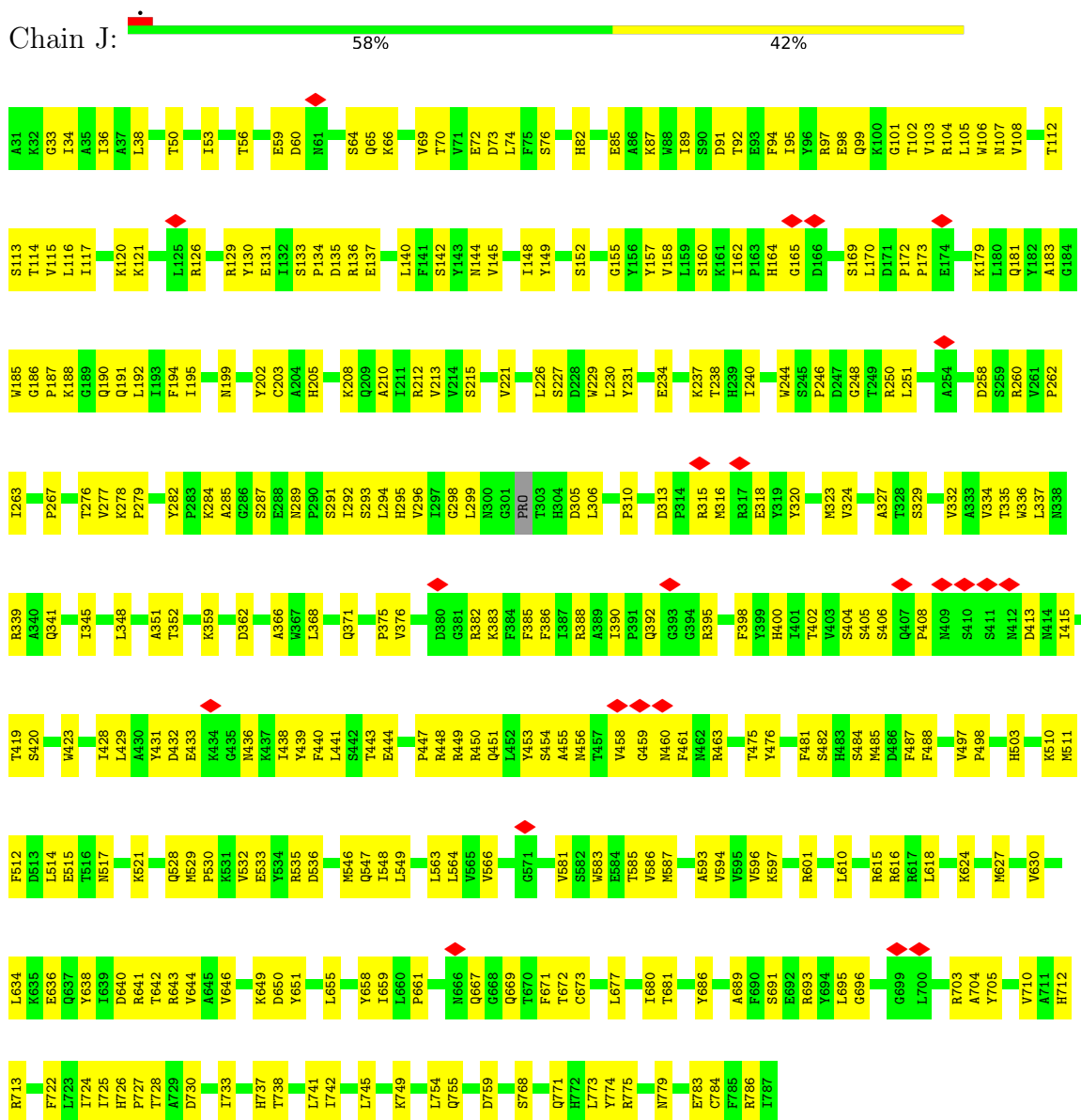
- Molecule 5 is a protein called Kv channel-interacting protein 1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | E     | 177      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1466  | 937 | 238 | 282 | 9 |         |       |
| 5   | G     | 177      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1466  | 937 | 238 | 282 | 9 |         |       |

### 3 Residue-property plots

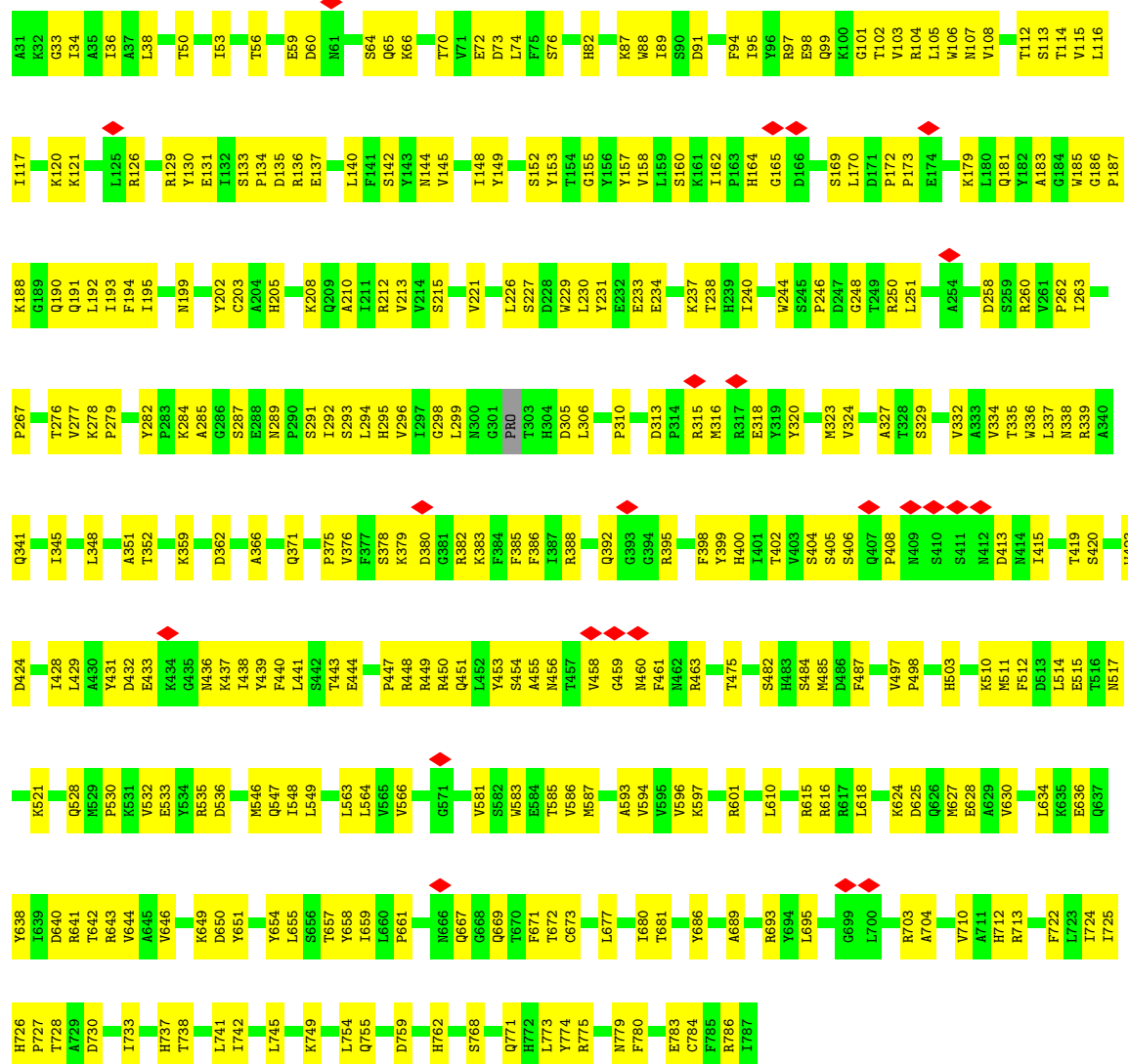
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Dipeptidyl aminopeptidase-like protein 6



- Molecule 1: Dipeptidyl aminopeptidase-like protein 6

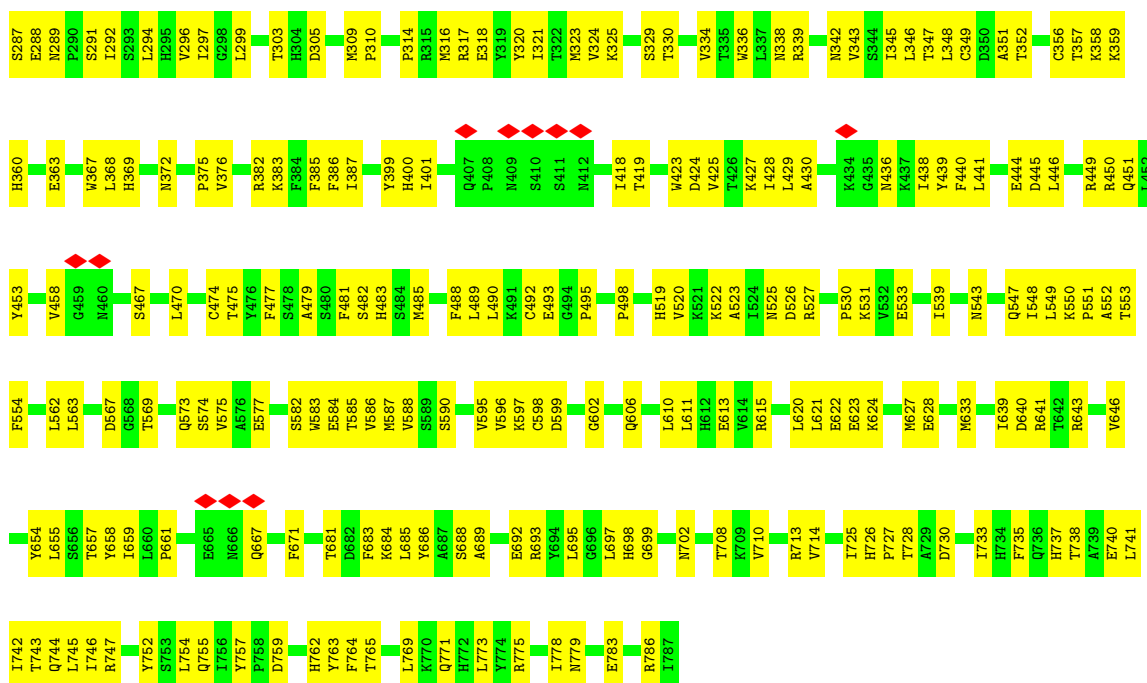
Chain L:  57% 43%



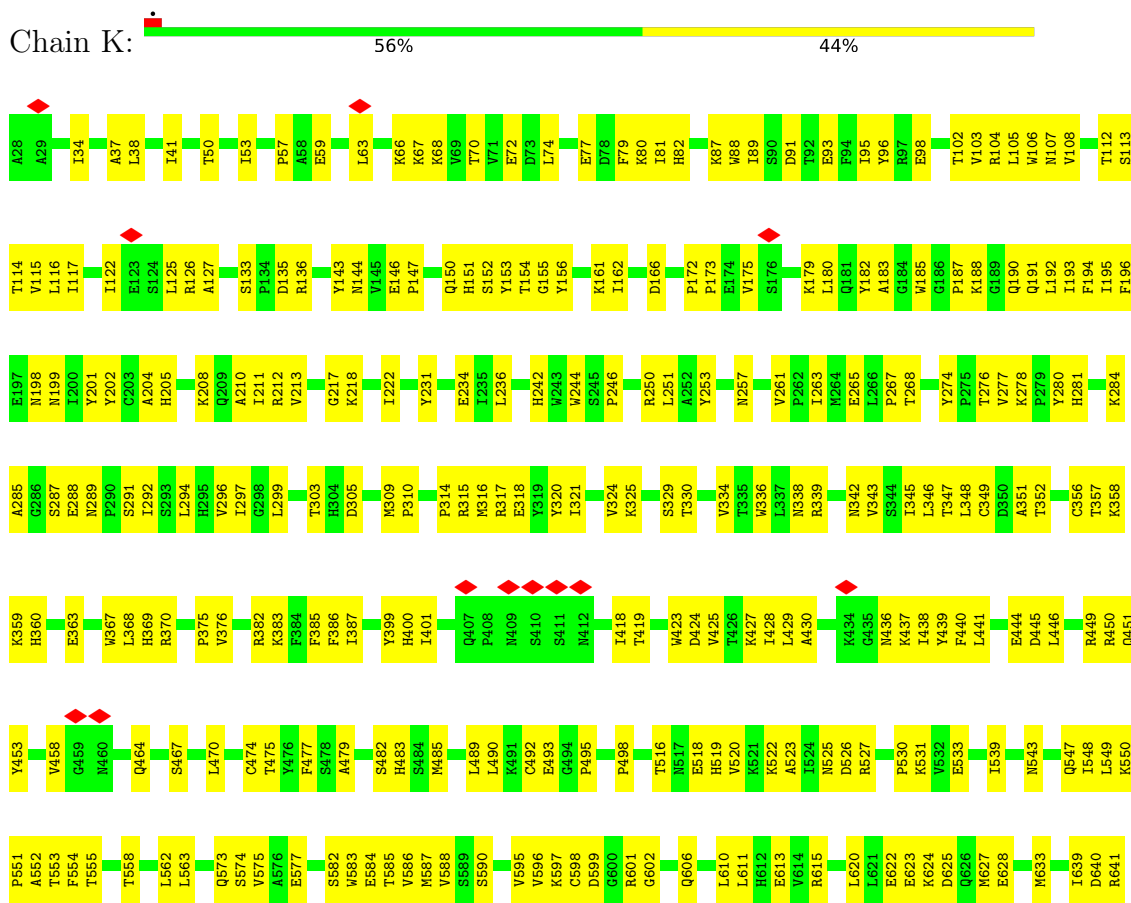
• Molecule 2: Dipeptidyl aminopeptidase-like protein 6

Chain I:  57% 43%

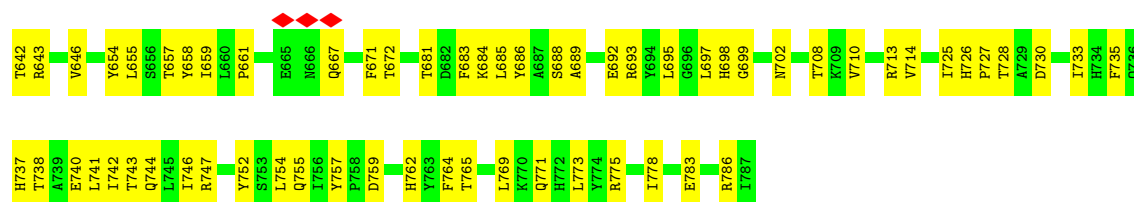




• Molecule 2: Dipeptidyl aminopeptidase-like protein 6



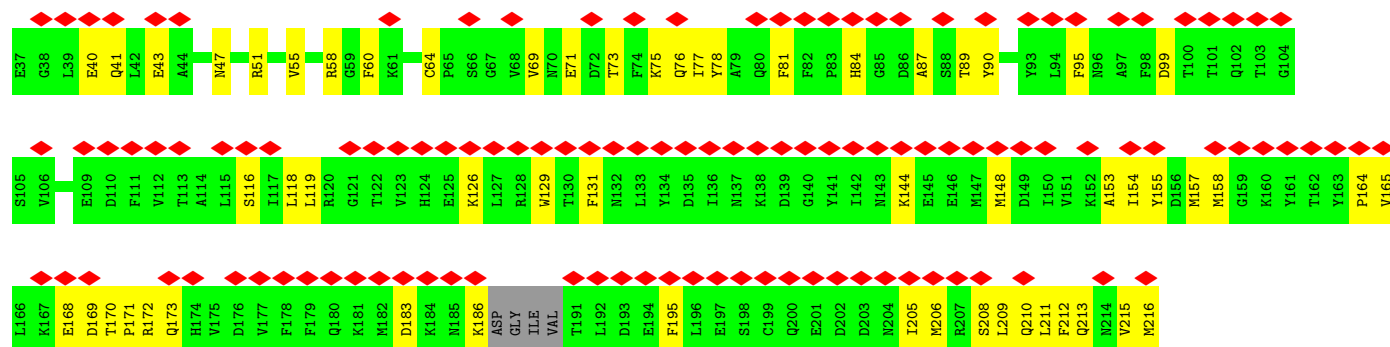




• Molecule 3: Kv channel-interacting protein 1

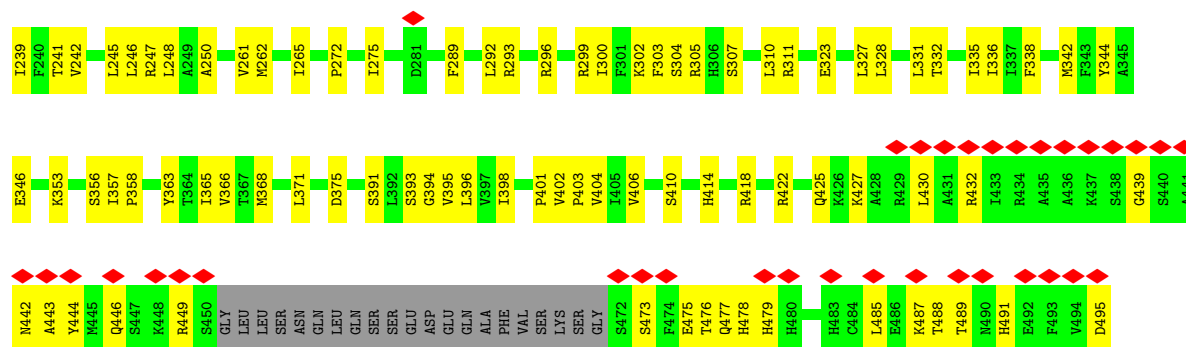


• Molecule 3: Kv channel-interacting protein 1

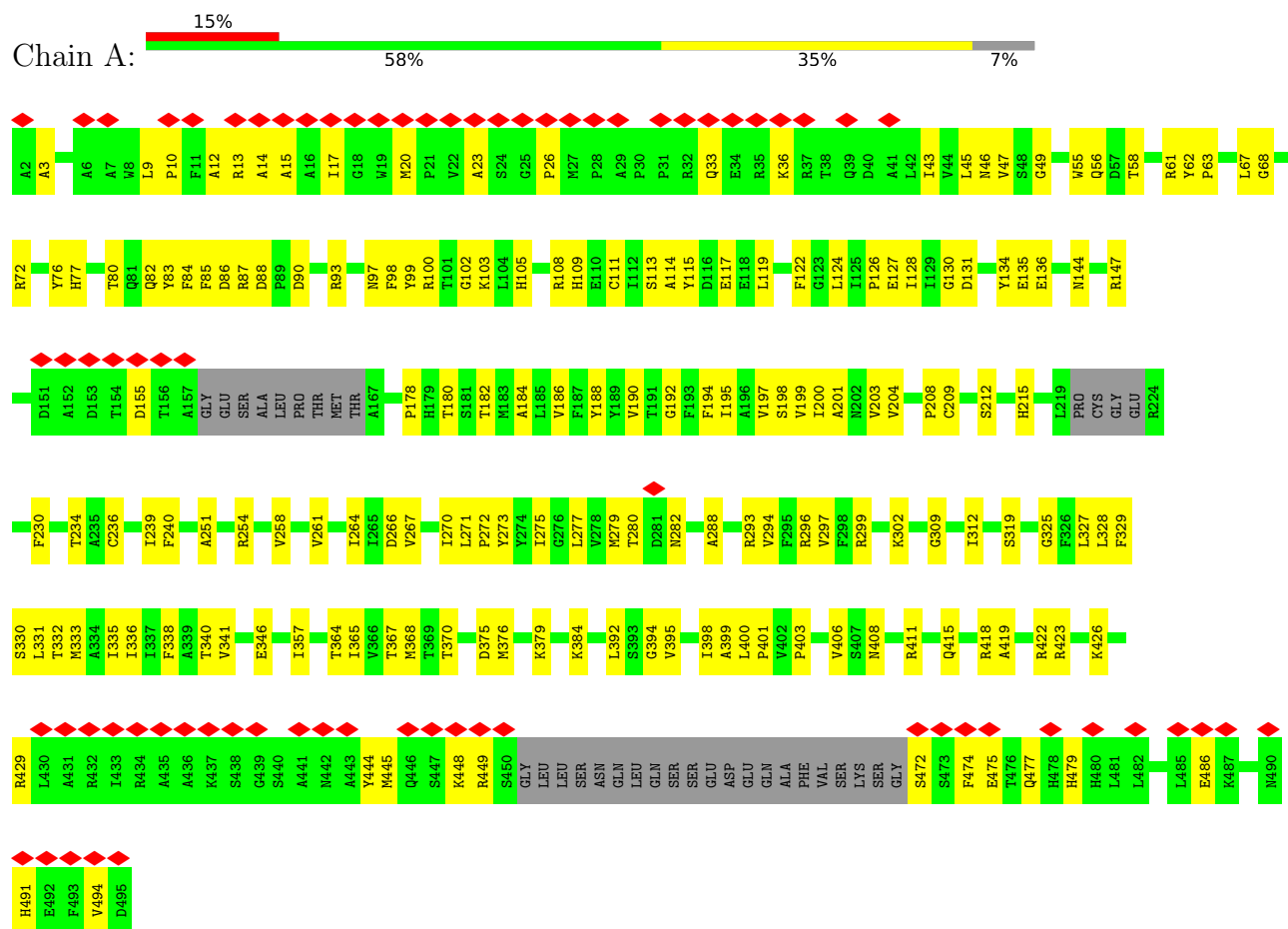


• Molecule 4: Potassium voltage-gated channel subfamily D member 2

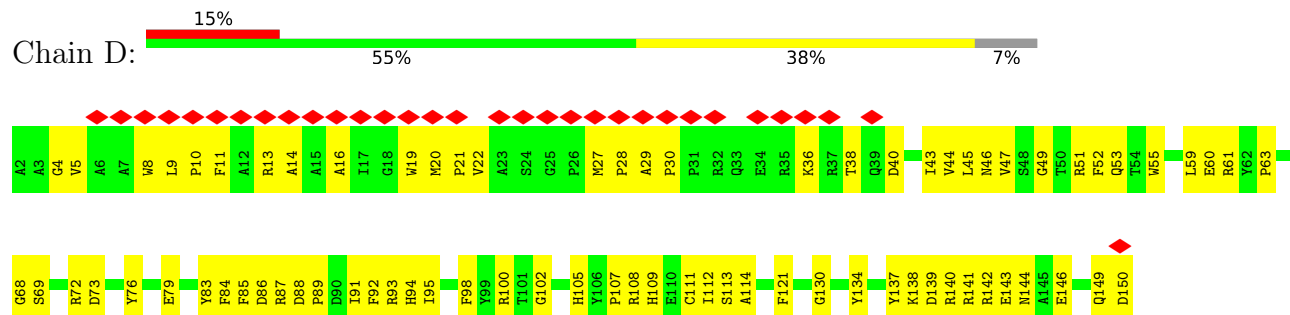


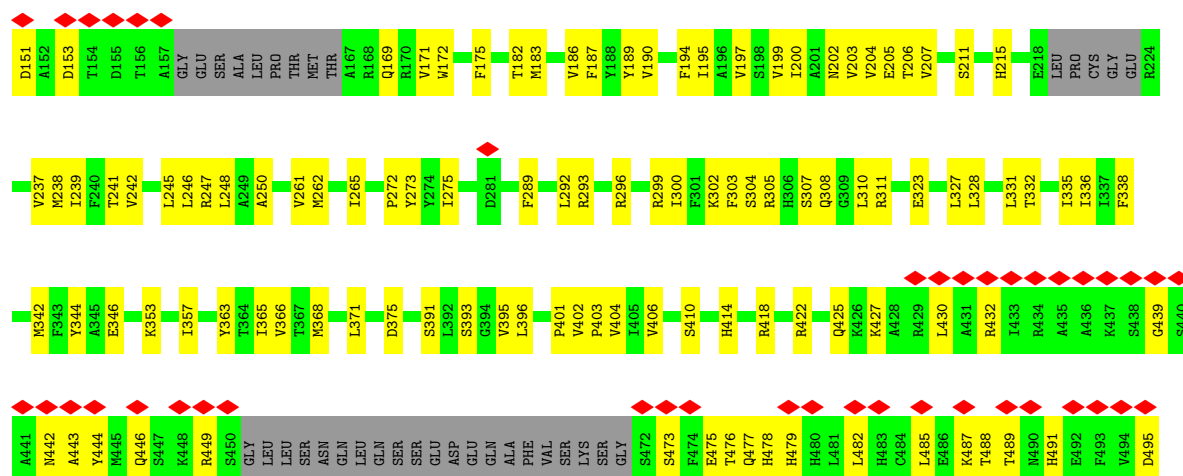


• Molecule 4: Potassium voltage-gated channel subfamily D member 2

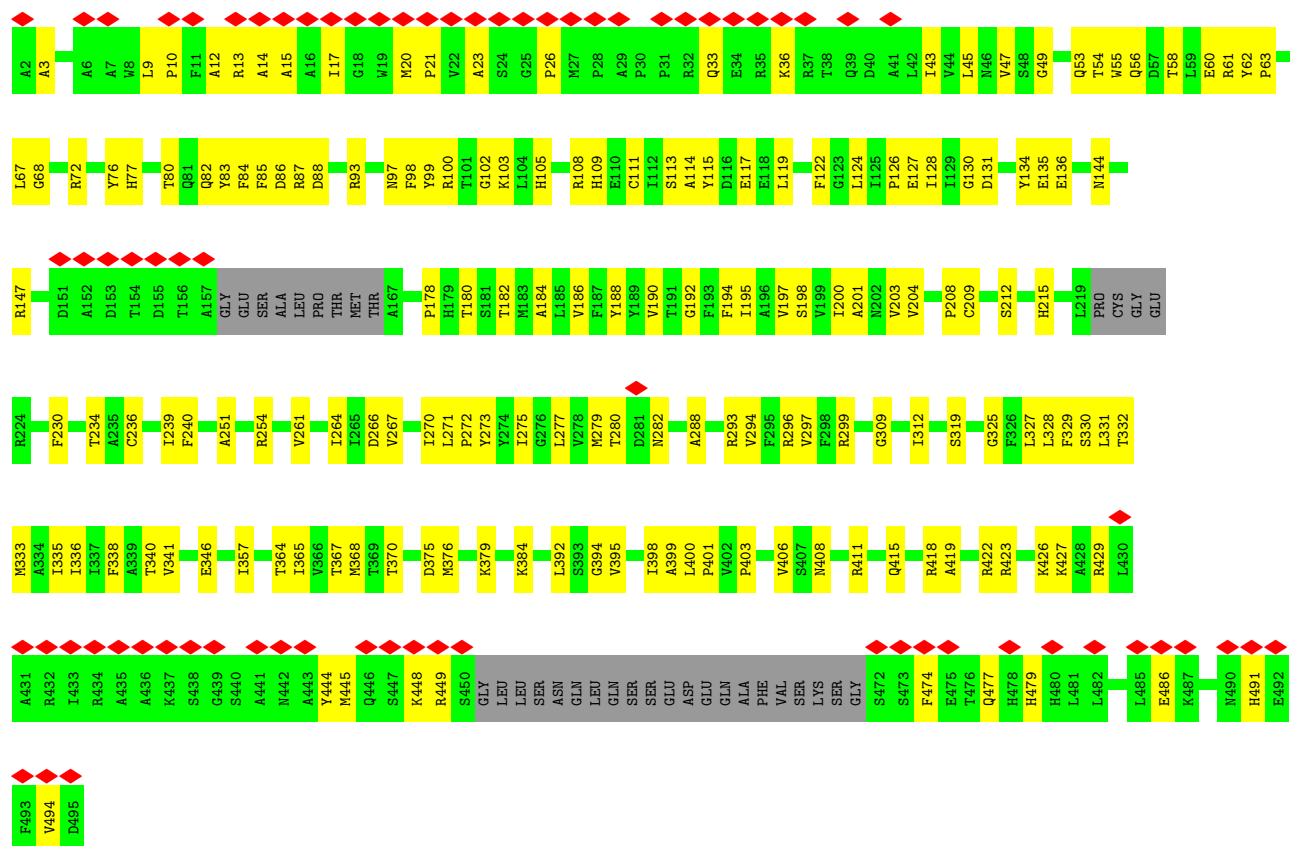


• Molecule 4: Potassium voltage-gated channel subfamily D member 2

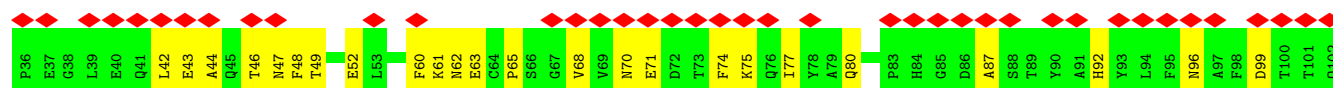
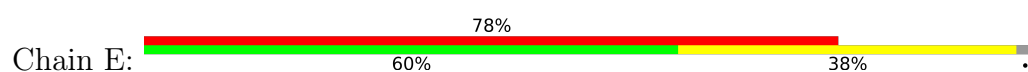


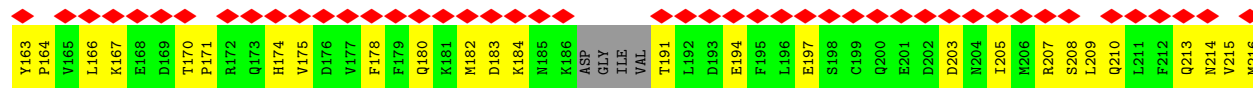
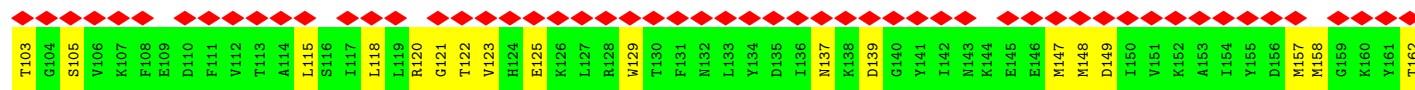


• Molecule 4: Potassium voltage-gated channel subfamily D member 2

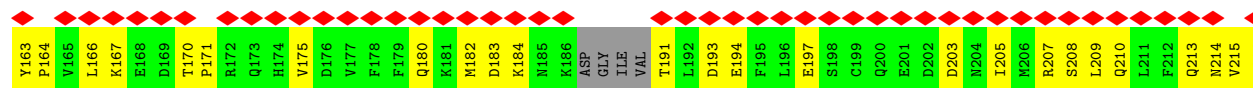
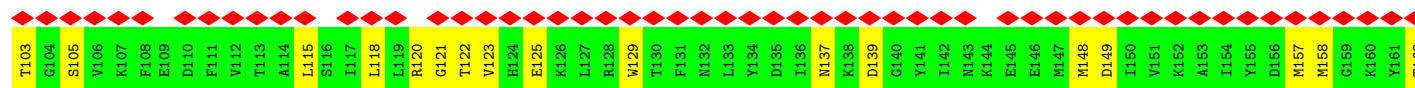
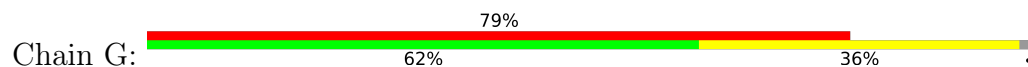


• Molecule 5: Kv channel-interacting protein 1





• Molecule 5: Kv channel-interacting protein 1



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 139524                                  | 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 ( $e^-/\text{\AA}^2$ ) | 48                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |
| Maximum map value                    | 0.041                                   | Depositor |
| Minimum map value                    | -0.016                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.002                                   | Depositor |
| Recommended contour level            | 0.0072                                  | Depositor |
| Map size ( $\text{\AA}$ )            | 298.7986, 298.7986, 298.7986            | wwPDB     |
| Map dimensions                       | 298, 298, 298                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.00268, 1.00268, 1.00268               | Depositor |

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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   | J     | 0.11         | 0/6220  | 0.32        | 0/8436  |
| 1   | L     | 0.11         | 0/6220  | 0.32        | 0/8436  |
| 2   | I     | 0.11         | 0/6244  | 0.34        | 0/8472  |
| 2   | K     | 0.11         | 0/6244  | 0.34        | 0/8472  |
| 3   | F     | 0.11         | 0/1490  | 0.32        | 0/2007  |
| 3   | H     | 0.11         | 0/1490  | 0.32        | 0/2007  |
| 4   | A     | 0.13         | 0/3776  | 0.38        | 0/5115  |
| 4   | B     | 0.14         | 0/3768  | 0.35        | 0/5104  |
| 4   | C     | 0.13         | 0/3776  | 0.38        | 0/5115  |
| 4   | D     | 0.14         | 0/3768  | 0.35        | 0/5104  |
| 5   | E     | 0.12         | 0/1498  | 0.34        | 0/2018  |
| 5   | G     | 0.12         | 0/1498  | 0.34        | 0/2018  |
| All | All   | 0.12         | 0/45992 | 0.34        | 0/62304 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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   | J     | 6071  | 0        | 5956     | 225     | 0            |
| 1   | L     | 6071  | 0        | 5956     | 230     | 0            |
| 2   | I     | 6093  | 0        | 5979     | 243     | 0            |
| 2   | K     | 6093  | 0        | 5979     | 247     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | F     | 1459  | 0        | 1400     | 48      | 0            |
| 3   | H     | 1459  | 0        | 1400     | 49      | 0            |
| 4   | A     | 3683  | 0        | 3650     | 160     | 0            |
| 4   | B     | 3675  | 0        | 3639     | 153     | 0            |
| 4   | C     | 3683  | 0        | 3650     | 158     | 0            |
| 4   | D     | 3675  | 0        | 3639     | 161     | 0            |
| 5   | E     | 1466  | 0        | 1408     | 54      | 0            |
| 5   | G     | 1466  | 0        | 1408     | 49      | 0            |
| All | All   | 44894 | 0        | 44064    | 1637    | 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 18.

All (1637) 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) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:147:PRO:HB3  | 2:I:152:SER:H    | 1.41                     | 0.86              |
| 2:K:296:VAL:O    | 2:K:305:ASP:HA   | 1.76                     | 0.85              |
| 5:E:92:HIS:O     | 5:E:96:ASN:ND2   | 2.10                     | 0.85              |
| 2:K:147:PRO:HB3  | 2:K:152:SER:H    | 1.41                     | 0.85              |
| 2:I:296:VAL:O    | 2:I:305:ASP:HA   | 1.76                     | 0.83              |
| 4:D:47:VAL:HG12  | 4:D:85:PHE:HB2   | 1.61                     | 0.82              |
| 4:B:47:VAL:HG12  | 4:B:85:PHE:HB2   | 1.61                     | 0.82              |
| 1:J:87:LYS:H     | 1:J:95:ILE:HG12  | 1.45                     | 0.81              |
| 4:B:100:ARG:HH12 | 4:C:87:ARG:HA    | 1.47                     | 0.80              |
| 2:I:38:LEU:HB3   | 4:A:186:VAL:HG22 | 1.63                     | 0.79              |
| 4:A:87:ARG:HA    | 4:D:100:ARG:HH12 | 1.47                     | 0.79              |
| 2:K:38:LEU:HB3   | 4:C:186:VAL:HG22 | 1.63                     | 0.79              |
| 1:J:103:VAL:HB   | 1:J:117:ILE:HB   | 1.66                     | 0.78              |
| 2:I:127:ALA:HA   | 2:I:143:TYR:HB3  | 1.66                     | 0.78              |
| 2:K:127:ALA:HA   | 2:K:143:TYR:HB3  | 1.66                     | 0.78              |
| 1:L:87:LYS:H     | 1:L:95:ILE:HG12  | 1.45                     | 0.78              |
| 1:L:103:VAL:HB   | 1:L:117:ILE:HB   | 1.65                     | 0.77              |
| 1:J:530:PRO:HB2  | 1:J:549:LEU:HD12 | 1.67                     | 0.75              |
| 1:L:38:LEU:HD22  | 4:D:186:VAL:HG23 | 1.67                     | 0.75              |
| 1:L:548:ILE:HD11 | 1:L:594:VAL:HB   | 1.68                     | 0.75              |
| 1:L:530:PRO:HB2  | 1:L:549:LEU:HD12 | 1.67                     | 0.75              |
| 2:K:533:GLU:HG2  | 2:K:548:ILE:HG23 | 1.68                     | 0.75              |
| 1:J:548:ILE:HD11 | 1:J:594:VAL:HB   | 1.68                     | 0.74              |
| 1:J:97:ARG:HH22  | 1:J:131:GLU:HA   | 1.53                     | 0.74              |
| 1:J:38:LEU:HD22  | 4:B:186:VAL:HG23 | 1.67                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:C:103:LYS:HE2  | 4:C:130:GLY:HA3  | 1.70                     | 0.73              |
| 2:I:533:GLU:HG2  | 2:I:548:ILE:HG23 | 1.68                     | 0.73              |
| 1:L:728:THR:HB   | 1:L:759:ASP:H    | 1.54                     | 0.73              |
| 4:A:103:LYS:HE2  | 4:A:130:GLY:HA3  | 1.70                     | 0.73              |
| 2:K:728:THR:HB   | 2:K:759:ASP:H    | 1.54                     | 0.73              |
| 1:L:97:ARG:HH22  | 1:L:131:GLU:HA   | 1.53                     | 0.73              |
| 1:L:250:ARG:HG2  | 1:L:298:GLY:HA2  | 1.72                     | 0.72              |
| 1:J:728:THR:HB   | 1:J:759:ASP:H    | 1.54                     | 0.72              |
| 2:I:726:HIS:ND1  | 2:I:738:THR:OG1  | 2.23                     | 0.72              |
| 2:I:728:THR:HB   | 2:I:759:ASP:H    | 1.53                     | 0.72              |
| 2:K:287:SER:O    | 2:K:339:ARG:NH2  | 2.23                     | 0.72              |
| 2:K:726:HIS:ND1  | 2:K:738:THR:OG1  | 2.23                     | 0.71              |
| 2:K:91:ASP:HA    | 2:K:482:SER:HB2  | 1.72                     | 0.71              |
| 1:J:104:ARG:HE   | 1:J:115:VAL:HA   | 1.54                     | 0.71              |
| 4:A:426:LYS:HA   | 4:A:429:ARG:HG2  | 1.73                     | 0.71              |
| 1:L:104:ARG:HE   | 1:L:115:VAL:HA   | 1.54                     | 0.71              |
| 4:C:63:PRO:HA    | 4:C:68:GLY:HA3   | 1.72                     | 0.71              |
| 1:J:250:ARG:HG2  | 1:J:298:GLY:HA2  | 1.72                     | 0.70              |
| 1:L:313:ASP:HB2  | 1:L:316:MET:HG2  | 1.73                     | 0.70              |
| 2:K:531:LYS:HG3  | 2:K:552:ALA:HA   | 1.73                     | 0.70              |
| 2:I:531:LYS:HG3  | 2:I:552:ALA:HA   | 1.73                     | 0.70              |
| 1:J:392:GLN:HG3  | 1:J:398:PHE:HB2  | 1.73                     | 0.70              |
| 2:K:551:PRO:HD2  | 2:K:554:PHE:HB2  | 1.74                     | 0.70              |
| 1:J:246:PRO:HD2  | 1:J:329:SER:HA   | 1.73                     | 0.70              |
| 2:K:201:TYR:HB3  | 2:K:210:ALA:HB1  | 1.74                     | 0.70              |
| 1:J:313:ASP:HB2  | 1:J:316:MET:HG2  | 1.73                     | 0.70              |
| 2:K:654:TYR:OH   | 2:K:708:THR:O    | 2.09                     | 0.70              |
| 2:K:655:LEU:O    | 2:K:659:ILE:HG12 | 1.92                     | 0.70              |
| 4:B:140:ARG:O    | 4:B:144:ASN:ND2  | 2.25                     | 0.70              |
| 4:A:63:PRO:HA    | 4:A:68:GLY:HA3   | 1.72                     | 0.70              |
| 4:D:140:ARG:O    | 4:D:144:ASN:ND2  | 2.25                     | 0.70              |
| 2:I:91:ASP:HA    | 2:I:482:SER:HB2  | 1.72                     | 0.69              |
| 2:I:287:SER:O    | 2:I:339:ARG:NH2  | 2.23                     | 0.69              |
| 2:I:201:TYR:HB3  | 2:I:210:ALA:HB1  | 1.74                     | 0.69              |
| 1:L:140:LEU:HD11 | 1:L:157:TYR:HB3  | 1.74                     | 0.69              |
| 4:C:426:LYS:HA   | 4:C:429:ARG:HG2  | 1.73                     | 0.69              |
| 1:L:202:TYR:HB3  | 1:L:213:VAL:HG21 | 1.74                     | 0.69              |
| 1:L:376:VAL:HB   | 1:L:385:PHE:HB2  | 1.75                     | 0.69              |
| 2:I:551:PRO:HD2  | 2:I:554:PHE:HB2  | 1.74                     | 0.69              |
| 4:A:236:CYS:HA   | 4:A:239:ILE:HD12 | 1.75                     | 0.69              |
| 4:D:108:ARG:O    | 4:C:108:ARG:NH2  | 2.25                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:655:LEU:O    | 2:I:659:ILE:HG12 | 1.92                     | 0.69              |
| 4:B:108:ARG:O    | 4:A:108:ARG:NH2  | 2.25                     | 0.69              |
| 2:K:382:ARG:HG3  | 2:K:383:LYS:H    | 1.57                     | 0.69              |
| 1:J:202:TYR:HB3  | 1:J:213:VAL:HG21 | 1.74                     | 0.69              |
| 2:K:201:TYR:HE1  | 2:K:212:ARG:HD3  | 1.58                     | 0.69              |
| 1:L:246:PRO:HD2  | 1:L:329:SER:HA   | 1.74                     | 0.69              |
| 2:K:367:TRP:HE1  | 2:K:369:HIS:HB2  | 1.58                     | 0.69              |
| 1:J:376:VAL:HB   | 1:J:385:PHE:HB2  | 1.75                     | 0.68              |
| 1:L:392:GLN:HG3  | 1:L:398:PHE:HB2  | 1.73                     | 0.68              |
| 1:J:436:ASN:O    | 1:J:456:ASN:ND2  | 2.26                     | 0.68              |
| 4:D:40:ASP:HB2   | 4:D:55:TRP:HD1   | 1.58                     | 0.68              |
| 2:I:367:TRP:HE1  | 2:I:369:HIS:HB2  | 1.58                     | 0.68              |
| 4:C:236:CYS:HA   | 4:C:239:ILE:HD12 | 1.75                     | 0.68              |
| 1:L:438:ILE:O    | 1:L:454:SER:HA   | 1.94                     | 0.68              |
| 2:K:285:ALA:HB3  | 2:K:684:LYS:HA   | 1.76                     | 0.68              |
| 1:L:296:VAL:HG11 | 1:L:351:ALA:HB1  | 1.76                     | 0.68              |
| 5:G:137:ASN:ND2  | 5:G:139:ASP:OD1  | 2.26                     | 0.68              |
| 1:J:140:LEU:HD11 | 1:J:157:TYR:HB3  | 1.74                     | 0.68              |
| 1:J:438:ILE:O    | 1:J:454:SER:HA   | 1.94                     | 0.68              |
| 2:I:695:LEU:O    | 2:I:702:ASN:ND2  | 2.27                     | 0.67              |
| 2:I:201:TYR:HE1  | 2:I:212:ARG:HD3  | 1.58                     | 0.67              |
| 4:D:410:SER:O    | 4:D:414:HIS:ND1  | 2.27                     | 0.67              |
| 2:I:150:GLN:HG2  | 2:I:151:HIS:HD1  | 1.60                     | 0.67              |
| 5:E:137:ASN:ND2  | 5:E:139:ASP:OD1  | 2.27                     | 0.67              |
| 1:L:436:ASN:O    | 1:L:456:ASN:ND2  | 2.26                     | 0.67              |
| 4:D:63:PRO:HA    | 4:D:68:GLY:HA3   | 1.77                     | 0.67              |
| 2:I:67:LYS:HG3   | 2:I:527:ARG:HG3  | 1.77                     | 0.67              |
| 1:J:726:HIS:ND1  | 1:J:738:THR:OG1  | 2.25                     | 0.67              |
| 2:I:382:ARG:HG3  | 2:I:383:LYS:H    | 1.58                     | 0.67              |
| 4:A:49:GLY:HA3   | 4:D:52:PHE:HA    | 1.76                     | 0.67              |
| 2:I:318:GLU:HB3  | 2:I:339:ARG:HB2  | 1.77                     | 0.67              |
| 4:B:52:PHE:HA    | 4:C:49:GLY:HA3   | 1.76                     | 0.67              |
| 1:L:221:VAL:HA   | 1:L:258:ASP:HB2  | 1.77                     | 0.67              |
| 2:K:318:GLU:HB3  | 2:K:339:ARG:HB2  | 1.77                     | 0.67              |
| 2:K:695:LEU:O    | 2:K:702:ASN:ND2  | 2.27                     | 0.67              |
| 1:J:296:VAL:HG11 | 1:J:351:ALA:HB1  | 1.76                     | 0.66              |
| 4:B:40:ASP:HB2   | 4:B:55:TRP:HD1   | 1.59                     | 0.66              |
| 2:I:285:ALA:HB3  | 2:I:684:LYS:HA   | 1.76                     | 0.66              |
| 2:I:661:PRO:HB3  | 2:I:713:ARG:HH22 | 1.60                     | 0.66              |
| 1:L:121:LYS:HG3  | 1:L:126:ARG:HH12 | 1.60                     | 0.66              |
| 1:J:121:LYS:HG3  | 1:J:126:ARG:HH12 | 1.60                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:4:GLY:HA2    | 4:B:61:ARG:HB2   | 1.78                     | 0.66              |
| 4:B:63:PRO:HA    | 4:B:68:GLY:HA3   | 1.77                     | 0.66              |
| 1:J:221:VAL:HA   | 1:J:258:ASP:HB2  | 1.77                     | 0.66              |
| 4:B:100:ARG:NH1  | 4:C:86:ASP:O     | 2.29                     | 0.66              |
| 2:K:661:PRO:HB3  | 2:K:713:ARG:HH22 | 1.60                     | 0.66              |
| 4:D:238:MET:O    | 4:D:241:THR:OG1  | 2.12                     | 0.66              |
| 4:B:10:PRO:O     | 4:B:13:ARG:HB2   | 1.96                     | 0.66              |
| 4:A:330:SER:HA   | 4:A:333:MET:HE2  | 1.78                     | 0.66              |
| 2:K:150:GLN:HG2  | 2:K:151:HIS:HD1  | 1.60                     | 0.66              |
| 4:B:410:SER:O    | 4:B:414:HIS:ND1  | 2.27                     | 0.66              |
| 1:J:105:LEU:HB3  | 1:J:114:THR:HB   | 1.77                     | 0.66              |
| 4:B:195:ILE:HG23 | 4:B:299:ARG:HB2  | 1.78                     | 0.66              |
| 4:A:86:ASP:O     | 4:D:100:ARG:NH1  | 2.29                     | 0.66              |
| 1:L:105:LEU:HB3  | 1:L:114:THR:HB   | 1.77                     | 0.66              |
| 4:A:47:VAL:HG12  | 4:A:85:PHE:HB2   | 1.78                     | 0.66              |
| 4:C:330:SER:HA   | 4:C:333:MET:HE2  | 1.78                     | 0.65              |
| 2:K:67:LYS:HG3   | 2:K:527:ARG:HG3  | 1.77                     | 0.65              |
| 4:D:111:CYS:SG   | 4:D:113:SER:OG   | 2.55                     | 0.65              |
| 4:D:4:GLY:HA2    | 4:D:61:ARG:HB2   | 1.78                     | 0.65              |
| 4:D:10:PRO:O     | 4:D:13:ARG:HB2   | 1.95                     | 0.65              |
| 4:D:304:SER:HA   | 4:D:310:LEU:HD23 | 1.77                     | 0.65              |
| 2:I:654:TYR:OH   | 2:I:708:THR:O    | 2.09                     | 0.65              |
| 4:B:353:LYS:NZ   | 4:B:375:ASP:O    | 2.26                     | 0.65              |
| 2:I:213:VAL:HG13 | 2:I:303:THR:HB   | 1.79                     | 0.65              |
| 3:H:164:PRO:HG2  | 4:D:491:HIS:HA   | 1.78                     | 0.65              |
| 3:H:216:MET:H    | 4:C:36:LYS:HB2   | 1.62                     | 0.65              |
| 4:B:150:ASP:OD2  | 4:B:418:ARG:NH1  | 2.27                     | 0.65              |
| 4:A:49:GLY:HA2   | 4:D:53:GLN:HG3   | 1.79                     | 0.65              |
| 1:L:134:PRO:O    | 1:L:136:ARG:NH1  | 2.30                     | 0.65              |
| 2:K:276:THR:O    | 2:K:278:LYS:NZ   | 2.30                     | 0.65              |
| 4:C:47:VAL:HG12  | 4:C:85:PHE:HB2   | 1.78                     | 0.65              |
| 1:J:134:PRO:O    | 1:J:136:ARG:NH1  | 2.30                     | 0.65              |
| 4:B:111:CYS:SG   | 4:B:113:SER:OG   | 2.55                     | 0.65              |
| 4:B:304:SER:HA   | 4:B:310:LEU:HD23 | 1.78                     | 0.65              |
| 2:I:91:ASP:HB3   | 2:I:483:HIS:HB2  | 1.79                     | 0.64              |
| 4:A:180:THR:H    | 4:A:184:ALA:HB3  | 1.62                     | 0.64              |
| 3:H:81:PHE:O     | 4:D:478:HIS:NE2  | 2.27                     | 0.64              |
| 4:D:195:ILE:HG23 | 4:D:299:ARG:HB2  | 1.78                     | 0.64              |
| 2:I:267:PRO:HA   | 2:I:277:VAL:HG12 | 1.80                     | 0.64              |
| 4:D:150:ASP:OD2  | 4:D:418:ARG:NH1  | 2.27                     | 0.64              |
| 5:G:121:GLY:O    | 5:G:213:GLN:NE2  | 2.29                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:267:PRO:HA   | 2:K:277:VAL:HG12 | 1.80                     | 0.64              |
| 4:B:53:GLN:HG3   | 4:C:49:GLY:HA2   | 1.79                     | 0.64              |
| 4:B:169:GLN:O    | 4:B:172:TRP:HB3  | 1.98                     | 0.64              |
| 4:D:353:LYS:NZ   | 4:D:375:ASP:O    | 2.26                     | 0.64              |
| 4:C:180:THR:H    | 4:C:184:ALA:HB3  | 1.62                     | 0.64              |
| 4:A:251:ALA:O    | 4:A:254:ARG:NH1  | 2.31                     | 0.64              |
| 1:L:548:ILE:HD13 | 1:L:596:VAL:HG22 | 1.80                     | 0.64              |
| 2:K:91:ASP:HB3   | 2:K:483:HIS:HB2  | 1.80                     | 0.64              |
| 3:F:90:TYR:HB2   | 3:F:153:ALA:HB1  | 1.80                     | 0.64              |
| 3:F:205:ILE:HG13 | 4:A:20:MET:HB3   | 1.80                     | 0.64              |
| 5:E:121:GLY:O    | 5:E:213:GLN:NE2  | 2.29                     | 0.64              |
| 2:K:213:VAL:HG13 | 2:K:303:THR:HB   | 1.79                     | 0.64              |
| 2:K:615:ARG:NH1  | 2:K:693:ARG:O    | 2.31                     | 0.64              |
| 2:I:276:THR:O    | 2:I:278:LYS:NZ   | 2.30                     | 0.63              |
| 3:F:216:MET:H    | 4:A:36:LYS:HB2   | 1.62                     | 0.63              |
| 4:A:277:LEU:O    | 4:A:280:THR:OG1  | 2.16                     | 0.63              |
| 3:H:90:TYR:HB2   | 3:H:153:ALA:HB1  | 1.80                     | 0.63              |
| 1:L:726:HIS:ND1  | 1:L:738:THR:OG1  | 2.25                     | 0.63              |
| 2:K:725:ILE:HD13 | 2:K:755:GLN:HB2  | 1.80                     | 0.63              |
| 4:C:251:ALA:O    | 4:C:254:ARG:NH1  | 2.31                     | 0.63              |
| 1:J:727:PRO:HG2  | 1:J:730:ASP:HB2  | 1.80                     | 0.63              |
| 2:I:547:GLN:HG3  | 2:I:597:LYS:HB2  | 1.79                     | 0.63              |
| 3:F:164:PRO:HG2  | 4:B:491:HIS:HA   | 1.78                     | 0.63              |
| 4:B:11:PHE:HD1   | 5:G:115:LEU:HD13 | 1.64                     | 0.63              |
| 4:B:239:ILE:O    | 4:B:242:VAL:HG12 | 1.99                     | 0.63              |
| 2:K:348:LEU:HG   | 2:K:359:LYS:HD3  | 1.79                     | 0.63              |
| 4:D:175:PHE:HE2  | 4:D:247:ARG:HE   | 1.46                     | 0.63              |
| 1:J:172:PRO:HB2  | 1:J:212:ARG:HH22 | 1.64                     | 0.63              |
| 5:G:87:ALA:HB2   | 5:G:157:MET:HE1  | 1.81                     | 0.63              |
| 2:K:547:GLN:HG3  | 2:K:597:LYS:HB2  | 1.79                     | 0.63              |
| 2:I:87:LYS:H     | 2:I:95:ILE:HG22  | 1.63                     | 0.63              |
| 2:I:348:LEU:HG   | 2:I:359:LYS:HD3  | 1.79                     | 0.63              |
| 2:I:615:ARG:NH1  | 2:I:693:ARG:O    | 2.31                     | 0.63              |
| 4:A:408:ASN:OD1  | 4:A:411:ARG:NH2  | 2.32                     | 0.63              |
| 1:L:172:PRO:HB2  | 1:L:212:ARG:HH22 | 1.64                     | 0.63              |
| 1:L:727:PRO:HG2  | 1:L:730:ASP:HB2  | 1.80                     | 0.63              |
| 2:K:87:LYS:H     | 2:K:95:ILE:HG22  | 1.63                     | 0.63              |
| 2:K:367:TRP:HZ3  | 2:K:615:ARG:HB2  | 1.63                     | 0.63              |
| 2:K:640:ASP:OD2  | 2:K:643:ARG:NE   | 2.31                     | 0.63              |
| 4:D:292:LEU:O    | 4:D:296:ARG:HG3  | 1.99                     | 0.63              |
| 1:L:498:PRO:O    | 1:L:517:ASN:ND2  | 2.32                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:H:205:ILE:HG13 | 4:C:20:MET:HB3   | 1.80                     | 0.63              |
| 4:D:169:GLN:O    | 4:D:172:TRP:HB3  | 1.98                     | 0.63              |
| 1:J:749:LYS:HZ3  | 2:I:775:ARG:HH22 | 1.47                     | 0.62              |
| 5:E:174:HIS:HE1  | 4:D:22:VAL:HG13  | 1.63                     | 0.62              |
| 2:I:367:TRP:HZ3  | 2:I:615:ARG:HB2  | 1.63                     | 0.62              |
| 4:B:238:MET:O    | 4:B:241:THR:OG1  | 2.11                     | 0.62              |
| 4:A:67:LEU:HD11  | 4:A:122:PHE:HD1  | 1.63                     | 0.62              |
| 1:L:749:LYS:HZ3  | 2:K:775:ARG:HH22 | 1.47                     | 0.62              |
| 1:J:548:ILE:HD13 | 1:J:596:VAL:HG22 | 1.80                     | 0.62              |
| 2:K:66:LYS:NZ    | 2:K:525:ASN:O    | 2.30                     | 0.62              |
| 1:J:498:PRO:O    | 1:J:517:ASN:ND2  | 2.32                     | 0.62              |
| 1:J:616:ARG:HA   | 1:J:695:LEU:HD23 | 1.82                     | 0.62              |
| 1:L:616:ARG:HA   | 1:L:695:LEU:HD23 | 1.81                     | 0.62              |
| 4:D:171:VAL:O    | 4:D:175:PHE:N    | 2.33                     | 0.62              |
| 1:J:260:ARG:NH1  | 1:J:291:SER:OG   | 2.32                     | 0.62              |
| 4:D:239:ILE:O    | 4:D:242:VAL:HG12 | 1.99                     | 0.62              |
| 4:B:112:ILE:HG13 | 4:B:140:ARG:HB3  | 1.82                     | 0.62              |
| 4:D:112:ILE:HG13 | 4:D:140:ARG:HB3  | 1.82                     | 0.62              |
| 5:G:148:MET:HG3  | 5:G:175:VAL:HG21 | 1.81                     | 0.62              |
| 5:G:162:THR:HG22 | 5:G:164:PRO:HD2  | 1.82                     | 0.62              |
| 2:I:38:LEU:HA    | 2:I:41:ILE:HG12  | 1.82                     | 0.62              |
| 2:I:640:ASP:OD2  | 2:I:643:ARG:NE   | 2.31                     | 0.62              |
| 4:B:175:PHE:HE2  | 4:B:247:ARG:HE   | 1.46                     | 0.62              |
| 5:E:147:MET:HE2  | 5:E:178:PHE:HB3  | 1.81                     | 0.62              |
| 5:E:162:THR:HG22 | 5:E:164:PRO:HD2  | 1.82                     | 0.62              |
| 1:L:98:GLU:HG3   | 1:L:101:GLY:H    | 1.65                     | 0.62              |
| 1:L:260:ARG:NH1  | 1:L:291:SER:OG   | 2.32                     | 0.62              |
| 2:I:725:ILE:HD13 | 2:I:755:GLN:HB2  | 1.80                     | 0.62              |
| 4:B:292:LEU:O    | 4:B:296:ARG:HG3  | 1.99                     | 0.62              |
| 4:B:487:LYS:HD2  | 4:A:26:PRO:HD2   | 1.82                     | 0.62              |
| 5:E:167:LYS:O    | 5:E:170:THR:OG1  | 2.16                     | 0.62              |
| 4:C:111:CYS:SG   | 4:C:113:SER:OG   | 2.57                     | 0.62              |
| 4:C:408:ASN:OD1  | 4:C:411:ARG:NH2  | 2.32                     | 0.62              |
| 1:J:91:ASP:HA    | 1:J:482:SER:HB2  | 1.81                     | 0.62              |
| 2:I:692:GLU:HG2  | 2:I:697:LEU:HA   | 1.82                     | 0.62              |
| 2:I:107:ASN:N    | 2:I:112:THR:O    | 2.28                     | 0.61              |
| 5:E:115:LEU:HD13 | 4:D:11:PHE:HD1   | 1.64                     | 0.61              |
| 4:D:487:LYS:HD2  | 4:C:26:PRO:HD2   | 1.82                     | 0.61              |
| 1:J:160:SER:OG   | 1:J:165:GLY:O    | 2.17                     | 0.61              |
| 3:H:216:MET:SD   | 4:C:13:ARG:NH2   | 2.71                     | 0.61              |
| 1:J:444:GLU:OE2  | 1:J:463:ARG:NH2  | 2.34                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:533:GLU:HG2  | 1:L:548:ILE:HG23 | 1.83                     | 0.61              |
| 2:K:38:LEU:HA    | 2:K:41:ILE:HG12  | 1.82                     | 0.61              |
| 4:C:67:LEU:HD11  | 4:C:122:PHE:HD1  | 1.63                     | 0.61              |
| 2:K:692:GLU:HG2  | 2:K:697:LEU:HA   | 1.83                     | 0.61              |
| 5:E:62:ASN:ND2   | 5:E:63:GLU:OE2   | 2.34                     | 0.61              |
| 5:E:215:VAL:HG21 | 4:D:30:PRO:HG2   | 1.83                     | 0.61              |
| 1:L:91:ASP:HA    | 1:L:482:SER:HB2  | 1.82                     | 0.61              |
| 5:E:87:ALA:HB2   | 5:E:157:MET:HE1  | 1.82                     | 0.61              |
| 1:J:187:PRO:HD2  | 1:J:191:GLN:HE21 | 1.66                     | 0.61              |
| 4:A:279:MET:HA   | 4:A:282:ASN:HB2  | 1.83                     | 0.61              |
| 5:G:167:LYS:O    | 5:G:170:THR:OG1  | 2.16                     | 0.61              |
| 1:J:98:GLU:HG3   | 1:J:101:GLY:H    | 1.65                     | 0.60              |
| 4:C:97:ASN:OD1   | 4:C:100:ARG:NH1  | 2.35                     | 0.60              |
| 1:J:383:LYS:HA   | 1:J:404:SER:O    | 2.01                     | 0.60              |
| 1:J:533:GLU:HG2  | 1:J:548:ILE:HG23 | 1.83                     | 0.60              |
| 4:C:279:MET:HA   | 4:C:282:ASN:HB2  | 1.83                     | 0.60              |
| 5:G:62:ASN:ND2   | 5:G:63:GLU:OE2   | 2.34                     | 0.60              |
| 4:C:319:SER:OG   | 4:C:408:ASN:ND2  | 2.34                     | 0.60              |
| 2:K:116:LEU:HD23 | 2:K:162:ILE:HD11 | 1.84                     | 0.60              |
| 1:L:383:LYS:HA   | 1:L:404:SER:O    | 2.01                     | 0.60              |
| 1:L:444:GLU:OE2  | 1:L:463:ARG:NH2  | 2.34                     | 0.60              |
| 3:F:216:MET:SD   | 4:A:13:ARG:NH2   | 2.71                     | 0.60              |
| 4:A:97:ASN:OD1   | 4:A:100:ARG:NH1  | 2.35                     | 0.60              |
| 1:L:160:SER:OG   | 1:L:165:GLY:O    | 2.17                     | 0.60              |
| 2:I:116:LEU:HD23 | 2:I:162:ILE:HD11 | 1.84                     | 0.60              |
| 1:J:655:LEU:O    | 1:J:659:ILE:HG13 | 2.02                     | 0.60              |
| 1:L:661:PRO:HA   | 1:L:713:ARG:HH12 | 1.67                     | 0.60              |
| 4:D:307:SER:HB2  | 4:C:329:PHE:HE2  | 1.67                     | 0.60              |
| 1:L:187:PRO:HD2  | 1:L:191:GLN:HE21 | 1.66                     | 0.59              |
| 1:L:655:LEU:O    | 1:L:659:ILE:HG13 | 2.02                     | 0.59              |
| 4:D:98:PHE:O     | 4:D:102:GLY:N    | 2.33                     | 0.59              |
| 1:J:97:ARG:NH1   | 1:J:130:TYR:O    | 2.34                     | 0.59              |
| 4:B:307:SER:HB2  | 4:A:329:PHE:HE2  | 1.67                     | 0.59              |
| 4:B:30:PRO:HG2   | 5:G:215:VAL:HG21 | 1.83                     | 0.59              |
| 4:A:319:SER:OG   | 4:A:408:ASN:ND2  | 2.34                     | 0.59              |
| 4:A:329:PHE:O    | 4:A:332:THR:OG1  | 2.20                     | 0.59              |
| 4:A:279:MET:HE1  | 4:A:288:ALA:HB3  | 1.85                     | 0.59              |
| 1:J:267:PRO:HA   | 1:J:277:VAL:HG12 | 1.83                     | 0.59              |
| 1:J:681:THR:HG23 | 1:J:710:VAL:H    | 1.68                     | 0.59              |
| 2:I:641:ARG:NH2  | 2:I:667:GLN:O    | 2.36                     | 0.59              |
| 4:A:338:PHE:HA   | 4:A:341:VAL:HG12 | 1.85                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:451:GLN:NE2  | 2:K:475:THR:O    | 2.36                     | 0.59              |
| 1:J:348:LEU:HD12 | 1:J:359:LYS:HE2  | 1.84                     | 0.59              |
| 1:J:661:PRO:HA   | 1:J:713:ARG:HH12 | 1.67                     | 0.59              |
| 2:I:451:GLN:NE2  | 2:I:475:THR:O    | 2.36                     | 0.59              |
| 1:L:641:ARG:NH2  | 1:L:669:GLN:OE1  | 2.36                     | 0.59              |
| 2:K:107:ASN:N    | 2:K:112:THR:O    | 2.28                     | 0.59              |
| 2:K:445:ASP:OD2  | 2:K:449:ARG:NH1  | 2.36                     | 0.59              |
| 3:F:81:PHE:O     | 4:B:478:HIS:NE2  | 2.27                     | 0.59              |
| 4:B:171:VAL:O    | 4:B:175:PHE:N    | 2.33                     | 0.59              |
| 4:C:277:LEU:O    | 4:C:280:THR:OG1  | 2.16                     | 0.58              |
| 2:I:602:GLY:HA2  | 2:I:611:LEU:HA   | 1.85                     | 0.58              |
| 1:L:267:PRO:HA   | 1:L:277:VAL:HG12 | 1.83                     | 0.58              |
| 1:J:641:ARG:NH2  | 1:J:669:GLN:OE1  | 2.36                     | 0.58              |
| 2:I:66:LYS:NZ    | 2:I:525:ASN:O    | 2.30                     | 0.58              |
| 2:I:445:ASP:OD2  | 2:I:449:ARG:NH1  | 2.36                     | 0.58              |
| 3:H:131:PHE:HE1  | 3:H:195:PHE:HD2  | 1.52                     | 0.58              |
| 4:D:202:ASN:HB2  | 4:D:299:ARG:HH21 | 1.69                     | 0.58              |
| 2:K:445:ASP:OD1  | 2:K:446:LEU:N    | 2.34                     | 0.58              |
| 1:L:66:LYS:HZ3   | 1:L:528:GLN:HA   | 1.69                     | 0.58              |
| 4:D:45:LEU:HB3   | 4:D:85:PHE:HE2   | 1.69                     | 0.58              |
| 5:G:125:GLU:HG3  | 5:G:129:TRP:HZ3  | 1.68                     | 0.58              |
| 1:J:181:GLN:HE21 | 1:J:226:LEU:HD12 | 1.69                     | 0.57              |
| 2:I:445:ASP:OD1  | 2:I:446:LEU:N    | 2.34                     | 0.57              |
| 5:E:125:GLU:HG3  | 5:E:129:TRP:HZ3  | 1.68                     | 0.57              |
| 4:D:272:PRO:HA   | 4:D:275:ILE:HG22 | 1.86                     | 0.57              |
| 4:C:338:PHE:HA   | 4:C:341:VAL:HG12 | 1.85                     | 0.57              |
| 4:A:88:ASP:OD1   | 4:D:93:ARG:NH1   | 2.38                     | 0.57              |
| 3:H:78:TYR:CD2   | 3:H:87:ALA:HB1   | 2.39                     | 0.57              |
| 1:L:181:GLN:HE21 | 1:L:226:LEU:HD12 | 1.69                     | 0.57              |
| 4:C:279:MET:HE1  | 4:C:288:ALA:HB3  | 1.85                     | 0.57              |
| 3:F:131:PHE:HE1  | 3:F:195:PHE:HD2  | 1.51                     | 0.57              |
| 4:B:45:LEU:HB3   | 4:B:85:PHE:HE2   | 1.69                     | 0.57              |
| 1:L:116:LEU:HB3  | 1:L:117:ILE:HD12 | 1.86                     | 0.57              |
| 1:L:348:LEU:HD12 | 1:L:359:LYS:HE2  | 1.84                     | 0.57              |
| 2:K:602:GLY:HA2  | 2:K:611:LEU:HA   | 1.84                     | 0.57              |
| 4:C:17:ILE:HA    | 4:C:20:MET:HE1   | 1.87                     | 0.57              |
| 1:J:66:LYS:HZ3   | 1:J:528:GLN:HA   | 1.69                     | 0.57              |
| 1:L:104:ARG:NH2  | 1:L:117:ILE:O    | 2.38                     | 0.57              |
| 2:I:104:ARG:HD2  | 2:I:115:VAL:HG22 | 1.86                     | 0.57              |
| 4:B:93:ARG:NH1   | 4:C:88:ASP:OD1   | 2.38                     | 0.57              |
| 4:A:264:ILE:HA   | 4:A:267:VAL:HG22 | 1.87                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:145:VAL:HG22 | 1:L:155:GLY:HA3  | 1.87                     | 0.57              |
| 1:L:199:ASN:HB3  | 1:L:215:SER:HA   | 1.87                     | 0.57              |
| 2:K:201:TYR:CE1  | 2:K:212:ARG:HD3  | 2.39                     | 0.57              |
| 3:F:78:TYR:CD2   | 3:F:87:ALA:HB1   | 2.39                     | 0.57              |
| 4:A:86:ASP:HB2   | 4:D:55:TRP:HZ3   | 1.70                     | 0.57              |
| 2:K:104:ARG:HD2  | 2:K:115:VAL:HG22 | 1.86                     | 0.57              |
| 3:H:95:PHE:O     | 3:H:99:ASP:N     | 2.36                     | 0.57              |
| 4:D:477:GLN:HE21 | 4:C:9:LEU:HG     | 1.69                     | 0.57              |
| 1:J:285:ALA:N    | 1:J:686:TYR:O    | 2.38                     | 0.57              |
| 4:D:338:PHE:O    | 4:D:342:MET:HG3  | 2.05                     | 0.57              |
| 4:B:338:PHE:O    | 4:B:342:MET:HG3  | 2.05                     | 0.56              |
| 2:K:623:GLU:HG3  | 2:K:658:TYR:CE2  | 2.40                     | 0.56              |
| 1:J:104:ARG:NH2  | 1:J:117:ILE:O    | 2.38                     | 0.56              |
| 3:F:126:LYS:HG2  | 3:F:209:LEU:HD11 | 1.87                     | 0.56              |
| 4:B:202:ASN:HB2  | 4:B:299:ARG:HH21 | 1.69                     | 0.56              |
| 1:L:120:LYS:HE2  | 1:L:164:HIS:HA   | 1.87                     | 0.56              |
| 1:L:681:THR:HG23 | 1:L:710:VAL:H    | 1.68                     | 0.56              |
| 4:C:264:ILE:HA   | 4:C:267:VAL:HG22 | 1.87                     | 0.56              |
| 1:J:116:LEU:HB3  | 1:J:117:ILE:HD12 | 1.86                     | 0.56              |
| 2:I:323:MET:HE1  | 2:I:372:ASN:HA   | 1.85                     | 0.56              |
| 4:B:477:GLN:HE21 | 4:A:9:LEU:HG     | 1.69                     | 0.56              |
| 4:A:17:ILE:HA    | 4:A:20:MET:HE1   | 1.87                     | 0.56              |
| 1:L:587:MET:HE1  | 1:L:593:ALA:HB3  | 1.87                     | 0.56              |
| 2:K:316:MET:HE3  | 2:K:343:VAL:HG12 | 1.86                     | 0.56              |
| 2:I:316:MET:HE3  | 2:I:343:VAL:HG12 | 1.86                     | 0.56              |
| 2:I:623:GLU:HG3  | 2:I:658:TYR:CE2  | 2.40                     | 0.56              |
| 4:B:272:PRO:HA   | 4:B:275:ILE:HG22 | 1.86                     | 0.56              |
| 4:A:77:HIS:ND1   | 4:A:80:THR:HG22  | 2.20                     | 0.56              |
| 2:K:173:PRO:HD3  | 2:K:210:ALA:HB3  | 1.88                     | 0.56              |
| 4:C:329:PHE:O    | 4:C:332:THR:OG1  | 2.20                     | 0.56              |
| 1:J:587:MET:HE1  | 1:J:593:ALA:HB3  | 1.87                     | 0.56              |
| 4:B:60:GLU:OE2   | 4:B:69:SER:N     | 2.38                     | 0.56              |
| 1:L:285:ALA:N    | 1:L:686:TYR:O    | 2.38                     | 0.56              |
| 1:J:120:LYS:HE2  | 1:J:164:HIS:HA   | 1.87                     | 0.56              |
| 1:L:276:THR:O    | 1:L:278:LYS:NZ   | 2.39                     | 0.56              |
| 1:L:649:LYS:NZ   | 1:L:650:ASP:OD2  | 2.39                     | 0.56              |
| 3:H:126:LYS:HG2  | 3:H:209:LEU:HD11 | 1.87                     | 0.56              |
| 4:C:77:HIS:ND1   | 4:C:80:THR:HG22  | 2.20                     | 0.56              |
| 2:K:658:TYR:O    | 2:K:713:ARG:NE   | 2.39                     | 0.56              |
| 4:B:55:TRP:HZ3   | 4:C:86:ASP:HB2   | 1.70                     | 0.56              |
| 1:L:97:ARG:NH1   | 1:L:130:TYR:O    | 2.34                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:276:THR:O    | 1:J:278:LYS:NZ   | 2.39                     | 0.56              |
| 4:B:432:ARG:NH1  | 4:A:127:GLU:O    | 2.39                     | 0.56              |
| 1:L:564:LEU:HD22 | 1:L:646:VAL:HG23 | 1.88                     | 0.56              |
| 2:K:250:ARG:HE   | 2:K:352:THR:HG22 | 1.71                     | 0.56              |
| 3:H:118:LEU:HD12 | 4:C:17:ILE:HG21  | 1.88                     | 0.56              |
| 5:E:42:LEU:HG    | 5:E:43:GLU:H     | 1.71                     | 0.56              |
| 2:K:555:THR:HG1  | 2:K:558:THR:HG1  | 1.54                     | 0.56              |
| 4:C:147:ARG:O    | 4:C:422:ARG:NH1  | 2.39                     | 0.56              |
| 1:J:145:VAL:HG22 | 1:J:155:GLY:HA3  | 1.87                     | 0.55              |
| 2:I:201:TYR:CE1  | 2:I:212:ARG:HD3  | 2.39                     | 0.55              |
| 4:B:5:VAL:HG21   | 5:G:80:GLN:HE22  | 1.71                     | 0.55              |
| 4:B:307:SER:O    | 4:B:311:ARG:NH1  | 2.39                     | 0.55              |
| 2:K:316:MET:HG2  | 2:K:338:ASN:HB3  | 1.88                     | 0.55              |
| 1:J:564:LEU:HD22 | 1:J:646:VAL:HG23 | 1.88                     | 0.55              |
| 2:I:147:PRO:HB3  | 2:I:152:SER:N    | 2.18                     | 0.55              |
| 2:K:234:GLU:HG2  | 2:K:689:ALA:HB3  | 1.88                     | 0.55              |
| 2:I:155:GLY:O    | 2:I:180:LEU:N    | 2.31                     | 0.55              |
| 2:I:234:GLU:HG2  | 2:I:689:ALA:HB3  | 1.88                     | 0.55              |
| 3:F:71:GLU:OE2   | 3:F:75:LYS:NZ    | 2.39                     | 0.55              |
| 2:K:427:LYS:HG2  | 2:K:441:LEU:HB2  | 1.87                     | 0.55              |
| 2:I:427:LYS:HG2  | 2:I:441:LEU:HB2  | 1.88                     | 0.55              |
| 5:E:70:ASN:OD1   | 5:E:71:GLU:N     | 2.37                     | 0.55              |
| 1:L:293:SER:OG   | 1:L:295:HIS:NE2  | 2.36                     | 0.55              |
| 3:H:71:GLU:OE2   | 3:H:75:LYS:NZ    | 2.39                     | 0.55              |
| 1:J:199:ASN:HB3  | 1:J:215:SER:HA   | 1.87                     | 0.55              |
| 4:A:368:MET:HG3  | 4:A:394:GLY:HA3  | 1.88                     | 0.55              |
| 2:K:641:ARG:NH2  | 2:K:667:GLN:O    | 2.36                     | 0.55              |
| 4:C:346:GLU:OE1  | 4:C:379:LYS:N    | 2.39                     | 0.55              |
| 2:I:451:GLN:HB2  | 2:I:453:TYR:CZ   | 2.41                     | 0.55              |
| 4:D:300:ILE:HG23 | 4:C:333:MET:HG3  | 1.88                     | 0.55              |
| 5:G:122:THR:HB   | 5:G:125:GLU:HB3  | 1.89                     | 0.55              |
| 1:J:95:ILE:HA    | 1:J:105:LEU:HD12 | 1.89                     | 0.55              |
| 2:I:103:VAL:HB   | 2:I:117:ILE:HB   | 1.89                     | 0.55              |
| 5:E:80:GLN:HE22  | 4:D:5:VAL:HG21   | 1.71                     | 0.55              |
| 4:A:119:LEU:HD11 | 4:A:126:PRO:HA   | 1.89                     | 0.55              |
| 4:A:346:GLU:OE1  | 4:A:379:LYS:N    | 2.39                     | 0.55              |
| 1:L:95:ILE:HA    | 1:L:105:LEU:HD12 | 1.89                     | 0.55              |
| 2:K:451:GLN:HB2  | 2:K:453:TYR:CZ   | 2.41                     | 0.55              |
| 2:I:173:PRO:HD3  | 2:I:210:ALA:HB3  | 1.88                     | 0.55              |
| 4:A:55:TRP:O     | 4:A:58:THR:OG1   | 2.24                     | 0.55              |
| 4:D:307:SER:O    | 4:D:311:ARG:NH1  | 2.39                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:G:68:VAL:HG12  | 5:G:105:SER:HB3  | 1.89                     | 0.55              |
| 4:A:147:ARG:O    | 4:A:422:ARG:NH1  | 2.40                     | 0.55              |
| 2:K:93:GLU:OE1   | 2:K:107:ASN:ND2  | 2.40                     | 0.55              |
| 2:K:598:CYS:SG   | 2:K:599:ASP:N    | 2.80                     | 0.55              |
| 5:G:210:GLN:HA   | 5:G:213:GLN:HB3  | 1.89                     | 0.55              |
| 4:C:119:LEU:HD11 | 4:C:126:PRO:HA   | 1.89                     | 0.55              |
| 1:J:144:ASN:O    | 1:J:179:LYS:NZ   | 2.40                     | 0.55              |
| 1:J:649:LYS:NZ   | 1:J:650:ASP:OD2  | 2.39                     | 0.55              |
| 2:K:744:GLN:OE1  | 2:K:747:ARG:NH1  | 2.40                     | 0.55              |
| 2:I:316:MET:HG2  | 2:I:338:ASN:HB3  | 1.88                     | 0.54              |
| 3:H:118:LEU:HD13 | 3:H:126:LYS:HG3  | 1.89                     | 0.54              |
| 1:J:262:PRO:HB2  | 2:I:274:TYR:CZ   | 2.43                     | 0.54              |
| 3:F:118:LEU:HD12 | 4:A:17:ILE:HG21  | 1.88                     | 0.54              |
| 5:E:210:GLN:HA   | 5:E:213:GLN:HB3  | 1.89                     | 0.54              |
| 1:L:144:ASN:O    | 1:L:179:LYS:NZ   | 2.40                     | 0.54              |
| 5:G:42:LEU:HG    | 5:G:43:GLU:H     | 1.71                     | 0.54              |
| 2:I:250:ARG:HE   | 2:I:352:THR:HG22 | 1.71                     | 0.54              |
| 2:I:339:ARG:HG2  | 2:I:697:LEU:HD21 | 1.89                     | 0.54              |
| 2:I:598:CYS:SG   | 2:I:599:ASP:N    | 2.80                     | 0.54              |
| 2:I:744:GLN:OE1  | 2:I:747:ARG:NH1  | 2.40                     | 0.54              |
| 3:F:58:ARG:NH1   | 4:B:84:PHE:O     | 2.40                     | 0.54              |
| 3:F:118:LEU:HD13 | 3:F:126:LYS:HG3  | 1.90                     | 0.54              |
| 4:B:98:PHE:O     | 4:B:102:GLY:N    | 2.33                     | 0.54              |
| 1:L:59:GLU:HG2   | 1:L:60:ASP:H     | 1.72                     | 0.54              |
| 1:L:563:LEU:HD13 | 1:L:587:MET:HE3  | 1.89                     | 0.54              |
| 2:K:449:ARG:HG2  | 2:K:577:GLU:HB2  | 1.89                     | 0.54              |
| 2:K:531:LYS:HB2  | 2:K:550:LYS:HB2  | 1.89                     | 0.54              |
| 4:B:444:TYR:HD1  | 4:B:479:HIS:HD2  | 1.55                     | 0.54              |
| 4:A:43:ILE:HG21  | 4:A:56:GLN:HE21  | 1.73                     | 0.54              |
| 4:D:444:TYR:HD1  | 4:D:479:HIS:HD2  | 1.55                     | 0.54              |
| 5:G:70:ASN:OD1   | 5:G:71:GLU:N     | 2.37                     | 0.54              |
| 1:J:547:GLN:HG3  | 1:J:597:LYS:HE2  | 1.90                     | 0.54              |
| 1:J:768:SER:O    | 1:J:771:GLN:NE2  | 2.41                     | 0.54              |
| 2:I:658:TYR:O    | 2:I:713:ARG:NE   | 2.39                     | 0.54              |
| 4:A:198:SER:HB3  | 4:A:236:CYS:SG   | 2.47                     | 0.54              |
| 2:K:77:GLU:OE2   | 2:K:82:HIS:NE2   | 2.31                     | 0.54              |
| 2:K:103:VAL:HB   | 2:K:117:ILE:HB   | 1.89                     | 0.54              |
| 5:G:180:GLN:O    | 5:G:184:LYS:NZ   | 2.40                     | 0.54              |
| 4:C:56:GLN:OE1   | 4:C:72:ARG:NH1   | 2.34                     | 0.54              |
| 4:C:368:MET:HG3  | 4:C:394:GLY:HA3  | 1.88                     | 0.54              |
| 1:J:59:GLU:HG2   | 1:J:60:ASP:H     | 1.73                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:144:ASN:HB3  | 2:I:155:GLY:HA3  | 1.89                     | 0.54              |
| 2:I:531:LYS:HB2  | 2:I:550:LYS:HB2  | 1.89                     | 0.54              |
| 4:B:108:ARG:HD2  | 4:A:108:ARG:HH21 | 1.71                     | 0.54              |
| 1:L:448:ARG:NH1  | 1:L:536:ASP:OD1  | 2.39                     | 0.54              |
| 4:D:108:ARG:HD2  | 4:C:108:ARG:HH21 | 1.71                     | 0.54              |
| 4:C:198:SER:HB3  | 4:C:236:CYS:SG   | 2.47                     | 0.54              |
| 3:F:169:ASP:CG   | 3:F:173:GLN:HE22 | 2.16                     | 0.54              |
| 4:B:357:ILE:HG21 | 4:C:203:VAL:HG13 | 1.90                     | 0.54              |
| 5:E:122:THR:HB   | 5:E:125:GLU:HB3  | 1.89                     | 0.54              |
| 5:E:123:VAL:HG13 | 5:E:209:LEU:HD22 | 1.89                     | 0.54              |
| 4:D:60:GLU:OE2   | 4:D:69:SER:N     | 2.38                     | 0.54              |
| 2:I:98:GLU:HG2   | 2:I:103:VAL:HG22 | 1.89                     | 0.54              |
| 2:I:376:VAL:HB   | 2:I:385:PHE:HB2  | 1.90                     | 0.54              |
| 2:I:449:ARG:HG2  | 2:I:577:GLU:HB2  | 1.89                     | 0.54              |
| 4:B:151:ASP:HA   | 4:B:422:ARG:HD2  | 1.89                     | 0.54              |
| 1:L:262:PRO:HB2  | 2:K:274:TYR:CZ   | 2.43                     | 0.54              |
| 1:L:441:LEU:HD12 | 1:L:450:ARG:HB3  | 1.89                     | 0.54              |
| 1:L:658:TYR:CE1  | 1:L:713:ARG:HG3  | 2.43                     | 0.54              |
| 4:D:44:VAL:HG12  | 4:D:53:GLN:HG2   | 1.89                     | 0.54              |
| 4:C:43:ILE:HG21  | 4:C:56:GLN:HE21  | 1.73                     | 0.54              |
| 4:A:67:LEU:HD11  | 4:A:122:PHE:CD1  | 2.42                     | 0.54              |
| 1:L:460:ASN:OD1  | 1:L:461:PHE:N    | 2.41                     | 0.54              |
| 1:L:768:SER:O    | 1:L:771:GLN:NE2  | 2.41                     | 0.54              |
| 2:K:324:VAL:HG12 | 2:K:334:VAL:HA   | 1.90                     | 0.54              |
| 4:D:59:LEU:HD23  | 4:D:72:ARG:HH11  | 1.73                     | 0.54              |
| 1:J:448:ARG:NH1  | 1:J:536:ASP:OD1  | 2.39                     | 0.54              |
| 2:I:685:LEU:O    | 2:I:737:HIS:NE2  | 2.40                     | 0.54              |
| 4:B:43:ILE:HD11  | 4:B:83:TYR:HE2   | 1.74                     | 0.54              |
| 4:B:300:ILE:HG23 | 4:A:333:MET:HG3  | 1.88                     | 0.54              |
| 4:B:344:TYR:CE2  | 4:C:293:ARG:HG3  | 2.43                     | 0.54              |
| 4:A:293:ARG:HG3  | 4:D:344:TYR:CE2  | 2.43                     | 0.54              |
| 2:K:98:GLU:HG2   | 2:K:103:VAL:HG22 | 1.90                     | 0.54              |
| 3:H:58:ARG:NH1   | 4:D:84:PHE:O     | 2.40                     | 0.54              |
| 4:D:203:VAL:HG23 | 4:C:357:ILE:HG21 | 1.89                     | 0.54              |
| 4:C:67:LEU:HD11  | 4:C:122:PHE:CD1  | 2.42                     | 0.54              |
| 2:I:93:GLU:OE1   | 2:I:107:ASN:ND2  | 2.40                     | 0.53              |
| 4:B:44:VAL:HG12  | 4:B:53:GLN:HG2   | 1.89                     | 0.53              |
| 4:A:445:MET:HE1  | 4:A:449:ARG:HH12 | 1.72                     | 0.53              |
| 2:K:685:LEU:O    | 2:K:737:HIS:NE2  | 2.40                     | 0.53              |
| 1:J:441:LEU:HD12 | 1:J:450:ARG:HB3  | 1.89                     | 0.53              |
| 2:I:523:ALA:HB1  | 2:I:527:ARG:HH22 | 1.74                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:203:VAL:HG23 | 4:A:357:ILE:HG21 | 1.89                     | 0.53              |
| 1:L:106:TRP:HA   | 1:L:113:SER:HA   | 1.90                     | 0.53              |
| 2:K:144:ASN:HB3  | 2:K:155:GLY:HA3  | 1.89                     | 0.53              |
| 2:K:339:ARG:HG2  | 2:K:697:LEU:HD21 | 1.89                     | 0.53              |
| 3:H:206:MET:O    | 3:H:210:GLN:NE2  | 2.41                     | 0.53              |
| 1:J:106:TRP:HA   | 1:J:113:SER:HA   | 1.90                     | 0.53              |
| 1:J:563:LEU:HD13 | 1:J:587:MET:HE3  | 1.89                     | 0.53              |
| 5:E:120:ARG:NE   | 5:E:213:GLN:O    | 2.40                     | 0.53              |
| 2:K:533:GLU:OE2  | 2:K:550:LYS:NZ   | 2.25                     | 0.53              |
| 2:I:623:GLU:O    | 2:I:627:MET:HG2  | 2.09                     | 0.53              |
| 5:E:68:VAL:HG12  | 5:E:105:SER:HB3  | 1.89                     | 0.53              |
| 1:L:190:GLN:HG3  | 1:L:205:HIS:HA   | 1.91                     | 0.53              |
| 1:L:677:LEU:HD11 | 1:L:773:LEU:HD11 | 1.90                     | 0.53              |
| 4:D:43:ILE:HD11  | 4:D:83:TYR:HE2   | 1.74                     | 0.53              |
| 1:J:658:TYR:CE1  | 1:J:713:ARG:HG3  | 2.43                     | 0.53              |
| 2:I:654:TYR:O    | 2:I:657:THR:OG1  | 2.26                     | 0.53              |
| 1:L:74:LEU:HD22  | 1:L:581:VAL:HB   | 1.90                     | 0.53              |
| 1:L:547:GLN:HG3  | 1:L:597:LYS:HE2  | 1.90                     | 0.53              |
| 2:K:376:VAL:HB   | 2:K:385:PHE:HB2  | 1.90                     | 0.53              |
| 2:K:523:ALA:HB1  | 2:K:527:ARG:HH22 | 1.73                     | 0.53              |
| 3:H:169:ASP:CG   | 3:H:173:GLN:HE22 | 2.16                     | 0.53              |
| 5:G:71:GLU:O     | 5:G:75:LYS:HG2   | 2.08                     | 0.53              |
| 4:B:289:PHE:O    | 4:B:293:ARG:HG2  | 2.09                     | 0.53              |
| 5:E:71:GLU:O     | 5:E:75:LYS:HG2   | 2.08                     | 0.53              |
| 5:E:180:GLN:O    | 5:E:184:LYS:NZ   | 2.40                     | 0.53              |
| 1:J:460:ASN:OD1  | 1:J:461:PHE:N    | 2.41                     | 0.53              |
| 2:I:324:VAL:HG12 | 2:I:334:VAL:HA   | 1.90                     | 0.53              |
| 3:F:206:MET:O    | 3:F:210:GLN:NE2  | 2.42                     | 0.53              |
| 4:B:109:HIS:HB2  | 4:A:109:HIS:ND1  | 2.24                     | 0.53              |
| 5:E:148:MET:HG3  | 5:E:175:VAL:HG21 | 1.91                     | 0.53              |
| 2:K:418:ILE:HG22 | 2:K:419:THR:HG23 | 1.91                     | 0.53              |
| 2:K:623:GLU:O    | 2:K:627:MET:HG2  | 2.08                     | 0.53              |
| 5:G:120:ARG:NH1  | 5:G:216:MET:O    | 2.42                     | 0.53              |
| 4:C:379:LYS:O    | 4:C:384:LYS:NZ   | 2.42                     | 0.53              |
| 4:B:59:LEU:HD23  | 4:B:72:ARG:HH11  | 1.73                     | 0.53              |
| 2:K:153:TYR:HE2  | 2:K:182:TYR:HD1  | 1.57                     | 0.53              |
| 4:D:151:ASP:HA   | 4:D:422:ARG:HD2  | 1.89                     | 0.53              |
| 1:J:428:ILE:HA   | 1:J:440:PHE:HB3  | 1.91                     | 0.53              |
| 1:L:33:GLY:HA2   | 1:L:36:ILE:HD12  | 1.91                     | 0.53              |
| 4:D:432:ARG:NH1  | 4:C:127:GLU:O    | 2.39                     | 0.53              |
| 1:J:74:LEU:HD22  | 1:J:581:VAL:HB   | 1.90                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:324:VAL:HG23 | 1:J:334:VAL:HG22 | 1.90                     | 0.53              |
| 5:E:120:ARG:NH1  | 5:E:216:MET:O    | 2.42                     | 0.53              |
| 2:K:246:PRO:HD2  | 2:K:329:SER:HA   | 1.91                     | 0.53              |
| 5:G:123:VAL:HG13 | 5:G:209:LEU:HD22 | 1.91                     | 0.53              |
| 1:J:677:LEU:HD11 | 1:J:773:LEU:HD11 | 1.90                     | 0.52              |
| 4:A:379:LYS:O    | 4:A:384:LYS:NZ   | 2.42                     | 0.52              |
| 4:C:445:MET:HE1  | 4:C:449:ARG:HH12 | 1.72                     | 0.52              |
| 1:J:190:GLN:HG3  | 1:J:205:HIS:HA   | 1.91                     | 0.52              |
| 2:I:153:TYR:HE2  | 2:I:182:TYR:HD1  | 1.57                     | 0.52              |
| 1:L:87:LYS:HE2   | 1:L:95:ILE:HD11  | 1.90                     | 0.52              |
| 4:D:109:HIS:HB2  | 4:C:109:HIS:ND1  | 2.24                     | 0.52              |
| 1:J:87:LYS:HE2   | 1:J:95:ILE:HD11  | 1.90                     | 0.52              |
| 1:J:191:GLN:HE22 | 1:J:248:GLY:HA3  | 1.74                     | 0.52              |
| 2:I:201:TYR:OH   | 2:I:212:ARG:NH1  | 2.41                     | 0.52              |
| 2:I:268:THR:OG1  | 2:I:278:LYS:NZ   | 2.39                     | 0.52              |
| 1:L:107:ASN:HB3  | 1:L:112:THR:HB   | 1.92                     | 0.52              |
| 1:J:107:ASN:HB3  | 1:J:112:THR:HB   | 1.91                     | 0.52              |
| 1:J:420:SER:O    | 1:J:423:TRP:NE1  | 2.42                     | 0.52              |
| 2:I:246:PRO:HD2  | 2:I:329:SER:HA   | 1.91                     | 0.52              |
| 2:I:583:TRP:HD1  | 2:I:587:MET:HE1  | 1.74                     | 0.52              |
| 4:A:271:LEU:HG   | 4:A:272:PRO:HD3  | 1.92                     | 0.52              |
| 1:L:191:GLN:HE22 | 1:L:248:GLY:HA3  | 1.74                     | 0.52              |
| 2:K:201:TYR:OH   | 2:K:212:ARG:NH1  | 2.41                     | 0.52              |
| 2:K:475:THR:H    | 2:K:495:PRO:HD3  | 1.75                     | 0.52              |
| 4:D:139:ASP:HA   | 4:D:142:ARG:NE   | 2.24                     | 0.52              |
| 4:D:289:PHE:O    | 4:D:293:ARG:HG2  | 2.09                     | 0.52              |
| 4:D:342:MET:O    | 4:D:346:GLU:HB2  | 2.10                     | 0.52              |
| 1:J:497:VAL:HG11 | 1:J:521:LYS:HG2  | 1.92                     | 0.52              |
| 2:K:583:TRP:HD1  | 2:K:587:MET:HE1  | 1.74                     | 0.52              |
| 2:K:622:GLU:OE1  | 2:K:622:GLU:N    | 2.37                     | 0.52              |
| 4:D:425:GLN:HG3  | 4:C:134:TYR:CE2  | 2.44                     | 0.52              |
| 4:C:14:ALA:HA    | 4:C:17:ILE:HD12  | 1.92                     | 0.52              |
| 4:C:147:ARG:HG3  | 4:C:422:ARG:HH12 | 1.74                     | 0.52              |
| 1:J:395:ARG:HB3  | 1:J:398:PHE:HE1  | 1.75                     | 0.52              |
| 2:I:172:PRO:HG2  | 2:I:175:VAL:HB   | 1.92                     | 0.52              |
| 2:I:574:SER:H    | 2:I:599:ASP:CG   | 2.18                     | 0.52              |
| 1:L:324:VAL:HG23 | 1:L:334:VAL:HG22 | 1.90                     | 0.52              |
| 2:K:338:ASN:ND2  | 2:K:342:ASN:OD1  | 2.36                     | 0.52              |
| 4:C:329:PHE:CD2  | 4:C:333:MET:HE1  | 2.45                     | 0.52              |
| 1:J:72:GLU:O     | 1:J:76:SER:N     | 2.43                     | 0.52              |
| 4:A:203:VAL:HG13 | 4:D:357:ILE:HG21 | 1.90                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:548:ILE:HD13 | 2:K:596:VAL:HG22 | 1.92                     | 0.52              |
| 3:F:95:PHE:O     | 3:F:99:ASP:N     | 2.36                     | 0.52              |
| 5:E:208:SER:HB3  | 4:D:27:MET:HE1   | 1.91                     | 0.52              |
| 4:D:194:PHE:CD2  | 4:D:239:ILE:HG21 | 2.45                     | 0.52              |
| 4:C:271:LEU:HG   | 4:C:272:PRO:HD3  | 1.92                     | 0.52              |
| 2:I:549:LEU:HD23 | 2:I:588:VAL:HG21 | 1.92                     | 0.52              |
| 4:B:194:PHE:CD2  | 4:B:239:ILE:HG21 | 2.45                     | 0.52              |
| 4:B:425:GLN:HG3  | 4:A:134:TYR:CE2  | 2.44                     | 0.52              |
| 2:K:68:LYS:HD2   | 2:K:590:SER:HA   | 1.92                     | 0.52              |
| 2:K:146:GLU:OE2  | 2:K:765:THR:OG1  | 2.28                     | 0.52              |
| 2:I:68:LYS:HD2   | 2:I:590:SER:HA   | 1.92                     | 0.51              |
| 2:I:77:GLU:OE2   | 2:I:82:HIS:NE2   | 2.31                     | 0.51              |
| 2:I:418:ILE:HG22 | 2:I:419:THR:HG23 | 1.91                     | 0.51              |
| 2:I:548:ILE:HD13 | 2:I:596:VAL:HG22 | 1.92                     | 0.51              |
| 4:B:139:ASP:HA   | 4:B:142:ARG:NE   | 2.24                     | 0.51              |
| 4:B:200:ILE:HA   | 4:B:203:VAL:HG12 | 1.93                     | 0.51              |
| 4:A:332:THR:HA   | 4:A:335:ILE:HG12 | 1.93                     | 0.51              |
| 4:A:477:GLN:HB2  | 4:D:9:LEU:HD21   | 1.91                     | 0.51              |
| 1:L:72:GLU:O     | 1:L:76:SER:N     | 2.43                     | 0.51              |
| 1:L:395:ARG:HB3  | 1:L:398:PHE:HE1  | 1.75                     | 0.51              |
| 2:K:698:HIS:CG   | 2:K:699:GLY:H    | 2.28                     | 0.51              |
| 1:J:323:MET:HE3  | 1:J:335:THR:OG1  | 2.10                     | 0.51              |
| 1:L:323:MET:HE3  | 1:L:335:THR:OG1  | 2.10                     | 0.51              |
| 2:K:314:PRO:O    | 2:K:317:ARG:NH1  | 2.36                     | 0.51              |
| 2:K:530:PRO:HG3  | 2:K:585:THR:HG23 | 1.93                     | 0.51              |
| 4:D:475:GLU:O    | 4:D:479:HIS:ND1  | 2.32                     | 0.51              |
| 4:A:14:ALA:HA    | 4:A:17:ILE:HD12  | 1.91                     | 0.51              |
| 1:L:428:ILE:HA   | 1:L:440:PHE:HB3  | 1.91                     | 0.51              |
| 2:K:654:TYR:O    | 2:K:657:THR:OG1  | 2.26                     | 0.51              |
| 3:H:144:LYS:HZ2  | 3:H:172:ARG:HH21 | 1.58                     | 0.51              |
| 1:J:33:GLY:HA2   | 1:J:36:ILE:HD12  | 1.91                     | 0.51              |
| 4:B:342:MET:O    | 4:B:346:GLU:HB2  | 2.10                     | 0.51              |
| 1:L:383:LYS:HB3  | 1:L:405:SER:HA   | 1.93                     | 0.51              |
| 2:K:539:ILE:HD11 | 2:K:628:GLU:HG2  | 1.92                     | 0.51              |
| 4:D:137:TYR:OH   | 4:D:141:ARG:NH2  | 2.43                     | 0.51              |
| 5:G:182:MET:SD   | 5:G:191:THR:N    | 2.84                     | 0.51              |
| 2:I:530:PRO:HG3  | 2:I:585:THR:HG23 | 1.92                     | 0.51              |
| 2:I:698:HIS:CG   | 2:I:699:GLY:H    | 2.28                     | 0.51              |
| 4:B:9:LEU:HD21   | 4:C:477:GLN:HB2  | 1.91                     | 0.51              |
| 1:L:659:ILE:C    | 1:L:661:PRO:HD3  | 2.36                     | 0.51              |
| 1:J:443:THR:HB   | 1:J:447:PRO:HA   | 1.93                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:88:TRP:HE1   | 2:I:489:LEU:H    | 1.58                     | 0.51              |
| 2:I:195:ILE:HD11 | 2:I:242:HIS:CE1  | 2.46                     | 0.51              |
| 3:F:144:LYS:HZ2  | 3:F:172:ARG:HH21 | 1.58                     | 0.51              |
| 4:D:141:ARG:HA   | 4:D:144:ASN:HD21 | 1.75                     | 0.51              |
| 4:D:242:VAL:O    | 4:D:246:LEU:N    | 2.40                     | 0.51              |
| 4:C:67:LEU:HD22  | 4:C:99:TYR:CE2   | 2.46                     | 0.51              |
| 2:I:257:ASN:HB3  | 2:I:291:SER:HB3  | 1.93                     | 0.51              |
| 2:I:429:LEU:H    | 2:I:440:PHE:HA   | 1.76                     | 0.51              |
| 2:I:654:TYR:CE1  | 2:I:710:VAL:HB   | 2.45                     | 0.51              |
| 4:B:137:TYR:OH   | 4:B:141:ARG:NH2  | 2.43                     | 0.51              |
| 4:B:473:SER:O    | 4:B:476:THR:OG1  | 2.23                     | 0.51              |
| 4:A:111:CYS:SG   | 4:A:113:SER:OG   | 2.57                     | 0.51              |
| 1:L:646:VAL:HB   | 1:L:671:PHE:CE2  | 2.45                     | 0.51              |
| 2:K:268:THR:OG1  | 2:K:278:LYS:NZ   | 2.39                     | 0.51              |
| 2:K:485:MET:HE2  | 2:K:485:MET:H    | 1.75                     | 0.51              |
| 5:G:120:ARG:NE   | 5:G:213:GLN:O    | 2.40                     | 0.51              |
| 1:J:722:PHE:CE2  | 1:J:724:ILE:HD11 | 2.46                     | 0.51              |
| 2:I:146:GLU:OE2  | 2:I:765:THR:OG1  | 2.28                     | 0.51              |
| 2:I:475:THR:H    | 2:I:495:PRO:HD3  | 1.74                     | 0.51              |
| 4:B:199:VAL:HG21 | 4:B:300:ILE:HD11 | 1.93                     | 0.51              |
| 1:L:102:THR:OG1  | 1:L:117:ILE:O    | 2.26                     | 0.51              |
| 2:K:72:GLU:OE2   | 2:K:771:GLN:NE2  | 2.44                     | 0.51              |
| 2:K:519:HIS:HA   | 2:K:522:LYS:HZ2  | 1.74                     | 0.51              |
| 2:K:574:SER:H    | 2:K:599:ASP:CG   | 2.18                     | 0.51              |
| 1:J:646:VAL:HB   | 1:J:671:PHE:CE2  | 2.45                     | 0.51              |
| 2:I:105:LEU:N    | 2:I:114:THR:O    | 2.44                     | 0.51              |
| 2:I:387:ILE:HB   | 2:I:428:ILE:HD11 | 1.93                     | 0.51              |
| 2:I:485:MET:HE2  | 2:I:485:MET:H    | 1.76                     | 0.51              |
| 2:I:539:ILE:HD11 | 2:I:628:GLU:HG2  | 1.92                     | 0.51              |
| 4:B:475:GLU:O    | 4:B:479:HIS:ND1  | 2.32                     | 0.51              |
| 5:E:103:THR:OG1  | 5:E:105:SER:O    | 2.29                     | 0.51              |
| 5:E:182:MET:SD   | 5:E:191:THR:N    | 2.84                     | 0.51              |
| 1:L:105:LEU:HB2  | 1:L:116:LEU:HD13 | 1.93                     | 0.51              |
| 2:K:105:LEU:N    | 2:K:114:THR:O    | 2.44                     | 0.51              |
| 4:C:55:TRP:O     | 4:C:58:THR:OG1   | 2.24                     | 0.51              |
| 1:J:383:LYS:HB3  | 1:J:405:SER:HA   | 1.93                     | 0.51              |
| 1:J:659:ILE:C    | 1:J:661:PRO:HD3  | 2.36                     | 0.51              |
| 1:L:443:THR:HB   | 1:L:447:PRO:HA   | 1.93                     | 0.51              |
| 2:K:387:ILE:HB   | 2:K:428:ILE:HD11 | 1.93                     | 0.51              |
| 2:K:654:TYR:CE1  | 2:K:710:VAL:HB   | 2.45                     | 0.51              |
| 1:J:686:TYR:HE1  | 1:J:733:ILE:HG12 | 1.76                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:775:ARG:NH1  | 1:J:779:ASN:OD1  | 2.44                     | 0.50              |
| 2:I:288:GLU:HA   | 2:I:339:ARG:HH12 | 1.76                     | 0.50              |
| 2:K:172:PRO:HG2  | 2:K:175:VAL:HB   | 1.92                     | 0.50              |
| 4:D:488:THR:HA   | 4:C:23:ALA:HA    | 1.93                     | 0.50              |
| 5:G:149:ASP:OD1  | 5:G:149:ASP:N    | 2.44                     | 0.50              |
| 1:J:515:GLU:OE2  | 1:J:517:ASN:N    | 2.41                     | 0.50              |
| 2:I:187:PRO:HD3  | 2:I:244:TRP:CE3  | 2.46                     | 0.50              |
| 2:I:710:VAL:HG22 | 2:I:714:VAL:HG13 | 1.94                     | 0.50              |
| 4:B:141:ARG:HA   | 4:B:144:ASN:HD21 | 1.75                     | 0.50              |
| 4:B:332:THR:O    | 4:B:336:ILE:HG12 | 2.11                     | 0.50              |
| 5:E:149:ASP:N    | 5:E:149:ASP:OD1  | 2.44                     | 0.50              |
| 5:E:164:PRO:HG2  | 4:A:491:HIS:CD2  | 2.46                     | 0.50              |
| 4:A:67:LEU:HD22  | 4:A:99:TYR:CE2   | 2.46                     | 0.50              |
| 4:A:147:ARG:HG3  | 4:A:422:ARG:HH12 | 1.75                     | 0.50              |
| 4:A:329:PHE:CD2  | 4:A:333:MET:HE1  | 2.45                     | 0.50              |
| 1:L:722:PHE:CE2  | 1:L:724:ILE:HD11 | 2.46                     | 0.50              |
| 1:L:775:ARG:NH1  | 1:L:779:ASN:OD1  | 2.44                     | 0.50              |
| 4:D:200:ILE:HA   | 4:D:203:VAL:HG12 | 1.93                     | 0.50              |
| 2:K:88:TRP:HE1   | 2:K:489:LEU:H    | 1.58                     | 0.50              |
| 2:I:338:ASN:ND2  | 2:I:342:ASN:OD1  | 2.36                     | 0.50              |
| 1:L:94:PHE:CE1   | 1:L:106:TRP:HB3  | 2.47                     | 0.50              |
| 2:K:155:GLY:O    | 2:K:180:LEU:N    | 2.31                     | 0.50              |
| 2:K:549:LEU:HD23 | 2:K:588:VAL:HG21 | 1.92                     | 0.50              |
| 1:J:105:LEU:HB2  | 1:J:116:LEU:HD13 | 1.93                     | 0.50              |
| 2:I:72:GLU:OE2   | 2:I:771:GLN:NE2  | 2.44                     | 0.50              |
| 2:K:193:ILE:HD13 | 2:K:251:LEU:HD21 | 1.93                     | 0.50              |
| 2:K:251:LEU:HB2  | 2:K:299:LEU:HD21 | 1.94                     | 0.50              |
| 2:K:429:LEU:H    | 2:K:440:PHE:HA   | 1.76                     | 0.50              |
| 2:I:193:ILE:HD13 | 2:I:251:LEU:HD21 | 1.93                     | 0.50              |
| 2:I:289:ASN:OD1  | 2:I:688:SER:OG   | 2.19                     | 0.50              |
| 4:D:114:ALA:HB2  | 4:C:105:HIS:CE1  | 2.47                     | 0.50              |
| 5:G:164:PRO:HG2  | 4:C:491:HIS:CD2  | 2.46                     | 0.50              |
| 2:I:251:LEU:HB2  | 2:I:299:LEU:HD21 | 1.94                     | 0.50              |
| 4:B:327:LEU:HD22 | 4:B:401:PRO:HG2  | 1.93                     | 0.50              |
| 5:E:49:THR:HG23  | 5:E:52:GLU:H     | 1.77                     | 0.50              |
| 5:E:77:ILE:HG13  | 5:E:80:GLN:NE2   | 2.27                     | 0.50              |
| 1:L:497:VAL:HG11 | 1:L:521:LYS:HG2  | 1.92                     | 0.50              |
| 2:K:195:ILE:HD11 | 2:K:242:HIS:CE1  | 2.46                     | 0.50              |
| 2:K:196:PHE:O    | 2:K:199:ASN:ND2  | 2.45                     | 0.50              |
| 2:K:257:ASN:HB3  | 2:K:291:SER:HB3  | 1.93                     | 0.50              |
| 2:K:740:GLU:O    | 2:K:743:THR:OG1  | 2.27                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:C:365:ILE:HA   | 4:C:368:MET:HE2  | 1.94                     | 0.50              |
| 1:J:107:ASN:N    | 1:J:112:THR:O    | 2.45                     | 0.50              |
| 2:I:196:PHE:O    | 2:I:199:ASN:ND2  | 2.45                     | 0.50              |
| 2:I:294:LEU:HD22 | 2:I:324:VAL:HG11 | 1.94                     | 0.50              |
| 2:I:562:LEU:HB2  | 2:I:639:ILE:HD11 | 1.94                     | 0.50              |
| 4:B:261:VAL:O    | 4:B:265:ILE:HG12 | 2.12                     | 0.50              |
| 4:A:234:THR:HG22 | 4:A:273:TYR:HE1  | 1.77                     | 0.50              |
| 1:L:642:THR:O    | 1:L:672:THR:OG1  | 2.22                     | 0.50              |
| 2:K:187:PRO:HD3  | 2:K:244:TRP:CE3  | 2.46                     | 0.50              |
| 3:H:215:VAL:HA   | 4:C:36:LYS:HD2   | 1.93                     | 0.50              |
| 4:D:199:VAL:HG21 | 4:D:300:ILE:HD11 | 1.93                     | 0.50              |
| 3:F:215:VAL:HA   | 4:A:36:LYS:HD2   | 1.93                     | 0.50              |
| 4:B:449:ARG:NH2  | 4:B:495:ASP:OD2  | 2.40                     | 0.50              |
| 4:A:234:THR:HG22 | 4:A:273:TYR:CE1  | 2.47                     | 0.50              |
| 1:L:503:HIS:CE1  | 1:L:510:LYS:HB2  | 2.47                     | 0.50              |
| 1:L:515:GLU:OE2  | 1:L:517:ASN:N    | 2.41                     | 0.50              |
| 1:L:686:TYR:HE1  | 1:L:733:ILE:HG12 | 1.76                     | 0.50              |
| 4:C:332:THR:HA   | 4:C:335:ILE:HG12 | 1.93                     | 0.50              |
| 2:I:451:GLN:HA   | 2:I:477:PHE:HB2  | 1.94                     | 0.49              |
| 4:D:261:VAL:O    | 4:D:265:ILE:HG12 | 2.12                     | 0.49              |
| 4:D:327:LEU:HD22 | 4:D:401:PRO:HG2  | 1.93                     | 0.49              |
| 4:C:379:LYS:C    | 4:C:384:LYS:HZ2  | 2.20                     | 0.49              |
| 5:E:118:LEU:HB3  | 4:D:14:ALA:HB1   | 1.94                     | 0.49              |
| 4:D:332:THR:O    | 4:D:336:ILE:HG12 | 2.11                     | 0.49              |
| 1:J:94:PHE:CE1   | 1:J:106:TRP:HB3  | 2.47                     | 0.49              |
| 1:J:102:THR:OG1  | 1:J:117:ILE:O    | 2.26                     | 0.49              |
| 1:J:227:SER:HB3  | 1:J:231:TYR:HB2  | 1.94                     | 0.49              |
| 2:I:310:PRO:HB3  | 2:I:336:TRP:CZ3  | 2.47                     | 0.49              |
| 4:B:27:MET:HE1   | 5:G:208:SER:HB3  | 1.93                     | 0.49              |
| 2:K:288:GLU:HA   | 2:K:339:ARG:HH12 | 1.76                     | 0.49              |
| 2:K:309:MET:HE2  | 2:K:309:MET:N    | 2.27                     | 0.49              |
| 5:G:103:THR:OG1  | 5:G:105:SER:O    | 2.29                     | 0.49              |
| 4:C:309:GLY:HA2  | 4:C:312:ILE:HD12 | 1.94                     | 0.49              |
| 1:J:323:MET:SD   | 1:J:375:PRO:HD3  | 2.53                     | 0.49              |
| 1:J:532:VAL:HG22 | 1:J:549:LEU:HD11 | 1.94                     | 0.49              |
| 1:L:107:ASN:N    | 1:L:112:THR:O    | 2.45                     | 0.49              |
| 1:L:640:ASP:OD2  | 1:L:643:ARG:NE   | 2.37                     | 0.49              |
| 1:J:104:ARG:NE   | 1:J:115:VAL:HA   | 2.24                     | 0.49              |
| 1:J:627:MET:HA   | 1:J:630:VAL:HG22 | 1.95                     | 0.49              |
| 4:B:323:GLU:HG2  | 4:B:404:VAL:HG11 | 1.95                     | 0.49              |
| 1:L:429:LEU:HD21 | 1:L:441:LEU:HD23 | 1.95                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:106:TRP:HA   | 2:K:113:SER:HA   | 1.94                     | 0.49              |
| 2:K:147:PRO:HB3  | 2:K:152:SER:N    | 2.18                     | 0.49              |
| 2:K:294:LEU:HD22 | 2:K:324:VAL:HG11 | 1.94                     | 0.49              |
| 4:D:204:VAL:O    | 4:D:207:VAL:HG12 | 2.12                     | 0.49              |
| 1:J:503:HIS:CE1  | 1:J:510:LYS:HB2  | 2.47                     | 0.49              |
| 1:L:327:ALA:H    | 1:L:332:VAL:HA   | 1.77                     | 0.49              |
| 2:K:161:LYS:NZ   | 2:K:166:ASP:OD2  | 2.34                     | 0.49              |
| 2:K:710:VAL:HG22 | 2:K:714:VAL:HG13 | 1.94                     | 0.49              |
| 4:D:391:SER:O    | 4:D:395:VAL:HG23 | 2.13                     | 0.49              |
| 2:I:399:TYR:N    | 2:I:424:ASP:OD1  | 2.45                     | 0.49              |
| 2:I:450:ARG:NH2  | 2:I:573:GLN:OE1  | 2.46                     | 0.49              |
| 4:B:14:ALA:HB1   | 5:G:118:LEU:HB3  | 1.94                     | 0.49              |
| 4:B:215:HIS:O    | 4:B:215:HIS:ND1  | 2.46                     | 0.49              |
| 4:A:365:ILE:HA   | 4:A:368:MET:HE2  | 1.94                     | 0.49              |
| 1:L:627:MET:HA   | 1:L:630:VAL:HG22 | 1.95                     | 0.49              |
| 2:K:562:LEU:HB2  | 2:K:639:ILE:HD11 | 1.94                     | 0.49              |
| 5:G:74:PHE:HA    | 5:G:77:ILE:HG22  | 1.95                     | 0.49              |
| 2:I:309:MET:HE2  | 2:I:309:MET:N    | 2.28                     | 0.49              |
| 4:B:105:HIS:CD2  | 4:C:114:ALA:HB2  | 2.48                     | 0.49              |
| 2:K:310:PRO:HB3  | 2:K:336:TRP:CZ3  | 2.47                     | 0.49              |
| 2:I:70:THR:HG23  | 2:I:72:GLU:H     | 1.78                     | 0.49              |
| 4:A:327:LEU:HD13 | 4:A:401:PRO:HG3  | 1.95                     | 0.49              |
| 4:A:375:ASP:OD1  | 4:A:376:MET:N    | 2.46                     | 0.49              |
| 1:L:227:SER:HB3  | 1:L:231:TYR:HB2  | 1.94                     | 0.49              |
| 2:K:399:TYR:N    | 2:K:424:ASP:OD1  | 2.46                     | 0.49              |
| 1:J:188:LYS:NZ   | 1:J:248:GLY:O    | 2.46                     | 0.49              |
| 1:J:429:LEU:HD21 | 1:J:441:LEU:HD23 | 1.95                     | 0.49              |
| 4:A:3:ALA:O      | 4:A:61:ARG:HG3   | 2.13                     | 0.49              |
| 4:A:98:PHE:O     | 4:A:102:GLY:N    | 2.46                     | 0.49              |
| 4:A:114:ALA:HB2  | 4:D:105:HIS:CD2  | 2.48                     | 0.49              |
| 1:L:108:VAL:HG11 | 1:L:487:PHE:CG   | 2.48                     | 0.49              |
| 5:G:77:ILE:HG13  | 5:G:80:GLN:NE2   | 2.27                     | 0.49              |
| 4:C:135:GLU:HG2  | 4:C:136:GLU:N    | 2.27                     | 0.49              |
| 2:I:191:GLN:NE2  | 2:I:202:TYR:OH   | 2.46                     | 0.48              |
| 2:I:587:MET:HE3  | 2:I:778:ILE:HG22 | 1.95                     | 0.48              |
| 4:A:309:GLY:HA2  | 4:A:312:ILE:HD12 | 1.94                     | 0.48              |
| 1:L:142:SER:HB2  | 1:L:145:VAL:HG21 | 1.94                     | 0.48              |
| 1:L:188:LYS:NZ   | 1:L:248:GLY:O    | 2.46                     | 0.48              |
| 4:C:3:ALA:O      | 4:C:61:ARG:HG3   | 2.13                     | 0.48              |
| 4:C:375:ASP:OD1  | 4:C:376:MET:N    | 2.46                     | 0.48              |
| 1:J:108:VAL:HG11 | 1:J:487:PHE:CG   | 2.48                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:348:LEU:N    | 2:I:357:THR:O    | 2.42                     | 0.48              |
| 4:B:488:THR:HA   | 4:A:23:ALA:HA    | 1.93                     | 0.48              |
| 5:E:61:LYS:NZ    | 5:E:65:PRO:O     | 2.43                     | 0.48              |
| 5:E:74:PHE:HA    | 5:E:77:ILE:HG22  | 1.95                     | 0.48              |
| 4:A:335:ILE:HG22 | 4:A:368:MET:HE3  | 1.95                     | 0.48              |
| 1:L:420:SER:O    | 1:L:423:TRP:NE1  | 2.42                     | 0.48              |
| 1:L:431:TYR:C    | 1:L:485:MET:HE1  | 2.38                     | 0.48              |
| 2:K:451:GLN:HA   | 2:K:477:PHE:HB2  | 1.94                     | 0.48              |
| 1:J:92:THR:O     | 1:J:108:VAL:N    | 2.37                     | 0.48              |
| 3:F:87:ALA:HB2   | 3:F:157:MET:HE1  | 1.96                     | 0.48              |
| 4:A:135:GLU:HG2  | 4:A:136:GLU:N    | 2.27                     | 0.48              |
| 4:A:296:ARG:O    | 4:A:299:ARG:NH1  | 2.46                     | 0.48              |
| 1:L:133:SER:OG   | 1:L:135:ASP:OD1  | 2.28                     | 0.48              |
| 2:K:623:GLU:HG3  | 2:K:658:TYR:HE2  | 1.79                     | 0.48              |
| 5:G:49:THR:HG23  | 5:G:52:GLU:H     | 1.77                     | 0.48              |
| 4:B:92:PHE:HA    | 4:B:95:ILE:HD12  | 1.96                     | 0.48              |
| 4:B:114:ALA:HB2  | 4:A:105:HIS:CE1  | 2.47                     | 0.48              |
| 4:B:204:VAL:O    | 4:B:207:VAL:HG12 | 2.12                     | 0.48              |
| 2:K:70:THR:HG23  | 2:K:72:GLU:H     | 1.78                     | 0.48              |
| 2:K:686:TYR:HE1  | 2:K:733:ILE:HG12 | 1.79                     | 0.48              |
| 4:C:296:ARG:O    | 4:C:299:ARG:NH1  | 2.46                     | 0.48              |
| 1:J:142:SER:HB2  | 1:J:145:VAL:HG21 | 1.94                     | 0.48              |
| 4:B:371:LEU:HD13 | 4:A:370:THR:HA   | 1.95                     | 0.48              |
| 4:B:391:SER:O    | 4:B:395:VAL:HG23 | 2.13                     | 0.48              |
| 4:A:56:GLN:OE1   | 4:A:72:ARG:NH1   | 2.34                     | 0.48              |
| 2:K:50:THR:HA    | 2:K:53:ILE:HG12  | 1.95                     | 0.48              |
| 2:K:191:GLN:NE2  | 2:K:202:TYR:OH   | 2.46                     | 0.48              |
| 5:G:164:PRO:HG2  | 4:C:491:HIS:CG   | 2.49                     | 0.48              |
| 4:C:119:LEU:HG   | 4:C:124:LEU:HD11 | 1.94                     | 0.48              |
| 4:C:234:THR:HG22 | 4:C:273:TYR:CE1  | 2.47                     | 0.48              |
| 1:J:327:ALA:H    | 1:J:332:VAL:HA   | 1.77                     | 0.48              |
| 1:J:382:ARG:HG3  | 1:J:383:LYS:HG3  | 1.96                     | 0.48              |
| 4:B:89:PRO:HD2   | 4:A:93:ARG:HD2   | 1.95                     | 0.48              |
| 5:E:174:HIS:CE1  | 4:D:22:VAL:HG13  | 2.45                     | 0.48              |
| 1:L:104:ARG:NE   | 1:L:115:VAL:HA   | 2.24                     | 0.48              |
| 1:L:624:LYS:HA   | 1:L:627:MET:CE   | 2.44                     | 0.48              |
| 4:C:234:THR:HG22 | 4:C:273:TYR:HE1  | 1.77                     | 0.48              |
| 1:J:149:TYR:HE2  | 1:J:229:TRP:HB2  | 1.79                     | 0.48              |
| 2:I:50:THR:HA    | 2:I:53:ILE:HG12  | 1.95                     | 0.48              |
| 2:I:106:TRP:HA   | 2:I:113:SER:HA   | 1.94                     | 0.48              |
| 2:I:485:MET:HE2  | 2:I:485:MET:N    | 2.29                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:43:GLU:OE2   | 3:F:47:ASN:ND2   | 2.46                     | 0.48              |
| 5:E:183:ASP:HB3  | 5:E:194:GLU:HG3  | 1.96                     | 0.48              |
| 1:L:323:MET:SD   | 1:L:375:PRO:HD3  | 2.53                     | 0.48              |
| 1:L:644:VAL:HG12 | 1:L:671:PHE:CD2  | 2.49                     | 0.48              |
| 2:K:587:MET:HE3  | 2:K:778:ILE:HG22 | 1.95                     | 0.48              |
| 3:H:170:THR:OG1  | 3:H:171:PRO:HD3  | 2.14                     | 0.48              |
| 4:C:98:PHE:O     | 4:C:102:GLY:N    | 2.46                     | 0.48              |
| 1:J:230:LEU:HD11 | 1:J:689:ALA:HB3  | 1.96                     | 0.48              |
| 2:I:265:GLU:HB2  | 2:I:277:VAL:HB   | 1.96                     | 0.48              |
| 2:I:623:GLU:HG3  | 2:I:658:TYR:HE2  | 1.78                     | 0.48              |
| 4:C:335:ILE:HG22 | 4:C:368:MET:HE3  | 1.95                     | 0.48              |
| 2:I:533:GLU:OE2  | 2:I:550:LYS:NZ   | 2.25                     | 0.48              |
| 5:E:203:ASP:OD2  | 5:E:207:ARG:NH1  | 2.47                     | 0.48              |
| 1:L:149:TYR:HE2  | 1:L:229:TRP:HB2  | 1.79                     | 0.48              |
| 1:L:532:VAL:HG22 | 1:L:549:LEU:HD11 | 1.94                     | 0.48              |
| 4:D:323:GLU:HG2  | 4:D:404:VAL:HG11 | 1.95                     | 0.48              |
| 1:J:431:TYR:C    | 1:J:485:MET:HE1  | 2.38                     | 0.48              |
| 4:B:8:TRP:CZ2    | 5:G:60:PHE:HA    | 2.49                     | 0.48              |
| 4:A:49:GLY:O     | 4:D:51:ARG:NH1   | 2.47                     | 0.48              |
| 4:A:119:LEU:HG   | 4:A:124:LEU:HD11 | 1.94                     | 0.48              |
| 2:K:348:LEU:N    | 2:K:357:THR:O    | 2.42                     | 0.48              |
| 2:I:201:TYR:HA   | 2:I:211:ILE:O    | 2.14                     | 0.47              |
| 5:E:99:ASP:OD1   | 5:E:103:THR:OG1  | 2.28                     | 0.47              |
| 1:L:641:ARG:NH1  | 1:L:667:GLN:OE1  | 2.47                     | 0.47              |
| 2:K:96:TYR:CD2   | 2:K:104:ARG:HB2  | 2.49                     | 0.47              |
| 4:D:92:PHE:HA    | 4:D:95:ILE:HD12  | 1.96                     | 0.47              |
| 5:G:203:ASP:OD2  | 5:G:207:ARG:NH1  | 2.46                     | 0.47              |
| 2:I:519:HIS:HA   | 2:I:522:LYS:NZ   | 2.28                     | 0.47              |
| 2:I:686:TYR:HE1  | 2:I:733:ILE:HG12 | 1.79                     | 0.47              |
| 5:E:60:PHE:HA    | 4:D:8:TRP:CZ2    | 2.49                     | 0.47              |
| 4:A:230:PHE:O    | 4:A:234:THR:HG23 | 2.14                     | 0.47              |
| 4:D:16:ALA:HA    | 4:D:19:TRP:CE2   | 2.50                     | 0.47              |
| 4:B:242:VAL:O    | 4:B:246:LEU:N    | 2.40                     | 0.47              |
| 5:E:164:PRO:HG2  | 4:A:491:HIS:CG   | 2.49                     | 0.47              |
| 4:A:415:GLN:HG2  | 4:A:418:ARG:NH2  | 2.28                     | 0.47              |
| 2:K:37:ALA:O     | 2:K:41:ILE:HG23  | 2.14                     | 0.47              |
| 2:K:450:ARG:NH2  | 2:K:573:GLN:OE1  | 2.46                     | 0.47              |
| 4:D:371:LEU:HD13 | 4:C:370:THR:HA   | 1.95                     | 0.47              |
| 3:F:47:ASN:HB2   | 3:F:116:SER:HB2  | 1.97                     | 0.47              |
| 2:K:265:GLU:HB2  | 2:K:277:VAL:HB   | 1.96                     | 0.47              |
| 2:K:485:MET:HE2  | 2:K:485:MET:N    | 2.29                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:H:87:ALA:HB2   | 3:H:157:MET:HE1  | 1.95                     | 0.47              |
| 4:D:427:LYS:O    | 4:D:430:LEU:HG   | 2.15                     | 0.47              |
| 4:D:473:SER:O    | 4:D:476:THR:OG1  | 2.23                     | 0.47              |
| 1:J:745:LEU:O    | 1:J:749:LYS:N    | 2.46                     | 0.47              |
| 4:B:51:ARG:NH1   | 4:C:49:GLY:O     | 2.47                     | 0.47              |
| 4:B:300:ILE:O    | 4:B:303:PHE:HB2  | 2.15                     | 0.47              |
| 1:L:230:LEU:HD11 | 1:L:689:ALA:HB3  | 1.96                     | 0.47              |
| 2:K:201:TYR:HA   | 2:K:211:ILE:O    | 2.14                     | 0.47              |
| 2:K:519:HIS:HA   | 2:K:522:LYS:NZ   | 2.28                     | 0.47              |
| 4:D:89:PRO:HD2   | 4:C:93:ARG:HD2   | 1.95                     | 0.47              |
| 4:C:230:PHE:O    | 4:C:234:THR:HG23 | 2.14                     | 0.47              |
| 4:C:327:LEU:HD13 | 4:C:401:PRO:HG3  | 1.95                     | 0.47              |
| 4:C:415:GLN:HG2  | 4:C:418:ARG:NH2  | 2.28                     | 0.47              |
| 4:C:423:ARG:HD2  | 4:C:426:LYS:HD3  | 1.96                     | 0.47              |
| 1:J:34:ILE:HG12  | 4:B:182:THR:HG23 | 1.96                     | 0.47              |
| 1:J:641:ARG:NH1  | 1:J:667:GLN:OE1  | 2.47                     | 0.47              |
| 3:F:183:ASP:OD1  | 3:F:183:ASP:N    | 2.47                     | 0.47              |
| 1:L:737:HIS:O    | 1:L:741:LEU:HD23 | 2.14                     | 0.47              |
| 2:K:444:GLU:HB3  | 2:K:453:TYR:CZ   | 2.50                     | 0.47              |
| 1:J:203:CYS:SG   | 1:J:210:ALA:HA   | 2.55                     | 0.47              |
| 1:J:624:LYS:HA   | 1:J:627:MET:CE   | 2.44                     | 0.47              |
| 1:J:644:VAL:HG12 | 1:J:671:PHE:CD2  | 2.49                     | 0.47              |
| 1:J:680:ILE:HD12 | 1:J:686:TYR:CD1  | 2.50                     | 0.47              |
| 1:J:737:HIS:O    | 1:J:741:LEU:HD23 | 2.14                     | 0.47              |
| 2:I:444:GLU:HB3  | 2:I:453:TYR:CZ   | 2.50                     | 0.47              |
| 2:I:764:PHE:CE1  | 2:I:769:LEU:HB3  | 2.50                     | 0.47              |
| 3:F:170:THR:OG1  | 3:F:171:PRO:HD3  | 2.14                     | 0.47              |
| 5:E:163:TYR:HB2  | 4:A:494:VAL:HG23 | 1.97                     | 0.47              |
| 4:A:294:VAL:O    | 4:A:297:VAL:HG22 | 2.15                     | 0.47              |
| 4:A:444:TYR:HD1  | 4:A:479:HIS:HD2  | 1.63                     | 0.47              |
| 1:L:173:PRO:HD3  | 1:L:210:ALA:HB3  | 1.96                     | 0.47              |
| 1:L:185:TRP:CZ3  | 1:L:192:LEU:HB3  | 2.50                     | 0.47              |
| 1:L:382:ARG:HG3  | 1:L:383:LYS:HG3  | 1.96                     | 0.47              |
| 2:K:346:LEU:HB2  | 2:K:360:HIS:HB3  | 1.97                     | 0.47              |
| 3:H:47:ASN:HB2   | 3:H:116:SER:HB2  | 1.97                     | 0.47              |
| 4:D:215:HIS:O    | 4:D:215:HIS:ND1  | 2.46                     | 0.47              |
| 4:C:261:VAL:O    | 4:C:264:ILE:HG22 | 2.15                     | 0.47              |
| 4:B:16:ALA:HA    | 4:B:19:TRP:CE2   | 2.50                     | 0.47              |
| 4:B:368:MET:HA   | 4:B:368:MET:HE2  | 1.96                     | 0.47              |
| 4:B:443:ALA:O    | 4:B:446:GLN:HG3  | 2.15                     | 0.47              |
| 4:B:487:LYS:HA   | 4:B:487:LYS:HD3  | 1.79                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:205:ILE:HD12 | 4:D:21:PRO:HA    | 1.95                     | 0.47              |
| 2:K:429:LEU:N    | 2:K:439:TYR:O    | 2.48                     | 0.47              |
| 1:J:432:ASP:HB2  | 1:J:485:MET:SD   | 2.55                     | 0.47              |
| 3:F:60:PHE:O     | 3:F:64:CYS:N     | 2.47                     | 0.47              |
| 4:A:261:VAL:O    | 4:A:264:ILE:HG22 | 2.15                     | 0.47              |
| 4:A:423:ARG:HD2  | 4:A:426:LYS:HD3  | 1.96                     | 0.47              |
| 1:L:137:GLU:HA   | 1:L:162:ILE:HB   | 1.97                     | 0.47              |
| 1:L:432:ASP:HB2  | 1:L:485:MET:SD   | 2.55                     | 0.47              |
| 2:K:263:ILE:HG13 | 2:K:280:TYR:C    | 2.40                     | 0.47              |
| 4:D:241:THR:O    | 4:D:245:LEU:HG   | 2.15                     | 0.47              |
| 5:G:183:ASP:HB3  | 5:G:194:GLU:HG3  | 1.96                     | 0.47              |
| 1:L:680:ILE:HD12 | 1:L:686:TYR:CD1  | 2.50                     | 0.47              |
| 2:K:289:ASN:OD1  | 2:K:688:SER:OG   | 2.19                     | 0.47              |
| 3:H:43:GLU:OE2   | 3:H:47:ASN:ND2   | 2.46                     | 0.47              |
| 1:J:173:PRO:HD3  | 1:J:210:ALA:HB3  | 1.96                     | 0.46              |
| 1:J:673:CYS:HB3  | 1:J:784:CYS:HB2  | 1.60                     | 0.46              |
| 2:I:96:TYR:CD2   | 2:I:104:ARG:HB2  | 2.49                     | 0.46              |
| 4:C:403:PRO:HA   | 4:C:406:VAL:HG22 | 1.96                     | 0.46              |
| 2:I:37:ALA:O     | 2:I:41:ILE:HG23  | 2.14                     | 0.46              |
| 2:I:346:LEU:HB2  | 2:I:360:HIS:HB3  | 1.97                     | 0.46              |
| 2:I:727:PRO:HA   | 2:I:757:TYR:HB2  | 1.98                     | 0.46              |
| 4:A:379:LYS:C    | 4:A:384:LYS:HZ2  | 2.22                     | 0.46              |
| 2:K:81:ILE:HD13  | 2:K:520:VAL:HG21 | 1.97                     | 0.46              |
| 2:K:727:PRO:HA   | 2:K:757:TYR:HB2  | 1.98                     | 0.46              |
| 4:D:443:ALA:O    | 4:D:446:GLN:HG3  | 2.15                     | 0.46              |
| 1:J:511:MET:HG3  | 1:J:512:PHE:HD1  | 1.80                     | 0.46              |
| 4:B:194:PHE:HA   | 4:B:197:VAL:HG12 | 1.97                     | 0.46              |
| 5:E:44:ALA:C     | 5:E:46:THR:H     | 2.24                     | 0.46              |
| 2:K:467:SER:HA   | 2:K:470:LEU:HB2  | 1.96                     | 0.46              |
| 2:K:764:PHE:CE1  | 2:K:769:LEU:HB3  | 2.50                     | 0.46              |
| 5:G:163:TYR:HB2  | 4:C:494:VAL:HG23 | 1.97                     | 0.46              |
| 4:C:294:VAL:O    | 4:C:297:VAL:HG22 | 2.15                     | 0.46              |
| 1:J:185:TRP:CZ3  | 1:J:192:LEU:HB3  | 2.50                     | 0.46              |
| 1:J:366:ALA:O    | 1:J:615:ARG:NH1  | 2.49                     | 0.46              |
| 2:I:429:LEU:N    | 2:I:439:TYR:O    | 2.48                     | 0.46              |
| 2:I:622:GLU:OE1  | 2:I:622:GLU:N    | 2.37                     | 0.46              |
| 1:L:203:CYS:SG   | 1:L:210:ALA:HA   | 2.55                     | 0.46              |
| 2:K:367:TRP:NE1  | 2:K:369:HIS:HB2  | 2.29                     | 0.46              |
| 4:D:194:PHE:HA   | 4:D:197:VAL:HG12 | 1.96                     | 0.46              |
| 4:C:33:GLN:NE2   | 4:C:36:LYS:HB3   | 2.31                     | 0.46              |
| 2:I:436:ASN:HD22 | 2:I:458:VAL:HG22 | 1.80                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:138:LYS:HA   | 4:B:138:LYS:HD3  | 1.71                     | 0.46              |
| 4:B:143:GLU:O    | 4:B:146:GLU:HG3  | 2.16                     | 0.46              |
| 4:D:86:ASP:O     | 4:C:100:ARG:NE   | 2.26                     | 0.46              |
| 4:C:335:ILE:HG13 | 4:C:336:ILE:N    | 2.31                     | 0.46              |
| 1:J:696:GLY:O    | 1:J:705:TYR:OH   | 2.28                     | 0.46              |
| 2:I:81:ILE:HD13  | 2:I:520:VAL:HG21 | 1.97                     | 0.46              |
| 3:F:148:MET:HE3  | 3:F:148:MET:O    | 2.16                     | 0.46              |
| 4:B:203:VAL:O    | 4:B:206:THR:OG1  | 2.32                     | 0.46              |
| 4:B:427:LYS:O    | 4:B:430:LEU:HG   | 2.15                     | 0.46              |
| 4:B:485:LEU:HA   | 4:B:488:THR:HG22 | 1.97                     | 0.46              |
| 4:A:87:ARG:HD2   | 4:D:100:ARG:NH1  | 2.31                     | 0.46              |
| 1:L:148:ILE:H    | 1:L:152:SER:HB3  | 1.81                     | 0.46              |
| 1:L:511:MET:HG3  | 1:L:512:PHE:HD1  | 1.80                     | 0.46              |
| 2:K:367:TRP:CZ3  | 2:K:615:ARG:HB2  | 2.47                     | 0.46              |
| 3:H:76:GLN:NE2   | 3:H:77:ILE:HG23  | 2.31                     | 0.46              |
| 3:H:208:SER:O    | 3:H:211:LEU:HD22 | 2.16                     | 0.46              |
| 4:D:203:VAL:O    | 4:D:206:THR:OG1  | 2.32                     | 0.46              |
| 4:D:368:MET:HE2  | 4:D:368:MET:HA   | 1.96                     | 0.46              |
| 2:I:284:LYS:O    | 2:I:287:SER:OG   | 2.33                     | 0.46              |
| 2:I:477:PHE:CE1  | 2:I:490:LEU:HD21 | 2.51                     | 0.46              |
| 2:I:522:LYS:O    | 2:I:526:ASP:HB2  | 2.16                     | 0.46              |
| 2:I:661:PRO:CB   | 2:I:713:ARG:HH22 | 2.28                     | 0.46              |
| 2:I:738:THR:O    | 2:I:742:ILE:HG12 | 2.16                     | 0.46              |
| 4:B:87:ARG:CZ    | 4:A:100:ARG:HD3  | 2.46                     | 0.46              |
| 4:B:406:VAL:HG21 | 4:A:403:PRO:HG3  | 1.97                     | 0.46              |
| 1:L:34:ILE:HG12  | 4:D:182:THR:HG23 | 1.96                     | 0.46              |
| 2:K:493:GLU:H    | 2:K:498:PRO:HA   | 1.81                     | 0.46              |
| 3:H:55:VAL:HG23  | 4:C:55:TRP:CZ3   | 2.51                     | 0.46              |
| 3:H:183:ASP:OD1  | 3:H:183:ASP:N    | 2.47                     | 0.46              |
| 4:D:143:GLU:O    | 4:D:146:GLU:HG3  | 2.16                     | 0.46              |
| 4:D:406:VAL:HG21 | 4:C:403:PRO:HG3  | 1.97                     | 0.46              |
| 4:D:449:ARG:NH2  | 4:D:495:ASP:OD2  | 2.40                     | 0.46              |
| 4:C:444:TYR:HD1  | 4:C:479:HIS:HD2  | 1.63                     | 0.46              |
| 3:F:76:GLN:NE2   | 3:F:77:ILE:HG23  | 2.31                     | 0.46              |
| 2:I:263:ILE:HG13 | 2:I:280:TYR:C    | 2.40                     | 0.46              |
| 2:I:474:CYS:HB2  | 2:I:492:CYS:HB3  | 1.61                     | 0.46              |
| 4:D:87:ARG:CZ    | 4:C:100:ARG:HD3  | 2.46                     | 0.46              |
| 4:C:340:THR:HA   | 4:C:357:ILE:HD11 | 1.98                     | 0.46              |
| 1:J:53:ILE:HA    | 1:J:56:THR:HG22  | 1.98                     | 0.46              |
| 1:J:250:ARG:NE   | 1:J:352:THR:HG22 | 2.31                     | 0.46              |
| 2:I:193:ILE:HG23 | 2:I:244:TRP:CH2  | 2.51                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:467:SER:HA   | 2:I:470:LEU:HB2  | 1.96                     | 0.46              |
| 4:A:403:PRO:HA   | 4:A:406:VAL:HG22 | 1.96                     | 0.46              |
| 1:L:50:THR:HA    | 1:L:53:ILE:HG12  | 1.98                     | 0.46              |
| 1:L:366:ALA:O    | 1:L:615:ARG:NH1  | 2.49                     | 0.46              |
| 2:K:477:PHE:CE1  | 2:K:490:LEU:HD21 | 2.51                     | 0.46              |
| 3:H:148:MET:HE3  | 3:H:148:MET:O    | 2.16                     | 0.46              |
| 3:H:212:PHE:CD2  | 4:C:13:ARG:HB3   | 2.51                     | 0.46              |
| 4:D:300:ILE:O    | 4:D:303:PHE:HB2  | 2.15                     | 0.46              |
| 5:G:44:ALA:C     | 5:G:46:THR:H     | 2.24                     | 0.46              |
| 1:J:137:GLU:HA   | 1:J:162:ILE:HB   | 1.97                     | 0.45              |
| 1:J:148:ILE:H    | 1:J:152:SER:HB3  | 1.81                     | 0.45              |
| 1:J:278:LYS:HA   | 1:J:278:LYS:HD3  | 1.74                     | 0.45              |
| 4:B:100:ARG:NH1  | 4:C:87:ARG:HD2   | 2.31                     | 0.45              |
| 4:B:169:GLN:NE2  | 4:B:250:ALA:HA   | 2.31                     | 0.45              |
| 4:A:17:ILE:HG23  | 4:A:20:MET:HE1   | 1.98                     | 0.45              |
| 4:A:340:THR:HA   | 4:A:357:ILE:HD11 | 1.98                     | 0.45              |
| 4:A:448:LYS:HZ1  | 4:A:486:GLU:CD   | 2.23                     | 0.45              |
| 1:L:250:ARG:NE   | 1:L:352:THR:HG22 | 2.31                     | 0.45              |
| 2:K:523:ALA:HB1  | 2:K:527:ARG:NH2  | 2.31                     | 0.45              |
| 2:K:726:HIS:CE1  | 2:K:735:PHE:HA   | 2.51                     | 0.45              |
| 4:C:392:LEU:O    | 4:C:395:VAL:HG12 | 2.17                     | 0.45              |
| 2:I:367:TRP:NE1  | 2:I:369:HIS:HB2  | 2.29                     | 0.45              |
| 2:I:683:PHE:HE2  | 2:I:708:THR:HB   | 1.81                     | 0.45              |
| 3:F:208:SER:O    | 3:F:211:LEU:HD22 | 2.16                     | 0.45              |
| 3:F:212:PHE:CD2  | 4:A:13:ARG:HB3   | 2.52                     | 0.45              |
| 4:B:21:PRO:HA    | 5:G:205:ILE:HD12 | 1.97                     | 0.45              |
| 2:K:193:ILE:HG23 | 2:K:244:TRP:CH2  | 2.51                     | 0.45              |
| 2:K:596:VAL:HG21 | 2:K:633:MET:HG3  | 1.98                     | 0.45              |
| 4:D:302:LYS:C    | 4:D:304:SER:H    | 2.25                     | 0.45              |
| 4:C:208:PRO:HA   | 4:C:212:SER:OG   | 2.16                     | 0.45              |
| 4:C:448:LYS:HZ1  | 4:C:486:GLU:CD   | 2.23                     | 0.45              |
| 1:J:99:GLN:NE2   | 1:J:514:LEU:O    | 2.49                     | 0.45              |
| 1:J:535:ARG:O    | 1:J:546:MET:HB3  | 2.16                     | 0.45              |
| 1:J:779:ASN:O    | 1:J:783:GLU:HG2  | 2.17                     | 0.45              |
| 2:I:596:VAL:HG21 | 2:I:633:MET:HG3  | 1.98                     | 0.45              |
| 2:I:726:HIS:CE1  | 2:I:735:PHE:HA   | 2.51                     | 0.45              |
| 4:B:241:THR:O    | 4:B:245:LEU:HG   | 2.15                     | 0.45              |
| 5:E:61:LYS:HG3   | 5:E:65:PRO:HA    | 1.99                     | 0.45              |
| 4:A:131:ASP:HA   | 4:A:134:TYR:HB3  | 1.99                     | 0.45              |
| 1:L:53:ILE:HA    | 1:L:56:THR:HG22  | 1.98                     | 0.45              |
| 1:L:318:GLU:HB3  | 1:L:339:ARG:HB2  | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:485:LEU:HA   | 4:D:488:THR:HG22 | 1.97                     | 0.45              |
| 1:J:203:CYS:HB3  | 1:J:208:LYS:HB3  | 1.98                     | 0.45              |
| 1:J:251:LEU:O    | 1:J:296:VAL:HA   | 2.17                     | 0.45              |
| 4:B:446:GLN:HA   | 4:B:449:ARG:HD2  | 1.98                     | 0.45              |
| 1:L:203:CYS:HB3  | 1:L:208:LYS:HB3  | 1.98                     | 0.45              |
| 2:K:436:ASN:HD22 | 2:K:458:VAL:HG22 | 1.80                     | 0.45              |
| 4:D:112:ILE:HG21 | 4:D:144:ASN:ND2  | 2.32                     | 0.45              |
| 4:D:130:GLY:O    | 4:D:134:TYR:N    | 2.48                     | 0.45              |
| 4:D:169:GLN:NE2  | 4:D:250:ALA:HA   | 2.31                     | 0.45              |
| 4:C:332:THR:O    | 4:C:336:ILE:HG12 | 2.17                     | 0.45              |
| 1:J:382:ARG:NH2  | 1:J:431:TYR:OH   | 2.32                     | 0.45              |
| 2:I:95:ILE:HA    | 2:I:105:LEU:HD12 | 1.98                     | 0.45              |
| 3:F:55:VAL:HG23  | 4:A:55:TRP:CZ3   | 2.51                     | 0.45              |
| 4:A:209:CYS:HA   | 4:A:215:HIS:ND1  | 2.32                     | 0.45              |
| 1:L:310:PRO:HB3  | 1:L:336:TRP:CE3  | 2.52                     | 0.45              |
| 1:L:535:ARG:O    | 1:L:546:MET:HB3  | 2.16                     | 0.45              |
| 1:L:779:ASN:O    | 1:L:783:GLU:HG2  | 2.16                     | 0.45              |
| 2:K:185:TRP:CZ3  | 2:K:192:LEU:HD23 | 2.52                     | 0.45              |
| 2:K:346:LEU:HB3  | 2:K:359:LYS:HE2  | 1.99                     | 0.45              |
| 2:K:543:ASN:O    | 2:K:606:GLN:NE2  | 2.49                     | 0.45              |
| 1:J:738:THR:O    | 1:J:742:ILE:HG12 | 2.17                     | 0.45              |
| 2:I:89:ILE:HG21  | 2:I:136:ARG:HH21 | 1.81                     | 0.45              |
| 2:I:523:ALA:HB1  | 2:I:527:ARG:NH2  | 2.31                     | 0.45              |
| 4:A:33:GLN:NE2   | 4:A:36:LYS:HB3   | 2.31                     | 0.45              |
| 1:L:601:ARG:HA   | 1:L:610:LEU:HD11 | 1.98                     | 0.45              |
| 2:K:204:ALA:H    | 2:K:208:LYS:HG2  | 1.82                     | 0.45              |
| 4:D:138:LYS:HA   | 4:D:138:LYS:HD3  | 1.71                     | 0.45              |
| 1:J:50:THR:HA    | 1:J:53:ILE:HG12  | 1.98                     | 0.45              |
| 1:J:408:PRO:HB3  | 1:J:413:ASP:HA   | 1.98                     | 0.45              |
| 2:I:742:ILE:O    | 2:I:746:ILE:HG12 | 2.17                     | 0.45              |
| 4:B:302:LYS:C    | 4:B:304:SER:H    | 2.25                     | 0.45              |
| 5:E:167:LYS:HB2  | 5:E:170:THR:HG23 | 1.99                     | 0.45              |
| 4:A:335:ILE:HG13 | 4:A:336:ILE:N    | 2.31                     | 0.45              |
| 1:L:64:SER:OG    | 1:L:65:GLN:N     | 2.50                     | 0.45              |
| 1:L:673:CYS:HB3  | 1:L:784:CYS:HB2  | 1.60                     | 0.45              |
| 2:I:204:ALA:H    | 2:I:208:LYS:HG2  | 1.82                     | 0.45              |
| 2:I:346:LEU:HB3  | 2:I:359:LYS:HE2  | 1.99                     | 0.45              |
| 3:F:89:THR:HG23  | 3:F:153:ALA:HB2  | 1.99                     | 0.45              |
| 1:L:263:ILE:HD11 | 1:L:279:PRO:HB2  | 1.99                     | 0.45              |
| 1:L:745:LEU:O    | 1:L:749:LYS:N    | 2.46                     | 0.45              |
| 5:G:167:LYS:HB2  | 5:G:170:THR:HG23 | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:310:PRO:HB3  | 1:J:336:TRP:CE3  | 2.52                     | 0.45              |
| 4:B:36:LYS:NZ    | 5:G:214:ASN:O    | 2.41                     | 0.45              |
| 4:B:88:ASP:OD1   | 4:A:93:ARG:NH1   | 2.50                     | 0.45              |
| 4:A:332:THR:O    | 4:A:336:ILE:HG12 | 2.17                     | 0.45              |
| 4:A:392:LEU:O    | 4:A:395:VAL:HG12 | 2.17                     | 0.45              |
| 1:L:530:PRO:HG2  | 1:L:585:THR:HG23 | 1.99                     | 0.45              |
| 2:K:429:LEU:HD11 | 2:K:479:ALA:HB3  | 1.98                     | 0.45              |
| 5:G:61:LYS:HG3   | 5:G:65:PRO:HA    | 1.99                     | 0.45              |
| 1:J:293:SER:OG   | 1:J:295:HIS:NE2  | 2.36                     | 0.45              |
| 2:I:34:ILE:HG12  | 4:A:182:THR:HA   | 1.99                     | 0.45              |
| 4:B:27:MET:C     | 4:B:29:ALA:H     | 2.25                     | 0.45              |
| 4:A:208:PRO:HA   | 4:A:212:SER:OG   | 2.16                     | 0.45              |
| 1:L:630:VAL:O    | 1:L:634:LEU:HB2  | 2.17                     | 0.45              |
| 1:L:738:THR:O    | 1:L:742:ILE:HG12 | 2.17                     | 0.45              |
| 2:K:686:TYR:CE1  | 2:K:733:ILE:HG12 | 2.52                     | 0.45              |
| 3:H:60:PHE:O     | 3:H:64:CYS:N     | 2.47                     | 0.45              |
| 5:G:99:ASP:OD1   | 5:G:103:THR:OG1  | 2.28                     | 0.45              |
| 4:C:124:LEU:HD13 | 4:C:128:ILE:HD11 | 1.99                     | 0.45              |
| 2:I:548:ILE:HD12 | 2:I:595:VAL:O    | 2.17                     | 0.44              |
| 1:L:244:TRP:HA   | 1:L:251:LEU:HD23 | 1.99                     | 0.44              |
| 1:L:278:LYS:HA   | 1:L:278:LYS:HD3  | 1.74                     | 0.44              |
| 1:L:429:LEU:N    | 1:L:439:TYR:O    | 2.50                     | 0.44              |
| 2:K:253:TYR:HE1  | 2:K:297:ILE:HG23 | 1.82                     | 0.44              |
| 2:K:775:ARG:HA   | 2:K:778:ILE:HG12 | 1.99                     | 0.44              |
| 4:D:169:GLN:HE22 | 4:D:250:ALA:HA   | 1.83                     | 0.44              |
| 2:I:183:ALA:HA   | 2:I:194:PHE:HA   | 2.00                     | 0.44              |
| 2:I:655:LEU:O    | 2:I:658:TYR:N    | 2.51                     | 0.44              |
| 4:A:144:ASN:HA   | 4:A:147:ARG:HB3  | 2.00                     | 0.44              |
| 4:A:364:THR:O    | 4:A:367:THR:HG22 | 2.17                     | 0.44              |
| 1:L:99:GLN:NE2   | 1:L:514:LEU:O    | 2.49                     | 0.44              |
| 1:L:395:ARG:HB3  | 1:L:398:PHE:CE1  | 2.52                     | 0.44              |
| 2:K:95:ILE:HA    | 2:K:105:LEU:HD12 | 1.98                     | 0.44              |
| 2:K:522:LYS:O    | 2:K:526:ASP:HB2  | 2.16                     | 0.44              |
| 4:C:105:HIS:O    | 4:C:115:TYR:OH   | 2.35                     | 0.44              |
| 1:J:238:THR:HG22 | 1:J:240:ILE:HG22 | 2.00                     | 0.44              |
| 2:I:429:LEU:HD11 | 2:I:479:ALA:HB3  | 1.98                     | 0.44              |
| 2:I:563:LEU:HD23 | 2:I:595:VAL:HG12 | 1.99                     | 0.44              |
| 1:L:251:LEU:O    | 1:L:296:VAL:HA   | 2.17                     | 0.44              |
| 1:L:408:PRO:HB3  | 1:L:413:ASP:HA   | 1.98                     | 0.44              |
| 1:L:654:TYR:O    | 1:L:657:THR:OG1  | 2.28                     | 0.44              |
| 2:K:738:THR:O    | 2:K:742:ILE:HG12 | 2.16                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:446:GLN:HA   | 4:D:449:ARG:HD2  | 1.98                     | 0.44              |
| 1:J:305:ASP:OD1  | 1:J:306:LEU:N    | 2.50                     | 0.44              |
| 1:J:630:VAL:O    | 1:J:634:LEU:HB2  | 2.16                     | 0.44              |
| 2:I:440:PHE:CE2  | 2:I:453:TYR:HB2  | 2.53                     | 0.44              |
| 2:I:775:ARG:HA   | 2:I:778:ILE:HG12 | 1.99                     | 0.44              |
| 4:B:27:MET:O     | 4:B:29:ALA:N     | 2.51                     | 0.44              |
| 4:B:439:GLY:HA2  | 4:B:442:ASN:HD21 | 1.82                     | 0.44              |
| 1:L:238:THR:HG22 | 1:L:240:ILE:HG22 | 2.00                     | 0.44              |
| 2:K:231:TYR:HB3  | 2:K:236:LEU:HB2  | 2.00                     | 0.44              |
| 2:K:363:GLU:HA   | 2:K:368:LEU:HD21 | 1.99                     | 0.44              |
| 2:K:563:LEU:HD23 | 2:K:595:VAL:HG12 | 1.99                     | 0.44              |
| 2:K:642:THR:O    | 2:K:672:THR:OG1  | 2.28                     | 0.44              |
| 2:K:742:ILE:O    | 2:K:746:ILE:HG12 | 2.17                     | 0.44              |
| 4:D:149:GLN:NE2  | 4:D:153:ASP:OD1  | 2.50                     | 0.44              |
| 4:D:262:MET:HE2  | 4:D:262:MET:N    | 2.32                     | 0.44              |
| 4:C:17:ILE:HG23  | 4:C:20:MET:HE1   | 1.98                     | 0.44              |
| 1:J:234:GLU:OE2  | 1:J:693:ARG:NH2  | 2.46                     | 0.44              |
| 1:J:244:TRP:CD2  | 1:J:251:LEU:HD21 | 2.53                     | 0.44              |
| 1:J:402:THR:HG21 | 1:J:415:ILE:HG13 | 1.99                     | 0.44              |
| 1:J:601:ARG:HA   | 1:J:610:LEU:HD11 | 1.98                     | 0.44              |
| 2:I:185:TRP:CZ3  | 2:I:192:LEU:HD23 | 2.52                     | 0.44              |
| 3:F:84:HIS:CE1   | 3:F:157:MET:HG3  | 2.53                     | 0.44              |
| 3:F:169:ASP:OD1  | 3:F:173:GLN:NE2  | 2.51                     | 0.44              |
| 5:E:75:LYS:HE3   | 5:E:92:HIS:HA    | 1.99                     | 0.44              |
| 4:A:331:LEU:O    | 4:A:335:ILE:HG23 | 2.18                     | 0.44              |
| 1:L:173:PRO:HD2  | 1:L:212:ARG:NH1  | 2.32                     | 0.44              |
| 2:K:89:ILE:HG21  | 2:K:136:ARG:HH21 | 1.81                     | 0.44              |
| 2:K:655:LEU:O    | 2:K:658:TYR:N    | 2.51                     | 0.44              |
| 5:G:46:THR:O     | 5:G:48:PHE:N     | 2.49                     | 0.44              |
| 4:C:209:CYS:HA   | 4:C:215:HIS:ND1  | 2.32                     | 0.44              |
| 1:J:173:PRO:HD2  | 1:J:212:ARG:NH1  | 2.32                     | 0.44              |
| 1:J:517:ASN:O    | 1:J:521:LYS:HG3  | 2.18                     | 0.44              |
| 2:I:198:ASN:ND2  | 2:I:222:ILE:O    | 2.51                     | 0.44              |
| 2:I:363:GLU:HA   | 2:I:368:LEU:HD21 | 1.99                     | 0.44              |
| 2:I:367:TRP:CZ3  | 2:I:615:ARG:HB2  | 2.47                     | 0.44              |
| 4:B:112:ILE:HG21 | 4:B:144:ASN:ND2  | 2.31                     | 0.44              |
| 1:L:305:ASP:OD1  | 1:L:306:LEU:N    | 2.50                     | 0.44              |
| 1:L:725:ILE:HD13 | 1:L:755:GLN:HB2  | 1.99                     | 0.44              |
| 2:K:261:VAL:O    | 2:K:281:HIS:ND1  | 2.51                     | 0.44              |
| 2:K:683:PHE:HE2  | 2:K:708:THR:HB   | 1.81                     | 0.44              |
| 4:D:402:VAL:N    | 4:D:403:PRO:HD2  | 2.32                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:487:LYS:HA   | 4:D:487:LYS:HD3  | 1.79                     | 0.44              |
| 1:J:133:SER:OG   | 1:J:135:ASP:OD1  | 2.28                     | 0.44              |
| 2:I:346:LEU:HD21 | 2:I:386:PHE:CZ   | 2.53                     | 0.44              |
| 2:I:633:MET:O    | 2:I:639:ILE:HG21 | 2.18                     | 0.44              |
| 4:B:130:GLY:O    | 4:B:134:TYR:N    | 2.48                     | 0.44              |
| 4:B:149:GLN:NE2  | 4:B:153:ASP:OD1  | 2.50                     | 0.44              |
| 4:B:169:GLN:HE22 | 4:B:250:ALA:HA   | 1.82                     | 0.44              |
| 2:K:183:ALA:HA   | 2:K:194:PHE:HA   | 2.00                     | 0.44              |
| 2:K:292:ILE:HG12 | 2:K:321:ILE:HD12 | 2.00                     | 0.44              |
| 2:K:474:CYS:HB2  | 2:K:492:CYS:HB3  | 1.61                     | 0.44              |
| 4:D:87:ARG:HD3   | 4:D:121:PHE:CZ   | 2.53                     | 0.44              |
| 5:G:75:LYS:HE3   | 5:G:92:HIS:HA    | 1.98                     | 0.44              |
| 1:J:104:ARG:HB3  | 1:J:113:SER:HB2  | 2.00                     | 0.44              |
| 1:J:438:ILE:O    | 1:J:438:ILE:HG13 | 2.18                     | 0.44              |
| 1:J:530:PRO:HG2  | 1:J:585:THR:HG23 | 1.99                     | 0.44              |
| 1:J:686:TYR:CE1  | 1:J:733:ILE:HG12 | 2.52                     | 0.44              |
| 2:I:63:LEU:HD11  | 2:I:553:THR:HG22 | 2.00                     | 0.44              |
| 2:I:182:TYR:HE2  | 2:I:242:HIS:CE1  | 2.36                     | 0.44              |
| 2:I:330:THR:O    | 2:I:351:ALA:N    | 2.41                     | 0.44              |
| 2:I:349:CYS:HA   | 2:I:356:CYS:HA   | 1.99                     | 0.44              |
| 2:I:757:TYR:HE2  | 2:I:773:LEU:HD12 | 1.82                     | 0.44              |
| 4:B:87:ARG:HD3   | 4:B:121:PHE:CZ   | 2.53                     | 0.44              |
| 4:A:46:ASN:O     | 4:A:85:PHE:N     | 2.44                     | 0.44              |
| 4:A:124:LEU:HD13 | 4:A:128:ILE:HD11 | 1.99                     | 0.44              |
| 2:K:244:TRP:HA   | 2:K:251:LEU:HD12 | 2.00                     | 0.44              |
| 2:K:440:PHE:CE2  | 2:K:453:TYR:HB2  | 2.53                     | 0.44              |
| 2:K:548:ILE:HD12 | 2:K:595:VAL:O    | 2.17                     | 0.44              |
| 2:K:757:TYR:HE2  | 2:K:773:LEU:HD12 | 1.82                     | 0.44              |
| 4:D:40:ASP:OD1   | 4:D:40:ASP:N     | 2.51                     | 0.44              |
| 4:D:46:ASN:O     | 4:D:84:PHE:HA    | 2.18                     | 0.44              |
| 4:C:131:ASP:HA   | 4:C:134:TYR:HB3  | 1.99                     | 0.44              |
| 1:J:263:ILE:HD11 | 1:J:279:PRO:HB2  | 1.99                     | 0.44              |
| 1:J:318:GLU:HB3  | 1:J:339:ARG:HB2  | 1.98                     | 0.44              |
| 1:J:725:ILE:HD13 | 1:J:755:GLN:HB2  | 1.99                     | 0.44              |
| 2:I:244:TRP:HA   | 2:I:251:LEU:HD12 | 2.00                     | 0.44              |
| 2:I:493:GLU:H    | 2:I:498:PRO:HA   | 1.81                     | 0.44              |
| 4:B:262:MET:HE2  | 4:B:262:MET:N    | 2.32                     | 0.44              |
| 4:A:302:LYS:HA   | 4:A:302:LYS:HD2  | 1.73                     | 0.44              |
| 1:L:438:ILE:O    | 1:L:438:ILE:HG13 | 2.18                     | 0.44              |
| 1:L:517:ASN:O    | 1:L:521:LYS:HG3  | 2.18                     | 0.44              |
| 2:K:34:ILE:HG12  | 4:C:182:THR:HA   | 1.99                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:284:LYS:O    | 2:K:287:SER:OG   | 2.33                     | 0.44              |
| 3:H:84:HIS:CE1   | 3:H:157:MET:HG3  | 2.53                     | 0.44              |
| 3:H:89:THR:HG23  | 3:H:153:ALA:HB2  | 1.99                     | 0.44              |
| 4:C:364:THR:O    | 4:C:367:THR:HG22 | 2.17                     | 0.44              |
| 1:J:284:LYS:O    | 1:J:287:SER:OG   | 2.29                     | 0.43              |
| 2:I:253:TYR:HE1  | 2:I:297:ILE:HG23 | 1.82                     | 0.43              |
| 3:F:73:THR:O     | 3:F:77:ILE:HG12  | 2.18                     | 0.43              |
| 4:B:150:ASP:HA   | 4:B:153:ASP:OD2  | 2.18                     | 0.43              |
| 4:A:105:HIS:O    | 4:A:115:TYR:OH   | 2.35                     | 0.43              |
| 4:A:201:ALA:HA   | 4:A:204:VAL:HG22 | 2.00                     | 0.43              |
| 1:L:564:LEU:HD21 | 1:L:566:VAL:HB   | 1.99                     | 0.43              |
| 2:K:349:CYS:HA   | 2:K:356:CYS:HA   | 1.99                     | 0.43              |
| 3:H:81:PHE:CE2   | 4:C:12:ALA:HB2   | 2.52                     | 0.43              |
| 4:D:27:MET:O     | 4:D:29:ALA:N     | 2.51                     | 0.43              |
| 4:D:150:ASP:HA   | 4:D:153:ASP:OD2  | 2.18                     | 0.43              |
| 4:D:293:ARG:HA   | 4:D:296:ARG:HD3  | 2.00                     | 0.43              |
| 4:D:335:ILE:HD11 | 4:D:365:ILE:HD13 | 2.00                     | 0.43              |
| 4:C:197:VAL:HA   | 4:C:200:ILE:HG22 | 1.99                     | 0.43              |
| 1:J:395:ARG:HB3  | 1:J:398:PHE:CE1  | 2.52                     | 0.43              |
| 1:J:564:LEU:HD12 | 1:J:630:VAL:HG11 | 2.00                     | 0.43              |
| 2:I:195:ILE:HD11 | 2:I:242:HIS:HE1  | 1.83                     | 0.43              |
| 2:I:289:ASN:ND2  | 2:I:320:TYR:OH   | 2.52                     | 0.43              |
| 2:I:314:PRO:O    | 2:I:317:ARG:NH1  | 2.36                     | 0.43              |
| 2:I:584:GLU:HA   | 2:I:587:MET:SD   | 2.58                     | 0.43              |
| 3:F:118:LEU:HD21 | 3:F:129:TRP:CG   | 2.52                     | 0.43              |
| 4:B:86:ASP:O     | 4:A:100:ARG:NE   | 2.26                     | 0.43              |
| 4:A:84:PHE:CE2   | 4:D:53:GLN:HB2   | 2.53                     | 0.43              |
| 1:L:400:HIS:ND1  | 1:L:419:THR:OG1  | 2.36                     | 0.43              |
| 1:L:583:TRP:HB3  | 1:L:774:TYR:CD1  | 2.54                     | 0.43              |
| 2:K:57:PRO:HB2   | 2:K:59:GLU:OE1   | 2.18                     | 0.43              |
| 2:K:133:SER:OG   | 2:K:135:ASP:OD1  | 2.31                     | 0.43              |
| 4:D:88:ASP:OD1   | 4:C:93:ARG:NH1   | 2.50                     | 0.43              |
| 5:G:194:GLU:HA   | 5:G:197:GLU:HG2  | 2.00                     | 0.43              |
| 1:J:429:LEU:N    | 1:J:439:TYR:O    | 2.50                     | 0.43              |
| 2:I:567:ASP:OD1  | 2:I:569:THR:OG1  | 2.31                     | 0.43              |
| 4:B:46:ASN:HA    | 4:B:51:ARG:HA    | 2.01                     | 0.43              |
| 4:B:53:GLN:HB2   | 4:C:84:PHE:CE2   | 2.53                     | 0.43              |
| 4:A:178:PRO:HA   | 4:A:188:TYR:CE2  | 2.54                     | 0.43              |
| 4:A:197:VAL:HA   | 4:A:200:ILE:HG22 | 1.99                     | 0.43              |
| 1:L:82:HIS:HD2   | 1:L:517:ASN:HA   | 1.83                     | 0.43              |
| 1:L:244:TRP:CD2  | 1:L:251:LEU:HD21 | 2.53                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:402:THR:HG21 | 1:L:415:ILE:HG13 | 1.99                     | 0.43              |
| 2:K:584:GLU:HA   | 2:K:587:MET:SD   | 2.58                     | 0.43              |
| 2:K:633:MET:O    | 2:K:639:ILE:HG21 | 2.18                     | 0.43              |
| 2:K:681:THR:HG21 | 2:K:741:LEU:HB2  | 2.00                     | 0.43              |
| 3:H:118:LEU:HD21 | 3:H:129:TRP:CG   | 2.53                     | 0.43              |
| 4:D:46:ASN:HA    | 4:D:51:ARG:HA    | 2.01                     | 0.43              |
| 4:D:393:SER:O    | 4:D:396:LEU:HG   | 2.18                     | 0.43              |
| 4:C:144:ASN:HA   | 4:C:147:ARG:HB3  | 2.00                     | 0.43              |
| 1:J:82:HIS:HD2   | 1:J:517:ASN:HA   | 1.83                     | 0.43              |
| 1:J:183:ALA:HA   | 1:J:194:PHE:HA   | 2.00                     | 0.43              |
| 1:J:244:TRP:HA   | 1:J:251:LEU:HD23 | 1.99                     | 0.43              |
| 1:J:282:TYR:HE1  | 1:J:284:LYS:HD3  | 1.84                     | 0.43              |
| 1:J:289:ASN:OD1  | 1:J:320:TYR:OH   | 2.36                     | 0.43              |
| 1:J:337:LEU:HD22 | 1:J:371:GLN:HG3  | 2.00                     | 0.43              |
| 1:J:640:ASP:OD2  | 1:J:643:ARG:NE   | 2.37                     | 0.43              |
| 2:I:231:TYR:HB3  | 2:I:236:LEU:HB2  | 2.00                     | 0.43              |
| 2:I:234:GLU:HG3  | 2:I:693:ARG:HH22 | 1.83                     | 0.43              |
| 3:F:81:PHE:CE2   | 4:A:12:ALA:HB2   | 2.52                     | 0.43              |
| 4:B:245:LEU:HA   | 4:B:248:LEU:HD12 | 2.00                     | 0.43              |
| 4:B:393:SER:O    | 4:B:396:LEU:HG   | 2.18                     | 0.43              |
| 1:L:337:LEU:HD22 | 1:L:371:GLN:HG3  | 2.01                     | 0.43              |
| 3:H:40:GLU:OE2   | 3:H:41:GLN:NE2   | 2.52                     | 0.43              |
| 4:C:445:MET:HE1  | 4:C:449:ARG:NH1  | 2.34                     | 0.43              |
| 1:J:187:PRO:HD2  | 1:J:191:GLN:NE2  | 2.31                     | 0.43              |
| 1:J:231:TYR:O    | 1:J:237:LYS:N    | 2.51                     | 0.43              |
| 2:I:292:ILE:HG12 | 2:I:321:ILE:HD12 | 2.01                     | 0.43              |
| 4:B:402:VAL:N    | 4:B:403:PRO:HD2  | 2.32                     | 0.43              |
| 4:A:10:PRO:HA    | 4:A:13:ARG:HG3   | 2.01                     | 0.43              |
| 1:L:282:TYR:HE1  | 1:L:284:LYS:HD3  | 1.83                     | 0.43              |
| 1:L:686:TYR:CE1  | 1:L:733:ILE:HG12 | 2.52                     | 0.43              |
| 2:K:292:ILE:HD13 | 2:K:321:ILE:H    | 1.83                     | 0.43              |
| 3:H:215:VAL:HG22 | 3:H:216:MET:HG3  | 2.01                     | 0.43              |
| 2:I:122:ILE:HA   | 2:I:126:ARG:HH11 | 1.84                     | 0.43              |
| 2:I:428:ILE:HA   | 2:I:440:PHE:HB3  | 2.01                     | 0.43              |
| 3:F:118:LEU:O    | 3:F:213:GLN:NE2  | 2.52                     | 0.43              |
| 4:B:46:ASN:O     | 4:B:84:PHE:HA    | 2.18                     | 0.43              |
| 4:B:293:ARG:HA   | 4:B:296:ARG:HD3  | 2.01                     | 0.43              |
| 1:L:170:LEU:HD21 | 1:L:194:PHE:HB3  | 2.00                     | 0.43              |
| 1:L:183:ALA:HA   | 1:L:194:PHE:HA   | 2.00                     | 0.43              |
| 1:L:231:TYR:O    | 1:L:237:LYS:N    | 2.51                     | 0.43              |
| 1:L:399:TYR:N    | 1:L:424:ASP:OD1  | 2.40                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:193:ILE:HD11 | 2:K:242:HIS:CE1  | 2.53                     | 0.43              |
| 2:K:198:ASN:ND2  | 2:K:222:ILE:O    | 2.51                     | 0.43              |
| 2:K:346:LEU:HD21 | 2:K:386:PHE:CZ   | 2.53                     | 0.43              |
| 3:H:73:THR:O     | 3:H:77:ILE:HG12  | 2.18                     | 0.43              |
| 4:D:261:VAL:HB   | 4:D:262:MET:HE2  | 2.01                     | 0.43              |
| 4:D:439:GLY:HA2  | 4:D:442:ASN:HD21 | 1.82                     | 0.43              |
| 4:C:201:ALA:HA   | 4:C:204:VAL:HG22 | 2.00                     | 0.43              |
| 2:I:193:ILE:HD11 | 2:I:242:HIS:CE1  | 2.54                     | 0.43              |
| 2:I:686:TYR:CE1  | 2:I:733:ILE:HG12 | 2.53                     | 0.43              |
| 4:B:94:HIS:NE2   | 4:B:107:PRO:HG3  | 2.34                     | 0.43              |
| 1:L:38:LEU:HD11  | 4:D:189:TYR:HB3  | 2.00                     | 0.43              |
| 1:L:382:ARG:NH2  | 1:L:431:TYR:OH   | 2.32                     | 0.43              |
| 2:K:289:ASN:ND2  | 2:K:320:TYR:OH   | 2.51                     | 0.43              |
| 3:H:60:PHE:HE1   | 3:H:69:VAL:HB    | 1.83                     | 0.43              |
| 3:H:169:ASP:OD1  | 3:H:173:GLN:NE2  | 2.51                     | 0.43              |
| 4:C:114:ALA:HA   | 4:C:117:GLU:CD   | 2.44                     | 0.43              |
| 1:J:64:SER:OG    | 1:J:65:GLN:N     | 2.50                     | 0.43              |
| 2:I:155:GLY:HA2  | 2:I:179:LYS:HE3  | 2.00                     | 0.43              |
| 2:I:573:GLN:NE2  | 2:I:575:VAL:O    | 2.52                     | 0.43              |
| 4:A:45:LEU:HB2   | 4:A:85:PHE:HE1   | 1.84                     | 0.43              |
| 4:A:67:LEU:O     | 4:A:72:ARG:HD3   | 2.19                     | 0.43              |
| 4:A:444:TYR:OH   | 4:A:486:GLU:OE2  | 2.35                     | 0.43              |
| 1:L:202:TYR:CZ   | 1:L:299:LEU:HB3  | 2.54                     | 0.43              |
| 2:K:143:TYR:CE2  | 2:K:156:TYR:HB2  | 2.54                     | 0.43              |
| 4:D:183:MET:HA   | 4:D:186:VAL:HG12 | 2.01                     | 0.43              |
| 5:G:158:MET:HE1  | 5:G:166:LEU:HD13 | 2.01                     | 0.43              |
| 4:C:195:ILE:HG22 | 4:C:240:PHE:HE1  | 1.84                     | 0.43              |
| 4:C:331:LEU:O    | 4:C:335:ILE:HG23 | 2.18                     | 0.43              |
| 1:J:564:LEU:HD21 | 1:J:566:VAL:HB   | 1.99                     | 0.43              |
| 1:J:583:TRP:HB3  | 1:J:774:TYR:CD1  | 2.53                     | 0.43              |
| 2:I:261:VAL:O    | 2:I:281:HIS:ND1  | 2.51                     | 0.43              |
| 2:I:543:ASN:O    | 2:I:606:GLN:NE2  | 2.49                     | 0.43              |
| 3:F:60:PHE:HE1   | 3:F:69:VAL:HB    | 1.83                     | 0.43              |
| 5:E:194:GLU:HA   | 5:E:197:GLU:HG2  | 2.00                     | 0.43              |
| 1:L:195:ILE:HD12 | 1:L:226:LEU:HG   | 2.01                     | 0.43              |
| 1:L:289:ASN:OD1  | 1:L:320:TYR:OH   | 2.36                     | 0.43              |
| 2:K:63:LEU:HD11  | 2:K:553:THR:HG22 | 2.00                     | 0.43              |
| 2:K:155:GLY:HA2  | 2:K:179:LYS:HE3  | 2.00                     | 0.43              |
| 2:K:330:THR:O    | 2:K:351:ALA:N    | 2.41                     | 0.43              |
| 4:D:94:HIS:NE2   | 4:D:107:PRO:HG3  | 2.34                     | 0.43              |
| 4:C:10:PRO:HA    | 4:C:13:ARG:HG3   | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:C:45:LEU:HB2   | 4:C:85:PHE:HE1   | 1.84                     | 0.43              |
| 2:I:57:PRO:HB2   | 2:I:59:GLU:OE1   | 2.18                     | 0.43              |
| 2:I:234:GLU:OE2  | 2:I:693:ARG:NH2  | 2.52                     | 0.43              |
| 2:I:681:THR:HG21 | 2:I:741:LEU:HB2  | 2.00                     | 0.43              |
| 4:B:47:VAL:HG21  | 4:B:92:PHE:HD1   | 1.84                     | 0.43              |
| 4:B:199:VAL:HA   | 4:B:299:ARG:HE   | 1.84                     | 0.43              |
| 4:B:335:ILE:HD11 | 4:B:365:ILE:HD13 | 2.00                     | 0.43              |
| 4:A:195:ILE:HG22 | 4:A:240:PHE:CE1  | 2.53                     | 0.43              |
| 2:K:74:LEU:HA    | 2:K:79:PHE:HD2   | 1.84                     | 0.43              |
| 2:K:423:TRP:CG   | 2:K:444:GLU:HA   | 2.54                     | 0.43              |
| 4:D:27:MET:C     | 4:D:29:ALA:H     | 2.26                     | 0.43              |
| 4:D:88:ASP:HA    | 4:D:89:PRO:HD3   | 1.91                     | 0.43              |
| 4:D:328:LEU:O    | 4:D:332:THR:HG23 | 2.19                     | 0.43              |
| 1:J:195:ILE:HD12 | 1:J:226:LEU:HG   | 2.01                     | 0.42              |
| 1:J:429:LEU:HG   | 1:J:440:PHE:HA   | 2.01                     | 0.42              |
| 1:J:616:ARG:NH2  | 1:J:704:ALA:HB2  | 2.34                     | 0.42              |
| 2:I:133:SER:OG   | 2:I:135:ASP:OD1  | 2.30                     | 0.42              |
| 2:I:325:LYS:HD3  | 2:I:375:PRO:HG2  | 2.00                     | 0.42              |
| 4:A:400:LEU:HB3  | 4:A:401:PRO:HD3  | 2.01                     | 0.42              |
| 1:L:564:LEU:HD12 | 1:L:630:VAL:HG11 | 2.00                     | 0.42              |
| 1:L:616:ARG:NH2  | 1:L:704:ALA:HB2  | 2.34                     | 0.42              |
| 2:K:91:ASP:N     | 2:K:91:ASP:OD1   | 2.52                     | 0.42              |
| 2:K:122:ILE:HA   | 2:K:126:ARG:HH11 | 1.84                     | 0.42              |
| 2:K:182:TYR:HE2  | 2:K:242:HIS:CE1  | 2.36                     | 0.42              |
| 2:K:428:ILE:HA   | 2:K:440:PHE:HB3  | 2.01                     | 0.42              |
| 1:J:170:LEU:HD21 | 1:J:194:PHE:HB3  | 2.00                     | 0.42              |
| 2:I:80:LYS:HD3   | 2:I:81:ILE:H     | 1.85                     | 0.42              |
| 2:I:143:TYR:CE2  | 2:I:156:TYR:HB2  | 2.54                     | 0.42              |
| 2:I:292:ILE:HD13 | 2:I:321:ILE:H    | 1.83                     | 0.42              |
| 3:F:215:VAL:HG22 | 3:F:216:MET:HG3  | 2.01                     | 0.42              |
| 4:B:73:ASP:HA    | 4:B:76:TYR:HB2   | 2.01                     | 0.42              |
| 4:A:109:HIS:HB2  | 4:D:109:HIS:ND1  | 2.34                     | 0.42              |
| 1:L:82:HIS:CD2   | 1:L:517:ASN:HA   | 2.54                     | 0.42              |
| 1:L:449:ARG:HG2  | 1:L:475:THR:HB   | 2.00                     | 0.42              |
| 2:K:234:GLU:HG3  | 2:K:693:ARG:HH22 | 1.83                     | 0.42              |
| 3:H:51:ARG:HH22  | 4:D:79:GLU:CD    | 2.27                     | 0.42              |
| 4:D:187:PHE:HA   | 4:D:190:VAL:HG12 | 2.02                     | 0.42              |
| 4:C:195:ILE:HG22 | 4:C:240:PHE:CE1  | 2.53                     | 0.42              |
| 1:J:38:LEU:HD11  | 4:B:189:TYR:HB3  | 2.00                     | 0.42              |
| 1:J:82:HIS:CD2   | 1:J:517:ASN:HA   | 2.54                     | 0.42              |
| 1:J:362:ASP:OD1  | 1:J:388:ARG:NE   | 2.53                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:449:ARG:HG2  | 1:J:475:THR:HB   | 2.00                     | 0.42              |
| 4:A:398:ILE:HG13 | 4:A:399:ALA:N    | 2.34                     | 0.42              |
| 2:K:80:LYS:HD3   | 2:K:81:ILE:H     | 1.85                     | 0.42              |
| 2:K:195:ILE:HD11 | 2:K:242:HIS:HE1  | 1.83                     | 0.42              |
| 4:D:245:LEU:HA   | 4:D:248:LEU:HD12 | 2.00                     | 0.42              |
| 1:J:129:ARG:HH21 | 1:J:157:TYR:HE1  | 1.66                     | 0.42              |
| 3:F:51:ARG:HH22  | 4:B:79:GLU:CD    | 2.27                     | 0.42              |
| 4:B:261:VAL:HB   | 4:B:262:MET:HE2  | 2.01                     | 0.42              |
| 4:B:327:LEU:HG   | 4:B:331:LEU:HD23 | 2.02                     | 0.42              |
| 5:E:47:ASN:ND2   | 5:E:120:ARG:O    | 2.53                     | 0.42              |
| 4:A:80:THR:HG23  | 4:A:82:GLN:HG3   | 2.01                     | 0.42              |
| 4:A:445:MET:HE1  | 4:A:449:ARG:NH1  | 2.34                     | 0.42              |
| 1:L:313:ASP:OD2  | 1:L:345:ILE:HD11 | 2.19                     | 0.42              |
| 1:L:362:ASP:OD1  | 1:L:388:ARG:NE   | 2.53                     | 0.42              |
| 1:L:429:LEU:HG   | 1:L:440:PHE:HA   | 2.01                     | 0.42              |
| 2:K:601:ARG:N    | 2:K:625:ASP:OD2  | 2.33                     | 0.42              |
| 2:K:620:LEU:HG   | 2:K:624:LYS:HE3  | 2.01                     | 0.42              |
| 3:H:47:ASN:H     | 3:H:116:SER:HB2  | 1.84                     | 0.42              |
| 4:C:67:LEU:O     | 4:C:72:ARG:HD3   | 2.19                     | 0.42              |
| 4:B:40:ASP:OD1   | 4:B:40:ASP:N     | 2.51                     | 0.42              |
| 4:B:183:MET:HA   | 4:B:186:VAL:HG12 | 2.01                     | 0.42              |
| 4:A:61:ARG:HG2   | 4:A:62:TYR:CZ    | 2.55                     | 0.42              |
| 1:L:91:ASP:HB2   | 1:L:484:SER:HB2  | 2.01                     | 0.42              |
| 1:L:104:ARG:HB3  | 1:L:113:SER:HB2  | 2.00                     | 0.42              |
| 1:L:438:ILE:HD11 | 1:L:455:ALA:HB3  | 2.02                     | 0.42              |
| 1:L:448:ARG:H    | 1:L:448:ARG:HG2  | 1.73                     | 0.42              |
| 2:K:154:THR:OG1  | 2:K:155:GLY:N    | 2.52                     | 0.42              |
| 4:C:178:PRO:HA   | 4:C:188:TYR:HE2  | 1.84                     | 0.42              |
| 4:C:272:PRO:HA   | 4:C:275:ILE:HG22 | 2.01                     | 0.42              |
| 1:J:313:ASP:OD2  | 1:J:345:ILE:HD11 | 2.19                     | 0.42              |
| 1:J:703:ARG:HA   | 1:J:703:ARG:HD2  | 1.89                     | 0.42              |
| 2:I:783:GLU:HA   | 2:I:786:ARG:HD2  | 2.02                     | 0.42              |
| 4:B:109:HIS:ND1  | 4:C:109:HIS:HB2  | 2.34                     | 0.42              |
| 4:B:233:ASP:OD1  | 4:B:233:ASP:N    | 2.53                     | 0.42              |
| 4:A:114:ALA:HA   | 4:A:117:GLU:CD   | 2.44                     | 0.42              |
| 1:L:234:GLU:OE2  | 1:L:693:ARG:NH2  | 2.46                     | 0.42              |
| 2:K:418:ILE:HD13 | 2:K:438:ILE:HG21 | 2.02                     | 0.42              |
| 4:C:61:ARG:HG2   | 4:C:62:TYR:CZ    | 2.55                     | 0.42              |
| 4:C:178:PRO:HA   | 4:C:188:TYR:CE2  | 2.54                     | 0.42              |
| 4:C:398:ILE:HG13 | 4:C:399:ALA:N    | 2.34                     | 0.42              |
| 1:J:642:THR:O    | 1:J:672:THR:OG1  | 2.23                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:74:LEU:HA    | 2:I:79:PHE:HD2   | 1.84                     | 0.42              |
| 2:I:190:GLN:HE21 | 2:I:205:HIS:HB3  | 1.85                     | 0.42              |
| 2:I:418:ILE:HD13 | 2:I:438:ILE:HG21 | 2.02                     | 0.42              |
| 2:I:439:TYR:HE2  | 2:I:485:MET:HG3  | 1.84                     | 0.42              |
| 2:I:763:TYR:HD1  | 2:I:763:TYR:HA   | 1.71                     | 0.42              |
| 4:A:178:PRO:HA   | 4:A:188:TYR:HE2  | 1.84                     | 0.42              |
| 1:L:153:TYR:O    | 1:L:157:TYR:OH   | 2.34                     | 0.42              |
| 1:L:730:ASP:OD2  | 1:L:762:HIS:ND1  | 2.45                     | 0.42              |
| 2:K:347:THR:HA   | 2:K:358:LYS:HA   | 2.02                     | 0.42              |
| 2:K:573:GLN:NE2  | 2:K:575:VAL:O    | 2.52                     | 0.42              |
| 2:K:610:LEU:HA   | 2:K:613:GLU:HG2  | 2.02                     | 0.42              |
| 2:K:726:HIS:HD2  | 2:K:727:PRO:HD2  | 1.85                     | 0.42              |
| 4:D:47:VAL:HG21  | 4:D:92:PHE:HD1   | 1.84                     | 0.42              |
| 4:C:97:ASN:HA    | 4:C:100:ARG:HH11 | 1.85                     | 0.42              |
| 1:J:382:ARG:HA   | 1:J:406:SER:HB2  | 2.01                     | 0.42              |
| 2:I:423:TRP:CG   | 2:I:444:GLU:HA   | 2.54                     | 0.42              |
| 4:B:88:ASP:HA    | 4:B:89:PRO:HD3   | 1.92                     | 0.42              |
| 4:B:328:LEU:O    | 4:B:332:THR:HG23 | 2.19                     | 0.42              |
| 4:A:192:GLY:O    | 4:A:195:ILE:HG12 | 2.20                     | 0.42              |
| 2:K:88:TRP:HH2   | 2:K:108:VAL:HG21 | 1.85                     | 0.42              |
| 5:G:47:ASN:ND2   | 5:G:120:ARG:O    | 2.53                     | 0.42              |
| 4:C:43:ILE:N     | 4:C:54:THR:O     | 2.48                     | 0.42              |
| 2:I:154:THR:OG1  | 2:I:155:GLY:N    | 2.52                     | 0.42              |
| 2:I:347:THR:HA   | 2:I:358:LYS:HA   | 2.02                     | 0.42              |
| 2:I:610:LEU:HA   | 2:I:613:GLU:HG2  | 2.02                     | 0.42              |
| 2:I:764:PHE:CE2  | 2:I:773:LEU:HD13 | 2.55                     | 0.42              |
| 3:F:55:VAL:HG23  | 4:A:55:TRP:HZ3   | 1.85                     | 0.42              |
| 4:B:91:ILE:O     | 4:B:95:ILE:HG13  | 2.20                     | 0.42              |
| 1:L:315:ARG:H    | 1:L:315:ARG:HD3  | 1.85                     | 0.42              |
| 2:K:382:ARG:HG3  | 2:K:383:LYS:N    | 2.30                     | 0.42              |
| 2:K:661:PRO:CB   | 2:K:713:ARG:HH22 | 2.28                     | 0.42              |
| 3:H:158:MET:HE1  | 4:D:489:THR:OG1  | 2.20                     | 0.42              |
| 3:F:158:MET:HE1  | 4:B:489:THR:OG1  | 2.20                     | 0.42              |
| 4:B:187:PHE:HA   | 4:B:190:VAL:HG12 | 2.02                     | 0.42              |
| 5:E:214:ASN:O    | 4:D:36:LYS:NZ    | 2.41                     | 0.42              |
| 1:L:187:PRO:HD2  | 1:L:191:GLN:NE2  | 2.31                     | 0.42              |
| 4:C:80:THR:HG23  | 4:C:82:GLN:HG3   | 2.01                     | 0.42              |
| 4:C:423:ARG:HA   | 4:C:426:LYS:HG2  | 2.02                     | 0.42              |
| 2:I:187:PRO:HB2  | 2:I:188:LYS:HZ1  | 1.85                     | 0.41              |
| 2:I:387:ILE:HG13 | 2:I:400:HIS:O    | 2.20                     | 0.41              |
| 2:I:726:HIS:HD2  | 2:I:727:PRO:HD2  | 1.85                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:47:ASN:H     | 3:F:116:SER:HB2  | 1.84                     | 0.41              |
| 4:A:474:PHE:CD1  | 4:D:9:LEU:HD22   | 2.55                     | 0.41              |
| 1:L:636:GLU:HB3  | 1:L:638:TYR:CE1  | 2.55                     | 0.41              |
| 2:K:190:GLN:HE21 | 2:K:205:HIS:HB3  | 1.85                     | 0.41              |
| 1:J:105:LEU:HD13 | 1:J:116:LEU:HD22 | 2.02                     | 0.41              |
| 2:I:88:TRP:HH2   | 2:I:108:VAL:HG21 | 1.85                     | 0.41              |
| 2:I:91:ASP:N     | 2:I:91:ASP:OD1   | 2.52                     | 0.41              |
| 3:F:40:GLU:OE2   | 3:F:41:GLN:NE2   | 2.52                     | 0.41              |
| 3:F:95:PHE:HZ    | 3:F:105:SER:HA   | 1.85                     | 0.41              |
| 4:A:195:ILE:HG22 | 4:A:240:PHE:HE1  | 1.84                     | 0.41              |
| 2:K:234:GLU:OE2  | 2:K:693:ARG:NH2  | 2.52                     | 0.41              |
| 2:K:387:ILE:HG13 | 2:K:400:HIS:O    | 2.21                     | 0.41              |
| 2:K:439:TYR:HE2  | 2:K:485:MET:HG3  | 1.84                     | 0.41              |
| 3:H:119:LEU:O    | 3:H:213:GLN:HA   | 2.20                     | 0.41              |
| 1:J:202:TYR:CZ   | 1:J:299:LEU:HB3  | 2.54                     | 0.41              |
| 3:F:87:ALA:HB2   | 3:F:157:MET:CE   | 2.50                     | 0.41              |
| 4:B:363:TYR:HA   | 4:B:366:VAL:HG22 | 2.02                     | 0.41              |
| 1:L:70:THR:HG22  | 1:L:73:ASP:CG    | 2.46                     | 0.41              |
| 1:L:129:ARG:HH21 | 1:L:157:TYR:HE1  | 1.67                     | 0.41              |
| 1:L:284:LYS:O    | 1:L:287:SER:OG   | 2.29                     | 0.41              |
| 4:D:199:VAL:HA   | 4:D:299:ARG:HE   | 1.84                     | 0.41              |
| 4:D:363:TYR:HA   | 4:D:366:VAL:HG22 | 2.02                     | 0.41              |
| 1:J:438:ILE:HD11 | 1:J:455:ALA:HB3  | 2.02                     | 0.41              |
| 1:J:440:PHE:CE2  | 1:J:453:TYR:HB2  | 2.56                     | 0.41              |
| 2:I:161:LYS:HD3  | 2:I:166:ASP:HB3  | 2.02                     | 0.41              |
| 2:I:198:ASN:HB3  | 2:I:217:GLY:HA3  | 2.03                     | 0.41              |
| 2:I:752:TYR:HE2  | 2:I:754:LEU:HB2  | 1.86                     | 0.41              |
| 4:A:266:ASP:O    | 4:A:270:ILE:HG23 | 2.21                     | 0.41              |
| 1:L:451:GLN:HB2  | 1:L:453:TYR:CZ   | 2.55                     | 0.41              |
| 2:K:250:ARG:HD3  | 2:K:296:VAL:HG11 | 2.02                     | 0.41              |
| 4:D:16:ALA:O     | 4:D:20:MET:N     | 2.53                     | 0.41              |
| 5:G:170:THR:N    | 5:G:171:PRO:HD2  | 2.36                     | 0.41              |
| 4:C:192:GLY:O    | 4:C:195:ILE:HG12 | 2.20                     | 0.41              |
| 4:C:400:LEU:HB3  | 4:C:401:PRO:HD3  | 2.01                     | 0.41              |
| 2:I:620:LEU:HG   | 2:I:624:LYS:HE3  | 2.01                     | 0.41              |
| 4:B:38:THR:HG23  | 5:G:52:GLU:HG3   | 2.02                     | 0.41              |
| 4:A:419:ALA:HA   | 4:A:422:ARG:HG2  | 2.02                     | 0.41              |
| 4:A:472:SER:OG   | 4:A:475:GLU:OE2  | 2.38                     | 0.41              |
| 1:L:783:GLU:HA   | 1:L:786:ARG:HG2  | 2.02                     | 0.41              |
| 4:C:266:ASP:O    | 4:C:270:ILE:HG23 | 2.21                     | 0.41              |
| 1:J:386:PHE:HE2  | 1:J:388:ARG:HD3  | 1.86                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:481:PHE:CD2  | 1:J:488:PHE:HB3  | 2.56                     | 0.41              |
| 1:J:529:MET:HA   | 1:J:530:PRO:HD3  | 1.94                     | 0.41              |
| 1:J:783:GLU:HA   | 1:J:786:ARG:HG2  | 2.02                     | 0.41              |
| 2:I:621:LEU:HA   | 2:I:624:LYS:HD2  | 2.02                     | 0.41              |
| 4:B:157:ALA:O    | 4:B:170:ARG:NH2  | 2.43                     | 0.41              |
| 5:E:46:THR:O     | 5:E:48:PHE:N     | 2.49                     | 0.41              |
| 5:E:170:THR:N    | 5:E:171:PRO:HD2  | 2.36                     | 0.41              |
| 4:A:12:ALA:O     | 4:A:15:ALA:HB3   | 2.21                     | 0.41              |
| 4:A:76:TYR:HA    | 4:A:83:TYR:HA    | 2.03                     | 0.41              |
| 4:A:113:SER:O    | 4:A:117:GLU:OE1  | 2.39                     | 0.41              |
| 4:A:272:PRO:HA   | 4:A:275:ILE:HG22 | 2.01                     | 0.41              |
| 1:L:294:LEU:HD12 | 1:L:294:LEU:HA   | 1.87                     | 0.41              |
| 1:L:378:SER:OG   | 1:L:382:ARG:HG2  | 2.21                     | 0.41              |
| 1:L:378:SER:OG   | 1:L:380:ASP:OD1  | 2.38                     | 0.41              |
| 1:L:386:PHE:HE2  | 1:L:388:ARG:HD3  | 1.86                     | 0.41              |
| 1:L:458:VAL:HG22 | 1:L:459:GLY:H    | 1.85                     | 0.41              |
| 2:K:325:LYS:HD3  | 2:K:375:PRO:HG2  | 2.02                     | 0.41              |
| 1:J:315:ARG:H    | 1:J:315:ARG:HD3  | 1.85                     | 0.41              |
| 4:A:190:VAL:HG22 | 4:A:194:PHE:CE2  | 2.55                     | 0.41              |
| 4:A:325:GLY:O    | 4:A:328:LEU:HG   | 2.20                     | 0.41              |
| 1:L:120:LYS:HE3  | 1:L:120:LYS:HB3  | 1.87                     | 0.41              |
| 1:L:170:LEU:HD11 | 1:L:194:PHE:CD1  | 2.56                     | 0.41              |
| 1:L:437:LYS:HA   | 1:L:437:LYS:HD3  | 1.69                     | 0.41              |
| 1:L:673:CYS:HB2  | 1:L:780:PHE:CZ   | 2.56                     | 0.41              |
| 2:K:582:SER:O    | 2:K:586:VAL:HG23 | 2.21                     | 0.41              |
| 2:K:659:ILE:C    | 2:K:661:PRO:HD3  | 2.46                     | 0.41              |
| 4:C:113:SER:O    | 4:C:117:GLU:OE1  | 2.39                     | 0.41              |
| 4:C:365:ILE:HA   | 4:C:365:ILE:HD12 | 1.96                     | 0.41              |
| 4:C:395:VAL:HA   | 4:C:398:ILE:HG12 | 2.03                     | 0.41              |
| 1:J:89:ILE:HD12  | 1:J:105:LEU:HD11 | 2.02                     | 0.41              |
| 1:J:186:GLY:HA2  | 1:J:244:TRP:CD2  | 2.56                     | 0.41              |
| 2:I:401:ILE:HG13 | 2:I:425:VAL:HG21 | 2.03                     | 0.41              |
| 5:E:147:MET:HE2  | 5:E:178:PHE:HD2  | 1.86                     | 0.41              |
| 4:A:61:ARG:HE    | 4:A:61:ARG:HB2   | 1.78                     | 0.41              |
| 1:L:158:VAL:HG12 | 1:L:169:SER:HA   | 2.02                     | 0.41              |
| 1:L:382:ARG:HA   | 1:L:406:SER:HB2  | 2.01                     | 0.41              |
| 2:K:430:ALA:O    | 2:K:438:ILE:HD12 | 2.21                     | 0.41              |
| 4:C:325:GLY:O    | 4:C:328:LEU:HG   | 2.20                     | 0.41              |
| 1:J:70:THR:HG22  | 1:J:73:ASP:CG    | 2.45                     | 0.41              |
| 1:J:85:GLU:O     | 1:J:87:LYS:NZ    | 2.46                     | 0.41              |
| 1:J:91:ASP:HB2   | 1:J:484:SER:HB2  | 2.01                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:195:ILE:HA   | 1:J:199:ASN:O    | 2.20                     | 0.41              |
| 1:J:339:ARG:O    | 1:J:341:GLN:HG3  | 2.21                     | 0.41              |
| 1:J:382:ARG:HH22 | 1:J:433:GLU:HB2  | 1.86                     | 0.41              |
| 1:J:390:ILE:HG13 | 1:J:392:GLN:HG2  | 2.03                     | 0.41              |
| 1:J:636:GLU:HB3  | 1:J:638:TYR:CE1  | 2.56                     | 0.41              |
| 1:J:712:HIS:CD2  | 1:J:713:ARG:HG2  | 2.56                     | 0.41              |
| 1:J:742:ILE:HD11 | 1:J:754:LEU:HD12 | 2.03                     | 0.41              |
| 2:I:102:THR:OG1  | 2:I:104:ARG:NE   | 2.53                     | 0.41              |
| 2:I:481:PHE:CD2  | 2:I:488:PHE:HB3  | 2.56                     | 0.41              |
| 4:B:9:LEU:HD22   | 4:C:474:PHE:CD1  | 2.55                     | 0.41              |
| 4:B:342:MET:HE1  | 4:B:363:TYR:HE2  | 1.85                     | 0.41              |
| 5:E:158:MET:HE1  | 5:E:166:LEU:HD13 | 2.02                     | 0.41              |
| 4:A:90:ASP:HB2   | 4:D:93:ARG:HH12  | 1.86                     | 0.41              |
| 4:A:97:ASN:HA    | 4:A:100:ARG:HH11 | 1.85                     | 0.41              |
| 4:A:199:VAL:O    | 4:A:203:VAL:HG23 | 2.20                     | 0.41              |
| 1:L:742:ILE:HD11 | 1:L:754:LEU:HD12 | 2.02                     | 0.41              |
| 2:K:102:THR:OG1  | 2:K:104:ARG:NE   | 2.53                     | 0.41              |
| 2:K:187:PRO:HB2  | 2:K:188:LYS:HZ2  | 1.86                     | 0.41              |
| 2:K:345:ILE:HG23 | 2:K:358:LYS:HG3  | 2.03                     | 0.41              |
| 2:K:574:SER:OG   | 2:K:598:CYS:O    | 2.36                     | 0.41              |
| 2:K:764:PHE:CE2  | 2:K:773:LEU:HD13 | 2.55                     | 0.41              |
| 3:H:51:ARG:HE    | 3:H:51:ARG:HB2   | 1.69                     | 0.41              |
| 3:H:87:ALA:HB2   | 3:H:157:MET:CE   | 2.50                     | 0.41              |
| 3:H:154:ILE:HG22 | 3:H:155:TYR:HD1  | 1.86                     | 0.41              |
| 4:D:91:ILE:O     | 4:D:95:ILE:HG13  | 2.20                     | 0.41              |
| 4:D:305:ARG:O    | 4:D:311:ARG:NH1  | 2.54                     | 0.41              |
| 4:D:342:MET:HE1  | 4:D:363:TYR:HE2  | 1.85                     | 0.41              |
| 5:G:193:ASP:OD1  | 5:G:193:ASP:N    | 2.54                     | 0.41              |
| 4:C:76:TYR:HA    | 4:C:83:TYR:HA    | 2.03                     | 0.41              |
| 4:C:190:VAL:HG22 | 4:C:194:PHE:CE2  | 2.55                     | 0.41              |
| 1:J:158:VAL:HG12 | 1:J:169:SER:HA   | 2.02                     | 0.41              |
| 1:J:170:LEU:HD11 | 1:J:194:PHE:CD1  | 2.56                     | 0.41              |
| 1:J:292:ILE:HG21 | 1:J:320:TYR:HA   | 2.03                     | 0.41              |
| 1:J:661:PRO:N    | 1:J:713:ARG:HH22 | 2.19                     | 0.41              |
| 2:I:250:ARG:HD3  | 2:I:296:VAL:HG11 | 2.02                     | 0.41              |
| 2:I:741:LEU:O    | 2:I:745:LEU:HG   | 2.21                     | 0.41              |
| 4:B:394:GLY:O    | 4:B:398:ILE:HG12 | 2.21                     | 0.41              |
| 4:A:87:ARG:HA    | 4:D:100:ARG:NH1  | 2.26                     | 0.41              |
| 4:A:328:LEU:HA   | 4:A:331:LEU:HG   | 2.02                     | 0.41              |
| 1:L:339:ARG:O    | 1:L:341:GLN:HG3  | 2.21                     | 0.41              |
| 1:L:703:ARG:HD2  | 1:L:703:ARG:HA   | 1.89                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:218:LYS:N    | 2:K:222:ILE:O    | 2.46                     | 0.41              |
| 2:K:324:VAL:HG12 | 2:K:334:VAL:HG13 | 2.03                     | 0.41              |
| 3:H:55:VAL:HG23  | 4:C:55:TRP:HZ3   | 1.85                     | 0.41              |
| 3:H:154:ILE:HD13 | 3:H:154:ILE:HA   | 1.91                     | 0.41              |
| 4:D:73:ASP:HA    | 4:D:76:TYR:HB2   | 2.01                     | 0.41              |
| 1:J:294:LEU:HD12 | 1:J:294:LEU:HA   | 1.87                     | 0.40              |
| 1:J:400:HIS:ND1  | 1:J:419:THR:OG1  | 2.36                     | 0.40              |
| 2:I:430:ALA:O    | 2:I:438:ILE:HD12 | 2.21                     | 0.40              |
| 2:I:562:LEU:HD13 | 2:I:639:ILE:HD11 | 2.03                     | 0.40              |
| 3:F:119:LEU:O    | 3:F:213:GLN:HA   | 2.20                     | 0.40              |
| 4:A:43:ILE:HD13  | 4:A:56:GLN:NE2   | 2.36                     | 0.40              |
| 4:A:147:ARG:HG3  | 4:A:422:ARG:NH1  | 2.36                     | 0.40              |
| 4:A:423:ARG:HA   | 4:A:426:LYS:HG2  | 2.02                     | 0.40              |
| 1:L:88:TRP:CG    | 1:L:482:SER:HA   | 2.56                     | 0.40              |
| 1:L:89:ILE:HD12  | 1:L:105:LEU:HD11 | 2.02                     | 0.40              |
| 1:L:186:GLY:HA2  | 1:L:244:TRP:CD2  | 2.56                     | 0.40              |
| 1:L:282:TYR:CE1  | 1:L:284:LYS:HD3  | 2.57                     | 0.40              |
| 1:L:379:LYS:HA   | 1:L:379:LYS:HD3  | 1.89                     | 0.40              |
| 1:L:440:PHE:CE2  | 1:L:453:TYR:HB2  | 2.55                     | 0.40              |
| 1:L:712:HIS:CD2  | 1:L:713:ARG:HG2  | 2.56                     | 0.40              |
| 2:K:106:TRP:CE3  | 2:K:113:SER:HB3  | 2.56                     | 0.40              |
| 2:K:198:ASN:HB3  | 2:K:217:GLY:HA3  | 2.03                     | 0.40              |
| 2:K:401:ILE:HG13 | 2:K:425:VAL:HG21 | 2.03                     | 0.40              |
| 2:K:783:GLU:HA   | 2:K:786:ARG:HD2  | 2.02                     | 0.40              |
| 4:C:427:LYS:HD3  | 4:C:427:LYS:HA   | 1.87                     | 0.40              |
| 1:J:97:ARG:HA    | 1:J:103:VAL:HG13 | 2.03                     | 0.40              |
| 1:J:450:ARG:HB2  | 1:J:476:TYR:HD1  | 1.86                     | 0.40              |
| 1:J:458:VAL:HG22 | 1:J:459:GLY:H    | 1.85                     | 0.40              |
| 1:J:618:LEU:HB3  | 1:J:651:TYR:OH   | 2.21                     | 0.40              |
| 2:I:88:TRP:CH2   | 2:I:108:VAL:HG21 | 2.57                     | 0.40              |
| 2:I:250:ARG:NE   | 2:I:352:THR:HG22 | 2.36                     | 0.40              |
| 2:I:757:TYR:CE2  | 2:I:773:LEU:HD12 | 2.56                     | 0.40              |
| 3:F:168:GLU:C    | 3:F:171:PRO:HD2  | 2.46                     | 0.40              |
| 4:B:305:ARG:O    | 4:B:311:ARG:NH1  | 2.54                     | 0.40              |
| 4:B:356:SER:HB2  | 4:B:358:PRO:HD2  | 2.03                     | 0.40              |
| 4:A:155:ASP:H    | 4:A:423:ARG:HH22 | 1.69                     | 0.40              |
| 1:L:70:THR:HA    | 1:L:586:VAL:HG13 | 2.03                     | 0.40              |
| 1:L:382:ARG:HH22 | 1:L:433:GLU:HB2  | 1.86                     | 0.40              |
| 1:L:625:ASP:O    | 1:L:628:GLU:HG3  | 2.22                     | 0.40              |
| 2:K:180:LEU:HD21 | 2:K:194:PHE:HB2  | 2.03                     | 0.40              |
| 2:K:516:THR:OG1  | 2:K:518:GLU:OE2  | 2.31                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:730:ASP:OD1  | 2:K:762:HIS:HB2  | 2.20                     | 0.40              |
| 2:K:752:TYR:HE2  | 2:K:754:LEU:HB2  | 1.86                     | 0.40              |
| 3:H:168:GLU:C    | 3:H:171:PRO:HD2  | 2.46                     | 0.40              |
| 4:D:205:GLU:O    | 4:D:211:SER:HB2  | 2.21                     | 0.40              |
| 4:D:327:LEU:HG   | 4:D:331:LEU:HD23 | 2.02                     | 0.40              |
| 4:C:56:GLN:HG3   | 4:C:60:GLU:OE1   | 2.21                     | 0.40              |
| 1:J:120:LYS:HE3  | 1:J:120:LYS:HB3  | 1.87                     | 0.40              |
| 1:J:691:SER:HB3  | 1:J:705:TYR:HE2  | 1.86                     | 0.40              |
| 2:I:345:ILE:HG23 | 2:I:358:LYS:HG3  | 2.03                     | 0.40              |
| 2:I:730:ASP:OD1  | 2:I:762:HIS:HB2  | 2.20                     | 0.40              |
| 2:I:740:GLU:O    | 2:I:743:THR:OG1  | 2.27                     | 0.40              |
| 4:B:100:ARG:HD3  | 4:C:87:ARG:NH1   | 2.36                     | 0.40              |
| 4:A:87:ARG:NH1   | 4:D:100:ARG:HD3  | 2.36                     | 0.40              |
| 1:L:292:ILE:HG21 | 1:L:320:TYR:HA   | 2.03                     | 0.40              |
| 1:L:316:MET:HB3  | 1:L:338:ASN:HB3  | 2.03                     | 0.40              |
| 1:L:564:LEU:HD12 | 1:L:630:VAL:CG1  | 2.52                     | 0.40              |
| 2:K:437:LYS:NZ   | 2:K:464:GLN:OE1  | 2.41                     | 0.40              |
| 2:K:646:VAL:HB   | 2:K:671:PHE:CE2  | 2.56                     | 0.40              |
| 4:D:49:GLY:HA2   | 4:C:53:GLN:H     | 1.86                     | 0.40              |
| 4:D:475:GLU:HB2  | 4:D:479:HIS:HE1  | 1.87                     | 0.40              |
| 1:J:69:VAL:HG12  | 1:J:586:VAL:HG22 | 2.04                     | 0.40              |
| 1:J:70:THR:HA    | 1:J:586:VAL:HG13 | 2.03                     | 0.40              |
| 1:J:368:LEU:HB3  | 1:J:371:GLN:OE1  | 2.22                     | 0.40              |
| 1:J:390:ILE:HD11 | 1:J:400:HIS:CD2  | 2.57                     | 0.40              |
| 2:I:324:VAL:HG12 | 2:I:334:VAL:HG13 | 2.03                     | 0.40              |
| 2:I:646:VAL:HB   | 2:I:671:PHE:CE2  | 2.57                     | 0.40              |
| 2:I:659:ILE:C    | 2:I:661:PRO:HD3  | 2.46                     | 0.40              |
| 3:F:154:ILE:HG22 | 3:F:155:TYR:HD1  | 1.86                     | 0.40              |
| 4:A:254:ARG:O    | 4:A:258:VAL:HG23 | 2.22                     | 0.40              |
| 1:L:97:ARG:HA    | 1:L:103:VAL:HG13 | 2.03                     | 0.40              |
| 1:L:229:TRP:O    | 1:L:233:GLU:HB2  | 2.21                     | 0.40              |
| 1:L:250:ARG:HE   | 1:L:352:THR:HG22 | 1.86                     | 0.40              |
| 1:L:618:LEU:HB3  | 1:L:651:TYR:OH   | 2.21                     | 0.40              |
| 2:K:125:LEU:HD23 | 2:K:143:TYR:CE2  | 2.57                     | 0.40              |
| 2:K:315:ARG:H    | 2:K:315:ARG:HG2  | 1.78                     | 0.40              |
| 3:H:186:LYS:HD2  | 3:H:186:LYS:HA   | 1.90                     | 0.40              |
| 4:D:308:GLN:O    | 4:D:308:GLN:NE2  | 2.54                     | 0.40              |
| 4:C:43:ILE:HD13  | 4:C:56:GLN:NE2   | 2.36                     | 0.40              |
| 4:C:368:MET:HE2  | 4:C:368:MET:HB2  | 1.97                     | 0.40              |
| 4:C:419:ALA:HA   | 4:C:422:ARG:HG2  | 2.02                     | 0.40              |
| 1:J:451:GLN:HB2  | 1:J:453:TYR:CZ   | 2.55                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:582:SER:O    | 2:I:586:VAL:HG23 | 2.21                     | 0.40              |
| 2:I:778:ILE:HG13 | 2:I:779:ASN:N    | 2.36                     | 0.40              |
| 5:E:52:GLU:HG3   | 4:D:38:THR:HG23  | 2.02                     | 0.40              |
| 1:L:193:ILE:HG21 | 1:L:251:LEU:HD11 | 2.03                     | 0.40              |
| 1:L:661:PRO:N    | 1:L:713:ARG:HH22 | 2.19                     | 0.40              |
| 2:K:88:TRP:CH2   | 2:K:108:VAL:HG21 | 2.57                     | 0.40              |
| 2:K:369:HIS:CE1  | 2:K:370:ARG:HG3  | 2.57                     | 0.40              |
| 4:D:108:ARG:HD2  | 4:C:108:ARG:NH2  | 2.36                     | 0.40              |
| 4:D:237:VAL:HG11 | 4:D:273:TYR:HD2  | 1.87                     | 0.40              |
| 4:D:444:TYR:CD1  | 4:D:482:LEU:HD13 | 2.57                     | 0.40              |
| 4:C:12:ALA:O     | 4:C:15:ALA:HB3   | 2.21                     | 0.40              |
| 4:C:20:MET:N     | 4:C:21:PRO:HD2   | 2.37                     | 0.40              |
| 4:C:335:ILE:HG22 | 4:C:368:MET:CE   | 2.52                     | 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   | J     | 752/757 (99%)  | 694 (92%) | 58 (8%) | 0        | 100         | 100 |
| 1   | L     | 752/757 (99%)  | 693 (92%) | 59 (8%) | 0        | 100         | 100 |
| 2   | I     | 758/760 (100%) | 688 (91%) | 70 (9%) | 0        | 100         | 100 |
| 2   | K     | 758/760 (100%) | 688 (91%) | 70 (9%) | 0        | 100         | 100 |
| 3   | F     | 172/180 (96%)  | 168 (98%) | 3 (2%)  | 1 (1%)   | 21          | 58  |
| 3   | H     | 172/180 (96%)  | 168 (98%) | 3 (2%)  | 1 (1%)   | 21          | 58  |
| 4   | A     | 452/494 (92%)  | 424 (94%) | 28 (6%) | 0        | 100         | 100 |
| 4   | B     | 451/494 (91%)  | 430 (95%) | 20 (4%) | 1 (0%)   | 43          | 77  |
| 4   | C     | 452/494 (92%)  | 423 (94%) | 29 (6%) | 0        | 100         | 100 |
| 4   | D     | 451/494 (91%)  | 430 (95%) | 20 (4%) | 1 (0%)   | 43          | 77  |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 5   | E     | 173/181 (96%)   | 163 (94%)  | 10 (6%)  | 0        | 100         | 100 |
| 5   | G     | 173/181 (96%)   | 163 (94%)  | 10 (6%)  | 0        | 100         | 100 |
| All | All   | 5516/5732 (96%) | 5132 (93%) | 380 (7%) | 4 (0%)   | 49          | 83  |

All (4) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | F     | 165 | VAL  |
| 4   | B     | 28  | PRO  |
| 3   | H     | 165 | VAL  |
| 4   | D     | 28  | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 1   | J     | 671/672 (100%)  | 671 (100%)  | 0        | 100         | 100 |
| 1   | L     | 671/672 (100%)  | 671 (100%)  | 0        | 100         | 100 |
| 2   | I     | 672/672 (100%)  | 672 (100%)  | 0        | 100         | 100 |
| 2   | K     | 672/672 (100%)  | 672 (100%)  | 0        | 100         | 100 |
| 3   | F     | 161/164 (98%)   | 161 (100%)  | 0        | 100         | 100 |
| 3   | H     | 161/164 (98%)   | 161 (100%)  | 0        | 100         | 100 |
| 4   | A     | 391/419 (93%)   | 391 (100%)  | 0        | 100         | 100 |
| 4   | B     | 390/419 (93%)   | 390 (100%)  | 0        | 100         | 100 |
| 4   | C     | 391/419 (93%)   | 391 (100%)  | 0        | 100         | 100 |
| 4   | D     | 390/419 (93%)   | 390 (100%)  | 0        | 100         | 100 |
| 5   | E     | 162/165 (98%)   | 162 (100%)  | 0        | 100         | 100 |
| 5   | G     | 162/165 (98%)   | 162 (100%)  | 0        | 100         | 100 |
| All | All   | 4894/5022 (98%) | 4894 (100%) | 0        | 100         | 100 |

There are no protein residues with a non-rotameric sidechain to report.



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 61  | ASN  |
| 1   | J     | 164 | HIS  |
| 1   | J     | 177 | ASN  |
| 1   | J     | 190 | GLN  |
| 1   | J     | 209 | GLN  |
| 2   | I     | 150 | GLN  |
| 2   | I     | 190 | GLN  |
| 2   | I     | 191 | GLN  |
| 2   | I     | 755 | GLN  |
| 3   | F     | 54  | GLN  |
| 3   | F     | 132 | ASN  |
| 3   | F     | 210 | GLN  |
| 3   | F     | 213 | GLN  |
| 4   | B     | 144 | ASN  |
| 4   | B     | 169 | GLN  |
| 4   | B     | 477 | GLN  |
| 5   | E     | 132 | ASN  |
| 5   | E     | 174 | HIS  |
| 5   | E     | 180 | GLN  |
| 1   | L     | 61  | ASN  |
| 1   | L     | 164 | HIS  |
| 1   | L     | 177 | ASN  |
| 1   | L     | 190 | GLN  |
| 1   | L     | 209 | GLN  |
| 2   | K     | 150 | GLN  |
| 2   | K     | 190 | GLN  |
| 2   | K     | 191 | GLN  |
| 2   | K     | 242 | HIS  |
| 2   | K     | 559 | HIS  |
| 2   | K     | 755 | GLN  |
| 3   | H     | 132 | ASN  |
| 3   | H     | 210 | GLN  |
| 4   | D     | 144 | ASN  |
| 4   | D     | 169 | GLN  |
| 4   | D     | 477 | GLN  |
| 5   | G     | 80  | GLN  |
| 5   | G     | 132 | ASN  |
| 5   | G     | 180 | GLN  |

### 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](#)

There are no ligands in this entry.

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

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

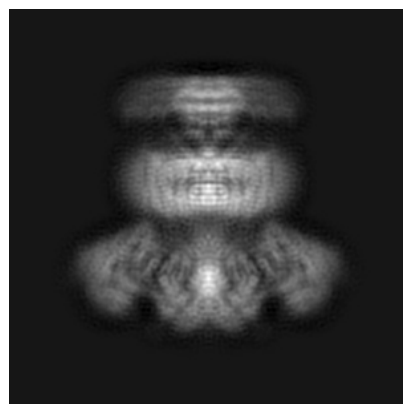
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31019. These allow visual inspection of the internal detail of the map and identification of artifacts.

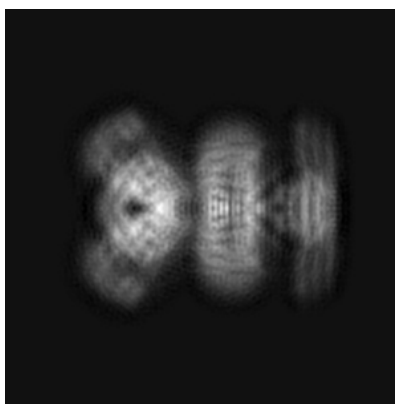
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

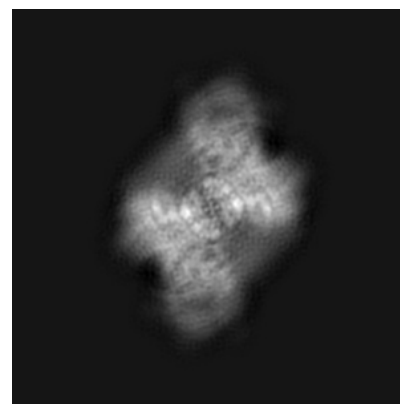
#### 6.1.1 Primary map



X

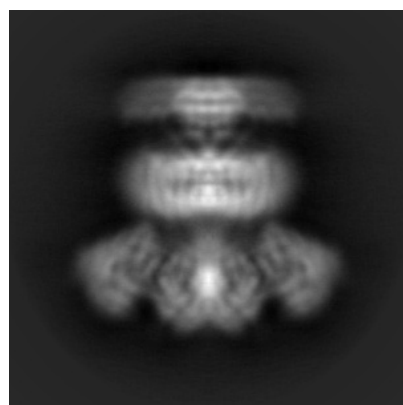


Y

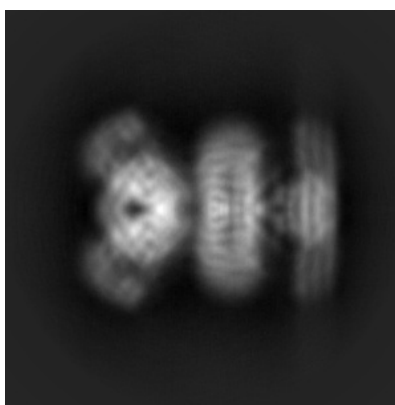


Z

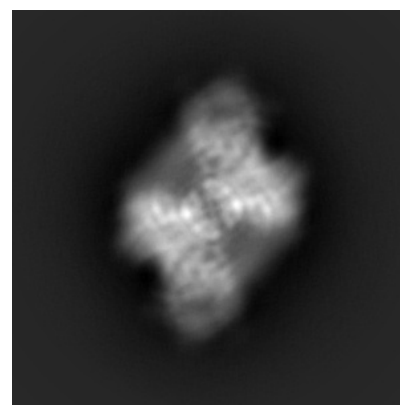
#### 6.1.2 Raw map



X



Y

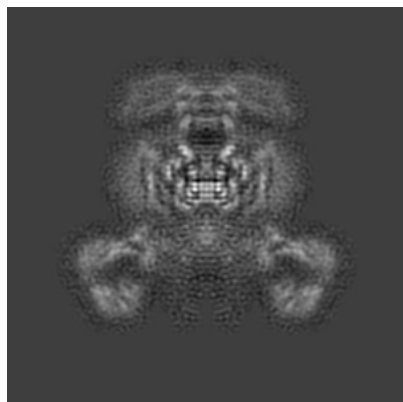


Z

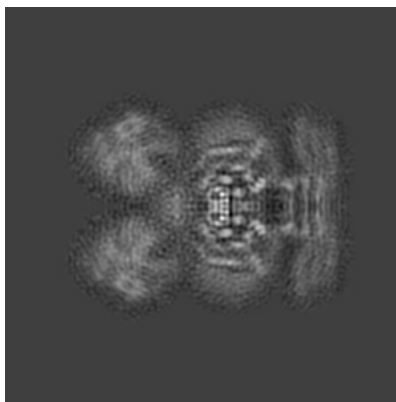
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

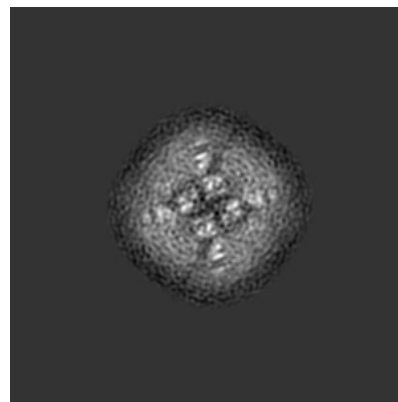
### 6.2.1 Primary map



X Index: 149

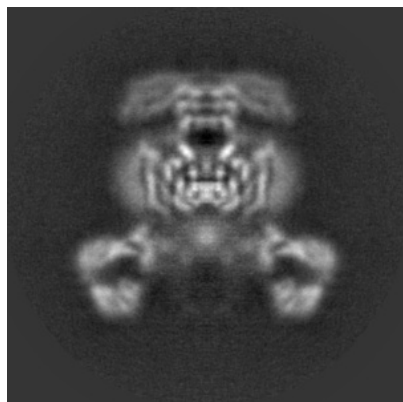


Y Index: 149

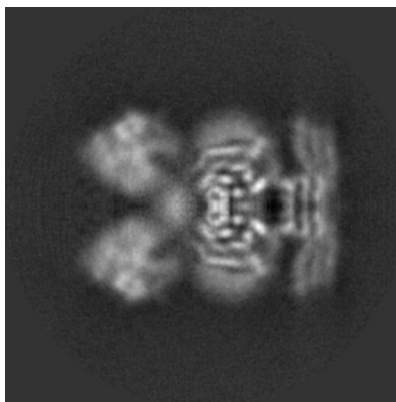


Z Index: 149

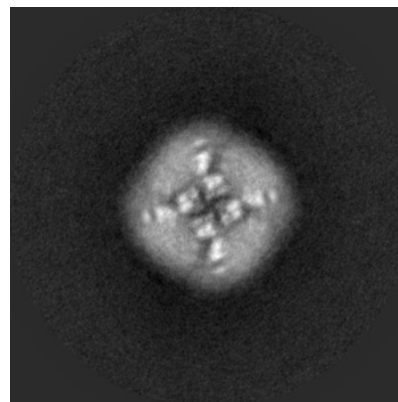
### 6.2.2 Raw map



X Index: 149



Y Index: 149

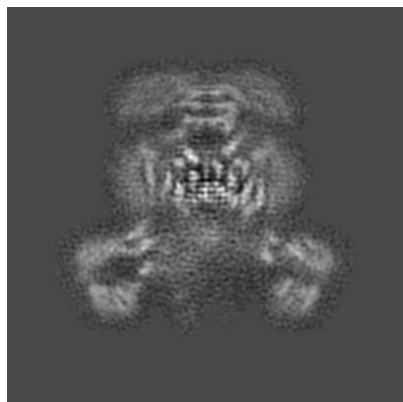


Z Index: 149

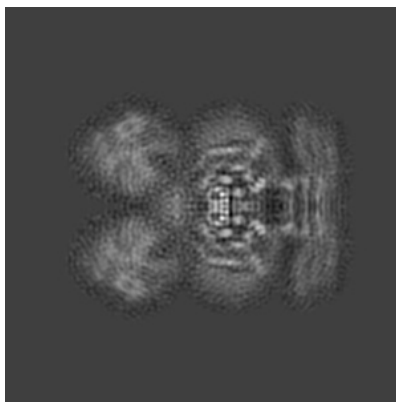
The images above show central slices of the map in three orthogonal directions.

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

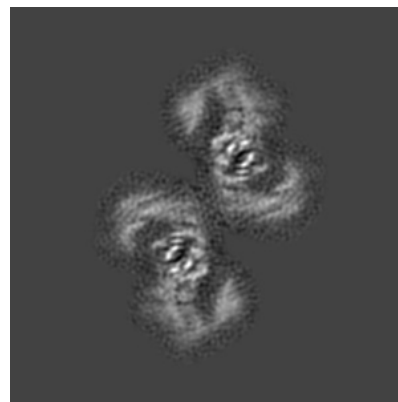
### 6.3.1 Primary map



X Index: 146

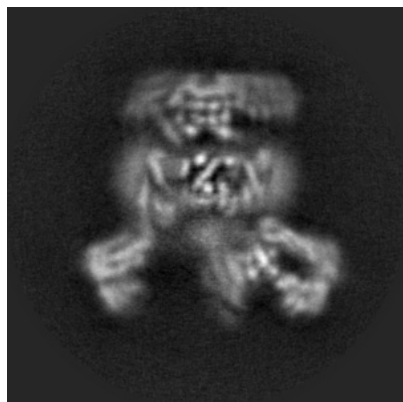


Y Index: 149

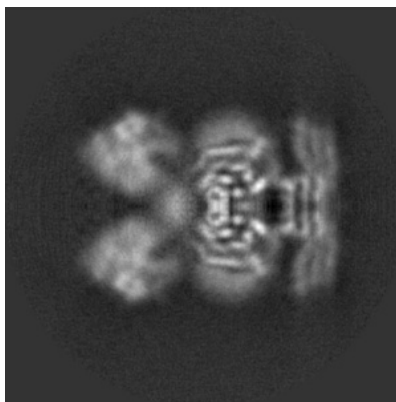


Z Index: 100

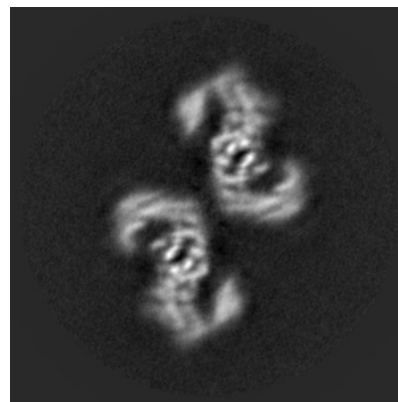
### 6.3.2 Raw map



X Index: 158



Y Index: 149

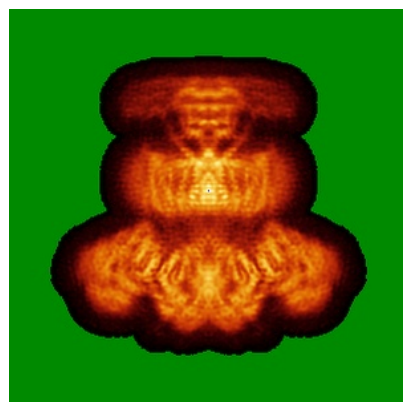


Z Index: 100

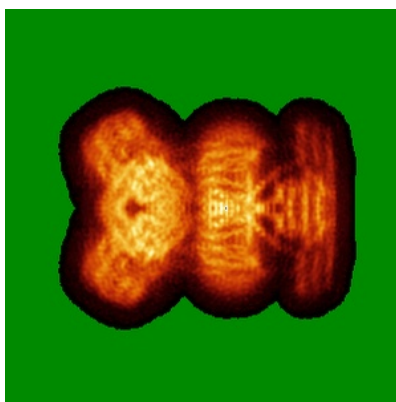
The images above show the largest variance slices of the map in three orthogonal directions.

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

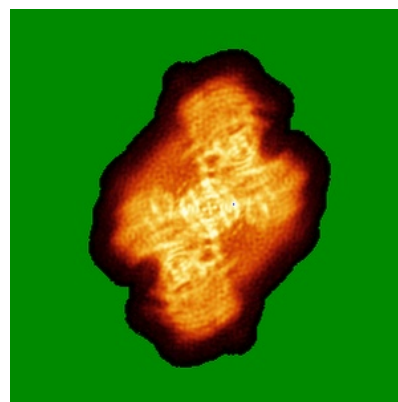
### 6.4.1 Primary map



X



Y

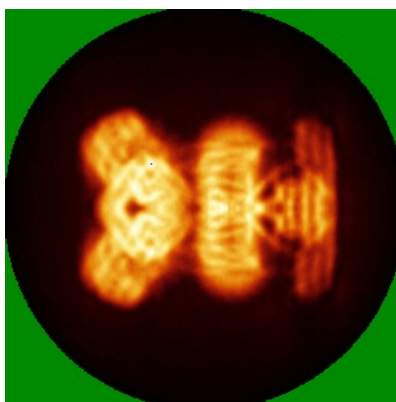


Z

### 6.4.2 Raw map



X



Y

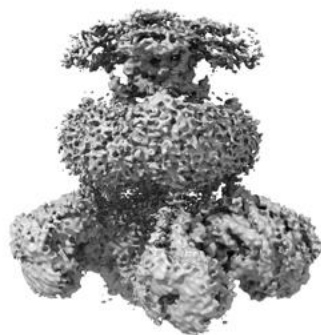


Z

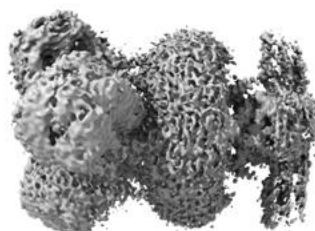
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0072. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

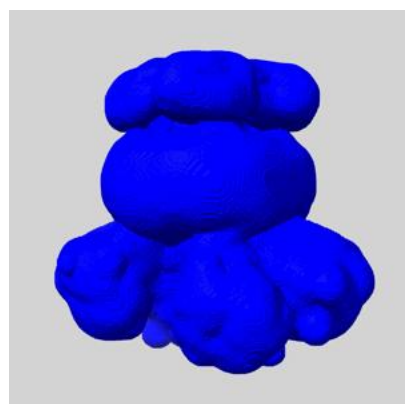
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

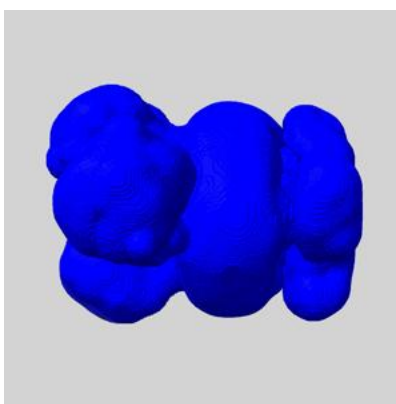
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

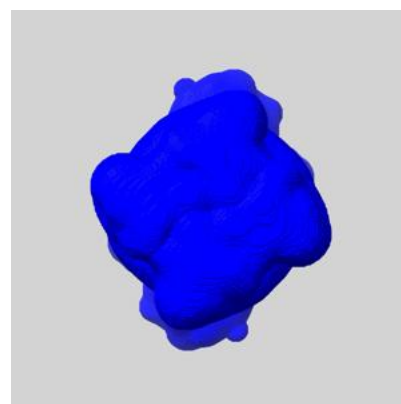
### 6.6.1 emd\_31019\_msk\_1.map [i](#)



X



Y



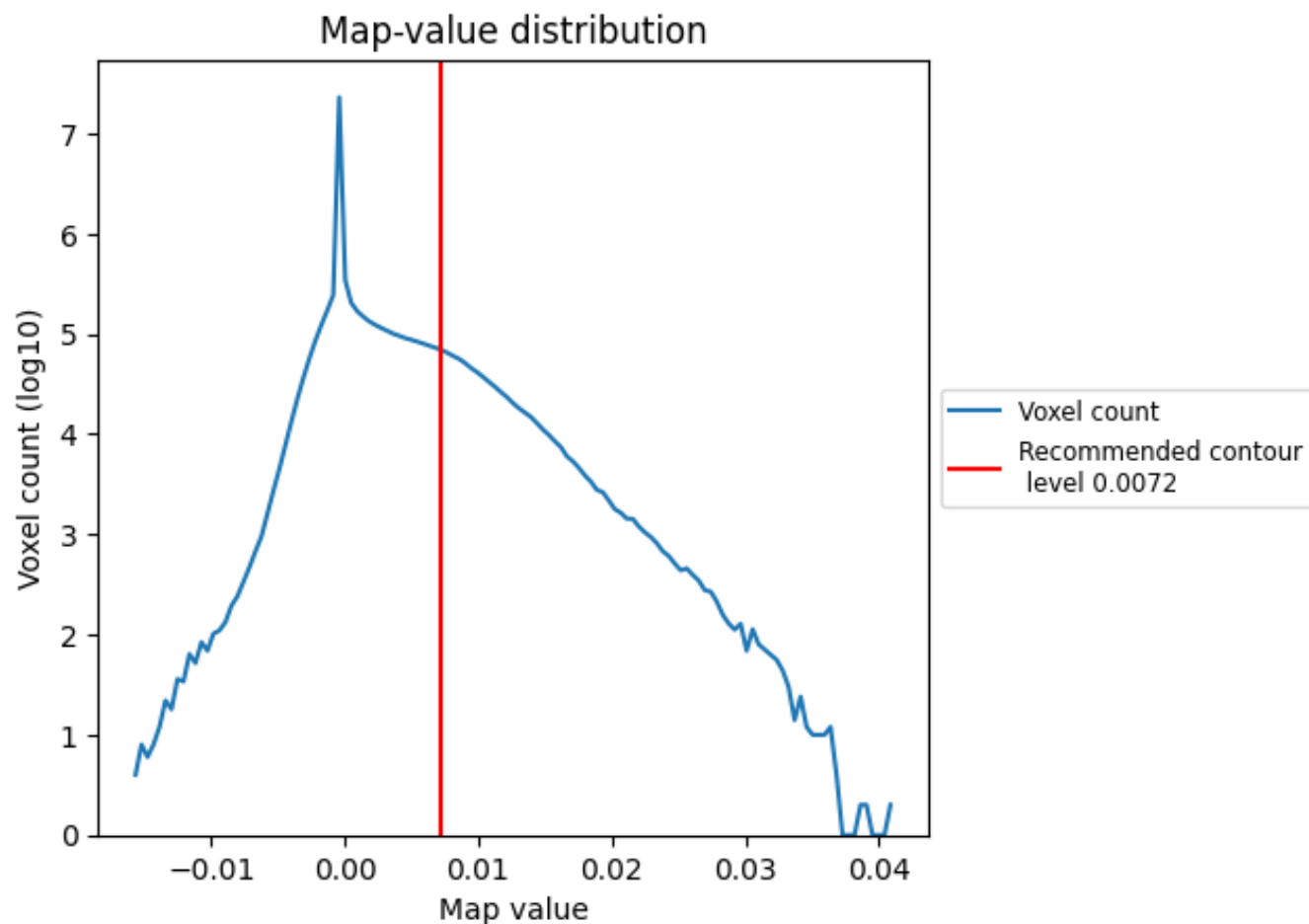
Z



## 7 Map analysis [i](#)

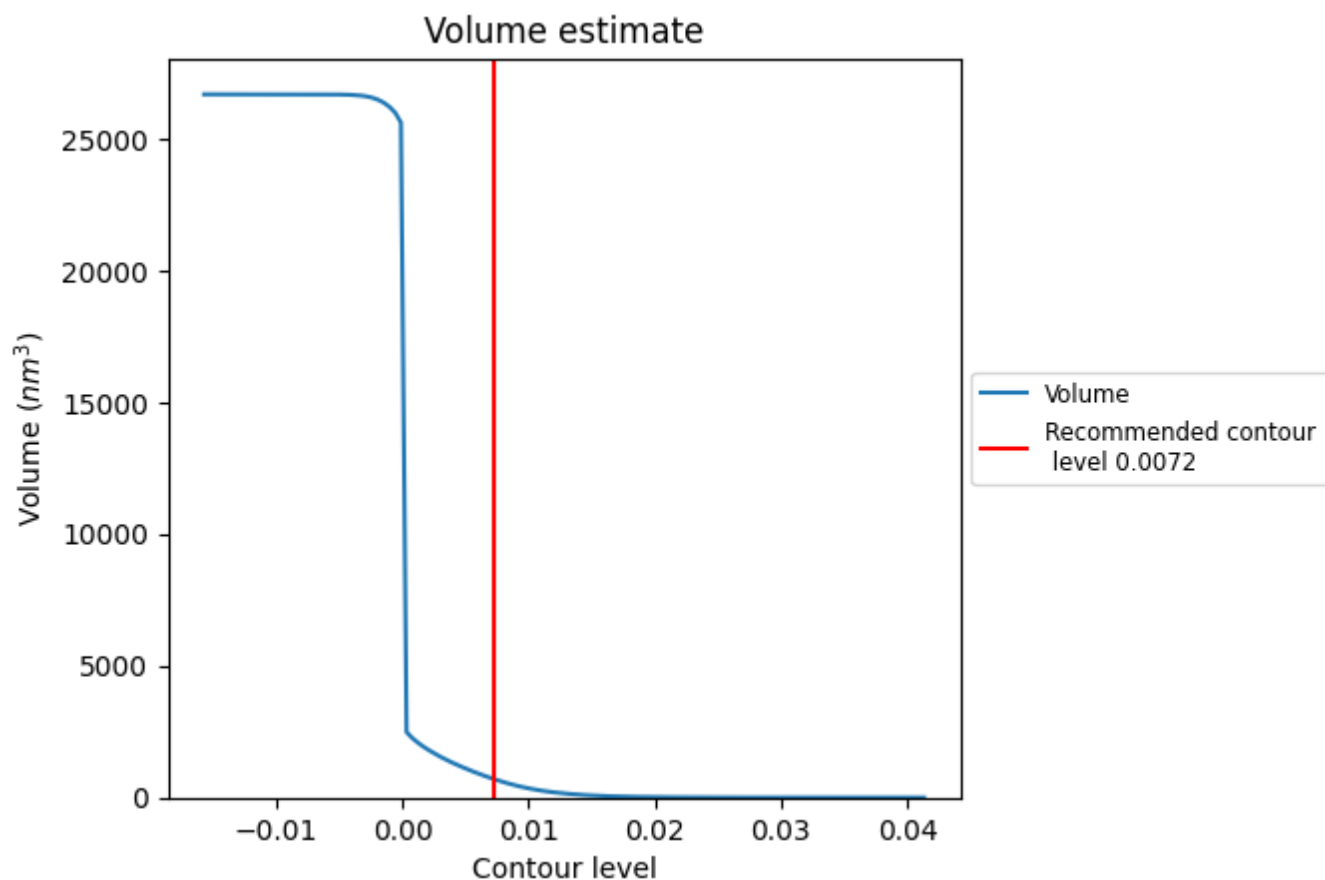
This section contains the results of statistical analysis of the map.

### 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.

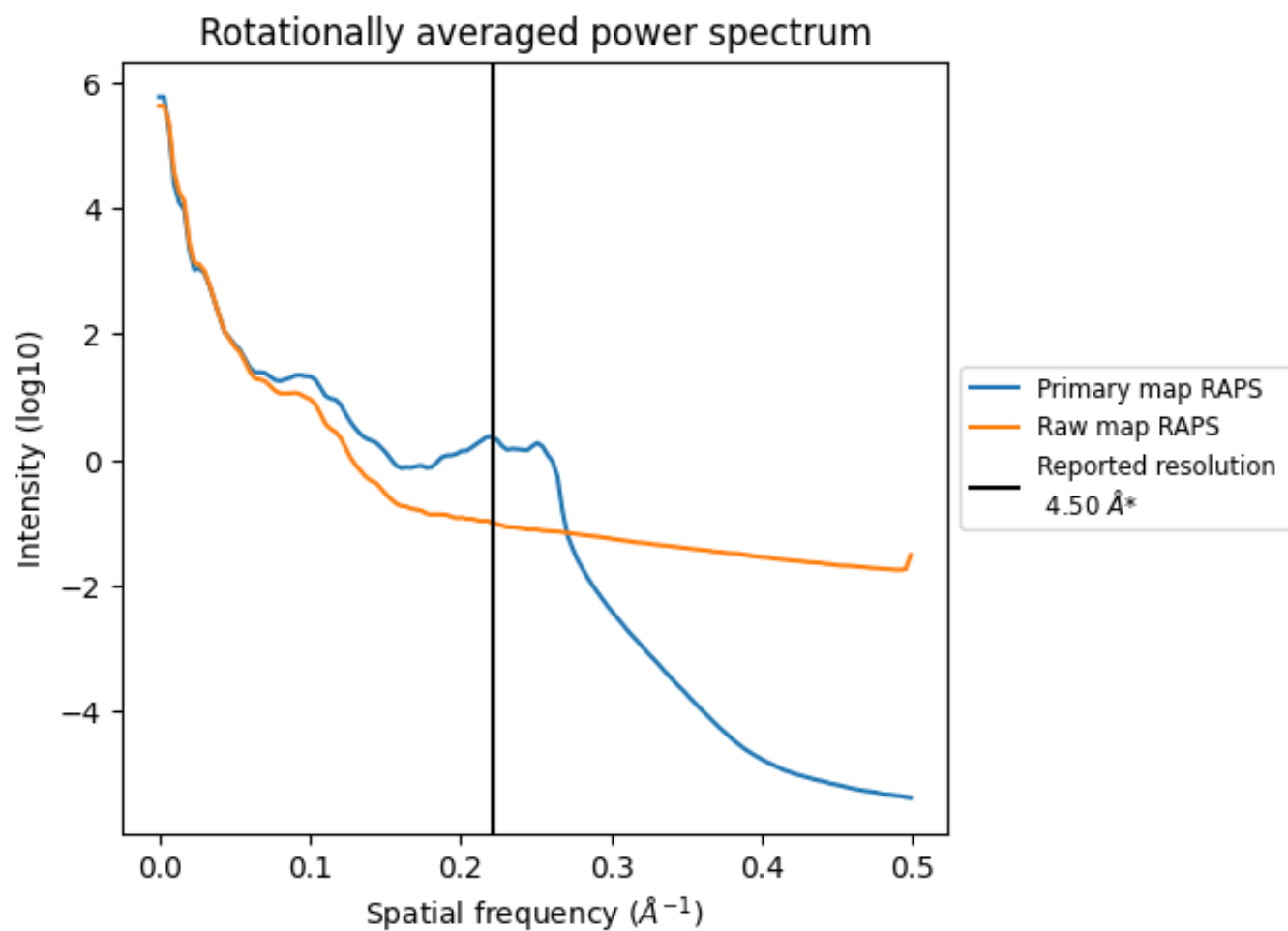
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 713 nm<sup>3</sup>; this corresponds to an approximate mass of 644 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 ⓘ

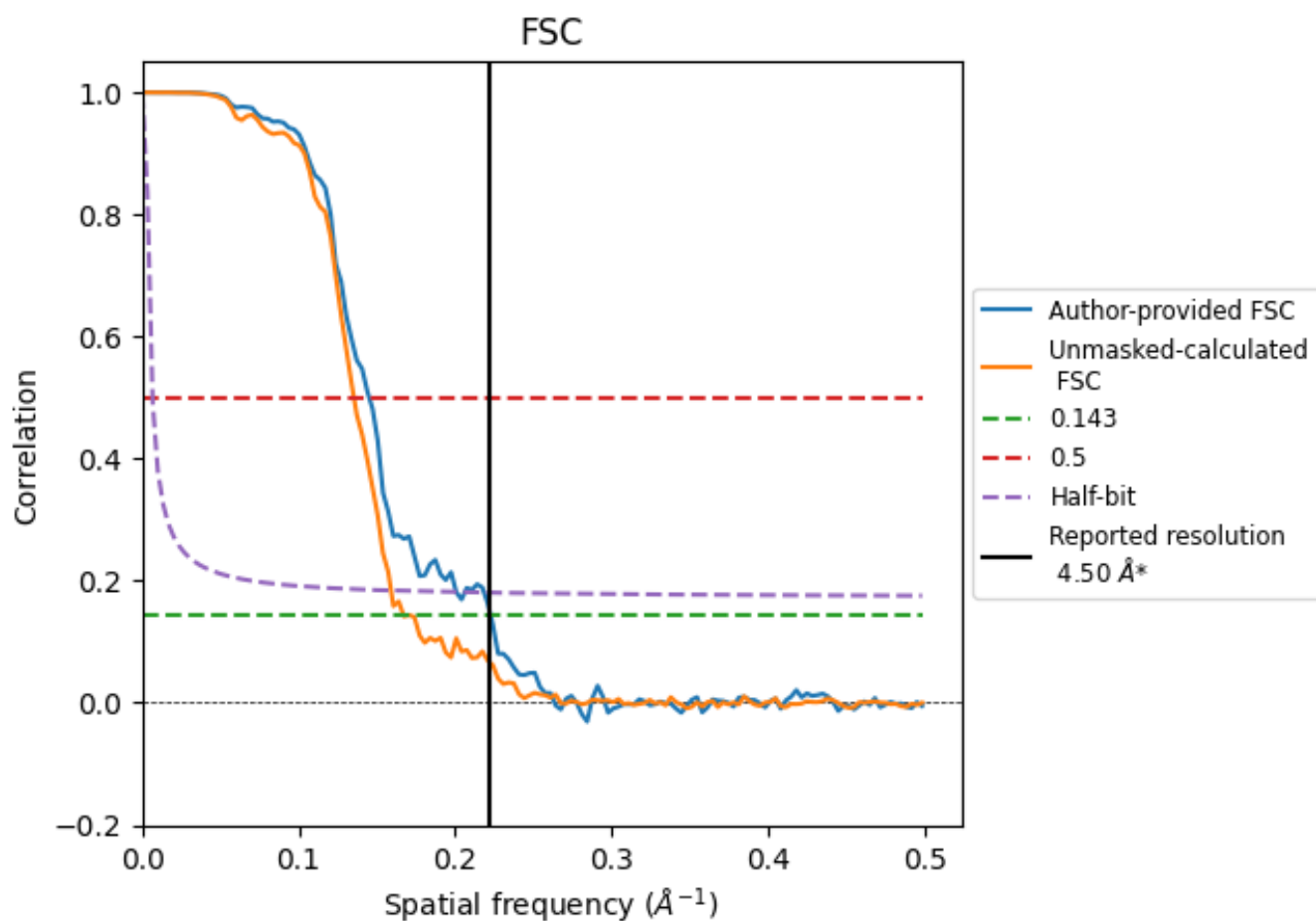


\*Reported resolution corresponds to spatial frequency of 0.222  $\text{\AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.222 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 4.50                               | -    | -        |
| Author-provided FSC curve | 4.49                               | 6.89 | 4.98     |
| Unmasked-calculated*      | 5.98                               | 7.39 | 6.29     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.98 differs from the reported value 4.5 by more than 10 %

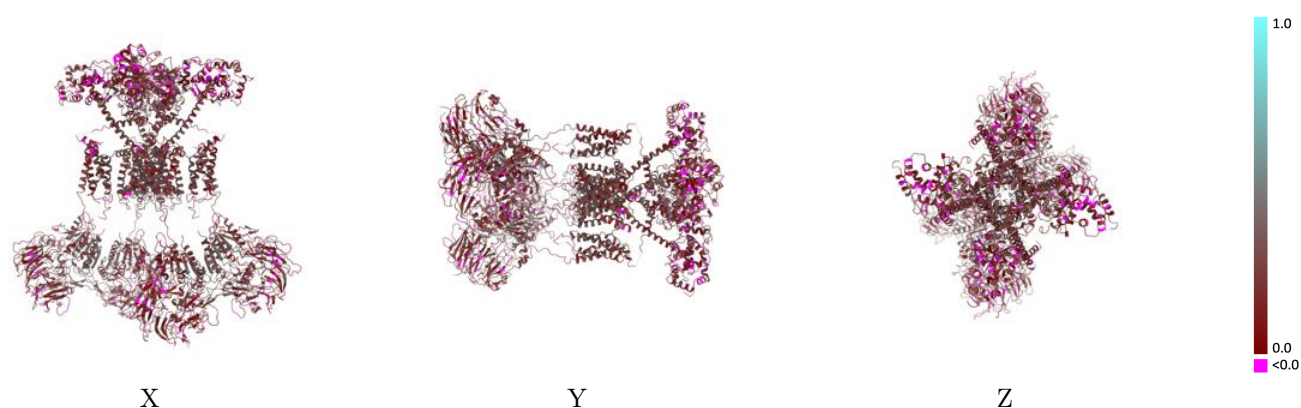
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31019 and PDB model 7E8H. Per-residue inclusion information can be found in section 3 on page 6.

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

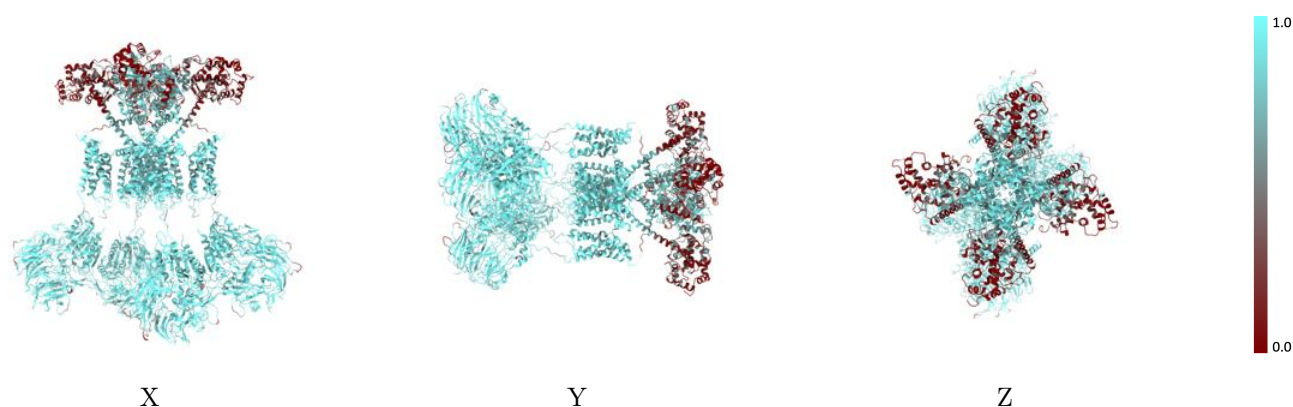
This section was not generated.

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



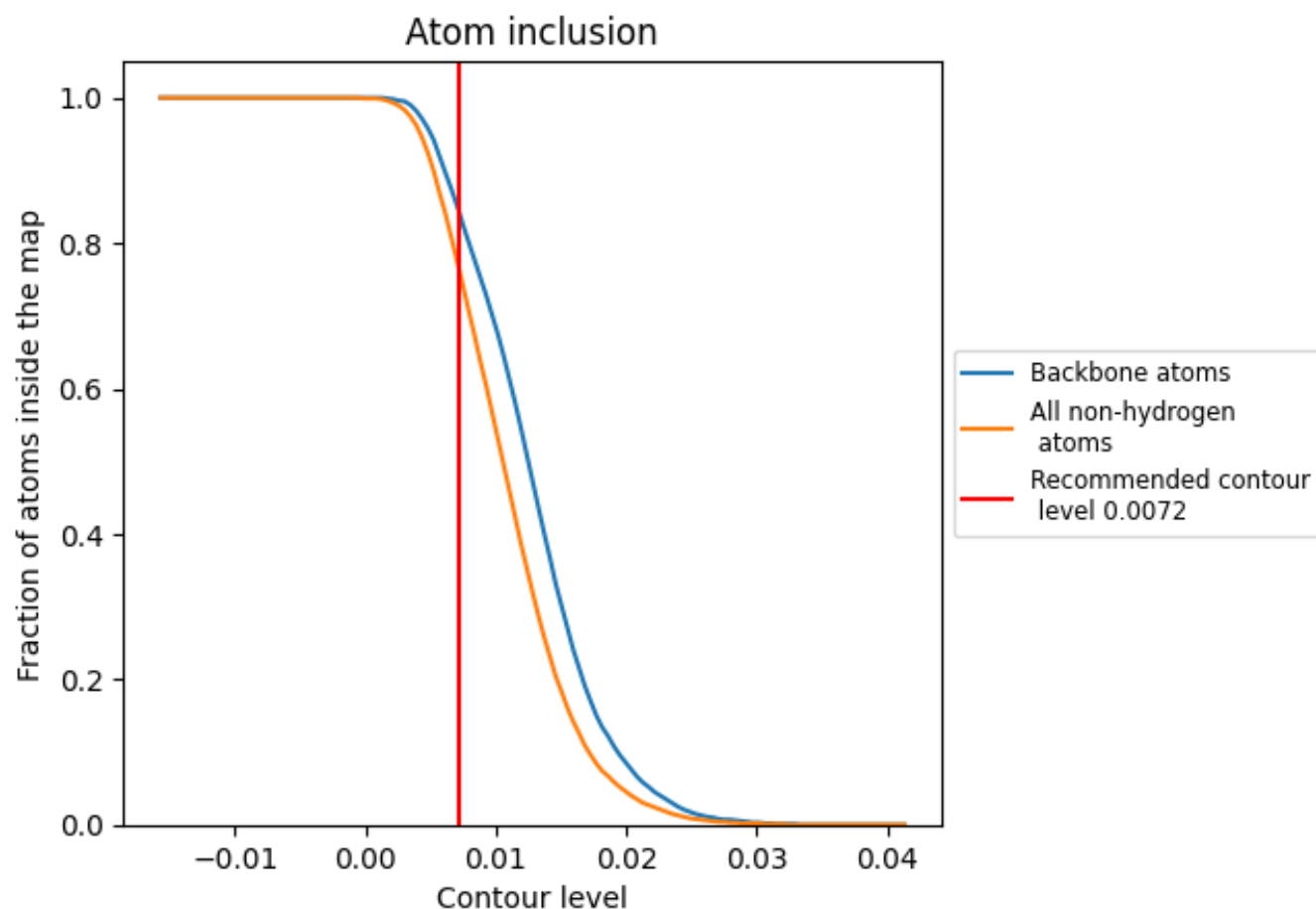
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0072).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 76% 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 (0.0072) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.7640 | <div></div> 0.2320 |
| A     | <div></div> 0.7460 | <div></div> 0.2490 |
| B     | <div></div> 0.7370 | <div></div> 0.2530 |
| C     | <div></div> 0.7460 | <div></div> 0.2500 |
| D     | <div></div> 0.7370 | <div></div> 0.2530 |
| E     | <div></div> 0.1990 | <div></div> 0.1450 |
| F     | <div></div> 0.2880 | <div></div> 0.1540 |
| G     | <div></div> 0.1960 | <div></div> 0.1450 |
| H     | <div></div> 0.2880 | <div></div> 0.1530 |
| I     | <div></div> 0.9120 | <div></div> 0.2500 |
| J     | <div></div> 0.8930 | <div></div> 0.2300 |
| K     | <div></div> 0.9120 | <div></div> 0.2530 |
| L     | <div></div> 0.8930 | <div></div> 0.2300 |

1.0

0.0

<0.0