



## Full wwPDB EM Validation Report ⓘ

Jan 21, 2025 – 07:16 pm GMT

PDB ID : 8PKP  
EMDB ID : EMD-17751  
Title : Cryo-EM structure of the apo Anaphase-promoting complex/cyclosome (APC/C) at 3.2 Angstrom resolution  
Authors : Hoefler, A.; Yu, J.; Chang, L.; Zhang, Z.; Yang, J.; Boland, A.; Barford, D.  
Deposited on : 2023-06-27  
Resolution : 3.20 Å(reported)  
Based on initial model : 5G05

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.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

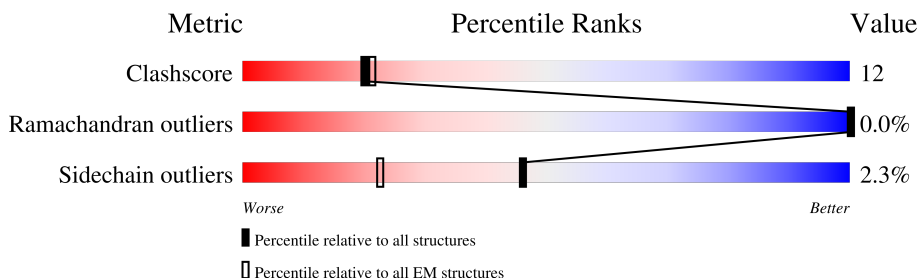
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 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) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 210492                      | 15764                       |
| Ramachandran outliers | 207382                      | 16835                       |
| Sidechain outliers    | 206894                      | 16415                       |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 1944   |                  |
| 2   | D     | 121    |                  |
| 3   | G     | 85     |                  |
| 3   | W     | 85     |                  |
| 4   | H     | 110    |                  |
| 5   | J     | 824    |                  |
| 5   | P     | 824    |                  |
| 6   | K     | 620    |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 6   | Q     | 620    |  |
| 7   | L     | 185    |  |
| 8   | M     | 74     |  |
| 9   | O     | 755    |  |
| 10  | U     | 597    |  |
| 10  | V     | 597    |  |
| 11  | Y     | 565    |  |
| 11  | Z     | 565    |  |
| 12  | I     | 814    |  |
| 13  | N     | 822    |  |
| 14  | C     | 84     |  |

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 63749 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 Anaphase-promoting complex subunit 1.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1   | A     | 1580     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 12284 | 7873 | 2074 | 2251 | 86 |         |       |

- Molecule 2 is a protein called Anaphase-promoting complex subunit 15.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 2   | D     | 56       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 458   | 291 | 77 | 89 | 1 |         |       |

- Molecule 3 is a protein called Anaphase-promoting complex subunit CDC26.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 3   | G     | 27       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 226   | 142 | 42 | 41 | 1 |         |       |
| 3   | W     | 25       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 217   | 136 | 41 | 39 | 1 |         |       |

- Molecule 4 is a protein called Anaphase-promoting complex subunit 16.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 4   | H     | 57       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 459   | 296 | 75 | 86 | 2 |         |       |

- Molecule 5 is a protein called Cell division cycle protein 27 homolog.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | J     | 476      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 3601  | 2300 | 615 | 662 | 24 |         |       |
| 5   | P     | 484      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3883  | 2497 | 653 | 707 | 26 |         |       |

- Molecule 6 is a protein called Cell division cycle protein 16 homolog.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6   | K     | 512      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4134  | 2657 | 697 | 755 | 25 |         |       |
| 6   | Q     | 504      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4049  | 2603 | 681 | 741 | 24 |         |       |

- Molecule 7 is a protein called Anaphase-promoting complex subunit 10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | L     | 179      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1446  | 906 | 263 | 270 | 7 |         |       |

- Molecule 8 is a protein called Anaphase-promoting complex subunit 13.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 8   | M     | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 478   | 301 | 78 | 97 | 2 |         |       |

- Molecule 9 is a protein called Anaphase-promoting complex subunit 5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9   | O     | 683      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5404  | 3444 | 941 | 993 | 26 |         |       |

- Molecule 10 is a protein called Cell division cycle protein 23 homolog.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 10  | U     | 503      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4121  | 2655 | 690 | 751 | 25 |         |       |
| 10  | V     | 534      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4393  | 2826 | 740 | 802 | 25 |         |       |

- Molecule 11 is a protein called Anaphase-promoting complex subunit 7.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 11  | Y     | 499      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 3907  | 2471 | 681 | 728 | 27 |         |       |
| 11  | Z     | 486      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 3807  | 2413 | 664 | 705 | 25 |         |       |

- Molecule 12 is a protein called Anaphase-promoting complex subunit 4.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 12  | I     | 718      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5705  | 3656 | 945 | 1070 | 34 |         |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| I     | 809     | GLU      | -      | expression tag | UNP Q9UJX5 |
| I     | 810     | ASN      | -      | expression tag | UNP Q9UJX5 |
| I     | 811     | LEU      | -      | expression tag | UNP Q9UJX5 |
| I     | 812     | TYR      | -      | expression tag | UNP Q9UJX5 |
| I     | 813     | PHE      | -      | expression tag | UNP Q9UJX5 |
| I     | 814     | GLN      | -      | expression tag | UNP Q9UJX5 |

- Molecule 13 is a protein called Anaphase-promoting complex subunit 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 13  | N     | 612      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4601  | 2913 | 805 | 858 | 25 |         |       |

- Molecule 14 is a protein called Anaphase-promoting complex subunit 11.

| Mol | Chain | Residues | Atoms |     |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---------|-------|
| 14  | C     | 83       | Total | C   | N   | O  | S  | 0       | 0     |
|     |       |          | 572   | 365 | 102 | 93 | 12 |         |       |

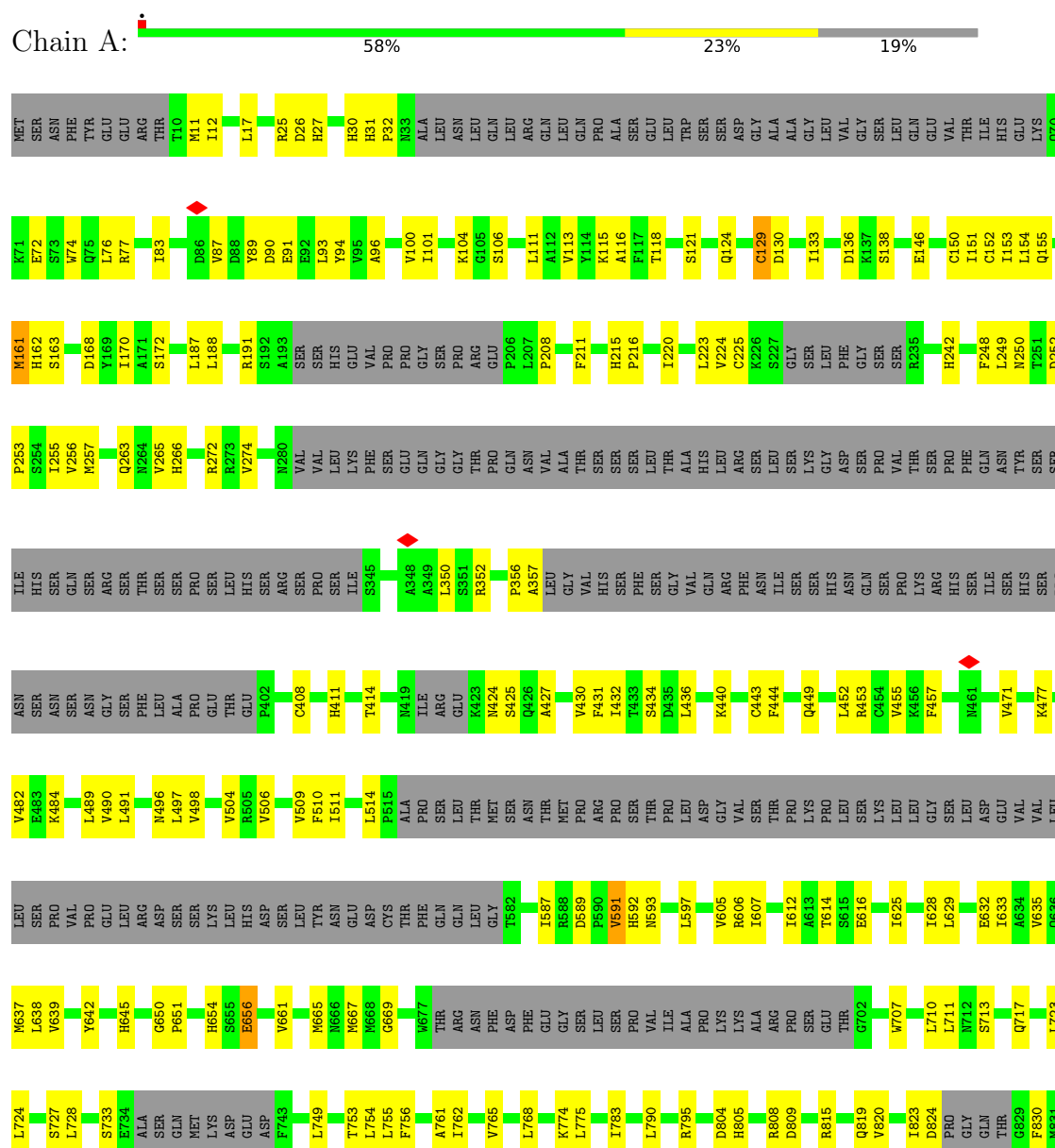
- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 15  | N     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 15  | C     | 3        | Total | Zn | 0       |
|     |       |          | 3     | 3  |         |

### 3 Residue-property plots

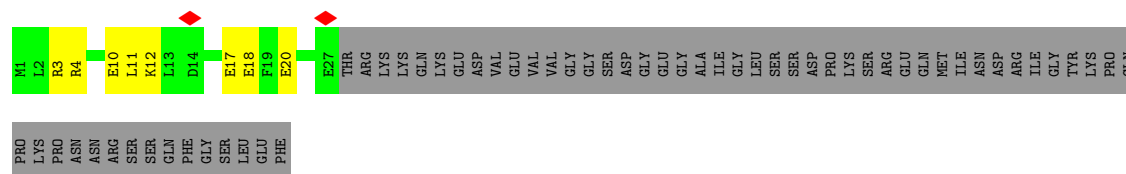
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Anaphase-promoting complex subunit 1

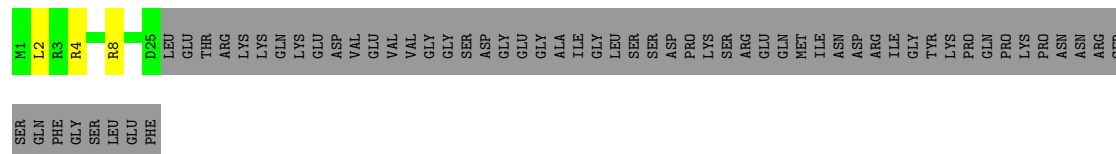




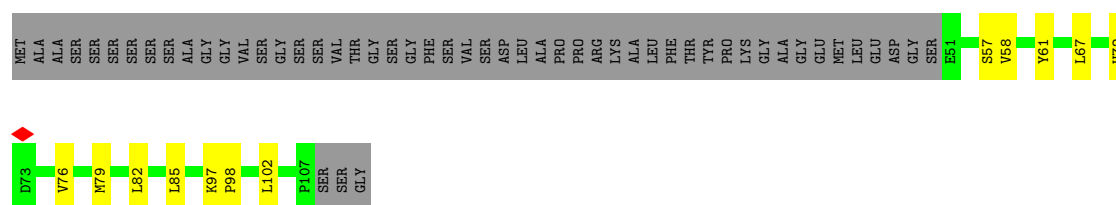




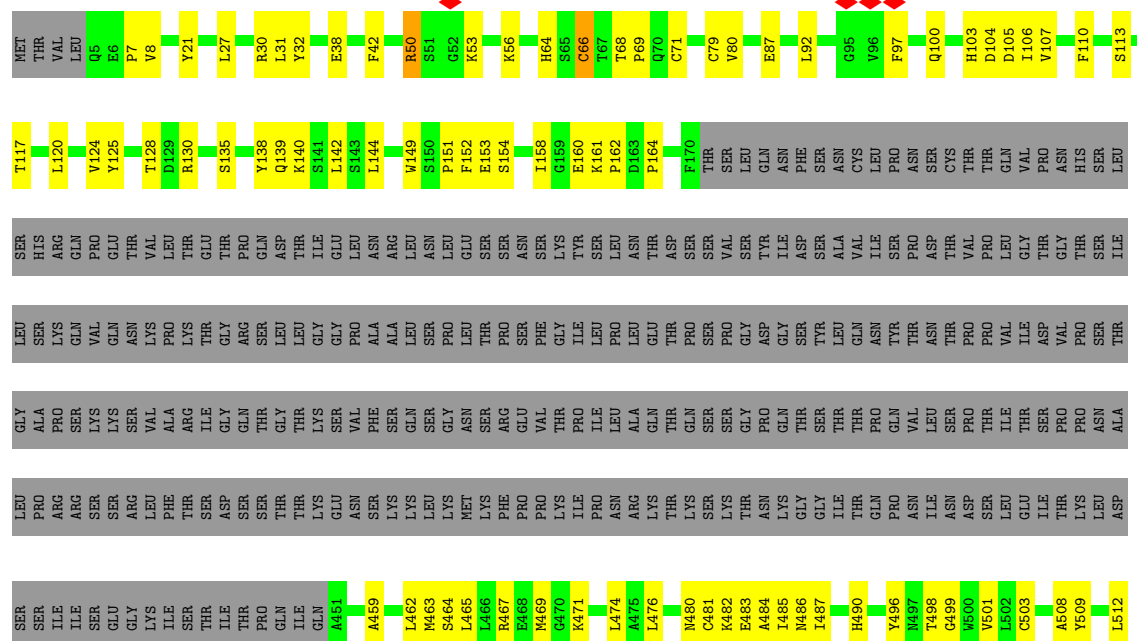
• Molecule 3: Anaphase-promoting complex subunit CDC26

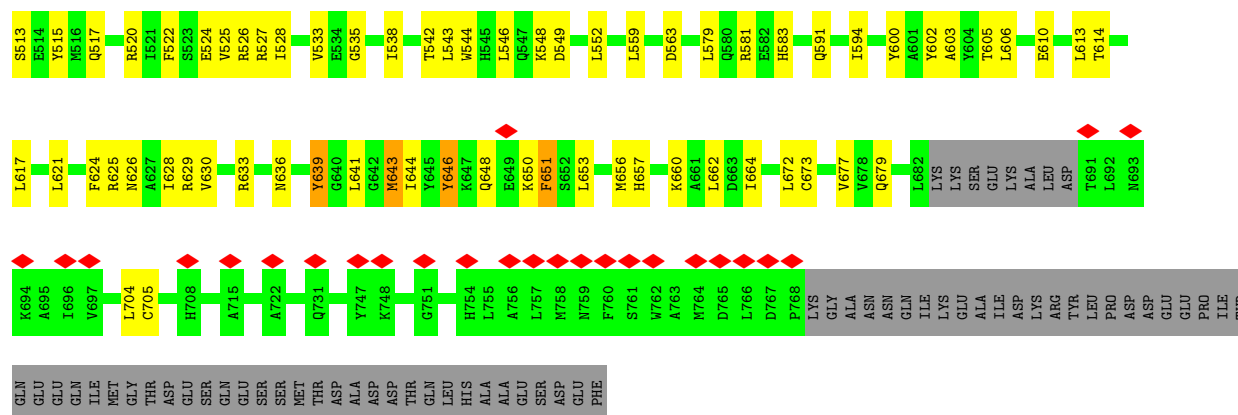


• Molecule 4: Anaphase-promoting complex subunit 16

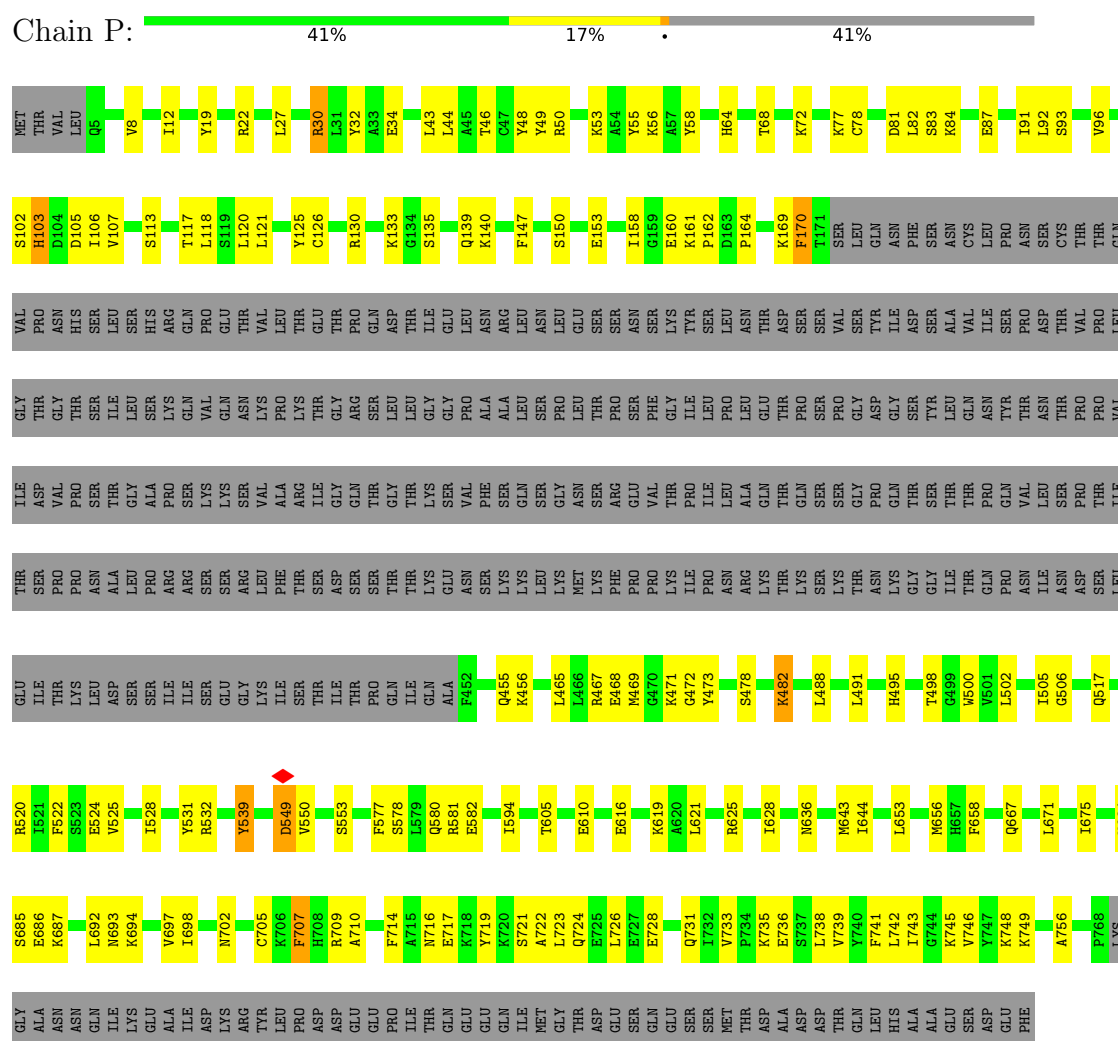


• Molecule 5: Cell division cycle protein 27 homolog



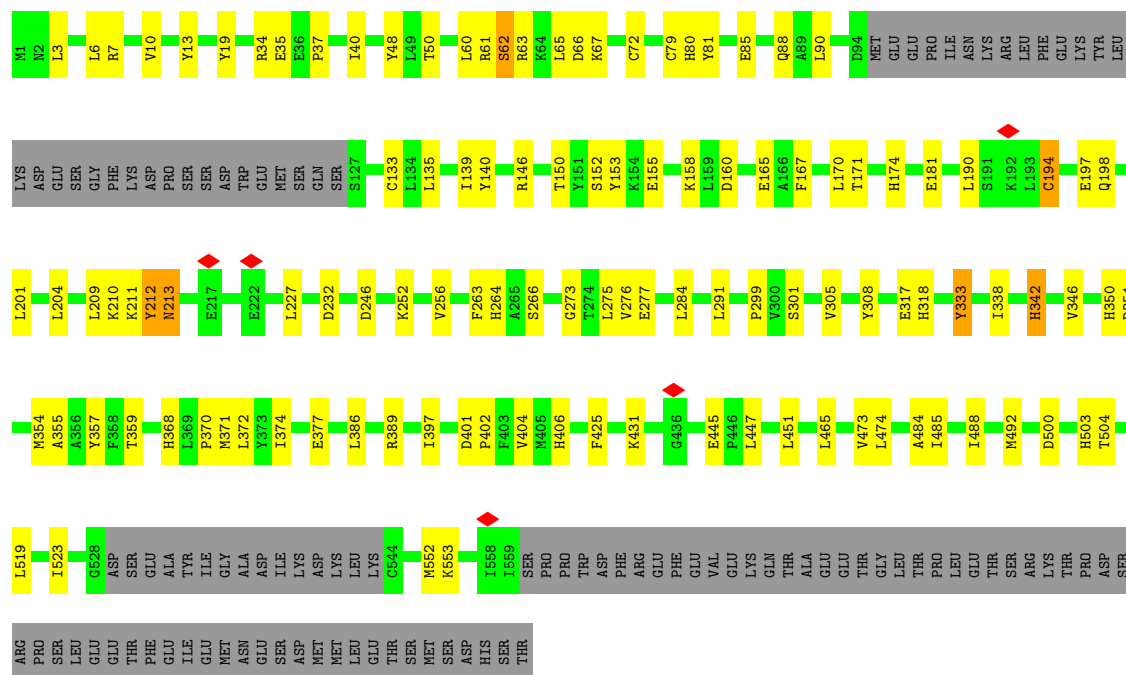


• Molecule 5: Cell division cycle protein 27 homolog



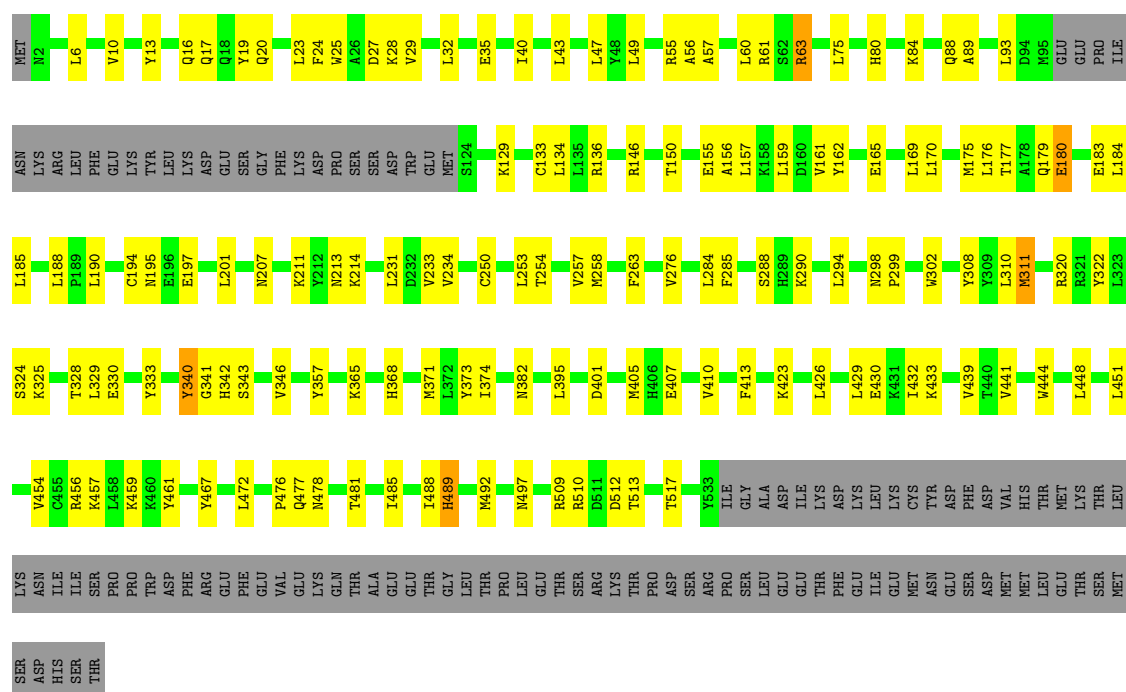
• Molecule 6: Cell division cycle protein 16 homolog





• Molecule 6: Cell division cycle protein 16 homolog

Chain Q: 58% 22% 19%

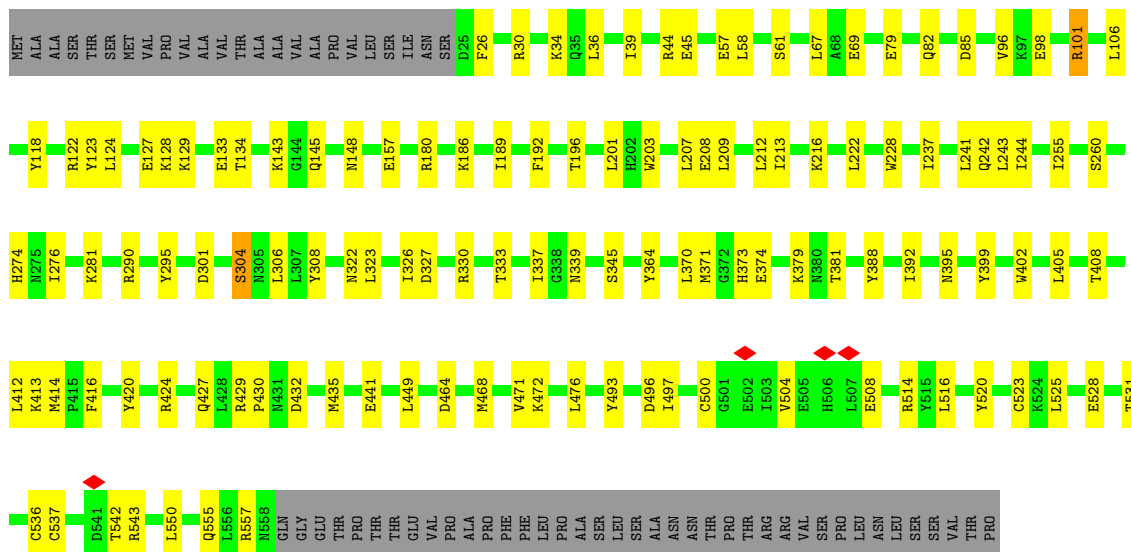


• Molecule 7: Anaphase-promoting complex subunit 10

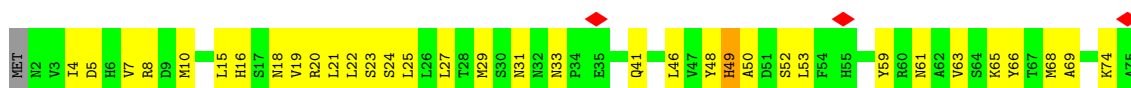
Chain L: 59% 35%

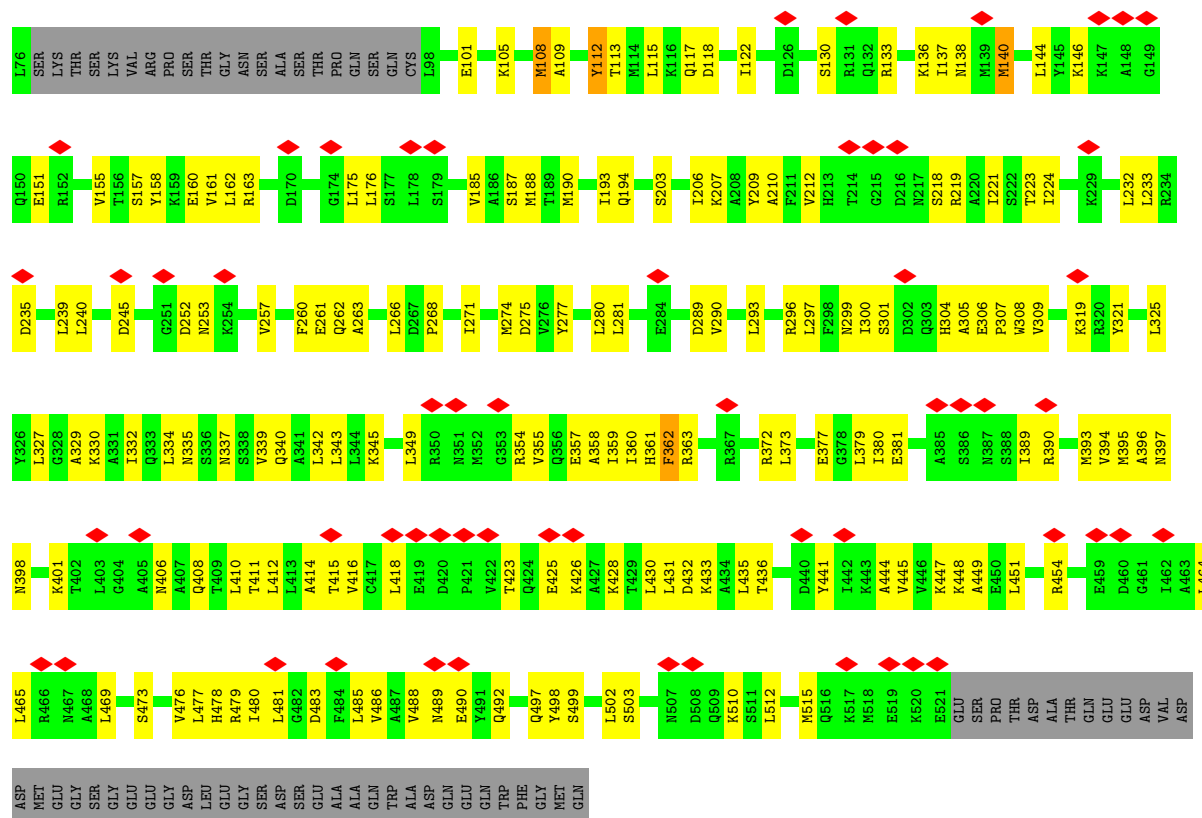


- Molecule 10: Cell division cycle protein 23 homolog

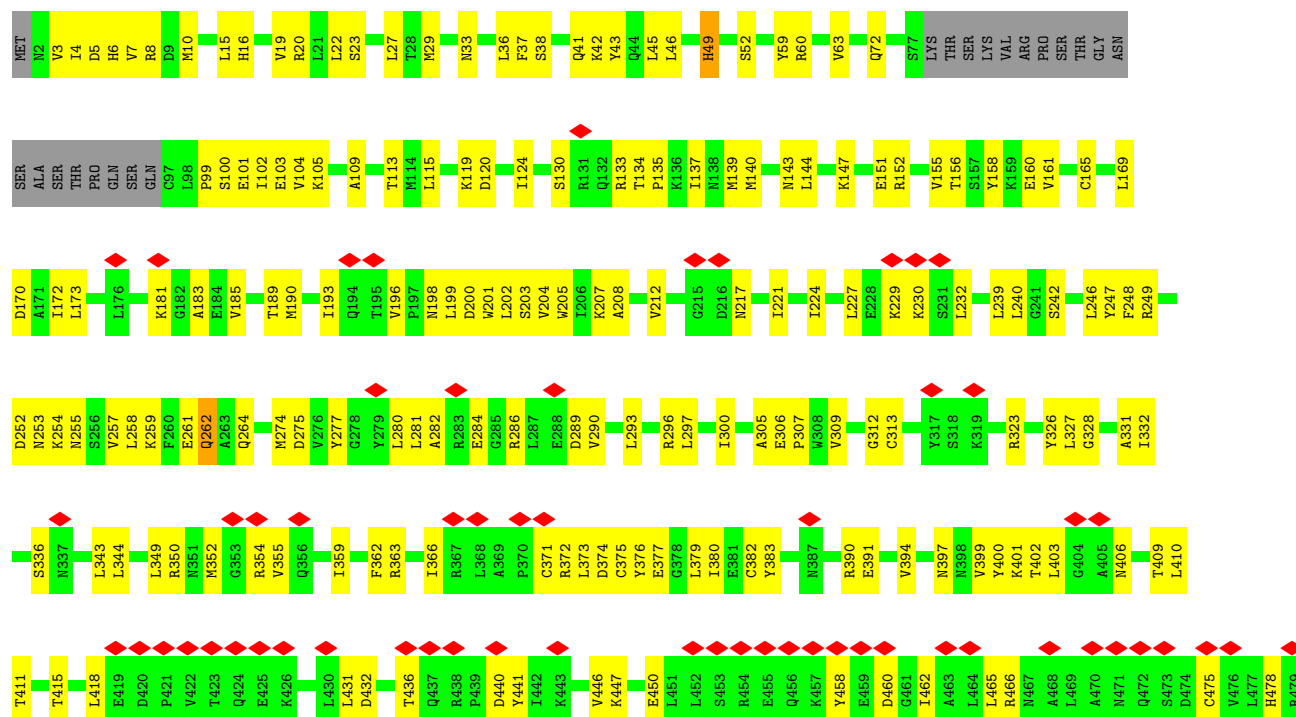


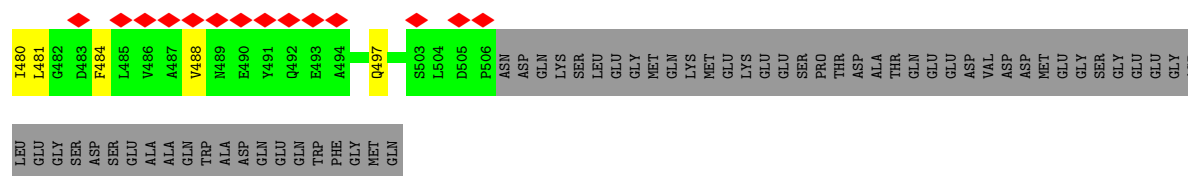
- Molecule 11: Anaphase-promoting complex subunit 7





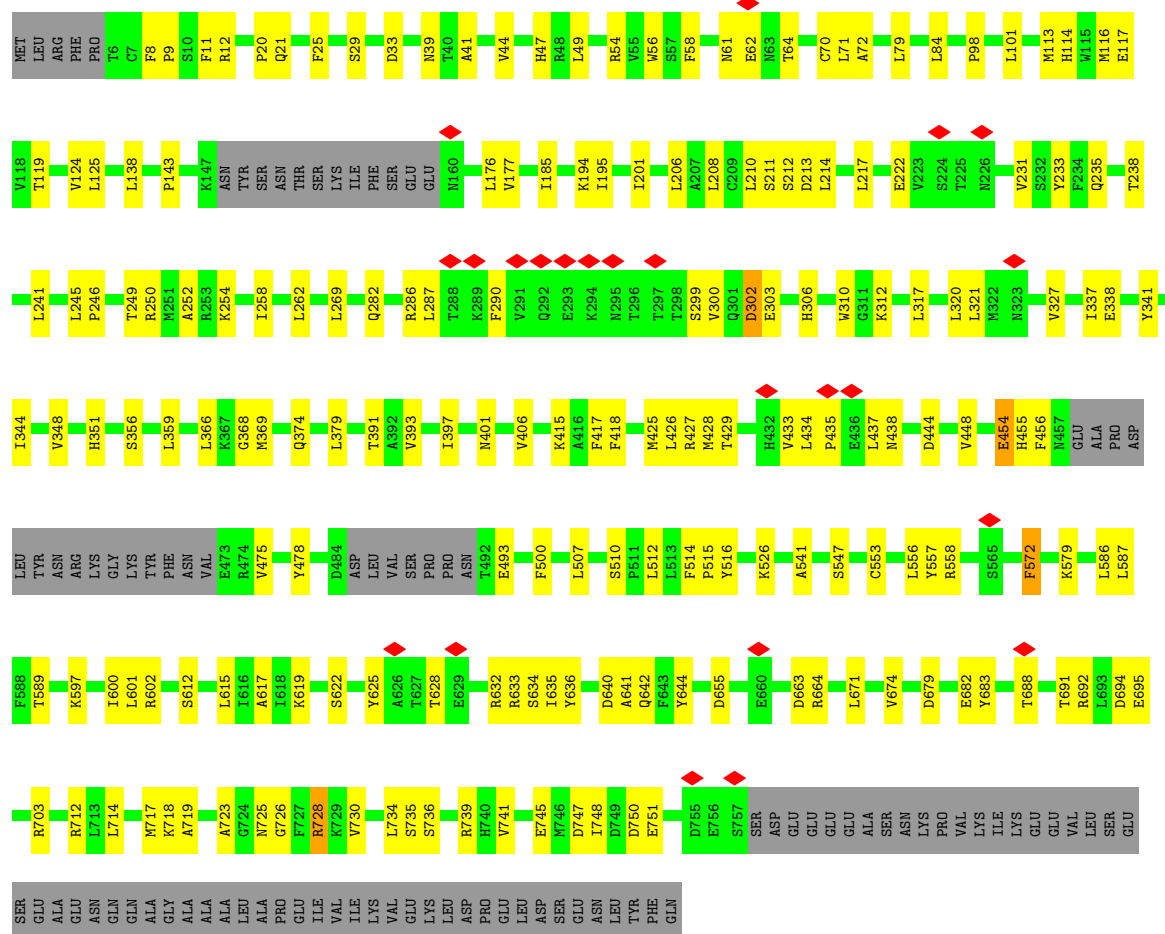
• Molecule 11: Anaphase-promoting complex subunit 7





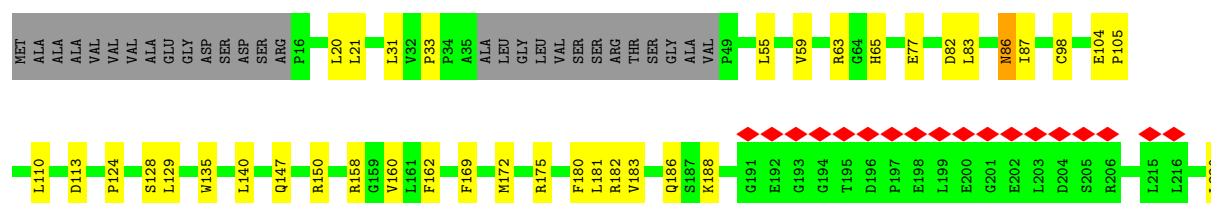
• Molecule 12: Anaphase-promoting complex subunit 4

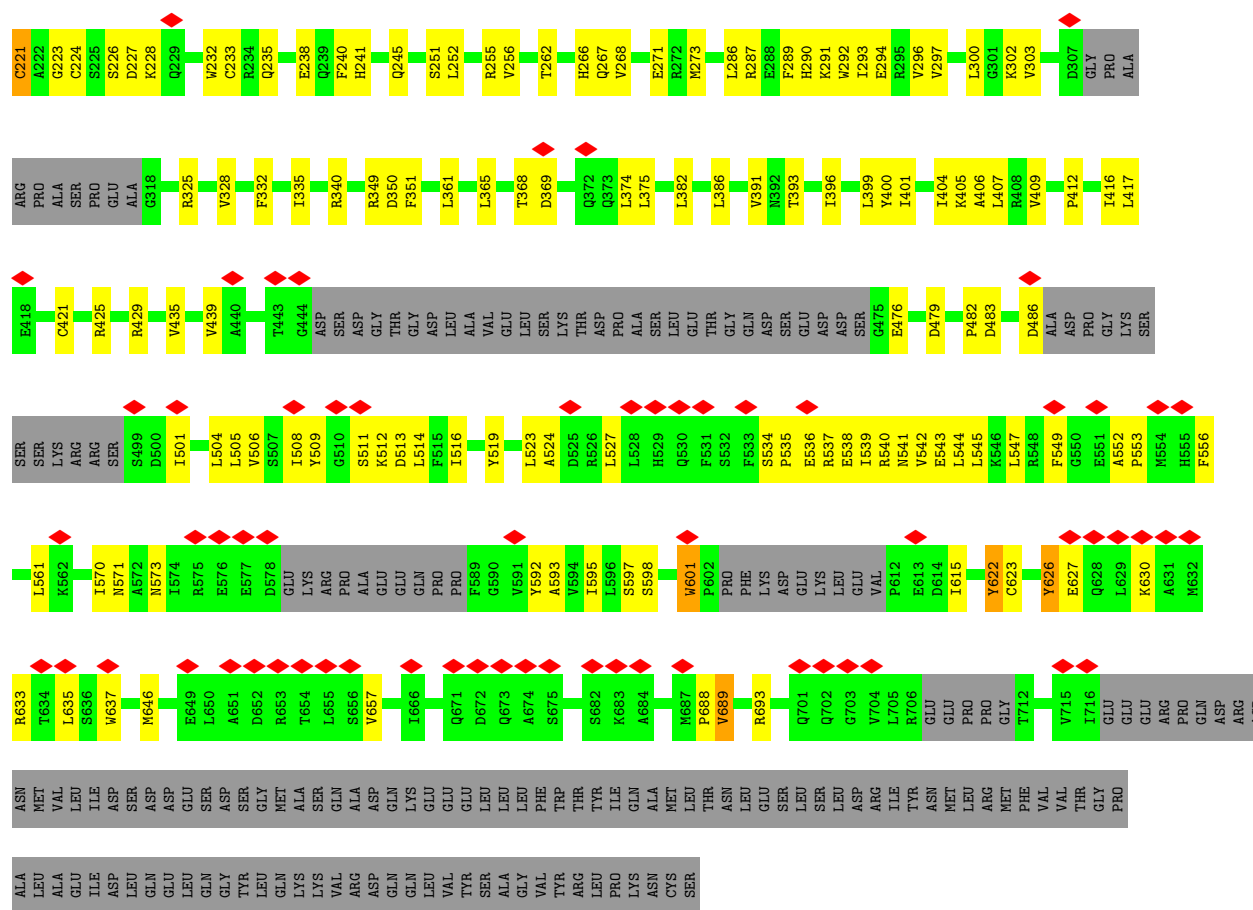
Chain I:



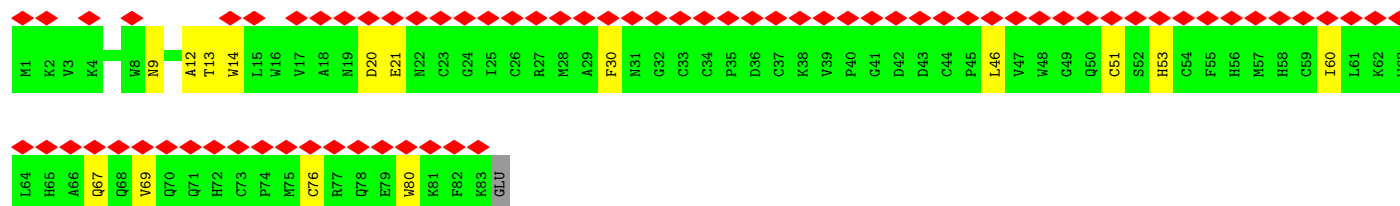
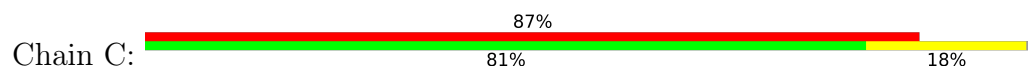
• Molecule 13: Anaphase-promoting complex subunit 2

Chain N:





● Molecule 14: Anaphase-promoting complex subunit 11





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 174356                                  | 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 ( $e^-/\text{\AA}^2$ ) | 40                                      | Depositor |
| Minimum defocus (nm)                 | 1500                                    | Depositor |
| Maximum defocus (nm)                 | 3500                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | FEI FALCON III (4k x 4k)                | Depositor |
| Maximum map value                    | 1.975                                   | Depositor |
| Minimum map value                    | -0.749                                  | Depositor |
| Average map value                    | 0.002                                   | Depositor |
| Map value standard deviation         | 0.083                                   | Depositor |
| Recommended contour level            | 0.4                                     | Depositor |
| Map size (Å)                         | 385.2, 385.2, 385.2                     | wwPDB     |
| Map dimensions                       | 360, 360, 360                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.07, 1.07, 1.07                        | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |             | Bond angles |             |
|-----|-------|--------------|-------------|-------------|-------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$ |
| 1   | A     | 0.29         | 0/12566     | 0.50        | 0/17085     |
| 2   | D     | 0.25         | 0/470       | 0.45        | 0/643       |
| 3   | G     | 0.24         | 0/227       | 0.55        | 0/302       |
| 3   | W     | 0.28         | 0/218       | 0.55        | 0/288       |
| 4   | H     | 0.27         | 0/468       | 0.45        | 0/631       |
| 5   | J     | 0.28         | 0/3686      | 0.49        | 0/5000      |
| 5   | P     | 0.29         | 0/3975      | 0.47        | 0/5371      |
| 6   | K     | 0.28         | 0/4233      | 0.47        | 0/5730      |
| 6   | Q     | 0.28         | 0/4148      | 0.49        | 0/5620      |
| 7   | L     | 0.27         | 0/1480      | 0.55        | 0/2005      |
| 8   | M     | 0.26         | 0/486       | 0.51        | 0/658       |
| 9   | O     | 0.32         | 0/5504      | 0.49        | 0/7435      |
| 10  | U     | 0.28         | 0/4218      | 0.48        | 0/5701      |
| 10  | V     | 0.31         | 0/4493      | 0.47        | 0/6065      |
| 11  | Y     | 0.27         | 0/3970      | 0.53        | 0/5365      |
| 11  | Z     | 0.25         | 0/3870      | 0.51        | 0/5233      |
| 12  | I     | 0.29         | 0/5824      | 0.50        | 0/7888      |
| 13  | N     | 0.28         | 0/4683      | 0.53        | 0/6369      |
| 14  | C     | 0.29         | 0/592       | 0.46        | 0/819       |
| All | All   | 0.29         | 0/65111     | 0.50        | 0/88208     |

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 ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 12284 | 0        | 12181    | 311     | 0            |
| 2   | D     | 458   | 0        | 434      | 13      | 0            |
| 3   | G     | 226   | 0        | 233      | 9       | 0            |
| 3   | W     | 217   | 0        | 231      | 3       | 0            |
| 4   | H     | 459   | 0        | 449      | 10      | 0            |
| 5   | J     | 3601  | 0        | 3314     | 99      | 0            |
| 5   | P     | 3883  | 0        | 3834     | 117     | 0            |
| 6   | K     | 4134  | 0        | 4060     | 85      | 0            |
| 6   | Q     | 4049  | 0        | 3948     | 108     | 0            |
| 7   | L     | 1446  | 0        | 1423     | 48      | 0            |
| 8   | M     | 478   | 0        | 454      | 15      | 0            |
| 9   | O     | 5404  | 0        | 5452     | 135     | 0            |
| 10  | U     | 4121  | 0        | 4046     | 81      | 0            |
| 10  | V     | 4393  | 0        | 4362     | 92      | 0            |
| 11  | Y     | 3907  | 0        | 3975     | 158     | 0            |
| 11  | Z     | 3807  | 0        | 3885     | 141     | 0            |
| 12  | I     | 5705  | 0        | 5655     | 130     | 0            |
| 13  | N     | 4601  | 0        | 4327     | 117     | 0            |
| 14  | C     | 572   | 0        | 452      | 9       | 0            |
| 15  | C     | 3     | 0        | 0        | 0       | 0            |
| 15  | N     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 63749 | 0        | 62715    | 1524    | 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 12.

All (1524) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 5:P:12:ILE:HG21  | 5:P:43:LEU:HD21   | 1.56                     | 0.86              |
| 12:I:719:ALA:HA  | 12:I:735:SER:HA   | 1.58                     | 0.83              |
| 1:A:83:ILE:HD11  | 9:O:541:ILE:HD13  | 1.61                     | 0.83              |
| 6:Q:161:VAL:HG23 | 6:Q:188:LEU:HD12  | 1.62                     | 0.81              |
| 11:Y:112:TYR:HB3 | 11:Y:117:GLN:HB2  | 1.60                     | 0.81              |
| 13:N:400:TYR:HE2 | 13:N:508:ILE:HG21 | 1.45                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:O:448:MET:SD    | 12:I:401:ASN:ND2  | 2.57                     | 0.77              |
| 9:O:430:ARG:HD3   | 9:O:476:LEU:HD11  | 1.67                     | 0.77              |
| 6:K:473:VAL:HG21  | 5:P:130:ARG:HH22  | 1.50                     | 0.77              |
| 6:Q:157:LEU:HG    | 6:Q:188:LEU:HD11  | 1.66                     | 0.77              |
| 7:L:83:TYR:HD2    | 7:L:115:GLU:HG3   | 1.50                     | 0.77              |
| 1:A:121:SER:HB2   | 1:A:155:GLN:HE21  | 1.50                     | 0.75              |
| 9:O:671:GLN:HE22  | 12:I:374:GLN:HE22 | 1.34                     | 0.75              |
| 7:L:34:SER:HB3    | 7:L:63:LEU:HB2    | 1.68                     | 0.75              |
| 10:V:536:CYS:SG   | 10:V:542:THR:OG1  | 2.45                     | 0.75              |
| 1:A:1354:GLU:HB3  | 7:L:30:VAL:HG13   | 1.69                     | 0.74              |
| 6:Q:23:LEU:HD11   | 6:Q:47:LEU:HD12   | 1.70                     | 0.74              |
| 11:Z:332:ILE:HD12 | 11:Z:336:SER:HA   | 1.69                     | 0.74              |
| 4:H:102:LEU:HD23  | 5:P:594:ILE:HG22  | 1.70                     | 0.74              |
| 7:L:48:ASP:OD1    | 7:L:157:LYS:NZ    | 2.20                     | 0.73              |
| 11:Y:50:ALA:HB1   | 11:Y:66:TYR:CE1   | 2.23                     | 0.73              |
| 12:I:692:ARG:HE   | 12:I:694:ASP:HB3  | 1.54                     | 0.73              |
| 11:Z:193:ILE:HG22 | 11:Z:199:LEU:HB2  | 1.70                     | 0.73              |
| 11:Y:271:ILE:HG22 | 11:Y:306:GLU:HG3  | 1.69                     | 0.73              |
| 6:Q:432:ILE:HD11  | 6:Q:444:TRP:CG    | 2.23                     | 0.73              |
| 6:K:474:LEU:HD21  | 5:P:96:VAL:HG21   | 1.69                     | 0.72              |
| 1:A:1193:ILE:HG23 | 1:A:1208:LEU:HD21 | 1.71                     | 0.72              |
| 9:O:329:ARG:NH2   | 10:V:413:LYS:O    | 2.23                     | 0.72              |
| 4:H:57:SER:OG     | 11:Z:323:ARG:NH2  | 2.23                     | 0.72              |
| 10:V:36:LEU:HD21  | 10:V:58:LEU:HB3   | 1.71                     | 0.72              |
| 12:I:556:LEU:HD21 | 12:I:586:LEU:HD21 | 1.71                     | 0.71              |
| 1:A:869:ARG:NH2   | 1:A:946:THR:OG1   | 2.23                     | 0.71              |
| 11:Z:193:ILE:HA   | 11:Z:199:LEU:HD13 | 1.71                     | 0.71              |
| 5:J:160:GLU:HG3   | 5:J:161:LYS:HG2   | 1.71                     | 0.71              |
| 13:N:539:ILE:HG22 | 13:N:561:LEU:HD23 | 1.71                     | 0.71              |
| 12:I:714:LEU:HB3  | 12:I:717:MET:HB2  | 1.73                     | 0.71              |
| 1:A:1910:SER:HB2  | 13:N:21:LEU:HD11  | 1.71                     | 0.71              |
| 11:Y:297:LEU:HB3  | 11:Y:307:PRO:HB3  | 1.72                     | 0.71              |
| 1:A:191:ARG:NH2   | 1:A:208:PRO:O     | 2.23                     | 0.71              |
| 10:U:159:SER:O    | 10:U:163:GLN:NE2  | 2.24                     | 0.70              |
| 11:Y:137:ILE:HA   | 11:Y:140:MET:SD   | 2.31                     | 0.70              |
| 5:P:684:LYS:HG3   | 5:P:687:LYS:HB2   | 1.72                     | 0.70              |
| 6:Q:478:ASN:HB3   | 6:Q:481:THR:HG22  | 1.73                     | 0.70              |
| 10:U:298:GLU:OE2  | 10:V:101:ARG:NH1  | 2.24                     | 0.70              |
| 1:A:1221:ASP:HB3  | 1:A:1224:ILE:HG22 | 1.74                     | 0.70              |
| 5:J:80:VAL:HG11   | 5:J:120:LEU:HD11  | 1.74                     | 0.70              |
| 11:Y:342:LEU:HA   | 11:Y:345:LYS:HD2  | 1.74                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:O:291:ASN:O     | 9:O:298:ARG:NH2   | 2.25                     | 0.69              |
| 11:Y:268:PRO:O    | 11:Y:296:ARG:NH1  | 2.23                     | 0.69              |
| 1:A:272:ARG:NH1   | 1:A:408:CYS:SG    | 2.66                     | 0.69              |
| 1:A:1096:PRO:HG2  | 9:O:347:LEU:HD21  | 1.74                     | 0.69              |
| 5:P:726:LEU:HD23  | 5:P:739:VAL:HG13  | 1.74                     | 0.69              |
| 6:Q:368:HIS:NE2   | 6:Q:401:ASP:OD2   | 2.25                     | 0.69              |
| 11:Z:130:SER:HA   | 11:Z:133:ARG:HE   | 1.56                     | 0.69              |
| 13:N:286:LEU:O    | 13:N:290:HIS:ND1  | 2.26                     | 0.69              |
| 6:K:232:ASP:OD2   | 6:Q:28:LYS:NZ     | 2.26                     | 0.69              |
| 5:P:549:ASP:OD1   | 5:P:550:VAL:N     | 2.26                     | 0.69              |
| 13:N:241:HIS:O    | 13:N:245:GLN:HG3  | 1.92                     | 0.69              |
| 5:J:591:GLN:HA    | 5:J:594:ILE:HD12  | 1.75                     | 0.69              |
| 11:Z:169:LEU:HA   | 11:Z:172:ILE:HD12 | 1.74                     | 0.69              |
| 5:J:651:PHE:HE1   | 5:J:705:CYS:HB3   | 1.58                     | 0.68              |
| 11:Y:335:ASN:OD1  | 11:Y:337:ASN:ND2  | 2.26                     | 0.68              |
| 1:A:356:PRO:O     | 10:V:242:GLN:NE2  | 2.26                     | 0.68              |
| 11:Y:448:LYS:HD3  | 11:Y:464:LEU:HD21 | 1.73                     | 0.68              |
| 5:P:707:PHE:CE2   | 5:P:738:LEU:HB3   | 2.29                     | 0.68              |
| 6:Q:509:ARG:HD3   | 6:Q:512:ASP:HB2   | 1.74                     | 0.68              |
| 10:U:161:LYS:HE3  | 10:U:166:GLU:HB2  | 1.74                     | 0.68              |
| 12:I:177:VAL:HG12 | 12:I:208:LEU:HD13 | 1.76                     | 0.68              |
| 9:O:459:GLN:NE2   | 12:I:493:GLU:O    | 2.26                     | 0.67              |
| 1:A:1713:MET:HB2  | 1:A:1715:TRP:CD1  | 2.29                     | 0.67              |
| 7:L:60:GLN:NE2    | 7:L:142:LEU:O     | 2.27                     | 0.67              |
| 10:U:242:GLN:HE22 | 10:U:429:ARG:HE   | 1.41                     | 0.67              |
| 1:A:1031:ASP:HB2  | 13:N:482:PRO:HB2  | 1.77                     | 0.67              |
| 1:A:1150:ALA:HB1  | 1:A:1187:LYS:HE2  | 1.76                     | 0.67              |
| 3:G:11:LEU:HD21   | 6:Q:456:ARG:HH12  | 1.60                     | 0.67              |
| 1:A:443:CYS:HB3   | 1:A:452:LEU:HD21  | 1.75                     | 0.67              |
| 10:V:237:ILE:O    | 10:V:241:LEU:HB2  | 1.95                     | 0.67              |
| 9:O:521:ASN:HD21  | 9:O:658:LEU:HD22  | 1.60                     | 0.67              |
| 2:D:20:LEU:HD21   | 9:O:252:GLU:HG2   | 1.75                     | 0.67              |
| 11:Y:444:ALA:O    | 11:Y:448:LYS:HG3  | 1.95                     | 0.67              |
| 1:A:352:ARG:NH1   | 10:V:339:ASN:OD1  | 2.28                     | 0.67              |
| 10:U:88:THR:HG23  | 10:V:44:ARG:HH22  | 1.58                     | 0.67              |
| 11:Z:37:PHE:HB3   | 11:Z:41:GLN:HG3   | 1.77                     | 0.67              |
| 1:A:1531:GLY:HA2  | 1:A:1565:LEU:HG   | 1.77                     | 0.66              |
| 11:Y:476:VAL:O    | 11:Y:480:ILE:HG13 | 1.95                     | 0.66              |
| 5:P:169:LYS:HB3   | 5:P:467:ARG:HH21  | 1.61                     | 0.66              |
| 1:A:629:LEU:HD23  | 1:A:762:ILE:HD11  | 1.77                     | 0.66              |
| 5:J:103:HIS:HB3   | 5:J:140:LYS:HE2   | 1.77                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:504:VAL:HG21  | 1:A:635:VAL:HG11  | 1.78                     | 0.66              |
| 1:A:1574:LEU:O    | 1:A:1617:ARG:NH2  | 2.29                     | 0.66              |
| 11:Y:232:LEU:HD21 | 11:Z:33:ASN:HB3   | 1.78                     | 0.66              |
| 1:A:1753:TYR:O    | 9:O:639:GLN:NE2   | 2.27                     | 0.66              |
| 8:M:35:GLU:OE2    | 8:M:35:GLU:N      | 2.21                     | 0.66              |
| 9:O:105:LEU:HD11  | 9:O:151:VAL:HG12  | 1.77                     | 0.66              |
| 11:Z:198:ASN:O    | 11:Z:201:TRP:NE1  | 2.28                     | 0.66              |
| 9:O:649:GLU:HG2   | 12:I:369:MET:HG2  | 1.77                     | 0.65              |
| 10:U:29:LEU:HB2   | 10:U:30:ARG:NH2   | 2.11                     | 0.65              |
| 1:A:1897:PRO:HA   | 1:A:1900:LEU:HD12 | 1.77                     | 0.65              |
| 7:L:96:VAL:HG21   | 7:L:122:VAL:HG11  | 1.77                     | 0.65              |
| 11:Y:300:ILE:HA   | 11:Z:60:ARG:HG3   | 1.78                     | 0.65              |
| 11:Y:515:MET:SD   | 11:Y:515:MET:N    | 2.70                     | 0.65              |
| 11:Z:399:VAL:HG22 | 11:Z:409:THR:HG22 | 1.79                     | 0.65              |
| 11:Z:257:VAL:HG11 | 11:Z:286:ARG:HH22 | 1.61                     | 0.65              |
| 13:N:232:TRP:HB2  | 13:N:235:GLN:HE21 | 1.60                     | 0.65              |
| 11:Y:53:LEU:HD21  | 11:Y:61:ASN:HB3   | 1.79                     | 0.65              |
| 9:O:736:LEU:O     | 9:O:740:LEU:HD12  | 1.97                     | 0.65              |
| 9:O:415:SER:HB2   | 9:O:451:LEU:HD12  | 1.79                     | 0.65              |
| 5:P:488:LEU:HD23  | 5:P:505:ILE:HG13  | 1.78                     | 0.65              |
| 11:Z:399:VAL:HG23 | 11:Z:403:LEU:HD13 | 1.78                     | 0.65              |
| 11:Y:162:LEU:HD23 | 11:Y:188:MET:HG2  | 1.78                     | 0.64              |
| 5:J:486:ASN:OD1   | 5:J:490:HIS:NE2   | 2.30                     | 0.64              |
| 9:O:694:LEU:HD11  | 9:O:716:PHE:HD2   | 1.62                     | 0.64              |
| 6:Q:439:VAL:HG21  | 6:Q:448:LEU:HD21  | 1.78                     | 0.64              |
| 1:A:733:SER:OG    | 9:O:719:ARG:NH1   | 2.30                     | 0.64              |
| 7:L:12:ASP:HB3    | 7:L:15:GLN:HG2    | 1.79                     | 0.64              |
| 1:A:506:VAL:HG22  | 1:A:639:VAL:HG22  | 1.79                     | 0.64              |
| 11:Z:411:THR:HG21 | 11:Z:441:TYR:HE2  | 1.61                     | 0.64              |
| 11:Y:435:LEU:HD12 | 11:Y:448:LYS:HE2  | 1.79                     | 0.64              |
| 11:Y:449:ALA:HB1  | 11:Y:480:ILE:HG21 | 1.78                     | 0.64              |
| 11:Z:23:SER:HB3   | 11:Z:49:HIS:HB2   | 1.78                     | 0.64              |
| 1:A:982:ASP:OD1   | 1:A:983:LEU:N     | 2.30                     | 0.64              |
| 9:O:106:LYS:O     | 10:U:344:ARG:NH2  | 2.30                     | 0.64              |
| 1:A:928:GLU:HG3   | 1:A:970:TRP:HZ2   | 1.63                     | 0.64              |
| 6:K:523:ILE:HG21  | 5:P:653:LEU:HD22  | 1.80                     | 0.64              |
| 7:L:96:VAL:HG11   | 7:L:124:LEU:HD22  | 1.80                     | 0.64              |
| 10:U:35:GLN:HB3   | 10:U:201:LEU:HD21 | 1.80                     | 0.64              |
| 11:Y:23:SER:HB2   | 11:Y:49:HIS:HD2   | 1.63                     | 0.64              |
| 11:Z:172:ILE:HG23 | 11:Z:185:VAL:HG11 | 1.80                     | 0.63              |
| 9:O:79:TYR:O      | 9:O:83:GLU:HG2    | 1.99                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:Z:432:ASP:O    | 11:Z:436:THR:HG23 | 1.98                     | 0.63              |
| 13:N:537:ARG:HH12 | 13:N:541:ASN:HB2  | 1.64                     | 0.63              |
| 5:J:69:PRO:HB3    | 5:J:110:PHE:HA    | 1.80                     | 0.63              |
| 5:J:543:LEU:HB2   | 5:J:552:LEU:HD13  | 1.78                     | 0.63              |
| 6:Q:35:GLU:OE2    | 6:Q:63:ARG:NH1    | 2.28                     | 0.63              |
| 12:I:269:LEU:HD23 | 12:I:526:LYS:HD3  | 1.80                     | 0.63              |
| 1:A:774:LYS:NZ    | 1:A:809:ASP:OD2   | 2.30                     | 0.63              |
| 6:Q:476:PRO:HG2   | 10:U:182:LEU:HD22 | 1.81                     | 0.63              |
| 11:Z:59:TYR:O     | 11:Z:63:VAL:HG23  | 1.99                     | 0.63              |
| 11:Y:66:TYR:CD2   | 11:Y:108:MET:HB3  | 2.34                     | 0.63              |
| 12:I:64:THR:HG22  | 12:I:84:LEU:HD11  | 1.80                     | 0.63              |
| 13:N:374:LEU:HD22 | 13:N:416:ILE:HD11 | 1.79                     | 0.63              |
| 1:A:1277:ILE:HG22 | 1:A:1363:THR:HG23 | 1.80                     | 0.63              |
| 6:K:401:ASP:HB3   | 6:K:404:VAL:HG12  | 1.81                     | 0.63              |
| 7:L:22:VAL:HB     | 7:L:159:TYR:HB3   | 1.81                     | 0.62              |
| 1:A:249:LEU:HG    | 1:A:256:VAL:HG22  | 1.82                     | 0.62              |
| 5:J:30:ARG:HH22   | 5:P:498:THR:HG21  | 1.64                     | 0.62              |
| 11:Y:373:LEU:HD11 | 11:Y:412:LEU:HD22 | 1.80                     | 0.62              |
| 6:Q:371:MET:HA    | 6:Q:374:ILE:HD12  | 1.81                     | 0.62              |
| 11:Z:200:ASP:OD2  | 11:Z:201:TRP:N    | 2.33                     | 0.62              |
| 6:Q:451:LEU:HB3   | 6:Q:467:TYR:HD2   | 1.65                     | 0.62              |
| 13:N:349:ARG:HE   | 13:N:399:LEU:HD12 | 1.63                     | 0.62              |
| 1:A:482:VAL:HG23  | 1:A:593:ASN:HA    | 1.82                     | 0.62              |
| 3:G:4:ARG:N       | 6:Q:373:TYR:OH    | 2.32                     | 0.62              |
| 5:J:465:LEU:HG    | 5:J:469:MET:HE2   | 1.80                     | 0.62              |
| 6:K:35:GLU:HG3    | 6:K:40:ILE:HD11   | 1.82                     | 0.62              |
| 10:U:106:LEU:HD11 | 10:U:117:LEU:HD23 | 1.82                     | 0.62              |
| 9:O:207:LEU:HB3   | 10:V:145:GLN:HE22 | 1.64                     | 0.62              |
| 11:Z:458:TYR:O    | 11:Z:462:ILE:HG12 | 2.00                     | 0.62              |
| 4:H:58:VAL:HA     | 11:Z:323:ARG:HH12 | 1.64                     | 0.62              |
| 5:P:693:ASN:OD1   | 5:P:709:ARG:NH1   | 2.32                     | 0.62              |
| 6:Q:179:GLN:NE2   | 6:Q:183:GLU:OE2   | 2.33                     | 0.62              |
| 12:I:356:SER:HB3  | 12:I:397:ILE:HG12 | 1.82                     | 0.62              |
| 9:O:648:ILE:HD12  | 9:O:663:ALA:HB1   | 1.82                     | 0.61              |
| 12:I:231:VAL:HG12 | 12:I:556:LEU:HD13 | 1.82                     | 0.61              |
| 10:U:475:LYS:O    | 10:U:479:GLN:NE2  | 2.33                     | 0.61              |
| 1:A:1912:ALA:HB3  | 13:N:21:LEU:HD12  | 1.81                     | 0.61              |
| 10:V:127:GLU:OE1  | 10:V:148:ASN:ND2  | 2.32                     | 0.61              |
| 11:Y:5:ASP:OD1    | 11:Y:8:ARG:NH2    | 2.33                     | 0.61              |
| 11:Y:257:VAL:O    | 11:Y:261:GLU:HG3  | 2.00                     | 0.61              |
| 13:N:407:LEU:HB2  | 13:N:417:LEU:HD13 | 1.82                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:P:32:TYR:OH     | 5:P:64:HIS:NE2    | 2.32                     | 0.61              |
| 13:N:129:LEU:HD11 | 13:N:150:ARG:HA   | 1.81                     | 0.61              |
| 6:K:81:TYR:HD2    | 6:K:139:ILE:HG12  | 1.65                     | 0.61              |
| 7:L:68:PHE:HE2    | 7:L:137:ILE:HD12  | 1.66                     | 0.61              |
| 1:A:1306:CYS:HB2  | 1:A:1374:ILE:HG12 | 1.83                     | 0.61              |
| 12:I:327:VAL:HG22 | 12:I:425:MET:HB3  | 1.82                     | 0.61              |
| 7:L:70:ARG:HG2    | 7:L:71:LYS:H      | 1.66                     | 0.61              |
| 7:L:173:CYS:HB3   | 7:L:178:PHE:HB3   | 1.81                     | 0.61              |
| 11:Z:284:GLU:OE1  | 11:Z:286:ARG:NH2  | 2.34                     | 0.61              |
| 12:I:29:SER:O     | 12:I:725:ASN:ND2  | 2.33                     | 0.61              |
| 6:K:85:GLU:OE2    | 6:K:88:GLN:NE2    | 2.34                     | 0.61              |
| 6:Q:401:ASP:O     | 6:Q:405:MET:HB3   | 2.01                     | 0.61              |
| 11:Z:281:LEU:HD21 | 11:Z:289:ASP:HB3  | 1.83                     | 0.61              |
| 12:I:338:GLU:OE1  | 12:I:415:LYS:NZ   | 2.34                     | 0.61              |
| 11:Y:46:LEU:HD22  | 11:Y:69:ALA:HB2   | 1.82                     | 0.61              |
| 5:J:162:PRO:HB2   | 5:J:474:LEU:HD21  | 1.82                     | 0.60              |
| 5:P:714:PHE:HD2   | 5:P:746:VAL:HG22  | 1.65                     | 0.60              |
| 13:N:623:CYS:SG   | 13:N:637:TRP:NE1  | 2.68                     | 0.60              |
| 5:P:517:GLN:OE1   | 5:P:520:ARG:NH1   | 2.34                     | 0.60              |
| 11:Y:253:ASN:HB3  | 11:Y:280:LEU:HD11 | 1.83                     | 0.60              |
| 12:I:11:PHE:O     | 12:I:712:ARG:NH1  | 2.34                     | 0.60              |
| 1:A:808:ARG:NH2   | 1:A:1894:VAL:O    | 2.28                     | 0.60              |
| 11:Y:29:MET:SD    | 11:Z:232:LEU:HB3  | 2.41                     | 0.60              |
| 13:N:571:ASN:ND2  | 13:N:593:ALA:O    | 2.26                     | 0.60              |
| 8:M:17:ASP:O      | 8:M:21:GLU:HG3    | 2.01                     | 0.60              |
| 11:Z:181:LYS:HE2  | 11:Z:183:ALA:HB3  | 1.84                     | 0.60              |
| 9:O:103:GLY:O     | 9:O:155:TYR:OH    | 2.20                     | 0.60              |
| 10:V:497:ILE:HB   | 10:V:504:VAL:HG21 | 1.84                     | 0.60              |
| 12:I:206:LEU:HD11 | 12:I:222:GLU:HB2  | 1.82                     | 0.60              |
| 13:N:386:LEU:HD22 | 13:N:399:LEU:HD22 | 1.83                     | 0.60              |
| 6:Q:254:THR:O     | 6:Q:258:MET:HG2   | 2.02                     | 0.60              |
| 10:V:30:ARG:O     | 10:V:34:LYS:HG3   | 2.01                     | 0.60              |
| 11:Y:137:ILE:HD12 | 11:Y:138:ASN:N    | 2.16                     | 0.60              |
| 13:N:429:ARG:N    | 13:N:509:TYR:OH   | 2.35                     | 0.60              |
| 7:L:154:ARG:O     | 7:L:155:GLN:NE2   | 2.35                     | 0.59              |
| 9:O:207:LEU:O     | 10:V:145:GLN:NE2  | 2.35                     | 0.59              |
| 1:A:591:VAL:HG22  | 1:A:606:ARG:NH2   | 2.17                     | 0.59              |
| 5:J:107:VAL:HG22  | 5:J:144:LEU:HD21  | 1.83                     | 0.59              |
| 10:V:255:ILE:HD13 | 10:V:260:SER:HA   | 1.84                     | 0.59              |
| 11:Y:349:LEU:HD13 | 11:Y:357:GLU:HB2  | 1.84                     | 0.59              |
| 5:J:641:LEU:HA    | 5:J:644:ILE:HG22  | 1.84                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:P:748:LYS:HG2   | 5:P:756:ALA:HB1   | 1.83                     | 0.59              |
| 12:I:303:GLU:HB3  | 12:I:317:LEU:HD12 | 1.84                     | 0.59              |
| 7:L:43:ASP:O      | 7:L:47:ASP:HB2    | 2.02                     | 0.59              |
| 1:A:1267:ARG:NH1  | 1:A:1315:GLY:O    | 2.36                     | 0.59              |
| 1:A:1431:PRO:HG2  | 1:A:1434:ILE:HG13 | 1.83                     | 0.59              |
| 10:V:388:TYR:O    | 10:V:392:ILE:HD12 | 2.02                     | 0.59              |
| 1:A:274:VAL:HG22  | 1:A:408:CYS:HB3   | 1.85                     | 0.59              |
| 1:A:1381:ARG:NH2  | 1:A:1418:ASP:OD2  | 2.36                     | 0.59              |
| 13:N:297:VAL:HG21 | 13:N:325:ARG:HB2  | 1.85                     | 0.59              |
| 1:A:411:HIS:NE2   | 1:A:414:THR:OG1   | 2.31                     | 0.59              |
| 5:P:53:LYS:HG2    | 5:P:56:LYS:HD2    | 1.85                     | 0.59              |
| 11:Y:359:ILE:O    | 11:Y:363:ARG:HG3  | 2.02                     | 0.59              |
| 11:Z:49:HIS:O     | 11:Z:49:HIS:ND1   | 2.35                     | 0.59              |
| 5:P:46:THR:O      | 5:P:50:ARG:HG2    | 2.03                     | 0.59              |
| 5:P:465:LEU:O     | 5:P:469:MET:HG2   | 2.03                     | 0.59              |
| 5:P:702:ASN:ND2   | 5:P:705:CYS:SG    | 2.75                     | 0.59              |
| 11:Z:383:TYR:OH   | 11:Z:391:GLU:HB3  | 2.02                     | 0.59              |
| 1:A:1016:MET:SD   | 1:A:1084:ARG:HG3  | 2.43                     | 0.59              |
| 1:A:1599:ASN:HD22 | 1:A:1603:LEU:HD12 | 1.68                     | 0.59              |
| 6:Q:477:GLN:OE1   | 10:U:148:ASN:ND2  | 2.36                     | 0.59              |
| 13:N:512:LYS:O    | 13:N:516:ILE:HG12 | 2.02                     | 0.59              |
| 5:J:610:GLU:O     | 5:J:614:THR:HG22  | 2.02                     | 0.58              |
| 6:Q:6:LEU:HG      | 6:Q:29:VAL:HG22   | 1.84                     | 0.58              |
| 12:I:664:ARG:NH1  | 12:I:719:ALA:O    | 2.36                     | 0.58              |
| 13:N:393:THR:HA   | 13:N:396:ILE:HB   | 1.84                     | 0.58              |
| 7:L:175:THR:HG23  | 7:L:178:PHE:H     | 1.68                     | 0.58              |
| 1:A:1864:GLY:O    | 1:A:1868:VAL:HG12 | 2.03                     | 0.58              |
| 5:P:728:GLU:HA    | 11:Z:152:ARG:HH22 | 1.68                     | 0.58              |
| 10:U:423:ARG:HG3  | 10:U:423:ARG:HH11 | 1.67                     | 0.58              |
| 1:A:1736:GLU:HG3  | 1:A:1756:LYS:HE2  | 1.84                     | 0.58              |
| 6:Q:429:LEU:O     | 6:Q:432:ILE:HG22  | 2.04                     | 0.58              |
| 10:V:180:ARG:NH2  | 10:V:208:GLU:OE2  | 2.35                     | 0.58              |
| 11:Y:109:ALA:O    | 11:Y:113:THR:HG23 | 2.04                     | 0.58              |
| 11:Y:465:LEU:HD21 | 11:Y:480:ILE:HB   | 1.83                     | 0.58              |
| 11:Z:240:LEU:HD11 | 11:Z:262:GLN:HE22 | 1.67                     | 0.58              |
| 5:P:684:LYS:NZ    | 5:P:686:GLU:OE1   | 2.30                     | 0.58              |
| 6:Q:325:LYS:HE2   | 6:Q:329:LEU:HD21  | 1.85                     | 0.58              |
| 12:I:9:PRO:HG2    | 12:I:750:ASP:HB3  | 1.84                     | 0.58              |
| 13:N:375:LEU:HD21 | 13:N:416:ILE:HG13 | 1.86                     | 0.58              |
| 1:A:497:LEU:HD11  | 1:A:587:ILE:HD11  | 1.85                     | 0.58              |
| 1:A:761:ALA:O     | 1:A:765:VAL:HG22  | 2.03                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:V:96:VAL:HG23  | 10:V:98:GLU:HG3   | 1.85                     | 0.58              |
| 1:A:880:TYR:HB2   | 1:A:930:LEU:HD22  | 1.86                     | 0.58              |
| 9:O:41:LEU:HD13   | 9:O:132:VAL:HG13  | 1.86                     | 0.58              |
| 1:A:1023:VAL:O    | 1:A:1027:ILE:HG13 | 2.04                     | 0.58              |
| 9:O:435:SER:HB3   | 9:O:654:ASP:HB3   | 1.84                     | 0.58              |
| 13:N:98:CYS:HA    | 13:N:110:LEU:HD23 | 1.86                     | 0.58              |
| 9:O:97:ILE:HD11   | 9:O:158:LEU:HD11  | 1.84                     | 0.58              |
| 11:Y:357:GLU:O    | 11:Y:361:HIS:ND1  | 2.36                     | 0.58              |
| 12:I:117:GLU:O    | 12:I:579:LYS:NZ   | 2.34                     | 0.58              |
| 1:A:76:LEU:HD12   | 1:A:589:ASP:HB3   | 1.84                     | 0.58              |
| 1:A:1635:GLU:HB2  | 1:A:1669:LYS:HD2  | 1.86                     | 0.58              |
| 9:O:344:LEU:HD22  | 9:O:359:VAL:HG21  | 1.85                     | 0.58              |
| 5:P:522:PHE:HB3   | 5:P:539:TYR:CD2   | 2.39                     | 0.58              |
| 12:I:393:VAL:O    | 12:I:397:ILE:HG13 | 2.04                     | 0.58              |
| 5:J:42:PHE:HB2    | 5:J:71:CYS:SG     | 2.44                     | 0.57              |
| 11:Z:203:SER:O    | 11:Z:207:LYS:HG2  | 2.04                     | 0.57              |
| 11:Z:350:ARG:NE   | 11:Z:382:CYS:SG   | 2.76                     | 0.57              |
| 11:Z:355:VAL:O    | 11:Z:359:ILE:HG13 | 2.04                     | 0.57              |
| 12:I:25:PHE:HD2   | 12:I:71:LEU:HB2   | 1.69                     | 0.57              |
| 6:K:174:HIS:NE2   | 6:K:211:LYS:HD2   | 2.20                     | 0.57              |
| 11:Y:394:VAL:HA   | 11:Y:397:ASN:HD21 | 1.69                     | 0.57              |
| 5:J:538:ILE:O     | 5:J:542:THR:HG23  | 2.05                     | 0.57              |
| 7:L:73:THR:O      | 7:L:160:THR:HG22  | 2.05                     | 0.57              |
| 6:Q:207:ASN:HD21  | 6:Q:233:VAL:HG13  | 1.69                     | 0.57              |
| 10:V:370:LEU:O    | 10:V:374:GLU:HG2  | 2.05                     | 0.57              |
| 11:Z:431:LEU:HD11 | 11:Z:447:LYS:HG3  | 1.87                     | 0.57              |
| 13:N:220:LEU:HA   | 13:N:227:ASP:HA   | 1.85                     | 0.57              |
| 5:P:130:ARG:HD2   | 5:P:133:LYS:HD2   | 1.85                     | 0.57              |
| 1:A:1095:VAL:HG23 | 1:A:1098:GLU:HB2  | 1.86                     | 0.57              |
| 2:D:48:ASP:N      | 2:D:48:ASP:OD1    | 2.36                     | 0.57              |
| 10:V:322:ASN:O    | 10:V:326:ILE:HG13 | 2.05                     | 0.57              |
| 11:Y:4:ILE:HG21   | 11:Y:41:GLN:HG2   | 1.87                     | 0.57              |
| 11:Y:377:GLU:O    | 11:Y:381:GLU:HG2  | 2.04                     | 0.57              |
| 11:Y:431:LEU:HD21 | 11:Y:448:LYS:HG2  | 1.87                     | 0.57              |
| 13:N:221:CYS:N    | 13:N:226:SER:O    | 2.35                     | 0.57              |
| 11:Y:425:GLU:HA   | 11:Y:428:LYS:HD2  | 1.86                     | 0.57              |
| 9:O:435:SER:H     | 9:O:654:ASP:HB3   | 1.69                     | 0.57              |
| 11:Y:218:SER:HA   | 11:Y:221:ILE:HD12 | 1.87                     | 0.57              |
| 11:Y:235:ASP:HB3  | 11:Y:266:LEU:HD21 | 1.86                     | 0.57              |
| 11:Z:217:ASN:O    | 11:Z:221:ILE:HG23 | 2.05                     | 0.57              |
| 7:L:82:ASP:HA     | 7:L:117:SER:HA    | 1.86                     | 0.57              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 10:U:33:LYS:HE2    | 10:U:64:ALA:HA    | 1.87                     | 0.57              |
| 1:A:612:ILE:HD13   | 1:A:642:TYR:HD1   | 1.69                     | 0.57              |
| 5:J:149:TRP:NE1    | 5:J:153:GLU:OE1   | 2.35                     | 0.57              |
| 11:Y:24:SER:HB3    | 11:Y:49:HIS:HE2   | 1.69                     | 0.57              |
| 11:Z:466[A]:ARG:HE | 11:Z:481:LEU:HD11 | 1.70                     | 0.57              |
| 1:A:1032:LEU:HD12  | 13:N:483:ASP:HB2  | 1.86                     | 0.56              |
| 10:V:34:LYS:NZ     | 10:V:69:GLU:O     | 2.27                     | 0.56              |
| 10:V:345:SER:O     | 10:V:345:SER:OG   | 2.21                     | 0.56              |
| 10:V:449:LEU:HD12  | 10:V:476:LEU:HD11 | 1.86                     | 0.56              |
| 11:Y:441:TYR:HD2   | 11:Y:444:ALA:H    | 1.53                     | 0.56              |
| 9:O:446:LEU:O      | 9:O:460:GLN:NE2   | 2.38                     | 0.56              |
| 6:Q:451:LEU:HB3    | 6:Q:467:TYR:CD2   | 2.39                     | 0.56              |
| 11:Y:260:PHE:HB3   | 11:Y:277:TYR:CD1  | 2.41                     | 0.56              |
| 11:Z:102:ILE:HG13  | 11:Z:103:GLU:N    | 2.19                     | 0.56              |
| 12:I:185:ILE:HD11  | 12:I:201:ILE:HG13 | 1.86                     | 0.56              |
| 1:A:1255:VAL:HG21  | 1:A:1606:LEU:HD11 | 1.86                     | 0.56              |
| 1:A:1634:LEU:O     | 1:A:1650:GLU:HA   | 2.05                     | 0.56              |
| 5:P:126:CYS:SG     | 5:P:158:ILE:HD11  | 2.44                     | 0.56              |
| 6:Q:146:ARG:O      | 6:Q:150:THR:HG23  | 2.06                     | 0.56              |
| 6:Q:177:THR:HG22   | 6:Q:180:GLU:HB2   | 1.86                     | 0.56              |
| 11:Z:400:TYR:HA    | 11:Z:409:THR:HB   | 1.86                     | 0.56              |
| 13:N:267:GLN:O     | 13:N:271:GLU:HG2  | 2.05                     | 0.56              |
| 1:A:872:LEU:HD11   | 1:A:937:VAL:HG11  | 1.88                     | 0.56              |
| 5:J:522:PHE:HA     | 5:J:525:VAL:HG12  | 1.87                     | 0.56              |
| 7:L:37:LYS:HG3     | 7:L:38:PRO:HD2    | 1.88                     | 0.56              |
| 10:V:34:LYS:NZ     | 10:V:69:GLU:OE2   | 2.36                     | 0.56              |
| 10:V:133:GLU:N     | 10:V:133:GLU:OE1  | 2.39                     | 0.56              |
| 10:V:213:ILE:HD11  | 10:V:222:LEU:HD12 | 1.87                     | 0.56              |
| 11:Z:100:SER:O     | 11:Z:104:VAL:HG23 | 2.05                     | 0.56              |
| 4:H:72:HIS:O       | 4:H:76:VAL:HG23   | 2.06                     | 0.56              |
| 11:Z:352:MET:SD    | 11:Z:354:ARG:NH2  | 2.78                     | 0.56              |
| 13:N:104:GLU:OE2   | 13:N:175:ARG:NH2  | 2.37                     | 0.56              |
| 1:A:1564:LEU:HD23  | 1:A:1567:LEU:HD13 | 1.87                     | 0.56              |
| 5:P:736:GLU:OE1    | 5:P:736:GLU:N     | 2.38                     | 0.56              |
| 6:Q:441:VAL:HG21   | 6:Q:444:TRP:HD1   | 1.70                     | 0.56              |
| 10:U:185:VAL:HG13  | 10:U:212:LEU:HD22 | 1.86                     | 0.56              |
| 11:Y:274:MET:HB3   | 11:Y:297:LEU:HD11 | 1.88                     | 0.56              |
| 12:I:717:MET:HG3   | 12:I:719:ALA:HB2  | 1.86                     | 0.56              |
| 13:N:181:LEU:HD23  | 13:N:268:VAL:HG21 | 1.86                     | 0.56              |
| 5:J:38:GLU:HG3     | 5:J:66:CYS:HB2    | 1.87                     | 0.56              |
| 5:P:158:ILE:HG22   | 5:P:160:GLU:H     | 1.70                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:Q:161:VAL:HG13  | 6:Q:162:TYR:HD2   | 1.71                     | 0.56              |
| 11:Y:339:VAL:O    | 11:Y:343:LEU:HG   | 2.05                     | 0.56              |
| 13:N:386:LEU:HD12 | 13:N:391:VAL:HG11 | 1.88                     | 0.56              |
| 1:A:985:LYS:O     | 1:A:989:GLU:HG2   | 2.06                     | 0.56              |
| 5:J:138:TYR:HD1   | 5:J:151:PRO:HB3   | 1.71                     | 0.56              |
| 10:U:520:TYR:HB3  | 10:U:529:ALA:HB2  | 1.88                     | 0.56              |
| 11:Z:38:SER:O     | 11:Z:42:LYS:HG3   | 2.05                     | 0.56              |
| 9:O:644:LEU:HD11  | 9:O:666:LEU:HG    | 1.88                     | 0.56              |
| 13:N:162:PHE:O    | 13:N:255:ARG:NH2  | 2.37                     | 0.56              |
| 1:A:851:CYS:SG    | 1:A:882:LEU:HD11  | 2.46                     | 0.55              |
| 9:O:44:MET:HG3    | 9:O:89:LEU:HD21   | 1.88                     | 0.55              |
| 11:Y:274:MET:HG3  | 11:Y:297:LEU:HD21 | 1.88                     | 0.55              |
| 7:L:45:LEU:HD21   | 7:L:153:MET:HG2   | 1.88                     | 0.55              |
| 5:P:605:THR:HG21  | 5:P:636:ASN:HB3   | 1.89                     | 0.55              |
| 11:Y:118:ASP:OD1  | 11:Y:118:ASP:N    | 2.39                     | 0.55              |
| 12:I:125:LEU:HD21 | 12:I:249:THR:HG21 | 1.87                     | 0.55              |
| 11:Z:259:LYS:HA   | 11:Z:262:GLN:HE21 | 1.72                     | 0.55              |
| 1:A:111:LEU:H     | 9:O:508:MET:HE2   | 1.71                     | 0.55              |
| 1:A:1525:MET:SD   | 1:A:1588:LEU:HD13 | 2.47                     | 0.55              |
| 1:A:1540:ARG:HG3  | 1:A:1540:ARG:HH11 | 1.72                     | 0.55              |
| 6:Q:341:GLY:HA3   | 6:Q:357:TYR:CE1   | 2.41                     | 0.55              |
| 10:V:244:ILE:HG21 | 10:V:276:ILE:HB   | 1.88                     | 0.55              |
| 11:Z:5:ASP:OD1    | 11:Z:8:ARG:NH2    | 2.39                     | 0.55              |
| 5:P:707:PHE:HE2   | 5:P:738:LEU:HB3   | 1.70                     | 0.55              |
| 11:Z:161:VAL:O    | 11:Z:165:CYS:HB3  | 2.07                     | 0.55              |
| 12:I:734:LEU:HD12 | 12:I:741:VAL:HG12 | 1.89                     | 0.55              |
| 7:L:78:CYS:SG     | 7:L:157:LYS:HB2   | 2.47                     | 0.55              |
| 11:Y:27:LEU:O     | 11:Y:31:ASN:ND2   | 2.40                     | 0.55              |
| 11:Y:359:ILE:HG22 | 11:Y:363:ARG:HE   | 1.72                     | 0.55              |
| 11:Z:140:MET:HA   | 11:Z:143:ASN:HD21 | 1.72                     | 0.55              |
| 13:N:262:THR:O    | 13:N:266:HIS:ND1  | 2.39                     | 0.55              |
| 10:V:26:PHE:HE1   | 10:V:228:TRP:HE3  | 1.55                     | 0.55              |
| 11:Y:469:LEU:HD12 | 11:Y:473:SER:HA   | 1.88                     | 0.55              |
| 6:K:212:TYR:HH    | 6:K:368:HIS:HD1   | 1.55                     | 0.55              |
| 9:O:536:THR:HB    | 9:O:543:GLY:HA3   | 1.88                     | 0.55              |
| 11:Y:65:LYS:HA    | 11:Y:68:MET:HG3   | 1.89                     | 0.55              |
| 1:A:430:VAL:HG13  | 1:A:444:PHE:HB3   | 1.89                     | 0.55              |
| 1:A:953:LEU:HD22  | 1:A:1817:VAL:HG22 | 1.89                     | 0.55              |
| 5:J:605:THR:HG23  | 5:J:606:LEU:HD22  | 1.89                     | 0.55              |
| 6:K:212:TYR:OH    | 6:K:368:HIS:ND1   | 2.40                     | 0.55              |
| 9:O:727:THR:HG22  | 9:O:731:ASN:HD21  | 1.71                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:V:301:ASP:OD1  | 10:V:301:ASP:N    | 2.38                     | 0.55              |
| 1:A:1100:LEU:HD13 | 1:A:1147:ILE:HD11 | 1.89                     | 0.54              |
| 6:K:338:ILE:HD11  | 6:K:370:PRO:HG3   | 1.89                     | 0.54              |
| 9:O:44:MET:HE2    | 12:I:310:TRP:HZ2  | 1.72                     | 0.54              |
| 6:Q:461:TYR:HD2   | 6:Q:492:MET:HG2   | 1.72                     | 0.54              |
| 11:Z:296:ARG:O    | 11:Z:300:ILE:HG12 | 2.07                     | 0.54              |
| 11:Z:373:LEU:O    | 11:Z:377:GLU:HG3  | 2.07                     | 0.54              |
| 13:N:504:LEU:O    | 13:N:508:ILE:HG23 | 2.07                     | 0.54              |
| 6:K:165:GLU:HG2   | 6:Q:20:GLN:HB3    | 1.89                     | 0.54              |
| 10:V:290:ARG:NH2  | 10:V:322:ASN:OD1  | 2.34                     | 0.54              |
| 13:N:83:LEU:HA    | 13:N:87:ILE:HB    | 1.89                     | 0.54              |
| 13:N:351:PHE:CE1  | 13:N:409:VAL:HG11 | 2.42                     | 0.54              |
| 1:A:1875:GLN:N    | 1:A:1875:GLN:OE1  | 2.40                     | 0.54              |
| 10:U:467:LYS:NZ   | 10:U:506:HIS:HB3  | 2.23                     | 0.54              |
| 13:N:626:TYR:CE2  | 13:N:635:LEU:HG   | 2.41                     | 0.54              |
| 1:A:170:ILE:HG21  | 10:V:427:GLN:HB2  | 1.90                     | 0.54              |
| 5:J:53:LYS:HZ1    | 5:J:56:LYS:HD2    | 1.73                     | 0.54              |
| 11:Y:105:LYS:HA   | 11:Y:108:MET:CG   | 2.38                     | 0.54              |
| 11:Y:305:ALA:O    | 11:Y:309:VAL:HG23 | 2.08                     | 0.54              |
| 12:I:601:LEU:HB2  | 12:I:615:LEU:HD13 | 1.89                     | 0.54              |
| 12:I:692:ARG:NH1  | 12:I:695:GLU:OE1  | 2.41                     | 0.54              |
| 10:V:471:VAL:HG11 | 10:V:508:GLU:HG3  | 1.90                     | 0.54              |
| 13:N:537:ARG:NH1  | 13:N:541:ASN:HB2  | 2.22                     | 0.54              |
| 1:A:1595:HIS:CE1  | 1:A:1598:ASP:HB2  | 2.43                     | 0.54              |
| 5:J:97:PHE:CD2    | 11:Y:252:ASP:HB3  | 2.42                     | 0.54              |
| 5:J:626:ASN:O     | 5:J:630:VAL:HG13  | 2.08                     | 0.54              |
| 10:U:410:GLU:HB2  | 10:U:418:CYS:SG   | 2.47                     | 0.54              |
| 10:V:216:LYS:HD3  | 10:V:243:LEU:HD11 | 1.89                     | 0.54              |
| 11:Z:372:ARG:HH21 | 11:Z:374:ASP:HB2  | 1.73                     | 0.54              |
| 1:A:252:ASP:HB2   | 1:A:253:PRO:HD3   | 1.90                     | 0.54              |
| 12:I:282:GLN:HB2  | 12:I:337:ILE:HD11 | 1.90                     | 0.54              |
| 12:I:640:ASP:OD1  | 12:I:641:ALA:N    | 2.40                     | 0.54              |
| 13:N:535:PRO:O    | 13:N:539:ILE:HG23 | 2.08                     | 0.54              |
| 1:A:768:LEU:HD21  | 1:A:861:PRO:HB2   | 1.90                     | 0.54              |
| 9:O:57:ARG:HH21   | 12:I:306:HIS:HE1  | 1.53                     | 0.54              |
| 10:V:58:LEU:O     | 10:V:61:SER:OG    | 2.26                     | 0.54              |
| 5:J:617:LEU:HG    | 5:J:644:ILE:HG13  | 1.90                     | 0.54              |
| 11:Y:19:VAL:HG23  | 11:Y:52:SER:HB3   | 1.90                     | 0.54              |
| 11:Z:465:LEU:HD21 | 11:Z:480:ILE:HB   | 1.90                     | 0.54              |
| 12:I:254:LYS:O    | 12:I:258:ILE:HG12 | 2.08                     | 0.54              |
| 1:A:1672:ARG:NH1  | 1:A:1706:LEU:O    | 2.41                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:P:53:LYS:HB3    | 5:P:56:LYS:HB2    | 1.89                     | 0.53              |
| 11:Z:41:GLN:O     | 11:Z:45:LEU:HG    | 2.08                     | 0.53              |
| 13:N:83:LEU:HB3   | 13:N:160:VAL:HG11 | 1.91                     | 0.53              |
| 1:A:862:TYR:CZ    | 1:A:864:PRO:HA    | 2.43                     | 0.53              |
| 1:A:1131:MET:HG2  | 1:A:1132:THR:HG23 | 1.90                     | 0.53              |
| 6:K:19:TYR:HB3    | 6:K:50:THR:HG22   | 1.90                     | 0.53              |
| 10:U:29:LEU:HB2   | 10:U:30:ARG:HH21  | 1.70                     | 0.53              |
| 10:V:381:THR:HG21 | 10:V:412:LEU:HD11 | 1.90                     | 0.53              |
| 11:Y:479:ARG:HD2  | 11:Y:510:LYS:HB3  | 1.90                     | 0.53              |
| 11:Z:3:VAL:O      | 11:Z:7:VAL:HG23   | 2.08                     | 0.53              |
| 11:Z:156:THR:O    | 11:Z:160:GLU:HG3  | 2.08                     | 0.53              |
| 5:J:515:TYR:HB3   | 5:J:546:LEU:HD11  | 1.91                     | 0.53              |
| 7:L:170:PHE:HB3   | 5:P:738:LEU:HD21  | 1.90                     | 0.53              |
| 11:Z:257:VAL:HG13 | 11:Z:277:TYR:HE1  | 1.73                     | 0.53              |
| 1:A:728:LEU:HD13  | 9:O:716:PHE:HE1   | 1.73                     | 0.53              |
| 1:A:765:VAL:HG12  | 1:A:863:LEU:HD21  | 1.90                     | 0.53              |
| 11:Z:227:LEU:HA   | 11:Z:230:LYS:HE3  | 1.89                     | 0.53              |
| 12:I:683:TYR:CE2  | 12:I:703:ARG:HB2  | 2.44                     | 0.53              |
| 1:A:965:GLN:HB2   | 1:A:1833:HIS:NE2  | 2.24                     | 0.53              |
| 9:O:73:ILE:O      | 9:O:161:TYR:OH    | 2.21                     | 0.53              |
| 13:N:400:TYR:HE1  | 13:N:421:CYS:HG   | 1.55                     | 0.53              |
| 6:K:90:LEU:HD21   | 6:K:140:TYR:CE1   | 2.44                     | 0.53              |
| 11:Y:257:VAL:HA   | 11:Y:260:PHE:HD1  | 1.73                     | 0.53              |
| 10:V:493:TYR:O    | 10:V:497:ILE:HG23 | 2.08                     | 0.53              |
| 12:I:425:MET:O    | 12:I:429:THR:HG22 | 2.09                     | 0.53              |
| 1:A:489:LEU:HD21  | 1:A:509:VAL:HG21  | 1.90                     | 0.53              |
| 4:H:61:TYR:HD1    | 11:Z:326:TYR:CG   | 2.26                     | 0.53              |
| 7:L:105:LEU:HD21  | 7:L:136:MET:HG2   | 1.89                     | 0.53              |
| 5:P:92:LEU:HD22   | 5:P:120:LEU:HD23  | 1.91                     | 0.53              |
| 10:U:190:ASP:O    | 10:U:194:GLU:HG3  | 2.09                     | 0.53              |
| 1:A:77:ARG:NE     | 1:A:91:GLU:OE2    | 2.32                     | 0.53              |
| 6:K:519:LEU:O     | 6:K:523:ILE:HG12  | 2.09                     | 0.53              |
| 11:Y:362:PHE:HB2  | 11:Y:379:LEU:HD13 | 1.90                     | 0.53              |
| 1:A:100:VAL:HG21  | 1:A:153:ILE:HG12  | 1.91                     | 0.53              |
| 9:O:378:SER:HB3   | 9:O:409:HIS:CE1   | 2.43                     | 0.53              |
| 5:P:93:SER:HB2    | 5:P:106:ILE:HD11  | 1.91                     | 0.53              |
| 10:U:327:ASP:O    | 10:U:333:THR:HG21 | 2.09                     | 0.53              |
| 10:V:429:ARG:HG2  | 10:V:432:ASP:HB2  | 1.91                     | 0.53              |
| 11:Z:7:VAL:HG22   | 11:Z:22:LEU:HD21  | 1.90                     | 0.53              |
| 11:Z:306:GLU:HA   | 11:Z:309:VAL:HG22 | 1.90                     | 0.53              |
| 1:A:449:GLN:OE1   | 1:A:453:ARG:NH2   | 2.42                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:L:113:LEU:HB3   | 7:L:116:PRO:HG3   | 1.91                     | 0.52              |
| 10:U:253:ASN:O    | 10:U:257:VAL:HG13 | 2.09                     | 0.52              |
| 1:A:632:GLU:HG2   | 1:A:633:ILE:N     | 2.24                     | 0.52              |
| 5:J:79:CYS:SG     | 5:J:87:GLU:HB2    | 2.48                     | 0.52              |
| 5:J:125:TYR:HD1   | 5:J:130:ARG:HE    | 1.57                     | 0.52              |
| 6:K:264:HIS:CE1   | 6:K:266:SER:HB3   | 2.44                     | 0.52              |
| 7:L:21:THR:HG23   | 7:L:22:VAL:HG13   | 1.89                     | 0.52              |
| 12:I:750:ASP:OD2  | 12:I:751:GLU:N    | 2.41                     | 0.52              |
| 1:A:27:HIS:HB3    | 1:A:101:ILE:HD13  | 1.91                     | 0.52              |
| 7:L:177:ASP:OD2   | 11:Z:119:LYS:NZ   | 2.34                     | 0.52              |
| 9:O:489:VAL:HG23  | 12:I:507:LEU:HD11 | 1.90                     | 0.52              |
| 9:O:562:LYS:O     | 9:O:566:LYS:HG3   | 2.10                     | 0.52              |
| 11:Y:176:LEU:HD21 | 11:Y:185:VAL:HG21 | 1.89                     | 0.52              |
| 12:I:557:TYR:HA   | 12:I:694:ASP:HB2  | 1.91                     | 0.52              |
| 1:A:1267:ARG:NE   | 1:A:1271:GLU:OE2  | 2.39                     | 0.52              |
| 5:J:113:SER:O     | 5:J:117:THR:HG23  | 2.09                     | 0.52              |
| 5:J:549:ASP:OD1   | 5:J:549:ASP:N     | 2.36                     | 0.52              |
| 6:K:37:PRO:HA     | 6:K:65:LEU:HD21   | 1.92                     | 0.52              |
| 9:O:504:ALA:HA    | 9:O:507:TRP:CD1   | 2.45                     | 0.52              |
| 5:P:55:TYR:HA     | 5:P:82:LEU:HD21   | 1.91                     | 0.52              |
| 6:Q:263:PHE:HE2   | 6:Q:294:LEU:HD13  | 1.74                     | 0.52              |
| 11:Y:18:ASN:OD1   | 11:Z:170:ASP:N    | 2.37                     | 0.52              |
| 13:N:626:TYR:OH   | 13:N:633:ARG:HB3  | 2.10                     | 0.52              |
| 1:A:614:THR:O     | 9:O:556:GLN:NE2   | 2.43                     | 0.52              |
| 1:A:884:ASP:OD1   | 1:A:884:ASP:N     | 2.42                     | 0.52              |
| 1:A:1197:LEU:HD12 | 1:A:1227:LEU:HD11 | 1.91                     | 0.52              |
| 1:A:1552:TYR:OH   | 1:A:1604:GLN:NE2  | 2.42                     | 0.52              |
| 5:J:662:LEU:HD12  | 5:J:704:LEU:HD13  | 1.90                     | 0.52              |
| 6:K:402:PRO:HG3   | 6:K:431:LYS:HB3   | 1.90                     | 0.52              |
| 5:P:472:GLY:HA3   | 5:P:488:LEU:HD13  | 1.92                     | 0.52              |
| 12:I:214:LEU:O    | 12:I:238:THR:OG1  | 2.27                     | 0.52              |
| 5:J:164:PRO:HB2   | 5:J:471:LYS:HG3   | 1.92                     | 0.52              |
| 9:O:378:SER:HB3   | 9:O:409:HIS:HE1   | 1.75                     | 0.52              |
| 12:I:417:PHE:HA   | 12:I:448:VAL:HG22 | 1.91                     | 0.52              |
| 9:O:109:GLU:HB2   | 10:U:344:ARG:NH2  | 2.25                     | 0.52              |
| 9:O:491:LYS:HZ1   | 12:I:500:PHE:HE1  | 1.57                     | 0.52              |
| 5:P:482:LYS:HE2   | 5:P:667:GLN:HE22  | 1.75                     | 0.52              |
| 6:Q:276:VAL:HA    | 6:Q:311:MET:HE2   | 1.92                     | 0.52              |
| 10:U:385:ILE:O    | 10:U:389:ARG:HG3  | 2.10                     | 0.52              |
| 12:I:586:LEU:HD23 | 12:I:601:LEU:HD23 | 1.92                     | 0.52              |
| 1:A:1201:HIS:HB3  | 1:A:1204:THR:HB   | 1.91                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:J:624:PHE:O     | 5:J:628:ILE:HG13  | 2.10                     | 0.52              |
| 7:L:78:CYS:HG     | 7:L:159:TYR:HE2   | 1.56                     | 0.52              |
| 9:O:625:LEU:HD22  | 9:O:666:LEU:HD23  | 1.91                     | 0.52              |
| 5:P:721:SER:O     | 5:P:724:GLN:HG2   | 2.10                     | 0.52              |
| 10:V:295:TYR:HA   | 10:V:326:ILE:HD13 | 1.92                     | 0.52              |
| 11:Y:7:VAL:HG12   | 11:Y:48:TYR:HD2   | 1.75                     | 0.52              |
| 11:Z:261:GLU:O    | 11:Z:264:GLN:NE2  | 2.43                     | 0.52              |
| 11:Z:458:TYR:HD1  | 11:Z:484:PHE:HD1  | 1.58                     | 0.52              |
| 1:A:116:ALA:O     | 9:O:267:VAL:HG23  | 2.10                     | 0.52              |
| 1:A:250:ASN:HD22  | 1:A:432:ILE:HD12  | 1.75                     | 0.52              |
| 6:K:357:TYR:HB3   | 6:K:374:ILE:HG13  | 1.91                     | 0.52              |
| 11:Z:15:LEU:HD23  | 11:Z:15:LEU:H     | 1.74                     | 0.52              |
| 5:J:533:VAL:HG23  | 5:J:559:LEU:HD22  | 1.91                     | 0.52              |
| 11:Y:277:TYR:HD2  | 11:Y:293:LEU:HD22 | 1.75                     | 0.52              |
| 12:I:61:ASN:CG    | 12:I:62:GLU:H     | 2.13                     | 0.52              |
| 13:N:412:PRO:HB2  | 13:N:486:ASP:HB2  | 1.92                     | 0.52              |
| 13:N:598:SER:HB3  | 14:C:13:THR:HB    | 1.91                     | 0.52              |
| 6:K:153:TYR:HB2   | 6:K:170:LEU:HD21  | 1.92                     | 0.51              |
| 6:K:167:PHE:CZ    | 6:K:209:LEU:HD13  | 2.46                     | 0.51              |
| 5:P:49:TYR:OH     | 5:P:81:ASP:OD2    | 2.23                     | 0.51              |
| 11:Y:406:ASN:O    | 11:Y:410:LEU:HG   | 2.10                     | 0.51              |
| 13:N:365:LEU:HD11 | 13:N:374:LEU:HD13 | 1.91                     | 0.51              |
| 13:N:435:VAL:O    | 13:N:439:VAL:HG13 | 2.11                     | 0.51              |
| 1:A:1914:LEU:HD21 | 1:A:1935:LEU:HB3  | 1.93                     | 0.51              |
| 5:J:656:MET:HG3   | 11:Y:492:GLN:HB2  | 1.92                     | 0.51              |
| 6:K:90:LEU:HD21   | 6:K:140:TYR:HE1   | 1.75                     | 0.51              |
| 6:K:500:ASP:O     | 6:K:504:THR:HG23  | 2.10                     | 0.51              |
| 10:U:373:HIS:ND1  | 10:U:388:TYR:OH   | 2.38                     | 0.51              |
| 1:A:514:LEU:HD21  | 1:A:605:VAL:HG11  | 1.93                     | 0.51              |
| 6:K:171:THR:HG21  | 6:K:209:LEU:HD11  | 1.92                     | 0.51              |
| 10:U:38:LEU:HB3   | 10:U:71:GLN:HE22  | 1.76                     | 0.51              |
| 1:A:637:MET:HG3   | 1:A:667:MET:HE1   | 1.92                     | 0.51              |
| 1:A:1797:ILE:HD13 | 1:A:1851:THR:HG21 | 1.93                     | 0.51              |
| 5:J:600:TYR:HD2   | 5:J:603:ALA:HB2   | 1.75                     | 0.51              |
| 8:M:31:ILE:HD13   | 6:Q:302:TRP:HZ3   | 1.75                     | 0.51              |
| 9:O:653:ALA:HB2   | 12:I:368:GLY:HA3  | 1.90                     | 0.51              |
| 10:V:333:THR:O    | 10:V:337:ILE:HG12 | 2.10                     | 0.51              |
| 13:N:570:ILE:HA   | 13:N:573:ASN:HD21 | 1.76                     | 0.51              |
| 13:N:595:ILE:HD12 | 14:C:12:ALA:HB3   | 1.93                     | 0.51              |
| 1:A:819:GLN:NE2   | 1:A:820:VAL:O     | 2.44                     | 0.51              |
| 10:U:471:VAL:HG21 | 10:U:508:GLU:HG3  | 1.90                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:Z:242:SER:O    | 11:Z:246:LEU:HG   | 2.11                     | 0.51              |
| 11:Z:411:THR:HG21 | 11:Z:441:TYR:CE2  | 2.44                     | 0.51              |
| 1:A:1086:MET:HG3  | 1:A:1610:TYR:CZ   | 2.46                     | 0.51              |
| 1:A:1815:LYS:O    | 1:A:1819:GLU:HG3  | 2.10                     | 0.51              |
| 12:I:434:LEU:HD12 | 12:I:435:PRO:HD2  | 1.92                     | 0.51              |
| 13:N:534:SER:HB2  | 13:N:537:ARG:HB3  | 1.92                     | 0.51              |
| 1:A:1865:ASP:HB3  | 1:A:1934:LEU:HD21 | 1.93                     | 0.51              |
| 5:J:613:LEU:HD12  | 5:J:679:GLN:HG2   | 1.93                     | 0.51              |
| 6:Q:133:CYS:HB3   | 6:Q:156:ALA:HB2   | 1.92                     | 0.51              |
| 10:U:429:ARG:HB2  | 10:U:435:MET:HE1  | 1.92                     | 0.51              |
| 11:Y:465:LEU:HD11 | 11:Y:477:LEU:HD22 | 1.93                     | 0.51              |
| 11:Z:362:PHE:O    | 11:Z:366:ILE:HG23 | 2.10                     | 0.51              |
| 5:J:673:CYS:O     | 5:J:677:VAL:HG23  | 2.10                     | 0.51              |
| 6:Q:320:ARG:NH1   | 6:Q:343:SER:OG    | 2.44                     | 0.51              |
| 1:A:1871:TYR:CZ   | 1:A:1889:LEU:HD21 | 2.45                     | 0.51              |
| 5:P:93:SER:O      | 5:P:93:SER:OG     | 2.26                     | 0.51              |
| 11:Z:275:ASP:HB2  | 11:Z:306:GLU:HG3  | 1.93                     | 0.51              |
| 4:H:82:LEU:O      | 4:H:85:LEU:HG     | 2.10                     | 0.51              |
| 6:K:473:VAL:HG23  | 5:P:130:ARG:HH12  | 1.75                     | 0.51              |
| 10:U:289:LEU:HD11 | 10:U:296:ARG:HD3  | 1.92                     | 0.51              |
| 10:V:106:LEU:HB3  | 10:V:118:TYR:HB2  | 1.92                     | 0.51              |
| 11:Z:394:VAL:HA   | 11:Z:397:ASN:HD21 | 1.76                     | 0.51              |
| 12:I:21:GLN:HG2   | 12:I:41:ALA:HB2   | 1.92                     | 0.51              |
| 13:N:540:ARG:O    | 13:N:543:GLU:HG3  | 2.11                     | 0.51              |
| 1:A:121:SER:HB2   | 1:A:155:GLN:NE2   | 2.23                     | 0.50              |
| 1:A:133:ILE:HG22  | 1:A:146:GLU:HA    | 1.92                     | 0.50              |
| 6:K:372:LEU:HD13  | 6:K:404:VAL:HG23  | 1.92                     | 0.50              |
| 10:V:464:ASP:OD1  | 10:V:464:ASP:N    | 2.38                     | 0.50              |
| 10:V:528:GLU:HA   | 10:V:531:THR:HG22 | 1.93                     | 0.50              |
| 11:Y:133:ARG:HB3  | 11:Y:137:ILE:HD11 | 1.93                     | 0.50              |
| 11:Z:43:TYR:HB2   | 11:Z:72:GLN:HG2   | 1.92                     | 0.50              |
| 1:A:434:SER:HB2   | 1:A:440:LYS:HD3   | 1.91                     | 0.50              |
| 1:A:942:ARG:NH1   | 9:O:603:MET:SD    | 2.85                     | 0.50              |
| 5:J:465:LEU:O     | 5:J:469:MET:HE3   | 2.11                     | 0.50              |
| 9:O:91:ASN:O      | 9:O:95:ILE:HG23   | 2.12                     | 0.50              |
| 9:O:467:ALA:HB1   | 9:O:506:LEU:HD11  | 1.93                     | 0.50              |
| 6:Q:213:ASN:OD1   | 6:Q:214:LYS:N     | 2.45                     | 0.50              |
| 13:N:180:PHE:HB2  | 13:N:240:PHE:CE2  | 2.47                     | 0.50              |
| 1:A:188:LEU:HD11  | 1:A:223:LEU:HD13  | 1.93                     | 0.50              |
| 1:A:490:VAL:HG13  | 1:A:498:VAL:HG23  | 1.92                     | 0.50              |
| 1:A:625:ILE:HG12  | 1:A:762:ILE:HD12  | 1.92                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1119:ASP:OD1  | 1:A:1120:LEU:N    | 2.45                     | 0.50              |
| 5:P:742:LEU:O     | 5:P:746:VAL:HG23  | 2.11                     | 0.50              |
| 11:Y:301:SER:HB2  | 11:Y:304:HIS:ND1  | 2.26                     | 0.50              |
| 11:Z:328:GLY:O    | 11:Z:332:ILE:HG22 | 2.12                     | 0.50              |
| 12:I:211:SER:OG   | 12:I:213:ASP:OD1  | 2.24                     | 0.50              |
| 12:I:674:VAL:HA   | 12:I:703:ARG:HD3  | 1.93                     | 0.50              |
| 1:A:1209:LEU:HD22 | 1:A:1228:LEU:HD23 | 1.93                     | 0.50              |
| 1:A:1713:MET:HB2  | 1:A:1715:TRP:HD1  | 1.77                     | 0.50              |
| 9:O:329:ARG:O     | 9:O:333:GLU:HG2   | 2.11                     | 0.50              |
| 11:Z:173:LEU:HD11 | 11:Z:205:TRP:CH2  | 2.46                     | 0.50              |
| 1:A:31:HIS:CD2    | 1:A:32:PRO:HD2    | 2.47                     | 0.50              |
| 1:A:455:VAL:HB    | 1:A:471:VAL:HG22  | 1.94                     | 0.50              |
| 5:J:650:LYS:HE2   | 5:J:653:LEU:HD12  | 1.92                     | 0.50              |
| 6:K:135:LEU:O     | 6:K:139:ILE:HG13  | 2.11                     | 0.50              |
| 11:Z:362:PHE:HB2  | 11:Z:379:LEU:HD13 | 1.94                     | 0.50              |
| 1:A:484:LYS:HB2   | 1:A:592:HIS:HD1   | 1.77                     | 0.50              |
| 1:A:484:LYS:HG3   | 1:A:592:HIS:CE1   | 2.46                     | 0.50              |
| 1:A:592:HIS:CG    | 1:A:592:HIS:O     | 2.65                     | 0.50              |
| 1:A:727:SER:O     | 1:A:728:LEU:HG    | 2.11                     | 0.50              |
| 1:A:805:HIS:NE2   | 1:A:843:SER:HB2   | 2.26                     | 0.50              |
| 11:Y:478:HIS:ND1  | 11:Y:497:GLN:OE1  | 2.38                     | 0.50              |
| 9:O:624:VAL:HG11  | 9:O:647:ALA:HB3   | 1.94                     | 0.50              |
| 5:P:731:GLN:HG2   | 11:Z:151:GLU:HB2  | 1.93                     | 0.50              |
| 11:Y:483:ASP:O    | 11:Y:486:VAL:HG12 | 2.12                     | 0.50              |
| 11:Y:485:LEU:HB3  | 11:Y:490:GLU:HG3  | 1.93                     | 0.50              |
| 11:Z:199:LEU:HB3  | 11:Z:202:LEU:HB3  | 1.94                     | 0.50              |
| 1:A:616:GLU:OE2   | 9:O:558:SER:OG    | 2.25                     | 0.50              |
| 1:A:1097:THR:HG23 | 9:O:340:LEU:HD22  | 1.93                     | 0.50              |
| 3:G:10:GLU:OE2    | 3:G:10:GLU:N      | 2.45                     | 0.50              |
| 9:O:38:LEU:HD11   | 9:O:139:MET:HB3   | 1.93                     | 0.50              |
| 9:O:439:LEU:HD23  | 9:O:473:LEU:HD12  | 1.93                     | 0.50              |
| 5:P:93:SER:HB3    | 5:P:121:LEU:HD21  | 1.94                     | 0.50              |
| 1:A:645:HIS:NE2   | 1:A:656:GLU:OE1   | 2.44                     | 0.50              |
| 1:A:1485:PHE:CG   | 6:K:552:MET:HE1   | 2.46                     | 0.50              |
| 11:Z:139:MET:O    | 11:Z:143:ASN:ND2  | 2.45                     | 0.50              |
| 13:N:186:GLN:HG3  | 13:N:223:GLY:HA3  | 1.94                     | 0.50              |
| 1:A:250:ASN:ND2   | 1:A:432:ILE:HD12  | 2.27                     | 0.49              |
| 1:A:1770:LEU:HD22 | 1:A:1794:ASP:OD2  | 2.11                     | 0.49              |
| 2:D:45:ALA:HA     | 10:U:378:MET:CE   | 2.42                     | 0.49              |
| 5:J:139:GLN:NE2   | 5:J:161:LYS:HB3   | 2.27                     | 0.49              |
| 10:U:388:TYR:HB3  | 10:U:405:LEU:HG   | 1.94                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:I:747:ASP:N    | 12:I:747:ASP:OD1  | 2.45                     | 0.49              |
| 13:N:646:MET:HG3  | 13:N:657:VAL:HG22 | 1.94                     | 0.49              |
| 1:A:724:LEU:HD21  | 9:O:597:PRO:HG2   | 1.95                     | 0.49              |
| 6:K:194:CYS:O     | 6:K:198:GLN:HB2   | 2.12                     | 0.49              |
| 5:P:719:TYR:HE2   | 5:P:749:LYS:HB3   | 1.77                     | 0.49              |
| 10:U:330:ARG:HB2  | 10:U:333:THR:HG22 | 1.94                     | 0.49              |
| 1:A:17:LEU:HD11   | 1:A:511:ILE:HG23  | 1.94                     | 0.49              |
| 1:A:1148:ALA:HB3  | 1:A:1153:ILE:HD13 | 1.94                     | 0.49              |
| 7:L:83:TYR:OH     | 7:L:146:GLN:NE2   | 2.46                     | 0.49              |
| 6:Q:284:LEU:O     | 6:Q:288:SER:OG    | 2.24                     | 0.49              |
| 6:Q:432:ILE:HD11  | 6:Q:444:TRP:CD2   | 2.47                     | 0.49              |
| 1:A:151:ILE:HG22  | 1:A:162:HIS:O     | 2.12                     | 0.49              |
| 6:K:3:LEU:O       | 6:K:7:ARG:HG3     | 2.13                     | 0.49              |
| 6:Q:413:PHE:CD2   | 6:Q:454:VAL:HG12  | 2.47                     | 0.49              |
| 11:Y:349:LEU:HB2  | 11:Y:358:ALA:HB2  | 1.93                     | 0.49              |
| 11:Y:393:MET:O    | 11:Y:397:ASN:ND2  | 2.45                     | 0.49              |
| 11:Z:406:ASN:O    | 11:Z:410:LEU:HG   | 2.13                     | 0.49              |
| 12:I:72:ALA:HB2   | 12:I:113:MET:HG2  | 1.94                     | 0.49              |
| 12:I:406:VAL:HG12 | 12:I:475:VAL:HG22 | 1.94                     | 0.49              |
| 1:A:118:THR:HG22  | 9:O:269:SER:HB3   | 1.93                     | 0.49              |
| 1:A:151:ILE:O     | 1:A:161:MET:HA    | 2.12                     | 0.49              |
| 1:A:1666:ILE:HG23 | 1:A:1678:ILE:HB   | 1.94                     | 0.49              |
| 5:J:464:SER:HA    | 5:J:467:ARG:HE    | 1.77                     | 0.49              |
| 6:K:146:ARG:O     | 6:K:150:THR:HG23  | 2.11                     | 0.49              |
| 6:Q:324:SER:HB3   | 6:Q:340:TYR:OH    | 2.13                     | 0.49              |
| 6:Q:342:HIS:O     | 6:Q:346:VAL:HG13  | 2.12                     | 0.49              |
| 6:Q:510:ARG:O     | 6:Q:510:ARG:HD3   | 2.12                     | 0.49              |
| 11:Z:397:ASN:OD1  | 11:Z:401:LYS:NZ   | 2.42                     | 0.49              |
| 4:H:97:LYS:HG2    | 4:H:98:PRO:HD2    | 1.94                     | 0.49              |
| 9:O:568:LEU:HB2   | 9:O:583:VAL:HG11  | 1.94                     | 0.49              |
| 11:Y:203:SER:O    | 11:Y:207:LYS:HG3  | 2.12                     | 0.49              |
| 11:Z:390:ARG:O    | 11:Z:394:VAL:HG13 | 2.13                     | 0.49              |
| 1:A:966:PRO:HG3   | 1:A:980:ARG:HH12  | 1.78                     | 0.49              |
| 6:K:386:LEU:HA    | 6:K:389:ARG:HG2   | 1.95                     | 0.49              |
| 7:L:88:SER:O      | 7:L:88:SER:OG     | 2.30                     | 0.49              |
| 10:U:423:ARG:O    | 10:U:427:GLN:HG3  | 2.13                     | 0.49              |
| 12:I:195:ILE:O    | 12:I:541:ALA:HA   | 2.12                     | 0.49              |
| 12:I:300:VAL:HG13 | 12:I:456:PHE:HB3  | 1.95                     | 0.49              |
| 13:N:252:LEU:O    | 13:N:256:VAL:HG12 | 2.12                     | 0.49              |
| 1:A:25:ARG:NH2    | 1:A:72:GLU:OE2    | 2.39                     | 0.49              |
| 5:P:578:SER:OG    | 5:P:610:GLU:OE1   | 2.27                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:Q:231:LEU:HA    | 6:Q:234:VAL:HG22  | 1.95                     | 0.49              |
| 10:U:403:TYR:CD2  | 10:U:422:TYR:HE1  | 2.31                     | 0.49              |
| 13:N:511:SER:HB3  | 13:N:514:LEU:HD22 | 1.95                     | 0.49              |
| 2:D:45:ALA:HA     | 10:U:378:MET:HE3  | 1.95                     | 0.49              |
| 7:L:144:ASN:ND2   | 7:L:150:ASP:O     | 2.45                     | 0.49              |
| 6:Q:324:SER:O     | 6:Q:328:THR:HG23  | 2.12                     | 0.49              |
| 10:V:468:MET:O    | 10:V:472:LYS:HG3  | 2.12                     | 0.49              |
| 11:Z:134:THR:HG23 | 11:Z:137:ILE:HD12 | 1.94                     | 0.49              |
| 13:N:476:GLU:N    | 13:N:479:ASP:OD2  | 2.46                     | 0.49              |
| 14:C:51:CYS:SG    | 14:C:53:HIS:HB2   | 2.52                     | 0.49              |
| 1:A:1137:PHE:CD1  | 1:A:1203:MET:HG2  | 2.48                     | 0.49              |
| 1:A:1621:PRO:HG3  | 1:A:1653:ALA:HB3  | 1.95                     | 0.49              |
| 1:A:1634:LEU:HD13 | 1:A:1666:ILE:HD11 | 1.94                     | 0.49              |
| 5:J:459:ALA:O     | 5:J:463:MET:HG3   | 2.12                     | 0.49              |
| 9:O:583:VAL:O     | 9:O:587:VAL:HG23  | 2.12                     | 0.49              |
| 12:I:194:LYS:HD2  | 12:I:541:ALA:HB1  | 1.94                     | 0.49              |
| 1:A:1843:GLU:HA   | 1:A:1846:PRO:HG2  | 1.95                     | 0.48              |
| 1:A:1859:TRP:HE1  | 1:A:1881:GLN:HG2  | 1.77                     | 0.48              |
| 5:J:651:PHE:CE1   | 5:J:705:CYS:HB3   | 2.43                     | 0.48              |
| 6:K:194:CYS:N     | 6:K:197:GLU:OE2   | 2.39                     | 0.48              |
| 6:K:401:ASP:O     | 6:K:404:VAL:HG12  | 2.13                     | 0.48              |
| 9:O:56:GLU:HB2    | 9:O:86:CYS:SG     | 2.53                     | 0.48              |
| 9:O:439:LEU:HG    | 9:O:476:LEU:HD22  | 1.94                     | 0.48              |
| 11:Z:6:HIS:O      | 11:Z:10:MET:HG2   | 2.13                     | 0.48              |
| 1:A:253:PRO:HB2   | 1:A:255:ILE:HG23  | 1.94                     | 0.48              |
| 1:A:1727:ASN:HB3  | 1:A:1843:GLU:OE1  | 2.14                     | 0.48              |
| 1:A:1825:SER:OG   | 1:A:1829:ARG:NH2  | 2.41                     | 0.48              |
| 5:J:135:SER:HB2   | 5:J:161:LYS:HE3   | 1.94                     | 0.48              |
| 9:O:621:SER:HB3   | 9:O:651:ILE:HG13  | 1.95                     | 0.48              |
| 5:P:84:LYS:HB3    | 5:P:87:GLU:HG3    | 1.95                     | 0.48              |
| 5:P:621:LEU:O     | 5:P:625:ARG:HG3   | 2.13                     | 0.48              |
| 5:P:739:VAL:O     | 5:P:743:ILE:HG13  | 2.13                     | 0.48              |
| 11:Y:389:ILE:O    | 11:Y:393:MET:HG2  | 2.13                     | 0.48              |
| 12:I:600:ILE:O    | 12:I:600:ILE:HG13 | 2.13                     | 0.48              |
| 13:N:20:LEU:HD13  | 13:N:65:HIS:CD2   | 2.49                     | 0.48              |
| 5:J:154:SER:O     | 5:J:158:ILE:HG12  | 2.13                     | 0.48              |
| 11:Y:232:LEU:HB3  | 11:Z:29:MET:CE    | 2.44                     | 0.48              |
| 13:N:31:LEU:O     | 13:N:128:SER:OG   | 2.22                     | 0.48              |
| 1:A:104:LYS:O     | 9:O:537:ALA:HB1   | 2.14                     | 0.48              |
| 1:A:633:ILE:HG23  | 1:A:754:LEU:HD21  | 1.95                     | 0.48              |
| 1:A:1521:LEU:HD22 | 1:A:1588:LEU:HD22 | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:O:55:MET:O      | 9:O:59:ARG:HG2    | 2.12                     | 0.48              |
| 9:O:439:LEU:HD11  | 12:I:512:LEU:HD13 | 1.96                     | 0.48              |
| 11:Y:15:LEU:HD11  | 11:Z:135:PRO:HB2  | 1.96                     | 0.48              |
| 11:Y:151:GLU:O    | 11:Y:155:VAL:HG12 | 2.13                     | 0.48              |
| 11:Z:343:LEU:HD11 | 11:Z:375:CYS:HA   | 1.96                     | 0.48              |
| 13:N:300:LEU:HA   | 13:N:303:VAL:HG12 | 1.96                     | 0.48              |
| 1:A:482:VAL:CG2   | 1:A:593:ASN:HA    | 2.44                     | 0.48              |
| 1:A:1074:CYS:O    | 1:A:1078:MET:HG3  | 2.13                     | 0.48              |
| 1:A:1886:ALA:O    | 1:A:1890:VAL:HG12 | 2.13                     | 0.48              |
| 5:P:685:SER:HB3   | 5:P:716:ASN:HD21  | 1.77                     | 0.48              |
| 6:Q:35:GLU:HG3    | 6:Q:40:ILE:HD11   | 1.96                     | 0.48              |
| 11:Y:308:TRP:HE3  | 11:Y:327:LEU:HD13 | 1.78                     | 0.48              |
| 12:I:597:LYS:HZ1  | 12:I:619:LYS:HB2  | 1.78                     | 0.48              |
| 13:N:129:LEU:HD21 | 13:N:150:ARG:HB2  | 1.95                     | 0.48              |
| 13:N:523:LEU:O    | 13:N:527:LEU:HG   | 2.13                     | 0.48              |
| 1:A:774:LYS:HG2   | 1:A:783:ILE:HD11  | 1.96                     | 0.48              |
| 6:K:88:GLN:N      | 6:K:88:GLN:OE1    | 2.44                     | 0.48              |
| 5:P:68:THR:O      | 5:P:72:LYS:HG3    | 2.13                     | 0.48              |
| 6:Q:61:ARG:HH22   | 6:Q:88:GLN:NE2    | 2.11                     | 0.48              |
| 10:U:106:LEU:HB2  | 10:U:118:TYR:HB2  | 1.95                     | 0.48              |
| 11:Y:20:ARG:O     | 11:Y:49:HIS:NE2   | 2.46                     | 0.48              |
| 11:Y:390:ARG:O    | 11:Y:394:VAL:HG13 | 2.13                     | 0.48              |
| 11:Y:431:LEU:HD13 | 11:Y:451:LEU:HD21 | 1.96                     | 0.48              |
| 11:Z:376:TYR:O    | 11:Z:380:ILE:HG12 | 2.13                     | 0.48              |
| 12:I:56:TRP:CE3   | 12:I:98:PRO:HB3   | 2.49                     | 0.48              |
| 12:I:246:PRO:O    | 12:I:250:ARG:HG3  | 2.14                     | 0.48              |
| 12:I:587:LEU:HD22 | 12:I:600:ILE:HG22 | 1.95                     | 0.48              |
| 1:A:850:SER:OG    | 1:A:857:MET:SD    | 2.58                     | 0.48              |
| 1:A:1658:PRO:HG2  | 1:A:1663:LEU:HD13 | 1.95                     | 0.48              |
| 1:A:1830:LEU:O    | 1:A:1831:GLN:HG2  | 2.14                     | 0.48              |
| 7:L:94:ILE:HG12   | 7:L:141:VAL:HG12  | 1.95                     | 0.48              |
| 5:P:726:LEU:HD22  | 5:P:743:ILE:HG13  | 1.94                     | 0.48              |
| 10:U:451:GLU:HA   | 10:U:454:LYS:HE3  | 1.96                     | 0.48              |
| 11:Y:136:LYS:HG3  | 11:Y:137:ILE:N    | 2.29                     | 0.48              |
| 11:Y:224:ILE:HD11 | 11:Y:239:LEU:HD11 | 1.95                     | 0.48              |
| 12:I:625:TYR:HB2  | 12:I:628:THR:HG23 | 1.96                     | 0.48              |
| 1:A:352:ARG:HH21  | 10:V:373:HIS:HD2  | 1.60                     | 0.48              |
| 5:J:643:MET:HA    | 5:J:646:TYR:HB3   | 1.96                     | 0.48              |
| 7:L:25:ILE:N      | 7:L:25:ILE:HD12   | 2.28                     | 0.48              |
| 9:O:706:CYS:O     | 9:O:710:ILE:HG13  | 2.14                     | 0.48              |
| 6:Q:25:TRP:O      | 6:Q:29:VAL:HG23   | 2.13                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:U:238:TYR:CD1  | 10:U:243:LEU:HD12 | 2.49                     | 0.48              |
| 11:Z:208:ALA:O    | 11:Z:212:VAL:HG23 | 2.14                     | 0.48              |
| 12:I:210:LEU:HD11 | 12:I:214:LEU:HD23 | 1.96                     | 0.48              |
| 1:A:823:ILE:HG22  | 1:A:824:ASP:H     | 1.78                     | 0.48              |
| 1:A:1103:PRO:HD2  | 1:A:1143:ALA:HB2  | 1.96                     | 0.48              |
| 1:A:1114:ARG:HB3  | 1:A:1116:THR:HG23 | 1.95                     | 0.48              |
| 1:A:1653:ALA:O    | 1:A:1655:THR:N    | 2.42                     | 0.48              |
| 1:A:1745:PRO:HB2  | 9:O:609:ALA:HB1   | 1.94                     | 0.48              |
| 5:J:617:LEU:HD23  | 5:J:648:GLN:HE21  | 1.79                     | 0.48              |
| 7:L:19:THR:HG23   | 7:L:21:THR:HG22   | 1.96                     | 0.48              |
| 7:L:79:ILE:HD11   | 7:L:153:MET:SD    | 2.53                     | 0.48              |
| 9:O:480:GLN:HG3   | 12:I:512:LEU:HD11 | 1.95                     | 0.48              |
| 11:Z:253:ASN:O    | 11:Z:257:VAL:HG23 | 2.14                     | 0.48              |
| 13:N:340:ARG:HB3  | 13:N:361:LEU:HD22 | 1.96                     | 0.48              |
| 13:N:538:GLU:O    | 13:N:542:VAL:HG13 | 2.12                     | 0.48              |
| 9:O:445:LEU:HD23  | 9:O:469:ALA:HB2   | 1.96                     | 0.48              |
| 5:P:502:LEU:HD23  | 5:P:502:LEU:HA    | 1.68                     | 0.48              |
| 6:Q:27:ASP:HA     | 6:Q:43:LEU:HD22   | 1.96                     | 0.48              |
| 11:Z:248:PHE:HB2  | 11:Z:280:LEU:HD11 | 1.95                     | 0.48              |
| 1:A:1033:ARG:HG2  | 1:A:1566:PHE:HZ   | 1.78                     | 0.47              |
| 9:O:477:HIS:NE2   | 12:I:510:SER:OG   | 2.33                     | 0.47              |
| 9:O:742:GLN:OE1   | 9:O:742:GLN:N     | 2.32                     | 0.47              |
| 13:N:63:ARG:HH12  | 13:N:140:LEU:HA   | 1.79                     | 0.47              |
| 13:N:512:LYS:HG2  | 13:N:549:PHE:CD1  | 2.49                     | 0.47              |
| 13:N:689:VAL:O    | 13:N:693:ARG:N    | 2.43                     | 0.47              |
| 1:A:857:MET:HE3   | 1:A:858:PRO:HD2   | 1.96                     | 0.47              |
| 1:A:1247:HIS:O    | 1:A:1251:VAL:HG12 | 2.14                     | 0.47              |
| 6:K:133:CYS:O     | 6:K:152:SER:OG    | 2.32                     | 0.47              |
| 12:I:113:MET:HG3  | 12:I:176:LEU:HD11 | 1.96                     | 0.47              |
| 1:A:968:SER:HB2   | 1:A:1677:LEU:HD23 | 1.96                     | 0.47              |
| 1:A:1520:LEU:HD22 | 1:A:1542:LEU:HD12 | 1.96                     | 0.47              |
| 1:A:1625:ASP:OD2  | 1:A:1700:LYS:NZ   | 2.40                     | 0.47              |
| 5:J:480:ASN:O     | 5:J:480:ASN:ND2   | 2.47                     | 0.47              |
| 6:K:445:GLU:OE1   | 3:W:8:ARG:NH1     | 2.48                     | 0.47              |
| 11:Y:59:TYR:HB2   | 11:Y:115:LEU:HD21 | 1.96                     | 0.47              |
| 11:Y:240:LEU:HD21 | 11:Y:262:GLN:HB3  | 1.95                     | 0.47              |
| 11:Z:27:LEU:HD12  | 11:Z:49:HIS:HD2   | 1.78                     | 0.47              |
| 12:I:634:SER:OG   | 12:I:635:ILE:N    | 2.48                     | 0.47              |
| 9:O:596:SER:O     | 9:O:596:SER:OG    | 2.30                     | 0.47              |
| 5:P:722:ALA:O     | 5:P:726:LEU:HD12  | 2.14                     | 0.47              |
| 6:Q:134:LEU:HD21  | 6:Q:165:GLU:HG2   | 1.97                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:Q:150:THR:HG22  | 6:Q:175:MET:HB3   | 1.96                     | 0.47              |
| 10:U:449:LEU:O    | 10:U:453:LYS:HG3  | 2.15                     | 0.47              |
| 1:A:129:CYS:HB3   | 1:A:187:LEU:HD21  | 1.97                     | 0.47              |
| 1:A:1221:ASP:HB3  | 1:A:1224:ILE:CG2  | 2.41                     | 0.47              |
| 1:A:1222:MET:SD   | 10:V:514:ARG:NE   | 2.88                     | 0.47              |
| 7:L:83:TYR:CD2    | 7:L:115:GLU:HG3   | 2.38                     | 0.47              |
| 9:O:330:ILE:HD11  | 10:V:414:MET:HG2  | 1.96                     | 0.47              |
| 11:Y:373:LEU:O    | 11:Y:377:GLU:HG2  | 2.15                     | 0.47              |
| 11:Y:394:VAL:HA   | 11:Y:397:ASN:ND2  | 2.29                     | 0.47              |
| 12:I:572:PHE:CE2  | 12:I:589:THR:HG23 | 2.49                     | 0.47              |
| 13:N:289:PHE:O    | 13:N:293:ILE:HG12 | 2.14                     | 0.47              |
| 11:Z:402:THR:HG23 | 11:Z:403:LEU:HD12 | 1.96                     | 0.47              |
| 14:C:20:ASP:OD1   | 14:C:21:GLU:N     | 2.47                     | 0.47              |
| 1:A:795:ARG:NH2   | 1:A:815:ARG:O     | 2.48                     | 0.47              |
| 1:A:1097:THR:O    | 9:O:332:GLN:NE2   | 2.48                     | 0.47              |
| 1:A:1301:ALA:O    | 1:A:1305:VAL:HG23 | 2.15                     | 0.47              |
| 1:A:1733:PHE:CD2  | 1:A:1776:TYR:HB2  | 2.50                     | 0.47              |
| 5:J:483:GLU:O     | 5:J:487:ILE:HG22  | 2.15                     | 0.47              |
| 5:J:621:LEU:HG    | 5:J:625:ARG:HH21  | 1.79                     | 0.47              |
| 9:O:430:ARG:CD    | 9:O:476:LEU:HD11  | 2.41                     | 0.47              |
| 10:U:490:TYR:O    | 10:U:494:ILE:HG12 | 2.13                     | 0.47              |
| 10:V:420:TYR:OH   | 10:V:424:ARG:NH1  | 2.48                     | 0.47              |
| 11:Y:50:ALA:HB1   | 11:Y:66:TYR:HE1   | 1.73                     | 0.47              |
| 11:Y:340:GLN:HE21 | 11:Y:372:ARG:HH12 | 1.63                     | 0.47              |
| 11:Y:355:VAL:O    | 11:Y:359:ILE:HG13 | 2.14                     | 0.47              |
| 11:Y:441:TYR:HB3  | 11:Y:444:ALA:HB3  | 1.97                     | 0.47              |
| 11:Z:293:LEU:O    | 11:Z:297:LEU:HG   | 2.15                     | 0.47              |
| 12:I:406:VAL:HG21 | 12:I:478:TYR:HE2  | 1.80                     | 0.47              |
| 13:N:571:ASN:OD1  | 13:N:622:TYR:OH   | 2.33                     | 0.47              |
| 1:A:89:TYR:HA     | 9:O:533:THR:HG23  | 1.95                     | 0.47              |
| 1:A:1128:PRO:HG2  | 1:A:1131:MET:HB2  | 1.96                     | 0.47              |
| 6:K:62:SER:O      | 6:K:63:ARG:HG2    | 2.15                     | 0.47              |
| 1:A:443:CYS:HB3   | 1:A:452:LEU:CD2   | 2.44                     | 0.47              |
| 5:J:21:TYR:HE1    | 5:J:50:ARG:HB3    | 1.80                     | 0.47              |
| 5:J:524:GLU:O     | 5:J:527:ARG:HG3   | 2.15                     | 0.47              |
| 9:O:492:HIS:HB2   | 12:I:500:PHE:CZ   | 2.50                     | 0.47              |
| 10:U:358:LEU:HD22 | 10:U:371:MET:HE1  | 1.97                     | 0.47              |
| 10:V:301:ASP:OD2  | 10:V:364:TYR:OH   | 2.33                     | 0.47              |
| 1:A:1014:ASP:HB3  | 1:A:1044:ALA:HB3  | 1.97                     | 0.47              |
| 1:A:1926:ARG:O    | 1:A:1930:ARG:NH2  | 2.48                     | 0.47              |
| 4:H:97:LYS:HB3    | 4:H:102:LEU:CD1   | 2.45                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:J:482:LYS:HD2   | 5:J:482:LYS:HA    | 1.73                     | 0.47              |
| 5:J:581:ARG:HA    | 5:J:583:HIS:CE1   | 2.50                     | 0.47              |
| 5:J:660:LYS:O     | 5:J:664:ILE:HD12  | 2.14                     | 0.47              |
| 6:K:275:LEU:HB2   | 6:K:284:LEU:HD12  | 1.97                     | 0.47              |
| 9:O:159:GLN:O     | 9:O:163:GLN:HG2   | 2.15                     | 0.47              |
| 9:O:349:VAL:O     | 9:O:353:LYS:HG2   | 2.15                     | 0.47              |
| 10:V:39:ILE:HG12  | 10:V:201:LEU:O    | 2.14                     | 0.47              |
| 10:V:79:GLU:HA    | 10:V:82:GLN:HG2   | 1.97                     | 0.47              |
| 12:I:119:THR:OG1  | 12:I:212:SER:OG   | 2.26                     | 0.47              |
| 5:J:32:TYR:HH     | 5:J:64:HIS:CE1    | 2.33                     | 0.46              |
| 5:P:524:GLU:O     | 5:P:528:ILE:HG23  | 2.14                     | 0.46              |
| 11:Y:122:ILE:HG23 | 11:Y:144:LEU:HD23 | 1.97                     | 0.46              |
| 11:Z:255:ASN:O    | 11:Z:258:LEU:HG   | 2.15                     | 0.46              |
| 13:N:232:TRP:HB2  | 13:N:235:GLN:NE2  | 2.28                     | 0.46              |
| 13:N:544:LEU:O    | 13:N:547:LEU:HG   | 2.15                     | 0.46              |
| 9:O:644:LEU:HD22  | 9:O:648:ILE:HD11  | 1.96                     | 0.46              |
| 5:P:48:TYR:CD1    | 5:P:56:LYS:HD3    | 2.50                     | 0.46              |
| 6:Q:426:LEU:O     | 6:Q:430:GLU:HG2   | 2.15                     | 0.46              |
| 10:U:93:TYR:OH    | 10:V:57:GLU:OE2   | 2.24                     | 0.46              |
| 10:U:526:TRP:HA   | 10:U:529:ALA:HB3  | 1.98                     | 0.46              |
| 11:Y:396:ALA:CB   | 11:Y:416:VAL:HG21 | 2.44                     | 0.46              |
| 11:Z:59:TYR:HB2   | 11:Z:115:LEU:HD21 | 1.96                     | 0.46              |
| 11:Z:147:LYS:HE2  | 11:Z:336:SER:HB3  | 1.97                     | 0.46              |
| 11:Z:446:VAL:O    | 11:Z:450:GLU:HG2  | 2.15                     | 0.46              |
| 13:N:405:LYS:O    | 13:N:409:VAL:HG12 | 2.15                     | 0.46              |
| 1:A:1091:SER:O    | 1:A:1091:SER:OG   | 2.28                     | 0.46              |
| 1:A:1619:LEU:HD21 | 1:A:1697:LEU:HD22 | 1.98                     | 0.46              |
| 5:P:92:LEU:HD23   | 5:P:121:LEU:HD22  | 1.97                     | 0.46              |
| 6:Q:184:LEU:O     | 6:Q:188:LEU:HD23  | 2.15                     | 0.46              |
| 6:Q:489:HIS:ND1   | 6:Q:497:ASN:HB2   | 2.30                     | 0.46              |
| 11:Y:190:MET:O    | 11:Y:194:GLN:NE2  | 2.44                     | 0.46              |
| 13:N:592:TYR:O    | 14:C:9:ASN:HA     | 2.15                     | 0.46              |
| 14:C:67:GLN:O     | 14:C:69:VAL:N     | 2.45                     | 0.46              |
| 1:A:723:LEU:HB3   | 1:A:724:LEU:HD12  | 1.96                     | 0.46              |
| 1:A:1078:MET:HE3  | 1:A:1132:THR:HG22 | 1.97                     | 0.46              |
| 1:A:1134:TRP:HD1  | 1:A:1597:THR:HA   | 1.80                     | 0.46              |
| 5:P:102:SER:OG    | 5:P:103:HIS:N     | 2.48                     | 0.46              |
| 5:P:473:TYR:HD2   | 5:P:500:TRP:HZ2   | 1.64                     | 0.46              |
| 6:Q:513:THR:O     | 6:Q:517:THR:HG23  | 2.16                     | 0.46              |
| 10:U:293:ASP:OD2  | 10:U:296:ARG:HB2  | 2.16                     | 0.46              |
| 12:I:114:HIS:NE2  | 12:I:116:MET:HB3  | 2.29                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:N:158:ARG:NH1  | 13:N:251:SER:O    | 2.48                     | 0.46              |
| 13:N:570:ILE:HA   | 13:N:573:ASN:ND2  | 2.31                     | 0.46              |
| 1:A:263:GLN:HB2   | 1:A:265:VAL:HG22  | 1.97                     | 0.46              |
| 5:J:142:LEU:HD21  | 5:J:151:PRO:HB2   | 1.96                     | 0.46              |
| 7:L:74:VAL:HG11   | 7:L:137:ILE:HD11  | 1.97                     | 0.46              |
| 8:M:35:GLU:C      | 6:Q:325:LYS:HZ2   | 2.19                     | 0.46              |
| 9:O:416:GLU:HG2   | 9:O:417:LEU:N     | 2.31                     | 0.46              |
| 5:P:55:TYR:CE2    | 5:P:56:LYS:HG3    | 2.50                     | 0.46              |
| 11:Y:101:GLU:O    | 11:Y:105:LYS:HG2  | 2.16                     | 0.46              |
| 11:Y:411:THR:O    | 11:Y:415:THR:HG23 | 2.15                     | 0.46              |
| 11:Z:323:ARG:HE   | 11:Z:327:LEU:HD11 | 1.81                     | 0.46              |
| 12:I:688:THR:HB   | 12:I:691:THR:HG23 | 1.97                     | 0.46              |
| 1:A:12:ILE:O      | 1:A:510:PHE:N     | 2.32                     | 0.46              |
| 9:O:700:TYR:O     | 9:O:704:VAL:HG12  | 2.16                     | 0.46              |
| 6:Q:253:LEU:O     | 6:Q:257:VAL:HG23  | 2.14                     | 0.46              |
| 10:U:26:PHE:CE1   | 10:U:228:TRP:HB2  | 2.50                     | 0.46              |
| 11:Y:23:SER:HB2   | 11:Y:49:HIS:CD2   | 2.48                     | 0.46              |
| 13:N:512:LYS:HG2  | 13:N:549:PHE:HD1  | 1.79                     | 0.46              |
| 1:A:161:MET:SD    | 1:A:216:PRO:HG3   | 2.56                     | 0.46              |
| 1:A:942:ARG:NH1   | 1:A:945:GLU:OE2   | 2.48                     | 0.46              |
| 1:A:1867:CYS:HB3  | 1:A:1885:LEU:HD13 | 1.97                     | 0.46              |
| 5:J:482:LYS:HD3   | 5:J:512:LEU:HD11  | 1.98                     | 0.46              |
| 7:L:46:ARG:NH1    | 7:L:156:ILE:O     | 2.47                     | 0.46              |
| 5:P:643:MET:HE2   | 5:P:658:PHE:HZ    | 1.80                     | 0.46              |
| 11:Y:329:ALA:O    | 11:Y:332:ILE:HG22 | 2.16                     | 0.46              |
| 12:I:238:THR:HB   | 12:I:241:LEU:HD13 | 1.98                     | 0.46              |
| 13:N:597:SER:O    | 13:N:601:TRP:HB2  | 2.16                     | 0.46              |
| 1:A:1084:ARG:NH1  | 1:A:1139:ASN:OD1  | 2.39                     | 0.46              |
| 1:A:1930:ARG:HH22 | 13:N:77:GLU:CD    | 2.17                     | 0.46              |
| 5:J:139:GLN:HG3   | 5:J:161:LYS:NZ    | 2.31                     | 0.46              |
| 6:K:160:ASP:OD2   | 6:Q:13:TYR:OH     | 2.23                     | 0.46              |
| 6:K:227:LEU:HG    | 6:Q:32:LEU:HD13   | 1.98                     | 0.46              |
| 6:K:301:SER:O     | 6:K:305:VAL:HG23  | 2.16                     | 0.46              |
| 9:O:95:ILE:HG13   | 9:O:96:ARG:N      | 2.31                     | 0.46              |
| 11:Z:173:LEU:HD11 | 11:Z:205:TRP:HH2  | 1.80                     | 0.46              |
| 12:I:33:ASP:HB3   | 12:I:728:ARG:HD3  | 1.98                     | 0.46              |
| 1:A:878:ALA:HA    | 1:A:882:LEU:HD13  | 1.98                     | 0.46              |
| 3:G:17:GLU:HA     | 3:G:20:GLU:CD     | 2.36                     | 0.46              |
| 8:M:49:SER:O      | 8:M:53:GLN:HG2    | 2.16                     | 0.46              |
| 5:P:671:LEU:O     | 5:P:675:ILE:HG13  | 2.15                     | 0.46              |
| 5:P:726:LEU:HD11  | 5:P:742:LEU:HD23  | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:Y:157:SER:O    | 11:Y:161:VAL:HG23 | 2.16                     | 0.46              |
| 11:Y:451:LEU:O    | 11:Y:454:ARG:HG2  | 2.14                     | 0.46              |
| 11:Z:359:ILE:O    | 11:Z:363:ARG:HG3  | 2.15                     | 0.46              |
| 11:Z:481:LEU:HD22 | 11:Z:497:GLN:HG3  | 1.98                     | 0.46              |
| 12:I:434:LEU:HG   | 12:I:437:LEU:H    | 1.80                     | 0.46              |
| 12:I:602:ARG:NH2  | 12:I:612:SER:O    | 2.40                     | 0.46              |
| 1:A:248:PHE:HB3   | 1:A:257:MET:HB3   | 1.98                     | 0.46              |
| 1:A:989:GLU:HG3   | 1:A:1698:TYR:CE2  | 2.51                     | 0.46              |
| 1:A:1803:ARG:HH12 | 1:A:1859:TRP:HD1  | 1.64                     | 0.46              |
| 2:D:45:ALA:O      | 10:U:380:ASN:ND2  | 2.49                     | 0.46              |
| 5:J:27:LEU:HD21   | 5:P:147:PHE:HB3   | 1.97                     | 0.46              |
| 1:A:11:MET:SD     | 1:A:510:PHE:HB2   | 2.56                     | 0.45              |
| 1:A:27:HIS:CD2    | 1:A:113:VAL:HG21  | 2.51                     | 0.45              |
| 1:A:90:ASP:OD1    | 1:A:106:SER:HB3   | 2.16                     | 0.45              |
| 1:A:211:PHE:HB3   | 1:A:220:ILE:HG22  | 1.98                     | 0.45              |
| 7:L:18:ARG:HD3    | 7:L:18:ARG:HA     | 1.80                     | 0.45              |
| 11:Y:430:LEU:HA   | 11:Y:433:LYS:HD3  | 1.98                     | 0.45              |
| 12:I:12:ARG:HH21  | 12:I:748:ILE:HD12 | 1.79                     | 0.45              |
| 12:I:21:GLN:HB3   | 12:I:39:ASN:HB2   | 1.99                     | 0.45              |
| 14:C:53:HIS:HE1   | 14:C:76:CYS:HB3   | 1.80                     | 0.45              |
| 1:A:597:LEU:HD11  | 1:A:607:ILE:HD13  | 1.98                     | 0.45              |
| 1:A:1134:TRP:CD1  | 1:A:1597:THR:HA   | 2.51                     | 0.45              |
| 1:A:1251:VAL:HG23 | 1:A:1297:ALA:HB2  | 1.98                     | 0.45              |
| 1:A:1925:VAL:HA   | 1:A:1928:LEU:HB2  | 1.98                     | 0.45              |
| 5:J:92:LEU:HD11   | 5:J:120:LEU:HG    | 1.97                     | 0.45              |
| 5:J:503:CYS:SG    | 5:J:535:GLY:HA3   | 2.56                     | 0.45              |
| 6:K:181:GLU:HG3   | 6:K:209:LEU:CD2   | 2.46                     | 0.45              |
| 9:O:323:ALA:HB2   | 10:V:416:PHE:CE2  | 2.52                     | 0.45              |
| 6:Q:330:GLU:HB3   | 6:Q:333:TYR:HB2   | 1.99                     | 0.45              |
| 6:Q:357:TYR:CE2   | 6:Q:373:TYR:HB3   | 2.51                     | 0.45              |
| 10:U:87:TYR:CZ    | 10:U:113:LYS:HD2  | 2.51                     | 0.45              |
| 11:Z:36:LEU:HG    | 11:Z:37:PHE:CD2   | 2.51                     | 0.45              |
| 1:A:115:LYS:HG2   | 9:O:267:VAL:HG22  | 1.99                     | 0.45              |
| 1:A:436:LEU:HB2   | 1:A:638:LEU:HD23  | 1.98                     | 0.45              |
| 5:P:44:LEU:O      | 5:P:48:TYR:HD2    | 1.99                     | 0.45              |
| 10:V:123:TYR:HD2  | 10:V:124:LEU:HD22 | 1.81                     | 0.45              |
| 10:V:129:LYS:HA   | 10:V:129:LYS:HD3  | 1.69                     | 0.45              |
| 11:Y:240:LEU:HG   | 11:Y:263:ALA:HB2  | 1.98                     | 0.45              |
| 1:A:87:VAL:HB     | 9:O:544:VAL:HG12  | 1.99                     | 0.45              |
| 1:A:710:LEU:HD11  | 9:O:715:TYR:CE1   | 2.51                     | 0.45              |
| 1:A:1351:GLN:H    | 1:A:1351:GLN:HG2  | 1.60                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1460:ALA:O    | 1:A:1464:ILE:HG13 | 2.16                     | 0.45              |
| 6:K:465:LEU:HD21  | 6:K:485:ILE:HG23  | 1.98                     | 0.45              |
| 9:O:320:ALA:HB3   | 9:O:350:LEU:HD21  | 1.98                     | 0.45              |
| 5:P:53:LYS:HG3    | 5:P:55:TYR:CE1    | 2.51                     | 0.45              |
| 5:P:506:GLY:HA3   | 5:P:522:PHE:CE1   | 2.52                     | 0.45              |
| 11:Y:16:HIS:HA    | 11:Y:19:VAL:HG22  | 1.98                     | 0.45              |
| 11:Y:209:TYR:O    | 11:Y:212:VAL:HG12 | 2.16                     | 0.45              |
| 11:Z:20:ARG:HB2   | 11:Z:52:SER:HB2   | 1.99                     | 0.45              |
| 12:I:558:ARG:HE   | 12:I:558:ARG:HB2  | 1.62                     | 0.45              |
| 5:P:741:PHE:CE2   | 5:P:745:LYS:HE3   | 2.52                     | 0.45              |
| 11:Z:158:TYR:HA   | 11:Z:161:VAL:HG12 | 1.98                     | 0.45              |
| 12:I:290:PHE:CZ   | 12:I:320:LEU:HD13 | 2.51                     | 0.45              |
| 13:N:401:ILE:HD11 | 13:N:501:ILE:HG23 | 1.98                     | 0.45              |
| 1:A:790:LEU:HA    | 1:A:790:LEU:HD23  | 1.76                     | 0.45              |
| 5:P:164:PRO:HG2   | 5:P:471:LYS:HG2   | 1.97                     | 0.45              |
| 11:Y:481:LEU:O    | 11:Y:485:LEU:HD13 | 2.17                     | 0.45              |
| 11:Z:109:ALA:O    | 11:Z:113:THR:HG23 | 2.17                     | 0.45              |
| 1:A:1078:MET:O    | 1:A:1081:PRO:HD2  | 2.17                     | 0.45              |
| 1:A:1794:ASP:O    | 1:A:1797:ILE:HG13 | 2.16                     | 0.45              |
| 1:A:1810:GLU:HA   | 1:A:1813:GLN:HG2  | 1.99                     | 0.45              |
| 5:P:170:PHE:O     | 5:P:456:LYS:NZ    | 2.40                     | 0.45              |
| 6:Q:129:LYS:HB3   | 6:Q:159:LEU:HD13  | 1.99                     | 0.45              |
| 10:V:122:ARG:NH2  | 10:V:157:GLU:OE1  | 2.50                     | 0.45              |
| 13:N:351:PHE:HE1  | 13:N:409:VAL:HG11 | 1.80                     | 0.45              |
| 14:C:30:PHE:HB3   | 14:C:46:LEU:HD11  | 1.99                     | 0.45              |
| 1:A:756:PHE:HE2   | 1:A:830:PHE:HB2   | 1.82                     | 0.45              |
| 1:A:966:PRO:HG3   | 1:A:980:ARG:NH1   | 2.32                     | 0.45              |
| 1:A:1729:GLU:H    | 1:A:1729:GLU:CD   | 2.19                     | 0.45              |
| 11:Y:50:ALA:HA    | 11:Y:65:LYS:HE3   | 1.98                     | 0.45              |
| 13:N:626:TYR:HE2  | 13:N:635:LEU:HG   | 1.82                     | 0.45              |
| 3:G:3:ARG:HG3     | 3:G:3:ARG:HH11    | 1.82                     | 0.45              |
| 5:J:103:HIS:HD1   | 5:J:140:LYS:HD3   | 1.81                     | 0.45              |
| 6:K:61:ARG:NH1    | 6:K:80:HIS:HE1    | 2.15                     | 0.45              |
| 6:K:273:GLY:O     | 6:K:277:GLU:HG2   | 2.16                     | 0.45              |
| 6:K:386:LEU:HD22  | 6:K:389:ARG:HH21  | 1.82                     | 0.45              |
| 9:O:727:THR:HG22  | 9:O:731:ASN:ND2   | 2.32                     | 0.45              |
| 5:P:93:SER:OG     | 5:P:121:LEU:HD11  | 2.16                     | 0.45              |
| 11:Y:158:TYR:HB3  | 11:Y:175:LEU:HG   | 1.98                     | 0.45              |
| 11:Y:176:LEU:HD12 | 11:Y:210:ALA:HA   | 1.99                     | 0.45              |
| 12:I:233:TYR:OH   | 12:I:235:GLN:OE1  | 2.30                     | 0.45              |
| 12:I:454:GLU:HB3  | 12:I:455:HIS:HD2  | 1.82                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:26:ASP:OD1    | 1:A:26:ASP:N      | 2.45                     | 0.45              |
| 1:A:1141:VAL:HG11 | 1:A:1608:HIS:CG   | 2.52                     | 0.45              |
| 1:A:1328:TYR:CD1  | 1:A:1363:THR:HG21 | 2.52                     | 0.45              |
| 1:A:1591:HIS:HD2  | 1:A:1601:TYR:CG   | 2.35                     | 0.45              |
| 5:J:97:PHE:CG     | 11:Y:252:ASP:HB3  | 2.52                     | 0.45              |
| 5:J:162:PRO:HB3   | 5:J:474:LEU:HD11  | 1.97                     | 0.45              |
| 6:K:342:HIS:O     | 6:K:346:VAL:HG13  | 2.17                     | 0.45              |
| 9:O:447:SER:HG    | 12:I:516:TYR:HH   | 1.54                     | 0.45              |
| 6:Q:16:GLN:O      | 6:Q:17:GLN:HG2    | 2.17                     | 0.45              |
| 6:Q:61:ARG:HG3    | 6:Q:61:ARG:HH11   | 1.82                     | 0.45              |
| 10:U:78:GLU:HA    | 10:V:67:LEU:HD21  | 1.99                     | 0.45              |
| 10:U:323:LEU:HB3  | 10:U:333:THR:HB   | 1.99                     | 0.45              |
| 11:Z:440:ASP:OD1  | 11:Z:440:ASP:N    | 2.50                     | 0.45              |
| 12:I:49:LEU:HD13  | 12:I:730:VAL:HG11 | 1.98                     | 0.45              |
| 1:A:707:TRP:CE3   | 9:O:730:ARG:HD3   | 2.52                     | 0.44              |
| 1:A:775:LEU:HD11  | 1:A:844:ILE:HD13  | 1.99                     | 0.44              |
| 6:K:190:LEU:O     | 6:K:198:GLN:NE2   | 2.25                     | 0.44              |
| 9:O:443:GLN:HE22  | 12:I:514:PHE:H    | 1.65                     | 0.44              |
| 11:Y:377:GLU:O    | 11:Y:380:ILE:HG12 | 2.17                     | 0.44              |
| 11:Z:23:SER:CB    | 11:Z:49:HIS:HB2   | 2.46                     | 0.44              |
| 11:Z:411:THR:O    | 11:Z:415:THR:OG1  | 2.30                     | 0.44              |
| 12:I:655:ASP:N    | 12:I:663:ASP:O    | 2.39                     | 0.44              |
| 13:N:169:PHE:O    | 13:N:172:MET:HG3  | 2.17                     | 0.44              |
| 13:N:351:PHE:HB2  | 13:N:406:ALA:HB2  | 1.99                     | 0.44              |
| 1:A:224:VAL:HG23  | 1:A:408:CYS:HB2   | 1.99                     | 0.44              |
| 3:G:11:LEU:HD23   | 3:G:11:LEU:HA     | 1.78                     | 0.44              |
| 7:L:37:LYS:NZ     | 7:L:57:ASP:HB3    | 2.33                     | 0.44              |
| 5:P:125:TYR:HE1   | 5:P:130:ARG:HH21  | 1.65                     | 0.44              |
| 5:P:150:SER:HA    | 5:P:153:GLU:HG2   | 1.98                     | 0.44              |
| 11:Z:297:LEU:HB2  | 11:Z:307:PRO:HG3  | 1.99                     | 0.44              |
| 12:I:9:PRO:O      | 12:I:750:ASP:N    | 2.43                     | 0.44              |
| 1:A:350:LEU:HD11  | 10:V:399:TYR:HE2  | 1.83                     | 0.44              |
| 1:A:953:LEU:HD21  | 1:A:1821:PHE:CE2  | 2.53                     | 0.44              |
| 1:A:1060:HIS:O    | 1:A:1063:ILE:HG22 | 2.18                     | 0.44              |
| 5:J:525:VAL:HA    | 5:J:528:ILE:HG22  | 1.98                     | 0.44              |
| 6:K:174:HIS:CE1   | 6:K:211:LYS:HD2   | 2.52                     | 0.44              |
| 6:K:503:HIS:O     | 5:P:625:ARG:HD3   | 2.17                     | 0.44              |
| 7:L:53:TYR:HA     | 7:L:153:MET:O     | 2.18                     | 0.44              |
| 6:Q:263:PHE:HZ    | 6:Q:290:LYS:HB3   | 1.83                     | 0.44              |
| 6:Q:407:GLU:O     | 6:Q:410:VAL:HG12  | 2.17                     | 0.44              |
| 10:V:520:TYR:HA   | 10:V:523:CYS:SG   | 2.57                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:89:TYR:HB3    | 9:O:536:THR:HG23  | 2.00                     | 0.44              |
| 1:A:1251:VAL:HG23 | 1:A:1297:ALA:CB   | 2.47                     | 0.44              |
| 1:A:1830:LEU:C    | 1:A:1831:GLN:HG2  | 2.38                     | 0.44              |
| 5:J:485:ILE:HD13  | 5:J:509:TYR:CE1   | 2.52                     | 0.44              |
| 5:J:641:LEU:HB3   | 5:J:657:HIS:CD2   | 2.53                     | 0.44              |
| 5:P:685:SER:OG    | 5:P:716:ASN:OD1   | 2.25                     | 0.44              |
| 6:Q:80:HIS:HB2    | 6:Q:89:ALA:HB2    | 1.99                     | 0.44              |
| 6:Q:325:LYS:HE2   | 6:Q:329:LEU:CD2   | 2.47                     | 0.44              |
| 10:U:358:LEU:CD2  | 10:U:371:MET:HE1  | 2.47                     | 0.44              |
| 10:V:516:LEU:HD23 | 10:V:516:LEU:HA   | 1.83                     | 0.44              |
| 11:Y:59:TYR:O     | 11:Y:63:VAL:HG22  | 2.17                     | 0.44              |
| 13:N:332:PHE:HA   | 13:N:335:ILE:HG22 | 1.99                     | 0.44              |
| 1:A:1851:THR:O    | 1:A:1855:THR:HG22 | 2.17                     | 0.44              |
| 6:K:317:GLU:HG2   | 6:K:318:HIS:N     | 2.33                     | 0.44              |
| 5:P:621:LEU:HD13  | 5:P:644:ILE:HG21  | 1.98                     | 0.44              |
| 5:P:692:LEU:HD12  | 5:P:705:CYS:O     | 2.18                     | 0.44              |
| 11:Y:10:MET:HB3   | 11:Y:19:VAL:HG12  | 2.00                     | 0.44              |
| 11:Y:512:LEU:HA   | 11:Y:515:MET:HG2  | 2.00                     | 0.44              |
| 11:Z:38:SER:O     | 11:Z:41:GLN:HG2   | 2.16                     | 0.44              |
| 12:I:8:PHE:HB3    | 12:I:750:ASP:O    | 2.18                     | 0.44              |
| 13:N:506:VAL:HG11 | 13:N:512:LYS:HG3  | 1.99                     | 0.44              |
| 1:A:94:TYR:CE1    | 1:A:96:ALA:HB2    | 2.53                     | 0.44              |
| 1:A:1109:GLY:C    | 1:A:1110:ARG:HD2  | 2.38                     | 0.44              |
| 5:J:526:ARG:HE    | 5:J:526:ARG:HB3   | 1.68                     | 0.44              |
| 7:L:76:THR:HG23   | 7:L:159:TYR:HB2   | 2.00                     | 0.44              |
| 5:P:733:VAL:HG22  | 5:P:736:GLU:OE1   | 2.17                     | 0.44              |
| 6:Q:60:LEU:HD11   | 6:Q:75:LEU:HD23   | 1.99                     | 0.44              |
| 10:V:134:THR:HG23 | 10:V:143:LYS:HG3  | 1.99                     | 0.44              |
| 10:V:327:ASP:O    | 10:V:333:THR:HG21 | 2.17                     | 0.44              |
| 11:Y:423:THR:HB   | 11:Y:426:LYS:HE2  | 1.98                     | 0.44              |
| 12:I:20:PRO:HA    | 12:I:739:ARG:HH21 | 1.83                     | 0.44              |
| 13:N:273:MET:HA   | 13:N:289:PHE:HZ   | 1.81                     | 0.44              |
| 6:K:155:GLU:O     | 6:K:158:LYS:HG2   | 2.18                     | 0.44              |
| 9:O:637:PRO:HB2   | 9:O:674:SER:HB3   | 1.98                     | 0.44              |
| 5:P:58:TYR:HB2    | 5:P:78:CYS:HB3    | 1.99                     | 0.44              |
| 5:P:161:LYS:HE2   | 5:P:478:SER:HB3   | 2.00                     | 0.44              |
| 6:Q:459:LYS:HA    | 6:Q:461:TYR:CE1   | 2.53                     | 0.44              |
| 6:Q:472:LEU:O     | 6:Q:476:PRO:HA    | 2.18                     | 0.44              |
| 10:V:186:LYS:HB3  | 10:V:186:LYS:HE2  | 1.93                     | 0.44              |
| 11:Y:232:LEU:HD21 | 11:Z:33:ASN:CB    | 2.47                     | 0.44              |
| 11:Z:101:GLU:O    | 11:Z:105:LYS:HG3  | 2.18                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:I:258:ILE:HD12 | 12:I:359:LEU:HD12 | 1.98                     | 0.44              |
| 1:A:83:ILE:HG21   | 9:O:544:VAL:HG21  | 1.99                     | 0.44              |
| 1:A:628:ILE:HD11  | 1:A:761:ALA:HB1   | 2.00                     | 0.44              |
| 1:A:853:LYS:HD3   | 1:A:1819:GLU:OE2  | 2.18                     | 0.44              |
| 5:J:27:LEU:HD11   | 5:P:147:PHE:O     | 2.18                     | 0.44              |
| 5:J:124:VAL:O     | 5:J:128:THR:HG22  | 2.18                     | 0.44              |
| 5:J:496:TYR:HA    | 5:J:501:VAL:HG21  | 2.00                     | 0.44              |
| 5:P:717:GLU:HA    | 5:P:719:TYR:CE1   | 2.52                     | 0.44              |
| 5:P:731:GLN:OE1   | 11:Z:152:ARG:NH2  | 2.50                     | 0.44              |
| 6:Q:61:ARG:HG3    | 6:Q:61:ARG:NH1    | 2.33                     | 0.44              |
| 11:Y:219:ARG:O    | 11:Y:223:THR:HG22 | 2.18                     | 0.44              |
| 11:Y:260:PHE:HB3  | 11:Y:277:TYR:HD1  | 1.82                     | 0.44              |
| 11:Z:189:THR:O    | 11:Z:193:ILE:HG12 | 2.17                     | 0.44              |
| 13:N:82:ASP:OD1   | 13:N:86:ASN:ND2   | 2.51                     | 0.44              |
| 13:N:404:ILE:HG12 | 13:N:417:LEU:HD21 | 1.99                     | 0.44              |
| 1:A:1012:GLU:OE1  | 1:A:1012:GLU:N    | 2.41                     | 0.44              |
| 1:A:1901:PRO:HD3  | 1:A:1921:LEU:HD11 | 2.00                     | 0.44              |
| 6:K:372:LEU:CD1   | 6:K:404:VAL:HG23  | 2.48                     | 0.44              |
| 9:O:708:GLU:OE1   | 9:O:711:ARG:NH2   | 2.51                     | 0.44              |
| 5:P:616:GLU:OE1   | 5:P:619:LYS:NZ    | 2.39                     | 0.44              |
| 6:Q:485:ILE:O     | 6:Q:488:ILE:HG22  | 2.18                     | 0.44              |
| 11:Z:100:SER:HB3  | 11:Z:103:GLU:HG3  | 2.00                     | 0.44              |
| 13:N:183:VAL:HG13 | 13:N:233:CYS:HB3  | 2.00                     | 0.44              |
| 1:A:30:HIS:O      | 9:O:233:PRO:HG2   | 2.18                     | 0.43              |
| 1:A:215:HIS:CG    | 1:A:216:PRO:HD2   | 2.53                     | 0.43              |
| 5:P:135:SER:O     | 5:P:139:GLN:HG3   | 2.17                     | 0.43              |
| 6:Q:365:LYS:HE2   | 6:Q:365:LYS:HB2   | 1.68                     | 0.43              |
| 6:Q:441:VAL:HG21  | 6:Q:444:TRP:CD1   | 2.52                     | 0.43              |
| 10:U:242:GLN:NE2  | 10:U:429:ARG:HE   | 2.11                     | 0.43              |
| 11:Z:4:ILE:HD12   | 11:Z:45:LEU:HD21  | 2.00                     | 0.43              |
| 11:Z:102:ILE:HG13 | 11:Z:103:GLU:H    | 1.83                     | 0.43              |
| 11:Z:224:ILE:HD11 | 11:Z:239:LEU:HD21 | 2.00                     | 0.43              |
| 13:N:505:LEU:O    | 13:N:508:ILE:HG12 | 2.18                     | 0.43              |
| 1:A:1076:ARG:HG3  | 1:A:1559:HIS:HE1  | 1.84                     | 0.43              |
| 1:A:1841:ASN:ND2  | 13:N:147:GLN:OE1  | 2.51                     | 0.43              |
| 5:J:629:ARG:HH21  | 11:Y:503:SER:HB2  | 1.84                     | 0.43              |
| 6:K:276:VAL:HG21  | 3:W:2:LEU:HD11    | 2.00                     | 0.43              |
| 9:O:378:SER:O     | 9:O:382:GLN:HG2   | 2.17                     | 0.43              |
| 6:Q:194:CYS:HB3   | 6:Q:197:GLU:OE1   | 2.18                     | 0.43              |
| 11:Y:138:ASN:HD21 | 11:Y:160:GLU:HB2  | 1.82                     | 0.43              |
| 11:Z:120:ASP:O    | 11:Z:124:ILE:HG22 | 2.18                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:Z:478:HIS:ND1  | 11:Z:497:GLN:OE1  | 2.50                     | 0.43              |
| 12:I:245:LEU:HB3  | 12:I:246:PRO:HD3  | 1.99                     | 0.43              |
| 12:I:287:LEU:HD21 | 12:I:456:PHE:CE1  | 2.53                     | 0.43              |
| 12:I:692:ARG:HG2  | 12:I:694:ASP:H    | 1.83                     | 0.43              |
| 13:N:688:PRO:O    | 13:N:689:VAL:C    | 2.56                     | 0.43              |
| 1:A:1137:PHE:O    | 1:A:1141:VAL:HG23 | 2.17                     | 0.43              |
| 1:A:1872:LEU:HD23 | 1:A:1900:LEU:HD11 | 1.99                     | 0.43              |
| 5:J:476:LEU:HD21  | 5:J:508:ALA:HB2   | 2.00                     | 0.43              |
| 6:K:65:LEU:HB3    | 6:K:72:CYS:SG     | 2.58                     | 0.43              |
| 6:K:425:PHE:HB3   | 6:K:451:LEU:HG    | 2.00                     | 0.43              |
| 8:M:5:VAL:O       | 8:M:7:ARG:HD2     | 2.17                     | 0.43              |
| 8:M:34:ASN:O      | 8:M:50:VAL:HG22   | 2.19                     | 0.43              |
| 10:V:186:LYS:O    | 10:V:189:ILE:HG22 | 2.19                     | 0.43              |
| 11:Y:281:LEU:HD21 | 11:Y:289:ASP:CG   | 2.38                     | 0.43              |
| 12:I:143:PRO:HG2  | 12:I:351:HIS:CD2  | 2.54                     | 0.43              |
| 12:I:444:ASP:O    | 12:I:448:VAL:HG23 | 2.17                     | 0.43              |
| 1:A:710:LEU:HD11  | 9:O:715:TYR:CD1   | 2.52                     | 0.43              |
| 2:D:20:LEU:HD23   | 2:D:20:LEU:HA     | 1.89                     | 0.43              |
| 6:K:523:ILE:HD12  | 5:P:656:MET:HE1   | 2.00                     | 0.43              |
| 9:O:646:MET:HG2   | 12:I:124:VAL:HG22 | 1.99                     | 0.43              |
| 10:V:180:ARG:NE   | 10:V:208:GLU:OE1  | 2.52                     | 0.43              |
| 11:Y:321:TYR:O    | 11:Y:325:LEU:HG   | 2.19                     | 0.43              |
| 11:Y:406:ASN:OD1  | 11:Y:408:GLN:HG2  | 2.18                     | 0.43              |
| 12:I:644:TYR:O    | 12:I:726:GLY:HA2  | 2.18                     | 0.43              |
| 13:N:523:LEU:HD12 | 13:N:524:ALA:N    | 2.33                     | 0.43              |
| 1:A:172:SER:HB3   | 10:V:430:PRO:HB3  | 2.00                     | 0.43              |
| 1:A:924:SER:OG    | 1:A:925:SER:N     | 2.51                     | 0.43              |
| 1:A:1103:PRO:O    | 1:A:1139:ASN:ND2  | 2.51                     | 0.43              |
| 3:G:11:LEU:HD21   | 6:Q:456:ARG:NH1   | 2.30                     | 0.43              |
| 5:J:56:LYS:NZ     | 5:P:531:TYR:O     | 2.50                     | 0.43              |
| 5:J:660:LYS:HE2   | 11:Y:492:GLN:NE2  | 2.33                     | 0.43              |
| 6:K:171:THR:O     | 6:K:171:THR:OG1   | 2.32                     | 0.43              |
| 6:K:204:LEU:HD12  | 6:Q:24:PHE:HZ     | 1.83                     | 0.43              |
| 9:O:581:ILE:HD13  | 9:O:611:SER:HB2   | 2.00                     | 0.43              |
| 5:P:710:ALA:HB1   | 5:P:726:LEU:HD11  | 1.99                     | 0.43              |
| 10:U:234:LEU:HA   | 10:U:237:ILE:HG22 | 2.01                     | 0.43              |
| 10:U:238:TYR:CE2  | 10:U:250:LYS:HE2  | 2.54                     | 0.43              |
| 10:V:180:ARG:HD3  | 10:V:212:LEU:HD21 | 1.99                     | 0.43              |
| 11:Y:118:ASP:O    | 11:Y:122:ILE:HG12 | 2.18                     | 0.43              |
| 11:Z:152:ARG:HA   | 11:Z:155:VAL:HG12 | 2.00                     | 0.43              |
| 12:I:286:ARG:HA   | 12:I:286:ARG:HD3  | 1.71                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:I:391:THR:HB   | 12:I:515:PRO:HD3  | 2.00                     | 0.43              |
| 1:A:1461:HIS:O    | 1:A:1465:ILE:HG23 | 2.18                     | 0.43              |
| 5:J:68:THR:OG1    | 5:J:71:CYS:SG     | 2.76                     | 0.43              |
| 6:K:6:LEU:HD23    | 6:K:6:LEU:HA      | 1.89                     | 0.43              |
| 9:O:229:LYS:NZ    | 9:O:458:VAL:HA    | 2.34                     | 0.43              |
| 9:O:348:TYR:CZ    | 9:O:361:LEU:HD11  | 2.53                     | 0.43              |
| 6:Q:357:TYR:HB3   | 6:Q:374:ILE:HG13  | 2.01                     | 0.43              |
| 10:V:304:SER:OG   | 10:V:339:ASN:ND2  | 2.36                     | 0.43              |
| 11:Y:395:MET:HA   | 11:Y:398:ASN:HD21 | 1.84                     | 0.43              |
| 12:I:663:ASP:OD1  | 12:I:663:ASP:N    | 2.38                     | 0.43              |
| 1:A:1503:ASN:O    | 1:A:1507:THR:HG22 | 2.19                     | 0.43              |
| 6:K:299:PRO:HB2   | 6:K:333:TYR:CD2   | 2.53                     | 0.43              |
| 6:K:371:MET:HE1   | 6:K:397:ILE:HD12  | 2.00                     | 0.43              |
| 8:M:63:GLN:HA     | 8:M:67:GLU:HA     | 2.00                     | 0.43              |
| 9:O:644:LEU:O     | 9:O:648:ILE:HG12  | 2.19                     | 0.43              |
| 5:P:87:GLU:O      | 5:P:91:ILE:HG22   | 2.18                     | 0.43              |
| 6:Q:19:TYR:CZ     | 6:Q:49:LEU:HD22   | 2.53                     | 0.43              |
| 10:U:124:LEU:HD23 | 10:U:124:LEU:HA   | 1.92                     | 0.43              |
| 10:U:295:TYR:HB2  | 10:V:101:ARG:HG3  | 2.00                     | 0.43              |
| 10:V:330:ARG:HB2  | 10:V:333:THR:HG23 | 2.01                     | 0.43              |
| 11:Y:252:ASP:OD1  | 11:Y:252:ASP:N    | 2.49                     | 0.43              |
| 11:Y:445:VAL:HA   | 11:Y:448:LYS:HD2  | 2.00                     | 0.43              |
| 1:A:1493:LYS:HD2  | 1:A:1493:LYS:HA   | 1.77                     | 0.43              |
| 5:P:522:PHE:O     | 5:P:525:VAL:HG12  | 2.19                     | 0.43              |
| 6:Q:451:LEU:HD13  | 6:Q:467:TYR:CE2   | 2.54                     | 0.43              |
| 10:U:418:CYS:HG   | 10:U:442:CYS:HG   | 1.67                     | 0.43              |
| 10:U:448:GLN:OE1  | 10:U:451:GLU:HG3  | 2.18                     | 0.43              |
| 11:Y:447:LYS:HZ3  | 11:Y:447:LYS:HG3  | 1.76                     | 0.43              |
| 11:Z:240:LEU:HD21 | 11:Z:262:GLN:NE2  | 2.34                     | 0.43              |
| 12:I:718:LYS:NZ   | 12:I:736:SER:HB3  | 2.34                     | 0.43              |
| 6:K:201:LEU:HD13  | 6:Q:25:TRP:HH2    | 1.84                     | 0.43              |
| 6:K:351:ASP:OD1   | 10:V:550:LEU:HD22 | 2.19                     | 0.43              |
| 8:M:31:ILE:HD13   | 6:Q:302:TRP:CZ3   | 2.52                     | 0.43              |
| 11:Z:140:MET:HA   | 11:Z:143:ASN:ND2  | 2.32                     | 0.43              |
| 1:A:352:ARG:NH2   | 10:V:374:GLU:OE2  | 2.49                     | 0.43              |
| 1:A:629:LEU:HD13  | 1:A:633:ILE:HG22  | 2.00                     | 0.43              |
| 1:A:1076:ARG:O    | 1:A:1080:LEU:HG   | 2.18                     | 0.43              |
| 1:A:1709:LYS:HE3  | 1:A:1709:LYS:HB2  | 1.87                     | 0.43              |
| 1:A:1730:ALA:HA   | 1:A:1776:TYR:CD2  | 2.53                     | 0.43              |
| 6:K:7:ARG:HA      | 6:K:10:VAL:HG12   | 2.01                     | 0.43              |
| 8:M:60:LEU:HD12   | 8:M:60:LEU:HA     | 1.86                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:P:465:LEU:HD13  | 5:P:495:HIS:CD2   | 2.54                     | 0.43              |
| 6:Q:170:LEU:HD22  | 6:Q:176:LEU:HD11  | 2.01                     | 0.43              |
| 6:Q:179:GLN:O     | 6:Q:183:GLU:HG2   | 2.18                     | 0.43              |
| 6:Q:190:LEU:HD11  | 6:Q:201:LEU:HD23  | 2.01                     | 0.43              |
| 10:U:404:GLY:O    | 10:U:408:THR:HG22 | 2.19                     | 0.43              |
| 11:Y:414:ALA:O    | 11:Y:418:LEU:HG   | 2.18                     | 0.43              |
| 11:Y:432:ASP:O    | 11:Y:436:THR:HG23 | 2.18                     | 0.43              |
| 12:I:671:LEU:HA   | 12:I:674:VAL:HG12 | 2.01                     | 0.43              |
| 12:I:730:VAL:HG22 | 12:I:745:GLU:HG2  | 2.00                     | 0.43              |
| 13:N:55:LEU:HD23  | 13:N:55:LEU:HA    | 1.88                     | 0.43              |
| 13:N:292:TRP:O    | 13:N:296:VAL:HG22 | 2.19                     | 0.43              |
| 1:A:1363:THR:O    | 1:A:1363:THR:HG22 | 2.19                     | 0.42              |
| 6:K:291:LEU:HB3   | 6:K:301:SER:HB2   | 2.00                     | 0.42              |
| 8:M:31:ILE:HD12   | 6:Q:322:TYR:CE1   | 2.54                     | 0.42              |
| 9:O:408:LEU:HD23  | 9:O:408:LEU:H     | 1.84                     | 0.42              |
| 9:O:422:ILE:HG21  | 9:O:445:LEU:HB2   | 2.01                     | 0.42              |
| 6:Q:47:LEU:HB3    | 6:Q:56:ALA:HB2    | 2.01                     | 0.42              |
| 6:Q:194:CYS:SG    | 6:Q:195:ASN:N     | 2.92                     | 0.42              |
| 10:V:58:LEU:HD23  | 10:V:58:LEU:HA    | 1.80                     | 0.42              |
| 11:Y:441:TYR:O    | 11:Y:445:VAL:HG23 | 2.19                     | 0.42              |
| 11:Z:140:MET:SD   | 11:Z:144:LEU:HD23 | 2.59                     | 0.42              |
| 11:Z:323:ARG:HH21 | 11:Z:327:LEU:HD21 | 1.84                     | 0.42              |
| 13:N:425:ARG:O    | 13:N:509:TYR:OH   | 2.21                     | 0.42              |
| 1:A:669:GLY:HA2   | 1:A:753:THR:HG21  | 2.00                     | 0.42              |
| 1:A:823:ILE:HG22  | 1:A:824:ASP:N     | 2.35                     | 0.42              |
| 1:A:1251:VAL:HG13 | 1:A:1603:LEU:HD22 | 2.00                     | 0.42              |
| 2:D:10:PRO:HG2    | 9:O:346:TRP:CE2   | 2.54                     | 0.42              |
| 5:J:544:TRP:CD1   | 5:J:579:LEU:HD13  | 2.54                     | 0.42              |
| 6:K:284:LEU:HD22  | 6:K:308:TYR:HB2   | 2.00                     | 0.42              |
| 6:Q:395:LEU:HD21  | 6:Q:405:MET:HB2   | 2.01                     | 0.42              |
| 10:V:281:LYS:HD2  | 10:V:281:LYS:HA   | 1.61                     | 0.42              |
| 12:I:366:LEU:HD23 | 12:I:366:LEU:HA   | 1.89                     | 0.42              |
| 12:I:597:LYS:HE3  | 12:I:617:ALA:HB1  | 2.01                     | 0.42              |
| 13:N:33:PRO:HG3   | 13:N:124:PRO:HB2  | 2.01                     | 0.42              |
| 1:A:1019:MET:HB3  | 1:A:1024:MET:HE3  | 2.00                     | 0.42              |
| 1:A:1396:LEU:HD23 | 1:A:1396:LEU:HA   | 1.89                     | 0.42              |
| 4:H:67:LEU:HD22   | 11:Y:308:TRP:CH2  | 2.54                     | 0.42              |
| 5:J:7:PRO:HG3     | 5:P:455:GLN:HG3   | 2.00                     | 0.42              |
| 7:L:82:ASP:N      | 7:L:82:ASP:OD1    | 2.51                     | 0.42              |
| 9:O:662:ARG:HG2   | 9:O:755:LEU:HD12  | 2.00                     | 0.42              |
| 5:P:522:PHE:HB3   | 5:P:539:TYR:CE2   | 2.54                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:P:577:PHE:HD2   | 5:P:582:GLU:HB3   | 1.84                     | 0.42              |
| 5:P:694:LYS:O     | 5:P:697:VAL:HG12  | 2.19                     | 0.42              |
| 6:Q:299:PRO:HG3   | 6:Q:330:GLU:HB2   | 2.01                     | 0.42              |
| 10:U:213:ILE:HG23 | 10:U:218:MET:HB3  | 2.00                     | 0.42              |
| 11:Z:43:TYR:HE1   | 11:Z:99:PRO:HD2   | 1.84                     | 0.42              |
| 1:A:633:ILE:HG23  | 1:A:754:LEU:CD2   | 2.49                     | 0.42              |
| 1:A:1599:ASN:N    | 1:A:1599:ASN:OD1  | 2.52                     | 0.42              |
| 5:J:546:LEU:HD23  | 5:J:548:LYS:HE3   | 2.01                     | 0.42              |
| 6:K:66:ASP:OD1    | 6:K:67:LYS:N      | 2.53                     | 0.42              |
| 7:L:80:TYR:CD2    | 7:L:154:ARG:HD2   | 2.54                     | 0.42              |
| 5:P:19:TYR:N      | 5:P:19:TYR:CD1    | 2.87                     | 0.42              |
| 6:Q:185:LEU:HA    | 6:Q:185:LEU:HD12  | 1.70                     | 0.42              |
| 6:Q:382:ASN:O     | 6:Q:382:ASN:ND2   | 2.52                     | 0.42              |
| 11:Y:8:ARG:HA     | 11:Y:48:TYR:CE2   | 2.55                     | 0.42              |
| 11:Y:357:GLU:O    | 11:Y:360:ILE:HG22 | 2.19                     | 0.42              |
| 11:Z:249:ARG:NH2  | 11:Z:371:CYS:O    | 2.51                     | 0.42              |
| 12:I:254:LYS:HA   | 12:I:254:LYS:HD2  | 1.87                     | 0.42              |
| 13:N:188:LYS:HA   | 13:N:188:LYS:HD3  | 1.69                     | 0.42              |
| 13:N:539:ILE:HA   | 13:N:542:VAL:HG22 | 2.02                     | 0.42              |
| 1:A:440:LYS:HB3   | 1:A:457:PHE:CE1   | 2.54                     | 0.42              |
| 1:A:1651:LEU:HD22 | 6:K:553:LYS:HB2   | 2.02                     | 0.42              |
| 10:U:200:PRO:O    | 10:U:201:LEU:HB2  | 2.19                     | 0.42              |
| 10:U:516:LEU:HB3  | 10:U:532:CYS:SG   | 2.59                     | 0.42              |
| 12:I:208:LEU:HD22 | 12:I:217:LEU:HD11 | 2.02                     | 0.42              |
| 13:N:294:GLU:O    | 13:N:297:VAL:HG12 | 2.19                     | 0.42              |
| 13:N:622:TYR:HD2  | 13:N:622:TYR:O    | 2.03                     | 0.42              |
| 1:A:707:TRP:CH2   | 1:A:711:LEU:HD21  | 2.55                     | 0.42              |
| 5:J:104:ASP:OD1   | 5:J:105:ASP:N     | 2.53                     | 0.42              |
| 5:J:552:LEU:HD12  | 5:J:552:LEU:HA    | 1.81                     | 0.42              |
| 6:K:406:HIS:HD2   | 6:K:447:LEU:HD13  | 1.84                     | 0.42              |
| 7:L:80:TYR:HB3    | 7:L:154:ARG:HB2   | 2.01                     | 0.42              |
| 9:O:326:GLU:OE2   | 10:V:416:PHE:N    | 2.43                     | 0.42              |
| 10:U:58:LEU:HD23  | 10:U:58:LEU:HA    | 1.76                     | 0.42              |
| 10:U:62:LEU:HD11  | 10:U:259:PHE:CE1  | 2.55                     | 0.42              |
| 11:Y:281:LEU:HG   | 11:Y:290:VAL:HG23 | 2.01                     | 0.42              |
| 11:Z:484:PHE:O    | 11:Z:488:VAL:HG23 | 2.20                     | 0.42              |
| 1:A:124:GLN:N     | 1:A:154:LEU:O     | 2.53                     | 0.42              |
| 1:A:168:ASP:OD1   | 1:A:168:ASP:N     | 2.42                     | 0.42              |
| 1:A:713:SER:O     | 1:A:717:GLN:HG2   | 2.19                     | 0.42              |
| 1:A:1751:ALA:HA   | 1:A:1755:CYS:SG   | 2.59                     | 0.42              |
| 2:D:49:ASN:OD1    | 2:D:49:ASN:N      | 2.52                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:J:513:SER:HA    | 5:J:515:TYR:CE1   | 2.54                     | 0.42              |
| 5:J:517:GLN:HG2   | 5:J:520:ARG:HE    | 1.85                     | 0.42              |
| 6:K:81:TYR:CD2    | 6:K:139:ILE:HG12  | 2.49                     | 0.42              |
| 9:O:392:GLY:H     | 9:O:615:ARG:NH2   | 2.18                     | 0.42              |
| 9:O:608:LEU:HA    | 9:O:623:THR:HG21  | 2.02                     | 0.42              |
| 5:P:473:TYR:CD2   | 5:P:500:TRP:HZ2   | 2.37                     | 0.42              |
| 10:U:242:GLN:OE1  | 10:U:429:ARG:NE   | 2.53                     | 0.42              |
| 13:N:536:GLU:O    | 13:N:539:ILE:HG12 | 2.19                     | 0.42              |
| 14:C:60:ILE:HG12  | 14:C:80:TRP:CZ2   | 2.54                     | 0.42              |
| 5:J:462:LEU:HD21  | 5:P:34:GLU:HG2    | 2.02                     | 0.42              |
| 7:L:71:LYS:HD2    | 7:L:135:PHE:CE2   | 2.54                     | 0.42              |
| 11:Y:410:LEU:HD13 | 11:Y:433:LYS:HB2  | 2.01                     | 0.42              |
| 11:Z:274:MET:HA   | 11:Z:277:TYR:HB3  | 2.02                     | 0.42              |
| 11:Z:406:ASN:OD1  | 11:Z:409:THR:HG23 | 2.19                     | 0.42              |
| 13:N:626:TYR:HE1  | 13:N:630:LYS:HD2  | 1.85                     | 0.42              |
| 1:A:424:ASN:OD1   | 1:A:425:SER:N     | 2.52                     | 0.42              |
| 1:A:628:ILE:CD1   | 1:A:761:ALA:HB1   | 2.50                     | 0.42              |
| 1:A:961:HIS:ND1   | 1:A:1830:LEU:HD11 | 2.35                     | 0.42              |
| 1:A:1208:LEU:O    | 1:A:1212:VAL:HG12 | 2.20                     | 0.42              |
| 5:J:639:TYR:HB3   | 5:J:672:LEU:HD13  | 2.01                     | 0.42              |
| 9:O:63:LEU:HD11   | 9:O:81:LEU:HB3    | 2.02                     | 0.42              |
| 6:Q:310:LEU:HD11  | 6:Q:343:SER:HB2   | 2.01                     | 0.42              |
| 6:Q:429:LEU:HD11  | 6:Q:433:LYS:HE2   | 2.02                     | 0.42              |
| 10:U:33:LYS:HB2   | 10:U:62:LEU:HD22  | 2.01                     | 0.42              |
| 11:Y:33:ASN:HD21  | 11:Z:232:LEU:HD23 | 1.85                     | 0.42              |
| 11:Y:431:LEU:HD11 | 11:Y:448:LYS:HG2  | 2.02                     | 0.42              |
| 12:I:417:PHE:HD1  | 12:I:448:VAL:HG13 | 1.84                     | 0.42              |
| 13:N:513:ASP:O    | 13:N:516:ILE:HG13 | 2.20                     | 0.42              |
| 1:A:804:ASP:O     | 1:A:808:ARG:HG3   | 2.20                     | 0.42              |
| 1:A:861:PRO:HB3   | 1:A:899:ILE:HD11  | 2.02                     | 0.42              |
| 1:A:1391:ASP:OD2  | 1:A:1391:ASP:N    | 2.38                     | 0.42              |
| 6:K:350:HIS:O     | 6:K:354:MET:HG2   | 2.20                     | 0.42              |
| 9:O:44:MET:CE     | 12:I:310:TRP:HZ2  | 2.33                     | 0.42              |
| 9:O:360:LEU:HD23  | 9:O:360:LEU:HA    | 1.79                     | 0.42              |
| 6:Q:285:PHE:HB2   | 6:Q:308:TYR:CE1   | 2.55                     | 0.42              |
| 10:U:397:ARG:HA   | 10:U:428:LEU:HD21 | 2.01                     | 0.42              |
| 10:V:379:LYS:HA   | 10:V:379:LYS:HD3  | 1.71                     | 0.42              |
| 11:Y:190:MET:HA   | 11:Y:193:ILE:HD12 | 2.01                     | 0.42              |
| 11:Y:319:LYS:HA   | 11:Y:319:LYS:HD2  | 1.85                     | 0.42              |
| 11:Y:349:LEU:HB3  | 11:Y:354:ARG:O    | 2.20                     | 0.42              |
| 11:Z:33:ASN:OD1   | 11:Z:36:LEU:HB2   | 2.20                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:Z:418:LEU:HD23 | 11:Z:418:LEU:HA   | 1.94                     | 0.42              |
| 12:I:79:LEU:HD11  | 12:I:101:LEU:HD12 | 2.01                     | 0.42              |
| 13:N:519:TYR:O    | 13:N:523:LEU:HG   | 2.20                     | 0.42              |
| 13:N:552:ALA:N    | 13:N:553:PRO:HD2  | 2.35                     | 0.42              |
| 1:A:115:LYS:HD3   | 9:O:267:VAL:HG21  | 2.02                     | 0.41              |
| 5:J:106:ILE:HD13  | 5:J:106:ILE:HA    | 1.93                     | 0.41              |
| 6:K:484:ALA:O     | 6:K:488:ILE:HG22  | 2.20                     | 0.41              |
| 5:P:468:GLU:HG2   | 5:P:491:LEU:HD23  | 2.01                     | 0.41              |
| 5:P:667:GLN:HG3   | 5:P:698:ILE:HD12  | 2.01                     | 0.41              |
| 10:V:405:LEU:HA   | 10:V:408:THR:HG22 | 2.01                     | 0.41              |
| 11:Z:196:VAL:HG12 | 11:Z:199:LEU:HD11 | 2.02                     | 0.41              |
| 11:Z:349:LEU:HD11 | 11:Z:354:ARG:HB2  | 2.02                     | 0.41              |
| 12:I:47:HIS:ND1   | 12:I:54:ARG:HA    | 2.35                     | 0.41              |
| 12:I:379:LEU:HA   | 12:I:379:LEU:HD12 | 1.85                     | 0.41              |
| 12:I:632:ARG:O    | 12:I:636:TYR:OH   | 2.38                     | 0.41              |
| 13:N:627:GLU:HG2  | 13:N:633:ARG:O    | 2.20                     | 0.41              |
| 1:A:74:TRP:HA     | 1:A:93:LEU:O      | 2.20                     | 0.41              |
| 1:A:357:ALA:HA    | 10:V:395:ASN:HD21 | 1.84                     | 0.41              |
| 1:A:650:GLY:N     | 1:A:651:PRO:HD3   | 2.34                     | 0.41              |
| 1:A:848:VAL:O     | 1:A:852:LEU:HG    | 2.21                     | 0.41              |
| 1:A:1631:TYR:HB2  | 1:A:1708:TYR:HB2  | 2.01                     | 0.41              |
| 3:G:18:GLU:OE1    | 6:Q:457:LYS:NZ    | 2.44                     | 0.41              |
| 4:H:79:MET:SD     | 5:P:580:GLN:NE2   | 2.93                     | 0.41              |
| 6:K:252:LYS:O     | 6:K:256:VAL:HG13  | 2.20                     | 0.41              |
| 7:L:12:ASP:OD2    | 7:L:14:LYS:HE3    | 2.20                     | 0.41              |
| 5:P:113:SER:O     | 5:P:117:THR:HG23  | 2.19                     | 0.41              |
| 6:Q:57:ALA:HB1    | 6:Q:80:HIS:NE2    | 2.35                     | 0.41              |
| 11:Y:330:LYS:O    | 11:Y:334:LEU:HG   | 2.20                     | 0.41              |
| 12:I:210:LEU:HB2  | 12:I:217:LEU:HD13 | 2.02                     | 0.41              |
| 12:I:262:LEU:HD23 | 12:I:262:LEU:HA   | 1.88                     | 0.41              |
| 13:N:293:ILE:HD12 | 13:N:328:VAL:HG12 | 2.02                     | 0.41              |
| 1:A:1084:ARG:NH2  | 1:A:1142:ALA:HB3  | 2.35                     | 0.41              |
| 1:A:1663:LEU:HB3  | 1:A:1680:LEU:HD22 | 2.02                     | 0.41              |
| 1:A:1860:LEU:HD22 | 1:A:1865:ASP:OD1  | 2.19                     | 0.41              |
| 9:O:283:LEU:HA    | 9:O:283:LEU:HD12  | 1.83                     | 0.41              |
| 9:O:365:VAL:O     | 9:O:369:VAL:HG22  | 2.20                     | 0.41              |
| 9:O:642:SER:O     | 9:O:646:MET:HG3   | 2.20                     | 0.41              |
| 6:Q:6:LEU:O       | 6:Q:10:VAL:HG12   | 2.20                     | 0.41              |
| 10:V:392:ILE:HG21 | 10:V:402:TRP:CZ2  | 2.55                     | 0.41              |
| 11:Y:46:LEU:HD11  | 11:Y:68:MET:HB2   | 2.02                     | 0.41              |
| 11:Y:498:TYR:HB3  | 11:Y:515:MET:SD   | 2.60                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:Y:499:SER:HA   | 11:Y:502:LEU:HG   | 2.02                     | 0.41              |
| 12:I:426:LEU:HB3  | 12:I:433:VAL:HG22 | 2.01                     | 0.41              |
| 1:A:352:ARG:HG3   | 10:V:308:TYR:HD2  | 1.86                     | 0.41              |
| 1:A:1328:TYR:HB3  | 1:A:1363:THR:HG22 | 2.02                     | 0.41              |
| 1:A:1369:LEU:HD22 | 1:A:1585:LEU:HD22 | 2.02                     | 0.41              |
| 5:J:138:TYR:CD1   | 5:J:151:PRO:HB3   | 2.52                     | 0.41              |
| 6:K:355:ALA:O     | 6:K:359:THR:HG22  | 2.21                     | 0.41              |
| 9:O:132:VAL:HG11  | 12:I:310:TRP:CZ3  | 2.55                     | 0.41              |
| 9:O:631:GLN:HB3   | 9:O:636:ILE:HG13  | 2.01                     | 0.41              |
| 6:Q:6:LEU:O       | 6:Q:6:LEU:HD12    | 2.20                     | 0.41              |
| 10:U:512:ALA:O    | 10:U:516:LEU:HG   | 2.21                     | 0.41              |
| 11:Y:25:LEU:HD21  | 11:Z:205:TRP:CD1  | 2.55                     | 0.41              |
| 11:Z:447:LYS:HD3  | 11:Z:447:LYS:HA   | 1.74                     | 0.41              |
| 12:I:195:ILE:HD11 | 12:I:252:ALA:HB2  | 2.02                     | 0.41              |
| 12:I:427:ARG:HH21 | 12:I:438:ASN:HD21 | 1.67                     | 0.41              |
| 13:N:105:PRO:HG3  | 13:N:232:TRP:CD2  | 2.55                     | 0.41              |
| 1:A:661:VAL:O     | 1:A:665:MET:HG3   | 2.21                     | 0.41              |
| 1:A:755:LEU:HD23  | 1:A:755:LEU:HA    | 1.92                     | 0.41              |
| 1:A:1033:ARG:HG2  | 1:A:1566:PHE:CZ   | 2.54                     | 0.41              |
| 5:J:8:VAL:HG12    | 5:J:31:LEU:HD22   | 2.02                     | 0.41              |
| 5:J:549:ASP:HB2   | 8:M:60:LEU:HD21   | 2.03                     | 0.41              |
| 6:K:60:LEU:HD22   | 6:K:72:CYS:SG     | 2.60                     | 0.41              |
| 6:K:473:VAL:CG2   | 5:P:130:ARG:HH12  | 2.32                     | 0.41              |
| 5:P:103:HIS:O     | 5:P:107:VAL:HG12  | 2.19                     | 0.41              |
| 10:U:31:GLU:HA    | 10:U:34:LYS:HG2   | 2.02                     | 0.41              |
| 11:Y:401:LYS:HA   | 11:Y:401:LYS:HD3  | 1.80                     | 0.41              |
| 12:I:299:SER:N    | 12:I:302:ASP:OD2  | 2.53                     | 0.41              |
| 13:N:350:ASP:OD1  | 13:N:350:ASP:N    | 2.53                     | 0.41              |
| 1:A:93:LEU:HD12   | 1:A:93:LEU:HA     | 1.67                     | 0.41              |
| 1:A:136:ASP:N     | 1:A:136:ASP:OD1   | 2.54                     | 0.41              |
| 1:A:444:PHE:CE2   | 1:A:453:ARG:HB2   | 2.55                     | 0.41              |
| 2:D:51:LEU:HD23   | 2:D:51:LEU:HA     | 1.83                     | 0.41              |
| 8:M:11:ILE:O      | 8:M:15:ILE:HD12   | 2.20                     | 0.41              |
| 5:P:102:SER:N     | 5:P:105:ASP:OD2   | 2.48                     | 0.41              |
| 10:V:123:TYR:CD2  | 10:V:124:LEU:HD22 | 2.55                     | 0.41              |
| 11:Z:204:VAL:HB   | 11:Z:227:LEU:HD21 | 2.02                     | 0.41              |
| 12:I:321:LEU:HD23 | 12:I:428:MET:HE1  | 2.02                     | 0.41              |
| 1:A:477:LYS:N     | 1:A:491:LEU:O     | 2.52                     | 0.41              |
| 1:A:1930:ARG:NH2  | 13:N:77:GLU:OE2   | 2.40                     | 0.41              |
| 5:J:142:LEU:CD2   | 5:J:151:PRO:HB2   | 2.51                     | 0.41              |
| 5:J:641:LEU:HA    | 5:J:644:ILE:CG2   | 2.49                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:L:75:LYS:HE3    | 7:L:161:PRO:HB3   | 2.03                     | 0.41              |
| 8:M:35:GLU:O      | 6:Q:325:LYS:NZ    | 2.49                     | 0.41              |
| 9:O:65:LEU:HB3    | 9:O:66:PRO:HD3    | 2.02                     | 0.41              |
| 10:U:379:LYS:HD2  | 10:U:379:LYS:HA   | 1.69                     | 0.41              |
| 11:Y:21:LEU:HG    | 11:Z:169:LEU:HD23 | 2.03                     | 0.41              |
| 11:Y:481:LEU:HD23 | 11:Y:485:LEU:HD13 | 2.02                     | 0.41              |
| 1:A:431:PHE:CE2   | 1:A:443:CYS:HB2   | 2.55                     | 0.41              |
| 1:A:591:VAL:HG22  | 1:A:606:ARG:HH22  | 1.84                     | 0.41              |
| 1:A:1811:LEU:HD12 | 1:A:1811:LEU:HA   | 1.86                     | 0.41              |
| 2:D:53:PRO:HB3    | 10:U:385:ILE:HG21 | 2.03                     | 0.41              |
| 5:J:8:VAL:HG22    | 5:P:147:PHE:HE2   | 1.86                     | 0.41              |
| 9:O:361:LEU:HB3   | 9:O:384:LEU:HG    | 2.02                     | 0.41              |
| 9:O:532:VAL:HG22  | 9:O:546:ARG:HB3   | 2.02                     | 0.41              |
| 6:Q:169:LEU:HD23  | 6:Q:169:LEU:HA    | 1.85                     | 0.41              |
| 10:V:203:TRP:CD1  | 10:V:207:LEU:HD12 | 2.56                     | 0.41              |
| 11:Y:275:ASP:HB2  | 11:Y:306:GLU:OE1  | 2.21                     | 0.41              |
| 1:A:266:HIS:CE1   | 1:A:427:ALA:HB2   | 2.56                     | 0.41              |
| 1:A:852:LEU:HB3   | 1:A:881:ILE:HD13  | 2.03                     | 0.41              |
| 2:D:37:HIS:NE2    | 9:O:144:SER:OG    | 2.53                     | 0.41              |
| 2:D:54:ILE:HG12   | 6:Q:510:ARG:NH2   | 2.35                     | 0.41              |
| 5:J:103:HIS:O     | 5:J:107:VAL:HG23  | 2.20                     | 0.41              |
| 6:K:263:PHE:O     | 6:Q:55:ARG:HD3    | 2.21                     | 0.41              |
| 6:K:377:GLU:OE2   | 3:W:4:ARG:NH2     | 2.40                     | 0.41              |
| 7:L:5:ASN:OD1     | 7:L:5:ASN:N       | 2.54                     | 0.41              |
| 9:O:509:LEU:HD13  | 9:O:538:LEU:HB2   | 2.03                     | 0.41              |
| 5:P:118:LEU:HD13  | 5:P:140:LYS:HG3   | 2.03                     | 0.41              |
| 5:P:707:PHE:C     | 5:P:707:PHE:CD1   | 2.95                     | 0.41              |
| 5:P:726:LEU:HD21  | 5:P:742:LEU:HD23  | 2.02                     | 0.41              |
| 5:P:749:LYS:HB2   | 5:P:749:LYS:HE2   | 1.75                     | 0.41              |
| 10:U:419:LEU:HD13 | 10:U:442:CYS:HB3  | 2.03                     | 0.41              |
| 10:U:460:TYR:HE2  | 10:U:470:LEU:HD21 | 1.85                     | 0.41              |
| 10:U:467:LYS:HZ2  | 10:U:506:HIS:HB3  | 1.86                     | 0.41              |
| 10:V:192:PHE:O    | 10:V:196:THR:HG23 | 2.21                     | 0.41              |
| 10:V:525:LEU:HB3  | 10:V:528:GLU:OE1  | 2.21                     | 0.41              |
| 11:Y:105:LYS:HA   | 11:Y:108:MET:HG3  | 2.03                     | 0.41              |
| 11:Y:332:ILE:HD12 | 11:Y:332:ILE:HA   | 1.82                     | 0.41              |
| 11:Z:305:ALA:HB1  | 11:Z:331:ALA:HB1  | 2.03                     | 0.41              |
| 12:I:44:VAL:HG22  | 12:I:58:PHE:HB3   | 2.03                     | 0.41              |
| 12:I:622:SER:HB3  | 12:I:633:ARG:HE   | 1.85                     | 0.41              |
| 12:I:679:ASP:OD1  | 12:I:682:GLU:HB3  | 2.20                     | 0.41              |
| 13:N:287:ARG:O    | 13:N:291:LYS:HD3  | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1053:GLN:HG3  | 1:A:1057:LEU:HD23 | 2.03                     | 0.41              |
| 1:A:1176:LEU:HD13 | 1:A:1208:LEU:HD13 | 2.03                     | 0.41              |
| 1:A:1617:ARG:HA   | 1:A:1691:LEU:HD13 | 2.03                     | 0.41              |
| 5:J:476:LEU:HG    | 5:J:484:ALA:HB1   | 2.02                     | 0.41              |
| 5:J:499:GLY:HA2   | 5:J:525:VAL:HG23  | 2.02                     | 0.41              |
| 5:J:653:LEU:HD23  | 5:J:653:LEU:HA    | 1.81                     | 0.41              |
| 9:O:33:TYR:CE2    | 9:O:73:ILE:HG12   | 2.56                     | 0.41              |
| 10:U:33:LYS:NZ    | 10:V:85:ASP:OD2   | 2.31                     | 0.41              |
| 11:Z:16:HIS:HA    | 11:Z:19:VAL:HG12  | 2.02                     | 0.41              |
| 12:I:344:ILE:O    | 12:I:348:VAL:HG23 | 2.21                     | 0.41              |
| 13:N:368:THR:HG22 | 13:N:369:ASP:N    | 2.36                     | 0.41              |
| 1:A:150:CYS:HA    | 1:A:163:SER:HA    | 2.03                     | 0.40              |
| 1:A:152:CYS:SG    | 1:A:187:LEU:HD11  | 2.60                     | 0.40              |
| 1:A:982:ASP:HB2   | 1:A:1698:TYR:O    | 2.20                     | 0.40              |
| 1:A:1390:PRO:HB2  | 1:A:1396:LEU:HD23 | 2.02                     | 0.40              |
| 3:G:12:LYS:HE3    | 3:G:12:LYS:HB2    | 1.87                     | 0.40              |
| 9:O:378:SER:HB2   | 9:O:417:LEU:HD13  | 2.03                     | 0.40              |
| 5:P:628:ILE:HD13  | 5:P:628:ILE:HA    | 1.79                     | 0.40              |
| 5:P:658:PHE:HB3   | 5:P:675:ILE:HG12  | 2.03                     | 0.40              |
| 6:Q:155:GLU:OE2   | 6:Q:159:LEU:HG    | 2.21                     | 0.40              |
| 10:V:228:TRP:HD1  | 10:V:228:TRP:H    | 1.68                     | 0.40              |
| 10:V:323:LEU:HD23 | 10:V:323:LEU:HA   | 1.87                     | 0.40              |
| 10:V:537:CYS:HA   | 10:V:543:ARG:HA   | 2.02                     | 0.40              |
| 11:Y:146:LYS:HE3  | 11:Y:146:LYS:HB2  | 1.75                     | 0.40              |
| 11:Y:206:ILE:HD12 | 11:Y:206:ILE:HA   | 1.93                     | 0.40              |
| 11:Z:282:ALA:HB2  | 11:Z:290:VAL:HG21 | 2.02                     | 0.40              |
| 11:Z:312:GLY:HA3  | 11:Z:344:LEU:HD21 | 2.03                     | 0.40              |
| 12:I:138:LEU:HA   | 12:I:138:LEU:HD23 | 1.87                     | 0.40              |
| 13:N:182:ARG:HB3  | 13:N:223:GLY:HA2  | 2.03                     | 0.40              |
| 1:A:953:LEU:HD21  | 1:A:1821:PHE:HE2  | 1.87                     | 0.40              |
| 6:K:48:TYR:HB2    | 6:K:79:CYS:SG     | 2.62                     | 0.40              |
| 6:K:232:ASP:OD1   | 6:K:264:HIS:NE2   | 2.54                     | 0.40              |
| 9:O:97:ILE:HD12   | 9:O:97:ILE:HA     | 1.94                     | 0.40              |
| 6:Q:84:LYS:HD3    | 6:Q:84:LYS:HA     | 1.83                     | 0.40              |
| 6:Q:93:LEU:HD13   | 6:Q:136:ARG:HG2   | 2.03                     | 0.40              |
| 6:Q:298:ASN:OD1   | 6:Q:299:PRO:HD2   | 2.22                     | 0.40              |
| 10:U:35:GLN:O     | 10:U:38:LEU:HG    | 2.21                     | 0.40              |
| 10:U:39:ILE:HG12  | 10:U:201:LEU:O    | 2.20                     | 0.40              |
| 10:V:45:GLU:OE2   | 10:V:45:GLU:HA    | 2.20                     | 0.40              |
| 10:V:209:LEU:HD12 | 10:V:209:LEU:HA   | 1.79                     | 0.40              |
| 10:V:441:GLU:HG2  | 10:V:472:LYS:HE2  | 2.01                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:I:321:LEU:HA   | 12:I:321:LEU:HD12 | 1.86                     | 0.40              |
| 13:N:59:VAL:HG21  | 13:N:135:TRP:CZ3  | 2.56                     | 0.40              |
| 13:N:228:LYS:N    | 13:N:228:LYS:HD3  | 2.36                     | 0.40              |
| 5:J:498:THR:HG21  | 5:P:30:ARG:HH12   | 1.86                     | 0.40              |
| 8:M:50:VAL:HA     | 8:M:53:GLN:HG2    | 2.03                     | 0.40              |
| 9:O:648:ILE:HD13  | 9:O:648:ILE:HA    | 1.85                     | 0.40              |
| 5:P:8:VAL:HG23    | 5:P:27:LEU:HD12   | 2.02                     | 0.40              |
| 5:P:473:TYR:HD2   | 5:P:500:TRP:CZ2   | 2.39                     | 0.40              |
| 10:U:318:TYR:HA   | 10:U:321:HIS:CD2  | 2.57                     | 0.40              |
| 11:Y:163:ARG:HD2  | 11:Y:163:ARG:C    | 2.41                     | 0.40              |
| 11:Y:232:LEU:HD11 | 11:Z:33:ASN:HB2   | 2.04                     | 0.40              |
| 11:Y:488:VAL:O    | 11:Y:489:ASN:HB2  | 2.22                     | 0.40              |
| 13:N:180:PHE:HB2  | 13:N:240:PHE:CZ   | 2.56                     | 0.40              |
| 1:A:1216:LYS:HB3  | 1:A:1219:THR:OG1  | 2.22                     | 0.40              |
| 1:A:1716:GLN:OE1  | 13:N:369:ASP:HB3  | 2.21                     | 0.40              |
| 2:D:37:HIS:HD2    | 9:O:145:LYS:HD3   | 1.87                     | 0.40              |
| 6:K:210:LYS:HB3   | 6:K:213:ASN:OD1   | 2.22                     | 0.40              |
| 7:L:73:THR:HG23   | 7:L:133:ARG:HG2   | 2.03                     | 0.40              |
| 9:O:422:ILE:CG2   | 9:O:445:LEU:HB2   | 2.52                     | 0.40              |
| 9:O:706:CYS:SG    | 9:O:709:ARG:HD3   | 2.62                     | 0.40              |
| 5:P:160:GLU:O     | 5:P:162:PRO:HD3   | 2.21                     | 0.40              |
| 10:U:29:LEU:HD12  | 10:U:62:LEU:HD21  | 2.04                     | 0.40              |
| 10:U:419:LEU:HD21 | 10:U:443:TYR:CE2  | 2.56                     | 0.40              |
| 10:V:180:ARG:HD3  | 10:V:212:LEU:CD2  | 2.50                     | 0.40              |
| 11:Y:25:LEU:HD23  | 11:Z:201:TRP:CZ3  | 2.57                     | 0.40              |
| 11:Z:46:LEU:HD23  | 11:Z:46:LEU:HA    | 1.89                     | 0.40              |
| 12:I:642:GLN:OE1  | 12:I:723:ALA:HA   | 2.21                     | 0.40              |
| 13:N:545:LEU:HD23 | 13:N:545:LEU:O    | 2.21                     | 0.40              |
| 1:A:27:HIS:O      | 1:A:27:HIS:ND1    | 2.54                     | 0.40              |
| 1:A:860:TYR:HE2   | 1:A:870:SER:HG    | 1.68                     | 0.40              |
| 1:A:1179:LEU:HD23 | 1:A:1179:LEU:HA   | 1.93                     | 0.40              |
| 1:A:1225:THR:HG21 | 1:A:1261:TYR:OH   | 2.22                     | 0.40              |
| 1:A:1416:TRP:CH2  | 1:A:1475:ARG:HA   | 2.57                     | 0.40              |
| 1:A:1702:ARG:HG2  | 1:A:1782:GLU:OE2  | 2.21                     | 0.40              |
| 6:K:284:LEU:O     | 6:K:284:LEU:HD23  | 2.21                     | 0.40              |
| 5:P:735:LYS:HA    | 5:P:735:LYS:HD2   | 1.83                     | 0.40              |
| 10:U:290:ARG:HD3  | 10:U:300:MET:SD   | 2.62                     | 0.40              |
| 10:U:423:ARG:HG3  | 10:U:423:ARG:NH1  | 2.35                     | 0.40              |
| 10:V:128:LYS:HB3  | 10:V:128:LYS:HE3  | 1.90                     | 0.40              |
| 10:V:274:HIS:ND1  | 10:V:306:LEU:HD21 | 2.37                     | 0.40              |
| 11:Y:22:LEU:HD12  | 11:Y:22:LEU:HA    | 1.82                     | 0.40              |

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| Atom-1            | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-----------------|--------------------------|-------------------|
| 13:N:615:ILE:HD13 | 13:N:615:ILE:HA | 1.92                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 1   | A     | 1546/1944 (80%) | 1493 (97%) | 52 (3%) | 1 (0%)   | 48          | 80  |
| 2   | D     | 54/121 (45%)    | 54 (100%)  | 0       | 0        | 100         | 100 |
| 3   | G     | 25/85 (29%)     | 25 (100%)  | 0       | 0        | 100         | 100 |
| 3   | W     | 23/85 (27%)     | 23 (100%)  | 0       | 0        | 100         | 100 |
| 4   | H     | 55/110 (50%)    | 55 (100%)  | 0       | 0        | 100         | 100 |
| 5   | J     | 471/824 (57%)   | 456 (97%)  | 15 (3%) | 0        | 100         | 100 |
| 5   | P     | 480/824 (58%)   | 467 (97%)  | 13 (3%) | 0        | 100         | 100 |
| 6   | K     | 506/620 (82%)   | 489 (97%)  | 17 (3%) | 0        | 100         | 100 |
| 6   | Q     | 500/620 (81%)   | 490 (98%)  | 10 (2%) | 0        | 100         | 100 |
| 7   | L     | 175/185 (95%)   | 167 (95%)  | 8 (5%)  | 0        | 100         | 100 |
| 8   | M     | 54/74 (73%)     | 51 (94%)   | 3 (6%)  | 0        | 100         | 100 |
| 9   | O     | 675/755 (89%)   | 664 (98%)  | 11 (2%) | 0        | 100         | 100 |
| 10  | U     | 499/597 (84%)   | 486 (97%)  | 13 (3%) | 0        | 100         | 100 |
| 10  | V     | 532/597 (89%)   | 519 (98%)  | 13 (2%) | 0        | 100         | 100 |
| 11  | Y     | 496/565 (88%)   | 486 (98%)  | 10 (2%) | 0        | 100         | 100 |
| 11  | Z     | 483/565 (86%)   | 475 (98%)  | 8 (2%)  | 0        | 100         | 100 |
| 12  | I     | 710/814 (87%)   | 695 (98%)  | 15 (2%) | 0        | 100         | 100 |
| 13  | N     | 596/822 (72%)   | 579 (97%)  | 16 (3%) | 1 (0%)   | 44          | 75  |
| 14  | C     | 81/84 (96%)     | 78 (96%)   | 3 (4%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| All | All   | 7961/10291 (77%) | 7752 (97%) | 207 (3%) | 2 (0%)   | 100         | 100 |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | N     | 689 | VAL  |
| 1   | A     | 591 | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 1   | A     | 1349/1720 (78%) | 1322 (98%) | 27 (2%)  | 50          | 75  |
| 2   | D     | 52/115 (45%)    | 51 (98%)   | 1 (2%)   | 52          | 76  |
| 3   | G     | 24/77 (31%)     | 24 (100%)  | 0        | 100         | 100 |
| 3   | W     | 24/77 (31%)     | 24 (100%)  | 0        | 100         | 100 |
| 4   | H     | 49/89 (55%)     | 49 (100%)  | 0        | 100         | 100 |
| 5   | J     | 343/727 (47%)   | 329 (96%)  | 14 (4%)  | 26          | 59  |
| 5   | P     | 414/727 (57%)   | 400 (97%)  | 14 (3%)  | 32          | 63  |
| 6   | K     | 439/548 (80%)   | 429 (98%)  | 10 (2%)  | 45          | 72  |
| 6   | Q     | 425/548 (78%)   | 417 (98%)  | 8 (2%)   | 52          | 76  |
| 7   | L     | 163/170 (96%)   | 156 (96%)  | 7 (4%)   | 25          | 57  |
| 8   | M     | 52/67 (78%)     | 49 (94%)   | 3 (6%)   | 17          | 49  |
| 9   | O     | 582/650 (90%)   | 568 (98%)  | 14 (2%)  | 44          | 71  |
| 10  | U     | 431/520 (83%)   | 422 (98%)  | 9 (2%)   | 48          | 74  |
| 10  | V     | 464/520 (89%)   | 456 (98%)  | 8 (2%)   | 56          | 78  |
| 11  | Y     | 423/484 (87%)   | 412 (97%)  | 11 (3%)  | 41          | 70  |
| 11  | Z     | 412/484 (85%)   | 402 (98%)  | 10 (2%)  | 44          | 71  |
| 12  | I     | 634/736 (86%)   | 624 (98%)  | 10 (2%)  | 58          | 79  |
| 13  | N     | 458/724 (63%)   | 447 (98%)  | 11 (2%)  | 44          | 71  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |
|-----|-------|-----------------|------------|----------|-------------|
| 14  | C     | 48/75 (64%)     | 47 (98%)   | 1 (2%)   | 48 74       |
| All | All   | 6786/9058 (75%) | 6628 (98%) | 158 (2%) | 46 72       |

All (158) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 129    | CYS  |
| 1   | A     | 130    | ASP  |
| 1   | A     | 138    | SER  |
| 1   | A     | 161    | MET  |
| 1   | A     | 225    | CYS  |
| 1   | A     | 242    | HIS  |
| 1   | A     | 496    | ASN  |
| 1   | A     | 654    | HIS  |
| 1   | A     | 656    | GLU  |
| 1   | A     | 749    | LEU  |
| 1   | A     | 832    | HIS  |
| 1   | A     | 837    | PHE  |
| 1   | A     | 840    | GLU  |
| 1   | A     | 843    | SER  |
| 1   | A     | 939    | PHE  |
| 1   | A     | 988    | CYS  |
| 1   | A     | 1072   | GLN  |
| 1   | A     | 1288   | CYS  |
| 1   | A     | 1291   | ARG  |
| 1   | A     | 1295   | SER  |
| 1   | A     | 1386   | TRP  |
| 1   | A     | 1391   | ASP  |
| 1   | A     | 1395   | LEU  |
| 1   | A     | 1475   | ARG  |
| 1   | A     | 1503   | ASN  |
| 1   | A     | 1599   | ASN  |
| 1   | A     | 1899   | HIS  |
| 2   | D     | 35     | GLN  |
| 5   | J     | 50     | ARG  |
| 5   | J     | 66     | CYS  |
| 5   | J     | 100    | GLN  |
| 5   | J     | 152    | PHE  |
| 5   | J     | 481    | CYS  |
| 5   | J     | 563    | ASP  |
| 5   | J     | 602    | TYR  |
| 5   | J     | 633[A] | ARG  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 5   | J     | 633[B] | ARG  |
| 5   | J     | 636    | ASN  |
| 5   | J     | 639    | TYR  |
| 5   | J     | 643    | MET  |
| 5   | J     | 646    | TYR  |
| 5   | J     | 651    | PHE  |
| 6   | K     | 13     | TYR  |
| 6   | K     | 34     | ARG  |
| 6   | K     | 62     | SER  |
| 6   | K     | 194    | CYS  |
| 6   | K     | 212    | TYR  |
| 6   | K     | 213    | ASN  |
| 6   | K     | 246    | ASP  |
| 6   | K     | 333    | TYR  |
| 6   | K     | 342    | HIS  |
| 6   | K     | 492    | MET  |
| 7   | L     | 48     | ASP  |
| 7   | L     | 83     | TYR  |
| 7   | L     | 84     | LYS  |
| 7   | L     | 88     | SER  |
| 7   | L     | 101    | ASN  |
| 7   | L     | 110    | GLN  |
| 7   | L     | 177    | ASP  |
| 8   | M     | 10     | ARG  |
| 8   | M     | 49     | SER  |
| 8   | M     | 62     | LEU  |
| 9   | O     | 57     | ARG  |
| 9   | O     | 106    | LYS  |
| 9   | O     | 250    | PHE  |
| 9   | O     | 267    | VAL  |
| 9   | O     | 306    | ASN  |
| 9   | O     | 462    | ASN  |
| 9   | O     | 487    | SER  |
| 9   | O     | 510    | CYS  |
| 9   | O     | 546    | ARG  |
| 9   | O     | 593    | ARG  |
| 9   | O     | 665    | PHE  |
| 9   | O     | 707    | LYS  |
| 9   | O     | 709    | ARG  |
| 9   | O     | 741    | HIS  |
| 5   | P     | 22     | ARG  |
| 5   | P     | 30     | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | P     | 77  | LYS  |
| 5   | P     | 83  | SER  |
| 5   | P     | 103 | HIS  |
| 5   | P     | 170 | PHE  |
| 5   | P     | 482 | LYS  |
| 5   | P     | 532 | ARG  |
| 5   | P     | 539 | TYR  |
| 5   | P     | 549 | ASP  |
| 5   | P     | 553 | SER  |
| 5   | P     | 581 | ARG  |
| 5   | P     | 707 | PHE  |
| 5   | P     | 723 | LEU  |
| 6   | Q     | 63  | ARG  |
| 6   | Q     | 180 | GLU  |
| 6   | Q     | 211 | LYS  |
| 6   | Q     | 250 | CYS  |
| 6   | Q     | 311 | MET  |
| 6   | Q     | 340 | TYR  |
| 6   | Q     | 423 | LYS  |
| 6   | Q     | 489 | HIS  |
| 10  | U     | 95  | ASP  |
| 10  | U     | 163 | GLN  |
| 10  | U     | 168 | ASP  |
| 10  | U     | 364 | TYR  |
| 10  | U     | 371 | MET  |
| 10  | U     | 376 | MET  |
| 10  | U     | 399 | TYR  |
| 10  | U     | 460 | TYR  |
| 10  | U     | 467 | LYS  |
| 10  | V     | 101 | ARG  |
| 10  | V     | 304 | SER  |
| 10  | V     | 371 | MET  |
| 10  | V     | 435 | MET  |
| 10  | V     | 496 | ASP  |
| 10  | V     | 500 | CYS  |
| 10  | V     | 555 | GLN  |
| 10  | V     | 557 | ARG  |
| 11  | Y     | 49  | HIS  |
| 11  | Y     | 74  | LYS  |
| 11  | Y     | 108 | MET  |
| 11  | Y     | 112 | TYR  |
| 11  | Y     | 130 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | Y     | 140 | MET  |
| 11  | Y     | 187 | SER  |
| 11  | Y     | 233 | LEU  |
| 11  | Y     | 245 | ASP  |
| 11  | Y     | 299 | ASN  |
| 11  | Y     | 362 | PHE  |
| 11  | Z     | 49  | HIS  |
| 11  | Z     | 190 | MET  |
| 11  | Z     | 229 | LYS  |
| 11  | Z     | 247 | TYR  |
| 11  | Z     | 252 | ASP  |
| 11  | Z     | 254 | LYS  |
| 11  | Z     | 262 | GLN  |
| 11  | Z     | 313 | CYS  |
| 11  | Z     | 460 | ASP  |
| 11  | Z     | 475 | CYS  |
| 12  | I     | 70  | CYS  |
| 12  | I     | 302 | ASP  |
| 12  | I     | 312 | LYS  |
| 12  | I     | 341 | TYR  |
| 12  | I     | 418 | PHE  |
| 12  | I     | 454 | GLU  |
| 12  | I     | 547 | SER  |
| 12  | I     | 553 | CYS  |
| 12  | I     | 572 | PHE  |
| 12  | I     | 728 | ARG  |
| 13  | N     | 86  | ASN  |
| 13  | N     | 113 | ASP  |
| 13  | N     | 221 | CYS  |
| 13  | N     | 224 | CYS  |
| 13  | N     | 238 | GLU  |
| 13  | N     | 302 | LYS  |
| 13  | N     | 382 | LEU  |
| 13  | N     | 556 | PHE  |
| 13  | N     | 601 | TRP  |
| 13  | N     | 622 | TYR  |
| 13  | N     | 626 | TYR  |
| 14  | C     | 14  | TRP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 18   | GLN  |
| 1   | A     | 155  | GLN  |
| 1   | A     | 266  | HIS  |
| 1   | A     | 1201 | HIS  |
| 1   | A     | 1351 | GLN  |
| 1   | A     | 1591 | HIS  |
| 1   | A     | 1604 | GLN  |
| 1   | A     | 1627 | ASN  |
| 1   | A     | 1763 | GLN  |
| 1   | A     | 1832 | ASN  |
| 5   | J     | 139  | GLN  |
| 5   | J     | 583  | HIS  |
| 5   | J     | 648  | GLN  |
| 6   | K     | 80   | HIS  |
| 6   | K     | 352  | GLN  |
| 6   | K     | 415  | ASN  |
| 7   | L     | 60   | GLN  |
| 7   | L     | 145  | HIS  |
| 7   | L     | 146  | GLN  |
| 8   | M     | 66   | HIS  |
| 9   | O     | 261  | ASN  |
| 9   | O     | 306  | ASN  |
| 9   | O     | 332  | GLN  |
| 9   | O     | 521  | ASN  |
| 9   | O     | 671  | GLN  |
| 9   | O     | 731  | ASN  |
| 5   | P     | 575  | ASN  |
| 5   | P     | 599  | ASN  |
| 5   | P     | 667  | GLN  |
| 5   | P     | 674  | HIS  |
| 5   | P     | 680  | HIS  |
| 5   | P     | 716  | ASN  |
| 6   | Q     | 20   | GLN  |
| 6   | Q     | 45   | GLN  |
| 6   | Q     | 88   | GLN  |
| 6   | Q     | 179  | GLN  |
| 6   | Q     | 449  | ASN  |
| 6   | Q     | 468  | HIS  |
| 10  | U     | 71   | GLN  |
| 10  | U     | 107  | HIS  |
| 10  | U     | 347  | HIS  |
| 10  | U     | 407  | GLN  |
| 10  | U     | 479  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | U     | 534 | GLN  |
| 10  | V     | 145 | GLN  |
| 10  | V     | 373 | HIS  |
| 11  | Y     | 213 | HIS  |
| 11  | Y     | 335 | ASN  |
| 11  | Y     | 337 | ASN  |
| 11  | Y     | 408 | GLN  |
| 11  | Y     | 516 | GLN  |
| 11  | Z     | 143 | ASN  |
| 11  | Z     | 213 | HIS  |
| 11  | Z     | 236 | ASN  |
| 11  | Z     | 262 | GLN  |
| 11  | Z     | 387 | ASN  |
| 12  | I     | 455 | HIS  |
| 12  | I     | 584 | HIS  |
| 13  | N     | 235 | GLN  |
| 13  | N     | 241 | HIS  |
| 13  | N     | 245 | 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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.



There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

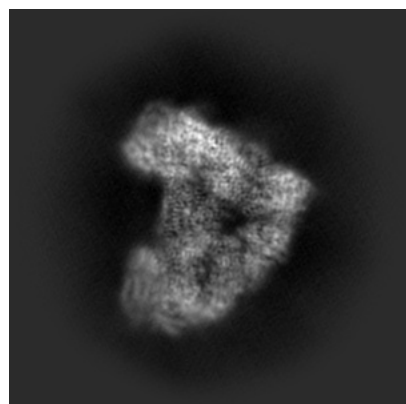
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17751. These allow visual inspection of the internal detail of the map and identification of artifacts.

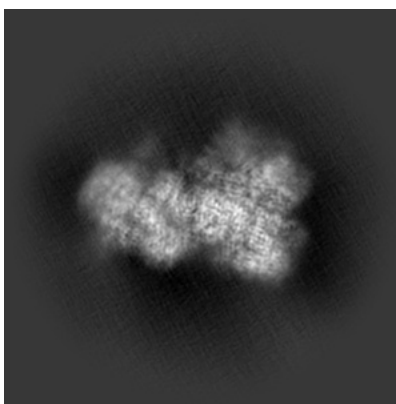
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

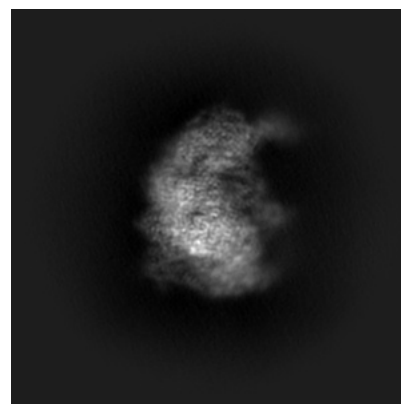
#### 6.1.1 Primary map



X

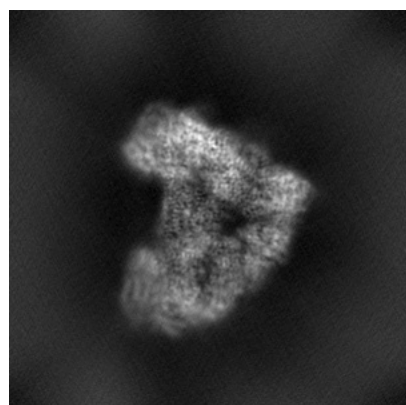


Y

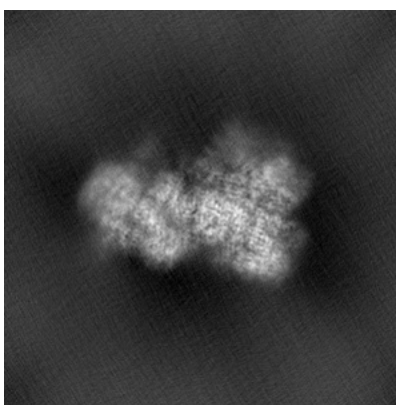


Z

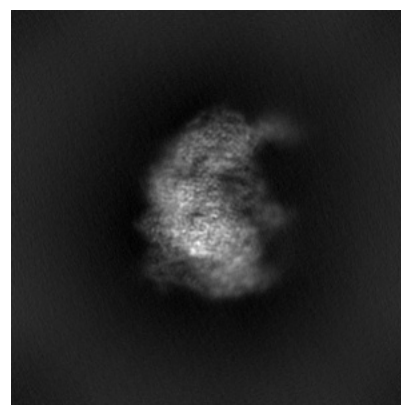
#### 6.1.2 Raw map



X



Y

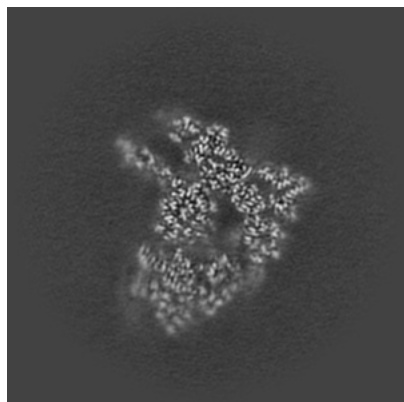


Z

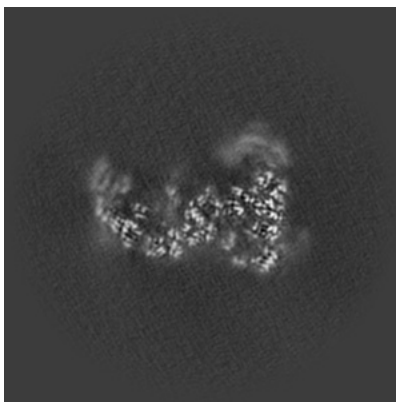
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

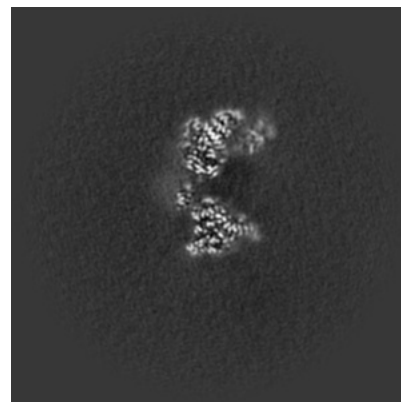
### 6.2.1 Primary map



X Index: 180

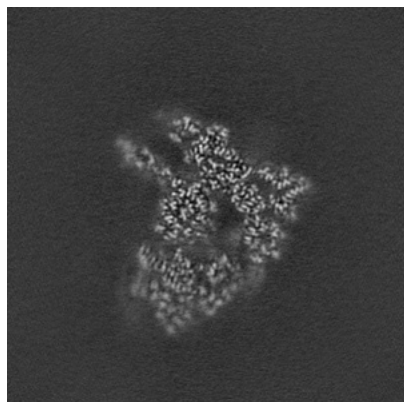


Y Index: 180

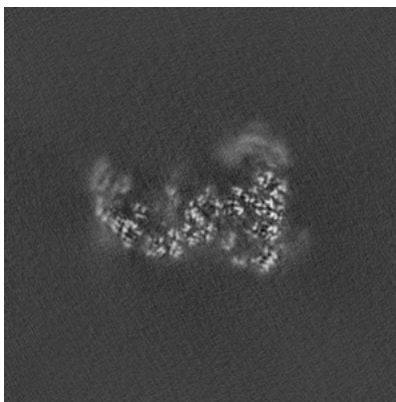


Z Index: 180

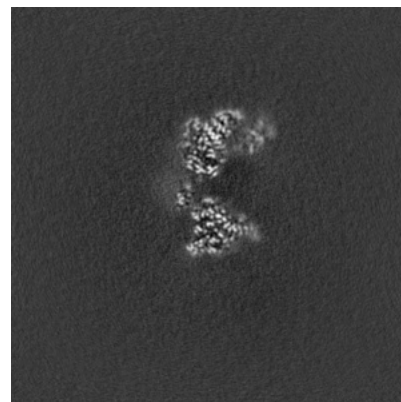
### 6.2.2 Raw map



X Index: 180



Y Index: 180

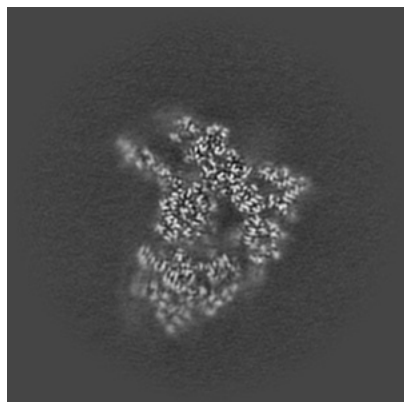


Z Index: 180

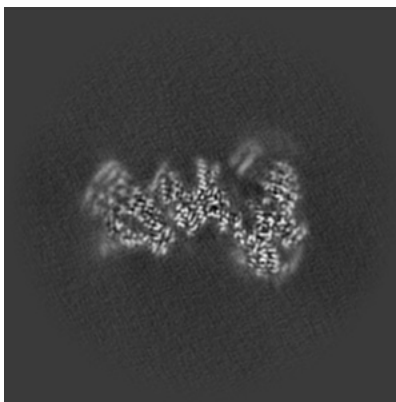
The images above show central slices of the map in three orthogonal directions.

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

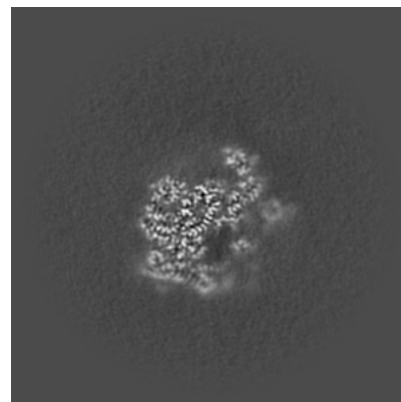
### 6.3.1 Primary map



X Index: 179

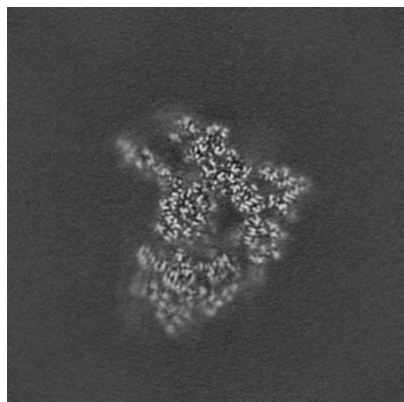


Y Index: 160

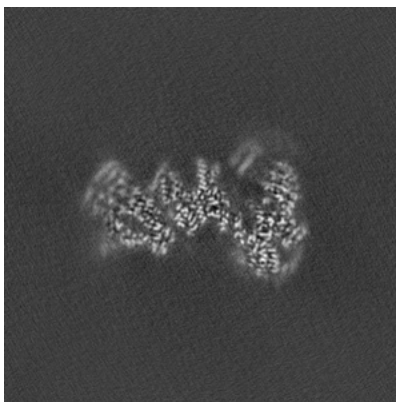


Z Index: 232

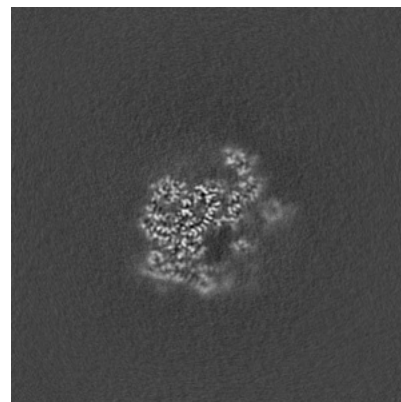
### 6.3.2 Raw map



X Index: 179



Y Index: 160

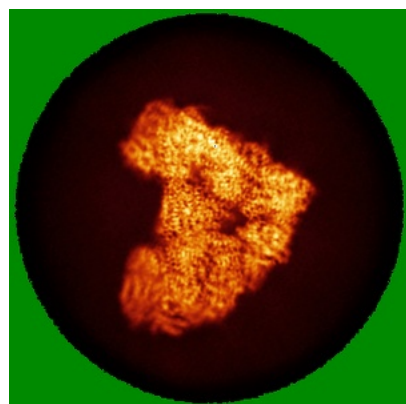


Z Index: 232

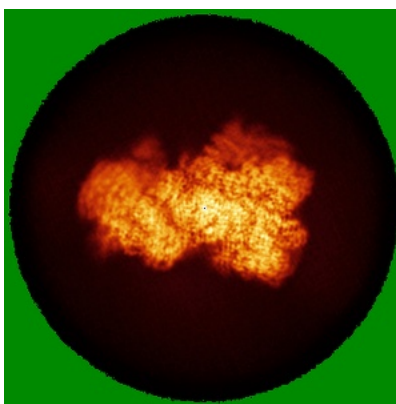
The images above show the largest variance slices of the map in three orthogonal directions.

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

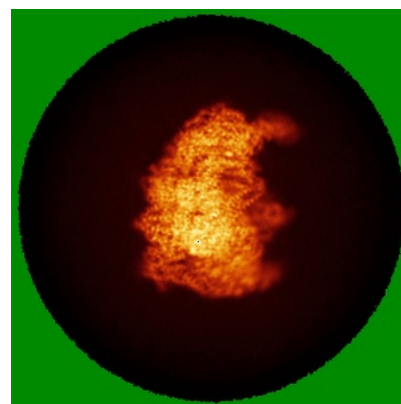
### 6.4.1 Primary map



X

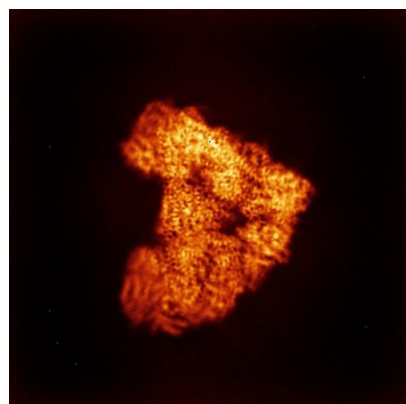


Y

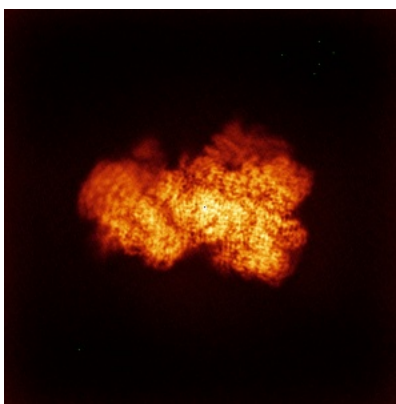


Z

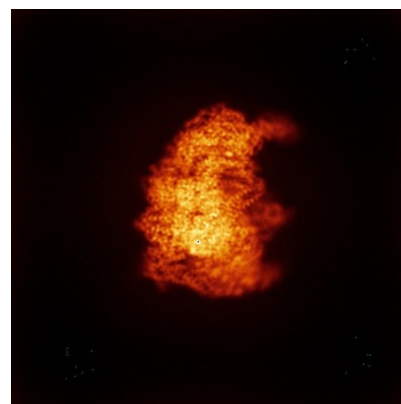
### 6.4.2 Raw map



X



Y

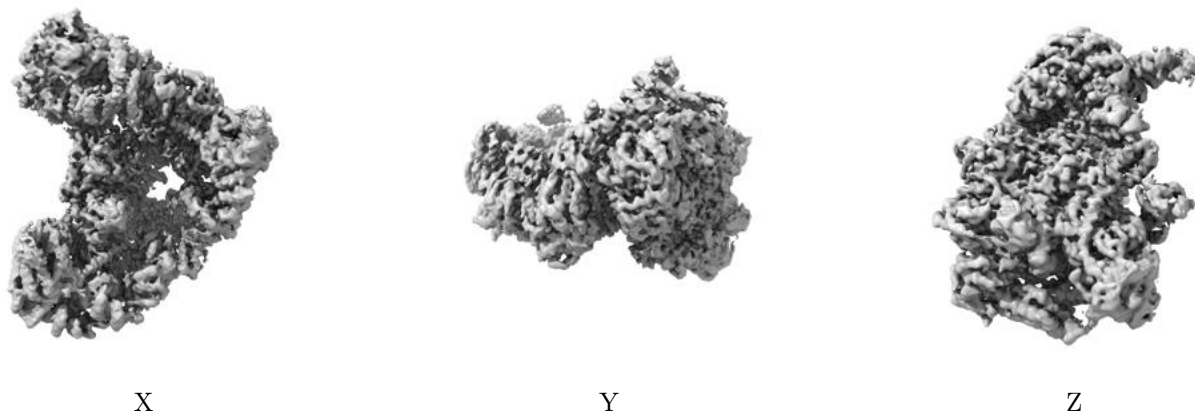


Z

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.

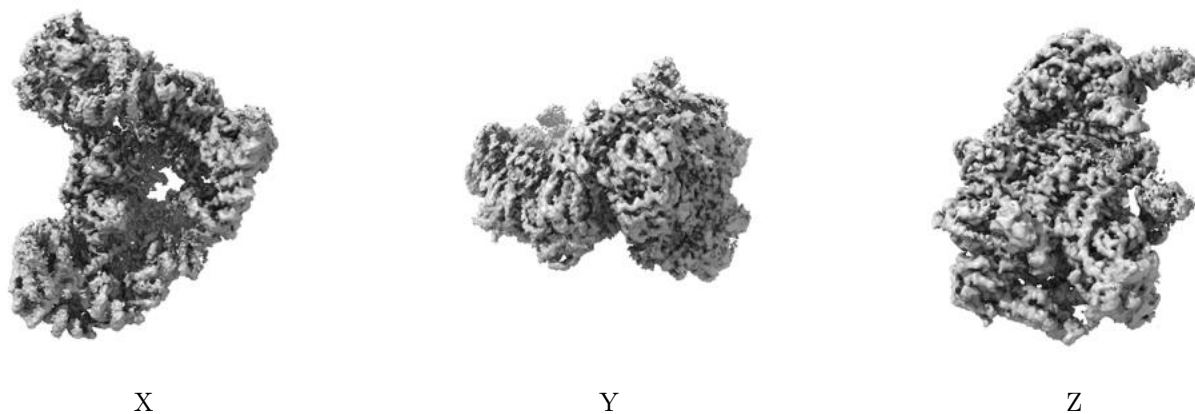
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

## 6.6 Mask visualisation [i](#)

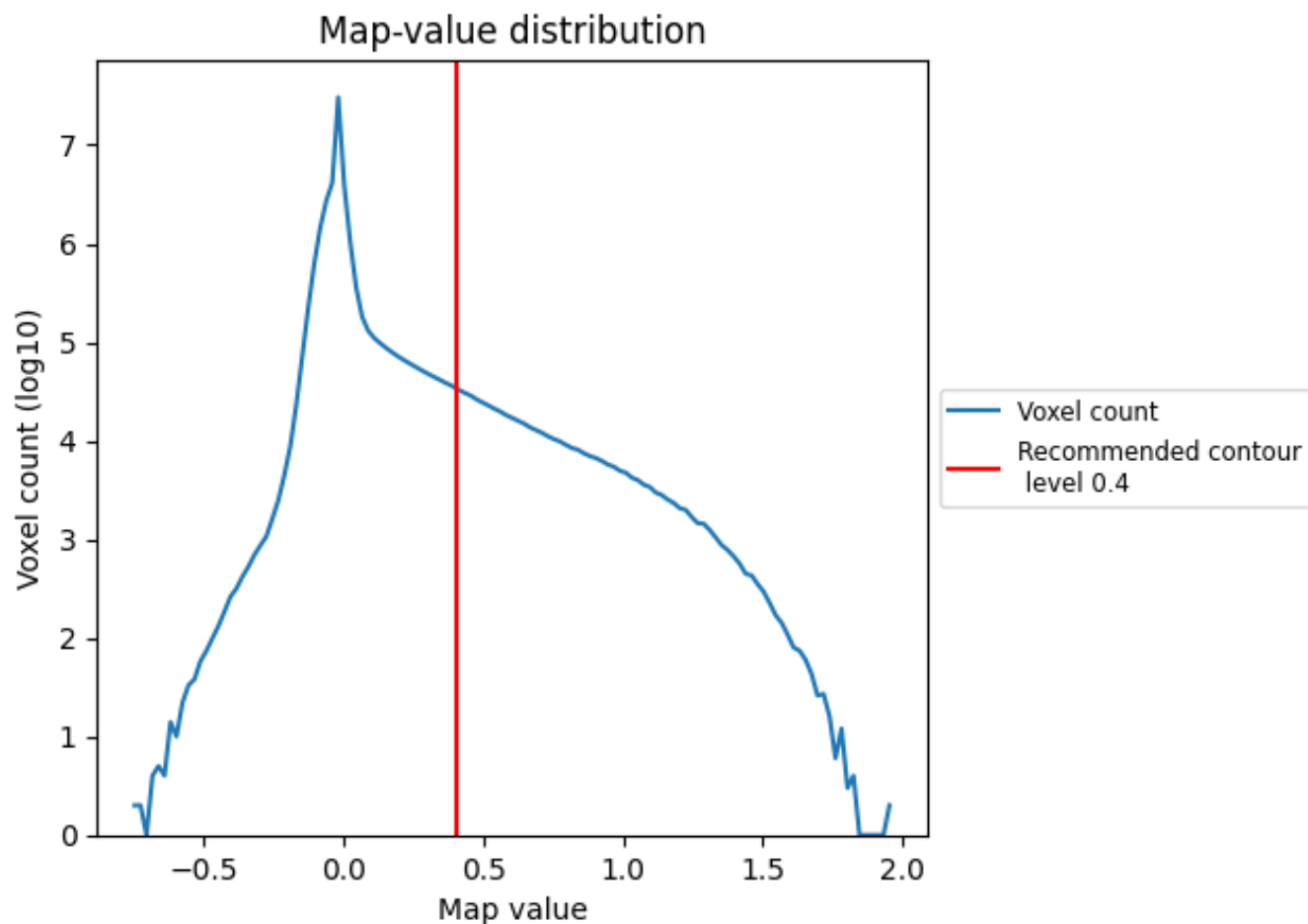
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

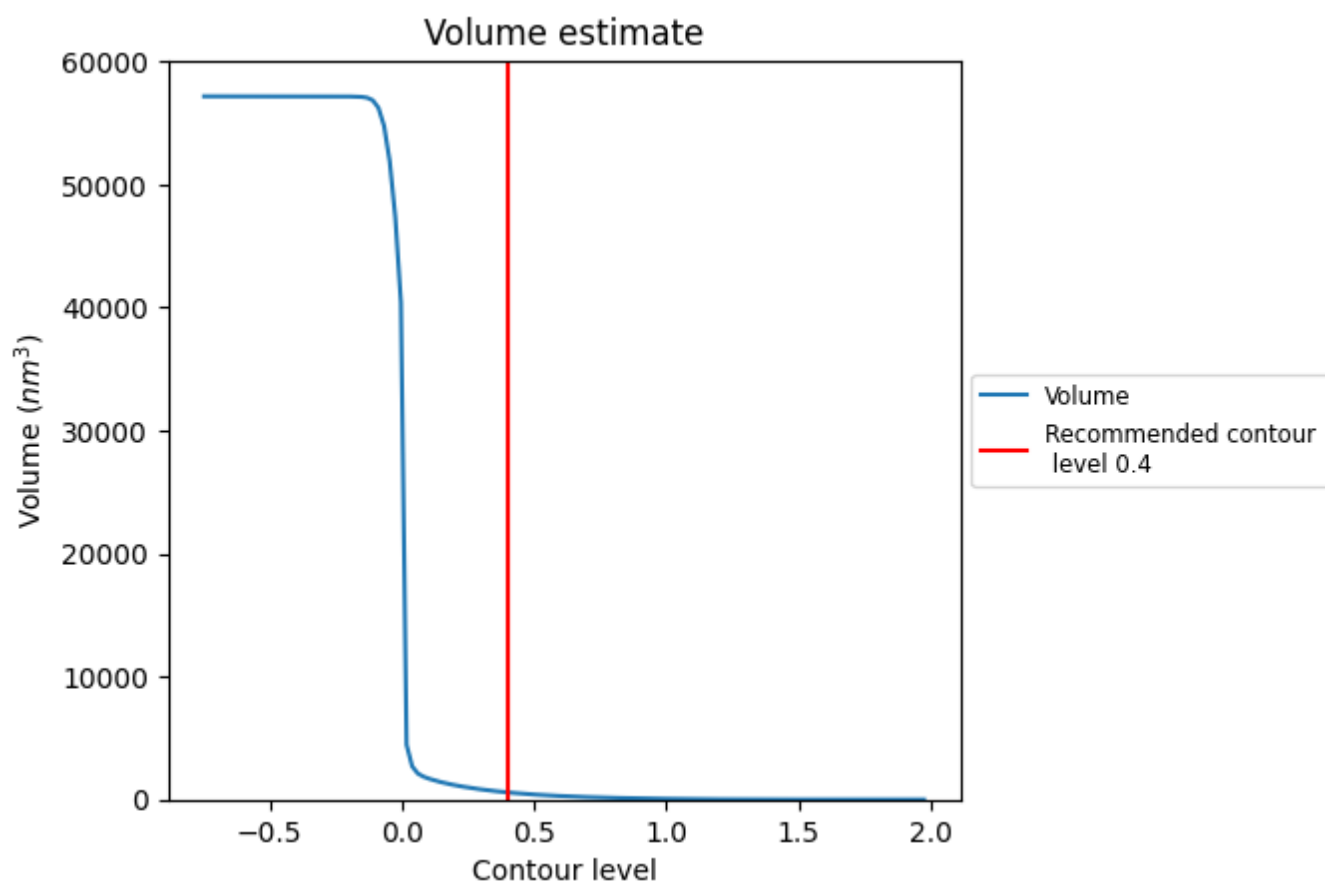
This section contains the results of statistical analysis of the map.

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



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

## 7.2 Volume estimate [i](#)

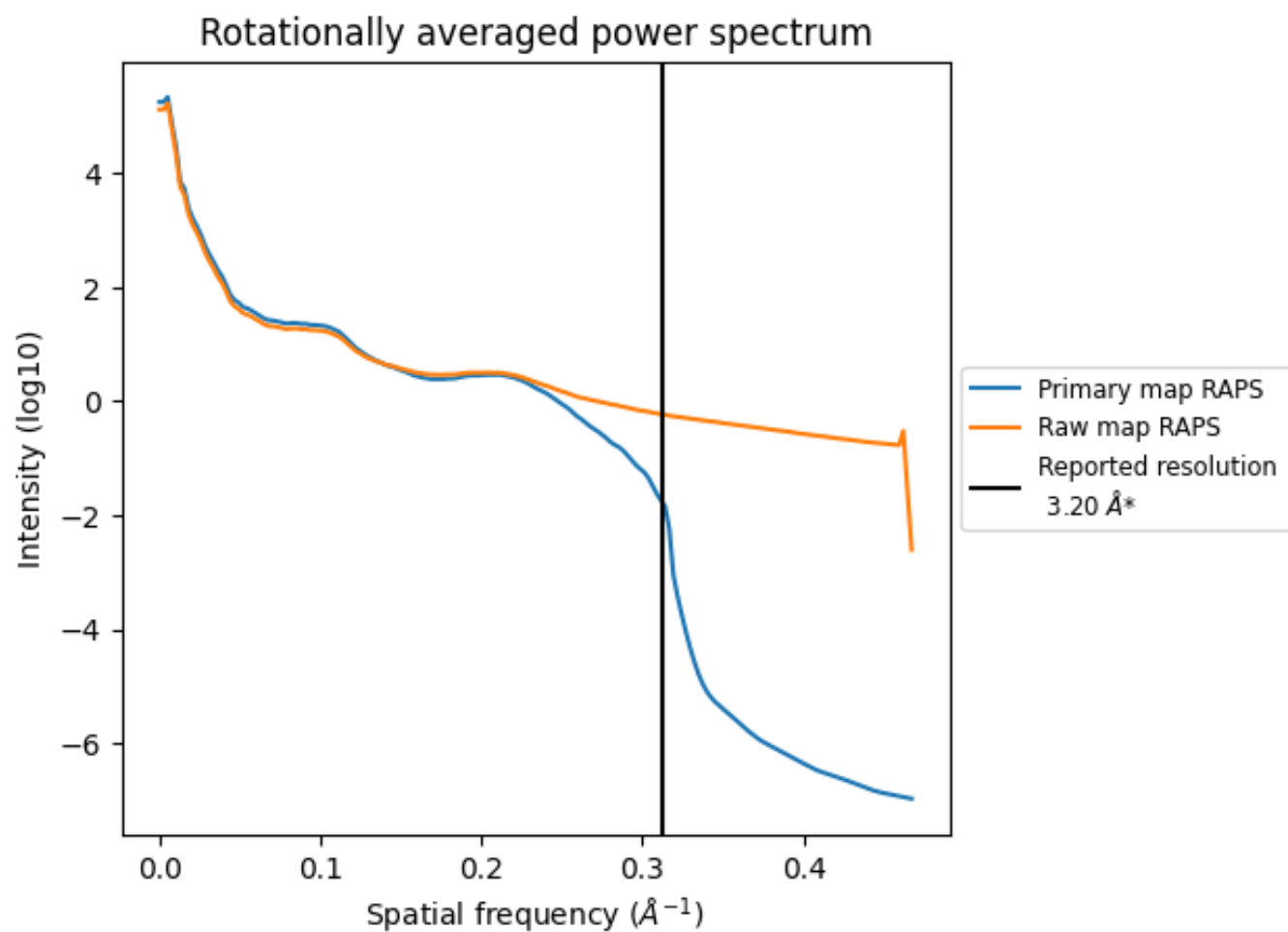


The volume at the recommended contour level is 582 nm<sup>3</sup>; this corresponds to an approximate mass of 526 kDa.

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 ⓘ

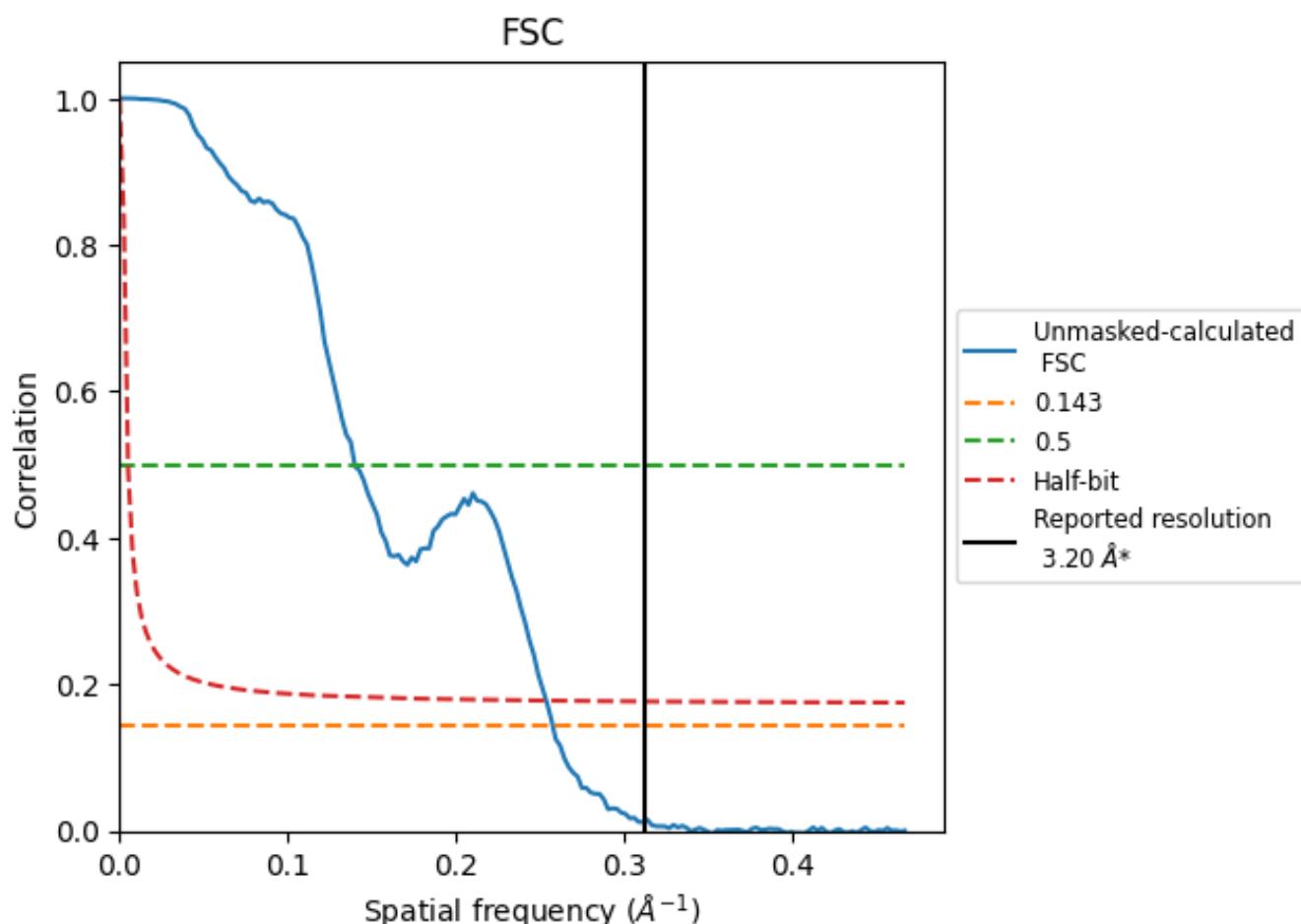


\*Reported resolution corresponds to spatial frequency of  $0.312 \text{ \AA}^{-1}$

## 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 0.312  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

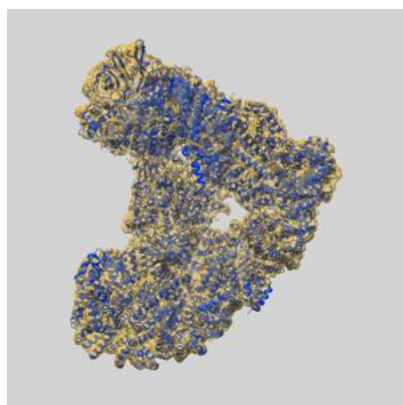
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.20                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 3.88                               | 7.14 | 3.94     |

\*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 3.88 differs from the reported value 3.2 by more than 10 %

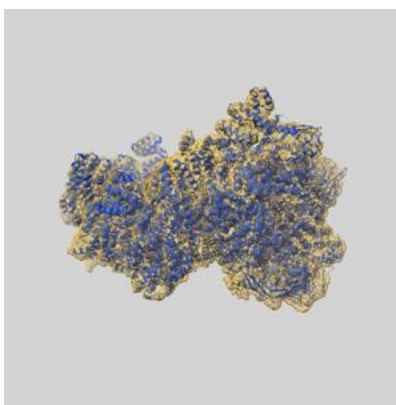
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17751 and PDB model 8PKP. Per-residue inclusion information can be found in section [3](#) on page [7](#).

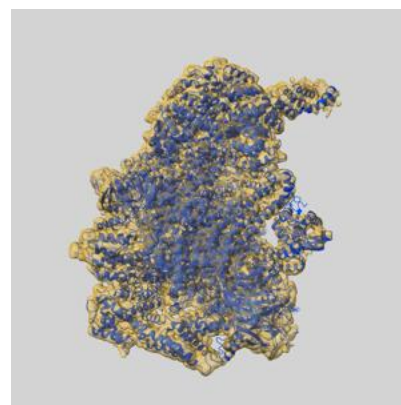
### 9.1 Map-model overlay [i](#)



X



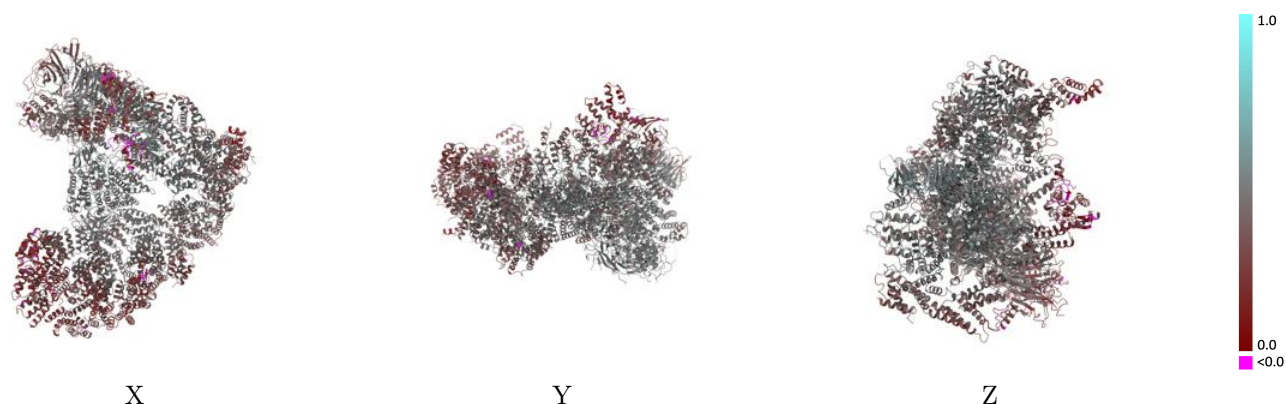
Y



Z

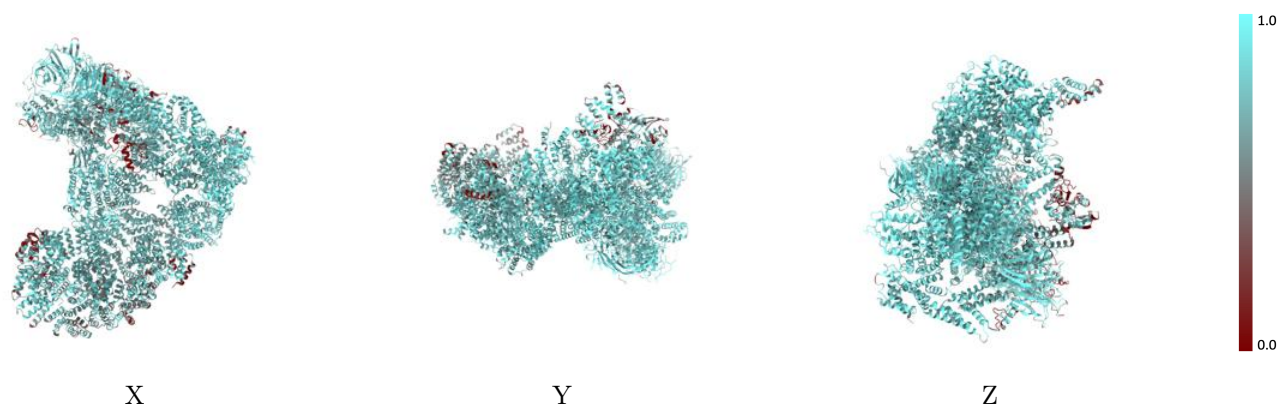
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



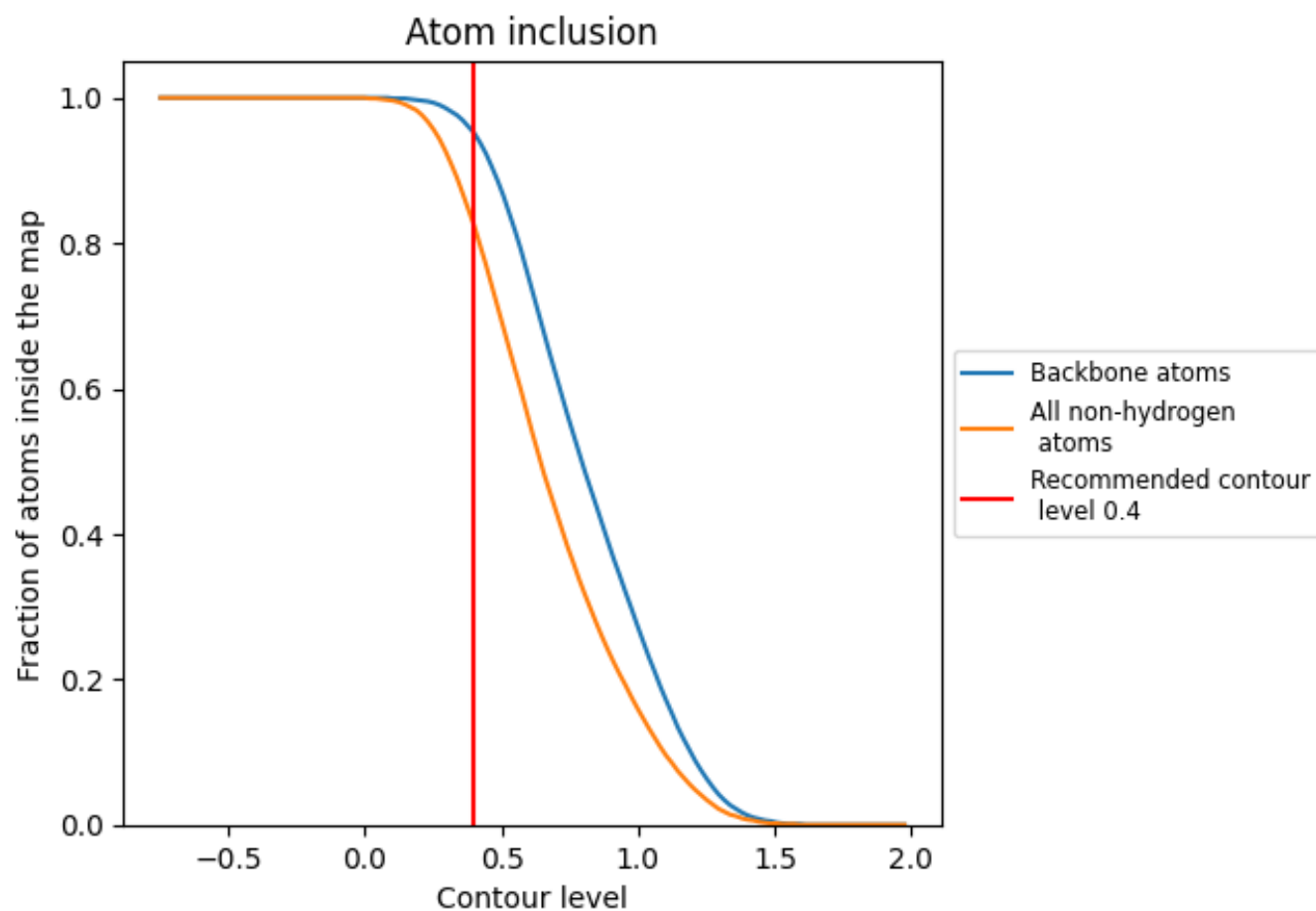
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).









































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 82% 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 (0.4) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.8230   |  0.4120   |
| A     |  0.8960   |  0.4790   |
| C     |  0.1200   |  0.0950   |
| D     |  0.7850   |  0.4610   |
| G     |  0.7750   |  0.4240   |
| H     |  0.7700   |  0.3860   |
| I     |  0.8440   |  0.4220   |
| J     |  0.7870   |  0.3830   |
| K     |  0.8610   |  0.4400   |
| L     |  0.8370   |  0.4390   |
| M     |  0.7270   |  0.4500   |
| N     |  0.7210   |  0.3460   |
| O     |  0.8840   |  0.4750   |
| P     |  0.8630   |  0.4310   |
| Q     |  0.8640  |  0.4160  |
| U     |  0.8490 |  0.4080 |
| V     |  0.8800 |  0.4690 |
| W     |  0.7800 |  0.4850 |
| Y     |  0.6740 |  0.2670 |
| Z     |  0.6870 |  0.2610 |

