



## Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 07:55 AM UTC

PDB ID : 5HNX / pdb\_00005hnx  
EMDB ID : EMD-8059  
Title : Structural basis of backwards motion in kinesin-14: minus-end directed nKn664 in the nucleotide-free state  
Authors : Shigematsu, H.; Yokoyama, T.; Kikkawa, M.; Shirouzu, M.; Nitta, R.  
Deposited on : 2016-01-19  
Resolution : 6.60 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

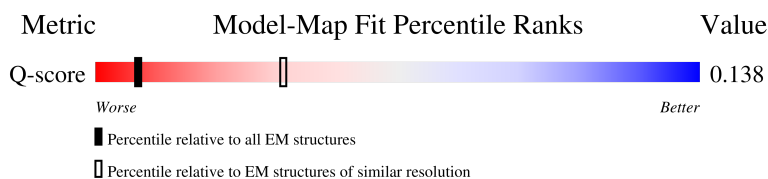
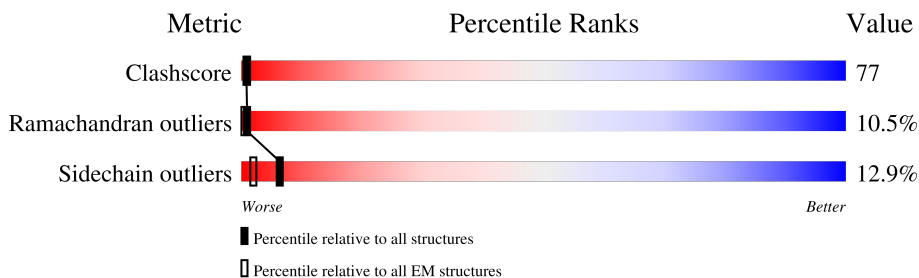
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 531 ( 6.10 - 7.10 )                                      |

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     | 451    |                  |
| 2   | B     | 445    |                  |
| 3   | K     | 371    |                  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 5   | GTP  | A     | 502 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 9198 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 Tubulin alpha-1B chain.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 412      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3227  | 2043 | 551 | 613 | 20 |         |       |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 136     | SER      | LEU    | conflict | UNP P81947 |
| A     | 232     | GLY      | SER    | conflict | UNP P81947 |
| A     | 265     | GLY      | ILE    | conflict | UNP P81947 |
| A     | 340     | THR      | SER    | conflict | UNP P81947 |
| A     | 358     | GLU      | GLN    | conflict | UNP P81947 |

- Molecule 2 is a protein called Tubulin beta-2B chain.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | B     | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3351  | 2105 | 575 | 646 | 25 |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| B     | 57      | ALA      | THR    | conflict | UNP Q6B856 |
| B     | 172     | VAL      | MET    | conflict | UNP Q6B856 |
| B     | 298     | ALA      | SER    | conflict | UNP Q6B856 |
| B     | 318     | VAL      | ILE    | conflict | UNP Q6B856 |

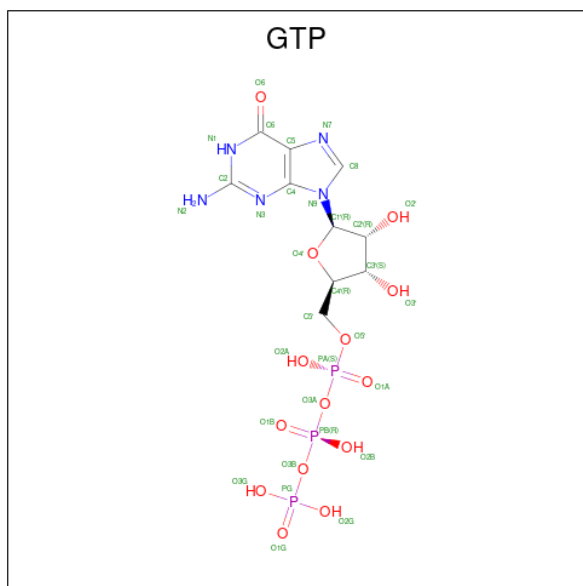
- Molecule 3 is a protein called Protein claret segregational,kinesin-1/kinesin-14,Protein claret segregational.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | K     | 320      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2497  | 1567 | 432 | 485 | 13 |         |       |

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

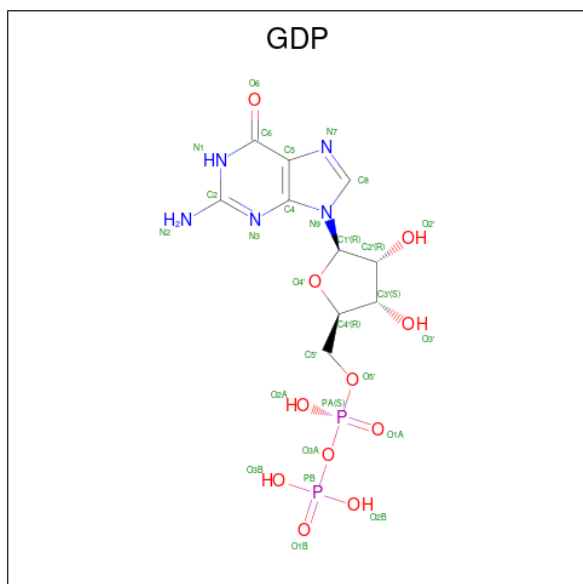
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 4   | A     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).

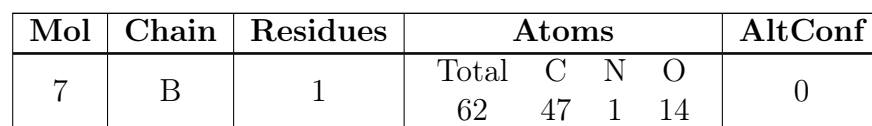


| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 5   | A     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



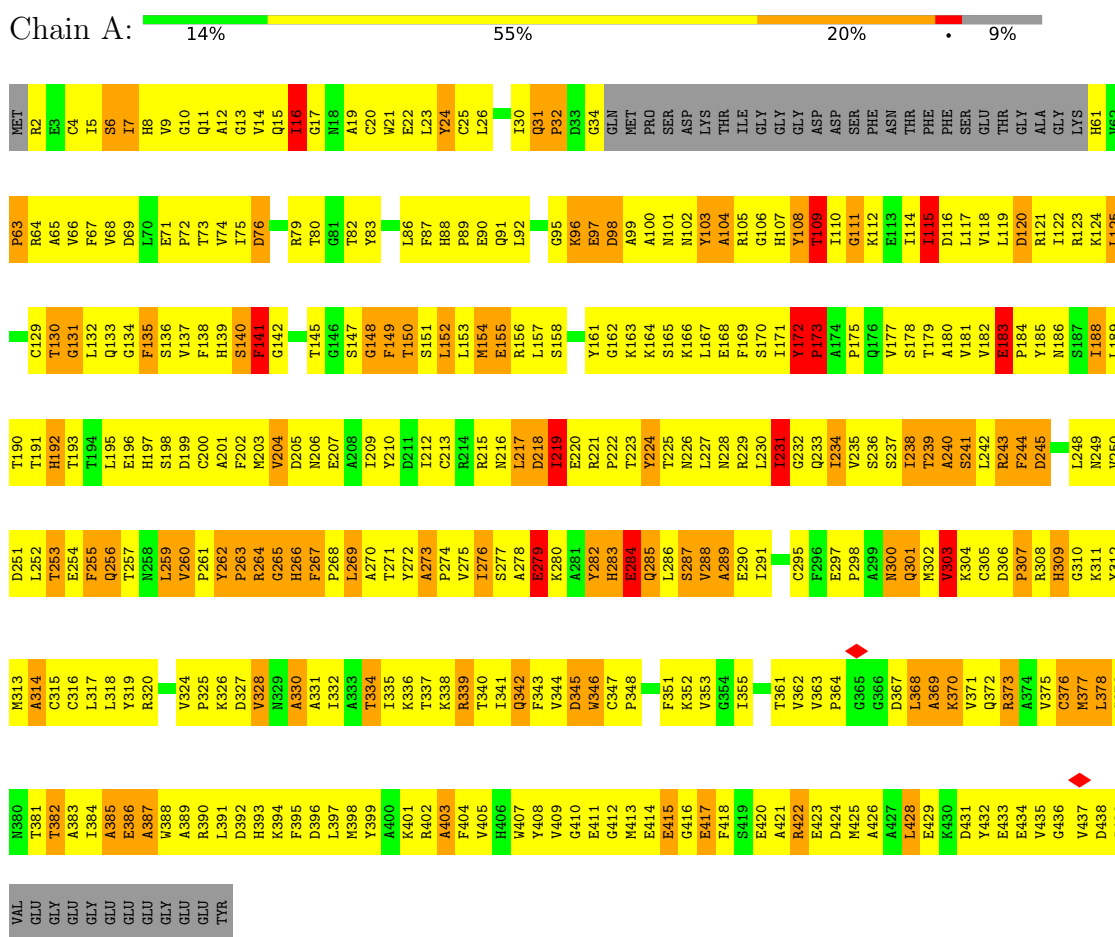
- Molecule 7 is TAXOL (CCD ID: TA1) (formula:  $C_{47}H_{51}NO_{14}$ ).



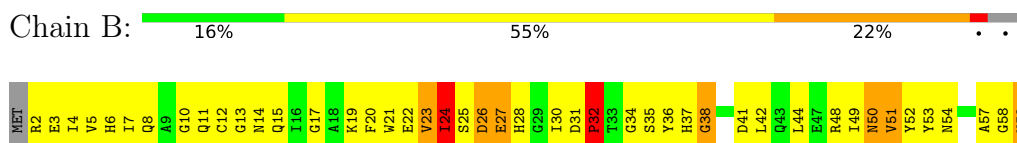
### 3 Residue-property plots

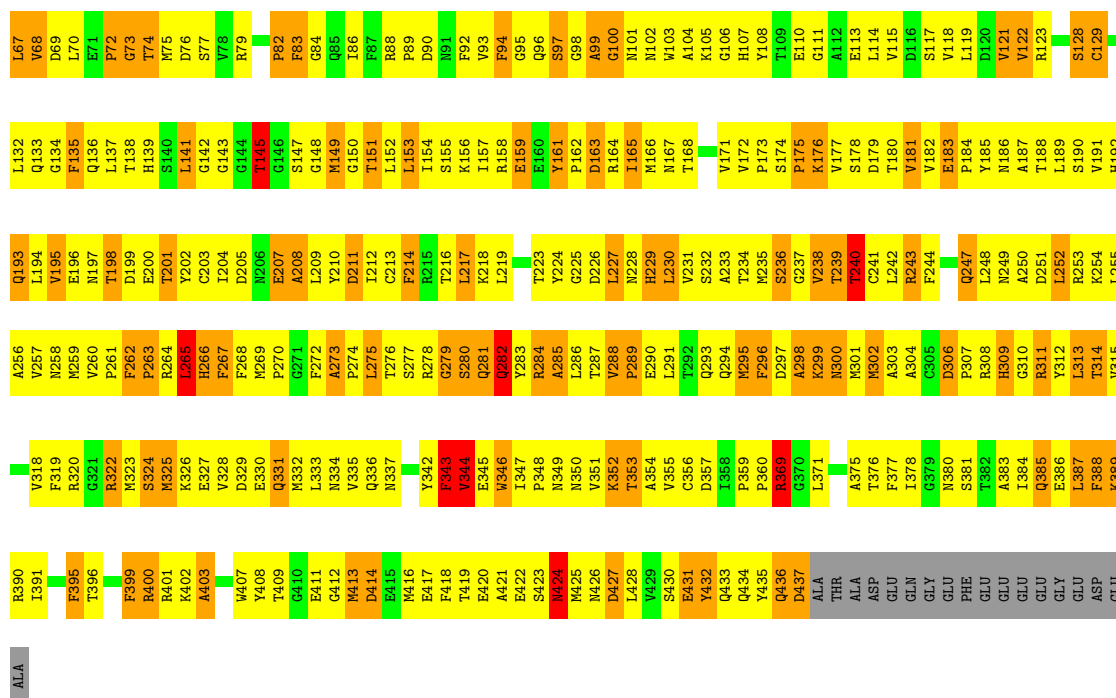
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

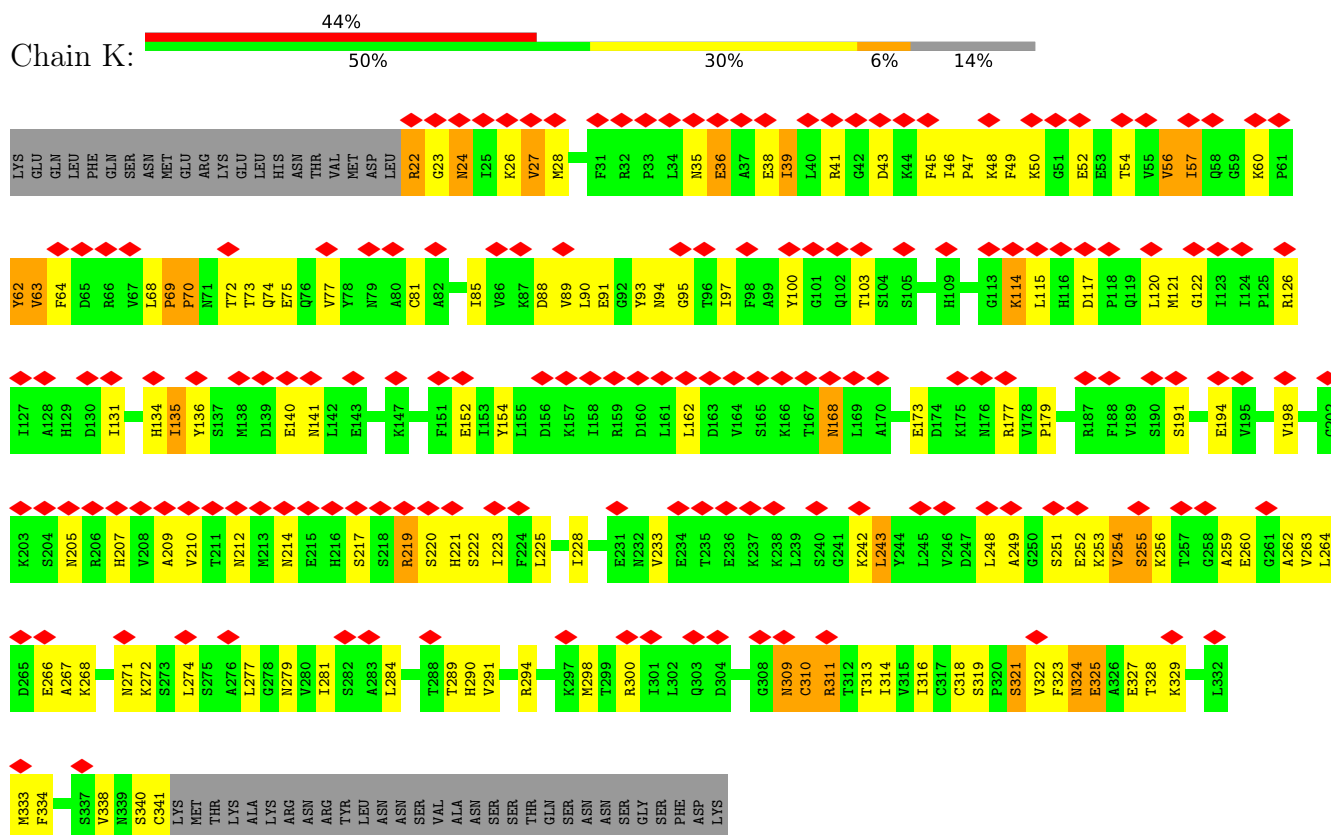


#### • Molecule 2: Tubulin beta-2B chain





- Molecule 3: Protein claret segregational,kinesin-1/kinesin-14,Protein claret segregational



## 4 Experimental information

| Property                           | Value                                                     | Source    |
|------------------------------------|-----------------------------------------------------------|-----------|
| EM reconstruction method           | HELICAL                                                   | Depositor |
| Imposed symmetry                   | HELICAL, twist=-25.725189°, rise=8.751208 Å, axial sym=C1 | Depositor |
| Number of segments used            | 229516                                                    | Depositor |
| Resolution determination method    | FSC 0.143 CUT-OFF                                         | Depositor |
| CTF correction method              | PHASE FLIPPING AND AMPLITUDE CORRECTION                   | Depositor |
| Microscope                         | FEI TECNAI ARCTICA                                        | Depositor |
| Voltage (kV)                       | 200                                                       | Depositor |
| Electron dose ( $e^-/\text{Å}^2$ ) | 30                                                        | Depositor |
| Minimum defocus (nm)               | Not provided                                              |           |
| Maximum defocus (nm)               | Not provided                                              |           |
| Magnification                      | Not provided                                              |           |
| Image detector                     | FEI FALCON II (4k x 4k)                                   | Depositor |
| Maximum map value                  | 18.355                                                    | Depositor |
| Minimum map value                  | -7.321                                                    | Depositor |
| Average map value                  | 1.121                                                     | Depositor |
| Map value standard deviation       | 3.360                                                     | Depositor |
| Recommended contour level          | 3.1                                                       | Depositor |
| Map size (Å)                       | 138.672, 138.672, 246.52802                               | wwPDB     |
| Map dimensions                     | 108, 108, 192                                             | wwPDB     |
| Map angles (°)                     | 90.0, 90.0, 90.0                                          | wwPDB     |
| Pixel spacing (Å)                  | 1.2839999, 1.2839999, 1.284                               | Depositor |

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: TA1, MG, GTP, GDP

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     | 0.62         | 1/3300 (0.0%) | 1.09        | 22/4482 (0.5%)  |
| 2   | B     | 0.63         | 0/3426        | 1.11        | 22/4642 (0.5%)  |
| 3   | K     | 1.17         | 5/2538 (0.2%) | 1.59        | 33/3425 (1.0%)  |
| All | All   | 0.81         | 6/9264 (0.1%) | 1.26        | 77/12549 (0.6%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 3   | K     | 0                   | 3                   |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | K     | 69  | PRO  | N-CD  | 25.17 | 1.82        | 1.47     |
| 3   | K     | 70  | PRO  | N-CD  | 21.21 | 1.77        | 1.47     |
| 3   | K     | 311 | ARG  | CA-C  | -9.12 | 1.42        | 1.53     |
| 3   | K     | 168 | ASN  | C-N   | 6.11  | 1.42        | 1.33     |
| 3   | K     | 327 | GLU  | C-N   | 5.82  | 1.41        | 1.33     |
| 1   | A     | 282 | TYR  | CA-C  | -5.54 | 1.48        | 1.53     |

All (77) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 3   | K     | 168 | ASN  | O-C-N  | -18.07 | 102.32      | 123.28   |
| 1   | A     | 172 | TYR  | CA-C-N | 10.71  | 133.23      | 119.84   |
| 1   | A     | 172 | TYR  | C-N-CA | 10.71  | 133.23      | 119.84   |
| 2   | B     | 262 | PHE  | CA-C-N | 9.97   | 132.30      | 119.84   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | B     | 262 | PHE  | C-N-CA   | 9.97  | 132.30      | 119.84   |
| 3   | K     | 24  | ASN  | CA-CB-CG | -9.67 | 102.93      | 112.60   |
| 1   | A     | 283 | HIS  | N-CA-C   | -8.22 | 101.28      | 113.61   |
| 3   | K     | 36  | GLU  | CA-C-N   | 7.95  | 130.93      | 120.28   |
| 3   | K     | 36  | GLU  | C-N-CA   | 7.95  | 130.93      | 120.28   |
| 2   | B     | 77  | SER  | N-CA-C   | -7.88 | 104.27      | 114.04   |
| 2   | B     | 159 | GLU  | N-CA-C   | -7.68 | 104.40      | 114.31   |
| 2   | B     | 313 | LEU  | N-CA-C   | -7.65 | 103.91      | 113.55   |
| 1   | A     | 428 | LEU  | N-CA-C   | -7.51 | 104.35      | 113.97   |
| 3   | K     | 309 | ASN  | CA-CB-CG | -7.48 | 105.12      | 112.60   |
| 2   | B     | 208 | ALA  | N-CA-C   | -7.46 | 102.83      | 112.23   |
| 3   | K     | 69  | PRO  | CA-N-CD  | -7.46 | 101.56      | 112.00   |
| 2   | B     | 293 | GLN  | N-CA-C   | -7.36 | 102.94      | 110.97   |
| 3   | K     | 35  | ASN  | CA-CB-CG | -7.18 | 105.42      | 112.60   |
| 3   | K     | 23  | GLY  | CA-C-N   | 7.11  | 133.72      | 122.21   |
| 3   | K     | 23  | GLY  | C-N-CA   | 7.11  | 133.72      | 122.21   |
| 2   | B     | 385 | GLN  | N-CA-C   | -7.08 | 103.49      | 111.14   |
| 2   | B     | 399 | PHE  | N-CA-C   | -7.03 | 103.54      | 111.07   |
| 2   | B     | 22  | GLU  | N-CA-C   | -7.02 | 103.32      | 110.97   |
| 3   | K     | 212 | ASN  | CA-CB-CG | -7.00 | 105.60      | 112.60   |
| 1   | A     | 301 | GLN  | N-CA-C   | 6.96  | 121.45      | 112.41   |
| 2   | B     | 388 | PHE  | N-CA-C   | -6.95 | 104.07      | 112.54   |
| 3   | K     | 205 | ASN  | CA-C-N   | 6.94  | 130.72      | 120.87   |
| 3   | K     | 205 | ASN  | C-N-CA   | 6.94  | 130.72      | 120.87   |
| 2   | B     | 389 | LYS  | N-CA-C   | -6.86 | 103.50      | 110.97   |
| 3   | K     | 217 | SER  | CA-C-N   | -6.83 | 113.48      | 123.05   |
| 3   | K     | 217 | SER  | C-N-CA   | -6.83 | 113.48      | 123.05   |
| 1   | A     | 422 | ARG  | N-CA-C   | -6.81 | 103.10      | 111.40   |
| 1   | A     | 385 | ALA  | N-CA-C   | -6.80 | 103.10      | 111.33   |
| 3   | K     | 62  | TYR  | CA-C-N   | 6.75  | 134.11      | 121.97   |
| 3   | K     | 62  | TYR  | C-N-CA   | 6.75  | 134.11      | 121.97   |
| 3   | K     | 69  | PRO  | N-CA-CB  | 6.74  | 109.62      | 103.08   |
| 1   | A     | 188 | ILE  | N-CA-C   | -6.65 | 103.25      | 113.16   |
| 3   | K     | 56  | VAL  | CA-C-N   | 6.55  | 133.11      | 122.69   |
| 3   | K     | 56  | VAL  | C-N-CA   | 6.55  | 133.11      | 122.69   |
| 2   | B     | 217 | LEU  | N-CA-C   | -6.48 | 96.41       | 107.23   |
| 1   | A     | 123 | ARG  | N-CA-C   | -6.46 | 105.98      | 114.31   |
| 3   | K     | 324 | ASN  | CA-C-O   | -6.36 | 113.83      | 120.32   |
| 2   | B     | 27  | GLU  | N-CA-C   | -6.35 | 105.91      | 113.21   |
| 3   | K     | 256 | LYS  | N-CA-C   | -6.30 | 102.05      | 110.55   |
| 3   | K     | 212 | ASN  | N-CA-C   | -6.03 | 100.18      | 109.52   |
| 3   | K     | 70  | PRO  | CA-N-CD  | -6.03 | 103.56      | 112.00   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | B     | 181 | VAL  | N-CA-C   | 6.01  | 116.77      | 111.90   |
| 2   | B     | 243 | ARG  | N-CA-C   | -6.01 | 106.60      | 112.97   |
| 2   | B     | 88  | ARG  | N-CA-C   | -5.96 | 102.25      | 109.83   |
| 1   | A     | 264 | ARG  | N-CA-C   | -5.96 | 101.48      | 110.24   |
| 1   | A     | 231 | ILE  | N-CA-C   | -5.88 | 103.92      | 110.62   |
| 3   | K     | 310 | CYS  | N-CA-CB  | 5.82  | 120.33      | 110.49   |
| 2   | B     | 296 | PHE  | N-CA-C   | 5.76  | 120.01      | 113.15   |
| 2   | B     | 247 | GLN  | N-CA-C   | -5.75 | 105.02      | 111.28   |
| 3   | K     | 214 | ASN  | CA-CB-CG | -5.68 | 106.92      | 112.60   |
| 3   | K     | 219 | ARG  | CB-CA-C  | -5.64 | 103.47      | 112.05   |
| 1   | A     | 415 | GLU  | N-CA-C   | -5.58 | 105.58      | 112.38   |
| 1   | A     | 262 | TYR  | CA-C-N   | 5.50  | 126.71      | 119.84   |
| 1   | A     | 262 | TYR  | C-N-CA   | 5.50  | 126.71      | 119.84   |
| 1   | A     | 297 | GLU  | N-CA-C   | -5.48 | 101.44      | 109.50   |
| 1   | A     | 75  | ILE  | N-CA-C   | -5.47 | 104.26      | 111.09   |
| 1   | A     | 259 | LEU  | N-CA-C   | 5.46  | 120.95      | 113.97   |
| 2   | B     | 59  | ASN  | N-CA-C   | -5.43 | 105.67      | 114.09   |
| 2   | B     | 436 | GLN  | N-CA-C   | -5.33 | 106.48      | 112.87   |
| 3   | K     | 70  | PRO  | N-CA-CB  | 5.31  | 109.17      | 103.33   |
| 1   | A     | 429 | GLU  | N-CA-C   | -5.28 | 105.98      | 112.90   |
| 3   | K     | 255 | SER  | N-CA-C   | -5.28 | 105.42      | 111.07   |
| 2   | B     | 289 | PRO  | N-CA-C   | -5.16 | 107.13      | 113.84   |
| 3   | K     | 57  | ILE  | N-CA-C   | -5.15 | 100.46      | 108.86   |
| 3   | K     | 168 | ASN  | CA-C-N   | 5.13  | 130.86      | 122.81   |
| 3   | K     | 168 | ASN  | C-N-CA   | 5.13  | 130.86      | 122.81   |
| 1   | A     | 241 | SER  | N-CA-C   | 5.10  | 116.84      | 111.28   |
| 1   | A     | 140 | SER  | N-CA-C   | 5.08  | 116.32      | 109.11   |
| 3   | K     | 27  | VAL  | N-CA-CB  | 5.07  | 120.20      | 111.39   |
| 1   | A     | 421 | ALA  | N-CA-C   | -5.06 | 107.14      | 113.72   |
| 1   | A     | 16  | ILE  | N-CA-C   | -5.03 | 105.49      | 110.62   |
| 3   | K     | 191 | SER  | N-CA-C   | 5.01  | 112.73      | 108.22   |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 3   | K     | 168 | ASN  | Mainchain,Peptide |
| 3   | K     | 22  | ARG  | Peptide           |

## 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     | 3227  | 0        | 3143     | 662     | 0            |
| 2   | B     | 3351  | 0        | 3229     | 669     | 0            |
| 3   | K     | 2497  | 0        | 2498     | 209     | 0            |
| 4   | A     | 1     | 0        | 0        | 0       | 0            |
| 5   | A     | 32    | 0        | 12       | 12      | 0            |
| 6   | B     | 28    | 0        | 12       | 2       | 0            |
| 7   | B     | 62    | 0        | 51       | 11      | 0            |
| All | All   | 9198  | 0        | 8945     | 1399    | 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 77.

All (1399) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:434:GLN:CD   | 3:K:290:HIS:HB2  | 1.38                     | 1.47              |
| 1:A:108:TYR:CE2  | 3:K:255:SER:HB2  | 1.50                     | 1.44              |
| 2:B:416:MET:HE1  | 3:K:173:GLU:CB   | 1.48                     | 1.43              |
| 2:B:416:MET:CE   | 3:K:173:GLU:HB2  | 1.46                     | 1.42              |
| 3:K:70:PRO:CD    | 3:K:70:PRO:N     | 1.77                     | 1.32              |
| 3:K:69:PRO:CD    | 3:K:69:PRO:N     | 1.83                     | 1.31              |
| 3:K:43:ASP:OD2   | 3:K:322:VAL:HG12 | 1.29                     | 1.25              |
| 2:B:434:GLN:CD   | 3:K:290:HIS:CB   | 2.10                     | 1.23              |
| 3:K:68:LEU:CD1   | 3:K:77:VAL:HG22  | 1.67                     | 1.23              |
| 1:A:410:GLY:O    | 3:K:268:LYS:HD3  | 1.39                     | 1.21              |
| 2:B:427:ASP:OD2  | 3:K:294:ARG:HD2  | 1.40                     | 1.17              |
| 3:K:27:VAL:HG22  | 3:K:314:ILE:HB   | 1.15                     | 1.15              |
| 2:B:234:THR:HG21 | 2:B:270:PRO:HB2  | 1.23                     | 1.15              |
| 1:A:243:ARG:NH2  | 1:A:252:LEU:H    | 1.45                     | 1.14              |
| 2:B:434:GLN:OE1  | 3:K:290:HIS:CB   | 1.96                     | 1.14              |
| 2:B:416:MET:HE2  | 3:K:173:GLU:N    | 1.62                     | 1.13              |
| 1:A:108:TYR:CE2  | 3:K:255:SER:CB   | 2.31                     | 1.13              |
| 3:K:68:LEU:HD22  | 3:K:72:THR:HG21  | 1.30                     | 1.13              |
| 1:A:407:TRP:HE1  | 2:B:260:VAL:HG23 | 1.14                     | 1.12              |
| 3:K:27:VAL:HB    | 3:K:338:VAL:HG11 | 1.27                     | 1.12              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:434:GLN:OE1  | 3:K:290:HIS:HB3  | 1.49                     | 1.12              |
| 1:A:410:GLY:HA3  | 3:K:272:LYS:CE   | 1.78                     | 1.11              |
| 2:B:93:VAL:HG11  | 2:B:118:VAL:HG22 | 1.30                     | 1.11              |
| 2:B:264:ARG:HH12 | 3:K:294:ARG:HD3  | 1.03                     | 1.09              |
| 2:B:264:ARG:NH1  | 3:K:294:ARG:HD3  | 1.68                     | 1.07              |
| 1:A:410:GLY:HA3  | 3:K:272:LYS:HE2  | 1.31                     | 1.07              |
| 3:K:68:LEU:HD13  | 3:K:77:VAL:HG22  | 1.09                     | 1.07              |
| 2:B:416:MET:HE2  | 3:K:173:GLU:H    | 0.95                     | 1.07              |
| 1:A:101:ASN:ND2  | 2:B:254:LYS:HD2  | 1.69                     | 1.06              |
| 3:K:68:LEU:HD13  | 3:K:77:VAL:CG2   | 1.86                     | 1.05              |
| 2:B:434:GLN:HG3  | 3:K:290:HIS:CG   | 1.93                     | 1.03              |
| 1:A:109:THR:HG22 | 1:A:110:ILE:N    | 1.70                     | 1.03              |
| 3:K:62:TYR:O     | 3:K:63:VAL:HG23  | 1.59                     | 1.02              |
| 2:B:172:VAL:HG11 | 2:B:387:LEU:HD21 | 1.37                     | 1.02              |
| 1:A:243:ARG:HH21 | 1:A:252:LEU:N    | 1.57                     | 1.01              |
| 1:A:11:GLN:N     | 5:A:502:GTP:O1B  | 1.94                     | 1.01              |
| 2:B:236:SER:O    | 2:B:240:THR:HG23 | 1.61                     | 1.00              |
| 2:B:416:MET:CE   | 3:K:173:GLU:CB   | 2.18                     | 1.00              |
| 1:A:108:TYR:CD2  | 3:K:255:SER:HB2  | 1.97                     | 1.00              |
| 1:A:11:GLN:HG3   | 1:A:74:VAL:HG11  | 1.43                     | 0.99              |
| 2:B:299:LYS:H    | 2:B:299:LYS:HD3  | 1.24                     | 0.99              |
| 1:A:407:TRP:HE1  | 2:B:260:VAL:CG2  | 1.76                     | 0.97              |
| 1:A:259:LEU:HD11 | 1:A:378:LEU:HD13 | 1.47                     | 0.97              |
| 2:B:434:GLN:NE2  | 3:K:290:HIS:HB2  | 1.81                     | 0.95              |
| 1:A:251:ASP:N    | 1:A:254:GLU:HG3  | 1.82                     | 0.95              |
| 2:B:273:ALA:HB3  | 2:B:274:PRO:HD3  | 1.48                     | 0.94              |
| 2:B:332:MET:HE3  | 2:B:351:VAL:HG11 | 1.45                     | 0.94              |
| 1:A:109:THR:HG22 | 1:A:110:ILE:H    | 1.33                     | 0.94              |
| 1:A:251:ASP:H    | 1:A:254:GLU:HG3  | 1.33                     | 0.94              |
| 2:B:132:LEU:HD23 | 2:B:164:ARG:HG3  | 1.50                     | 0.94              |
| 2:B:281:GLN:O    | 2:B:283:TYR:N    | 2.00                     | 0.93              |
| 1:A:237:SER:HB2  | 1:A:376:CYS:SG   | 2.08                     | 0.93              |
| 1:A:316:CYS:HB3  | 1:A:378:LEU:HD11 | 1.48                     | 0.93              |
| 1:A:98:ASP:HB2   | 1:A:105:ARG:HH21 | 1.31                     | 0.93              |
| 1:A:31:GLN:HB3   | 1:A:32:PRO:HD2   | 1.51                     | 0.92              |
| 2:B:264:ARG:O    | 2:B:265:LEU:HB3  | 1.69                     | 0.92              |
| 2:B:70:LEU:H     | 2:B:145:THR:HG21 | 1.33                     | 0.91              |
| 1:A:151:SER:HB3  | 1:A:193:THR:HG21 | 1.51                     | 0.91              |
| 1:A:177:VAL:CG1  | 2:B:329:ASP:HB3  | 2.00                     | 0.91              |
| 1:A:177:VAL:HG11 | 2:B:329:ASP:HB3  | 1.53                     | 0.90              |
| 1:A:119:LEU:HD23 | 1:A:122:ILE:HD11 | 1.53                     | 0.90              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:323:MET:HE2  | 2:B:328:VAL:HG22 | 1.54                     | 0.90              |
| 1:A:11:GLN:HE22  | 2:B:249:ASN:ND2  | 1.68                     | 0.90              |
| 3:K:57:ILE:HD11  | 3:K:325:GLU:HG2  | 1.54                     | 0.90              |
| 1:A:412:GLY:HA3  | 3:K:254:VAL:HG11 | 1.54                     | 0.89              |
| 1:A:407:TRP:NE1  | 2:B:260:VAL:HG23 | 1.86                     | 0.89              |
| 3:K:27:VAL:HB    | 3:K:338:VAL:CG1  | 2.00                     | 0.89              |
| 1:A:401:LYS:HZ2  | 2:B:346:TRP:CD1  | 1.91                     | 0.89              |
| 2:B:147:SER:O    | 2:B:151:THR:HB   | 1.71                     | 0.89              |
| 1:A:343:PHE:CZ   | 1:A:351:PHE:CE2  | 2.60                     | 0.89              |
| 2:B:8:GLN:OE1    | 2:B:67:LEU:HD22  | 1.73                     | 0.88              |
| 2:B:101:ASN:HD21 | 2:B:143:GLY:HA2  | 1.38                     | 0.88              |
| 1:A:410:GLY:HA2  | 3:K:272:LYS:HD2  | 1.55                     | 0.88              |
| 2:B:93:VAL:HG11  | 2:B:118:VAL:CG2  | 2.03                     | 0.88              |
| 1:A:122:ILE:HD12 | 1:A:157:LEU:HD21 | 1.54                     | 0.88              |
| 2:B:419:THR:HG22 | 3:K:173:GLU:OE1  | 1.72                     | 0.88              |
| 2:B:10:GLY:HA2   | 2:B:145:THR:HB   | 1.55                     | 0.88              |
| 2:B:264:ARG:HB2  | 2:B:266:HIS:CD2  | 2.08                     | 0.88              |
| 3:K:45:PHE:O     | 3:K:48:LYS:NZ    | 2.05                     | 0.88              |
| 2:B:102:ASN:HD21 | 2:B:408:TYR:HA   | 1.38                     | 0.88              |
| 1:A:147:SER:HB2  | 1:A:190:THR:OG1  | 1.73                     | 0.87              |
| 2:B:360:PRO:HG2  | 2:B:371:LEU:HB3  | 1.56                     | 0.87              |
| 3:K:27:VAL:CG2   | 3:K:314:ILE:HB   | 2.02                     | 0.87              |
| 1:A:110:ILE:HG23 | 1:A:111:GLY:H    | 1.38                     | 0.87              |
| 2:B:311:ARG:HD3  | 2:B:342:TYR:HA   | 1.56                     | 0.87              |
| 2:B:153:LEU:O    | 2:B:157:ILE:HG12 | 1.75                     | 0.86              |
| 2:B:6:HIS:CE1    | 2:B:8:GLN:HG2    | 2.10                     | 0.86              |
| 2:B:276:THR:HB   | 2:B:281:GLN:HG3  | 1.56                     | 0.86              |
| 1:A:410:GLY:CA   | 3:K:272:LYS:CE   | 2.54                     | 0.85              |
| 1:A:220:GLU:C    | 1:A:222:PRO:HD3  | 2.01                     | 0.85              |
| 2:B:264:ARG:HH12 | 3:K:294:ARG:CD   | 1.87                     | 0.85              |
| 1:A:179:THR:HG21 | 2:B:248:LEU:CD2  | 2.06                     | 0.85              |
| 1:A:264:ARG:O    | 1:A:266:HIS:N    | 2.09                     | 0.85              |
| 3:K:38:GLU:O     | 3:K:39:ILE:HG13  | 1.76                     | 0.85              |
| 1:A:101:ASN:CG   | 2:B:254:LYS:HD2  | 2.01                     | 0.84              |
| 2:B:242:LEU:HD22 | 2:B:250:ALA:H    | 1.42                     | 0.84              |
| 1:A:204:VAL:HG11 | 1:A:231:ILE:HD12 | 1.60                     | 0.84              |
| 1:A:234:ILE:HG13 | 1:A:270:ALA:HB1  | 1.59                     | 0.84              |
| 2:B:19:LYS:HG3   | 2:B:228:ASN:HB3  | 1.57                     | 0.84              |
| 2:B:150:GLY:HA2  | 2:B:153:LEU:HD22 | 1.59                     | 0.84              |
| 1:A:264:ARG:HB2  | 1:A:266:HIS:CD2  | 2.13                     | 0.84              |
| 2:B:20:PHE:CD1   | 2:B:235:MET:SD   | 2.71                     | 0.84              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:22:ARG:CZ    | 3:K:93:TYR:CD1   | 2.59                     | 0.84              |
| 1:A:106:GLY:O    | 1:A:111:GLY:HA3  | 1.78                     | 0.84              |
| 1:A:316:CYS:HB3  | 1:A:378:LEU:CD1  | 2.08                     | 0.84              |
| 2:B:4:ILE:HD13   | 2:B:136:GLN:HE21 | 1.42                     | 0.84              |
| 2:B:234:THR:HG21 | 2:B:270:PRO:CB   | 2.06                     | 0.84              |
| 3:K:43:ASP:CG    | 3:K:322:VAL:HG12 | 2.02                     | 0.84              |
| 2:B:195:VAL:HG13 | 2:B:196:GLU:HG2  | 1.57                     | 0.84              |
| 2:B:324:SER:HB3  | 2:B:327:GLU:HG2  | 1.60                     | 0.83              |
| 1:A:172:TYR:C    | 1:A:172:TYR:HD1  | 1.87                     | 0.83              |
| 2:B:147:SER:HB2  | 2:B:190:SER:HB3  | 1.60                     | 0.83              |
| 1:A:101:ASN:ND2  | 2:B:254:LYS:CD   | 2.42                     | 0.83              |
| 2:B:209:LEU:HB3  | 2:B:227:LEU:HD22 | 1.59                     | 0.83              |
| 2:B:3:GLU:O      | 2:B:133:GLN:HB3  | 1.78                     | 0.83              |
| 3:K:89:VAL:HG12  | 3:K:228:ILE:HD12 | 1.61                     | 0.83              |
| 2:B:287:THR:O    | 2:B:288:VAL:HG23 | 1.78                     | 0.82              |
| 1:A:151:SER:CB   | 1:A:193:THR:HG21 | 2.09                     | 0.82              |
| 2:B:110:GLU:O    | 2:B:113:GLU:HG2  | 1.79                     | 0.82              |
| 2:B:148:GLY:O    | 2:B:151:THR:HG22 | 1.79                     | 0.82              |
| 1:A:23:LEU:HD23  | 1:A:236:SER:HB2  | 1.60                     | 0.82              |
| 3:K:28:MET:SD    | 3:K:81:CYS:SG    | 2.78                     | 0.82              |
| 2:B:191:VAL:HG11 | 2:B:425:MET:HG3  | 1.60                     | 0.82              |
| 2:B:424:ASN:HA   | 3:K:294:ARG:NH2  | 1.94                     | 0.82              |
| 2:B:101:ASN:ND2  | 2:B:143:GLY:HA2  | 1.94                     | 0.81              |
| 2:B:20:PHE:CZ    | 2:B:24:ILE:HD12  | 2.15                     | 0.81              |
| 2:B:156:LYS:HE2  | 2:B:156:LYS:HA   | 1.61                     | 0.80              |
| 1:A:248:LEU:HD23 | 1:A:353:VAL:O    | 1.80                     | 0.80              |
| 1:A:179:THR:HG21 | 2:B:248:LEU:HD21 | 1.61                     | 0.80              |
| 1:A:411:GLU:HA   | 3:K:268:LYS:HE2  | 1.62                     | 0.80              |
| 3:K:85:ILE:HD11  | 3:K:311:ARG:O    | 1.81                     | 0.80              |
| 1:A:109:THR:CG2  | 1:A:110:ILE:N    | 2.44                     | 0.80              |
| 1:A:234:ILE:HD13 | 1:A:234:ILE:O    | 1.81                     | 0.80              |
| 2:B:413:MET:HG3  | 2:B:414:ASP:H    | 1.47                     | 0.80              |
| 2:B:68:VAL:HG12  | 2:B:149:MET:SD   | 2.22                     | 0.80              |
| 3:K:284:LEU:HD23 | 3:K:291:VAL:HG21 | 1.64                     | 0.80              |
| 1:A:402:ARG:HG3  | 3:K:279:ASN:OD1  | 1.81                     | 0.80              |
| 1:A:132:LEU:HD23 | 1:A:132:LEU:H    | 1.46                     | 0.79              |
| 1:A:313:MET:HB3  | 1:A:344:VAL:HG21 | 1.63                     | 0.79              |
| 1:A:267:PHE:N    | 1:A:267:PHE:CD1  | 2.49                     | 0.79              |
| 2:B:264:ARG:HB2  | 2:B:266:HIS:HD2  | 1.45                     | 0.79              |
| 1:A:224:TYR:HD2  | 2:B:247:GLN:HB3  | 1.47                     | 0.79              |
| 2:B:236:SER:O    | 2:B:240:THR:CG2  | 2.29                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:234:THR:CG2  | 2:B:270:PRO:HB2  | 2.11                     | 0.79              |
| 2:B:217:LEU:C    | 2:B:219:LEU:H    | 1.91                     | 0.79              |
| 1:A:241:SER:O    | 1:A:244:PHE:HB3  | 1.82                     | 0.79              |
| 2:B:54:ASN:HD21  | 2:B:64:ARG:HD3   | 1.46                     | 0.79              |
| 3:K:22:ARG:NH2   | 3:K:93:TYR:CE1   | 2.51                     | 0.79              |
| 1:A:6:SER:HB3    | 1:A:136:SER:OG   | 1.82                     | 0.78              |
| 1:A:410:GLY:O    | 3:K:268:LYS:CD   | 2.28                     | 0.78              |
| 1:A:69:ASP:HA    | 1:A:145:THR:HG21 | 1.65                     | 0.78              |
| 1:A:184:PRO:HG2  | 1:A:398:MET:HE1  | 1.64                     | 0.78              |
| 2:B:242:LEU:HD13 | 2:B:250:ALA:C    | 2.08                     | 0.78              |
| 2:B:396:THR:HG23 | 2:B:422:GLU:OE2  | 1.83                     | 0.78              |
| 2:B:8:GLN:CD     | 2:B:67:LEU:HD22  | 2.08                     | 0.78              |
| 2:B:265:LEU:HD12 | 2:B:265:LEU:O    | 1.83                     | 0.78              |
| 3:K:69:PRO:HD2   | 3:K:72:THR:OG1   | 1.84                     | 0.78              |
| 1:A:7:ILE:HG22   | 1:A:66:VAL:HG22  | 1.63                     | 0.78              |
| 1:A:264:ARG:C    | 1:A:266:HIS:H    | 1.91                     | 0.78              |
| 1:A:11:GLN:HG3   | 1:A:74:VAL:CG1   | 2.14                     | 0.77              |
| 1:A:155:GLU:HA   | 1:A:197:HIS:ND1  | 1.99                     | 0.77              |
| 1:A:199:ASP:HB3  | 1:A:256:GLN:NE2  | 1.98                     | 0.77              |
| 1:A:223:THR:HB   | 1:A:225:THR:HG22 | 1.67                     | 0.77              |
| 1:A:231:ILE:HA   | 1:A:234:ILE:HG22 | 1.66                     | 0.77              |
| 2:B:35:SER:HB3   | 2:B:59:ASN:HA    | 1.65                     | 0.77              |
| 2:B:427:ASP:CG   | 3:K:294:ARG:HD2  | 2.10                     | 0.77              |
| 2:B:205:ASP:OD2  | 2:B:304:ALA:HB2  | 1.84                     | 0.77              |
| 1:A:204:VAL:HG13 | 1:A:209:ILE:HD11 | 1.66                     | 0.77              |
| 2:B:198:THR:O    | 2:B:265:LEU:HD22 | 1.85                     | 0.77              |
| 2:B:192:HIS:ND1  | 2:B:424:ASN:OD1  | 2.18                     | 0.77              |
| 2:B:259:MET:HA   | 2:B:314:THR:HG21 | 1.65                     | 0.76              |
| 1:A:362:VAL:HG13 | 1:A:368:LEU:HD12 | 1.68                     | 0.76              |
| 1:A:108:TYR:HE2  | 3:K:255:SER:CB   | 1.94                     | 0.76              |
| 1:A:163:LYS:O    | 1:A:164:LYS:HG2  | 1.86                     | 0.76              |
| 1:A:344:VAL:HG11 | 1:A:346:TRP:CE2  | 2.21                     | 0.76              |
| 2:B:259:MET:HG2  | 2:B:314:THR:HG21 | 1.67                     | 0.76              |
| 1:A:7:ILE:HD12   | 1:A:153:LEU:HD21 | 1.67                     | 0.75              |
| 2:B:168:THR:HB   | 2:B:201:THR:HG23 | 1.68                     | 0.75              |
| 1:A:221:ARG:O    | 1:A:221:ARG:HD3  | 1.85                     | 0.75              |
| 1:A:276:ILE:HG23 | 1:A:369:ALA:CB   | 2.16                     | 0.75              |
| 1:A:172:TYR:OH   | 1:A:387:ALA:HB1  | 1.87                     | 0.75              |
| 3:K:50:LYS:CE    | 3:K:56:VAL:HG21  | 2.16                     | 0.75              |
| 1:A:110:ILE:HG23 | 1:A:111:GLY:N    | 1.99                     | 0.75              |
| 1:A:167:LEU:HG   | 1:A:200:CYS:HB3  | 1.69                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:225:THR:O    | 1:A:229:ARG:HG3  | 1.85                     | 0.75              |
| 2:B:19:LYS:HG3   | 2:B:228:ASN:CB   | 2.17                     | 0.75              |
| 2:B:325:MET:HE1  | 2:B:355:VAL:HG11 | 1.67                     | 0.75              |
| 1:A:172:TYR:C    | 1:A:172:TYR:CD1  | 2.61                     | 0.75              |
| 1:A:331:ALA:O    | 1:A:335:ILE:HG12 | 1.86                     | 0.75              |
| 2:B:250:ALA:HA   | 2:B:254:LYS:HE2  | 1.68                     | 0.75              |
| 2:B:176:LYS:HE3  | 2:B:207:GLU:HG3  | 1.68                     | 0.75              |
| 1:A:306:ASP:O    | 1:A:308:ARG:N    | 2.20                     | 0.74              |
| 1:A:410:GLY:CA   | 3:K:272:LYS:HE2  | 2.15                     | 0.74              |
| 2:B:103:TRP:CZ3  | 2:B:108:TYR:HE1  | 2.05                     | 0.74              |
| 1:A:205:ASP:CB   | 1:A:303:VAL:HA   | 2.17                     | 0.74              |
| 1:A:88:HIS:C     | 1:A:90:GLU:H     | 1.95                     | 0.74              |
| 1:A:317:LEU:HB3  | 1:A:319:TYR:HE1  | 1.52                     | 0.74              |
| 2:B:6:HIS:HE1    | 2:B:8:GLN:HG2    | 1.52                     | 0.74              |
| 1:A:63:PRO:C     | 1:A:64:ARG:HG2   | 2.12                     | 0.74              |
| 2:B:274:PRO:HG2  | 2:B:371:LEU:HD21 | 1.69                     | 0.74              |
| 3:K:22:ARG:NH1   | 3:K:88:ASP:CG    | 2.45                     | 0.74              |
| 2:B:434:GLN:CG   | 3:K:290:HIS:CG   | 2.71                     | 0.74              |
| 2:B:209:LEU:HG   | 2:B:230:LEU:HD22 | 1.69                     | 0.74              |
| 1:A:4:CYS:SG     | 1:A:252:LEU:HD11 | 2.27                     | 0.74              |
| 3:K:68:LEU:HD12  | 3:K:77:VAL:HG22  | 1.68                     | 0.74              |
| 1:A:412:GLY:HA3  | 3:K:254:VAL:CG1  | 2.17                     | 0.73              |
| 1:A:104:ALA:CB   | 1:A:413:MET:HG3  | 2.18                     | 0.73              |
| 2:B:76:ASP:HA    | 2:B:79:ARG:HG2   | 1.71                     | 0.73              |
| 1:A:31:GLN:HB3   | 1:A:32:PRO:CD    | 2.18                     | 0.73              |
| 3:K:254:VAL:HG23 | 3:K:267:ALA:CB   | 2.18                     | 0.73              |
| 1:A:381:THR:C    | 1:A:383:ALA:H    | 1.95                     | 0.73              |
| 1:A:154:MET:HE1  | 1:A:166:LYS:HB3  | 1.70                     | 0.73              |
| 2:B:217:LEU:O    | 2:B:219:LEU:N    | 2.22                     | 0.73              |
| 1:A:242:LEU:HG   | 1:A:250:VAL:O    | 1.88                     | 0.73              |
| 1:A:414:GLU:OE2  | 3:K:253:LYS:HA   | 1.89                     | 0.73              |
| 1:A:25:CYS:HB2   | 1:A:30:ILE:O     | 1.89                     | 0.73              |
| 2:B:356:CYS:SG   | 2:B:357:ASP:N    | 2.62                     | 0.72              |
| 2:B:427:ASP:OD2  | 3:K:294:ARG:CD   | 2.31                     | 0.72              |
| 2:B:108:TYR:CD1  | 2:B:413:MET:HE1  | 2.24                     | 0.72              |
| 2:B:299:LYS:HD3  | 2:B:299:LYS:N    | 2.04                     | 0.72              |
| 1:A:103:TYR:CD2  | 1:A:189:LEU:HD13 | 2.24                     | 0.72              |
| 1:A:224:TYR:CD2  | 2:B:247:GLN:HB3  | 2.23                     | 0.72              |
| 1:A:242:LEU:HD21 | 1:A:250:VAL:HB   | 1.71                     | 0.72              |
| 1:A:228:ASN:OD1  | 5:A:502:GTP:N1   | 2.21                     | 0.72              |
| 1:A:410:GLY:HA2  | 3:K:272:LYS:CD   | 2.19                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:66:ILE:C     | 2:B:67:LEU:HD23  | 2.15                     | 0.72              |
| 1:A:63:PRO:O     | 1:A:64:ARG:HG2   | 1.88                     | 0.72              |
| 1:A:105:ARG:O    | 1:A:110:ILE:HG22 | 1.89                     | 0.72              |
| 2:B:416:MET:HE2  | 3:K:173:GLU:CA   | 2.18                     | 0.72              |
| 1:A:7:ILE:HD11   | 1:A:137:VAL:HG22 | 1.71                     | 0.72              |
| 1:A:7:ILE:CG1    | 1:A:137:VAL:HG22 | 2.20                     | 0.72              |
| 1:A:243:ARG:HH21 | 1:A:252:LEU:H    | 0.79                     | 0.72              |
| 2:B:70:LEU:HG    | 2:B:145:THR:CG2  | 2.20                     | 0.72              |
| 1:A:112:LYS:O    | 1:A:115:ILE:HG22 | 1.89                     | 0.71              |
| 2:B:111:GLY:O    | 2:B:115:VAL:HG23 | 1.89                     | 0.71              |
| 2:B:191:VAL:CG1  | 2:B:425:MET:HG3  | 2.19                     | 0.71              |
| 1:A:11:GLN:NE2   | 2:B:249:ASN:ND2  | 2.38                     | 0.71              |
| 1:A:317:LEU:HD12 | 1:A:351:PHE:HD1  | 1.55                     | 0.71              |
| 2:B:269:MET:HE2  | 2:B:381:SER:OG   | 1.91                     | 0.71              |
| 1:A:410:GLY:HA3  | 3:K:272:LYS:HE3  | 1.72                     | 0.71              |
| 2:B:325:MET:HE3  | 2:B:325:MET:HA   | 1.72                     | 0.71              |
| 3:K:73:THR:HG22  | 3:K:75:GLU:H     | 1.54                     | 0.71              |
| 1:A:166:LYS:HE3  | 1:A:199:ASP:OD1  | 1.90                     | 0.71              |
| 1:A:104:ALA:HB2  | 1:A:413:MET:HG3  | 1.71                     | 0.71              |
| 1:A:343:PHE:CZ   | 1:A:351:PHE:HE2  | 2.08                     | 0.71              |
| 2:B:431:GLU:OE1  | 2:B:432:TYR:HA   | 1.91                     | 0.71              |
| 3:K:90:LEU:HD22  | 3:K:134:HIS:CD2  | 2.26                     | 0.71              |
| 2:B:175:PRO:HD2  | 2:B:207:GLU:OE2  | 1.91                     | 0.71              |
| 1:A:234:ILE:HG21 | 1:A:302:MET:HE1  | 1.73                     | 0.71              |
| 2:B:291:LEU:O    | 2:B:295:MET:HG3  | 1.91                     | 0.71              |
| 1:A:12:ALA:HB3   | 1:A:140:SER:OG   | 1.91                     | 0.70              |
| 1:A:148:GLY:O    | 1:A:151:SER:HB2  | 1.91                     | 0.70              |
| 2:B:8:GLN:NE2    | 2:B:17:GLY:HA3   | 2.06                     | 0.70              |
| 2:B:10:GLY:O     | 2:B:14:ASN:HB2   | 1.90                     | 0.70              |
| 2:B:201:THR:OG1  | 2:B:265:LEU:HD11 | 1.90                     | 0.70              |
| 2:B:48:ARG:HG2   | 2:B:243:ARG:O    | 1.90                     | 0.70              |
| 2:B:243:ARG:NH2  | 2:B:252:LEU:HG   | 2.05                     | 0.70              |
| 3:K:114:LYS:HB2  | 3:K:120:LEU:CB   | 2.21                     | 0.70              |
| 1:A:259:LEU:HD11 | 1:A:378:LEU:CD1  | 2.20                     | 0.70              |
| 1:A:312:TYR:O    | 1:A:344:VAL:HG23 | 1.90                     | 0.70              |
| 2:B:234:THR:O    | 2:B:238:VAL:HG23 | 1.92                     | 0.70              |
| 2:B:230:LEU:HD21 | 2:B:302:MET:HE2  | 1.73                     | 0.70              |
| 1:A:133:GLN:HG2  | 1:A:243:ARG:HH22 | 1.57                     | 0.70              |
| 1:A:410:GLY:CA   | 3:K:272:LYS:CD   | 2.70                     | 0.70              |
| 2:B:237:GLY:O    | 2:B:241:CYS:HB3  | 1.90                     | 0.70              |
| 2:B:424:ASN:HA   | 3:K:294:ARG:HH22 | 1.55                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:209:ALA:HB2  | 3:K:219:ARG:HD2  | 1.72                     | 0.70              |
| 1:A:6:SER:HB3    | 1:A:136:SER:HG   | 1.56                     | 0.70              |
| 2:B:23:VAL:HA    | 7:B:902:TA1:C32  | 2.22                     | 0.70              |
| 2:B:265:LEU:HD12 | 2:B:265:LEU:C    | 2.16                     | 0.70              |
| 1:A:109:THR:OG1  | 3:K:268:LYS:CE   | 2.40                     | 0.69              |
| 1:A:244:PHE:HD1  | 1:A:245:ASP:N    | 1.89                     | 0.69              |
| 1:A:99:ALA:H     | 2:B:2:ARG:HH22   | 1.37                     | 0.69              |
| 1:A:371:VAL:HG12 | 1:A:372:GLN:H    | 1.57                     | 0.69              |
| 2:B:255:LEU:O    | 2:B:259:MET:HG3  | 1.91                     | 0.69              |
| 1:A:298:PRO:HB3  | 1:A:307:PRO:HD2  | 1.74                     | 0.69              |
| 3:K:284:LEU:CD2  | 3:K:291:VAL:HG21 | 2.21                     | 0.69              |
| 1:A:199:ASP:HB3  | 1:A:256:GLN:HE21 | 1.57                     | 0.69              |
| 1:A:409:VAL:CG1  | 3:K:271:ASN:C    | 2.65                     | 0.69              |
| 1:A:5:ILE:HG22   | 1:A:6:SER:N      | 2.07                     | 0.69              |
| 2:B:434:GLN:HG3  | 3:K:290:HIS:CD2  | 2.28                     | 0.69              |
| 2:B:70:LEU:HG    | 2:B:145:THR:HG23 | 1.74                     | 0.69              |
| 2:B:359:PRO:HB2  | 2:B:360:PRO:HD2  | 1.74                     | 0.69              |
| 2:B:416:MET:CE   | 3:K:173:GLU:CG   | 2.70                     | 0.69              |
| 3:K:26:LYS:HD2   | 3:K:28:MET:HE3   | 1.75                     | 0.69              |
| 2:B:257:VAL:O    | 2:B:257:VAL:HG12 | 1.93                     | 0.69              |
| 2:B:301:MET:HE1  | 2:B:377:PHE:HE2  | 1.58                     | 0.69              |
| 3:K:22:ARG:HH12  | 3:K:88:ASP:HA    | 1.57                     | 0.69              |
| 1:A:180:ALA:HA   | 2:B:352:LYS:NZ   | 2.08                     | 0.69              |
| 1:A:221:ARG:N    | 1:A:222:PRO:HD3  | 2.09                     | 0.68              |
| 1:A:141:PHE:O    | 1:A:147:SER:HB3  | 1.94                     | 0.68              |
| 1:A:205:ASP:HB3  | 1:A:303:VAL:HA   | 1.73                     | 0.68              |
| 1:A:402:ARG:O    | 1:A:403:ALA:C    | 2.36                     | 0.68              |
| 2:B:250:ALA:HB1  | 2:B:254:LYS:HB2  | 1.75                     | 0.68              |
| 3:K:73:THR:HG22  | 3:K:74:GLN:N     | 2.09                     | 0.68              |
| 1:A:71:GLU:HG3   | 2:B:2:ARG:HH21   | 1.59                     | 0.68              |
| 1:A:210:TYR:OH   | 2:B:325:MET:HB3  | 1.93                     | 0.68              |
| 2:B:416:MET:HE1  | 3:K:173:GLU:CG   | 2.24                     | 0.68              |
| 1:A:234:ILE:HD13 | 1:A:234:ILE:C    | 2.18                     | 0.68              |
| 2:B:242:LEU:CD2  | 2:B:250:ALA:H    | 2.07                     | 0.68              |
| 2:B:256:ALA:O    | 2:B:260:VAL:HG22 | 1.93                     | 0.68              |
| 1:A:115:ILE:CD1  | 1:A:119:LEU:HG   | 2.23                     | 0.68              |
| 1:A:343:PHE:HZ   | 1:A:351:PHE:CE2  | 2.10                     | 0.68              |
| 2:B:24:ILE:HD11  | 2:B:52:TYR:CE2   | 2.28                     | 0.68              |
| 2:B:209:LEU:HD23 | 2:B:227:LEU:HB3  | 1.75                     | 0.68              |
| 1:A:102:ASN:HB2  | 1:A:408:TYR:CE1  | 2.29                     | 0.68              |
| 1:A:217:LEU:HD12 | 1:A:277:SER:HB3  | 1.75                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:237:SER:CB   | 1:A:376:CYS:SG   | 2.80                     | 0.68              |
| 2:B:180:THR:HG22 | 2:B:181:VAL:N    | 2.07                     | 0.68              |
| 2:B:251:ASP:O    | 2:B:253:ARG:N    | 2.26                     | 0.68              |
| 2:B:325:MET:CE   | 2:B:355:VAL:HG21 | 2.24                     | 0.68              |
| 3:K:22:ARG:HH11  | 3:K:88:ASP:CG    | 2.00                     | 0.68              |
| 1:A:414:GLU:OE2  | 3:K:253:LYS:CB   | 2.41                     | 0.68              |
| 2:B:4:ILE:HG21   | 2:B:136:GLN:HG2  | 1.76                     | 0.68              |
| 1:A:224:TYR:CD2  | 2:B:325:MET:HG2  | 2.29                     | 0.67              |
| 2:B:103:TRP:HZ3  | 2:B:108:TYR:HE1  | 1.42                     | 0.67              |
| 2:B:107:HIS:CD2  | 2:B:151:THR:CG2  | 2.78                     | 0.67              |
| 2:B:267:PHE:N    | 2:B:267:PHE:CD1  | 2.62                     | 0.67              |
| 1:A:234:ILE:CB   | 1:A:302:MET:HE1  | 2.24                     | 0.67              |
| 3:K:60:LYS:HE2   | 3:K:333:MET:SD   | 2.34                     | 0.67              |
| 1:A:152:LEU:HA   | 1:A:155:GLU:HB2  | 1.77                     | 0.67              |
| 2:B:44:LEU:HD12  | 2:B:49:ILE:HD13  | 1.76                     | 0.67              |
| 1:A:7:ILE:HD12   | 1:A:153:LEU:CD2  | 2.24                     | 0.67              |
| 1:A:251:ASP:O    | 1:A:254:GLU:HB2  | 1.94                     | 0.67              |
| 2:B:204:ILE:HD13 | 2:B:231:VAL:HG22 | 1.76                     | 0.67              |
| 1:A:73:THR:OG1   | 2:B:48:ARG:NE    | 2.28                     | 0.67              |
| 1:A:166:LYS:H    | 1:A:199:ASP:CG   | 2.03                     | 0.67              |
| 2:B:230:LEU:HD23 | 2:B:231:VAL:N    | 2.10                     | 0.67              |
| 1:A:414:GLU:OE2  | 3:K:253:LYS:HB2  | 1.94                     | 0.67              |
| 3:K:50:LYS:NZ    | 3:K:56:VAL:HG21  | 2.10                     | 0.67              |
| 2:B:328:VAL:O    | 2:B:332:MET:HG2  | 1.95                     | 0.67              |
| 1:A:95:GLY:O     | 1:A:97:GLU:N     | 2.27                     | 0.67              |
| 1:A:276:ILE:O    | 1:A:369:ALA:HB2  | 1.95                     | 0.66              |
| 1:A:175:PRO:HG3  | 1:A:304:LYS:HG2  | 1.76                     | 0.66              |
| 2:B:243:ARG:HH22 | 2:B:252:LEU:HG   | 1.59                     | 0.66              |
| 3:K:22:ARG:NH2   | 3:K:93:TYR:CD1   | 2.64                     | 0.66              |
| 1:A:68:VAL:HG11  | 1:A:149:PHE:CZ   | 2.30                     | 0.66              |
| 1:A:345:ASP:C    | 1:A:347:CYS:H    | 2.04                     | 0.66              |
| 1:A:407:TRP:NE1  | 2:B:260:VAL:CG2  | 2.49                     | 0.66              |
| 1:A:315:CYS:HB3  | 1:A:377:MET:HE1  | 1.78                     | 0.66              |
| 2:B:182:VAL:HG23 | 2:B:186:ASN:HD21 | 1.60                     | 0.66              |
| 1:A:172:TYR:HD1  | 1:A:173:PRO:N    | 1.93                     | 0.66              |
| 3:K:26:LYS:HD2   | 3:K:28:MET:CE    | 2.26                     | 0.66              |
| 1:A:313:MET:HB3  | 1:A:344:VAL:CG2  | 2.26                     | 0.66              |
| 2:B:242:LEU:CD1  | 2:B:255:LEU:HD11 | 2.25                     | 0.66              |
| 2:B:324:SER:C    | 2:B:326:LYS:H    | 2.03                     | 0.66              |
| 1:A:394:LYS:HG2  | 2:B:348:PRO:HG3  | 1.79                     | 0.65              |
| 2:B:35:SER:HB3   | 2:B:59:ASN:CA    | 2.26                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:434:GLN:OE1  | 3:K:290:HIS:HB2  | 1.68                     | 0.65              |
| 2:B:310:GLY:HA3  | 2:B:436:GLN:HE21 | 1.59                     | 0.65              |
| 1:A:217:LEU:HD11 | 1:A:367:ASP:O    | 1.96                     | 0.65              |
| 1:A:234:ILE:CG2  | 1:A:302:MET:HE1  | 2.27                     | 0.65              |
| 2:B:66:ILE:CD1   | 2:B:122:VAL:HG12 | 2.26                     | 0.65              |
| 1:A:206:ASN:OD1  | 1:A:227:LEU:HD13 | 1.96                     | 0.65              |
| 1:A:341:ILE:HG12 | 1:A:341:ILE:O    | 1.95                     | 0.65              |
| 2:B:282:GLN:O    | 2:B:282:GLN:HG2  | 1.97                     | 0.65              |
| 1:A:100:ALA:CB   | 1:A:105:ARG:HD3  | 2.26                     | 0.65              |
| 2:B:66:ILE:HD13  | 2:B:122:VAL:HG12 | 1.79                     | 0.65              |
| 2:B:281:GLN:O    | 2:B:283:TYR:HB2  | 1.96                     | 0.65              |
| 1:A:317:LEU:HD12 | 1:A:351:PHE:CD1  | 2.32                     | 0.65              |
| 3:K:114:LYS:HB2  | 3:K:120:LEU:HB3  | 1.78                     | 0.65              |
| 1:A:115:ILE:HG23 | 1:A:116:ASP:N    | 2.12                     | 0.65              |
| 1:A:344:VAL:HG12 | 1:A:345:ASP:N    | 2.12                     | 0.65              |
| 1:A:372:GLN:O    | 1:A:373:ARG:HB3  | 1.96                     | 0.65              |
| 2:B:158:ARG:NE   | 2:B:197:ASN:O    | 2.30                     | 0.65              |
| 2:B:242:LEU:HD12 | 2:B:255:LEU:HD11 | 1.78                     | 0.65              |
| 1:A:271:THR:HG23 | 1:A:300:ASN:O    | 1.97                     | 0.64              |
| 1:A:305:CYS:SG   | 1:A:384:ILE:HD13 | 2.37                     | 0.64              |
| 2:B:229:HIS:HD1  | 2:B:229:HIS:C    | 2.05                     | 0.64              |
| 2:B:413:MET:HG2  | 2:B:418:PHE:HE1  | 1.61                     | 0.64              |
| 1:A:311:LYS:HE3  | 1:A:342:GLN:CD   | 2.22                     | 0.64              |
| 2:B:180:THR:CG2  | 2:B:181:VAL:N    | 2.61                     | 0.64              |
| 2:B:63:PRO:HD2   | 2:B:86:ILE:HG12  | 1.80                     | 0.64              |
| 2:B:276:THR:HB   | 2:B:281:GLN:CG   | 2.25                     | 0.64              |
| 2:B:284:ARG:O    | 2:B:286:LEU:N    | 2.31                     | 0.64              |
| 1:A:71:GLU:HG3   | 2:B:2:ARG:NH2    | 2.13                     | 0.64              |
| 1:A:317:LEU:HB3  | 1:A:319:TYR:CE1  | 2.33                     | 0.64              |
| 1:A:209:ILE:HG23 | 1:A:230:LEU:HD23 | 1.79                     | 0.64              |
| 2:B:241:CYS:O    | 2:B:244:PHE:HB2  | 1.97                     | 0.64              |
| 2:B:422:GLU:O    | 2:B:426:ASN:HB2  | 1.97                     | 0.64              |
| 3:K:179:PRO:HG2  | 3:K:300:ARG:NH2  | 2.12                     | 0.64              |
| 1:A:7:ILE:HG22   | 1:A:66:VAL:CG2   | 2.28                     | 0.64              |
| 2:B:114:LEU:O    | 2:B:118:VAL:HG23 | 1.97                     | 0.64              |
| 1:A:386:GLU:O    | 1:A:389:ALA:N    | 2.31                     | 0.64              |
| 1:A:179:THR:HG22 | 2:B:352:LYS:NZ   | 2.12                     | 0.63              |
| 1:A:388:TRP:CE3  | 1:A:425:MET:HE1  | 2.32                     | 0.63              |
| 2:B:105:LYS:O    | 2:B:110:GLU:HB2  | 1.97                     | 0.63              |
| 1:A:394:LYS:HG2  | 2:B:348:PRO:CG   | 2.27                     | 0.63              |
| 2:B:133:GLN:HG3  | 2:B:165:ILE:HD11 | 1.80                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:318:VAL:HA   | 2:B:354:ALA:HB3  | 1.80                     | 0.63              |
| 3:K:262:ALA:O    | 3:K:266:GLU:HG3  | 1.98                     | 0.63              |
| 1:A:381:THR:C    | 1:A:383:ALA:N    | 2.56                     | 0.63              |
| 3:K:117:ASP:OD2  | 3:K:120:LEU:HG   | 1.98                     | 0.63              |
| 3:K:318:CYS:SG   | 3:K:328:THR:HG23 | 2.38                     | 0.63              |
| 1:A:155:GLU:HA   | 1:A:197:HIS:HD1  | 1.63                     | 0.63              |
| 2:B:70:LEU:N     | 2:B:145:THR:HG21 | 2.11                     | 0.63              |
| 1:A:411:GLU:HA   | 3:K:268:LYS:CE   | 2.27                     | 0.63              |
| 2:B:349:ASN:C    | 2:B:349:ASN:HD22 | 2.07                     | 0.63              |
| 2:B:427:ASP:O    | 2:B:430:SER:HB3  | 1.97                     | 0.63              |
| 2:B:137:LEU:HD22 | 2:B:154:ILE:CG2  | 2.28                     | 0.63              |
| 1:A:267:PHE:HD1  | 1:A:267:PHE:H    | 1.47                     | 0.63              |
| 1:A:276:ILE:HG23 | 1:A:369:ALA:HB2  | 1.79                     | 0.63              |
| 2:B:107:HIS:HD2  | 2:B:151:THR:CG2  | 2.12                     | 0.63              |
| 3:K:259:ALA:O    | 3:K:260:GLU:HG3  | 1.97                     | 0.63              |
| 1:A:175:PRO:HG2  | 1:A:207:GLU:OE1  | 1.98                     | 0.63              |
| 2:B:416:MET:CE   | 3:K:173:GLU:CA   | 2.76                     | 0.63              |
| 3:K:94:ASN:HB2   | 3:K:309:ASN:CG   | 2.24                     | 0.63              |
| 1:A:151:SER:O    | 1:A:155:GLU:HB2  | 1.98                     | 0.62              |
| 2:B:154:ILE:HG22 | 2:B:166:MET:HE2  | 1.81                     | 0.62              |
| 2:B:161:TYR:C    | 2:B:163:ASP:H    | 2.05                     | 0.62              |
| 2:B:192:HIS:O    | 2:B:195:VAL:HG12 | 1.98                     | 0.62              |
| 3:K:22:ARG:NH1   | 3:K:88:ASP:CB    | 2.62                     | 0.62              |
| 1:A:7:ILE:CD1    | 1:A:137:VAL:HG22 | 2.29                     | 0.62              |
| 1:A:102:ASN:OD1  | 1:A:105:ARG:HB3  | 1.99                     | 0.62              |
| 7:B:902:TA1:H463 | 7:B:902:TA1:H261 | 1.80                     | 0.62              |
| 1:A:11:GLN:HB3   | 5:A:502:GTP:O1B  | 1.98                     | 0.62              |
| 1:A:273:ALA:HB3  | 1:A:274:PRO:HD3  | 1.81                     | 0.62              |
| 2:B:115:VAL:HG21 | 2:B:152:LEU:CD2  | 2.30                     | 0.62              |
| 2:B:172:VAL:HG11 | 2:B:387:LEU:CD2  | 2.22                     | 0.62              |
| 2:B:315:VAL:HG13 | 2:B:377:PHE:CE1  | 2.34                     | 0.62              |
| 1:A:101:ASN:HD21 | 2:B:254:LYS:NZ   | 1.98                     | 0.62              |
| 1:A:315:CYS:HB3  | 1:A:377:MET:CE   | 2.29                     | 0.62              |
| 1:A:317:LEU:HD11 | 1:A:351:PHE:HE1  | 1.63                     | 0.62              |
| 1:A:23:LEU:HD22  | 1:A:232:GLY:O    | 1.99                     | 0.62              |
| 2:B:253:ARG:O    | 2:B:256:ALA:N    | 2.33                     | 0.62              |
| 2:B:299:LYS:O    | 2:B:300:ASN:HB2  | 1.97                     | 0.62              |
| 1:A:152:LEU:HD12 | 1:A:153:LEU:N    | 2.14                     | 0.62              |
| 1:A:236:SER:O    | 1:A:240:ALA:HB3  | 1.99                     | 0.62              |
| 1:A:278:ALA:HA   | 1:A:282:TYR:OH   | 2.00                     | 0.62              |
| 2:B:243:ARG:HH21 | 2:B:252:LEU:H    | 1.45                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:427:ASP:CG   | 3:K:294:ARG:CD   | 2.73                     | 0.62              |
| 1:A:115:ILE:HG13 | 1:A:152:LEU:HD13 | 1.81                     | 0.62              |
| 1:A:269:LEU:O    | 1:A:378:LEU:HA   | 1.99                     | 0.62              |
| 3:K:60:LYS:HE3   | 3:K:62:TYR:CE1   | 2.34                     | 0.62              |
| 2:B:4:ILE:HG23   | 2:B:134:GLY:O    | 2.00                     | 0.62              |
| 2:B:70:LEU:C     | 2:B:99:ALA:HB2   | 2.24                     | 0.62              |
| 1:A:118:VAL:HG11 | 1:A:149:PHE:HZ   | 1.65                     | 0.61              |
| 1:A:119:LEU:CD2  | 1:A:122:ILE:HD11 | 2.28                     | 0.61              |
| 1:A:409:VAL:HG12 | 3:K:272:LYS:N    | 2.14                     | 0.61              |
| 2:B:4:ILE:HA     | 2:B:134:GLY:O    | 1.99                     | 0.61              |
| 2:B:230:LEU:O    | 2:B:233:ALA:HB3  | 2.00                     | 0.61              |
| 1:A:205:ASP:HB2  | 1:A:303:VAL:HA   | 1.82                     | 0.61              |
| 2:B:205:ASP:OD2  | 2:B:304:ALA:N    | 2.32                     | 0.61              |
| 2:B:211:ASP:OD1  | 2:B:212:ILE:N    | 2.33                     | 0.61              |
| 2:B:70:LEU:CG    | 2:B:145:THR:HG23 | 2.30                     | 0.61              |
| 1:A:229:ARG:NH1  | 1:A:363:VAL:HG21 | 2.16                     | 0.61              |
| 3:K:43:ASP:OD2   | 3:K:322:VAL:CG1  | 2.25                     | 0.61              |
| 3:K:284:LEU:HD21 | 3:K:291:VAL:HG11 | 1.82                     | 0.61              |
| 1:A:11:GLN:HE21  | 1:A:74:VAL:HG22  | 1.66                     | 0.61              |
| 1:A:436:GLY:C    | 1:A:438:ASP:H    | 2.08                     | 0.61              |
| 2:B:204:ILE:CD1  | 2:B:231:VAL:HG13 | 2.30                     | 0.61              |
| 2:B:283:TYR:C    | 2:B:284:ARG:HG2  | 2.24                     | 0.61              |
| 3:K:131:ILE:CD1  | 3:K:228:ILE:HD11 | 2.30                     | 0.61              |
| 1:A:288:VAL:O    | 1:A:290:GLU:N    | 2.33                     | 0.61              |
| 2:B:253:ARG:O    | 2:B:254:LYS:C    | 2.42                     | 0.61              |
| 3:K:38:GLU:C     | 3:K:39:ILE:HG13  | 2.24                     | 0.61              |
| 1:A:248:LEU:CD2  | 1:A:353:VAL:O    | 2.49                     | 0.61              |
| 1:A:88:HIS:O     | 1:A:90:GLU:N     | 2.33                     | 0.61              |
| 1:A:168:GLU:OE1  | 1:A:198:SER:HB2  | 2.01                     | 0.61              |
| 1:A:414:GLU:OE2  | 3:K:253:LYS:CA   | 2.48                     | 0.61              |
| 1:A:109:THR:OG1  | 3:K:268:LYS:HE2  | 2.01                     | 0.60              |
| 2:B:324:SER:CB   | 2:B:327:GLU:HG2  | 2.30                     | 0.60              |
| 1:A:169:PHE:CE2  | 1:A:235:VAL:HG22 | 2.36                     | 0.60              |
| 2:B:70:LEU:H     | 2:B:145:THR:CG2  | 2.10                     | 0.60              |
| 2:B:115:VAL:HG21 | 2:B:152:LEU:HD23 | 1.84                     | 0.60              |
| 2:B:324:SER:C    | 2:B:326:LYS:N    | 2.59                     | 0.60              |
| 1:A:344:VAL:HG11 | 1:A:346:TRP:NE1  | 2.16                     | 0.60              |
| 1:A:362:VAL:HG13 | 1:A:368:LEU:HB2  | 1.83                     | 0.60              |
| 2:B:188:THR:HA   | 2:B:425:MET:HE2  | 1.83                     | 0.60              |
| 2:B:285:ALA:HB1  | 2:B:290:GLU:HG2  | 1.82                     | 0.60              |
| 2:B:434:GLN:CG   | 3:K:290:HIS:CB   | 2.78                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:191:THR:HG21 | 1:A:425:MET:SD   | 2.41                     | 0.60              |
| 2:B:114:LEU:HD23 | 2:B:149:MET:CE   | 2.30                     | 0.60              |
| 1:A:177:VAL:HG13 | 2:B:329:ASP:O    | 2.02                     | 0.60              |
| 2:B:279:GLY:O    | 2:B:282:GLN:HB3  | 2.01                     | 0.60              |
| 2:B:204:ILE:HG21 | 2:B:231:VAL:HG22 | 1.84                     | 0.60              |
| 2:B:217:LEU:C    | 2:B:219:LEU:N    | 2.55                     | 0.60              |
| 2:B:230:LEU:CD2  | 2:B:302:MET:HE2  | 2.31                     | 0.60              |
| 1:A:409:VAL:C    | 1:A:411:GLU:H    | 2.09                     | 0.60              |
| 1:A:242:LEU:C    | 1:A:244:PHE:H    | 2.09                     | 0.60              |
| 1:A:243:ARG:NH2  | 1:A:252:LEU:N    | 2.28                     | 0.60              |
| 2:B:324:SER:O    | 2:B:328:VAL:HG23 | 2.01                     | 0.60              |
| 1:A:435:VAL:HG12 | 1:A:435:VAL:O    | 2.01                     | 0.60              |
| 2:B:54:ASN:ND2   | 2:B:64:ARG:HD3   | 2.15                     | 0.60              |
| 2:B:102:ASN:ND2  | 2:B:407:TRP:O    | 2.35                     | 0.60              |
| 1:A:413:MET:O    | 1:A:414:GLU:HG3  | 2.02                     | 0.59              |
| 1:A:371:VAL:HG12 | 1:A:372:GLN:N    | 2.17                     | 0.59              |
| 1:A:407:TRP:O    | 1:A:411:GLU:HG2  | 2.02                     | 0.59              |
| 2:B:205:ASP:OD2  | 2:B:304:ALA:CB   | 2.50                     | 0.59              |
| 2:B:408:TYR:CG   | 2:B:418:PHE:HZ   | 2.20                     | 0.59              |
| 2:B:424:ASN:C    | 2:B:424:ASN:HD22 | 2.09                     | 0.59              |
| 1:A:167:LEU:HA   | 1:A:200:CYS:O    | 2.01                     | 0.59              |
| 3:K:131:ILE:HD13 | 3:K:228:ILE:HD11 | 1.83                     | 0.59              |
| 1:A:369:ALA:O    | 1:A:370:LYS:HB3  | 2.03                     | 0.59              |
| 2:B:49:ILE:O     | 2:B:51:VAL:N     | 2.35                     | 0.59              |
| 1:A:115:ILE:HD13 | 1:A:115:ILE:O    | 2.02                     | 0.59              |
| 1:A:202:PHE:CE1  | 1:A:378:LEU:HD22 | 2.38                     | 0.59              |
| 1:A:284:GLU:O    | 1:A:286:LEU:N    | 2.35                     | 0.59              |
| 2:B:31:ASP:O     | 2:B:32:PRO:C     | 2.44                     | 0.59              |
| 2:B:114:LEU:HD23 | 2:B:149:MET:HE1  | 1.85                     | 0.59              |
| 2:B:172:VAL:CG1  | 2:B:387:LEU:HD21 | 2.24                     | 0.59              |
| 1:A:339:ARG:C    | 1:A:341:ILE:H    | 2.11                     | 0.59              |
| 2:B:141:LEU:CD1  | 2:B:141:LEU:N    | 2.65                     | 0.59              |
| 1:A:6:SER:HA     | 1:A:136:SER:O    | 2.02                     | 0.59              |
| 1:A:110:ILE:CG2  | 1:A:111:GLY:H    | 2.15                     | 0.59              |
| 1:A:409:VAL:HG11 | 3:K:272:LYS:HA   | 1.85                     | 0.58              |
| 2:B:30:ILE:HD13  | 2:B:53:TYR:CE2   | 2.38                     | 0.58              |
| 3:K:50:LYS:HE3   | 3:K:56:VAL:HG21  | 1.84                     | 0.58              |
| 1:A:88:HIS:C     | 1:A:90:GLU:N     | 2.57                     | 0.58              |
| 1:A:119:LEU:O    | 1:A:122:ILE:HG12 | 2.02                     | 0.58              |
| 1:A:278:ALA:HB2  | 1:A:369:ALA:HA   | 1.85                     | 0.58              |
| 3:K:141:ASN:O    | 3:K:233:VAL:HG22 | 2.02                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:221:HIS:HD2  | 3:K:249:ALA:H    | 1.50                     | 0.58              |
| 1:A:264:ARG:HB2  | 1:A:266:HIS:HD2  | 1.67                     | 0.58              |
| 2:B:68:VAL:CG1   | 2:B:149:MET:SD   | 2.90                     | 0.58              |
| 2:B:179:ASP:HB2  | 6:B:901:GDP:H3'  | 1.84                     | 0.58              |
| 2:B:226:ASP:O    | 2:B:227:LEU:C    | 2.46                     | 0.58              |
| 2:B:229:HIS:C    | 2:B:229:HIS:ND1  | 2.62                     | 0.58              |
| 3:K:259:ALA:HB1  | 3:K:263:VAL:C    | 2.27                     | 0.58              |
| 1:A:234:ILE:HB   | 1:A:302:MET:HE1  | 1.85                     | 0.58              |
| 2:B:89:PRO:HA    | 2:B:92:PHE:CD2   | 2.38                     | 0.58              |
| 1:A:2:ARG:N      | 1:A:131:GLY:O    | 2.36                     | 0.58              |
| 1:A:268:PRO:HA   | 1:A:379:SER:O    | 2.03                     | 0.58              |
| 1:A:317:LEU:HD11 | 1:A:351:PHE:CE1  | 2.38                     | 0.58              |
| 3:K:114:LYS:HB2  | 3:K:120:LEU:HB2  | 1.84                     | 0.58              |
| 1:A:215:ARG:C    | 1:A:216:ASN:HD22 | 2.12                     | 0.58              |
| 1:A:218:ASP:O    | 1:A:219:ILE:HG23 | 2.04                     | 0.58              |
| 2:B:307:PRO:HB3  | 2:B:312:TYR:OH   | 2.04                     | 0.58              |
| 1:A:63:PRO:HD3   | 1:A:86:LEU:O     | 2.04                     | 0.58              |
| 1:A:102:ASN:HB3  | 2:B:257:VAL:HG11 | 1.83                     | 0.58              |
| 2:B:19:LYS:CG    | 2:B:228:ASN:HB3  | 2.31                     | 0.58              |
| 1:A:412:GLY:H    | 3:K:268:LYS:HG2  | 1.68                     | 0.58              |
| 2:B:151:THR:OG1  | 2:B:193:GLN:HB3  | 2.03                     | 0.58              |
| 2:B:183:GLU:HB3  | 2:B:184:PRO:CD   | 2.33                     | 0.58              |
| 2:B:319:PHE:HA   | 2:B:375:ALA:HA   | 1.86                     | 0.58              |
| 1:A:15:GLN:NE2   | 5:A:502:GTP:N7   | 2.52                     | 0.58              |
| 2:B:93:VAL:CG1   | 2:B:118:VAL:HG22 | 2.19                     | 0.58              |
| 1:A:11:GLN:NE2   | 2:B:249:ASN:HD21 | 2.02                     | 0.57              |
| 1:A:99:ALA:H     | 2:B:2:ARG:NH2    | 2.02                     | 0.57              |
| 1:A:115:ILE:HD13 | 1:A:115:ILE:C    | 2.28                     | 0.57              |
| 1:A:166:LYS:HD2  | 1:A:197:HIS:O    | 2.04                     | 0.57              |
| 1:A:196:GLU:C    | 1:A:197:HIS:CD2  | 2.82                     | 0.57              |
| 2:B:194:LEU:C    | 2:B:196:GLU:H    | 2.11                     | 0.57              |
| 1:A:181:VAL:HG21 | 2:B:258:ASN:O    | 2.04                     | 0.57              |
| 1:A:345:ASP:O    | 1:A:347:CYS:N    | 2.38                     | 0.57              |
| 1:A:179:THR:HG22 | 2:B:352:LYS:HZ1  | 1.68                     | 0.57              |
| 3:K:259:ALA:HB1  | 3:K:264:LEU:N    | 2.18                     | 0.57              |
| 2:B:320:ARG:O    | 2:B:359:PRO:HA   | 2.04                     | 0.57              |
| 2:B:6:HIS:HB3    | 2:B:65:ALA:HB2   | 1.87                     | 0.57              |
| 2:B:198:THR:HG22 | 2:B:265:LEU:HD22 | 1.86                     | 0.57              |
| 2:B:299:LYS:O    | 2:B:300:ASN:CB   | 2.51                     | 0.57              |
| 1:A:165:SER:HA   | 1:A:199:ASP:OD2  | 2.04                     | 0.57              |
| 1:A:224:TYR:CG   | 2:B:325:MET:HG2  | 2.39                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:286:LEU:HD12 | 1:A:290:GLU:HG2  | 1.87                     | 0.57              |
| 1:A:362:VAL:CG1  | 1:A:368:LEU:HB2  | 2.35                     | 0.57              |
| 2:B:180:THR:CG2  | 2:B:181:VAL:H    | 2.17                     | 0.57              |
| 2:B:274:PRO:CG   | 2:B:371:LEU:HD21 | 2.34                     | 0.57              |
| 2:B:345:GLU:C    | 2:B:347:ILE:H    | 2.12                     | 0.57              |
| 1:A:152:LEU:HA   | 1:A:155:GLU:CB   | 2.35                     | 0.57              |
| 1:A:209:ILE:CG2  | 1:A:227:LEU:HD22 | 2.35                     | 0.57              |
| 1:A:210:TYR:CE1  | 1:A:227:LEU:HD11 | 2.40                     | 0.57              |
| 1:A:216:ASN:O    | 1:A:217:LEU:HB2  | 2.05                     | 0.57              |
| 2:B:301:MET:CE   | 2:B:377:PHE:HE2  | 2.18                     | 0.57              |
| 2:B:209:LEU:O    | 2:B:210:TYR:C    | 2.48                     | 0.57              |
| 1:A:139:HIS:CE1  | 1:A:170:SER:HB3  | 2.40                     | 0.57              |
| 1:A:150:THR:O    | 1:A:151:SER:C    | 2.47                     | 0.57              |
| 2:B:319:PHE:CD2  | 2:B:375:ALA:HB2  | 2.40                     | 0.57              |
| 2:B:424:ASN:C    | 2:B:424:ASN:ND2  | 2.62                     | 0.57              |
| 1:A:362:VAL:HG11 | 1:A:368:LEU:O    | 2.04                     | 0.56              |
| 2:B:14:ASN:OD1   | 2:B:75:MET:HG2   | 2.05                     | 0.56              |
| 2:B:30:ILE:HA    | 2:B:35:SER:O     | 2.04                     | 0.56              |
| 2:B:128:SER:OG   | 2:B:129:CYS:N    | 2.34                     | 0.56              |
| 1:A:117:LEU:HD11 | 1:A:121:ARG:HH22 | 1.69                     | 0.56              |
| 2:B:5:VAL:CG2    | 2:B:135:PHE:HD2  | 2.18                     | 0.56              |
| 3:K:221:HIS:CD2  | 3:K:249:ALA:H    | 2.22                     | 0.56              |
| 1:A:409:VAL:CG1  | 3:K:272:LYS:N    | 2.68                     | 0.56              |
| 2:B:50:ASN:O     | 2:B:64:ARG:NH2   | 2.38                     | 0.56              |
| 2:B:70:LEU:CD1   | 2:B:145:THR:HG23 | 2.35                     | 0.56              |
| 2:B:270:PRO:HA   | 2:B:377:PHE:O    | 2.04                     | 0.56              |
| 1:A:175:PRO:HG3  | 1:A:304:LYS:CG   | 2.35                     | 0.56              |
| 1:A:313:MET:O    | 1:A:314:ALA:HB2  | 2.04                     | 0.56              |
| 2:B:216:THR:O    | 2:B:217:LEU:HD12 | 2.05                     | 0.56              |
| 1:A:253:THR:O    | 1:A:256:GLN:HG2  | 2.06                     | 0.56              |
| 1:A:283:HIS:O    | 1:A:284:GLU:C    | 2.47                     | 0.56              |
| 2:B:139:HIS:HE1  | 2:B:168:THR:HG23 | 1.71                     | 0.56              |
| 2:B:149:MET:O    | 2:B:153:LEU:HD13 | 2.05                     | 0.56              |
| 2:B:251:ASP:O    | 2:B:252:LEU:C    | 2.48                     | 0.56              |
| 2:B:108:TYR:CE1  | 2:B:413:MET:HE1  | 2.41                     | 0.56              |
| 2:B:273:ALA:HB3  | 2:B:274:PRO:CD   | 2.29                     | 0.56              |
| 2:B:311:ARG:HD2  | 2:B:344:VAL:H    | 1.71                     | 0.56              |
| 2:B:311:ARG:HG2  | 2:B:311:ARG:HH11 | 1.71                     | 0.56              |
| 2:B:23:VAL:HA    | 7:B:902:TA1:C33  | 2.36                     | 0.56              |
| 2:B:182:VAL:HG23 | 2:B:186:ASN:ND2  | 2.20                     | 0.56              |
| 1:A:244:PHE:CD1  | 1:A:244:PHE:C    | 2.83                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:272:PHE:HB3  | 2:B:275:LEU:HD22 | 1.88                     | 0.56              |
| 1:A:19:ALA:CB    | 1:A:228:ASN:HB3  | 2.35                     | 0.56              |
| 1:A:408:TYR:O    | 1:A:411:GLU:N    | 2.39                     | 0.56              |
| 2:B:119:LEU:O    | 2:B:123:ARG:HG3  | 2.06                     | 0.56              |
| 2:B:190:SER:O    | 2:B:194:LEU:HG   | 2.06                     | 0.56              |
| 2:B:204:ILE:HG21 | 2:B:231:VAL:CG2  | 2.36                     | 0.56              |
| 2:B:427:ASP:CG   | 3:K:294:ARG:NH1  | 2.64                     | 0.56              |
| 1:A:179:THR:HG21 | 2:B:248:LEU:HD22 | 1.84                     | 0.56              |
| 2:B:166:MET:HB3  | 2:B:198:THR:OG1  | 2.06                     | 0.56              |
| 1:A:108:TYR:HE2  | 3:K:255:SER:HB3  | 1.69                     | 0.55              |
| 1:A:228:ASN:ND2  | 5:A:502:GTP:O6   | 2.39                     | 0.55              |
| 1:A:305:CYS:O    | 1:A:306:ASP:C    | 2.49                     | 0.55              |
| 2:B:312:TYR:O    | 2:B:344:VAL:HB   | 2.05                     | 0.55              |
| 1:A:239:THR:O    | 1:A:240:ALA:C    | 2.48                     | 0.55              |
| 1:A:331:ALA:O    | 1:A:334:THR:HG22 | 2.05                     | 0.55              |
| 2:B:151:THR:OG1  | 2:B:193:GLN:CB   | 2.54                     | 0.55              |
| 2:B:223:THR:HG22 | 2:B:224:TYR:N    | 2.21                     | 0.55              |
| 2:B:297:ASP:OD1  | 2:B:298:ALA:N    | 2.39                     | 0.55              |
| 3:K:252:GLU:O    | 3:K:271:ASN:ND2  | 2.31                     | 0.55              |
| 1:A:209:ILE:HG22 | 1:A:227:LEU:HD22 | 1.88                     | 0.55              |
| 2:B:5:VAL:HG22   | 2:B:135:PHE:CD2  | 2.42                     | 0.55              |
| 2:B:239:THR:HG22 | 2:B:240:THR:N    | 2.22                     | 0.55              |
| 2:B:250:ALA:CA   | 2:B:254:LYS:HE2  | 2.35                     | 0.55              |
| 2:B:369:ARG:C    | 2:B:369:ARG:HD2  | 2.32                     | 0.55              |
| 3:K:219:ARG:HE   | 3:K:266:GLU:CD   | 2.14                     | 0.55              |
| 1:A:16:ILE:HD12  | 1:A:171:ILE:HD11 | 1.87                     | 0.55              |
| 1:A:388:TRP:CE3  | 1:A:388:TRP:HA   | 2.41                     | 0.55              |
| 2:B:165:ILE:HD13 | 2:B:165:ILE:H    | 1.71                     | 0.55              |
| 1:A:6:SER:O      | 1:A:65:ALA:HB1   | 2.07                     | 0.55              |
| 2:B:4:ILE:HD13   | 2:B:136:GLN:NE2  | 2.17                     | 0.55              |
| 1:A:5:ILE:CG2    | 1:A:6:SER:N      | 2.70                     | 0.55              |
| 1:A:150:THR:O    | 1:A:153:LEU:N    | 2.40                     | 0.55              |
| 2:B:19:LYS:O     | 2:B:23:VAL:HG23  | 2.06                     | 0.55              |
| 2:B:253:ARG:O    | 2:B:257:VAL:N    | 2.33                     | 0.55              |
| 3:K:260:GLU:H    | 3:K:263:VAL:HB   | 1.72                     | 0.55              |
| 2:B:204:ILE:HD13 | 2:B:231:VAL:HG13 | 1.89                     | 0.54              |
| 2:B:259:MET:CG   | 2:B:314:THR:HG21 | 2.36                     | 0.54              |
| 3:K:254:VAL:CG2  | 3:K:267:ALA:HB3  | 2.37                     | 0.54              |
| 1:A:408:TYR:CD2  | 1:A:418:PHE:HZ   | 2.24                     | 0.54              |
| 1:A:381:THR:OG1  | 1:A:383:ALA:HB3  | 2.07                     | 0.54              |
| 1:A:407:TRP:CZ2  | 2:B:260:VAL:HG21 | 2.43                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:254:VAL:HG22 | 3:K:259:ALA:HB3  | 1.90                     | 0.54              |
| 1:A:382:THR:O    | 1:A:382:THR:HG22 | 2.06                     | 0.54              |
| 2:B:67:LEU:HD23  | 2:B:67:LEU:N     | 2.22                     | 0.54              |
| 2:B:107:HIS:HD2  | 2:B:151:THR:HG22 | 1.72                     | 0.54              |
| 2:B:210:TYR:HD1  | 2:B:227:LEU:HD21 | 1.71                     | 0.54              |
| 2:B:310:GLY:CA   | 2:B:436:GLN:HE21 | 2.19                     | 0.54              |
| 1:A:118:VAL:HG21 | 1:A:149:PHE:CZ   | 2.42                     | 0.54              |
| 2:B:49:ILE:O     | 2:B:50:ASN:C     | 2.48                     | 0.54              |
| 2:B:242:LEU:HD22 | 2:B:250:ALA:N    | 2.19                     | 0.54              |
| 2:B:298:ALA:O    | 2:B:299:LYS:C    | 2.50                     | 0.54              |
| 2:B:331:GLN:O    | 2:B:335:VAL:HG23 | 2.08                     | 0.54              |
| 1:A:17:GLY:O     | 1:A:21:TRP:HB2   | 2.08                     | 0.54              |
| 1:A:108:TYR:CD2  | 3:K:255:SER:CB   | 2.81                     | 0.54              |
| 1:A:110:ILE:O    | 1:A:112:LYS:N    | 2.41                     | 0.54              |
| 1:A:115:ILE:O    | 1:A:116:ASP:C    | 2.51                     | 0.54              |
| 1:A:328:VAL:C    | 1:A:330:ALA:H    | 2.16                     | 0.54              |
| 2:B:213:CYS:SG   | 2:B:219:LEU:HD23 | 2.48                     | 0.54              |
| 2:B:383:ALA:C    | 2:B:385:GLN:H    | 2.15                     | 0.54              |
| 1:A:231:ILE:HA   | 1:A:234:ILE:CG2  | 2.36                     | 0.54              |
| 2:B:191:VAL:HA   | 2:B:194:LEU:HD12 | 1.88                     | 0.54              |
| 1:A:409:VAL:HG11 | 3:K:271:ASN:C    | 2.32                     | 0.54              |
| 2:B:44:LEU:O     | 2:B:49:ILE:HG12  | 2.07                     | 0.54              |
| 2:B:36:TYR:CZ    | 2:B:38:GLY:HA3   | 2.43                     | 0.54              |
| 1:A:5:ILE:O      | 1:A:135:PHE:HA   | 2.09                     | 0.53              |
| 1:A:180:ALA:HA   | 2:B:352:LYS:HZ2  | 1.72                     | 0.53              |
| 1:A:324:VAL:O    | 1:A:327:ASP:HB2  | 2.08                     | 0.53              |
| 1:A:163:LYS:C    | 1:A:164:LYS:HG2  | 2.33                     | 0.53              |
| 2:B:179:ASP:HB2  | 6:B:901:GDP:C3'  | 2.37                     | 0.53              |
| 2:B:239:THR:O    | 2:B:241:CYS:N    | 2.41                     | 0.53              |
| 2:B:259:MET:CA   | 2:B:314:THR:HG21 | 2.35                     | 0.53              |
| 1:A:121:ARG:O    | 1:A:125:LEU:HB2  | 2.08                     | 0.53              |
| 1:A:173:PRO:HB2  | 1:A:391:LEU:CD1  | 2.38                     | 0.53              |
| 2:B:191:VAL:HG11 | 2:B:425:MET:HE2  | 1.89                     | 0.53              |
| 2:B:343:PHE:O    | 2:B:344:VAL:O    | 2.26                     | 0.53              |
| 3:K:277:LEU:HD23 | 3:K:334:PHE:HZ   | 1.73                     | 0.53              |
| 2:B:20:PHE:CE1   | 2:B:24:ILE:HD12  | 2.42                     | 0.53              |
| 2:B:133:GLN:HE21 | 2:B:252:LEU:HB2  | 1.73                     | 0.53              |
| 2:B:427:ASP:OD1  | 2:B:428:LEU:N    | 2.41                     | 0.53              |
| 2:B:434:GLN:CD   | 3:K:290:HIS:CG   | 2.86                     | 0.53              |
| 2:B:4:ILE:CG2    | 2:B:136:GLN:HG2  | 2.38                     | 0.53              |
| 2:B:323:MET:HG3  | 2:B:328:VAL:HG21 | 1.90                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:9:VAL:CG1    | 1:A:139:HIS:HB3  | 2.38                     | 0.53              |
| 1:A:163:LYS:O    | 1:A:163:LYS:HG2  | 2.08                     | 0.53              |
| 2:B:8:GLN:OE1    | 2:B:14:ASN:ND2   | 2.42                     | 0.53              |
| 2:B:168:THR:CB   | 2:B:201:THR:HG23 | 2.38                     | 0.53              |
| 2:B:325:MET:O    | 2:B:329:ASP:HB2  | 2.07                     | 0.53              |
| 1:A:98:ASP:O     | 1:A:110:ILE:HD13 | 2.08                     | 0.53              |
| 1:A:275:VAL:HG21 | 1:A:300:ASN:OD1  | 2.09                     | 0.53              |
| 2:B:263:PRO:O    | 2:B:264:ARG:C    | 2.52                     | 0.53              |
| 2:B:322:ARG:HG3  | 2:B:322:ARG:HH11 | 1.73                     | 0.53              |
| 2:B:31:ASP:HB3   | 2:B:32:PRO:HD2   | 1.89                     | 0.53              |
| 2:B:68:VAL:HG12  | 2:B:149:MET:CE   | 2.38                     | 0.53              |
| 2:B:259:MET:HG2  | 2:B:314:THR:CG2  | 2.38                     | 0.53              |
| 3:K:38:GLU:HB3   | 3:K:41:ARG:NH2   | 2.24                     | 0.53              |
| 1:A:101:ASN:HD21 | 2:B:254:LYS:CD   | 2.22                     | 0.53              |
| 1:A:173:PRO:HB2  | 1:A:391:LEU:HD11 | 1.91                     | 0.53              |
| 1:A:338:LYS:O    | 1:A:340:THR:N    | 2.34                     | 0.53              |
| 2:B:27:GLU:O     | 2:B:27:GLU:HG2   | 2.08                     | 0.53              |
| 2:B:176:LYS:CE   | 2:B:207:GLU:HG3  | 2.39                     | 0.53              |
| 2:B:212:ILE:O    | 2:B:216:THR:HB   | 2.09                     | 0.53              |
| 3:K:121:MET:HE3  | 3:K:126:ARG:HG3  | 1.91                     | 0.53              |
| 1:A:248:LEU:HB3  | 1:A:355:ILE:H    | 1.72                     | 0.53              |
| 2:B:5:VAL:HG23   | 2:B:5:VAL:O      | 2.09                     | 0.53              |
| 2:B:70:LEU:HD12  | 2:B:145:THR:HG23 | 1.91                     | 0.53              |
| 2:B:132:LEU:CD2  | 2:B:164:ARG:HG3  | 2.32                     | 0.53              |
| 2:B:288:VAL:HG22 | 2:B:323:MET:HE3  | 1.90                     | 0.53              |
| 1:A:231:ILE:CA   | 1:A:234:ILE:HG22 | 2.38                     | 0.52              |
| 2:B:210:TYR:CD1  | 2:B:227:LEU:HD21 | 2.44                     | 0.52              |
| 2:B:281:GLN:C    | 2:B:283:TYR:N    | 2.67                     | 0.52              |
| 1:A:24:TYR:CE1   | 1:A:240:ALA:HB2  | 2.45                     | 0.52              |
| 1:A:182:VAL:O    | 1:A:184:PRO:N    | 2.41                     | 0.52              |
| 2:B:264:ARG:HE   | 2:B:264:ARG:HA   | 1.74                     | 0.52              |
| 1:A:206:ASN:OD1  | 1:A:227:LEU:CD1  | 2.57                     | 0.52              |
| 3:K:46:ILE:N     | 3:K:47:PRO:CD    | 2.73                     | 0.52              |
| 1:A:119:LEU:HD11 | 1:A:156:ARG:CD   | 2.40                     | 0.52              |
| 1:A:243:ARG:CZ   | 1:A:252:LEU:HG   | 2.39                     | 0.52              |
| 1:A:251:ASP:OD1  | 1:A:252:LEU:N    | 2.43                     | 0.52              |
| 2:B:103:TRP:CE2  | 2:B:189:LEU:HB3  | 2.45                     | 0.52              |
| 2:B:320:ARG:HA   | 2:B:356:CYS:HB3  | 1.92                     | 0.52              |
| 3:K:73:THR:CG2   | 3:K:74:GLN:N     | 2.72                     | 0.52              |
| 2:B:149:MET:O    | 2:B:149:MET:HG2  | 2.10                     | 0.52              |
| 2:B:288:VAL:CG2  | 2:B:323:MET:HE3  | 2.40                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:399:PHE:O    | 2:B:400:ARG:C    | 2.52                     | 0.52              |
| 2:B:422:GLU:O    | 2:B:426:ASN:N    | 2.37                     | 0.52              |
| 2:B:425:MET:O    | 2:B:428:LEU:HB3  | 2.09                     | 0.52              |
| 1:A:8:HIS:HB3    | 1:A:13:GLY:O     | 2.09                     | 0.52              |
| 3:K:22:ARG:CZ    | 3:K:93:TYR:CE1   | 2.90                     | 0.52              |
| 2:B:141:LEU:HA   | 2:B:147:SER:HB3  | 1.91                     | 0.52              |
| 2:B:198:THR:HG22 | 2:B:265:LEU:CD2  | 2.39                     | 0.52              |
| 2:B:277:SER:OG   | 2:B:281:GLN:HB2  | 2.10                     | 0.52              |
| 2:B:314:THR:CG2  | 2:B:315:VAL:N    | 2.73                     | 0.52              |
| 2:B:325:MET:CE   | 2:B:355:VAL:HG11 | 2.38                     | 0.52              |
| 1:A:253:THR:O    | 1:A:254:GLU:C    | 2.52                     | 0.52              |
| 2:B:226:ASP:O    | 2:B:229:HIS:N    | 2.42                     | 0.52              |
| 2:B:307:PRO:C    | 2:B:309:HIS:H    | 2.18                     | 0.52              |
| 2:B:107:HIS:CD2  | 2:B:151:THR:HG22 | 2.45                     | 0.52              |
| 2:B:149:MET:O    | 2:B:153:LEU:HD22 | 2.10                     | 0.52              |
| 2:B:200:GLU:N    | 2:B:265:LEU:HD13 | 2.25                     | 0.52              |
| 2:B:295:MET:SD   | 2:B:375:ALA:O    | 2.68                     | 0.52              |
| 2:B:21:TRP:HZ2   | 2:B:65:ALA:HB2   | 1.75                     | 0.51              |
| 2:B:21:TRP:CZ2   | 2:B:65:ALA:HB2   | 2.44                     | 0.51              |
| 2:B:346:TRP:CD1  | 2:B:346:TRP:H    | 2.27                     | 0.51              |
| 2:B:431:GLU:OE1  | 2:B:432:TYR:CA   | 2.57                     | 0.51              |
| 3:K:41:ARG:HH12  | 3:K:323:PHE:HB2  | 1.75                     | 0.51              |
| 3:K:154:TYR:HD1  | 3:K:219:ARG:O    | 1.92                     | 0.51              |
| 1:A:34:GLY:C     | 1:A:61:HIS:N     | 2.68                     | 0.51              |
| 1:A:172:TYR:OH   | 1:A:387:ALA:O    | 2.24                     | 0.51              |
| 1:A:201:ALA:O    | 1:A:267:PHE:HA   | 2.10                     | 0.51              |
| 3:K:43:ASP:CB    | 3:K:321:SER:HB2  | 2.41                     | 0.51              |
| 3:K:100:TYR:HB3  | 3:K:316:ILE:HG22 | 1.92                     | 0.51              |
| 1:A:9:VAL:HG21   | 1:A:149:PHE:CD1  | 2.46                     | 0.51              |
| 1:A:22:GLU:O     | 1:A:23:LEU:C     | 2.54                     | 0.51              |
| 1:A:345:ASP:OD2  | 1:A:439:SER:HB3  | 2.10                     | 0.51              |
| 1:A:396:ASP:O    | 1:A:397:LEU:C    | 2.53                     | 0.51              |
| 1:A:417:GLU:HA   | 1:A:417:GLU:OE1  | 2.10                     | 0.51              |
| 3:K:117:ASP:OD2  | 3:K:120:LEU:CG   | 2.58                     | 0.51              |
| 1:A:11:GLN:CG    | 1:A:74:VAL:HG11  | 2.28                     | 0.51              |
| 1:A:11:GLN:CA    | 5:A:502:GTP:O1B  | 2.58                     | 0.51              |
| 1:A:231:ILE:HD13 | 1:A:231:ILE:N    | 2.25                     | 0.51              |
| 2:B:175:PRO:O    | 2:B:176:LYS:C    | 2.52                     | 0.51              |
| 2:B:188:THR:HA   | 2:B:425:MET:CE   | 2.40                     | 0.51              |
| 1:A:151:SER:HB3  | 1:A:193:THR:CG2  | 2.34                     | 0.51              |
| 1:A:242:LEU:C    | 1:A:244:PHE:N    | 2.66                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:243:ARG:NH2  | 1:A:251:ASP:OD1  | 2.43                     | 0.51              |
| 1:A:255:PHE:O    | 1:A:256:GLN:C    | 2.53                     | 0.51              |
| 1:A:402:ARG:O    | 1:A:403:ALA:O    | 2.29                     | 0.51              |
| 2:B:103:TRP:HZ3  | 2:B:108:TYR:CE1  | 2.27                     | 0.51              |
| 1:A:238:ILE:O    | 1:A:242:LEU:HB2  | 2.11                     | 0.51              |
| 1:A:310:GLY:HA3  | 1:A:383:ALA:N    | 2.26                     | 0.51              |
| 1:A:434:GLU:C    | 1:A:436:GLY:H    | 2.18                     | 0.51              |
| 2:B:240:THR:HG23 | 2:B:241:CYS:H    | 1.76                     | 0.51              |
| 1:A:133:GLN:CB   | 1:A:243:ARG:HH12 | 2.24                     | 0.51              |
| 1:A:171:ILE:O    | 1:A:171:ILE:HG22 | 2.11                     | 0.51              |
| 2:B:49:ILE:HG13  | 2:B:50:ASN:H     | 1.76                     | 0.51              |
| 1:A:119:LEU:HA   | 1:A:122:ILE:HG12 | 1.93                     | 0.51              |
| 2:B:265:LEU:O    | 2:B:266:HIS:O    | 2.29                     | 0.51              |
| 3:K:22:ARG:HH12  | 3:K:88:ASP:CA    | 2.24                     | 0.51              |
| 1:A:180:ALA:HA   | 2:B:352:LYS:HZ3  | 1.75                     | 0.50              |
| 2:B:5:VAL:CG2    | 2:B:135:PHE:CD2  | 2.94                     | 0.50              |
| 3:K:210:VAL:O    | 3:K:210:VAL:HG13 | 2.11                     | 0.50              |
| 1:A:115:ILE:CG2  | 1:A:116:ASP:N    | 2.75                     | 0.50              |
| 1:A:148:GLY:O    | 1:A:149:PHE:C    | 2.55                     | 0.50              |
| 1:A:362:VAL:HG13 | 1:A:368:LEU:CD1  | 2.38                     | 0.50              |
| 2:B:333:LEU:O    | 2:B:336:GLN:N    | 2.44                     | 0.50              |
| 3:K:22:ARG:O     | 3:K:311:ARG:HB2  | 2.11                     | 0.50              |
| 1:A:11:GLN:O     | 1:A:14:VAL:HB    | 2.12                     | 0.50              |
| 1:A:132:LEU:CD2  | 1:A:164:LYS:HE3  | 2.42                     | 0.50              |
| 2:B:147:SER:O    | 2:B:151:THR:CB   | 2.51                     | 0.50              |
| 2:B:224:TYR:O    | 2:B:225:GLY:C    | 2.53                     | 0.50              |
| 2:B:260:VAL:HG23 | 2:B:260:VAL:O    | 2.11                     | 0.50              |
| 3:K:254:VAL:HG21 | 3:K:264:LEU:HD12 | 1.93                     | 0.50              |
| 1:A:4:CYS:HA     | 1:A:134:GLY:O    | 2.10                     | 0.50              |
| 1:A:23:LEU:HD23  | 1:A:236:SER:CB   | 2.37                     | 0.50              |
| 1:A:95:GLY:C     | 1:A:97:GLU:N     | 2.69                     | 0.50              |
| 1:A:222:PRO:HD2  | 2:B:326:LYS:HB3  | 1.92                     | 0.50              |
| 2:B:332:MET:CE   | 2:B:351:VAL:HG11 | 2.32                     | 0.50              |
| 2:B:360:PRO:O    | 2:B:369:ARG:C    | 2.54                     | 0.50              |
| 1:A:5:ILE:O      | 1:A:136:SER:N    | 2.40                     | 0.50              |
| 1:A:147:SER:CB   | 1:A:190:THR:OG1  | 2.52                     | 0.50              |
| 1:A:407:TRP:HZ2  | 2:B:260:VAL:HG21 | 1.75                     | 0.50              |
| 2:B:175:PRO:HD2  | 2:B:207:GLU:CD   | 2.36                     | 0.50              |
| 2:B:416:MET:HE1  | 3:K:173:GLU:HB2  | 0.61                     | 0.50              |
| 1:A:206:ASN:ND2  | 5:A:502:GTP:O2'  | 2.45                     | 0.50              |
| 1:A:412:GLY:N    | 3:K:268:LYS:HG2  | 2.26                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:3:GLU:HA     | 2:B:51:VAL:HA    | 1.93                     | 0.50              |
| 2:B:4:ILE:HD12   | 2:B:239:THR:CG2  | 2.42                     | 0.50              |
| 2:B:173:PRO:HB3  | 2:B:183:GLU:CG   | 2.42                     | 0.50              |
| 2:B:265:LEU:HD12 | 2:B:266:HIS:O    | 2.12                     | 0.50              |
| 2:B:325:MET:HE2  | 2:B:355:VAL:HG21 | 1.92                     | 0.50              |
| 2:B:420:GLU:HA   | 3:K:173:GLU:CD   | 2.36                     | 0.50              |
| 1:A:140:SER:O    | 1:A:142:GLY:N    | 2.44                     | 0.50              |
| 1:A:218:ASP:C    | 1:A:219:ILE:HG12 | 2.37                     | 0.50              |
| 1:A:413:MET:C    | 1:A:414:GLU:HG3  | 2.36                     | 0.50              |
| 2:B:24:ILE:HG22  | 2:B:25:SER:N     | 2.27                     | 0.50              |
| 2:B:82:PRO:C     | 2:B:84:GLY:H     | 2.20                     | 0.50              |
| 2:B:387:LEU:HD23 | 2:B:388:PHE:CD1  | 2.47                     | 0.50              |
| 1:A:196:GLU:O    | 1:A:197:HIS:CD2  | 2.64                     | 0.50              |
| 1:A:339:ARG:C    | 1:A:341:ILE:N    | 2.68                     | 0.50              |
| 3:K:38:GLU:O     | 3:K:39:ILE:CG1   | 2.55                     | 0.50              |
| 3:K:284:LEU:HG   | 3:K:291:VAL:CG1  | 2.42                     | 0.50              |
| 1:A:67:PHE:HE2   | 1:A:87:PHE:CE2   | 2.29                     | 0.50              |
| 1:A:261:PRO:HB2  | 1:A:262:TYR:CD2  | 2.46                     | 0.50              |
| 2:B:23:VAL:HG13  | 7:B:902:TA1:H321 | 1.94                     | 0.50              |
| 2:B:416:MET:HE2  | 3:K:173:GLU:CB   | 2.15                     | 0.50              |
| 1:A:181:VAL:HG23 | 2:B:258:ASN:HB3  | 1.93                     | 0.49              |
| 1:A:191:THR:HG23 | 1:A:192:HIS:N    | 2.25                     | 0.49              |
| 1:A:414:GLU:OE1  | 1:A:414:GLU:N    | 2.45                     | 0.49              |
| 2:B:280:SER:O    | 2:B:282:GLN:N    | 2.45                     | 0.49              |
| 2:B:296:PHE:CZ   | 2:B:315:VAL:HG11 | 2.46                     | 0.49              |
| 2:B:323:MET:HG3  | 2:B:328:VAL:CG2  | 2.41                     | 0.49              |
| 2:B:345:GLU:O    | 2:B:347:ILE:N    | 2.45                     | 0.49              |
| 1:A:244:PHE:CD1  | 1:A:245:ASP:N    | 2.76                     | 0.49              |
| 1:A:283:HIS:O    | 1:A:285:GLN:N    | 2.45                     | 0.49              |
| 1:A:11:GLN:CB    | 5:A:502:GTP:O1B  | 2.60                     | 0.49              |
| 1:A:16:ILE:HG23  | 1:A:17:GLY:N     | 2.26                     | 0.49              |
| 1:A:133:GLN:HB3  | 1:A:243:ARG:HH12 | 1.76                     | 0.49              |
| 2:B:113:GLU:HG3  | 2:B:114:LEU:N    | 2.26                     | 0.49              |
| 2:B:299:LYS:H    | 2:B:299:LYS:CD   | 2.07                     | 0.49              |
| 2:B:332:MET:HE3  | 2:B:351:VAL:CG1  | 2.32                     | 0.49              |
| 2:B:168:THR:O    | 2:B:201:THR:HA   | 2.12                     | 0.49              |
| 2:B:242:LEU:C    | 2:B:244:PHE:H    | 2.19                     | 0.49              |
| 3:K:27:VAL:CB    | 3:K:338:VAL:CG1  | 2.82                     | 0.49              |
| 1:A:115:ILE:HD11 | 1:A:119:LEU:HG   | 1.92                     | 0.49              |
| 1:A:230:LEU:O    | 1:A:233:GLN:N    | 2.35                     | 0.49              |
| 2:B:69:ASP:HA    | 2:B:145:THR:HG21 | 1.95                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:133:GLN:NE2  | 2:B:252:LEU:HB2  | 2.27                     | 0.49              |
| 2:B:173:PRO:HB3  | 2:B:183:GLU:HG2  | 1.93                     | 0.49              |
| 2:B:176:LYS:HG3  | 2:B:177:VAL:H    | 1.78                     | 0.49              |
| 1:A:63:PRO:C     | 1:A:64:ARG:CG    | 2.83                     | 0.49              |
| 1:A:188:ILE:O    | 1:A:191:THR:HG22 | 2.13                     | 0.49              |
| 1:A:252:LEU:O    | 1:A:253:THR:C    | 2.56                     | 0.49              |
| 2:B:199:ASP:O    | 2:B:200:GLU:HG3  | 2.13                     | 0.49              |
| 1:A:152:LEU:HD12 | 1:A:152:LEU:C    | 2.38                     | 0.49              |
| 1:A:158:SER:OG   | 1:A:197:HIS:HB3  | 2.13                     | 0.49              |
| 1:A:192:HIS:CD2  | 1:A:424:ASP:OD2  | 2.66                     | 0.49              |
| 1:A:241:SER:C    | 1:A:244:PHE:HB3  | 2.36                     | 0.49              |
| 1:A:274:PRO:CB   | 1:A:371:VAL:HG21 | 2.43                     | 0.49              |
| 2:B:175:PRO:CD   | 2:B:207:GLU:OE1  | 2.61                     | 0.49              |
| 2:B:273:ALA:CB   | 2:B:274:PRO:HD3  | 2.30                     | 0.49              |
| 2:B:336:GLN:HE22 | 2:B:349:ASN:ND2  | 2.10                     | 0.49              |
| 2:B:431:GLU:OE1  | 2:B:432:TYR:N    | 2.46                     | 0.49              |
| 1:A:12:ALA:HB2   | 5:A:502:GTP:C8   | 2.48                     | 0.49              |
| 1:A:118:VAL:HG21 | 1:A:149:PHE:CE2  | 2.48                     | 0.49              |
| 1:A:203:MET:SD   | 1:A:267:PHE:HB3  | 2.53                     | 0.49              |
| 1:A:227:LEU:O    | 1:A:231:ILE:HG12 | 2.12                     | 0.49              |
| 1:A:286:LEU:O    | 1:A:287:SER:C    | 2.55                     | 0.49              |
| 2:B:211:ASP:OD1  | 2:B:212:ILE:HG13 | 2.13                     | 0.49              |
| 2:B:239:THR:O    | 2:B:240:THR:C    | 2.56                     | 0.49              |
| 1:A:10:GLY:O     | 1:A:11:GLN:C     | 2.54                     | 0.49              |
| 1:A:234:ILE:C    | 1:A:234:ILE:CD1  | 2.86                     | 0.49              |
| 1:A:344:VAL:HG12 | 1:A:345:ASP:H    | 1.74                     | 0.49              |
| 2:B:137:LEU:HD22 | 2:B:154:ILE:HG21 | 1.95                     | 0.49              |
| 2:B:360:PRO:HG2  | 2:B:371:LEU:CB   | 2.38                     | 0.49              |
| 1:A:13:GLY:C     | 1:A:16:ILE:HG22  | 2.38                     | 0.48              |
| 2:B:262:PHE:O    | 2:B:264:ARG:N    | 2.45                     | 0.48              |
| 1:A:9:VAL:HG11   | 1:A:150:THR:OG1  | 2.13                     | 0.48              |
| 1:A:99:ALA:O     | 1:A:100:ALA:HB3  | 2.13                     | 0.48              |
| 1:A:104:ALA:CB   | 1:A:408:TYR:HD1  | 2.26                     | 0.48              |
| 2:B:2:ARG:NH1    | 2:B:251:ASP:OD2  | 2.46                     | 0.48              |
| 2:B:142:GLY:HA3  | 2:B:183:GLU:OE2  | 2.13                     | 0.48              |
| 2:B:191:VAL:HG13 | 2:B:192:HIS:N    | 2.28                     | 0.48              |
| 2:B:194:LEU:C    | 2:B:196:GLU:N    | 2.71                     | 0.48              |
| 2:B:264:ARG:HA   | 2:B:264:ARG:NE   | 2.28                     | 0.48              |
| 2:B:419:THR:HG23 | 3:K:177:ARG:NH1  | 2.28                     | 0.48              |
| 1:A:98:ASP:CB    | 1:A:105:ARG:HH21 | 2.14                     | 0.48              |
| 1:A:149:PHE:HE1  | 1:A:153:LEU:HD22 | 1.77                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:155:GLU:OE1  | 1:A:197:HIS:HE1  | 1.96                     | 0.48              |
| 1:A:392:ASP:O    | 1:A:395:PHE:HB3  | 2.13                     | 0.48              |
| 2:B:26:ASP:C     | 2:B:28:HIS:H     | 2.21                     | 0.48              |
| 2:B:269:MET:HB3  | 2:B:303:ALA:HB2  | 1.94                     | 0.48              |
| 3:K:24:ASN:HB2   | 3:K:311:ARG:HH12 | 1.78                     | 0.48              |
| 1:A:115:ILE:HG23 | 1:A:116:ASP:H    | 1.79                     | 0.48              |
| 1:A:196:GLU:C    | 1:A:197:HIS:HD2  | 2.19                     | 0.48              |
| 1:A:224:TYR:HD2  | 2:B:247:GLN:CB   | 2.22                     | 0.48              |
| 1:A:263:PRO:O    | 1:A:264:ARG:C    | 2.56                     | 0.48              |
| 2:B:296:PHE:HZ   | 2:B:315:VAL:HG11 | 1.78                     | 0.48              |
| 3:K:24:ASN:HB2   | 3:K:311:ARG:NH1  | 2.26                     | 0.48              |
| 2:B:4:ILE:HG22   | 2:B:5:VAL:N      | 2.27                     | 0.48              |
| 2:B:8:GLN:HB3    | 2:B:14:ASN:HA    | 1.94                     | 0.48              |
| 2:B:12:CYS:C     | 2:B:14:ASN:N     | 2.71                     | 0.48              |
| 2:B:154:ILE:HG22 | 2:B:166:MET:CE   | 2.44                     | 0.48              |
| 3:K:262:ALA:O    | 3:K:266:GLU:CG   | 2.61                     | 0.48              |
| 2:B:20:PHE:CG    | 2:B:235:MET:SD   | 3.07                     | 0.48              |
| 2:B:49:ILE:HG13  | 2:B:50:ASN:N     | 2.28                     | 0.48              |
| 2:B:102:ASN:HB3  | 2:B:105:LYS:HB2  | 1.95                     | 0.48              |
| 1:A:6:SER:OG     | 1:A:65:ALA:HB2   | 2.14                     | 0.48              |
| 1:A:147:SER:O    | 1:A:190:THR:HG23 | 2.14                     | 0.48              |
| 1:A:180:ALA:CA   | 2:B:352:LYS:NZ   | 2.77                     | 0.48              |
| 1:A:231:ILE:O    | 1:A:235:VAL:HG23 | 2.12                     | 0.48              |
| 1:A:384:ILE:HG22 | 1:A:388:TRP:CD1  | 2.49                     | 0.48              |
| 2:B:115:VAL:CG2  | 2:B:152:LEU:HD23 | 2.44                     | 0.48              |
| 2:B:161:TYR:C    | 2:B:163:ASP:N    | 2.72                     | 0.48              |
| 1:A:317:LEU:CD1  | 1:A:351:PHE:CD1  | 2.97                     | 0.48              |
| 1:A:386:GLU:O    | 1:A:388:TRP:N    | 2.47                     | 0.48              |
| 1:A:105:ARG:HH11 | 1:A:105:ARG:HG3  | 1.78                     | 0.48              |
| 1:A:401:LYS:HD2  | 2:B:346:TRP:CD2  | 2.49                     | 0.48              |
| 2:B:192:HIS:HD1  | 2:B:424:ASN:CG   | 2.20                     | 0.48              |
| 2:B:307:PRO:C    | 2:B:309:HIS:N    | 2.71                     | 0.48              |
| 1:A:217:LEU:CD1  | 1:A:277:SER:HA   | 2.44                     | 0.48              |
| 1:A:286:LEU:CD1  | 1:A:290:GLU:HG2  | 2.44                     | 0.48              |
| 2:B:243:ARG:N    | 2:B:243:ARG:HD3  | 2.26                     | 0.48              |
| 3:K:325:GLU:OE1  | 3:K:329:LYS:HD2  | 2.14                     | 0.48              |
| 1:A:97:GLU:HB2   | 1:A:110:ILE:HD11 | 1.96                     | 0.47              |
| 1:A:191:THR:CG2  | 1:A:192:HIS:N    | 2.76                     | 0.47              |
| 1:A:210:TYR:CE1  | 1:A:227:LEU:HD21 | 2.49                     | 0.47              |
| 1:A:5:ILE:HG22   | 1:A:6:SER:H      | 1.78                     | 0.47              |
| 1:A:96:LYS:O     | 1:A:97:GLU:O     | 2.31                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:148:GLY:O    | 1:A:151:SER:CB   | 2.61                     | 0.47              |
| 1:A:335:ILE:O    | 1:A:337:THR:N    | 2.47                     | 0.47              |
| 2:B:101:ASN:ND2  | 2:B:101:ASN:O    | 2.47                     | 0.47              |
| 2:B:301:MET:HE1  | 2:B:377:PHE:CE2  | 2.43                     | 0.47              |
| 2:B:360:PRO:HB2  | 7:B:902:TA1:H281 | 1.95                     | 0.47              |
| 2:B:409:THR:C    | 2:B:411:GLU:H    | 2.22                     | 0.47              |
| 3:K:277:LEU:HG   | 3:K:281:ILE:HD11 | 1.96                     | 0.47              |
| 3:K:284:LEU:HG   | 3:K:291:VAL:HG13 | 1.96                     | 0.47              |
| 1:A:241:SER:HB3  | 1:A:320:ARG:NH2  | 2.30                     | 0.47              |
| 2:B:20:PHE:O     | 2:B:24:ILE:HB    | 2.15                     | 0.47              |
| 2:B:226:ASP:O    | 2:B:229:HIS:HB3  | 2.15                     | 0.47              |
| 1:A:151:SER:OG   | 1:A:193:THR:HG21 | 2.13                     | 0.47              |
| 1:A:154:MET:HA   | 1:A:157:LEU:HD12 | 1.96                     | 0.47              |
| 1:A:260:VAL:O    | 1:A:260:VAL:CG2  | 2.63                     | 0.47              |
| 1:A:401:LYS:O    | 2:B:262:PHE:CZ   | 2.67                     | 0.47              |
| 2:B:209:LEU:CD2  | 2:B:227:LEU:HD13 | 2.44                     | 0.47              |
| 2:B:297:ASP:OD2  | 2:B:299:LYS:HE2  | 2.14                     | 0.47              |
| 2:B:307:PRO:HB3  | 2:B:312:TYR:CZ   | 2.49                     | 0.47              |
| 3:K:318:CYS:HB3  | 3:K:328:THR:HG23 | 1.96                     | 0.47              |
| 1:A:117:LEU:HD12 | 1:A:121:ARG:HH12 | 1.80                     | 0.47              |
| 1:A:388:TRP:HA   | 1:A:388:TRP:HE3  | 1.79                     | 0.47              |
| 2:B:185:TYR:HD1  | 2:B:395:PHE:CE1  | 2.33                     | 0.47              |
| 2:B:264:ARG:NH1  | 3:K:294:ARG:CD   | 2.57                     | 0.47              |
| 2:B:274:PRO:HG2  | 2:B:371:LEU:CD2  | 2.43                     | 0.47              |
| 2:B:384:ILE:O    | 2:B:384:ILE:HG23 | 2.14                     | 0.47              |
| 1:A:120:ASP:O    | 1:A:124:LYS:HB2  | 2.15                     | 0.47              |
| 1:A:132:LEU:HD21 | 1:A:164:LYS:HE3  | 1.96                     | 0.47              |
| 2:B:187:ALA:O    | 2:B:188:THR:C    | 2.57                     | 0.47              |
| 2:B:308:ARG:HG3  | 2:B:342:TYR:OH   | 2.13                     | 0.47              |
| 1:A:7:ILE:HD11   | 1:A:137:VAL:CG2  | 2.44                     | 0.47              |
| 1:A:25:CYS:SG    | 1:A:83:TYR:HE2   | 2.38                     | 0.47              |
| 1:A:103:TYR:O    | 1:A:104:ALA:C    | 2.57                     | 0.47              |
| 1:A:149:PHE:O    | 1:A:150:THR:C    | 2.56                     | 0.47              |
| 1:A:166:LYS:CE   | 1:A:199:ASP:OD1  | 2.62                     | 0.47              |
| 1:A:178:SER:HG   | 2:B:349:ASN:CG   | 2.20                     | 0.47              |
| 1:A:204:VAL:CG1  | 1:A:209:ILE:HD11 | 2.42                     | 0.47              |
| 1:A:256:GLN:HA   | 1:A:260:VAL:HG13 | 1.97                     | 0.47              |
| 1:A:404:PHE:CD1  | 1:A:404:PHE:N    | 2.83                     | 0.47              |
| 1:A:407:TRP:O    | 1:A:411:GLU:CG   | 2.63                     | 0.47              |
| 2:B:23:VAL:HA    | 7:B:902:TA1:H321 | 1.94                     | 0.47              |
| 2:B:209:LEU:O    | 2:B:213:CYS:N    | 2.47                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:242:LEU:CD1  | 2:B:250:ALA:HB3  | 2.45                     | 0.47              |
| 2:B:383:ALA:C    | 2:B:385:GLN:N    | 2.72                     | 0.47              |
| 3:K:309:ASN:HB3  | 3:K:310:CYS:H    | 1.53                     | 0.47              |
| 1:A:436:GLY:C    | 1:A:438:ASP:N    | 2.72                     | 0.47              |
| 2:B:210:TYR:O    | 2:B:211:ASP:C    | 2.57                     | 0.47              |
| 1:A:12:ALA:CB    | 1:A:140:SER:OG   | 2.60                     | 0.47              |
| 1:A:107:HIS:CE1  | 1:A:152:LEU:HB3  | 2.49                     | 0.47              |
| 1:A:288:VAL:C    | 1:A:290:GLU:N    | 2.71                     | 0.47              |
| 1:A:401:LYS:O    | 2:B:262:PHE:CE1  | 2.68                     | 0.47              |
| 3:K:64:PHE:CD1   | 3:K:338:VAL:HG21 | 2.50                     | 0.47              |
| 3:K:251:SER:HB3  | 3:K:274:LEU:HD13 | 1.96                     | 0.47              |
| 1:A:19:ALA:HB2   | 1:A:228:ASN:HB3  | 1.96                     | 0.47              |
| 1:A:115:ILE:CD1  | 1:A:115:ILE:C    | 2.88                     | 0.47              |
| 1:A:191:THR:O    | 1:A:195:LEU:HB2  | 2.15                     | 0.47              |
| 1:A:265:GLY:O    | 1:A:266:HIS:O    | 2.33                     | 0.47              |
| 1:A:344:VAL:CG1  | 1:A:345:ASP:N    | 2.78                     | 0.47              |
| 1:A:369:ALA:O    | 1:A:370:LYS:CB   | 2.62                     | 0.47              |
| 2:B:182:VAL:O    | 2:B:183:GLU:C    | 2.56                     | 0.47              |
| 1:A:11:GLN:NE2   | 1:A:74:VAL:HG22  | 2.30                     | 0.46              |
| 1:A:145:THR:O    | 1:A:149:PHE:HB3  | 2.15                     | 0.46              |
| 1:A:155:GLU:HG2  | 1:A:197:HIS:CE1  | 2.49                     | 0.46              |
| 1:A:278:ALA:O    | 1:A:279:GLU:HG2  | 2.15                     | 0.46              |
| 2:B:2:ARG:NH1    | 2:B:251:ASP:CG   | 2.73                     | 0.46              |
| 2:B:199:ASP:C    | 2:B:265:LEU:HD13 | 2.41                     | 0.46              |
| 2:B:236:SER:OG   | 7:B:902:TA1:C40  | 2.63                     | 0.46              |
| 2:B:242:LEU:HD11 | 2:B:250:ALA:HB3  | 1.97                     | 0.46              |
| 3:K:294:ARG:HG2  | 3:K:300:ARG:HD2  | 1.97                     | 0.46              |
| 1:A:9:VAL:HG21   | 1:A:149:PHE:HD1  | 1.80                     | 0.46              |
| 1:A:110:ILE:O    | 1:A:111:GLY:C    | 2.57                     | 0.46              |
| 1:A:114:ILE:O    | 1:A:118:VAL:HG23 | 2.16                     | 0.46              |
| 1:A:175:PRO:HD2  | 1:A:207:GLU:HB3  | 1.96                     | 0.46              |
| 1:A:210:TYR:CZ   | 1:A:227:LEU:HD11 | 2.51                     | 0.46              |
| 1:A:409:VAL:C    | 1:A:411:GLU:N    | 2.72                     | 0.46              |
| 2:B:133:GLN:O    | 2:B:165:ILE:CD1  | 2.64                     | 0.46              |
| 2:B:259:MET:HE1  | 2:B:378:ILE:CG2  | 2.45                     | 0.46              |
| 2:B:282:GLN:HB3  | 2:B:282:GLN:HE21 | 1.50                     | 0.46              |
| 1:A:119:LEU:HD11 | 1:A:156:ARG:HD2  | 1.97                     | 0.46              |
| 1:A:381:THR:O    | 1:A:383:ALA:N    | 2.49                     | 0.46              |
| 2:B:250:ALA:HB1  | 2:B:254:LYS:CB   | 2.44                     | 0.46              |
| 2:B:287:THR:N    | 2:B:290:GLU:OE1  | 2.48                     | 0.46              |
| 2:B:427:ASP:OD1  | 2:B:427:ASP:C    | 2.57                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:11:GLN:HE21  | 1:A:74:VAL:CG2   | 2.29                     | 0.46              |
| 1:A:185:TYR:OH   | 1:A:399:TYR:HA   | 2.15                     | 0.46              |
| 1:A:230:LEU:O    | 1:A:231:ILE:C    | 2.57                     | 0.46              |
| 2:B:70:LEU:O     | 2:B:99:ALA:HB2   | 2.15                     | 0.46              |
| 2:B:154:ILE:HD12 | 2:B:155:SER:N    | 2.31                     | 0.46              |
| 2:B:198:THR:HG23 | 2:B:200:GLU:H    | 1.79                     | 0.46              |
| 2:B:409:THR:C    | 2:B:411:GLU:N    | 2.73                     | 0.46              |
| 2:B:421:ALA:O    | 2:B:422:GLU:C    | 2.58                     | 0.46              |
| 2:B:435:TYR:C    | 2:B:437:ASP:N    | 2.72                     | 0.46              |
| 3:K:152:GLU:OE2  | 3:K:207:HIS:HD2  | 1.98                     | 0.46              |
| 3:K:254:VAL:HG23 | 3:K:267:ALA:HB1  | 1.94                     | 0.46              |
| 1:A:11:GLN:O     | 1:A:15:GLN:HG3   | 2.15                     | 0.46              |
| 1:A:228:ASN:OD1  | 5:A:502:GTP:C6   | 2.69                     | 0.46              |
| 1:A:243:ARG:NH2  | 1:A:252:LEU:HB2  | 2.31                     | 0.46              |
| 1:A:278:ALA:HB2  | 1:A:369:ALA:CA   | 2.45                     | 0.46              |
| 1:A:392:ASP:OD1  | 1:A:422:ARG:NE   | 2.48                     | 0.46              |
| 1:A:409:VAL:HG12 | 3:K:271:ASN:C    | 2.38                     | 0.46              |
| 2:B:208:ALA:O    | 2:B:212:ILE:HG13 | 2.16                     | 0.46              |
| 2:B:310:GLY:HA3  | 2:B:436:GLN:NE2  | 2.29                     | 0.46              |
| 1:A:328:VAL:O    | 1:A:330:ALA:N    | 2.39                     | 0.46              |
| 2:B:103:TRP:CE3  | 2:B:189:LEU:HD13 | 2.50                     | 0.46              |
| 2:B:230:LEU:CG   | 2:B:302:MET:HE2  | 2.46                     | 0.46              |
| 2:B:237:GLY:HA3  | 2:B:376:THR:OG1  | 2.15                     | 0.46              |
| 2:B:259:MET:HE1  | 2:B:378:ILE:HG21 | 1.98                     | 0.46              |
| 2:B:288:VAL:C    | 2:B:290:GLU:N    | 2.70                     | 0.46              |
| 7:B:902:TA1:H463 | 7:B:902:TA1:C26  | 2.46                     | 0.46              |
| 1:A:226:ASN:O    | 1:A:227:LEU:C    | 2.59                     | 0.46              |
| 2:B:72:PRO:O     | 2:B:73:GLY:C     | 2.58                     | 0.46              |
| 1:A:130:THR:O    | 1:A:131:GLY:C    | 2.59                     | 0.46              |
| 1:A:243:ARG:NH2  | 1:A:252:LEU:CB   | 2.79                     | 0.46              |
| 1:A:324:VAL:HG12 | 1:A:326:LYS:H    | 1.81                     | 0.46              |
| 1:A:436:GLY:O    | 1:A:438:ASP:N    | 2.48                     | 0.46              |
| 2:B:11:GLN:O     | 2:B:14:ASN:HB3   | 2.16                     | 0.46              |
| 2:B:242:LEU:HD23 | 2:B:242:LEU:HA   | 1.76                     | 0.46              |
| 3:K:254:VAL:HG23 | 3:K:267:ALA:HB3  | 1.94                     | 0.46              |
| 1:A:210:TYR:CD1  | 1:A:227:LEU:HD21 | 2.51                     | 0.46              |
| 1:A:286:LEU:O    | 1:A:287:SER:O    | 2.34                     | 0.46              |
| 1:A:401:LYS:HD2  | 2:B:346:TRP:CG   | 2.51                     | 0.46              |
| 1:A:401:LYS:C    | 1:A:403:ALA:H    | 2.24                     | 0.46              |
| 1:A:5:ILE:CG2    | 1:A:6:SER:H      | 2.29                     | 0.46              |
| 1:A:7:ILE:HG13   | 1:A:137:VAL:HG22 | 1.98                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:181:VAL:CG2  | 2:B:258:ASN:HB3  | 2.47                     | 0.46              |
| 1:A:184:PRO:HG2  | 1:A:398:MET:CE   | 2.40                     | 0.46              |
| 1:A:226:ASN:O    | 1:A:229:ARG:N    | 2.48                     | 0.46              |
| 1:A:384:ILE:HG22 | 1:A:384:ILE:O    | 2.15                     | 0.46              |
| 2:B:4:ILE:HD12   | 2:B:239:THR:HG21 | 1.98                     | 0.46              |
| 2:B:113:GLU:CG   | 2:B:114:LEU:N    | 2.79                     | 0.46              |
| 2:B:273:ALA:CB   | 2:B:274:PRO:CD   | 2.93                     | 0.46              |
| 1:A:152:LEU:C    | 1:A:152:LEU:CD1  | 2.89                     | 0.45              |
| 1:A:256:GLN:O    | 1:A:260:VAL:HG13 | 2.15                     | 0.45              |
| 1:A:288:VAL:HA   | 1:A:291:ILE:HG12 | 1.97                     | 0.45              |
| 1:A:316:CYS:HB3  | 1:A:378:LEU:HD12 | 1.95                     | 0.45              |
| 2:B:209:LEU:HD23 | 2:B:227:LEU:HD13 | 1.98                     | 0.45              |
| 2:B:333:LEU:O    | 2:B:334:ASN:C    | 2.58                     | 0.45              |
| 2:B:67:LEU:HD12  | 2:B:92:PHE:CD1   | 2.51                     | 0.45              |
| 2:B:135:PHE:CD1  | 2:B:135:PHE:N    | 2.84                     | 0.45              |
| 2:B:210:TYR:CE1  | 2:B:227:LEU:HD11 | 2.51                     | 0.45              |
| 2:B:408:TYR:O    | 2:B:411:GLU:HB2  | 2.15                     | 0.45              |
| 2:B:431:GLU:O    | 2:B:434:GLN:HB2  | 2.16                     | 0.45              |
| 1:A:95:GLY:C     | 1:A:97:GLU:H     | 2.23                     | 0.45              |
| 1:A:204:VAL:HG21 | 1:A:231:ILE:HG23 | 1.97                     | 0.45              |
| 1:A:224:TYR:CE2  | 2:B:325:MET:HG2  | 2.51                     | 0.45              |
| 1:A:264:ARG:C    | 1:A:266:HIS:N    | 2.60                     | 0.45              |
| 1:A:335:ILE:C    | 1:A:337:THR:N    | 2.73                     | 0.45              |
| 1:A:345:ASP:C    | 1:A:347:CYS:N    | 2.68                     | 0.45              |
| 2:B:72:PRO:O     | 2:B:74:THR:N     | 2.50                     | 0.45              |
| 2:B:134:GLY:HA3  | 2:B:165:ILE:HG12 | 1.97                     | 0.45              |
| 2:B:156:LYS:HA   | 2:B:156:LYS:CE   | 2.38                     | 0.45              |
| 2:B:196:GLU:O    | 2:B:197:ASN:OD1  | 2.34                     | 0.45              |
| 3:K:284:LEU:CD2  | 3:K:291:VAL:HG11 | 2.44                     | 0.45              |
| 1:A:155:GLU:HA   | 1:A:197:HIS:CE1  | 2.49                     | 0.45              |
| 1:A:203:MET:SD   | 1:A:267:PHE:CB   | 3.04                     | 0.45              |
| 1:A:231:ILE:C    | 1:A:233:GLN:N    | 2.73                     | 0.45              |
| 2:B:24:ILE:CD1   | 2:B:52:TYR:CE2   | 2.97                     | 0.45              |
| 2:B:313:LEU:O    | 2:B:347:ILE:HD12 | 2.16                     | 0.45              |
| 3:K:318:CYS:CB   | 3:K:328:THR:HG23 | 2.46                     | 0.45              |
| 1:A:100:ALA:C    | 1:A:102:ASN:H    | 2.24                     | 0.45              |
| 1:A:108:TYR:CE2  | 3:K:255:SER:HB3  | 2.38                     | 0.45              |
| 1:A:303:VAL:O    | 1:A:303:VAL:CG1  | 2.65                     | 0.45              |
| 1:A:308:ARG:O    | 1:A:309:HIS:HB3  | 2.16                     | 0.45              |
| 1:A:317:LEU:CD1  | 1:A:351:PHE:CE1  | 2.99                     | 0.45              |
| 1:A:334:THR:CG2  | 1:A:335:ILE:N    | 2.79                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:106:GLY:O    | 2:B:149:MET:HB2  | 2.17                     | 0.45              |
| 2:B:194:LEU:O    | 2:B:265:LEU:HD23 | 2.16                     | 0.45              |
| 2:B:275:LEU:HD12 | 2:B:275:LEU:HA   | 1.78                     | 0.45              |
| 3:K:194:GLU:O    | 3:K:198:VAL:HG23 | 2.17                     | 0.45              |
| 1:A:23:LEU:CD2   | 1:A:232:GLY:O    | 2.64                     | 0.45              |
| 1:A:286:LEU:HG   | 1:A:290:GLU:HB2  | 1.97                     | 0.45              |
| 1:A:346:TRP:HZ2  | 1:A:435:VAL:HG12 | 1.81                     | 0.45              |
| 1:A:413:MET:C    | 1:A:414:GLU:CG   | 2.90                     | 0.45              |
| 2:B:23:VAL:O     | 2:B:24:ILE:C     | 2.60                     | 0.45              |
| 2:B:175:PRO:HG2  | 2:B:207:GLU:OE1  | 2.16                     | 0.45              |
| 2:B:188:THR:HG23 | 2:B:425:MET:HE3  | 1.98                     | 0.45              |
| 2:B:237:GLY:O    | 2:B:241:CYS:CB   | 2.61                     | 0.45              |
| 2:B:288:VAL:N    | 2:B:289:PRO:CD   | 2.80                     | 0.45              |
| 3:K:43:ASP:HB3   | 3:K:321:SER:HB2  | 1.98                     | 0.45              |
| 3:K:46:ILE:HD12  | 3:K:46:ILE:C     | 2.42                     | 0.45              |
| 1:A:103:TYR:CD1  | 1:A:148:GLY:HA2  | 2.52                     | 0.45              |
| 1:A:117:LEU:HD11 | 1:A:121:ARG:NH2  | 2.31                     | 0.45              |
| 1:A:122:ILE:CD1  | 1:A:157:LEU:HD21 | 2.35                     | 0.45              |
| 1:A:268:PRO:CA   | 1:A:379:SER:O    | 2.65                     | 0.45              |
| 1:A:328:VAL:C    | 1:A:330:ALA:N    | 2.73                     | 0.45              |
| 1:A:408:TYR:CG   | 1:A:418:PHE:HZ   | 2.34                     | 0.45              |
| 1:A:423:GLU:O    | 1:A:426:ALA:HB3  | 2.16                     | 0.45              |
| 2:B:319:PHE:CD2  | 2:B:323:MET:HE1  | 2.52                     | 0.45              |
| 2:B:324:SER:OG   | 2:B:326:LYS:HB3  | 2.16                     | 0.45              |
| 1:A:23:LEU:O     | 1:A:26:LEU:HB3   | 2.17                     | 0.45              |
| 1:A:283:HIS:O    | 1:A:283:HIS:ND1  | 2.49                     | 0.45              |
| 1:A:287:SER:O    | 1:A:288:VAL:C    | 2.60                     | 0.45              |
| 1:A:425:MET:O    | 1:A:426:ALA:C    | 2.60                     | 0.45              |
| 2:B:35:SER:CB    | 2:B:59:ASN:HA    | 2.42                     | 0.45              |
| 2:B:288:VAL:N    | 2:B:289:PRO:HD2  | 2.32                     | 0.45              |
| 2:B:427:ASP:CG   | 3:K:294:ARG:HH11 | 2.24                     | 0.45              |
| 1:A:177:VAL:HG12 | 2:B:329:ASP:HB3  | 1.90                     | 0.45              |
| 1:A:276:ILE:HG12 | 1:A:277:SER:N    | 2.32                     | 0.45              |
| 1:A:388:TRP:CD2  | 1:A:425:MET:HE1  | 2.52                     | 0.45              |
| 1:A:410:GLY:C    | 3:K:268:LYS:HG2  | 2.42                     | 0.45              |
| 2:B:102:ASN:ND2  | 2:B:104:ALA:HB3  | 2.31                     | 0.45              |
| 2:B:137:LEU:HD22 | 2:B:154:ILE:HG23 | 1.98                     | 0.45              |
| 2:B:324:SER:O    | 2:B:326:LYS:N    | 2.50                     | 0.45              |
| 3:K:97:ILE:HD12  | 3:K:243:LEU:HD21 | 1.99                     | 0.45              |
| 2:B:8:GLN:CG     | 2:B:67:LEU:HD22  | 2.47                     | 0.45              |
| 1:A:182:VAL:O    | 1:A:184:PRO:CD   | 2.65                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:231:ILE:HD13 | 1:A:231:ILE:H    | 1.82                     | 0.44              |
| 1:A:409:VAL:CG1  | 3:K:272:LYS:HA   | 2.46                     | 0.44              |
| 1:A:425:MET:O    | 1:A:428:LEU:N    | 2.45                     | 0.44              |
| 2:B:95:GLY:C     | 2:B:97:SER:H     | 2.25                     | 0.44              |
| 2:B:99:ALA:O     | 2:B:100:GLY:C    | 2.60                     | 0.44              |
| 2:B:243:ARG:HH21 | 2:B:252:LEU:N    | 2.13                     | 0.44              |
| 2:B:287:THR:O    | 2:B:288:VAL:CG2  | 2.58                     | 0.44              |
| 2:B:312:TYR:HA   | 2:B:381:SER:HA   | 1.99                     | 0.44              |
| 2:B:413:MET:HG3  | 2:B:414:ASP:N    | 2.22                     | 0.44              |
| 1:A:108:TYR:O    | 1:A:109:THR:C    | 2.61                     | 0.44              |
| 1:A:210:TYR:OH   | 2:B:325:MET:CB   | 2.64                     | 0.44              |
| 1:A:288:VAL:O    | 1:A:289:ALA:C    | 2.59                     | 0.44              |
| 1:A:393:HIS:O    | 1:A:394:LYS:C    | 2.59                     | 0.44              |
| 2:B:14:ASN:O     | 2:B:17:GLY:N     | 2.50                     | 0.44              |
| 2:B:52:TYR:HE2   | 2:B:240:THR:HB   | 1.82                     | 0.44              |
| 1:A:271:THR:O    | 1:A:376:CYS:HA   | 2.17                     | 0.44              |
| 2:B:102:ASN:OD1  | 2:B:408:TYR:CZ   | 2.70                     | 0.44              |
| 1:A:8:HIS:HA     | 1:A:138:PHE:HB2  | 2.00                     | 0.44              |
| 1:A:119:LEU:O    | 1:A:120:ASP:C    | 2.61                     | 0.44              |
| 1:A:234:ILE:CG1  | 1:A:270:ALA:HB1  | 2.38                     | 0.44              |
| 1:A:343:PHE:CE1  | 1:A:351:PHE:HE2  | 2.36                     | 0.44              |
| 1:A:434:GLU:C    | 1:A:436:GLY:N    | 2.74                     | 0.44              |
| 2:B:189:LEU:HD23 | 2:B:421:ALA:CB   | 2.48                     | 0.44              |
| 2:B:239:THR:CG2  | 2:B:240:THR:N    | 2.80                     | 0.44              |
| 2:B:380:ASN:C    | 2:B:380:ASN:HD22 | 2.24                     | 0.44              |
| 2:B:423:SER:O    | 2:B:424:ASN:C    | 2.60                     | 0.44              |
| 1:A:12:ALA:C     | 1:A:14:VAL:N     | 2.75                     | 0.44              |
| 1:A:272:TYR:CE2  | 1:A:274:PRO:HD2  | 2.53                     | 0.44              |
| 1:A:274:PRO:HB2  | 1:A:371:VAL:HG21 | 1.98                     | 0.44              |
| 1:A:362:VAL:HG13 | 1:A:368:LEU:CG   | 2.48                     | 0.44              |
| 1:A:384:ILE:O    | 1:A:385:ALA:C    | 2.59                     | 0.44              |
| 1:A:392:ASP:OD1  | 1:A:422:ARG:CZ   | 2.65                     | 0.44              |
| 2:B:70:LEU:HD21  | 2:B:149:MET:HE3  | 1.98                     | 0.44              |
| 3:K:62:TYR:C     | 3:K:63:VAL:HG23  | 2.38                     | 0.44              |
| 2:B:23:VAL:O     | 2:B:25:SER:N     | 2.50                     | 0.44              |
| 2:B:295:MET:SD   | 2:B:375:ALA:HB3  | 2.57                     | 0.44              |
| 1:A:21:TRP:HE1   | 1:A:63:PRO:HB3   | 1.83                     | 0.44              |
| 1:A:212:ILE:HD11 | 1:A:302:MET:H    | 1.82                     | 0.44              |
| 2:B:42:LEU:C     | 2:B:44:LEU:H     | 2.26                     | 0.44              |
| 2:B:67:LEU:HD12  | 2:B:92:PHE:CE1   | 2.52                     | 0.44              |
| 2:B:212:ILE:O    | 2:B:212:ILE:HG22 | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:257:VAL:O    | 2:B:257:VAL:CG1  | 2.64                     | 0.44              |
| 2:B:280:SER:OG   | 2:B:281:GLN:N    | 2.49                     | 0.44              |
| 2:B:282:GLN:O    | 2:B:282:GLN:CG   | 2.65                     | 0.44              |
| 2:B:167:ASN:HD21 | 2:B:252:LEU:HD22 | 1.82                     | 0.44              |
| 2:B:301:MET:O    | 2:B:303:ALA:N    | 2.51                     | 0.44              |
| 2:B:409:THR:HA   | 2:B:413:MET:HB3  | 1.98                     | 0.44              |
| 1:A:390:ARG:HG3  | 1:A:390:ARG:HH11 | 1.83                     | 0.44              |
| 2:B:6:HIS:HB3    | 2:B:65:ALA:CB    | 2.48                     | 0.44              |
| 2:B:6:HIS:HB3    | 2:B:21:TRP:HZ2   | 1.81                     | 0.44              |
| 2:B:98:GLY:C     | 2:B:100:GLY:H    | 2.24                     | 0.44              |
| 2:B:168:THR:CG2  | 2:B:201:THR:HG23 | 2.48                     | 0.44              |
| 2:B:352:LYS:HD3  | 2:B:352:LYS:C    | 2.43                     | 0.44              |
| 1:A:229:ARG:NH1  | 1:A:229:ARG:HG2  | 2.31                     | 0.43              |
| 1:A:291:ILE:HD12 | 1:A:375:VAL:HG23 | 1.99                     | 0.43              |
| 1:A:402:ARG:CG   | 3:K:279:ASN:OD1  | 2.60                     | 0.43              |
| 2:B:24:ILE:CG2   | 2:B:25:SER:N     | 2.80                     | 0.43              |
| 2:B:70:LEU:HB2   | 2:B:99:ALA:CB    | 2.48                     | 0.43              |
| 2:B:105:LYS:HG2  | 2:B:110:GLU:CG   | 2.49                     | 0.43              |
| 2:B:167:ASN:HA   | 2:B:200:GLU:O    | 2.17                     | 0.43              |
| 1:A:172:TYR:CD1  | 1:A:173:PRO:N    | 2.80                     | 0.43              |
| 2:B:7:ILE:N      | 2:B:136:GLN:O    | 2.51                     | 0.43              |
| 2:B:240:THR:HG23 | 2:B:241:CYS:N    | 2.33                     | 0.43              |
| 2:B:269:MET:HB2  | 2:B:301:MET:HE3  | 2.00                     | 0.43              |
| 1:A:153:LEU:O    | 1:A:157:LEU:HG   | 2.18                     | 0.43              |
| 1:A:204:VAL:O    | 1:A:204:VAL:HG12 | 2.17                     | 0.43              |
| 1:A:295:CYS:HB3  | 1:A:377:MET:HG2  | 1.99                     | 0.43              |
| 1:A:301:GLN:O    | 1:A:302:MET:C    | 2.61                     | 0.43              |
| 1:A:343:PHE:HZ   | 1:A:351:PHE:CZ   | 2.36                     | 0.43              |
| 1:A:414:GLU:HG3  | 3:K:271:ASN:ND2  | 2.33                     | 0.43              |
| 2:B:37:HIS:O     | 2:B:38:GLY:C     | 2.61                     | 0.43              |
| 1:A:402:ARG:O    | 1:A:405:VAL:N    | 2.49                     | 0.43              |
| 2:B:68:VAL:HG11  | 2:B:153:LEU:HD21 | 2.00                     | 0.43              |
| 2:B:156:LYS:NZ   | 2:B:159:GLU:OE1  | 2.47                     | 0.43              |
| 2:B:161:TYR:CD1  | 2:B:161:TYR:N    | 2.86                     | 0.43              |
| 2:B:161:TYR:O    | 2:B:163:ASP:N    | 2.51                     | 0.43              |
| 2:B:330:GLU:O    | 2:B:331:GLN:C    | 2.61                     | 0.43              |
| 2:B:399:PHE:O    | 2:B:402:LYS:N    | 2.29                     | 0.43              |
| 3:K:69:PRO:CD    | 3:K:72:THR:OG1   | 2.62                     | 0.43              |
| 3:K:223:ILE:HD11 | 3:K:298:MET:HG3  | 2.00                     | 0.43              |
| 1:A:115:ILE:CG1  | 1:A:152:LEU:HD13 | 2.46                     | 0.43              |
| 1:A:121:ARG:NH1  | 1:A:121:ARG:HG2  | 2.33                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:182:VAL:O    | 1:A:183:GLU:C    | 2.61                     | 0.43              |
| 1:A:287:SER:N    | 1:A:290:GLU:OE1  | 2.51                     | 0.43              |
| 2:B:242:LEU:HD22 | 2:B:250:ALA:O    | 2.17                     | 0.43              |
| 2:B:345:GLU:C    | 2:B:347:ILE:N    | 2.76                     | 0.43              |
| 1:A:63:PRO:HG2   | 1:A:91:GLN:OE1   | 2.17                     | 0.43              |
| 1:A:310:GLY:HA3  | 1:A:383:ALA:CA   | 2.49                     | 0.43              |
| 1:A:377:MET:O    | 1:A:377:MET:HG3  | 2.18                     | 0.43              |
| 2:B:192:HIS:NE2  | 2:B:420:GLU:HG2  | 2.34                     | 0.43              |
| 2:B:236:SER:HB2  | 7:B:902:TA1:H401 | 2.01                     | 0.43              |
| 3:K:26:LYS:HE2   | 3:K:311:ARG:HG2  | 1.99                     | 0.43              |
| 1:A:104:ALA:HB3  | 1:A:408:TYR:HD1  | 1.84                     | 0.43              |
| 1:A:121:ARG:HG2  | 1:A:121:ARG:HH11 | 1.83                     | 0.43              |
| 1:A:209:ILE:CD1  | 1:A:231:ILE:HD11 | 2.47                     | 0.43              |
| 2:B:103:TRP:HB2  | 2:B:186:ASN:HA   | 2.01                     | 0.43              |
| 2:B:402:LYS:O    | 2:B:403:ALA:C    | 2.61                     | 0.43              |
| 1:A:16:ILE:CG2   | 1:A:17:GLY:N     | 2.82                     | 0.43              |
| 1:A:140:SER:O    | 1:A:141:PHE:C    | 2.62                     | 0.43              |
| 1:A:268:PRO:C    | 1:A:269:LEU:HD23 | 2.44                     | 0.43              |
| 1:A:304:LYS:O    | 1:A:304:LYS:HG3  | 2.19                     | 0.43              |
| 2:B:72:PRO:HG2   | 2:B:73:GLY:H     | 1.83                     | 0.43              |
| 2:B:390:ARG:O    | 2:B:391:ILE:C    | 2.61                     | 0.43              |
| 2:B:409:THR:O    | 2:B:412:GLY:N    | 2.48                     | 0.43              |
| 1:A:4:CYS:SG     | 1:A:252:LEU:CD1  | 3.02                     | 0.43              |
| 1:A:8:HIS:CD2    | 1:A:138:PHE:CD2  | 3.07                     | 0.43              |
| 1:A:278:ALA:CA   | 1:A:282:TYR:OH   | 2.65                     | 0.43              |
| 2:B:94:PHE:CD1   | 2:B:94:PHE:N     | 2.84                     | 0.43              |
| 2:B:306:ASP:HA   | 2:B:307:PRO:HD3  | 1.91                     | 0.43              |
| 1:A:132:LEU:H    | 1:A:132:LEU:CD2  | 2.23                     | 0.42              |
| 1:A:409:VAL:HG11 | 3:K:272:LYS:CA   | 2.49                     | 0.42              |
| 3:K:340:SER:HA   | 3:K:341:CYS:HA   | 1.66                     | 0.42              |
| 1:A:104:ALA:HB1  | 1:A:413:MET:HG3  | 1.95                     | 0.42              |
| 1:A:147:SER:HB2  | 1:A:186:ASN:O    | 2.19                     | 0.42              |
| 1:A:209:ILE:CD1  | 1:A:231:ILE:CD1  | 2.97                     | 0.42              |
| 1:A:363:VAL:CG1  | 1:A:364:PRO:HD2  | 2.48                     | 0.42              |
| 1:A:411:GLU:CA   | 3:K:268:LYS:HE2  | 2.41                     | 0.42              |
| 1:A:72:PRO:HG2   | 1:A:73:THR:H     | 1.83                     | 0.42              |
| 1:A:265:GLY:O    | 1:A:266:HIS:C    | 2.63                     | 0.42              |
| 1:A:413:MET:O    | 3:K:271:ASN:ND2  | 2.52                     | 0.42              |
| 2:B:12:CYS:O     | 2:B:13:GLY:C     | 2.59                     | 0.42              |
| 2:B:141:LEU:N    | 2:B:141:LEU:HD12 | 2.32                     | 0.42              |
| 2:B:250:ALA:CB   | 2:B:254:LYS:HE2  | 2.49                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:435:TYR:C    | 2:B:437:ASP:H    | 2.27                     | 0.42              |
| 2:B:115:VAL:HG21 | 2:B:152:LEU:HD21 | 1.98                     | 0.42              |
| 2:B:261:PRO:HB2  | 2:B:262:PHE:CD2  | 2.54                     | 0.42              |
| 2:B:272:PHE:CE1  | 7:B:902:TA1:H391 | 2.54                     | 0.42              |
| 3:K:22:ARG:HH11  | 3:K:88:ASP:CB    | 2.28                     | 0.42              |
| 1:A:224:TYR:OH   | 5:A:502:GTP:H2'  | 2.18                     | 0.42              |
| 1:A:238:ILE:HD11 | 1:A:378:LEU:HD23 | 2.01                     | 0.42              |
| 2:B:333:LEU:HD11 | 2:B:337:ASN:HD21 | 1.85                     | 0.42              |
| 2:B:387:LEU:O    | 2:B:387:LEU:HG   | 2.15                     | 0.42              |
| 1:A:378:LEU:HD12 | 1:A:378:LEU:O    | 2.19                     | 0.42              |
| 2:B:48:ARG:HG2   | 2:B:243:ARG:HB3  | 2.01                     | 0.42              |
| 2:B:165:ILE:H    | 2:B:165:ILE:CD1  | 2.31                     | 0.42              |
| 2:B:175:PRO:O    | 2:B:177:VAL:N    | 2.53                     | 0.42              |
| 2:B:297:ASP:CG   | 2:B:299:LYS:HE2  | 2.45                     | 0.42              |
| 2:B:343:PHE:CD1  | 2:B:350:ASN:ND2  | 2.88                     | 0.42              |
| 1:A:213:CYS:O    | 1:A:219:ILE:HG13 | 2.20                     | 0.42              |
| 1:A:238:ILE:O    | 1:A:242:LEU:CB   | 2.67                     | 0.42              |
| 3:K:54:THR:HG23  | 3:K:62:TYR:O     | 2.20                     | 0.42              |
| 2:B:178:SER:C    | 2:B:180:THR:H    | 2.26                     | 0.42              |
| 2:B:204:ILE:HD13 | 2:B:231:VAL:CG2  | 2.45                     | 0.42              |
| 2:B:210:TYR:O    | 2:B:214:PHE:N    | 2.52                     | 0.42              |
| 2:B:301:MET:C    | 2:B:303:ALA:N    | 2.77                     | 0.42              |
| 1:A:25:CYS:SG    | 1:A:26:LEU:N     | 2.92                     | 0.42              |
| 1:A:409:VAL:HG13 | 3:K:271:ASN:HB3  | 2.02                     | 0.42              |
| 2:B:118:VAL:O    | 2:B:122:VAL:HG13 | 2.19                     | 0.42              |
| 2:B:273:ALA:HB1  | 2:B:291:LEU:HG   | 2.02                     | 0.42              |
| 2:B:307:PRO:O    | 2:B:309:HIS:N    | 2.53                     | 0.42              |
| 3:K:26:LYS:HE3   | 3:K:313:THR:OG1  | 2.19                     | 0.42              |
| 1:A:161:TYR:C    | 1:A:163:LYS:N    | 2.77                     | 0.42              |
| 1:A:255:PHE:O    | 1:A:259:LEU:N    | 2.50                     | 0.42              |
| 1:A:363:VAL:HG13 | 1:A:364:PRO:HD2  | 2.02                     | 0.42              |
| 1:A:398:MET:HE3  | 1:A:398:MET:HB2  | 1.78                     | 0.42              |
| 2:B:19:LYS:HG3   | 2:B:228:ASN:HB2  | 2.01                     | 0.42              |
| 2:B:202:TYR:CE2  | 2:B:268:PHE:HD2  | 2.38                     | 0.42              |
| 3:K:254:VAL:CG2  | 3:K:267:ALA:CB   | 2.89                     | 0.42              |
| 1:A:24:TYR:O     | 1:A:25:CYS:C     | 2.63                     | 0.41              |
| 1:A:173:PRO:HG3  | 1:A:183:GLU:CD   | 2.45                     | 0.41              |
| 1:A:223:THR:CG2  | 2:B:247:GLN:NE2  | 2.83                     | 0.41              |
| 1:A:383:ALA:C    | 1:A:385:ALA:N    | 2.78                     | 0.41              |
| 2:B:121:VAL:C    | 2:B:123:ARG:N    | 2.77                     | 0.41              |
| 2:B:431:GLU:O    | 2:B:434:GLN:N    | 2.48                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:99:ALA:HB1   | 5:A:502:GTP:O2G  | 2.20                     | 0.41              |
| 1:A:175:PRO:HG3  | 1:A:304:LYS:CB   | 2.50                     | 0.41              |
| 1:A:243:ARG:NH2  | 1:A:252:LEU:HG   | 2.35                     | 0.41              |
| 1:A:318:LEU:HB2  | 1:A:376:CYS:SG   | 2.61                     | 0.41              |
| 1:A:335:ILE:C    | 1:A:337:THR:H    | 2.28                     | 0.41              |
| 1:A:362:VAL:HG13 | 1:A:368:LEU:CB   | 2.50                     | 0.41              |
| 2:B:417:GLU:O    | 2:B:420:GLU:HB3  | 2.21                     | 0.41              |
| 1:A:242:LEU:HD11 | 1:A:250:VAL:HG23 | 2.02                     | 0.41              |
| 1:A:262:TYR:HB3  | 1:A:263:PRO:HD2  | 2.00                     | 0.41              |
| 1:A:332:ILE:CD1  | 1:A:353:VAL:HG22 | 2.51                     | 0.41              |
| 2:B:98:GLY:O     | 2:B:100:GLY:N    | 2.49                     | 0.41              |
| 2:B:118:VAL:O    | 2:B:121:VAL:N    | 2.54                     | 0.41              |
| 2:B:153:LEU:HD13 | 2:B:153:LEU:N    | 2.34                     | 0.41              |
| 2:B:389:LYS:O    | 2:B:390:ARG:C    | 2.62                     | 0.41              |
| 1:A:108:TYR:OH   | 3:K:253:LYS:HE3  | 2.20                     | 0.41              |
| 1:A:119:LEU:HD11 | 1:A:156:ARG:HD3  | 2.01                     | 0.41              |
| 1:A:166:LYS:HB2  | 1:A:199:ASP:OD1  | 2.20                     | 0.41              |
| 1:A:244:PHE:HD1  | 1:A:244:PHE:C    | 2.24                     | 0.41              |
| 1:A:386:GLU:O    | 1:A:387:ALA:C    | 2.63                     | 0.41              |
| 1:A:394:LYS:HG2  | 2:B:348:PRO:CB   | 2.51                     | 0.41              |
| 2:B:106:GLY:O    | 2:B:149:MET:CA   | 2.68                     | 0.41              |
| 2:B:138:THR:O    | 2:B:139:HIS:HB3  | 2.20                     | 0.41              |
| 3:K:46:ILE:N     | 3:K:47:PRO:HD3   | 2.35                     | 0.41              |
| 1:A:13:GLY:HA2   | 1:A:16:ILE:CG2   | 2.50                     | 0.41              |
| 1:A:23:LEU:HD11  | 1:A:361:THR:O    | 2.21                     | 0.41              |
| 1:A:67:PHE:CE2   | 1:A:87:PHE:CE2   | 3.08                     | 0.41              |
| 1:A:98:ASP:HB3   | 2:B:253:ARG:HD2  | 2.03                     | 0.41              |
| 1:A:273:ALA:HB2  | 1:A:375:VAL:HB   | 2.03                     | 0.41              |
| 2:B:25:SER:O     | 2:B:28:HIS:N     | 2.53                     | 0.41              |
| 2:B:143:GLY:O    | 2:B:147:SER:OG   | 2.38                     | 0.41              |
| 1:A:105:ARG:O    | 1:A:110:ILE:CG2  | 2.65                     | 0.41              |
| 1:A:132:LEU:HD23 | 1:A:132:LEU:N    | 2.25                     | 0.41              |
| 1:A:255:PHE:O    | 1:A:257:THR:N    | 2.53                     | 0.41              |
| 2:B:102:ASN:ND2  | 2:B:408:TYR:HA   | 2.20                     | 0.41              |
| 2:B:399:PHE:O    | 2:B:401:ARG:N    | 2.53                     | 0.41              |
| 3:K:85:ILE:HG23  | 3:K:95:GLY:HA3   | 2.03                     | 0.41              |
| 3:K:259:ALA:CB   | 3:K:263:VAL:HG12 | 2.50                     | 0.41              |
| 1:A:76:ASP:O     | 1:A:80:THR:N     | 2.53                     | 0.41              |
| 1:A:305:CYS:SG   | 1:A:383:ALA:HB1  | 2.60                     | 0.41              |
| 1:A:355:ILE:HD13 | 1:A:355:ILE:HG21 | 1.90                     | 0.41              |
| 1:A:399:TYR:C    | 1:A:401:LYS:N    | 2.77                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:414:GLU:C    | 1:A:416:GLY:N    | 2.74                     | 0.41              |
| 2:B:11:GLN:O     | 2:B:15:GLN:N     | 2.41                     | 0.41              |
| 2:B:48:ARG:CG    | 2:B:243:ARG:O    | 2.67                     | 0.41              |
| 2:B:118:VAL:O    | 2:B:119:LEU:C    | 2.62                     | 0.41              |
| 2:B:238:VAL:HB   | 2:B:239:THR:H    | 1.65                     | 0.41              |
| 2:B:242:LEU:HB3  | 2:B:250:ALA:O    | 2.20                     | 0.41              |
| 3:K:50:LYS:HB2   | 3:K:54:THR:HB    | 2.02                     | 0.41              |
| 3:K:284:LEU:CG   | 3:K:291:VAL:HG11 | 2.51                     | 0.41              |
| 1:A:428:LEU:HD12 | 1:A:428:LEU:HA   | 1.79                     | 0.41              |
| 2:B:20:PHE:CD1   | 2:B:235:MET:CG   | 3.04                     | 0.41              |
| 2:B:82:PRO:HB2   | 2:B:83:PHE:H     | 1.55                     | 0.41              |
| 2:B:135:PHE:CD1  | 2:B:166:MET:SD   | 3.14                     | 0.41              |
| 2:B:182:VAL:O    | 2:B:184:PRO:N    | 2.54                     | 0.41              |
| 2:B:259:MET:HE3  | 2:B:268:PHE:CZ   | 2.56                     | 0.41              |
| 3:K:319:SER:HB3  | 3:K:324:ASN:HB2  | 2.02                     | 0.41              |
| 1:A:30:ILE:O     | 1:A:30:ILE:HG22  | 2.21                     | 0.41              |
| 1:A:67:PHE:HB2   | 1:A:92:LEU:HD23  | 2.02                     | 0.41              |
| 1:A:100:ALA:O    | 1:A:102:ASN:N    | 2.49                     | 0.41              |
| 1:A:115:ILE:CG2  | 1:A:116:ASP:H    | 2.32                     | 0.41              |
| 1:A:161:TYR:O    | 1:A:162:GLY:C    | 2.64                     | 0.41              |
| 1:A:207:GLU:C    | 1:A:209:ILE:H    | 2.29                     | 0.41              |
| 1:A:401:LYS:O    | 1:A:402:ARG:HB2  | 2.21                     | 0.41              |
| 1:A:412:GLY:CA   | 3:K:254:VAL:CG1  | 2.96                     | 0.41              |
| 2:B:70:LEU:HB2   | 2:B:99:ALA:HB2   | 2.03                     | 0.41              |
| 2:B:105:LYS:HG2  | 2:B:110:GLU:HG3  | 2.03                     | 0.41              |
| 2:B:119:LEU:O    | 2:B:122:VAL:HG22 | 2.21                     | 0.41              |
| 3:K:122:GLY:O    | 3:K:126:ARG:HD2  | 2.21                     | 0.41              |
| 3:K:221:HIS:HD2  | 3:K:248:LEU:HA   | 1.86                     | 0.41              |
| 1:A:147:SER:OG   | 1:A:148:GLY:N    | 2.54                     | 0.41              |
| 1:A:179:THR:HG23 | 2:B:353:THR:O    | 2.20                     | 0.41              |
| 1:A:217:LEU:HD12 | 1:A:277:SER:CB   | 2.49                     | 0.41              |
| 1:A:231:ILE:C    | 1:A:233:GLN:H    | 2.28                     | 0.41              |
| 1:A:272:TYR:O    | 1:A:300:ASN:ND2  | 2.54                     | 0.41              |
| 1:A:392:ASP:OD1  | 1:A:392:ASP:C    | 2.64                     | 0.41              |
| 2:B:114:LEU:HD12 | 2:B:117:SER:OG   | 2.21                     | 0.41              |
| 2:B:132:LEU:O    | 2:B:164:ARG:HD2  | 2.21                     | 0.41              |
| 2:B:171:VAL:HG12 | 2:B:171:VAL:O    | 2.20                     | 0.41              |
| 2:B:236:SER:CB   | 7:B:902:TA1:H401 | 2.51                     | 0.41              |
| 2:B:420:GLU:HA   | 3:K:173:GLU:OE2  | 2.21                     | 0.41              |
| 1:A:149:PHE:CD1  | 1:A:150:THR:N    | 2.89                     | 0.40              |
| 1:A:273:ALA:O    | 1:A:275:VAL:N    | 2.54                     | 0.40              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:B:11:GLN:HA   | 2:B:74:THR:HG21  | 2.03                     | 0.40              |
| 2:B:52:TYR:C    | 2:B:53:TYR:CD1   | 2.99                     | 0.40              |
| 2:B:168:THR:HB  | 2:B:198:THR:HG21 | 2.03                     | 0.40              |
| 2:B:288:VAL:O   | 2:B:289:PRO:C    | 2.64                     | 0.40              |
| 3:K:22:ARG:NH1  | 3:K:88:ASP:HB3   | 2.36                     | 0.40              |
| 3:K:135:ILE:O   | 3:K:136:TYR:HB3  | 2.21                     | 0.40              |
| 1:A:119:LEU:O   | 1:A:122:ILE:N    | 2.55                     | 0.40              |
| 1:A:286:LEU:HG  | 1:A:290:GLU:CB   | 2.52                     | 0.40              |
| 1:A:384:ILE:C   | 1:A:386:GLU:N    | 2.72                     | 0.40              |
| 2:B:311:ARG:HG2 | 2:B:311:ARG:NH1  | 2.34                     | 0.40              |
| 1:A:76:ASP:O    | 1:A:79:ARG:N     | 2.52                     | 0.40              |
| 1:A:184:PRO:O   | 1:A:185:TYR:C    | 2.62                     | 0.40              |
| 2:B:103:TRP:HD1 | 2:B:147:SER:OG   | 2.04                     | 0.40              |
| 2:B:359:PRO:CB  | 2:B:360:PRO:HD2  | 2.45                     | 0.40              |
| 2:B:427:ASP:CB  | 3:K:294:ARG:NH1  | 2.84                     | 0.40              |
| 1:A:100:ALA:HB2 | 1:A:105:ARG:HD3  | 2.03                     | 0.40              |
| 1:A:289:ALA:HB3 | 1:A:290:GLU:OE2  | 2.21                     | 0.40              |
| 2:B:12:CYS:O    | 2:B:14:ASN:N     | 2.55                     | 0.40              |
| 2:B:150:GLY:HA2 | 2:B:153:LEU:CD2  | 2.41                     | 0.40              |
| 2:B:185:TYR:HD1 | 2:B:185:TYR:HA   | 1.76                     | 0.40              |
| 2:B:422:GLU:O   | 2:B:423:SER:C    | 2.64                     | 0.40              |
| 2:B:427:ASP:OD1 | 3:K:294:ARG:CD   | 2.69                     | 0.40              |
| 1:A:95:GLY:O    | 1:A:96:LYS:C     | 2.64                     | 0.40              |
| 2:B:26:ASP:C    | 2:B:26:ASP:OD1   | 2.64                     | 0.40              |
| 2:B:175:PRO:HG2 | 2:B:207:GLU:CD   | 2.47                     | 0.40              |
| 2:B:385:GLN:OE1 | 2:B:433:GLN:HB2  | 2.22                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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     | 408/451 (90%)   | 265 (65%) | 84 (21%)  | 59 (14%)  | 0           | 3  |
| 2   | B     | 424/445 (95%)   | 273 (64%) | 95 (22%)  | 56 (13%)  | 0           | 4  |
| 3   | K     | 318/371 (86%)   | 287 (90%) | 25 (8%)   | 6 (2%)    | 6           | 32 |
| All | All   | 1150/1267 (91%) | 825 (72%) | 204 (18%) | 121 (10%) | 1           | 6  |

All (121) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 96  | LYS  |
| 1   | A     | 97  | GLU  |
| 1   | A     | 108 | TYR  |
| 1   | A     | 109 | THR  |
| 1   | A     | 141 | PHE  |
| 1   | A     | 183 | GLU  |
| 1   | A     | 217 | LEU  |
| 1   | A     | 240 | ALA  |
| 1   | A     | 249 | ASN  |
| 1   | A     | 255 | PHE  |
| 1   | A     | 266 | HIS  |
| 1   | A     | 280 | LYS  |
| 1   | A     | 284 | GLU  |
| 1   | A     | 285 | GLN  |
| 1   | A     | 289 | ALA  |
| 1   | A     | 309 | HIS  |
| 1   | A     | 346 | TRP  |
| 1   | A     | 370 | LYS  |
| 1   | A     | 387 | ALA  |
| 1   | A     | 403 | ALA  |
| 1   | A     | 437 | VAL  |
| 2   | B     | 23  | VAL  |
| 2   | B     | 24  | ILE  |
| 2   | B     | 32  | PRO  |
| 2   | B     | 50  | ASN  |
| 2   | B     | 82  | PRO  |
| 2   | B     | 97  | SER  |
| 2   | B     | 128 | SER  |
| 2   | B     | 176 | LYS  |
| 2   | B     | 183 | GLU  |
| 2   | B     | 218 | LYS  |
| 2   | B     | 238 | VAL  |
| 2   | B     | 239 | THR  |
| 2   | B     | 240 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 252 | LEU  |
| 2   | B     | 263 | PRO  |
| 2   | B     | 266 | HIS  |
| 2   | B     | 273 | ALA  |
| 2   | B     | 278 | ARG  |
| 2   | B     | 280 | SER  |
| 2   | B     | 281 | GLN  |
| 2   | B     | 282 | GLN  |
| 2   | B     | 288 | VAL  |
| 2   | B     | 294 | GLN  |
| 2   | B     | 295 | MET  |
| 2   | B     | 343 | PHE  |
| 2   | B     | 344 | VAL  |
| 2   | B     | 346 | TRP  |
| 2   | B     | 369 | ARG  |
| 2   | B     | 403 | ALA  |
| 3   | K     | 321 | SER  |
| 1   | A     | 24  | TYR  |
| 1   | A     | 63  | PRO  |
| 1   | A     | 103 | TYR  |
| 1   | A     | 111 | GLY  |
| 1   | A     | 131 | GLY  |
| 1   | A     | 218 | ASP  |
| 1   | A     | 219 | ILE  |
| 1   | A     | 238 | ILE  |
| 1   | A     | 265 | GLY  |
| 1   | A     | 287 | SER  |
| 1   | A     | 314 | ALA  |
| 1   | A     | 339 | ARG  |
| 1   | A     | 342 | GLN  |
| 1   | A     | 373 | ARG  |
| 1   | A     | 386 | GLU  |
| 2   | B     | 38  | GLY  |
| 2   | B     | 73  | GLY  |
| 2   | B     | 175 | PRO  |
| 2   | B     | 265 | LEU  |
| 2   | B     | 279 | GLY  |
| 2   | B     | 298 | ALA  |
| 2   | B     | 300 | ASN  |
| 2   | B     | 311 | ARG  |
| 3   | K     | 39  | ILE  |
| 3   | K     | 63  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | K     | 115 | LEU  |
| 1   | A     | 104 | ALA  |
| 1   | A     | 148 | GLY  |
| 1   | A     | 149 | PHE  |
| 1   | A     | 173 | PRO  |
| 1   | A     | 239 | THR  |
| 1   | A     | 245 | ASP  |
| 1   | A     | 263 | PRO  |
| 1   | A     | 279 | GLU  |
| 1   | A     | 288 | VAL  |
| 1   | A     | 330 | ALA  |
| 1   | A     | 336 | LYS  |
| 1   | A     | 369 | ALA  |
| 2   | B     | 34  | GLY  |
| 2   | B     | 83  | PHE  |
| 2   | B     | 99  | ALA  |
| 2   | B     | 100 | GLY  |
| 2   | B     | 302 | MET  |
| 2   | B     | 386 | GLU  |
| 3   | K     | 220 | SER  |
| 1   | A     | 89  | PRO  |
| 1   | A     | 129 | CYS  |
| 1   | A     | 300 | ASN  |
| 1   | A     | 348 | PRO  |
| 2   | B     | 96  | GLN  |
| 2   | B     | 395 | PHE  |
| 3   | K     | 49  | PHE  |
| 1   | A     | 256 | GLN  |
| 1   | A     | 303 | VAL  |
| 1   | A     | 307 | PRO  |
| 1   | A     | 382 | THR  |
| 2   | B     | 57  | ALA  |
| 2   | B     | 74  | THR  |
| 2   | B     | 285 | ALA  |
| 2   | B     | 424 | ASN  |
| 1   | A     | 31  | GLN  |
| 1   | A     | 273 | ALA  |
| 2   | B     | 51  | VAL  |
| 2   | B     | 58  | GLY  |
| 2   | B     | 145 | THR  |
| 2   | B     | 162 | PRO  |
| 2   | B     | 400 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 195 | VAL  |
| 1   | A     | 115 | ILE  |
| 2   | B     | 72  | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers  | Percentiles |    |
|-----|-------|----------------|-----------|-----------|-------------|----|
| 1   | A     | 347/377 (92%)  | 294 (85%) | 53 (15%)  | 3           | 12 |
| 2   | B     | 367/381 (96%)  | 307 (84%) | 60 (16%)  | 2           | 10 |
| 3   | K     | 280/330 (85%)  | 265 (95%) | 15 (5%)   | 20          | 41 |
| All | All   | 994/1088 (91%) | 866 (87%) | 128 (13%) | 6           | 15 |

All (128) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 6   | SER  |
| 1   | A     | 7   | ILE  |
| 1   | A     | 16  | ILE  |
| 1   | A     | 20  | CYS  |
| 1   | A     | 32  | PRO  |
| 1   | A     | 76  | ASP  |
| 1   | A     | 82  | THR  |
| 1   | A     | 98  | ASP  |
| 1   | A     | 109 | THR  |
| 1   | A     | 115 | ILE  |
| 1   | A     | 120 | ASP  |
| 1   | A     | 125 | LEU  |
| 1   | A     | 130 | THR  |
| 1   | A     | 135 | PHE  |
| 1   | A     | 141 | PHE  |
| 1   | A     | 150 | THR  |
| 1   | A     | 152 | LEU  |
| 1   | A     | 154 | MET  |
| 1   | A     | 155 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 172 | TYR  |
| 1   | A     | 173 | PRO  |
| 1   | A     | 183 | GLU  |
| 1   | A     | 192 | HIS  |
| 1   | A     | 204 | VAL  |
| 1   | A     | 219 | ILE  |
| 1   | A     | 224 | TYR  |
| 1   | A     | 231 | ILE  |
| 1   | A     | 234 | ILE  |
| 1   | A     | 243 | ARG  |
| 1   | A     | 244 | PHE  |
| 1   | A     | 253 | THR  |
| 1   | A     | 260 | VAL  |
| 1   | A     | 267 | PHE  |
| 1   | A     | 269 | LEU  |
| 1   | A     | 276 | ILE  |
| 1   | A     | 279 | GLU  |
| 1   | A     | 284 | GLU  |
| 1   | A     | 303 | VAL  |
| 1   | A     | 325 | PRO  |
| 1   | A     | 328 | VAL  |
| 1   | A     | 334 | THR  |
| 1   | A     | 345 | ASP  |
| 1   | A     | 352 | LYS  |
| 1   | A     | 368 | LEU  |
| 1   | A     | 376 | CYS  |
| 1   | A     | 377 | MET  |
| 1   | A     | 378 | LEU  |
| 1   | A     | 415 | GLU  |
| 1   | A     | 417 | GLU  |
| 1   | A     | 420 | GLU  |
| 1   | A     | 431 | ASP  |
| 1   | A     | 432 | TYR  |
| 1   | A     | 433 | GLU  |
| 2   | B     | 24  | ILE  |
| 2   | B     | 26  | ASP  |
| 2   | B     | 32  | PRO  |
| 2   | B     | 41  | ASP  |
| 2   | B     | 67  | LEU  |
| 2   | B     | 68  | VAL  |
| 2   | B     | 90  | ASP  |
| 2   | B     | 94  | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 121 | VAL  |
| 2   | B     | 122 | VAL  |
| 2   | B     | 129 | CYS  |
| 2   | B     | 135 | PHE  |
| 2   | B     | 141 | LEU  |
| 2   | B     | 145 | THR  |
| 2   | B     | 149 | MET  |
| 2   | B     | 151 | THR  |
| 2   | B     | 153 | LEU  |
| 2   | B     | 161 | TYR  |
| 2   | B     | 163 | ASP  |
| 2   | B     | 165 | ILE  |
| 2   | B     | 174 | SER  |
| 2   | B     | 193 | GLN  |
| 2   | B     | 198 | THR  |
| 2   | B     | 201 | THR  |
| 2   | B     | 203 | CYS  |
| 2   | B     | 207 | GLU  |
| 2   | B     | 211 | ASP  |
| 2   | B     | 214 | PHE  |
| 2   | B     | 227 | LEU  |
| 2   | B     | 229 | HIS  |
| 2   | B     | 230 | LEU  |
| 2   | B     | 232 | SER  |
| 2   | B     | 236 | SER  |
| 2   | B     | 240 | THR  |
| 2   | B     | 265 | LEU  |
| 2   | B     | 267 | PHE  |
| 2   | B     | 275 | LEU  |
| 2   | B     | 282 | GLN  |
| 2   | B     | 284 | ARG  |
| 2   | B     | 299 | LYS  |
| 2   | B     | 306 | ASP  |
| 2   | B     | 309 | HIS  |
| 2   | B     | 314 | THR  |
| 2   | B     | 322 | ARG  |
| 2   | B     | 324 | SER  |
| 2   | B     | 325 | MET  |
| 2   | B     | 331 | GLN  |
| 2   | B     | 343 | PHE  |
| 2   | B     | 344 | VAL  |
| 2   | B     | 352 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 353 | THR  |
| 2   | B     | 369 | ARG  |
| 2   | B     | 387 | LEU  |
| 2   | B     | 413 | MET  |
| 2   | B     | 414 | ASP  |
| 2   | B     | 424 | ASN  |
| 2   | B     | 427 | ASP  |
| 2   | B     | 431 | GLU  |
| 2   | B     | 432 | TYR  |
| 2   | B     | 437 | ASP  |
| 3   | K     | 36  | GLU  |
| 3   | K     | 52  | GLU  |
| 3   | K     | 91  | GLU  |
| 3   | K     | 103 | THR  |
| 3   | K     | 114 | LYS  |
| 3   | K     | 135 | ILE  |
| 3   | K     | 140 | GLU  |
| 3   | K     | 162 | LEU  |
| 3   | K     | 222 | SER  |
| 3   | K     | 225 | LEU  |
| 3   | K     | 242 | LYS  |
| 3   | K     | 243 | LEU  |
| 3   | K     | 254 | VAL  |
| 3   | K     | 289 | THR  |
| 3   | K     | 325 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 11  | GLN  |
| 1   | A     | 15  | GLN  |
| 1   | A     | 28  | HIS  |
| 1   | A     | 128 | GLN  |
| 1   | A     | 133 | GLN  |
| 1   | A     | 139 | HIS  |
| 1   | A     | 176 | GLN  |
| 1   | A     | 197 | HIS  |
| 1   | A     | 216 | ASN  |
| 1   | A     | 226 | ASN  |
| 1   | A     | 256 | GLN  |
| 1   | A     | 309 | HIS  |
| 2   | B     | 43  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 91  | ASN  |
| 2   | B     | 101 | ASN  |
| 2   | B     | 102 | ASN  |
| 2   | B     | 133 | GLN  |
| 2   | B     | 136 | GLN  |
| 2   | B     | 139 | HIS  |
| 2   | B     | 186 | ASN  |
| 2   | B     | 249 | ASN  |
| 2   | B     | 266 | HIS  |
| 2   | B     | 282 | GLN  |
| 2   | B     | 331 | GLN  |
| 2   | B     | 334 | ASN  |
| 2   | B     | 336 | GLN  |
| 2   | B     | 337 | ASN  |
| 2   | B     | 380 | ASN  |
| 2   | B     | 385 | GLN  |
| 2   | B     | 406 | HIS  |
| 2   | B     | 436 | GLN  |
| 3   | K     | 24  | ASN  |
| 3   | K     | 79  | ASN  |
| 3   | K     | 134 | HIS  |
| 3   | K     | 216 | HIS  |
| 3   | K     | 221 | HIS  |
| 3   | K     | 232 | ASN  |

### 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, 1 is monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 7   | TA1  | B     | 902 | -    | 68,68,68     | 2.21 | 26 (38%)    | 105,105,105 | 1.50 | 14 (13%)    |
| 6   | GDP  | B     | 901 | -    | 29,30,30     | 2.87 | 11 (37%)    | 45,47,47    | 3.48 | 16 (35%)    |
| 5   | GTP  | A     | 502 | 4    | 33,34,34     | 1.87 | 3 (9%)      | 50,54,54    | 0.91 | 3 (6%)      |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions     | Rings   |
|-----|------|-------|-----|------|---------|--------------|---------|
| 7   | TA1  | B     | 902 | -    | -       | 9/41/127/127 | 0/7/7/7 |
| 6   | GDP  | B     | 901 | -    | -       | 4/16/32/32   | 0/3/3/3 |
| 5   | GTP  | A     | 502 | 4    | -       | 4/22/38/38   | 0/3/3/3 |

All (40) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | B     | 901 | GDP  | PA-O3A  | 7.65  | 1.67        | 1.59     |
| 7   | B     | 902 | TA1  | C06-C05 | 6.53  | 1.50        | 1.38     |
| 6   | B     | 901 | GDP  | O6-C6   | 5.92  | 1.34        | 1.23     |
| 5   | A     | 502 | GTP  | PA-O3A  | -5.91 | 1.53        | 1.59     |
| 6   | B     | 901 | GDP  | C8-N9   | 5.86  | 1.50        | 1.37     |
| 7   | B     | 902 | TA1  | C08-C07 | -5.68 | 1.25        | 1.38     |
| 5   | A     | 502 | GTP  | PB-O3A  | -5.67 | 1.53        | 1.59     |
| 5   | A     | 502 | GTP  | PB-O3B  | 5.38  | 1.65        | 1.59     |
| 7   | B     | 902 | TA1  | C18-C10 | 5.35  | 1.69        | 1.57     |
| 7   | B     | 902 | TA1  | C05-C04 | 4.86  | 1.46        | 1.39     |
| 6   | B     | 901 | GDP  | C2-N1   | 4.81  | 1.49        | 1.37     |
| 7   | B     | 902 | TA1  | C45-C24 | 4.29  | 1.61        | 1.54     |
| 6   | B     | 901 | GDP  | PB-O2B  | -3.93 | 1.40        | 1.54     |
| 7   | B     | 902 | TA1  | C36-C31 | 3.71  | 1.45        | 1.39     |
| 7   | B     | 902 | TA1  | O02-C03 | 3.57  | 1.42        | 1.34     |
| 6   | B     | 901 | GDP  | O4'-C1' | 3.47  | 1.50        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 7   | B     | 902 | TA1  | C25-C24 | 3.41  | 1.39        | 1.34     |
| 7   | B     | 902 | TA1  | C43-C01 | 3.24  | 1.61        | 1.54     |
| 7   | B     | 902 | TA1  | C46-C45 | 3.24  | 1.60        | 1.53     |
| 6   | B     | 901 | GDP  | C8-N7   | 3.07  | 1.41        | 1.32     |
| 7   | B     | 902 | TA1  | C11-C10 | 3.05  | 1.61        | 1.54     |
| 7   | B     | 902 | TA1  | C43-C26 | 2.84  | 1.58        | 1.52     |
| 6   | B     | 901 | GDP  | C5-N7   | -2.84 | 1.33        | 1.39     |
| 6   | B     | 901 | GDP  | C5-C4   | 2.66  | 1.46        | 1.38     |
| 7   | B     | 902 | TA1  | C26-C25 | 2.60  | 1.56        | 1.51     |
| 7   | B     | 902 | TA1  | C01-C45 | 2.53  | 1.66        | 1.56     |
| 7   | B     | 902 | TA1  | C18-C20 | 2.52  | 1.62        | 1.55     |
| 7   | B     | 902 | TA1  | C04-C03 | -2.45 | 1.44        | 1.50     |
| 6   | B     | 901 | GDP  | C2-N3   | -2.44 | 1.27        | 1.33     |
| 6   | B     | 901 | GDP  | PB-O3B  | 2.44  | 1.63        | 1.54     |
| 7   | B     | 902 | TA1  | C41-C42 | 2.43  | 1.43        | 1.38     |
| 7   | B     | 902 | TA1  | C16-C15 | 2.32  | 1.56        | 1.52     |
| 7   | B     | 902 | TA1  | C08-C09 | 2.20  | 1.42        | 1.38     |
| 7   | B     | 902 | TA1  | O09-C21 | 2.17  | 1.49        | 1.44     |
| 7   | B     | 902 | TA1  | C10-C02 | 2.15  | 1.62        | 1.57     |
| 7   | B     | 902 | TA1  | C37-C29 | 2.13  | 1.54        | 1.52     |
| 7   | B     | 902 | TA1  | C34-C33 | 2.11  | 1.42        | 1.38     |
| 7   | B     | 902 | TA1  | C39-C38 | 2.10  | 1.42        | 1.38     |
| 7   | B     | 902 | TA1  | C33-C32 | 2.08  | 1.42        | 1.38     |
| 7   | B     | 902 | TA1  | O02-C02 | 2.02  | 1.48        | 1.45     |

All (33) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 6   | B     | 901 | GDP  | N9-C8-N7    | -10.76 | 93.44       | 113.40   |
| 6   | B     | 901 | GDP  | C8-N7-C5    | 9.23   | 120.71      | 104.26   |
| 6   | B     | 901 | GDP  | C6-C5-N7    | 8.58   | 145.91      | 130.29   |
| 6   | B     | 901 | GDP  | N2-C2-N3    | 6.34   | 132.04      | 119.67   |
| 6   | B     | 901 | GDP  | C6-C5-C4    | -6.16  | 109.56      | 118.83   |
| 6   | B     | 901 | GDP  | C8-N9-C4    | 5.86   | 117.01      | 106.03   |
| 7   | B     | 902 | TA1  | C06-C05-C04 | -5.84  | 114.63      | 120.36   |
| 7   | B     | 902 | TA1  | C07-C08-C09 | 5.76   | 127.34      | 120.24   |
| 6   | B     | 901 | GDP  | C5-C6-N1    | 4.51   | 124.74      | 113.25   |
| 6   | B     | 901 | GDP  | N2-C2-N1    | -4.29  | 107.71      | 116.76   |
| 6   | B     | 901 | GDP  | C2-N3-C4    | 4.13   | 119.41      | 112.30   |
| 7   | B     | 902 | TA1  | C05-C04-C03 | -4.05  | 111.46      | 120.40   |
| 6   | B     | 901 | GDP  | O6-C6-C5    | -3.94  | 116.14      | 126.53   |
| 6   | B     | 901 | GDP  | C4-C5-N7    | -3.88  | 104.52      | 110.67   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | B     | 901 | GDP  | C2-N1-C6    | -3.85 | 118.12      | 125.11   |
| 7   | B     | 902 | TA1  | C09-C04-C03 | 3.60  | 128.33      | 120.40   |
| 6   | B     | 901 | GDP  | C2'-C3'-C4' | 3.45  | 109.27      | 102.61   |
| 7   | B     | 902 | TA1  | C17-C18-C20 | 3.20  | 109.76      | 102.58   |
| 7   | B     | 902 | TA1  | O04-C11-C14 | -3.05 | 101.67      | 108.13   |
| 7   | B     | 902 | TA1  | C45-C01-C02 | 2.94  | 115.16      | 111.93   |
| 6   | B     | 901 | GDP  | C1'-N9-C8   | -2.65 | 119.20      | 126.73   |
| 5   | A     | 502 | GTP  | O2G-PG-O3B  | 2.63  | 113.46      | 104.64   |
| 7   | B     | 902 | TA1  | O01-C01-C43 | 2.47  | 113.36      | 107.04   |
| 7   | B     | 902 | TA1  | C08-C09-C04 | -2.44 | 117.97      | 120.36   |
| 6   | B     | 901 | GDP  | O2'-C2'-C3' | 2.30  | 119.19      | 111.82   |
| 7   | B     | 902 | TA1  | C14-C11-C15 | -2.27 | 83.04       | 85.38    |
| 7   | B     | 902 | TA1  | O06-C15-C11 | 2.25  | 93.04       | 90.58    |
| 7   | B     | 902 | TA1  | C10-C18-C17 | -2.23 | 102.32      | 106.55   |
| 5   | A     | 502 | GTP  | O5'-C5'-C4' | 2.11  | 116.18      | 108.99   |
| 6   | B     | 901 | GDP  | C4'-O4'-C1' | 2.07  | 114.05      | 109.47   |
| 7   | B     | 902 | TA1  | C21-O09-C22 | 2.04  | 120.17      | 115.95   |
| 5   | A     | 502 | GTP  | O3G-PG-O3B  | 2.02  | 111.42      | 104.64   |
| 7   | B     | 902 | TA1  | O04-C11-C10 | 2.00  | 112.35      | 109.24   |

There are no chirality outliers.

All (17) torsion outliers are listed below:

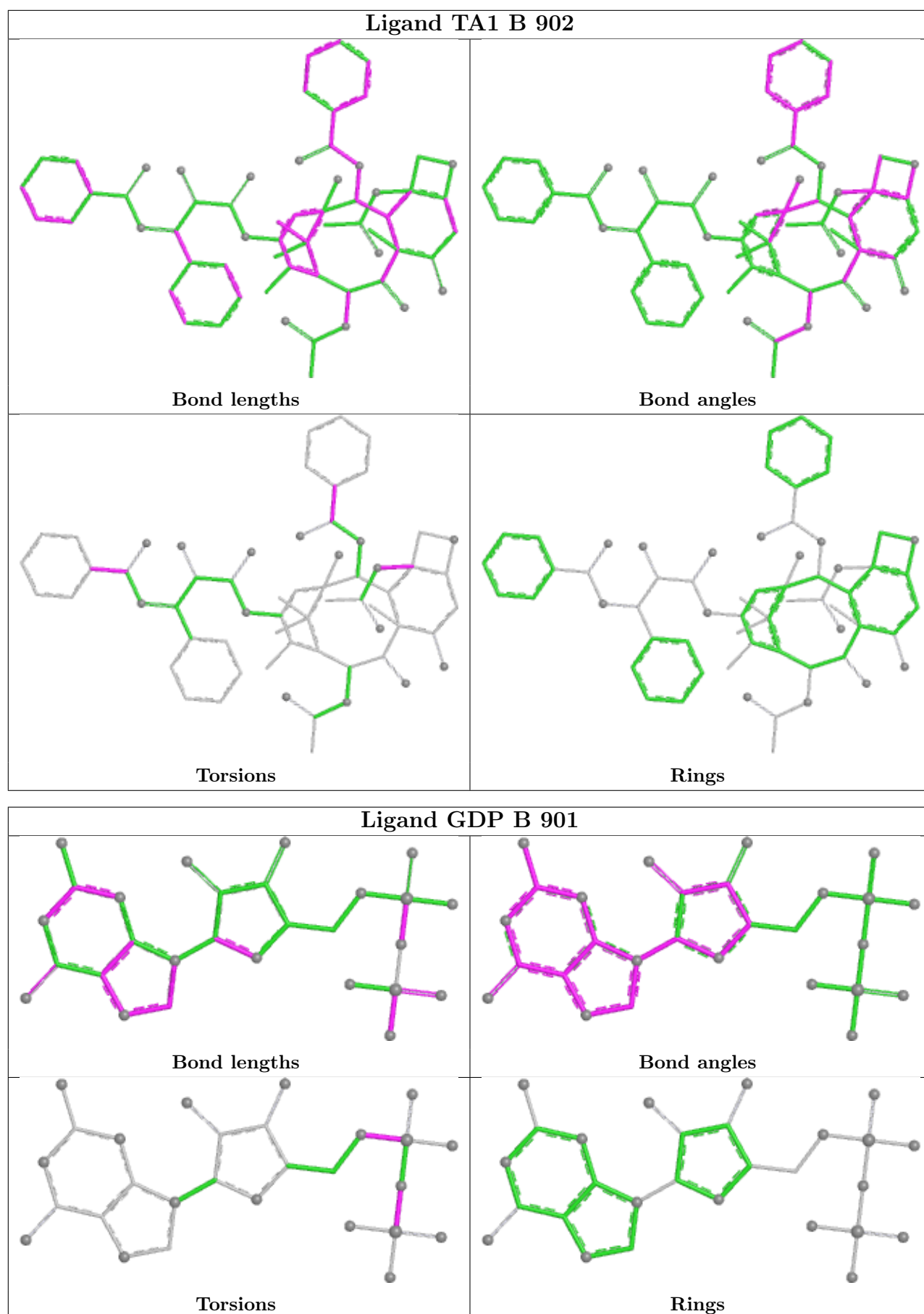
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 6   | B     | 901 | GDP  | PA-O3A-PB-O2B   |
| 6   | B     | 901 | GDP  | C5'-O5'-PA-O3A  |
| 6   | B     | 901 | GDP  | C5'-O5'-PA-O1A  |
| 7   | B     | 902 | TA1  | O02-C03-C04-C05 |
| 7   | B     | 902 | TA1  | O02-C03-C04-C09 |
| 7   | B     | 902 | TA1  | O03-C03-C04-C09 |
| 7   | B     | 902 | TA1  | O03-C03-C04-C05 |
| 7   | B     | 902 | TA1  | N01-C30-C31-C36 |
| 7   | B     | 902 | TA1  | O14-C30-C31-C36 |
| 7   | B     | 902 | TA1  | N01-C30-C31-C32 |
| 7   | B     | 902 | TA1  | O14-C30-C31-C32 |
| 5   | A     | 502 | GTP  | C3'-C4'-C5'-O5' |
| 5   | A     | 502 | GTP  | O4'-C4'-C5'-O5' |
| 5   | A     | 502 | GTP  | C5'-O5'-PA-O1A  |
| 6   | B     | 901 | GDP  | PA-O3A-PB-O3B   |
| 7   | B     | 902 | TA1  | C15-C11-O04-C12 |
| 5   | A     | 502 | GTP  | PG-O3B-PB-O2B   |

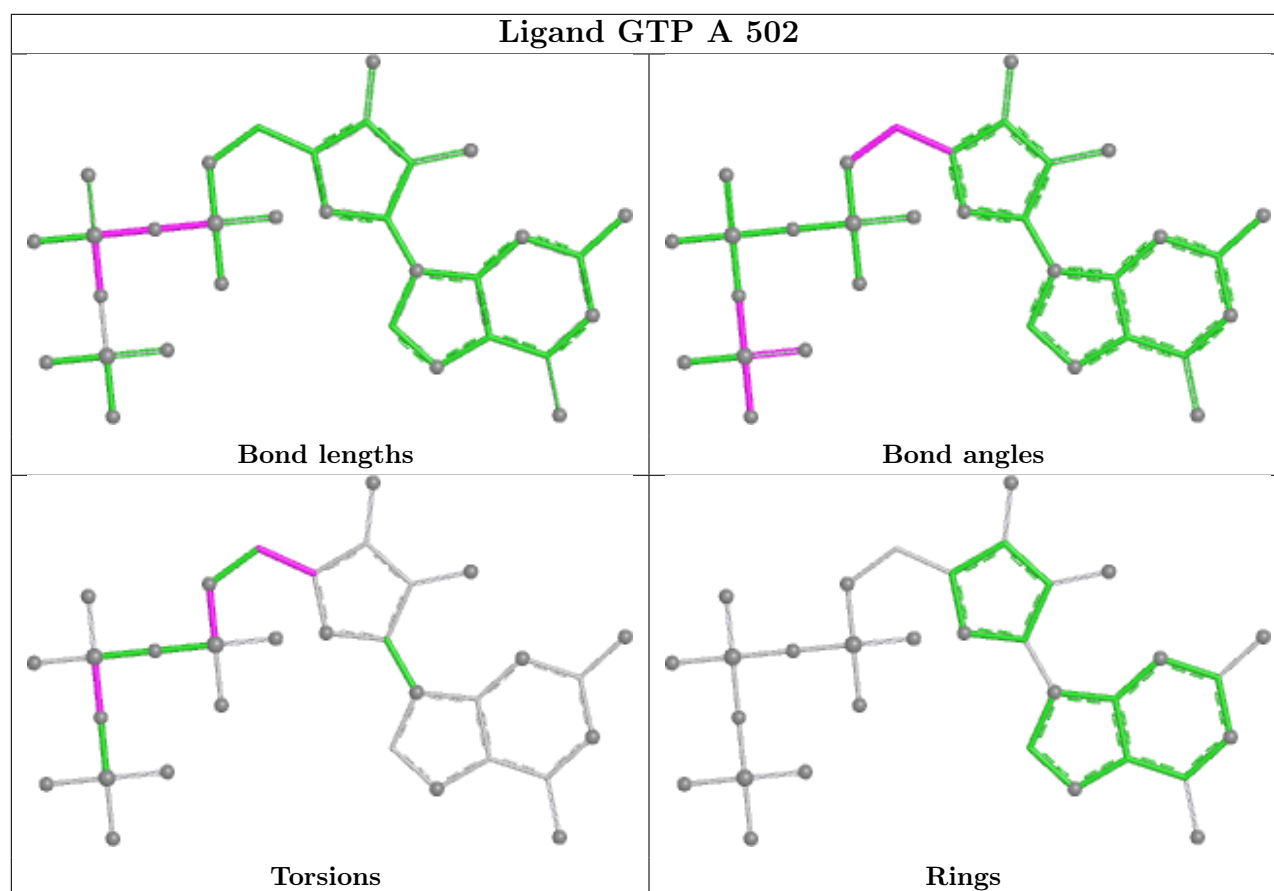
There are no ring outliers.

3 monomers are involved in 25 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 7   | B     | 902 | TA1  | 11      | 0            |
| 6   | B     | 901 | GDP  | 2       | 0            |
| 5   | A     | 502 | GTP  | 12      | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

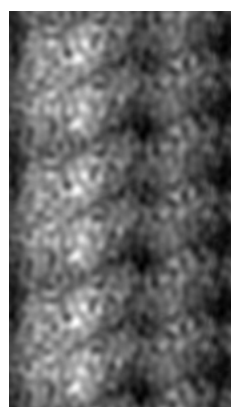
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8059. These allow visual inspection of the internal detail of the map and identification of artifacts.

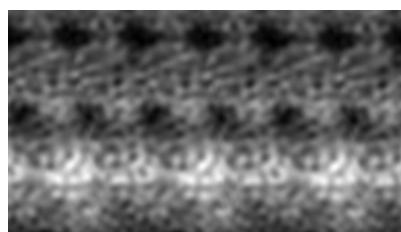
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

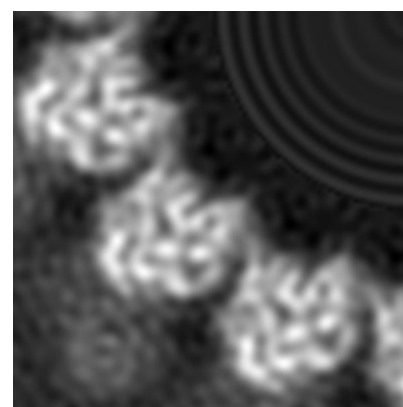
#### 6.1.1 Primary map



X



Y

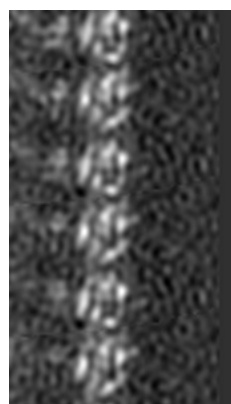


Z

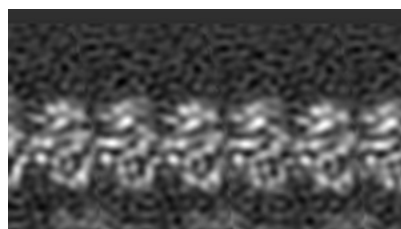
The images above show the map projected in three orthogonal directions.

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

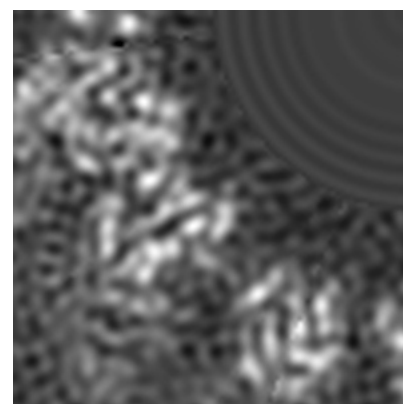
#### 6.2.1 Primary map



X Index: 54



Y Index: 54

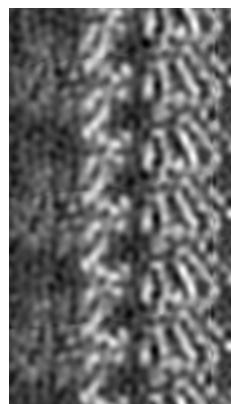


Z Index: 96

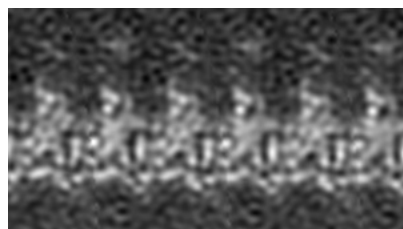
The images above show central slices of the map in three orthogonal directions.

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

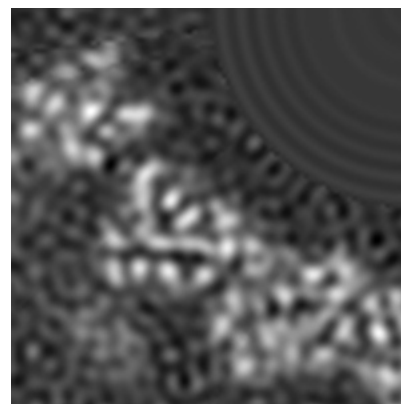
### 6.3.1 Primary map



X Index: 26



Y Index: 43

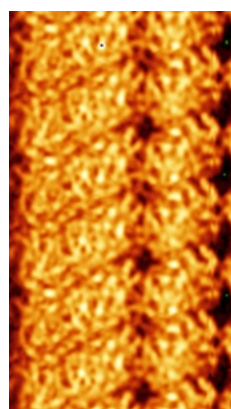


Z Index: 175

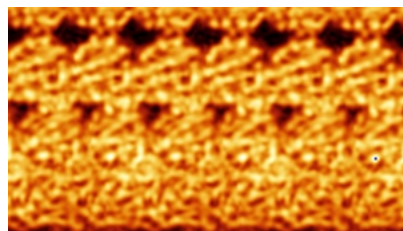
The images above show the largest variance slices of the map in three orthogonal directions.

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

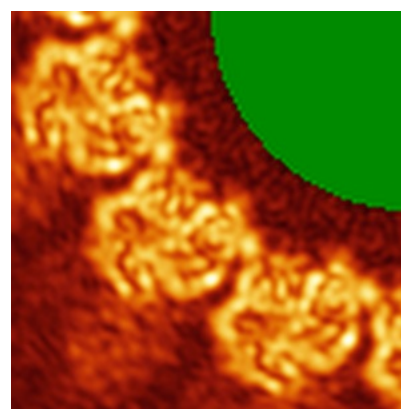
### 6.4.1 Primary map



X



Y

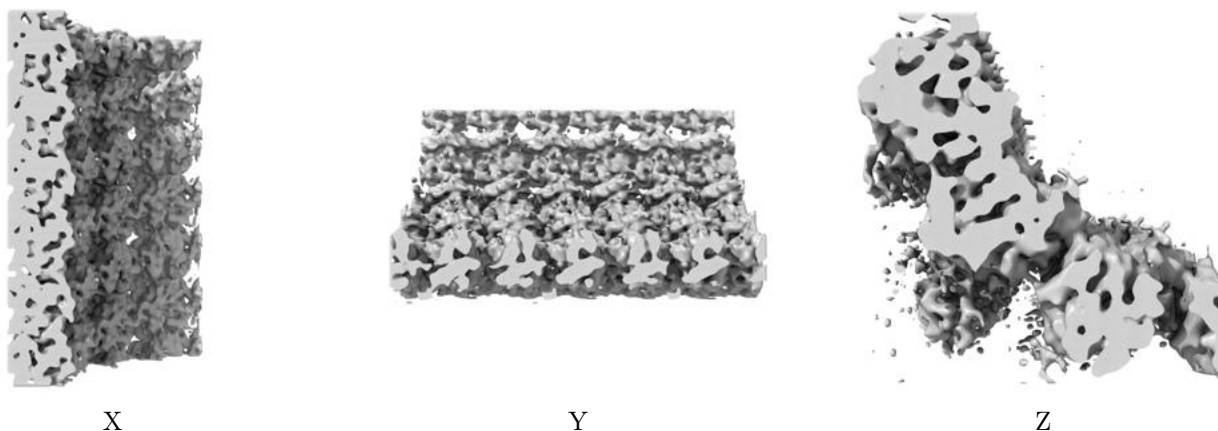


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

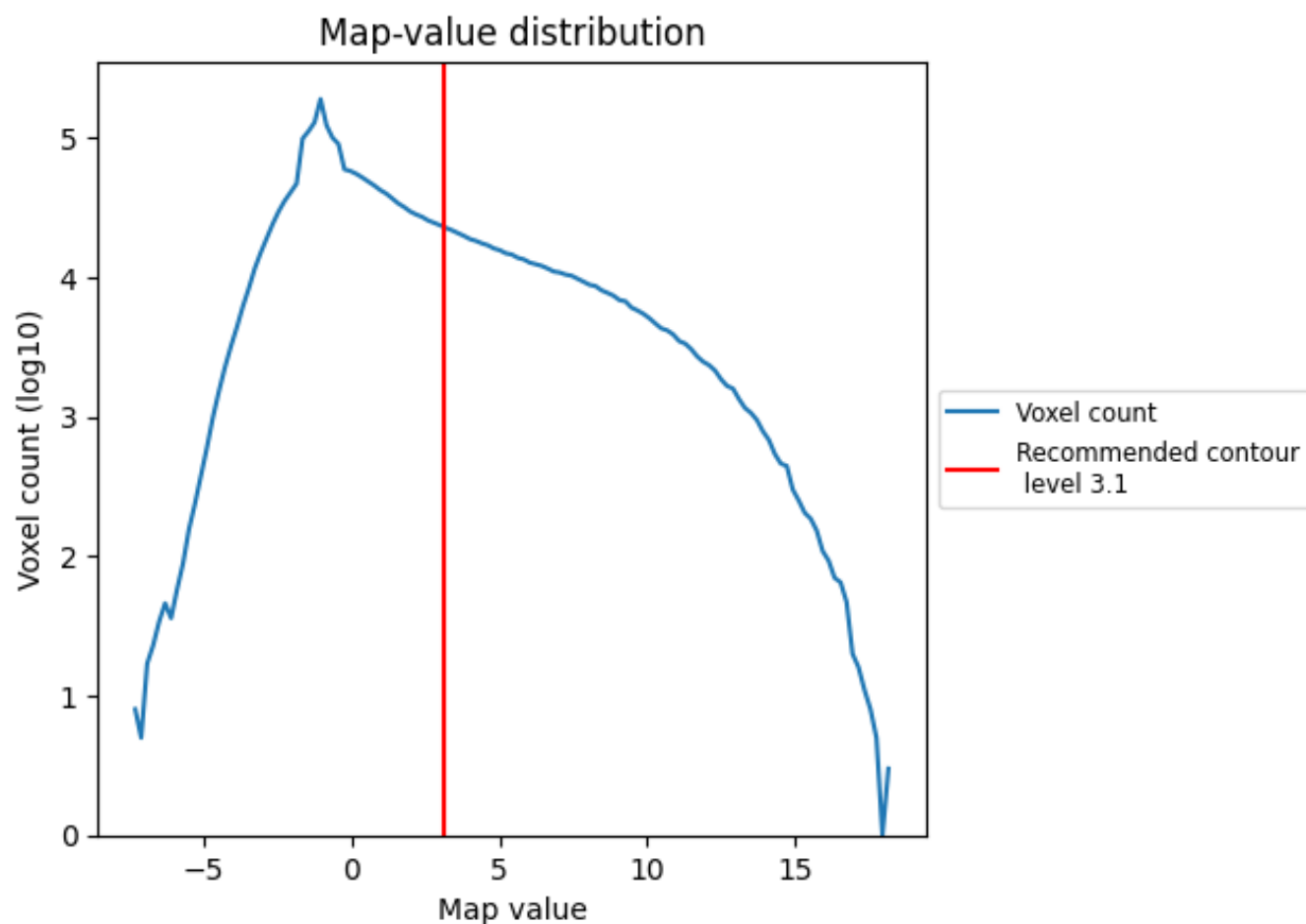
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

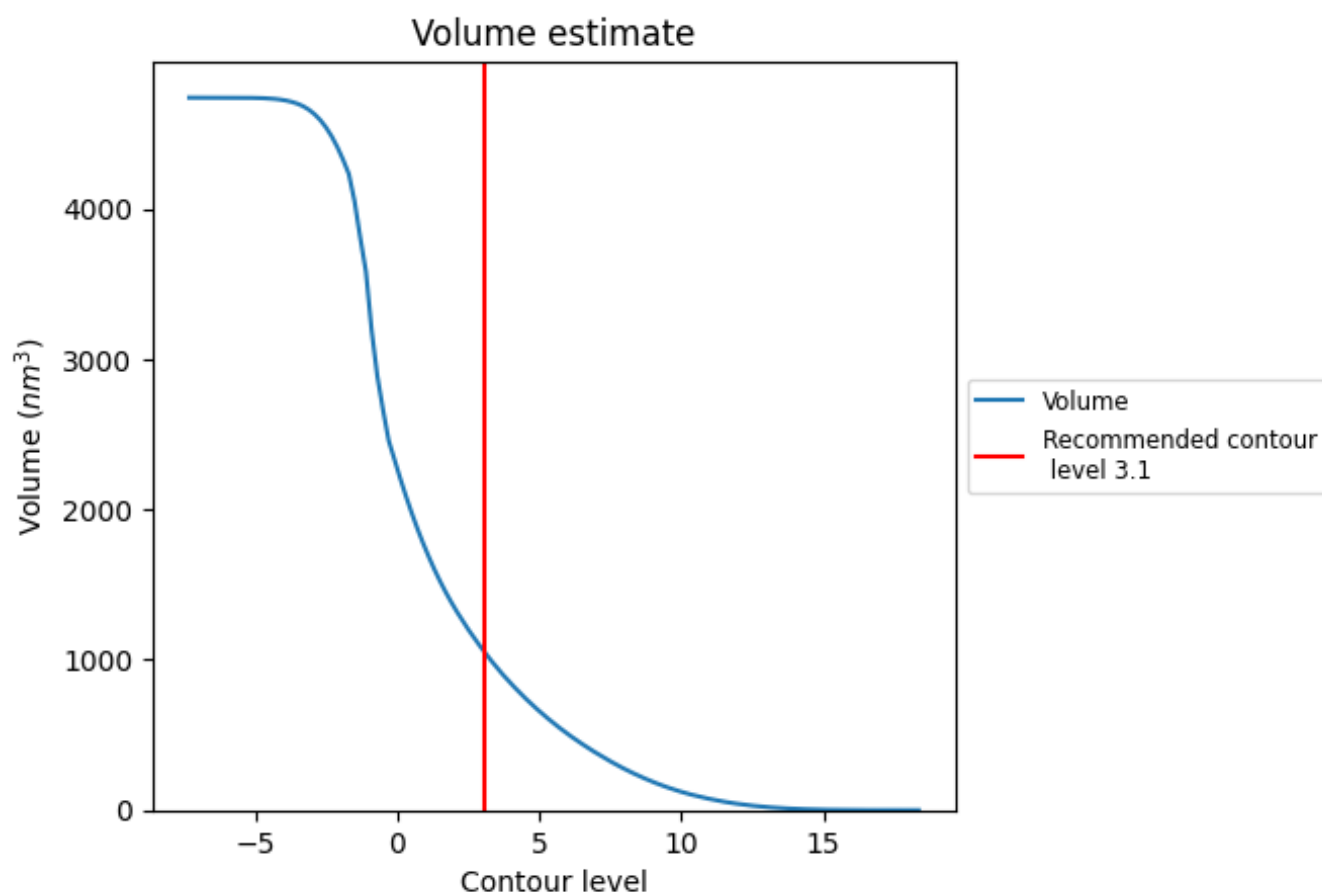
This section contains the results of statistical analysis of the map.

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



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

## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1045  $\text{nm}^3$ ; this corresponds to an approximate mass of 944 kDa.

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

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

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

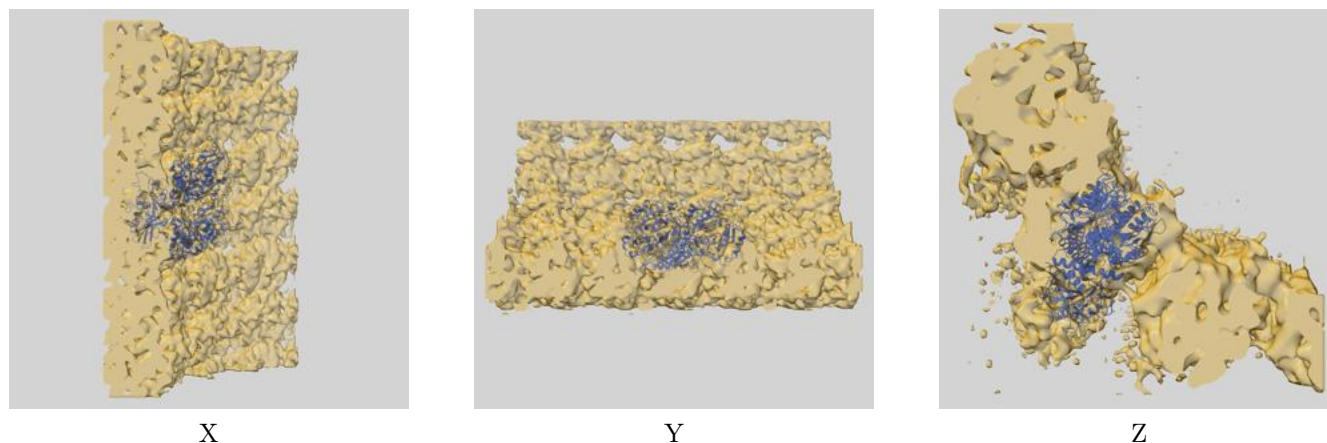
## 8 Fourier-Shell correlation

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

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

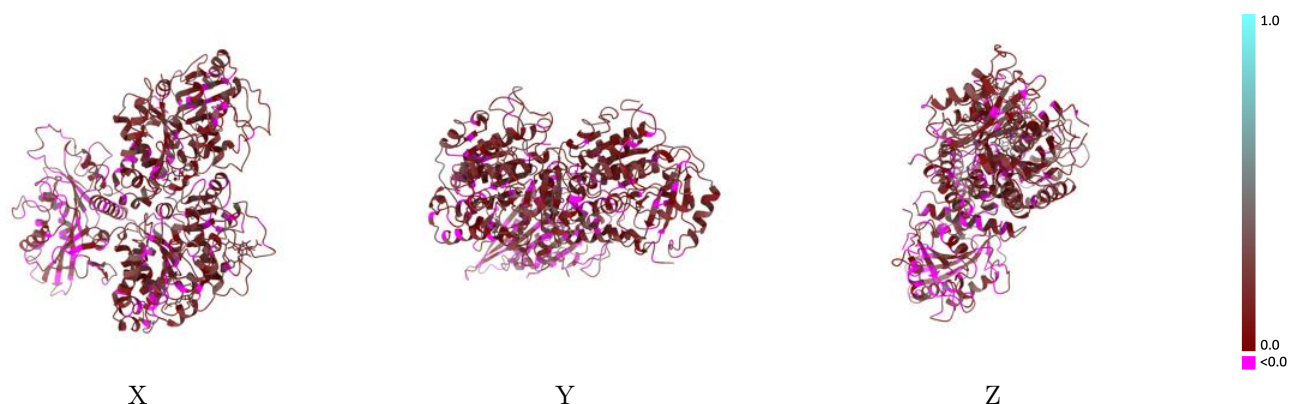
This section contains information regarding the fit between EMDB map EMD-8059 and PDB model 5HNX. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

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



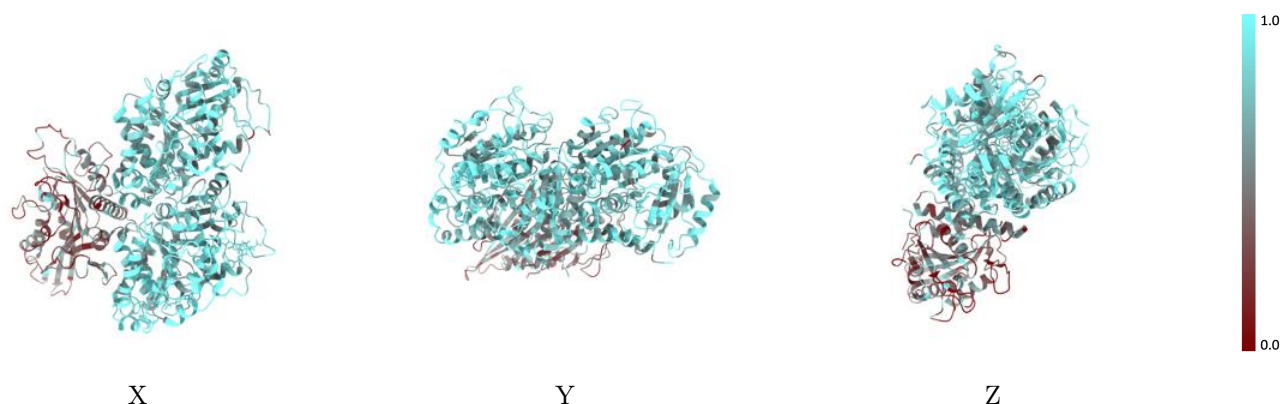
The images above show the 3D surface view of the map at the recommended contour level 3.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



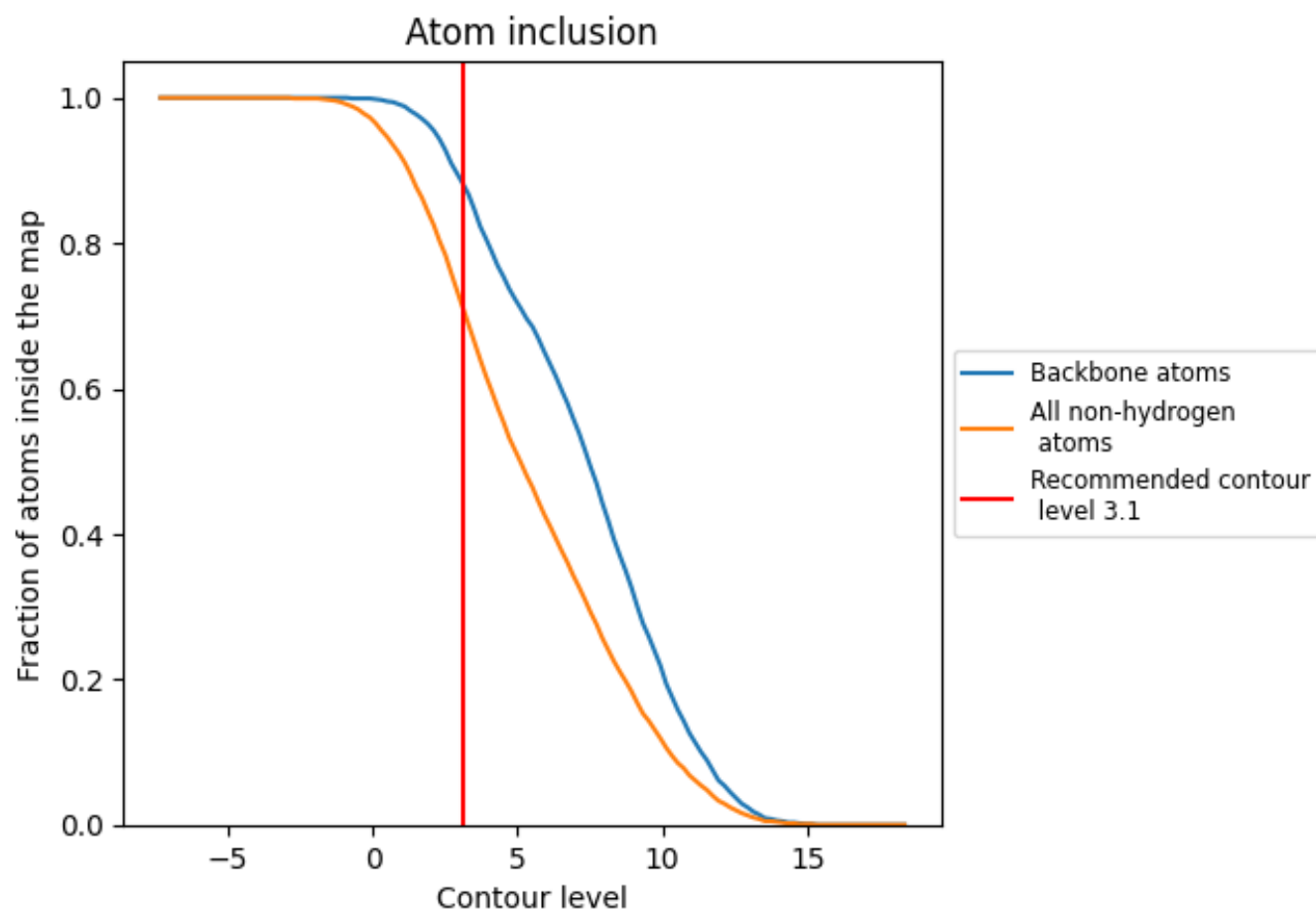
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.1).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 71% 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 (3.1) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.7120 | <div></div> 0.1380 |
| A     | <div></div> 0.8210 | <div></div> 0.1570 |
| B     | <div></div> 0.8430 | <div></div> 0.1520 |
| K     | <div></div> 0.3920 | <div></div> 0.0940 |

