



## Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 10:20 PM UTC

PDB ID : 6OUL / pdb\_00006oul  
EMDB ID : EMD-20203  
Title : Cryo-EM structure of Escherichia coli RNAP polymerase bound to rpsTP2 promoter DNA  
Authors : Chen, J.; Chiu, C.E.; Campbell, E.A.; Darst, S.A.  
Deposited on : 2019-05-04  
Resolution : 3.40 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:

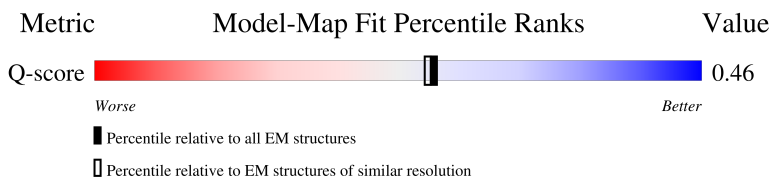
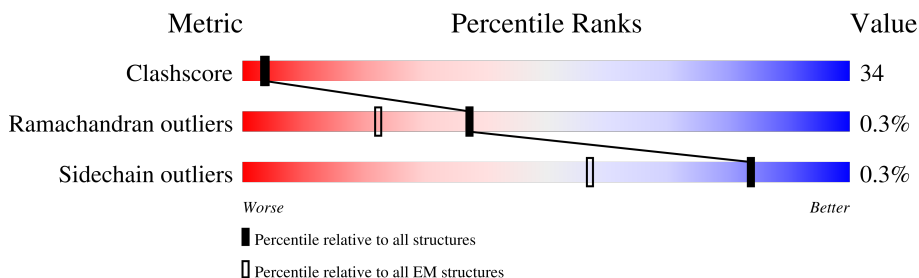
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 3.40 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                       | 14717 ( 2.90 - 3.90 )                                    |

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   | G     | 329    |                  |
| 1   | H     | 329    |                  |
| 1   | R     | 329    |                  |
| 2   | I     | 1342   |                  |

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| Mol | Chain | Length | Quality of chain                                                               |
|-----|-------|--------|--------------------------------------------------------------------------------|
| 3   | J     | 1430   | <div><div></div><div>14%</div><div>42%</div><div>51%</div><div>7%</div></div>  |
| 4   | K     | 91     | <div><div></div><div>11%</div><div>53%</div><div>34%</div><div>13%</div></div> |
| 5   | L     | 616    | <div><div></div><div>30%</div><div>32%</div><div>44%</div><div>24%</div></div> |
| 6   | P     | 85     | <div><div></div><div>20%</div><div>15%</div><div>56%</div><div>28%</div></div> |
| 7   | Q     | 85     | <div><div></div><div>24%</div><div>15%</div><div>51%</div><div>34%</div></div> |

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 32044 atoms, of which 117 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | G     | 231      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1785  | 1112 | 318 | 349 | 6 |         |       |
| 1   | H     | 219      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1681  | 1050 | 295 | 330 | 6 |         |       |
| 1   | R     | 73       | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 572   | 362  | 100 | 108 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 2   | I     | 1341     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10575 | 6634 | 1842 | 2056 | 43 |         |       |

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

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 3   | J     | 1337     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10386 | 6525 | 1851 | 1961 | 49 |         |       |

There are 24 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| J     | 1       | VAL      | -      | expression tag | UNP U9YPW3 |
| J     | 1408    | LEU      | -      | expression tag | UNP U9YPW3 |
| J     | 1409    | GLU      | -      | expression tag | UNP U9YPW3 |
| J     | 1410    | LEU      | -      | expression tag | UNP U9YPW3 |
| J     | 1411    | GLU      | -      | expression tag | UNP U9YPW3 |
| J     | 1412    | VAL      | -      | expression tag | UNP U9YPW3 |
| J     | 1413    | LEU      | -      | expression tag | UNP U9YPW3 |
| J     | 1414    | PHE      | -      | expression tag | UNP U9YPW3 |
| J     | 1415    | GLN      | -      | expression tag | UNP U9YPW3 |
| J     | 1416    | GLY      | -      | expression tag | UNP U9YPW3 |
| J     | 1417    | PRO      | -      | expression tag | UNP U9YPW3 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| J     | 1418    | SER      | -      | expression tag | UNP U9YPW3 |
| J     | 1419    | SER      | -      | expression tag | UNP U9YPW3 |
| J     | 1420    | GLY      | -      | expression tag | UNP U9YPW3 |
| J     | 1421    | HIS      | -      | expression tag | UNP U9YPW3 |
| J     | 1422    | HIS      | -      | expression tag | UNP U9YPW3 |
| J     | 1423    | HIS      | -      | expression tag | UNP U9YPW3 |
| J     | 1424    | HIS      | -      | expression tag | UNP U9YPW3 |
| J     | 1425    | HIS      | -      | expression tag | UNP U9YPW3 |
| J     | 1426    | HIS      | -      | expression tag | UNP U9YPW3 |
| J     | 1427    | HIS      | -      | expression tag | UNP U9YPW3 |
| J     | 1428    | HIS      | -      | expression tag | UNP U9YPW3 |
| J     | 1429    | HIS      | -      | expression tag | UNP U9YPW3 |
| J     | 1430    | HIS      | -      | expression tag | UNP U9YPW3 |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | K     | 79       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 627   | 382 | 118 | 126 | 1 |         |       |

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | L     | 471      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3821  | 2397 | 681 | 720 | 23 |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| L     | -2      | SER      | -      | expression tag | UNP Q0P6L9 |
| L     | -1      | GLU      | -      | expression tag | UNP Q0P6L9 |
| L     | 0       | PHE      | -      | expression tag | UNP Q0P6L9 |

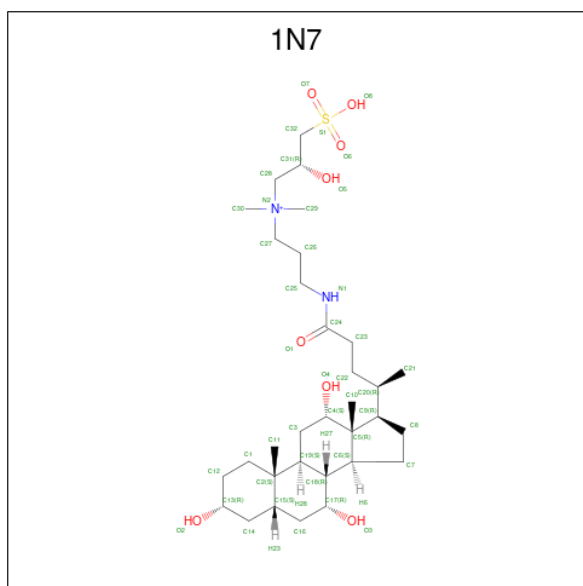
- Molecule 6 is a DNA chain called Non-template strand of rpsTP2 DNA promoter.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 6   | P     | 61       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1253  | 599 | 235 | 358 | 61 |         |       |

- Molecule 7 is a DNA chain called Template strand of rpsTP2 DNA promoter.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 7   | Q     | 56       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1143  | 549 | 192 | 346 | 56 |         |       |

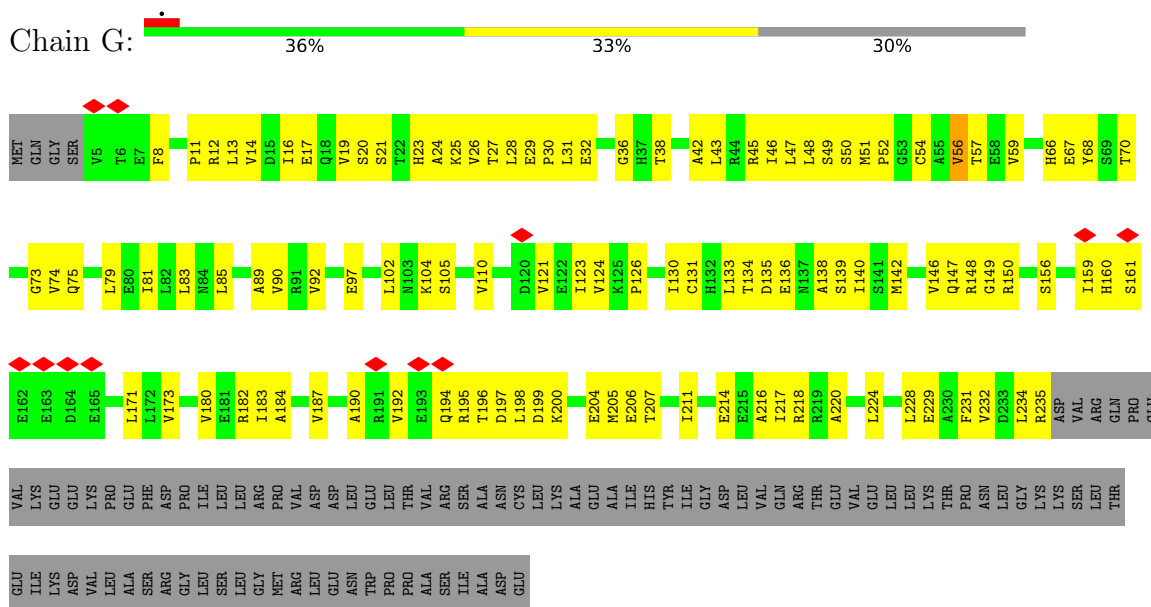
- Molecule 8 is CHAPSO (CCD ID: 1N7) (formula:  $C_{32}H_{59}N_2O_8S$ ).



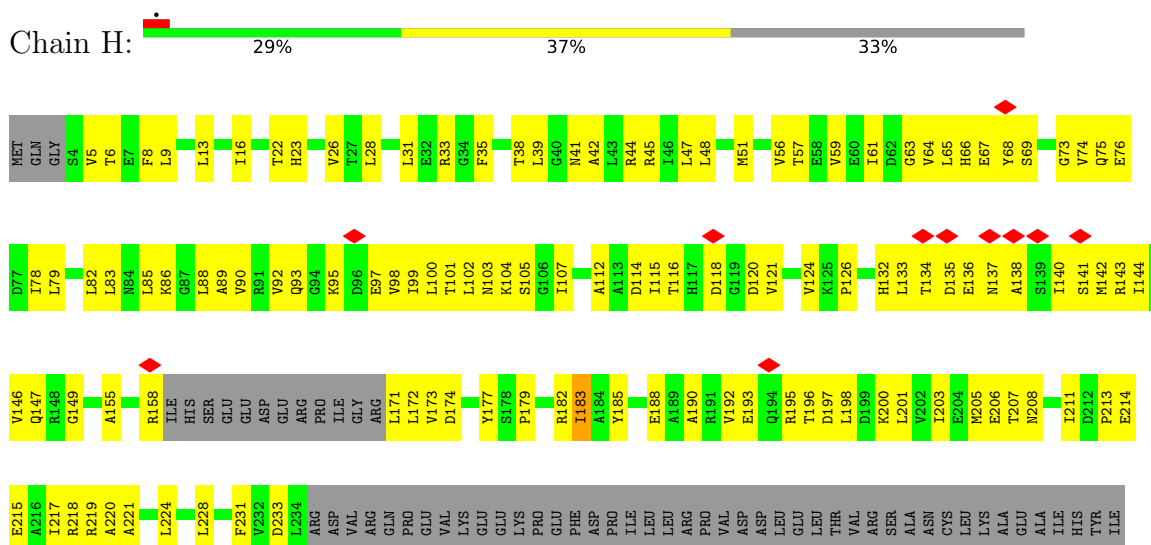
### 3 Residue-property plots

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

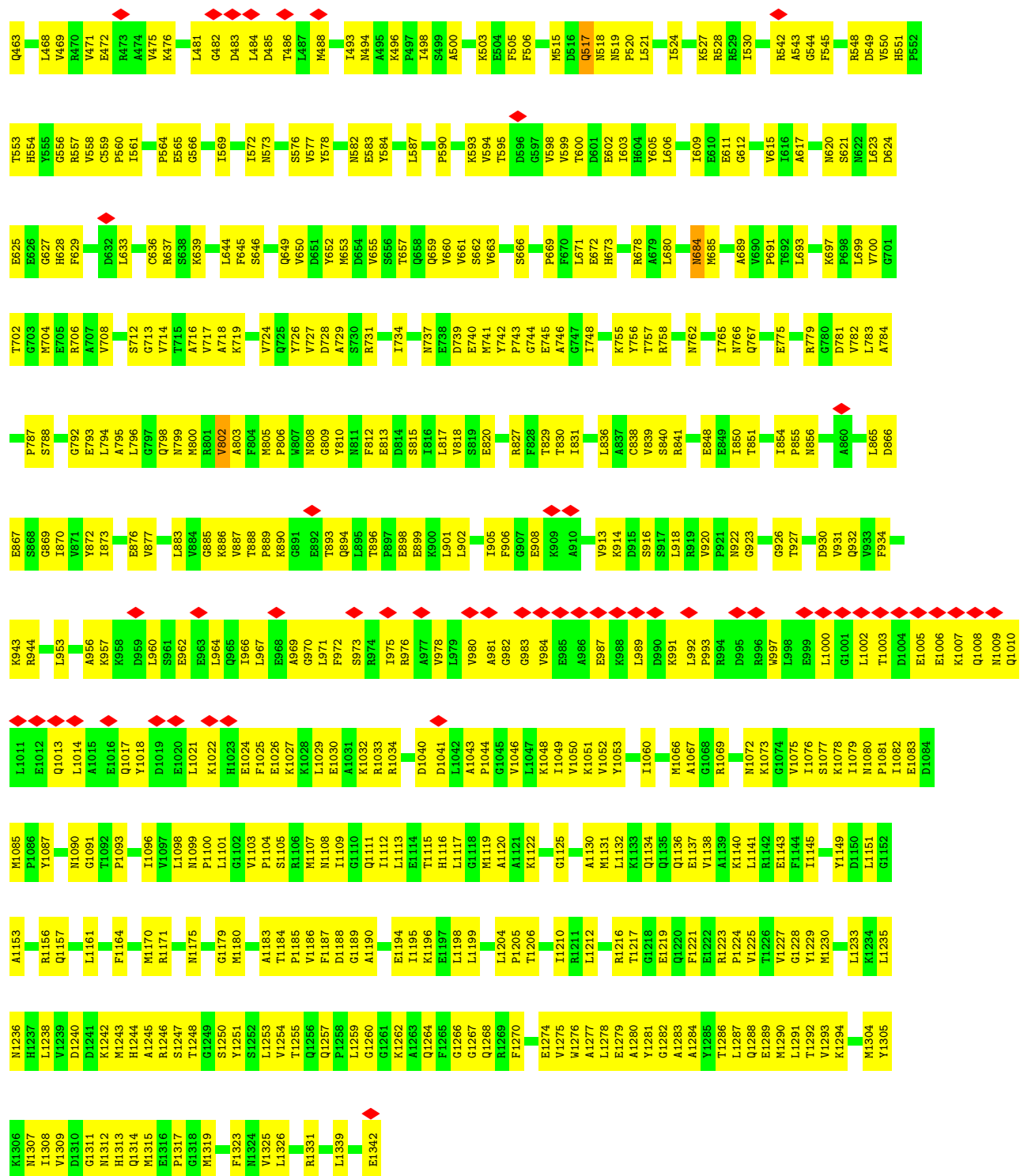
#### • Molecule 1: DNA-directed RNA polymerase subunit alpha



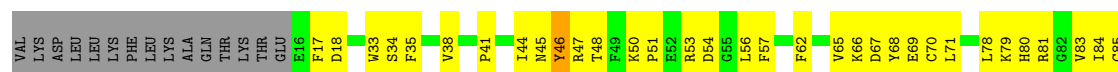
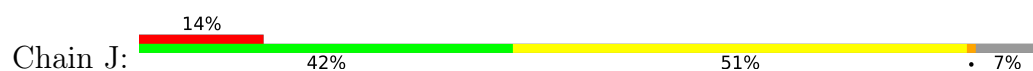
#### • Molecule 1: DNA-directed RNA polymerase subunit alpha

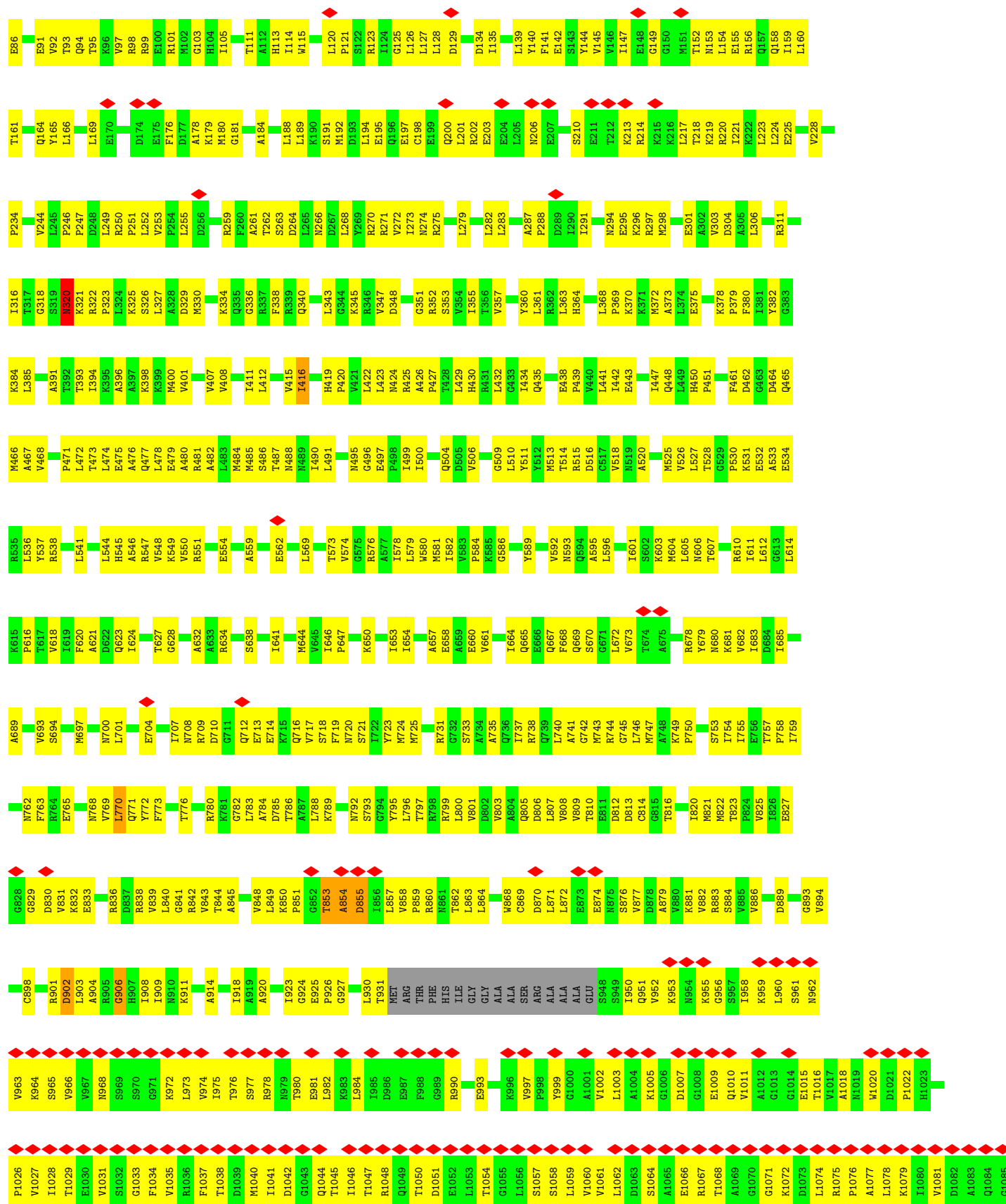


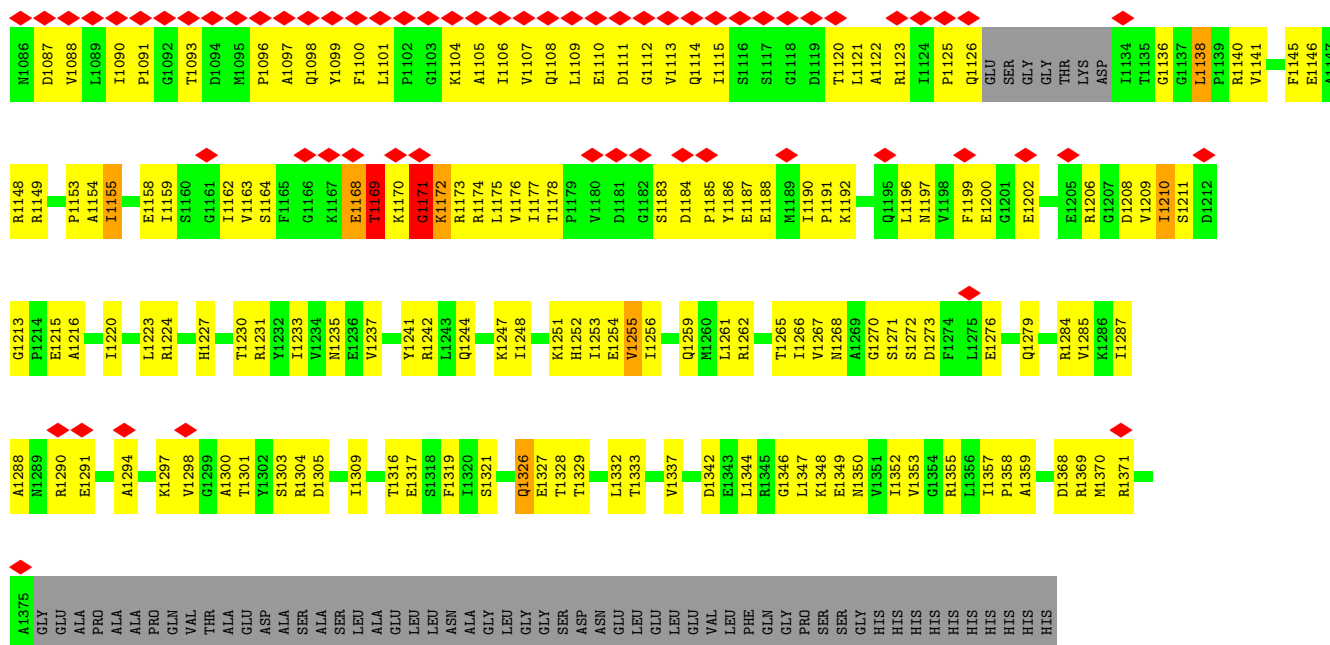




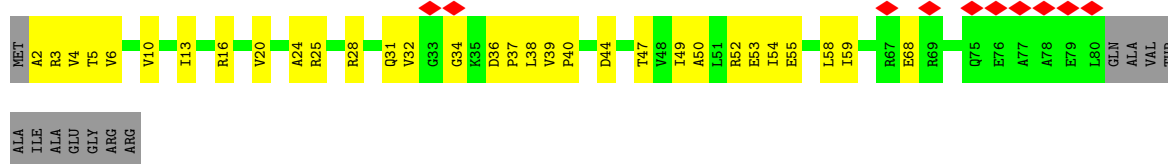
• Molecule 3: DNA-directed RNA polymerase subunit beta'



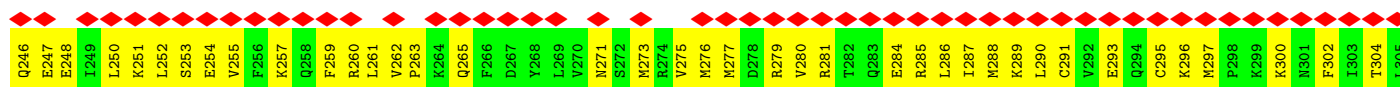
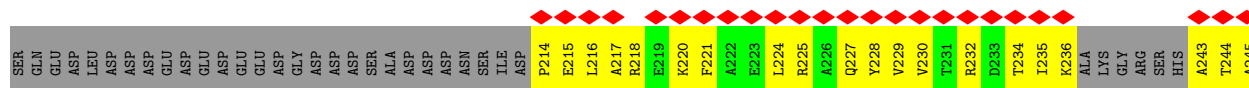
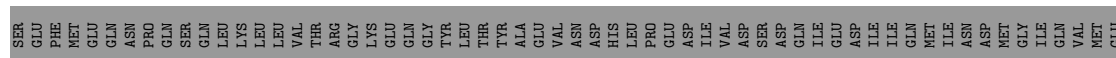


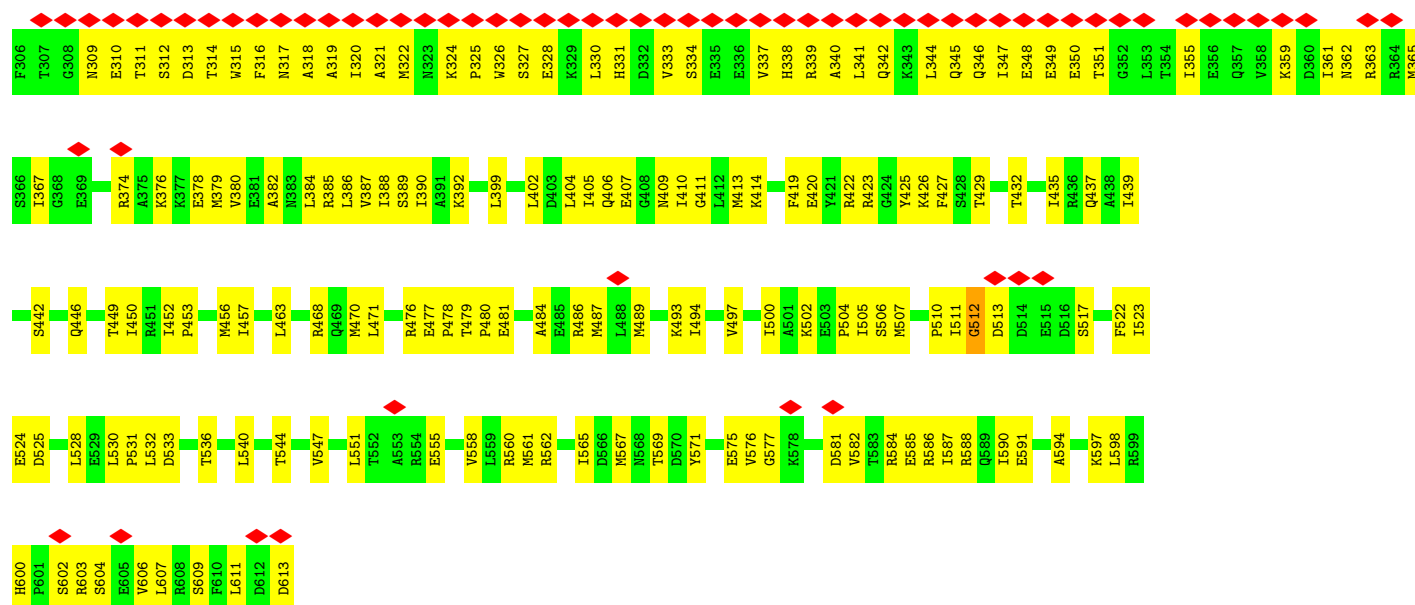


• Molecule 4: DNA-directed RNA polymerase subunit omega

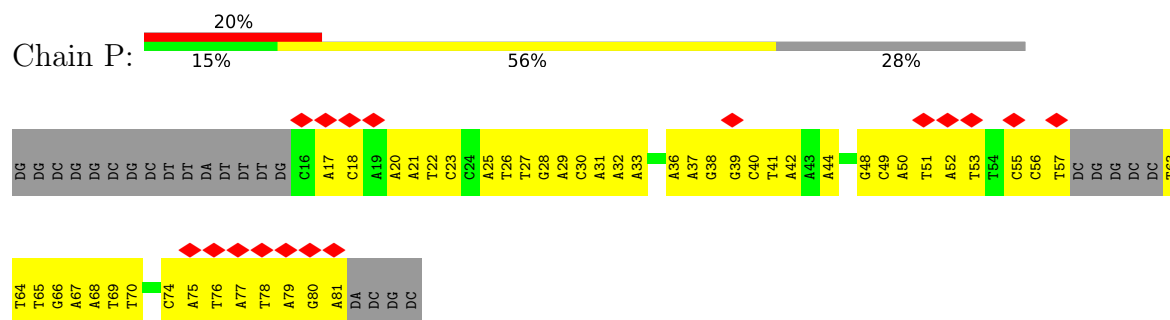


• Molecule 5: RNA polymerase sigma factor RpoD

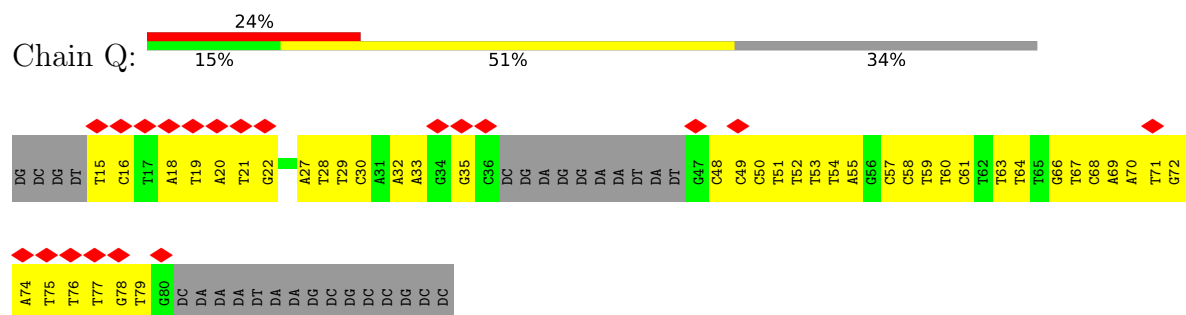




- Molecule 6: Non-template strand of rpsTP2 DNA promoter



- Molecule 7: Template strand of rpsTP2 DNA promoter



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 289670                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 1.0                                     | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 0.251                                   | Depositor |
| Minimum map value                    | -0.158                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.007                                   | Depositor |
| Recommended contour level            | 0.025                                   | Depositor |
| Map size (Å)                         | 332.8, 332.8, 332.8                     | wwPDB     |
| Map dimensions                       | 256, 256, 256                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.3, 1.3, 1.3                           | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 1N7, ZN

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

| Mol | Chain | Bond lengths |         | Bond angles |                |
|-----|-------|--------------|---------|-------------|----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5        |
| 1   | G     | 0.68         | 0/1807  | 0.76        | 0/2449         |
| 1   | H     | 0.54         | 0/1700  | 0.68        | 0/2305         |
| 1   | R     | 0.19         | 0/579   | 0.48        | 0/784          |
| 2   | I     | 0.70         | 0/10744 | 0.75        | 2/14496 (0.0%) |
| 3   | J     | 0.65         | 0/10543 | 0.73        | 5/14239 (0.0%) |
| 4   | K     | 0.47         | 0/629   | 0.59        | 0/847          |
| 5   | L     | 0.39         | 0/3872  | 0.57        | 2/5204 (0.0%)  |
| 6   | P     | 0.31         | 0/1407  | 0.45        | 0/2166         |
| 7   | Q     | 0.31         | 0/1276  | 0.45        | 0/1965         |
| All | All   | 0.61         | 0/32557 | 0.69        | 9/44455 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | I     | 0                   | 1                   |
| 3   | J     | 0                   | 10                  |
| All | All   | 0                   | 11                  |

There are no bond length outliers.

All (9) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | I     | 517 | GLN  | N-CA-C | 6.86  | 119.91      | 109.62   |
| 3   | J     | 765 | GLU  | CA-C-N | -6.48 | 116.71      | 122.73   |
| 3   | J     | 765 | GLU  | C-N-CA | -6.48 | 116.71      | 122.73   |
| 5   | L     | 512 | GLY  | CA-C-N | 5.73  | 132.02      | 121.70   |
| 5   | L     | 512 | GLY  | C-N-CA | 5.73  | 132.02      | 121.70   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 3   | J     | 1171 | GLY  | CA-C-N | 5.58  | 131.74      | 121.70   |
| 3   | J     | 1171 | GLY  | C-N-CA | 5.58  | 131.74      | 121.70   |
| 3   | J     | 1210 | ILE  | N-CA-C | -5.56 | 105.99      | 111.77   |
| 2   | I     | 482  | GLY  | N-CA-C | 5.05  | 117.28      | 111.36   |

There are no chirality outliers.

All (11) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 2   | I     | 1185 | PRO  | Peptide |
| 3   | J     | 1138 | LEU  | Peptide |
| 3   | J     | 1168 | GLU  | Peptide |
| 3   | J     | 1169 | THR  | Peptide |
| 3   | J     | 1171 | GLY  | Peptide |
| 3   | J     | 1326 | GLN  | Peptide |
| 3   | J     | 320  | ASN  | Peptide |
| 3   | J     | 416  | ILE  | Peptide |
| 3   | J     | 853  | THR  | Peptide |
| 3   | J     | 855  | ASP  | Peptide |
| 3   | J     | 902  | ASP  | 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   | G     | 1785  | 0        | 1806     | 122     | 0            |
| 1   | H     | 1681  | 0        | 1708     | 150     | 0            |
| 1   | R     | 572   | 0        | 602      | 85      | 0            |
| 2   | I     | 10575 | 0        | 10584    | 707     | 0            |
| 3   | J     | 10386 | 0        | 10594    | 806     | 0            |
| 4   | K     | 627   | 0        | 634      | 39      | 0            |
| 5   | L     | 3821  | 0        | 3891     | 325     | 0            |
| 6   | P     | 1253  | 0        | 689      | 73      | 0            |
| 7   | Q     | 1143  | 0        | 640      | 52      | 0            |
| 8   | I     | 27    | 39       | 37       | 6       | 0            |
| 8   | J     | 27    | 39       | 37       | 4       | 0            |
| 8   | L     | 27    | 39       | 38       | 4       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 9   | J     | 1     | 0        | 0        | 0       | 0            |
| 10  | J     | 2     | 0        | 0        | 0       | 0            |
| All | All   | 31927 | 117      | 31260    | 2170    | 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 34.

All (2170) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:I:1401:1N7:C3   | 8:I:1401:1N7:C19  | 1.83                     | 1.55              |
| 8:J:1504:1N7:C19  | 8:J:1504:1N7:C3   | 1.84                     | 1.54              |
| 8:L:701:1N7:C19   | 8:L:701:1N7:C3    | 1.84                     | 1.52              |
| 1:H:105:SER:HA    | 1:H:138:ALA:HB2   | 1.42                     | 1.01              |
| 2:I:75:LEU:HD11   | 2:I:127:ILE:HD11  | 1.43                     | 1.00              |
| 5:L:98:VAL:HG22   | 5:L:402:LEU:HD11  | 1.46                     | 0.98              |
| 2:I:13:LYS:HB2    | 2:I:1180:MET:HE2  | 1.44                     | 0.97              |
| 5:L:277:MET:HE1   | 5:L:359:LYS:HG2   | 1.44                     | 0.97              |
| 3:J:1081:VAL:HG12 | 3:J:1087:ASP:HA   | 1.43                     | 0.97              |
| 2:I:1212:LEU:HD22 | 2:I:1225:VAL:HG21 | 1.48                     | 0.96              |
| 1:H:74:VAL:HG12   | 1:H:76:GLU:H      | 1.30                     | 0.96              |
| 5:L:262:VAL:HB    | 5:L:265:GLN:HG2   | 1.48                     | 0.95              |
| 5:L:135:ALA:HB1   | 5:L:253:SER:HB3   | 1.48                     | 0.95              |
| 3:J:155:GLU:HB2   | 3:J:158:GLN:HB2   | 1.48                     | 0.94              |
| 2:I:718:ALA:HB2   | 2:I:783:LEU:HD21  | 1.48                     | 0.94              |
| 2:I:1120:ALA:HB1  | 2:I:1198:LEU:HD12 | 1.50                     | 0.94              |
| 1:H:103:ASN:HB3   | 1:H:141:SER:HA    | 1.49                     | 0.92              |
| 3:J:518:VAL:HG11  | 3:J:707:ILE:HD13  | 1.47                     | 0.92              |
| 2:I:1136:GLN:HE21 | 2:I:1140:LYS:HD3  | 1.34                     | 0.91              |
| 3:J:1090:ILE:HD11 | 3:J:1097:ALA:HB2  | 1.53                     | 0.91              |
| 3:J:271:ARG:HH11  | 3:J:316:ILE:HD12  | 1.35                     | 0.90              |
| 3:J:960:LEU:HD23  | 3:J:963:VAL:HG21  | 1.51                     | 0.90              |
| 3:J:1079:LYS:HD3  | 3:J:1098:GLN:HB3  | 1.50                     | 0.90              |
| 1:R:300:LEU:HA    | 1:R:303:ILE:HD12  | 1.50                     | 0.90              |
| 3:J:559:ALA:HB3   | 3:J:562:GLU:HB2   | 1.51                     | 0.90              |
| 3:J:797:THR:HG22  | 3:J:924:GLY:HA3   | 1.54                     | 0.90              |
| 2:I:870:ILE:HG21  | 2:I:931:VAL:HG11  | 1.55                     | 0.89              |
| 3:J:693:VAL:HG21  | 3:J:743:MET:HE3   | 1.52                     | 0.89              |
| 3:J:547:ARG:HA    | 3:J:573:THR:HG22  | 1.52                     | 0.89              |
| 3:J:141:PHE:HA    | 3:J:180:MET:HE2   | 1.55                     | 0.89              |
| 5:L:290:LEU:HB3   | 5:L:333:VAL:HG21  | 1.55                     | 0.89              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:1060:VAL:HG22 | 3:J:1106:ILE:HG12 | 1.52                     | 0.88              |
| 1:R:287:VAL:HG12  | 1:R:291:LYS:HE3   | 1.53                     | 0.88              |
| 5:L:309:ASN:HD21  | 5:L:312:SER:HB3   | 1.39                     | 0.88              |
| 3:J:311:ARG:HH22  | 3:J:1329:THR:HG21 | 1.38                     | 0.88              |
| 1:H:44:ARG:HB2    | 1:H:183:ILE:HD13  | 1.55                     | 0.87              |
| 2:I:1279:GLU:HG2  | 3:J:1357:ILE:HD13 | 1.57                     | 0.87              |
| 5:L:151:VAL:HG22  | 5:L:156:ALA:HB3   | 1.56                     | 0.87              |
| 3:J:1272:SER:HB3  | 3:J:1273:ASP:HB3  | 1.56                     | 0.86              |
| 2:I:806:PRO:HD3   | 2:I:1100:PRO:HG2  | 1.57                     | 0.86              |
| 1:H:205:MET:HE1   | 1:H:217:ILE:HG13  | 1.57                     | 0.86              |
| 2:I:748:ILE:HD11  | 2:I:966:ILE:HG12  | 1.58                     | 0.86              |
| 2:I:1151:LEU:HD22 | 2:I:1198:LEU:HD23 | 1.56                     | 0.86              |
| 1:R:283:GLN:HE21  | 1:R:318:LEU:HD22  | 1.41                     | 0.86              |
| 3:J:527:LEU:HB2   | 3:J:550:VAL:HG12  | 1.58                     | 0.86              |
| 2:I:251:ALA:HB2   | 2:I:269:ILE:HD11  | 1.57                     | 0.85              |
| 3:J:1104:LYS:HD2  | 3:J:1125:PRO:HG2  | 1.55                     | 0.85              |
| 2:I:519:ASN:HD21  | 2:I:796:LEU:HG    | 1.41                     | 0.85              |
| 5:L:318:ALA:HA    | 5:L:321:ALA:HB3   | 1.57                     | 0.84              |
| 2:I:452:ARG:NH1   | 2:I:584:TYR:O     | 2.10                     | 0.84              |
| 3:J:520:ALA:HB3   | 3:J:546:ALA:HB2   | 1.58                     | 0.84              |
| 1:R:283:GLN:HG2   | 1:R:318:LEU:HD13  | 1.58                     | 0.84              |
| 3:J:974:VAL:HG12  | 3:J:1002:VAL:HG22 | 1.60                     | 0.84              |
| 3:J:514:THR:HG21  | 3:J:596:LEU:HB2   | 1.58                     | 0.83              |
| 5:L:218:ARG:HA    | 5:L:221:PHE:HD2   | 1.43                     | 0.83              |
| 1:G:16:ILE:HD13   | 1:G:214:GLU:HB2   | 1.60                     | 0.83              |
| 5:L:313:ASP:HA    | 5:L:316:PHE:HB3   | 1.61                     | 0.83              |
| 4:K:2:ALA:HB1     | 4:K:3:ARG:HB2     | 1.60                     | 0.82              |
| 3:J:1061:VAL:HG11 | 3:J:1101:LEU:HB2  | 1.60                     | 0.82              |
| 3:J:128:LEU:HA    | 3:J:192:MET:HE1   | 1.61                     | 0.82              |
| 5:L:248:GLU:HA    | 5:L:251:LYS:HZ2   | 1.43                     | 0.82              |
| 5:L:588:ARG:HD3   | 7:Q:67:DT:H73     | 1.62                     | 0.82              |
| 2:I:600:THR:HG22  | 2:I:602:GLU:H     | 1.43                     | 0.81              |
| 5:L:148:TYR:OH    | 5:L:218:ARG:HG2   | 1.80                     | 0.81              |
| 1:R:260:LEU:HD21  | 1:R:278:ILE:HG12  | 1.63                     | 0.81              |
| 3:J:741:ALA:O     | 3:J:762:ASN:ND2   | 2.12                     | 0.81              |
| 5:L:215:GLU:HG2   | 5:L:218:ARG:HH21  | 1.44                     | 0.81              |
| 3:J:475:GLU:HG3   | 4:K:24:ALA:HB1    | 1.63                     | 0.81              |
| 2:I:980:VAL:HG22  | 2:I:984:VAL:HG23  | 1.62                     | 0.80              |
| 1:R:250:ASP:HB3   | 1:R:253:LEU:HB2   | 1.64                     | 0.80              |
| 3:J:56:LEU:HD11   | 3:J:273:ILE:HD12  | 1.64                     | 0.80              |
| 3:J:984:LEU:HB3   | 3:J:993:GLU:HB2   | 1.64                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:H:112:ALA:HB3   | 1:H:126:PRO:HA    | 1.63                     | 0.79              |
| 3:J:1173:ARG:HE   | 3:J:1192:LYS:HA   | 1.47                     | 0.79              |
| 1:G:70:THR:HG21   | 2:I:755:LYS:HE2   | 1.64                     | 0.79              |
| 3:J:950:ILE:HB    | 3:J:1018:ALA:HB3  | 1.64                     | 0.79              |
| 2:I:103:VAL:HG12  | 2:I:117:ILE:HG22  | 1.64                     | 0.79              |
| 3:J:202:ARG:NH2   | 3:J:225:GLU:OE2   | 2.14                     | 0.79              |
| 2:I:528:ARG:NH2   | 2:I:576:SER:O     | 2.16                     | 0.79              |
| 1:G:182:ARG:NH1   | 2:I:1090:ASN:O    | 2.14                     | 0.79              |
| 3:J:1075:ARG:HH21 | 3:J:1168:GLU:HG2  | 1.46                     | 0.79              |
| 3:J:1078:LEU:HD11 | 3:J:1101:LEU:HD11 | 1.62                     | 0.79              |
| 3:J:1046:ILE:HD12 | 3:J:1059:LEU:HD13 | 1.65                     | 0.79              |
| 2:I:617:ALA:HB3   | 2:I:653:MET:HA    | 1.63                     | 0.78              |
| 2:I:400:VAL:HG22  | 2:I:584:TYR:HB3   | 1.64                     | 0.78              |
| 3:J:833:GLU:OE1   | 3:J:1242:ARG:NH2  | 2.17                     | 0.78              |
| 2:I:1210:ILE:HD12 | 2:I:1227:VAL:HG21 | 1.65                     | 0.78              |
| 5:L:105:MET:HE3   | 5:L:388:ILE:HD12  | 1.65                     | 0.78              |
| 2:I:1280:ALA:HB1  | 3:J:918:ILE:HG22  | 1.64                     | 0.78              |
| 3:J:322:ARG:HG3   | 3:J:323:PRO:HD2   | 1.64                     | 0.78              |
| 2:I:887:VAL:HG22  | 2:I:913:VAL:HG22  | 1.64                     | 0.77              |
| 1:R:269:CYS:HB3   | 1:R:295:LEU:HD12  | 1.64                     | 0.77              |
| 3:J:576:ARG:HD3   | 3:J:593:ASN:HA    | 1.65                     | 0.77              |
| 3:J:1344:LEU:HD22 | 3:J:1349:GLU:HB3  | 1.67                     | 0.77              |
| 3:J:201:LEU:HD11  | 3:J:220:ARG:HH11  | 1.49                     | 0.77              |
| 2:I:590:PRO:HB2   | 2:I:655:VAL:HG21  | 1.67                     | 0.77              |
| 1:G:211:ILE:HG21  | 1:G:216:ALA:HB2   | 1.66                     | 0.77              |
| 7:Q:60:DT:H1'     | 7:Q:61:DC:H5'     | 1.66                     | 0.77              |
| 2:I:39:ILE:HD11   | 2:I:75:LEU:HG     | 1.66                     | 0.77              |
| 5:L:392:LYS:HD3   | 6:P:56:DC:H5''    | 1.65                     | 0.77              |
| 2:I:257:ALA:HB3   | 2:I:262:TYR:HE2   | 1.48                     | 0.76              |
| 5:L:585:GLU:OE2   | 5:L:588:ARG:NH2   | 2.16                     | 0.76              |
| 3:J:91:GLU:OE1    | 3:J:101:ARG:NH2   | 2.18                     | 0.76              |
| 1:H:214:GLU:HG2   | 1:H:218:ARG:HH12  | 1.49                     | 0.76              |
| 3:J:789:LYS:NZ    | 3:J:931:THR:O     | 2.18                     | 0.76              |
| 1:G:110:VAL:HG21  | 1:G:133:LEU:HD23  | 1.67                     | 0.76              |
| 3:J:401:VAL:HA    | 3:J:408:VAL:HG11  | 1.68                     | 0.76              |
| 3:J:518:VAL:HG11  | 3:J:707:ILE:CD1   | 2.16                     | 0.76              |
| 3:J:1081:VAL:HA   | 3:J:1088:VAL:HG23 | 1.66                     | 0.76              |
| 5:L:277:MET:SD    | 5:L:362:ASN:ND2   | 2.58                     | 0.76              |
| 2:I:883:LEU:HD11  | 2:I:920:VAL:HG22  | 1.68                     | 0.75              |
| 3:J:1220:ILE:HD12 | 3:J:1224:ARG:HH21 | 1.51                     | 0.75              |
| 3:J:1268:ASN:OD1  | 3:J:1301:THR:OG1  | 2.01                     | 0.75              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:L:402:LEU:HA   | 5:L:405:ILE:HG12  | 1.66                     | 0.75              |
| 2:I:238:GLN:HG2  | 2:I:286:GLU:HG2   | 1.67                     | 0.75              |
| 2:I:515:MET:HE3  | 2:I:517:GLN:HB3   | 1.67                     | 0.75              |
| 2:I:980:VAL:HA   | 2:I:984:VAL:HB    | 1.68                     | 0.75              |
| 2:I:1006:GLU:HA  | 2:I:1009:ASN:HB3  | 1.69                     | 0.75              |
| 3:J:799:ARG:NH1  | 3:J:1146:GLU:OE2  | 2.20                     | 0.75              |
| 3:J:807:LEU:HD11 | 3:J:894:VAL:HG23  | 1.67                     | 0.75              |
| 3:J:1199:PHE:HB2 | 3:J:1202:GLU:HG2  | 1.67                     | 0.75              |
| 3:J:363:LEU:HD21 | 3:J:618:VAL:HG13  | 1.68                     | 0.75              |
| 5:L:429:THR:HA   | 6:P:53:DT:H72     | 1.67                     | 0.75              |
| 1:H:107:ILE:HG12 | 1:H:135:ASP:HA    | 1.67                     | 0.75              |
| 3:J:510:LEU:O    | 3:J:514:THR:HG22  | 1.86                     | 0.75              |
| 3:J:857:LEU:HG   | 3:J:858:VAL:H     | 1.51                     | 0.75              |
| 1:G:140:ILE:HD12 | 1:G:142:MET:HE3   | 1.69                     | 0.75              |
| 1:H:190:ALA:HB2  | 1:H:200:LYS:HB2   | 1.69                     | 0.75              |
| 1:R:270:LEU:O    | 1:R:274:ALA:N     | 2.17                     | 0.75              |
| 1:H:206:GLU:OE1  | 3:J:531:LYS:NZ    | 2.20                     | 0.74              |
| 2:I:742:TYR:HB3  | 2:I:743:PRO:HD2   | 1.67                     | 0.74              |
| 3:J:1042:ASP:HA  | 3:J:1046:ILE:HG13 | 1.66                     | 0.74              |
| 1:G:83:LEU:HD21  | 2:I:693:LEU:HD21  | 1.68                     | 0.74              |
| 2:I:44:GLU:HG3   | 2:I:46:GLN:HG2    | 1.69                     | 0.74              |
| 3:J:141:PHE:HE2  | 3:J:296:LYS:HB2   | 1.51                     | 0.74              |
| 3:J:429:LEU:HB3  | 3:J:925:GLU:HB2   | 1.67                     | 0.74              |
| 3:J:982:LEU:HB2  | 3:J:997:VAL:HG23  | 1.67                     | 0.74              |
| 6:P:63:DT:H4'    | 6:P:64:DT:H5'     | 1.68                     | 0.74              |
| 3:J:902:ASP:HA   | 3:J:903:LEU:HG    | 1.69                     | 0.74              |
| 3:J:255:LEU:HD23 | 3:J:261:ALA:HB2   | 1.68                     | 0.74              |
| 1:H:205:MET:HE3  | 1:H:213:PRO:HA    | 1.70                     | 0.74              |
| 5:L:407:GLU:OE2  | 5:L:446:GLN:NE2   | 2.21                     | 0.74              |
| 1:H:196:THR:HG21 | 3:J:443:GLU:HG2   | 1.70                     | 0.73              |
| 5:L:387:VAL:HG22 | 5:L:435:ILE:HD13  | 1.70                     | 0.73              |
| 1:G:90:VAL:HG11  | 1:G:146:VAL:HG11  | 1.70                     | 0.73              |
| 1:H:22:THR:OG1   | 1:H:207:THR:O     | 2.06                     | 0.73              |
| 3:J:859:PRO:HD2  | 3:J:862:THR:HG21  | 1.70                     | 0.73              |
| 1:R:250:ASP:OD2  | 1:R:253:LEU:N     | 2.16                     | 0.73              |
| 2:I:471:VAL:HG21 | 2:I:493:ILE:HG13  | 1.71                     | 0.73              |
| 2:I:1085:MET:HE2 | 2:I:1085:MET:HA   | 1.71                     | 0.73              |
| 3:J:1041:ILE:N   | 3:J:1045:THR:OG1  | 2.22                     | 0.73              |
| 2:I:972:PHE:HA   | 2:I:975:ILE:HD12  | 1.69                     | 0.73              |
| 3:J:279:LEU:HD12 | 3:J:295:GLU:HG3   | 1.70                     | 0.73              |
| 3:J:822:MET:HE3  | 3:J:838:ARG:HB3   | 1.71                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:H:13:LEU:HA     | 1:H:28:LEU:HD23   | 1.70                     | 0.72              |
| 5:L:147:GLN:HB3   | 5:L:161:LEU:HD11  | 1.70                     | 0.72              |
| 2:I:11:ILE:O      | 2:I:1149:TYR:OH   | 2.06                     | 0.72              |
| 2:I:817:LEU:HD11  | 2:I:1080:ASN:HD22 | 1.52                     | 0.72              |
| 2:I:1117:LEU:HD12 | 2:I:1195:ILE:HG12 | 1.71                     | 0.72              |
| 2:I:302:ILE:HG22  | 2:I:309:LEU:HA    | 1.69                     | 0.72              |
| 2:I:758:ARG:NH2   | 2:I:762:ASN:OD1   | 2.20                     | 0.72              |
| 2:I:953:LEU:HD11  | 2:I:1033:ARG:HG2  | 1.71                     | 0.72              |
| 3:J:1061:VAL:HG21 | 3:J:1101:LEU:HD12 | 1.71                     | 0.72              |
| 2:I:621:SER:HB2   | 2:I:653:MET:HE3   | 1.72                     | 0.72              |
| 2:I:12:ARG:NH2    | 2:I:793:GLU:OE1   | 2.23                     | 0.72              |
| 3:J:958:ILE:HD13  | 3:J:984:LEU:HD13  | 1.71                     | 0.72              |
| 2:I:303:ASP:HB2   | 2:I:310:ILE:HD11  | 1.72                     | 0.72              |
| 3:J:1057:SER:OG   | 3:J:1110:GLU:OE2  | 2.08                     | 0.71              |
| 2:I:689:ALA:CB    | 2:I:1233:LEU:HD12 | 2.21                     | 0.71              |
| 3:J:1326:GLN:HE21 | 7:Q:32:DA:H5"     | 1.56                     | 0.71              |
| 5:L:320:ILE:HG23  | 5:L:327:SER:HB3   | 1.72                     | 0.71              |
| 1:H:35:PHE:HA     | 1:H:38:THR:HG22   | 1.72                     | 0.71              |
| 3:J:902:ASP:HA    | 3:J:903:LEU:CG    | 2.20                     | 0.71              |
| 3:J:844:THR:OG1   | 3:J:860:ARG:O     | 2.08                     | 0.71              |
| 5:L:163:THR:O     | 5:L:260:ARG:NE    | 2.23                     | 0.71              |
| 7:Q:77:DT:H3'     | 1:R:296:GLY:HA3   | 1.72                     | 0.71              |
| 1:G:38:THR:OG1    | 1:H:45:ARG:NH1    | 2.23                     | 0.71              |
| 3:J:697:MET:HE2   | 3:J:741:ALA:HB3   | 1.71                     | 0.71              |
| 2:I:617:ALA:N     | 2:I:652:TYR:O     | 2.22                     | 0.71              |
| 4:K:25:ARG:NH2    | 4:K:68:GLU:OE1    | 2.23                     | 0.71              |
| 2:I:22:LEU:HD13   | 2:I:603:ILE:HD13  | 1.73                     | 0.71              |
| 3:J:665:GLN:OE1   | 3:J:678:ARG:NH2   | 2.21                     | 0.71              |
| 5:L:533:ASP:HA    | 5:L:536:THR:HG22  | 1.71                     | 0.71              |
| 1:G:135:ASP:HB3   | 1:G:138:ALA:HB3   | 1.73                     | 0.71              |
| 3:J:680:ASN:HA    | 3:J:683:ILE:HG22  | 1.73                     | 0.70              |
| 3:J:1107:VAL:HG22 | 3:J:1122:ALA:HB2  | 1.73                     | 0.70              |
| 2:I:254:ASP:OD1   | 2:I:265:LYS:N     | 2.24                     | 0.70              |
| 2:I:594:VAL:HG22  | 2:I:599:VAL:HG22  | 1.72                     | 0.70              |
| 3:J:1031:VAL:HG12 | 3:J:1091:PRO:HD3  | 1.73                     | 0.70              |
| 3:J:1109:LEU:HD23 | 3:J:1113:VAL:HG12 | 1.74                     | 0.70              |
| 2:I:1254:VAL:O    | 3:J:99:ARG:NH2    | 2.23                     | 0.70              |
| 5:L:151:VAL:HG21  | 5:L:161:LEU:HB2   | 1.74                     | 0.70              |
| 2:I:560:PRO:O     | 3:J:780:ARG:NH2   | 2.25                     | 0.70              |
| 2:I:975:ILE:HG12  | 2:I:1014:LEU:HG   | 1.75                     | 0.69              |
| 3:J:977:SER:OG    | 3:J:980:THR:OG1   | 2.09                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:1062:LEU:O    | 3:J:1067:ARG:NH2  | 2.25                     | 0.69              |
| 3:J:1174:ARG:NH2  | 3:J:1187:GLU:OE1  | 2.25                     | 0.69              |
| 3:J:930:LEU:HD11  | 3:J:1241:TYR:CE1  | 2.27                     | 0.69              |
| 2:I:1103:VAL:HG22 | 2:I:1111:GLN:HE21 | 1.57                     | 0.69              |
| 2:I:1219:GLU:OE2  | 3:J:538:ARG:NH1   | 2.26                     | 0.69              |
| 3:J:218:THR:HA    | 3:J:221:ILE:HG22  | 1.75                     | 0.69              |
| 1:G:23:HIS:HB2    | 1:G:205:MET:O     | 1.92                     | 0.69              |
| 2:I:817:LEU:HD11  | 2:I:1085:MET:HE1  | 1.72                     | 0.69              |
| 3:J:951:GLN:OE1   | 3:J:1016:THR:OG1  | 2.10                     | 0.69              |
| 3:J:963:VAL:HG23  | 3:J:975:ILE:HG12  | 1.75                     | 0.69              |
| 3:J:1206:ARG:HH21 | 3:J:1223:LEU:HD13 | 1.56                     | 0.69              |
| 2:I:1122:LYS:HG2  | 2:I:1229:TYR:CZ   | 2.28                     | 0.69              |
| 1:R:273:GLU:OE1   | 1:R:284:ARG:NH1   | 2.26                     | 0.69              |
| 1:H:105:SER:HA    | 1:H:138:ALA:CB    | 2.21                     | 0.69              |
| 2:I:657:THR:HG21  | 2:I:1188:ASP:HB2  | 1.73                     | 0.69              |
| 3:J:872:LEU:HD23  | 3:J:877:VAL:HG21  | 1.75                     | 0.69              |
| 5:L:598:LEU:O     | 5:L:604:SER:OG    | 2.05                     | 0.69              |
| 3:J:270:ARG:NH1   | 5:L:449:THR:OG1   | 2.25                     | 0.69              |
| 2:I:176:ILE:HD11  | 2:I:428:VAL:HG21  | 1.74                     | 0.69              |
| 3:J:318:GLY:N     | 3:J:322:ARG:O     | 2.16                     | 0.69              |
| 3:J:1038:THR:OG1  | 3:J:1077:ALA:O    | 2.11                     | 0.69              |
| 3:J:1072:LYS:O    | 3:J:1075:ARG:NH1  | 2.24                     | 0.69              |
| 7:Q:19:DT:H3'     | 7:Q:19:DT:OP2     | 1.93                     | 0.69              |
| 2:I:214:ASN:HB3   | 2:I:359:ARG:HD2   | 1.75                     | 0.68              |
| 5:L:137:TYR:CE2   | 5:L:139:GLU:HB2   | 2.27                     | 0.68              |
| 5:L:512:GLY:HA3   | 5:L:513:ASP:CG    | 2.18                     | 0.68              |
| 1:R:255:ARG:HB3   | 1:R:278:ILE:HD12  | 1.75                     | 0.68              |
| 2:I:60:GLN:O      | 2:I:476:LYS:NZ    | 2.25                     | 0.68              |
| 3:J:385:LEU:HD21  | 3:J:411:ILE:HG13  | 1.75                     | 0.68              |
| 1:G:90:VAL:HG23   | 1:G:123:ILE:HD13  | 1.74                     | 0.68              |
| 3:J:255:LEU:HD11  | 3:J:259:ARG:HB2   | 1.74                     | 0.68              |
| 3:J:1108:GLN:HG3  | 3:J:1109:LEU:HD12 | 1.75                     | 0.68              |
| 2:I:714:VAL:HB    | 2:I:787:PRO:HD2   | 1.73                     | 0.68              |
| 5:L:606:VAL:O     | 5:L:609:SER:OG    | 2.11                     | 0.68              |
| 2:I:1116:HIS:HE1  | 3:J:641:ILE:H     | 1.41                     | 0.68              |
| 2:I:1304:MET:HE3  | 2:I:1308:ILE:HD11 | 1.75                     | 0.68              |
| 2:I:453:ILE:HD11  | 2:I:587:LEU:HD11  | 1.73                     | 0.68              |
| 3:J:930:LEU:HD11  | 3:J:1241:TYR:HE1  | 1.58                     | 0.68              |
| 3:J:438:GLU:HG3   | 3:J:485:MET:HE1   | 1.76                     | 0.68              |
| 3:J:554:GLU:OE1   | 3:J:589:TYR:N     | 2.24                     | 0.68              |
| 5:L:261:LEU:HD23  | 5:L:265:GLN:HB3   | 1.76                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:P:39:DG:H1'     | 6:P:40:DC:H5'     | 1.76                     | 0.68              |
| 1:H:64:VAL:HG12   | 1:H:66:HIS:H      | 1.57                     | 0.68              |
| 3:J:1028:ILE:HG22 | 3:J:1120:THR:HA   | 1.75                     | 0.68              |
| 2:I:704:MET:O     | 2:I:708:VAL:HG23  | 1.93                     | 0.68              |
| 3:J:490:ILE:HG13  | 3:J:491:LEU:HD12  | 1.76                     | 0.68              |
| 2:I:1212:LEU:HD11 | 2:I:1227:VAL:HG11 | 1.75                     | 0.67              |
| 3:J:134:ASP:OD1   | 3:J:159:ILE:HD12  | 1.93                     | 0.67              |
| 3:J:1046:ILE:HB   | 3:J:1059:LEU:HB3  | 1.76                     | 0.67              |
| 3:J:513:MET:HE1   | 3:J:579:LEU:HB2   | 1.76                     | 0.67              |
| 1:G:192:VAL:HG11  | 1:G:198:LEU:HD12  | 1.76                     | 0.67              |
| 3:J:807:LEU:HD23  | 3:J:1255:VAL:HG23 | 1.75                     | 0.67              |
| 2:I:46:GLN:O      | 2:I:51:ALA:HB2    | 1.94                     | 0.67              |
| 2:I:483:ASP:HB2   | 2:I:486:THR:HG22  | 1.76                     | 0.67              |
| 2:I:131:THR:HG22  | 2:I:132:ASP:H     | 1.60                     | 0.67              |
| 3:J:914:ALA:HB2   | 3:J:1359:ALA:HB1  | 1.76                     | 0.67              |
| 4:K:3:ARG:NH2     | 4:K:55:GLU:OE1    | 2.22                     | 0.67              |
| 2:I:5:TYR:OH      | 2:I:1171:ARG:NH1  | 2.23                     | 0.67              |
| 2:I:1314:GLN:HG2  | 4:K:28:ARG:NH2    | 2.08                     | 0.67              |
| 3:J:514:THR:CG2   | 3:J:596:LEU:HB2   | 2.25                     | 0.67              |
| 3:J:1233:ILE:O    | 3:J:1237:VAL:HG12 | 1.95                     | 0.67              |
| 5:L:456:MET:CE    | 5:L:497:VAL:HG22  | 2.24                     | 0.67              |
| 3:J:801:VAL:HG12  | 3:J:920:ALA:HB3   | 1.77                     | 0.67              |
| 3:J:1175:LEU:HD22 | 3:J:1190:ILE:HD11 | 1.76                     | 0.67              |
| 2:I:877:VAL:HG21  | 2:I:920:VAL:HG21  | 1.77                     | 0.66              |
| 5:L:162:ILE:HD13  | 5:L:221:PHE:HZ    | 1.60                     | 0.66              |
| 2:I:975:ILE:HG23  | 2:I:1014:LEU:HD21 | 1.77                     | 0.66              |
| 5:L:287:ILE:HD13  | 5:L:341:LEU:HD12  | 1.77                     | 0.66              |
| 2:I:810:TYR:O     | 2:I:1077:SER:OG   | 2.12                     | 0.66              |
| 2:I:838:CYS:HB2   | 2:I:918:LEU:HD22  | 1.78                     | 0.66              |
| 2:I:902:LEU:HD21  | 5:L:611:LEU:HD21  | 1.76                     | 0.66              |
| 3:J:697:MET:HE1   | 3:J:737:ILE:HG22  | 1.76                     | 0.66              |
| 3:J:759:ILE:HG23  | 3:J:771:GLN:HB3   | 1.77                     | 0.66              |
| 3:J:964:LYS:O     | 3:J:976:THR:OG1   | 2.11                     | 0.66              |
| 5:L:98:VAL:O      | 5:L:102:MET:HG2   | 1.95                     | 0.66              |
| 2:I:207:THR:OG1   | 2:I:354:ASP:OD2   | 2.12                     | 0.66              |
| 3:J:1031:VAL:CG1  | 3:J:1090:ILE:HA   | 2.25                     | 0.66              |
| 3:J:1044:GLN:HG2  | 3:J:1068:THR:OG1  | 1.95                     | 0.66              |
| 2:I:30:ILE:HD12   | 2:I:30:ILE:H      | 1.60                     | 0.66              |
| 2:I:565:GLU:HA    | 2:I:569:ILE:HG12  | 1.78                     | 0.66              |
| 3:J:79:LYS:HG2    | 5:L:569:THR:HG22  | 1.77                     | 0.66              |
| 3:J:334:LYS:NZ    | 7:Q:35:DG:OP2     | 2.24                     | 0.66              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:L:309:ASN:ND2  | 5:L:312:SER:HB3   | 2.10                     | 0.66              |
| 2:I:484:LEU:HD12 | 2:I:485:ASP:HB2   | 1.77                     | 0.66              |
| 3:J:822:MET:CE   | 3:J:838:ARG:HB3   | 2.26                     | 0.66              |
| 2:I:840:SER:HB2  | 2:I:850:ILE:HD11  | 1.78                     | 0.66              |
| 3:J:1199:PHE:HB2 | 3:J:1202:GLU:CG   | 2.26                     | 0.66              |
| 2:I:1080:ASN:HB2 | 2:I:1085:MET:HE3  | 1.78                     | 0.66              |
| 3:J:1348:LYS:O   | 3:J:1352:ILE:HG12 | 1.95                     | 0.66              |
| 1:G:218:ARG:NH2  | 1:H:233:ASP:OD1   | 2.28                     | 0.66              |
| 2:I:590:PRO:HG3  | 2:I:605:TYR:CE1   | 2.31                     | 0.66              |
| 3:J:141:PHE:CE1  | 3:J:181:GLY:HA3   | 2.31                     | 0.66              |
| 3:J:515:ARG:HG2  | 3:J:516:ASP:H     | 1.61                     | 0.66              |
| 4:K:38:LEU:HD22  | 4:K:58:LEU:HD13   | 1.76                     | 0.66              |
| 5:L:420:GLU:HG3  | 5:L:422:ARG:HH21  | 1.61                     | 0.65              |
| 2:I:744:GLY:O    | 2:I:745:GLU:HG3   | 1.95                     | 0.65              |
| 2:I:983:GLY:HA3  | 2:I:1002:LEU:HD11 | 1.78                     | 0.65              |
| 3:J:357:VAL:HG22 | 3:J:461:PHE:CD2   | 2.31                     | 0.65              |
| 3:J:650:LYS:HE3  | 3:J:654:ILE:HD11  | 1.77                     | 0.65              |
| 5:L:227:GLN:HA   | 5:L:230:VAL:HG12  | 1.78                     | 0.65              |
| 5:L:289:LYS:HA   | 5:L:293:GLU:OE1   | 1.95                     | 0.65              |
| 2:I:324:LYS:O    | 2:I:327:GLN:NE2   | 2.23                     | 0.65              |
| 3:J:384:LYS:HE3  | 3:J:415:VAL:HG12  | 1.78                     | 0.65              |
| 2:I:269:ILE:HG23 | 2:I:273:HIS:HB2   | 1.77                     | 0.65              |
| 3:J:510:LEU:HD22 | 3:J:601:ILE:HD11  | 1.78                     | 0.65              |
| 3:J:516:ASP:HA   | 3:J:545:HIS:HB2   | 1.79                     | 0.65              |
| 5:L:470:MET:SD   | 5:L:486:ARG:NH1   | 2.70                     | 0.65              |
| 2:I:1283:ALA:HB1 | 2:I:1286:THR:HB   | 1.77                     | 0.65              |
| 1:R:257:VAL:HG12 | 1:R:260:LEU:HD11  | 1.78                     | 0.65              |
| 2:I:794:LEU:HG   | 2:I:796:LEU:HD13  | 1.79                     | 0.65              |
| 3:J:966:VAL:O    | 3:J:974:VAL:HG22  | 1.97                     | 0.65              |
| 7:Q:27:DA:H2''   | 7:Q:28:DT:H5'     | 1.77                     | 0.65              |
| 2:I:975:ILE:CG2  | 2:I:1014:LEU:HD21 | 2.27                     | 0.65              |
| 1:R:297:LYS:O    | 1:R:301:THR:OG1   | 2.07                     | 0.65              |
| 1:G:110:VAL:CG2  | 1:G:133:LEU:HD23  | 2.27                     | 0.65              |
| 2:I:1006:GLU:O   | 2:I:1009:ASN:C    | 2.40                     | 0.65              |
| 2:I:559:CYS:HB2  | 2:I:662:SER:HB3   | 1.78                     | 0.64              |
| 3:J:264:ASP:OD1  | 5:L:506:SER:OG    | 2.14                     | 0.64              |
| 3:J:156:ARG:NH2  | 3:J:191:SER:OG    | 2.27                     | 0.64              |
| 3:J:430:HIS:HB3  | 3:J:925:GLU:HG2   | 1.78                     | 0.64              |
| 3:J:863:LEU:HD22 | 3:J:908:ILE:HG23  | 1.79                     | 0.64              |
| 5:L:113:ARG:O    | 5:L:117:ILE:HG12  | 1.97                     | 0.64              |
| 2:I:796:LEU:HB3  | 2:I:1233:LEU:CD1  | 2.27                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:J:527:LEU:HD13 | 3:J:548:VAL:CG1  | 2.27                     | 0.64              |
| 3:J:1022:PRO:O   | 3:J:1126:GLN:NE2 | 2.30                     | 0.64              |
| 2:I:9:LYS:NZ     | 2:I:775:GLU:OE2  | 2.26                     | 0.64              |
| 3:J:661:VAL:HG12 | 3:J:685:ILE:HG21 | 1.80                     | 0.64              |
| 4:K:36:ASP:OD1   | 4:K:37:PRO:HD2   | 1.97                     | 0.64              |
| 3:J:511:TYR:OH   | 3:J:515:ARG:NH1  | 2.31                     | 0.64              |
| 3:J:697:MET:CE   | 3:J:741:ALA:HB3  | 2.28                     | 0.64              |
| 5:L:300:LYS:O    | 5:L:304:THR:OG1  | 2.14                     | 0.64              |
| 1:G:135:ASP:HB3  | 1:G:138:ALA:CB   | 2.28                     | 0.64              |
| 3:J:214:ARG:NH2  | 3:J:1276:GLU:OE2 | 2.31                     | 0.64              |
| 3:J:385:LEU:CD2  | 3:J:411:ILE:HG13 | 2.28                     | 0.64              |
| 3:J:520:ALA:HB3  | 3:J:546:ALA:CB   | 2.28                     | 0.64              |
| 3:J:1267:VAL:O   | 3:J:1276:GLU:HB2 | 1.98                     | 0.64              |
| 2:I:518:ASN:O    | 2:I:691:PRO:HD3  | 1.98                     | 0.64              |
| 2:I:673:HIS:HB3  | 2:I:1109:ILE:CG2 | 2.28                     | 0.64              |
| 3:J:848:VAL:O    | 3:J:857:LEU:HB3  | 1.97                     | 0.64              |
| 5:L:234:THR:OG1  | 5:L:248:GLU:OE1  | 2.07                     | 0.64              |
| 5:L:463:LEU:HD23 | 5:L:487:MET:SD   | 2.38                     | 0.64              |
| 1:H:82:LEU:HD22  | 1:H:173:VAL:HG22 | 1.80                     | 0.64              |
| 1:H:107:ILE:CG1  | 1:H:135:ASP:HA   | 2.27                     | 0.64              |
| 2:I:240:GLU:CG   | 2:I:284:LEU:HD13 | 2.28                     | 0.64              |
| 6:P:56:DC:H2'    | 6:P:57:DT:H71    | 1.80                     | 0.64              |
| 2:I:1130:ALA:O   | 2:I:1134:GLN:NE2 | 2.30                     | 0.64              |
| 1:H:69:SER:HB2   | 1:H:78:ILE:CD1   | 2.28                     | 0.63              |
| 3:J:510:LEU:HD22 | 3:J:601:ILE:CD1  | 2.28                     | 0.63              |
| 2:I:1223:ARG:NH2 | 3:J:721:SER:OG   | 2.31                     | 0.63              |
| 3:J:259:ARG:NH1  | 5:L:502:LYS:HB2  | 2.14                     | 0.63              |
| 3:J:423:LEU:HB3  | 3:J:466:MET:CE   | 2.29                     | 0.63              |
| 6:P:27:DT:H1'    | 6:P:28:DG:H5'    | 1.81                     | 0.63              |
| 1:G:187:VAL:HA   | 1:G:200:LYS:O    | 1.98                     | 0.63              |
| 2:I:3:TYR:OH     | 2:I:1157:GLN:OE1 | 2.17                     | 0.63              |
| 2:I:149:LEU:HD12 | 2:I:452:ARG:O    | 1.98                     | 0.63              |
| 2:I:241:LEU:N    | 2:I:283:LYS:O    | 2.28                     | 0.63              |
| 2:I:373:GLY:O    | 5:L:103:ARG:HD3  | 1.99                     | 0.63              |
| 3:J:823:THR:HG22 | 3:J:879:ALA:HB1  | 1.80                     | 0.63              |
| 5:L:246:GLN:O    | 5:L:250:LEU:HG   | 1.98                     | 0.63              |
| 2:I:930:ASP:HB3  | 2:I:1053:TYR:HD2 | 1.63                     | 0.63              |
| 3:J:80:HIS:O     | 3:J:83:VAL:HG12  | 1.99                     | 0.63              |
| 3:J:1090:ILE:CD1 | 3:J:1097:ALA:HB2 | 2.28                     | 0.63              |
| 5:L:314:THR:O    | 5:L:318:ALA:HB3  | 1.98                     | 0.63              |
| 1:H:69:SER:HB2   | 1:H:78:ILE:HD12  | 1.80                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:H:83:LEU:HD11   | 3:J:526:VAL:HB    | 1.80                     | 0.63              |
| 3:J:416:ILE:HG13  | 3:J:441:LEU:HD21  | 1.81                     | 0.63              |
| 1:G:45:ARG:HH21   | 2:I:1216:ARG:HA   | 1.64                     | 0.63              |
| 2:I:1066:MET:HE2  | 2:I:1076:ILE:CG1  | 2.28                     | 0.63              |
| 3:J:1259:GLN:OE1  | 3:J:1262:ARG:NH1  | 2.31                     | 0.63              |
| 1:G:29:GLU:HB2    | 1:G:30:PRO:HD3    | 1.79                     | 0.63              |
| 3:J:850:LYS:HB3   | 3:J:854:ALA:HB3   | 1.80                     | 0.63              |
| 2:I:865:LEU:HD22  | 2:I:869:GLY:O     | 1.98                     | 0.62              |
| 5:L:338:HIS:O     | 5:L:342:GLN:HG2   | 1.98                     | 0.62              |
| 1:H:98:VAL:HG11   | 1:H:121:VAL:HG22  | 1.81                     | 0.62              |
| 2:I:56:VAL:HG11   | 2:I:468:LEU:HB3   | 1.79                     | 0.62              |
| 2:I:960:LEU:HB3   | 2:I:1025:PHE:CE1  | 2.33                     | 0.62              |
| 3:J:853:THR:O     | 3:J:855:ASP:N     | 2.32                     | 0.62              |
| 2:I:699:LEU:HB2   | 2:I:799:ASN:ND2   | 2.14                     | 0.62              |
| 3:J:210:SER:HB3   | 3:J:213:LYS:HB3   | 1.81                     | 0.62              |
| 3:J:1033:GLY:C    | 3:J:1114:GLN:HG3  | 2.24                     | 0.62              |
| 5:L:420:GLU:HG3   | 5:L:422:ARG:HE    | 1.63                     | 0.62              |
| 1:G:45:ARG:NH2    | 2:I:1216:ARG:HA   | 2.14                     | 0.62              |
| 5:L:437:GLN:HB2   | 6:P:49:DC:N4      | 2.15                     | 0.62              |
| 1:G:235:ARG:H     | 1:H:13:LEU:HD23   | 1.64                     | 0.62              |
| 2:I:594:VAL:HG22  | 2:I:599:VAL:HA    | 1.81                     | 0.62              |
| 2:I:1242:LYS:HD2  | 3:J:465:GLN:NE2   | 2.14                     | 0.62              |
| 3:J:810:THR:HG22  | 3:J:893:GLY:HA3   | 1.81                     | 0.62              |
| 3:J:962:ASN:O     | 3:J:980:THR:OG1   | 2.13                     | 0.62              |
| 5:L:561:MET:HA    | 5:L:567:MET:CE    | 2.29                     | 0.62              |
| 1:R:257:VAL:HG13  | 1:R:276:HIS:O     | 2.00                     | 0.62              |
| 1:G:57:THR:HG21   | 1:G:147:GLN:HE21  | 1.63                     | 0.62              |
| 3:J:259:ARG:HH12  | 5:L:502:LYS:HB2   | 1.64                     | 0.62              |
| 1:G:59:VAL:HG21   | 1:G:85:LEU:HD12   | 1.81                     | 0.62              |
| 2:I:593:LYS:HA    | 2:I:652:TYR:CD1   | 2.34                     | 0.62              |
| 5:L:493:LYS:O     | 5:L:497:VAL:HG23  | 2.00                     | 0.62              |
| 2:I:1060:ILE:HD11 | 2:I:1076:ILE:HD11 | 1.81                     | 0.62              |
| 2:I:1259:LEU:HD23 | 2:I:1264:GLN:HB3  | 1.80                     | 0.62              |
| 5:L:165:PHE:HD1   | 5:L:259:PHE:HA    | 1.65                     | 0.62              |
| 5:L:333:VAL:HG22  | 5:L:337:VAL:HG23  | 1.82                     | 0.62              |
| 1:G:51:MET:HE1    | 1:G:216:ALA:HA    | 1.81                     | 0.62              |
| 3:J:872:LEU:CD2   | 3:J:877:VAL:HG21  | 2.30                     | 0.62              |
| 3:J:1175:LEU:HB2  | 3:J:1190:ILE:HD12 | 1.80                     | 0.62              |
| 7:Q:32:DA:H2''    | 7:Q:33:DA:C5'     | 2.29                     | 0.62              |
| 1:H:59:VAL:O      | 1:H:171:LEU:HB2   | 2.00                     | 0.61              |
| 3:J:1077:ALA:HB2  | 3:J:1100:PHE:CE1  | 2.35                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:1162:ILE:HG22 | 3:J:1178:THR:O    | 1.99                     | 0.61              |
| 5:L:547:VAL:HG21  | 5:L:607:LEU:HD21  | 1.82                     | 0.61              |
| 3:J:141:PHE:CA    | 3:J:180:MET:HE2   | 2.29                     | 0.61              |
| 2:I:854:ILE:HD11  | 2:I:885:GLY:HA2   | 1.81                     | 0.61              |
| 2:I:1277:ALA:HB3  | 3:J:434:ILE:HD12  | 1.82                     | 0.61              |
| 7:Q:15:DT:H2"     | 7:Q:16:DC:OP2     | 1.99                     | 0.61              |
| 1:R:275:ILE:HG23  | 1:R:280:ASP:HB3   | 1.82                     | 0.61              |
| 1:G:8:PHE:HA      | 1:G:32:GLU:OE2    | 2.01                     | 0.61              |
| 2:I:235:ASN:OD1   | 2:I:236:LYS:HG2   | 2.01                     | 0.61              |
| 2:I:1018:TYR:O    | 2:I:1022:LYS:HG2  | 1.99                     | 0.61              |
| 3:J:1186:TYR:OH   | 3:J:1188:GLU:OE1  | 2.18                     | 0.61              |
| 2:I:229:ILE:HG23  | 2:I:332:ARG:HD2   | 1.82                     | 0.61              |
| 2:I:1248:THR:HG21 | 5:L:531:PRO:HG3   | 1.82                     | 0.61              |
| 3:J:1347:LEU:HG   | 3:J:1357:ILE:HG23 | 1.83                     | 0.61              |
| 7:Q:21:DT:H2"     | 7:Q:22:DG:C8      | 2.36                     | 0.61              |
| 1:G:12:ARG:O      | 1:G:14:VAL:HG23   | 2.00                     | 0.61              |
| 1:G:224:LEU:HD22  | 1:H:228:LEU:CD1   | 2.30                     | 0.61              |
| 3:J:1046:ILE:CD1  | 3:J:1059:LEU:HD13 | 2.31                     | 0.61              |
| 1:R:300:LEU:CD1   | 1:R:304:LYS:HE2   | 2.31                     | 0.61              |
| 2:I:611:GLU:OE2   | 2:I:637:ARG:NH2   | 2.31                     | 0.61              |
| 3:J:1355:ARG:HH12 | 3:J:1369:ARG:HH22 | 1.47                     | 0.61              |
| 1:R:300:LEU:HD21  | 1:R:314:LEU:HD11  | 1.82                     | 0.61              |
| 2:I:726:TYR:CE2   | 2:I:728:ASP:HB2   | 2.35                     | 0.61              |
| 2:I:817:LEU:HD11  | 2:I:1080:ASN:ND2  | 2.15                     | 0.61              |
| 3:J:368:LEU:CD2   | 3:J:373:ALA:HB2   | 2.30                     | 0.61              |
| 2:I:796:LEU:HB3   | 2:I:1233:LEU:HD11 | 1.82                     | 0.61              |
| 3:J:253:VAL:HG11  | 5:L:523:ILE:HG21  | 1.81                     | 0.61              |
| 3:J:268:LEU:HB3   | 3:J:306:LEU:HD23  | 1.82                     | 0.61              |
| 3:J:975:ILE:HD13  | 3:J:980:THR:HG21  | 1.82                     | 0.61              |
| 5:L:261:LEU:HB3   | 5:L:265:GLN:HB2   | 1.83                     | 0.61              |
| 1:G:13:LEU:CD2    | 1:G:214:GLU:HG3   | 2.30                     | 0.61              |
| 1:G:81:ILE:HG12   | 1:G:131:CYS:HB3   | 1.81                     | 0.61              |
| 1:H:33:ARG:NH1    | 2:I:1081:PRO:HG3  | 2.15                     | 0.61              |
| 2:I:992:LEU:HB2   | 2:I:993:PRO:HD2   | 1.82                     | 0.61              |
| 3:J:1173:ARG:HG3  | 3:J:1190:ILE:HB   | 1.81                     | 0.61              |
| 2:I:6:THR:OG1     | 2:I:781:ASP:OD1   | 2.02                     | 0.60              |
| 2:I:1113:LEU:HD11 | 3:J:641:ILE:HD13  | 1.83                     | 0.60              |
| 5:L:216:LEU:O     | 5:L:220:LYS:HG2   | 2.01                     | 0.60              |
| 5:L:287:ILE:HG23  | 5:L:337:VAL:HG13  | 1.83                     | 0.60              |
| 2:I:560:PRO:HB3   | 3:J:776:THR:HG21  | 1.83                     | 0.60              |
| 3:J:68:TYR:HA     | 3:J:92:VAL:HG23   | 1.82                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:971:LEU:HD23  | 2:I:975:ILE:HD11  | 1.83                     | 0.60              |
| 2:I:1305:TYR:CE1  | 3:J:379:PRO:HG3   | 2.37                     | 0.60              |
| 2:I:1312:ASN:OD1  | 2:I:1314:GLN:HG3  | 2.01                     | 0.60              |
| 4:K:3:ARG:HD2     | 4:K:5:THR:O       | 2.01                     | 0.60              |
| 1:G:42:ALA:O      | 1:G:46:ILE:HG12   | 2.00                     | 0.60              |
| 1:H:101:THR:HG22  | 1:H:116:THR:HG21  | 1.82                     | 0.60              |
| 2:I:216:THR:OG1   | 2:I:219:GLN:OE1   | 2.19                     | 0.60              |
| 2:I:517:GLN:O     | 2:I:517:GLN:HG3   | 2.00                     | 0.60              |
| 2:I:805:MET:HE1   | 2:I:1221:PHE:CZ   | 2.37                     | 0.60              |
| 2:I:1132:LEU:HD21 | 2:I:1141:LEU:HD21 | 1.82                     | 0.60              |
| 5:L:101:TYR:CE2   | 5:L:405:ILE:HD12  | 2.36                     | 0.60              |
| 5:L:297:MET:HE2   | 5:L:302:PHE:HA    | 1.82                     | 0.60              |
| 7:Q:74:DA:C8      | 7:Q:75:DT:H72     | 2.37                     | 0.60              |
| 2:I:296:VAL:HA    | 2:I:316:GLU:HA    | 1.82                     | 0.60              |
| 1:H:102:LEU:HD23  | 1:H:142:MET:SD    | 2.42                     | 0.60              |
| 2:I:118:LYS:CE    | 2:I:488:MET:HG2   | 2.32                     | 0.60              |
| 3:J:38:VAL:HG11   | 3:J:56:LEU:HD12   | 1.83                     | 0.60              |
| 3:J:1148:ARG:NH1  | 6:P:66:DG:H5"     | 2.17                     | 0.60              |
| 5:L:463:LEU:HD21  | 5:L:494:ILE:HG12  | 1.83                     | 0.60              |
| 2:I:150:HIS:NE2   | 2:I:454:ARG:HG3   | 2.16                     | 0.60              |
| 2:I:1243:MET:HA   | 3:J:353:SER:HB3   | 1.82                     | 0.60              |
| 3:J:800:LEU:HB3   | 3:J:920:ALA:HB1   | 1.83                     | 0.60              |
| 3:J:1071:GLY:HA2  | 3:J:1074:LEU:HB2  | 1.83                     | 0.60              |
| 3:J:1267:VAL:N    | 3:J:1301:THR:O    | 2.33                     | 0.60              |
| 5:L:271:ASN:O     | 5:L:275:VAL:HG23  | 2.02                     | 0.60              |
| 1:R:290:LEU:HA    | 1:R:295:LEU:HD22  | 1.84                     | 0.60              |
| 2:I:1109:ILE:HD11 | 3:J:644:MET:HE1   | 1.82                     | 0.60              |
| 3:J:279:LEU:HD11  | 3:J:296:LYS:HG2   | 1.83                     | 0.60              |
| 3:J:407:VAL:O     | 3:J:411:ILE:HG12  | 2.01                     | 0.60              |
| 3:J:98:ARG:O      | 3:J:247:PRO:HD2   | 2.02                     | 0.60              |
| 3:J:823:THR:HG22  | 3:J:879:ALA:CB    | 2.32                     | 0.60              |
| 3:J:1149:ARG:NH2  | 3:J:1153:PRO:HG3  | 2.17                     | 0.60              |
| 2:I:269:ILE:HG23  | 2:I:273:HIS:CB    | 2.31                     | 0.60              |
| 3:J:646:ILE:HD12  | 3:J:762:ASN:HD21  | 1.65                     | 0.60              |
| 5:L:137:TYR:HE2   | 5:L:139:GLU:HB2   | 1.66                     | 0.60              |
| 5:L:561:MET:HG2   | 5:L:576:VAL:HG22  | 1.83                     | 0.60              |
| 3:J:398:LYS:HD2   | 5:L:532:LEU:CD2   | 2.31                     | 0.59              |
| 3:J:1227:HIS:HA   | 3:J:1230:THR:HG22 | 1.84                     | 0.59              |
| 5:L:339:ARG:HA    | 5:L:342:GLN:CG    | 2.31                     | 0.59              |
| 1:G:68:TYR:HB3    | 2:I:756:TYR:HD2   | 1.66                     | 0.59              |
| 2:I:27:LEU:HB2    | 2:I:524:ILE:HD11  | 1.82                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:118:LYS:HE2   | 2:I:488:MET:HA    | 1.84                     | 0.59              |
| 1:G:224:LEU:HD22  | 1:H:228:LEU:HD11  | 1.84                     | 0.59              |
| 3:J:268:LEU:CB    | 3:J:306:LEU:HD23  | 2.31                     | 0.59              |
| 3:J:1109:LEU:HD22 | 3:J:1115:ILE:HG22 | 1.84                     | 0.59              |
| 5:L:148:TYR:CE1   | 5:L:158:LEU:HD21  | 2.37                     | 0.59              |
| 1:H:35:PHE:HA     | 1:H:38:THR:CG2    | 2.31                     | 0.59              |
| 2:I:33:ASP:O      | 2:I:37:LYS:HG2    | 2.02                     | 0.59              |
| 2:I:905:ILE:HG22  | 2:I:906:PHE:CD1   | 2.36                     | 0.59              |
| 3:J:197:GLU:OE2   | 3:J:220:ARG:NH2   | 2.29                     | 0.59              |
| 5:L:505:ILE:H     | 5:L:505:ILE:HD12  | 1.66                     | 0.59              |
| 1:G:234:LEU:HD22  | 1:H:13:LEU:HD22   | 1.85                     | 0.59              |
| 2:I:854:ILE:HD11  | 2:I:885:GLY:CA    | 2.33                     | 0.59              |
| 2:I:1293:VAL:HG21 | 2:I:1315:MET:HE3  | 1.83                     | 0.59              |
| 1:R:260:LEU:HD13  | 1:R:281:LEU:HD22  | 1.82                     | 0.59              |
| 7:Q:50:DC:H2'     | 7:Q:51:DT:H71     | 1.84                     | 0.59              |
| 2:I:145:ILE:CG2   | 2:I:456:VAL:HG22  | 2.33                     | 0.59              |
| 3:J:114:ILE:HD12  | 3:J:304:ASP:OD1   | 2.02                     | 0.59              |
| 3:J:515:ARG:NH2   | 3:J:718:SER:O     | 2.36                     | 0.59              |
| 3:J:682:VAL:O     | 3:J:685:ILE:HG22  | 2.02                     | 0.59              |
| 3:J:1155:ILE:HD12 | 3:J:1210:ILE:HB   | 1.83                     | 0.59              |
| 6:P:21:DA:H2''    | 6:P:22:DT:H5'     | 1.83                     | 0.59              |
| 1:G:160:HIS:CD2   | 1:G:161:SER:HB2   | 2.38                     | 0.59              |
| 1:H:56:VAL:HG22   | 1:H:146:VAL:HG12  | 1.83                     | 0.59              |
| 1:H:158:ARG:CB    | 1:H:172:LEU:HD23  | 2.33                     | 0.59              |
| 2:I:1131:MET:HE3  | 2:I:1140:LYS:HG2  | 1.85                     | 0.59              |
| 3:J:641:ILE:HD12  | 3:J:644:MET:HE3   | 1.84                     | 0.59              |
| 3:J:1058:SER:HB3  | 3:J:1106:ILE:HG23 | 1.83                     | 0.59              |
| 3:J:1170:LYS:CB   | 6:P:75:DA:H3'     | 2.33                     | 0.59              |
| 5:L:584:ARG:O     | 5:L:587:ILE:HG22  | 2.02                     | 0.59              |
| 7:Q:52:DT:H2''    | 7:Q:53:DT:C6      | 2.38                     | 0.59              |
| 2:I:719:LYS:O     | 2:I:779:ARG:HG3   | 2.03                     | 0.59              |
| 3:J:546:ALA:O     | 3:J:548:VAL:HG23  | 2.03                     | 0.59              |
| 3:J:641:ILE:HD12  | 3:J:644:MET:CE    | 2.33                     | 0.59              |
| 5:L:309:ASN:HB3   | 5:L:315:TRP:CD1   | 2.37                     | 0.59              |
| 2:I:564:PRO:CG    | 2:I:572:ILE:HB    | 2.33                     | 0.59              |
| 2:I:817:LEU:CD1   | 2:I:1085:MET:HE1  | 2.32                     | 0.59              |
| 3:J:1287:ILE:HG22 | 3:J:1290:ARG:NH2  | 2.18                     | 0.59              |
| 4:K:38:LEU:HB2    | 4:K:53:GLU:OE1    | 2.03                     | 0.59              |
| 5:L:110:LEU:HD21  | 5:L:385:ARG:HD2   | 1.85                     | 0.58              |
| 2:I:1255:THR:O    | 2:I:1257:GLN:N    | 2.36                     | 0.58              |
| 3:J:282:LEU:HD21  | 5:L:410:ILE:HG12  | 1.85                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:1155:ILE:CD1  | 3:J:1210:ILE:HB   | 2.33                     | 0.58              |
| 1:R:252:ILE:O     | 1:R:278:ILE:HB    | 2.03                     | 0.58              |
| 2:I:130:MET:CG    | 2:I:134:GLY:HA2   | 2.33                     | 0.58              |
| 2:I:424:ASP:O     | 2:I:428:VAL:HG23  | 2.03                     | 0.58              |
| 2:I:447:HIS:HE1   | 2:I:609:ILE:HG22  | 1.68                     | 0.58              |
| 3:J:301:GLU:OE1   | 5:L:97:PRO:HG2    | 2.02                     | 0.58              |
| 5:L:148:TYR:CE1   | 5:L:158:LEU:CD2   | 2.86                     | 0.58              |
| 5:L:311:THR:O     | 5:L:341:LEU:HD23  | 2.04                     | 0.58              |
| 2:I:594:VAL:CG2   | 2:I:599:VAL:HG22  | 2.33                     | 0.58              |
| 3:J:1155:ILE:HD12 | 3:J:1155:ILE:O    | 2.03                     | 0.58              |
| 5:L:295:CYS:SG    | 5:L:330:LEU:HD23  | 2.44                     | 0.58              |
| 2:I:556:GLY:HA2   | 2:I:659:GLN:O     | 2.03                     | 0.58              |
| 2:I:1278:LEU:HB2  | 2:I:1287:LEU:HD12 | 1.84                     | 0.58              |
| 3:J:140:TYR:CE2   | 5:L:100:MET:HE1   | 2.38                     | 0.58              |
| 3:J:475:GLU:OE2   | 4:K:28:ARG:NH1    | 2.36                     | 0.58              |
| 3:J:1216:ALA:O    | 3:J:1220:ILE:HG12 | 2.03                     | 0.58              |
| 1:H:82:LEU:HD22   | 1:H:173:VAL:CG2   | 2.33                     | 0.58              |
| 2:I:297:VAL:HG12  | 2:I:315:MET:H     | 1.68                     | 0.58              |
| 2:I:798:GLN:NE2   | 2:I:827:ARG:O     | 2.36                     | 0.58              |
| 2:I:1260:GLY:O    | 2:I:1266:GLY:HA3  | 2.04                     | 0.58              |
| 3:J:51:PRO:HB3    | 3:J:57:PHE:O      | 2.03                     | 0.58              |
| 5:L:288:MET:HA    | 5:L:302:PHE:CZ    | 2.39                     | 0.58              |
| 7:Q:54:DT:H2''    | 7:Q:55:DA:C8      | 2.38                     | 0.58              |
| 1:G:23:HIS:CB     | 1:G:206:GLU:HA    | 2.34                     | 0.58              |
| 2:I:551:HIS:HB3   | 2:I:554:HIS:CE1   | 2.37                     | 0.58              |
| 3:J:195:GLU:OE2   | 3:J:228:VAL:HG11  | 2.03                     | 0.58              |
| 3:J:984:LEU:CB    | 3:J:993:GLU:HB2   | 2.33                     | 0.58              |
| 1:H:211:ILE:HD11  | 1:H:215:GLU:OE1   | 2.03                     | 0.58              |
| 2:I:240:GLU:HG3   | 2:I:284:LEU:HD13  | 1.86                     | 0.58              |
| 2:I:1294:LYS:HG2  | 3:J:472:LEU:HD11  | 1.86                     | 0.58              |
| 3:J:473:THR:HG23  | 3:J:476:ALA:H     | 1.68                     | 0.58              |
| 3:J:490:ILE:C     | 3:J:491:LEU:HD12  | 2.29                     | 0.58              |
| 2:I:1161:LEU:HA   | 2:I:1164:PHE:CD2  | 2.38                     | 0.58              |
| 3:J:44:ILE:HG12   | 5:L:450:ILE:HG22  | 1.86                     | 0.58              |
| 3:J:1048:ARG:HD2  | 3:J:1059:LEU:HD21 | 1.85                     | 0.58              |
| 5:L:315:TRP:HZ2   | 5:L:341:LEU:HD21  | 1.68                     | 0.58              |
| 6:P:29:DA:H1'     | 6:P:30:DC:H5'     | 1.86                     | 0.58              |
| 2:I:802:VAL:HG21  | 2:I:1098:LEU:HD22 | 1.86                     | 0.58              |
| 2:I:1005:GLU:H    | 2:I:1008:GLN:HB3  | 1.68                     | 0.58              |
| 2:I:1111:GLN:HB2  | 2:I:1230:MET:HE1  | 1.86                     | 0.58              |
| 2:I:1275:VAL:O    | 2:I:1279:GLU:HG3  | 2.03                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:322:ARG:HH12  | 5:L:510:PRO:HG3   | 1.69                     | 0.58              |
| 4:K:32:VAL:O      | 4:K:34:GLY:N      | 2.37                     | 0.58              |
| 5:L:253:SER:O     | 5:L:257:LYS:HG3   | 2.04                     | 0.58              |
| 5:L:530:LEU:HD23  | 5:L:530:LEU:H     | 1.69                     | 0.58              |
| 1:R:317:ARG:C     | 1:R:318:LEU:HD12  | 2.29                     | 0.58              |
| 3:J:271:ARG:NH1   | 3:J:316:ILE:HD12  | 2.13                     | 0.57              |
| 3:J:1034:PHE:HD1  | 3:J:1114:GLN:HB2  | 1.69                     | 0.57              |
| 5:L:577:GLY:O     | 5:L:581:ASP:N     | 2.37                     | 0.57              |
| 1:G:134:THR:HG21  | 2:I:727:VAL:O     | 2.04                     | 0.57              |
| 5:L:571:TYR:HD1   | 5:L:575:GLU:HG2   | 1.68                     | 0.57              |
| 1:G:140:ILE:HD12  | 1:G:142:MET:CE    | 2.33                     | 0.57              |
| 2:I:184:LEU:HB2   | 2:I:389:PHE:CE1   | 2.39                     | 0.57              |
| 3:J:200:GLN:O     | 3:J:203:GLU:HG2   | 2.05                     | 0.57              |
| 5:L:324:LYS:HB3   | 5:L:325:PRO:HD2   | 1.86                     | 0.57              |
| 5:L:555:GLU:HA    | 5:L:558:VAL:HG12  | 1.86                     | 0.57              |
| 1:H:61:ILE:HG22   | 1:H:63:GLY:H      | 1.69                     | 0.57              |
| 2:I:4:SER:HB2     | 2:I:7:GLU:HB2     | 1.86                     | 0.57              |
| 2:I:22:LEU:HB3    | 2:I:655:VAL:HG11  | 1.86                     | 0.57              |
| 2:I:184:LEU:HD13  | 2:I:389:PHE:CZ    | 2.39                     | 0.57              |
| 2:I:232:ILE:HG12  | 2:I:237:LEU:CD2   | 2.34                     | 0.57              |
| 2:I:322:LEU:O     | 2:I:325:LEU:HG    | 2.04                     | 0.57              |
| 3:J:527:LEU:HD13  | 3:J:548:VAL:HG11  | 1.85                     | 0.57              |
| 3:J:744:ARG:O     | 3:J:744:ARG:HD3   | 2.04                     | 0.57              |
| 5:L:426:LYS:NZ    | 6:P:53:DT:OP1     | 2.37                     | 0.57              |
| 6:P:20:DA:H2''    | 6:P:21:DA:C8      | 2.39                     | 0.57              |
| 1:R:283:GLN:CG    | 1:R:318:LEU:HD13  | 2.32                     | 0.57              |
| 1:R:318:LEU:HD23  | 1:R:321:TRP:CB    | 2.34                     | 0.57              |
| 1:G:235:ARG:N     | 1:H:13:LEU:HD23   | 2.19                     | 0.57              |
| 2:I:302:ILE:HD12  | 2:I:302:ILE:O     | 2.05                     | 0.57              |
| 2:I:1073:LYS:HG3  | 3:J:462:ASP:HB2   | 1.87                     | 0.57              |
| 2:I:1082:ILE:H    | 2:I:1082:ILE:HD12 | 1.69                     | 0.57              |
| 2:I:1212:LEU:HD13 | 2:I:1225:VAL:CG2  | 2.35                     | 0.57              |
| 3:J:840:LEU:HD13  | 3:J:869:CYS:SG    | 2.45                     | 0.57              |
| 3:J:883:ARG:NH2   | 3:J:898:CYS:SG    | 2.77                     | 0.57              |
| 4:K:3:ARG:HD3     | 4:K:4:VAL:H       | 1.70                     | 0.57              |
| 5:L:328:GLU:HA    | 5:L:331:HIS:HD2   | 1.68                     | 0.57              |
| 8:L:701:1N7:C3    | 8:L:701:1N7:C2    | 2.74                     | 0.57              |
| 1:R:302:GLU:HA    | 1:R:305:ASP:OD2   | 2.05                     | 0.57              |
| 1:R:318:LEU:HD23  | 1:R:321:TRP:HB3   | 1.87                     | 0.57              |
| 2:I:748:ILE:HD11  | 2:I:966:ILE:CG1   | 2.33                     | 0.57              |
| 2:I:1009:ASN:O    | 2:I:1010:GLN:HG2  | 2.04                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:478:LEU:HG    | 4:K:47:THR:HG23   | 1.87                     | 0.57              |
| 3:J:1319:PHE:CE1  | 3:J:1342:ASP:HB2  | 2.40                     | 0.57              |
| 2:I:184:LEU:HB2   | 2:I:389:PHE:HE1   | 1.70                     | 0.57              |
| 2:I:289:VAL:HG22  | 2:I:322:LEU:HD13  | 1.87                     | 0.57              |
| 2:I:371:ARG:NH1   | 6:P:57:DT:O4      | 2.37                     | 0.57              |
| 2:I:672:GLU:HB3   | 2:I:1187:PHE:HD1  | 1.69                     | 0.57              |
| 2:I:700:VAL:HG22  | 2:I:1117:LEU:HD23 | 1.86                     | 0.57              |
| 2:I:1246:ARG:NH1  | 2:I:1266:GLY:HA2  | 2.19                     | 0.57              |
| 3:J:667:GLN:O     | 3:J:673:VAL:HG22  | 2.05                     | 0.57              |
| 3:J:1173:ARG:NE   | 3:J:1192:LYS:HA   | 2.18                     | 0.57              |
| 5:L:345:GLN:O     | 5:L:349:GLU:HG3   | 2.05                     | 0.57              |
| 2:I:1040:ASP:OD1  | 2:I:1041:ASP:N    | 2.36                     | 0.57              |
| 2:I:1119:MET:CE   | 2:I:1210:ILE:HD11 | 2.34                     | 0.57              |
| 5:L:313:ASP:CA    | 5:L:316:PHE:HB3   | 2.34                     | 0.57              |
| 1:H:136:GLU:HG2   | 1:H:137:ASN:H     | 1.69                     | 0.56              |
| 3:J:432:LEU:O     | 3:J:435:GLN:NE2   | 2.37                     | 0.56              |
| 3:J:1215:GLU:HB3  | 3:J:1220:ILE:HD11 | 1.86                     | 0.56              |
| 5:L:318:ALA:HA    | 5:L:321:ALA:CB    | 2.30                     | 0.56              |
| 1:R:282:VAL:HG11  | 1:R:312:LEU:HD22  | 1.87                     | 0.56              |
| 2:I:712:SER:OG    | 2:I:713:GLY:N     | 2.35                     | 0.56              |
| 3:J:201:LEU:HD11  | 3:J:220:ARG:NH1   | 2.19                     | 0.56              |
| 3:J:559:ALA:CB    | 3:J:562:GLU:HB2   | 2.31                     | 0.56              |
| 3:J:901:ARG:HD3   | 3:J:906:GLY:O     | 2.05                     | 0.56              |
| 2:I:130:MET:SD    | 2:I:134:GLY:HA2   | 2.45                     | 0.56              |
| 2:I:646:SER:HB3   | 2:I:649:GLN:HG3   | 1.86                     | 0.56              |
| 2:I:728:ASP:OD1   | 2:I:729:ALA:N     | 2.38                     | 0.56              |
| 2:I:877:VAL:CG2   | 2:I:920:VAL:HG21  | 2.36                     | 0.56              |
| 3:J:347:VAL:HG12  | 3:J:348:ASP:O     | 2.05                     | 0.56              |
| 3:J:475:GLU:HG3   | 4:K:24:ALA:CB     | 2.35                     | 0.56              |
| 3:J:701:LEU:CD1   | 3:J:723:TYR:HB2   | 2.35                     | 0.56              |
| 3:J:746:LEU:HG    | 3:J:758:PRO:HG3   | 1.87                     | 0.56              |
| 3:J:810:THR:CG2   | 3:J:893:GLY:HA3   | 2.35                     | 0.56              |
| 3:J:952:VAL:HG12  | 3:J:1015:GLU:O    | 2.05                     | 0.56              |
| 3:J:965:SER:HA    | 3:J:975:ILE:HA    | 1.86                     | 0.56              |
| 3:J:1159:ILE:O    | 3:J:1177:ILE:HG21 | 2.05                     | 0.56              |
| 3:J:1183:SER:OG   | 3:J:1185:PRO:HD3  | 2.05                     | 0.56              |
| 3:J:1261:LEU:HD13 | 3:J:1304:ARG:HH11 | 1.70                     | 0.56              |
| 3:J:1326:GLN:HG2  | 3:J:1327:GLU:H    | 1.71                     | 0.56              |
| 5:L:392:LYS:CD    | 6:P:56:DC:H5"     | 2.32                     | 0.56              |
| 5:L:456:MET:HE1   | 5:L:497:VAL:HG22  | 1.85                     | 0.56              |
| 1:G:25:LYS:HE2    | 1:G:204:GLU:OE1   | 2.06                     | 0.56              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:I:289:VAL:CG2   | 2:I:322:LEU:HD13 | 2.35                     | 0.56              |
| 3:J:180:MET:N     | 3:J:184:ALA:HB2  | 2.20                     | 0.56              |
| 3:J:697:MET:O     | 3:J:701:LEU:HB2  | 2.06                     | 0.56              |
| 3:J:805:GLN:OE1   | 3:J:1321:SER:OG  | 2.24                     | 0.56              |
| 3:J:1031:VAL:HG11 | 3:J:1090:ILE:HA  | 1.88                     | 0.56              |
| 3:J:1220:ILE:HD12 | 3:J:1224:ARG:NH2 | 2.21                     | 0.56              |
| 5:L:286:LEU:HD23  | 5:L:340:ALA:HB2  | 1.87                     | 0.56              |
| 1:R:260:LEU:O     | 1:R:306:VAL:HG21 | 2.06                     | 0.56              |
| 2:I:629:PHE:CZ    | 2:I:650:VAL:HG21 | 2.40                     | 0.56              |
| 2:I:953:LEU:CD1   | 2:I:1033:ARG:HG2 | 2.36                     | 0.56              |
| 3:J:532:GLU:O     | 3:J:536:LEU:HD23 | 2.04                     | 0.56              |
| 3:J:821:MET:SD    | 3:J:881:LYS:HB2  | 2.46                     | 0.56              |
| 3:J:863:LEU:HD22  | 3:J:908:ILE:CG2  | 2.35                     | 0.56              |
| 3:J:1162:ILE:CG2  | 3:J:1178:THR:HB  | 2.35                     | 0.56              |
| 5:L:148:TYR:HE1   | 5:L:158:LEU:CD2  | 2.18                     | 0.56              |
| 5:L:310:GLU:OE1   | 5:L:355:ILE:HG21 | 2.06                     | 0.56              |
| 5:L:320:ILE:HD13  | 5:L:331:HIS:CE1  | 2.39                     | 0.56              |
| 2:I:498:ILE:H     | 2:I:498:ILE:HD12 | 1.71                     | 0.56              |
| 2:I:908:GLU:OE2   | 5:L:611:LEU:HD13 | 2.06                     | 0.56              |
| 2:I:1313:HIS:HE2  | 3:J:380:PHE:HE1  | 1.52                     | 0.56              |
| 3:J:70:CYS:SG     | 3:J:71:LEU:N     | 2.78                     | 0.56              |
| 5:L:522:PHE:HB3   | 8:L:701:1N7:H17  | 1.88                     | 0.56              |
| 5:L:586:ARG:HB2   | 6:P:26:DT:C7     | 2.36                     | 0.56              |
| 2:I:123:TYR:OH    | 2:I:126:GLU:HG3  | 2.06                     | 0.56              |
| 2:I:494:ASN:OD1   | 5:L:468:ARG:HD2  | 2.05                     | 0.56              |
| 2:I:564:PRO:CD    | 2:I:572:ILE:HB   | 2.35                     | 0.56              |
| 3:J:287:ALA:HA    | 5:L:413:MET:HE1  | 1.88                     | 0.56              |
| 5:L:319:ALA:HB1   | 5:L:326:TRP:HZ3  | 1.71                     | 0.56              |
| 2:I:318:SER:OG    | 2:I:320:ASP:OD1  | 2.12                     | 0.56              |
| 2:I:805:MET:HE1   | 2:I:1221:PHE:CE1 | 2.41                     | 0.56              |
| 2:I:1072:ASN:ND2  | 2:I:1111:GLN:OE1 | 2.38                     | 0.56              |
| 6:P:26:DT:H2''    | 6:P:27:DT:O5'    | 2.06                     | 0.56              |
| 2:I:866:ASP:HB3   | 2:I:872:TYR:CE1  | 2.40                     | 0.56              |
| 2:I:876:GLU:HG2   | 2:I:927:THR:OG1  | 2.06                     | 0.56              |
| 2:I:1326:LEU:HD21 | 3:J:338:PHE:CZ   | 2.41                     | 0.56              |
| 3:J:825:VAL:HG22  | 3:J:833:GLU:HB3  | 1.87                     | 0.56              |
| 3:J:959:LYS:HD2   | 3:J:1007:ASP:OD1 | 2.06                     | 0.56              |
| 1:R:257:VAL:N     | 1:R:276:HIS:O    | 2.38                     | 0.56              |
| 2:I:888:THR:HG23  | 2:I:916:SER:HB2  | 1.87                     | 0.56              |
| 3:J:1079:LYS:HB2  | 3:J:1098:GLN:HA  | 1.86                     | 0.56              |
| 1:G:13:LEU:HB2    | 1:H:231:PHE:HE1  | 1.71                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:H:51:MET:HE1    | 1:H:219:ARG:HD2   | 1.88                     | 0.55              |
| 1:H:112:ALA:HB3   | 1:H:126:PRO:CA    | 2.36                     | 0.55              |
| 2:I:1103:VAL:HG22 | 2:I:1111:GLN:NE2  | 2.20                     | 0.55              |
| 3:J:972:LYS:HE2   | 3:J:972:LYS:HA    | 1.87                     | 0.55              |
| 3:J:1047:THR:O    | 3:J:1059:LEU:HA   | 2.05                     | 0.55              |
| 4:K:58:LEU:HD12   | 4:K:59:ILE:HG12   | 1.88                     | 0.55              |
| 5:L:290:LEU:HD13  | 5:L:333:VAL:CG2   | 2.36                     | 0.55              |
| 1:H:44:ARG:HH22   | 3:J:538:ARG:HB3   | 1.71                     | 0.55              |
| 2:I:38:PHE:CZ     | 2:I:49:LEU:HD21   | 2.41                     | 0.55              |
| 2:I:848:GLU:OE1   | 2:I:886:LYS:NZ    | 2.28                     | 0.55              |
| 3:J:839:VAL:HG12  | 3:J:864:LEU:HD12  | 1.89                     | 0.55              |
| 3:J:848:VAL:HB    | 3:J:858:VAL:CG2   | 2.36                     | 0.55              |
| 5:L:148:TYR:HE1   | 5:L:158:LEU:HD22  | 1.71                     | 0.55              |
| 5:L:582:VAL:HG21  | 5:L:586:ARG:HG2   | 1.88                     | 0.55              |
| 7:Q:50:DC:C2'     | 7:Q:51:DT:H71     | 2.36                     | 0.55              |
| 7:Q:77:DT:P       | 1:R:298:LYS:HD3   | 2.47                     | 0.55              |
| 1:R:255:ARG:O     | 1:R:278:ILE:HG13  | 2.05                     | 0.55              |
| 1:G:19:VAL:HG11   | 1:G:23:HIS:CE1    | 2.41                     | 0.55              |
| 2:I:435:ILE:HD11  | 2:I:442:VAL:HG12  | 1.88                     | 0.55              |
| 2:I:1029:LEU:HD21 | 2:I:1033:ARG:HD2  | 1.88                     | 0.55              |
| 3:J:255:LEU:CD1   | 3:J:259:ARG:HB2   | 2.35                     | 0.55              |
| 3:J:384:LYS:CE    | 3:J:415:VAL:HG12  | 2.36                     | 0.55              |
| 3:J:694:SER:O     | 3:J:697:MET:HG3   | 2.07                     | 0.55              |
| 3:J:749:LYS:HG2   | 3:J:753:SER:O     | 2.06                     | 0.55              |
| 3:J:902:ASP:HB2   | 3:J:903:LEU:C     | 2.31                     | 0.55              |
| 3:J:1173:ARG:HD2  | 3:J:1196:LEU:HD21 | 1.87                     | 0.55              |
| 8:J:1504:1N7:C3   | 8:J:1504:1N7:C18  | 2.75                     | 0.55              |
| 1:R:255:ARG:HD3   | 1:R:256:PRO:HD2   | 1.87                     | 0.55              |
| 1:R:292:THR:OG1   | 1:R:295:LEU:HD13  | 2.07                     | 0.55              |
| 2:I:902:LEU:CD2   | 5:L:611:LEU:HD21  | 2.36                     | 0.55              |
| 3:J:262:THR:O     | 5:L:507:MET:HB2   | 2.06                     | 0.55              |
| 3:J:709:ARG:NH1   | 3:J:710:ASP:HB3   | 2.21                     | 0.55              |
| 3:J:1035:VAL:O    | 3:J:1111:ASP:HA   | 2.07                     | 0.55              |
| 6:P:64:DT:C2'     | 6:P:65:DT:H71     | 2.36                     | 0.55              |
| 1:R:279:GLY:O     | 1:R:283:GLN:HG3   | 2.07                     | 0.55              |
| 1:G:13:LEU:HD21   | 1:G:214:GLU:HG3   | 1.87                     | 0.55              |
| 2:I:680:LEU:HD13  | 3:J:783:LEU:CD1   | 2.36                     | 0.55              |
| 2:I:983:GLY:HA3   | 2:I:1002:LEU:CD1  | 2.36                     | 0.55              |
| 3:J:525:MET:O     | 3:J:548:VAL:HG13  | 2.07                     | 0.55              |
| 3:J:1061:VAL:HG13 | 3:J:1076:PRO:CG   | 2.36                     | 0.55              |
| 3:J:1090:ILE:HB   | 3:J:1093:THR:OG1  | 2.06                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:L:280:VAL:O    | 5:L:284:GLU:HG3   | 2.06                     | 0.55              |
| 7:Q:28:DT:C2'    | 7:Q:29:DT:H71     | 2.36                     | 0.55              |
| 1:R:254:LEU:HB3  | 1:R:321:TRP:CH2   | 2.42                     | 0.55              |
| 1:H:179:PRO:HA   | 1:H:208:ASN:HD22  | 1.72                     | 0.55              |
| 2:I:91:THR:HG22  | 2:I:138:ILE:O     | 2.06                     | 0.55              |
| 2:I:193:ASN:OD1  | 2:I:349:GLU:HG2   | 2.06                     | 0.55              |
| 2:I:957:LYS:HG3  | 2:I:1029:LEU:HD11 | 1.88                     | 0.55              |
| 3:J:103:GLY:O    | 3:J:244:VAL:N     | 2.27                     | 0.55              |
| 3:J:149:GLY:O    | 3:J:152:THR:OG1   | 2.22                     | 0.55              |
| 1:G:17:GLU:O     | 1:G:24:ALA:HB1    | 2.07                     | 0.55              |
| 1:G:23:HIS:HB2   | 1:G:206:GLU:HA    | 1.89                     | 0.55              |
| 1:G:184:ALA:O    | 1:G:204:GLU:HG2   | 2.05                     | 0.55              |
| 2:I:629:PHE:CE2  | 2:I:650:VAL:HG21  | 2.42                     | 0.55              |
| 2:I:1120:ALA:CB  | 2:I:1198:LEU:HD12 | 2.31                     | 0.55              |
| 3:J:336:GLY:O    | 3:J:340:GLN:HB3   | 2.07                     | 0.55              |
| 3:J:528:THR:HG22 | 3:J:532:GLU:CD    | 2.32                     | 0.55              |
| 3:J:836:ARG:HG3  | 3:J:869:CYS:HB3   | 1.89                     | 0.55              |
| 3:J:1347:LEU:HG  | 3:J:1357:ILE:CG2  | 2.37                     | 0.55              |
| 4:K:39:VAL:HG12  | 4:K:53:GLU:OE2    | 2.06                     | 0.55              |
| 5:L:328:GLU:HA   | 5:L:331:HIS:CD2   | 2.41                     | 0.55              |
| 5:L:450:ILE:HG13 | 5:L:450:ILE:O     | 2.07                     | 0.55              |
| 2:I:98:VAL:HB    | 2:I:124:MET:HE3   | 1.88                     | 0.55              |
| 2:I:901:LEU:HD11 | 2:I:905:ILE:HD11  | 1.89                     | 0.55              |
| 2:I:901:LEU:HD22 | 5:L:565:ILE:HD11  | 1.88                     | 0.55              |
| 1:G:89:ALA:O     | 1:G:124:VAL:HG22  | 2.07                     | 0.55              |
| 2:I:9:LYS:O      | 2:I:1175:ASN:ND2  | 2.37                     | 0.55              |
| 2:I:256:GLU:CB   | 2:I:261:VAL:HA    | 2.36                     | 0.55              |
| 2:I:316:GLU:OE1  | 2:I:316:GLU:N     | 2.33                     | 0.55              |
| 2:I:548:ARG:HG2  | 2:I:569:ILE:O     | 2.07                     | 0.55              |
| 3:J:93:THR:HG22  | 3:J:94:GLN:H      | 1.72                     | 0.55              |
| 3:J:782:GLY:O    | 3:J:786:THR:HG23  | 2.07                     | 0.55              |
| 3:J:1075:ARG:NH2 | 3:J:1168:GLU:HG2  | 2.20                     | 0.55              |
| 5:L:135:ALA:O    | 5:L:253:SER:OG    | 2.11                     | 0.55              |
| 5:L:165:PHE:CD1  | 5:L:259:PHE:HA    | 2.42                     | 0.55              |
| 2:I:1066:MET:HE2 | 2:I:1076:ILE:HG12 | 1.87                     | 0.55              |
| 3:J:355:ILE:HG12 | 3:J:464:ASP:O     | 2.07                     | 0.55              |
| 3:J:1327:GLU:OE1 | 3:J:1327:GLU:N    | 2.40                     | 0.55              |
| 5:L:423:ARG:HG2  | 5:L:425:TYR:CE2   | 2.42                     | 0.55              |
| 2:I:447:HIS:O    | 2:I:450:ASN:N     | 2.28                     | 0.54              |
| 2:I:1161:LEU:HA  | 2:I:1164:PHE:HD2  | 1.72                     | 0.54              |
| 3:J:527:LEU:HD23 | 3:J:533:ALA:HB2   | 1.88                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:J:707:ILE:O    | 3:J:713:GLU:HA    | 2.08                     | 0.54              |
| 5:L:470:MET:SD   | 5:L:486:ARG:HG3   | 2.47                     | 0.54              |
| 7:Q:32:DA:H2''   | 7:Q:33:DA:H5'     | 1.88                     | 0.54              |
| 1:R:286:GLU:O    | 1:R:290:LEU:HG    | 2.07                     | 0.54              |
| 1:G:73:GLY:O     | 1:G:134:THR:HG22  | 2.07                     | 0.54              |
| 1:G:228:LEU:HD11 | 1:H:224:LEU:HD23  | 1.90                     | 0.54              |
| 2:I:13:LYS:HB2   | 2:I:1180:MET:CE   | 2.27                     | 0.54              |
| 3:J:378:LYS:HE3  | 3:J:382:TYR:OH    | 2.07                     | 0.54              |
| 8:J:1504:1N7:C3  | 8:J:1504:1N7:C2   | 2.75                     | 0.54              |
| 3:J:147:ILE:HG22 | 3:J:188:LEU:HD21  | 1.89                     | 0.54              |
| 4:K:10:VAL:HG21  | 4:K:16:ARG:HD3    | 1.90                     | 0.54              |
| 5:L:134:VAL:HA   | 5:L:273:MET:HE1   | 1.88                     | 0.54              |
| 1:G:156:SER:O    | 1:G:159:ILE:HG22  | 2.06                     | 0.54              |
| 2:I:1067:ALA:HB3 | 2:I:1235:LEU:HD11 | 1.88                     | 0.54              |
| 3:J:1081:VAL:CA  | 3:J:1088:VAL:HG23 | 2.34                     | 0.54              |
| 2:I:39:ILE:HD11  | 2:I:75:LEU:CG     | 2.36                     | 0.54              |
| 2:I:887:VAL:HG22 | 2:I:913:VAL:CG2   | 2.34                     | 0.54              |
| 3:J:679:TYR:OH   | 3:J:754:ILE:HG23  | 2.08                     | 0.54              |
| 3:J:974:VAL:CG1  | 3:J:1002:VAL:HG22 | 2.34                     | 0.54              |
| 5:L:136:GLU:OE1  | 5:L:361:ILE:HG12  | 2.08                     | 0.54              |
| 7:Q:63:DT:H2'    | 7:Q:64:DT:H72     | 1.89                     | 0.54              |
| 2:I:519:ASN:ND2  | 2:I:796:LEU:HG    | 2.18                     | 0.54              |
| 3:J:255:LEU:CD2  | 3:J:261:ALA:HB2   | 2.38                     | 0.54              |
| 1:R:284:ARG:HG3  | 1:R:289:LEU:HD21  | 1.90                     | 0.54              |
| 2:I:163:LYS:HA   | 2:I:163:LYS:HE2   | 1.89                     | 0.54              |
| 2:I:549:ASP:OD2  | 3:J:750:PRO:HB3   | 2.08                     | 0.54              |
| 3:J:41:PRO:HG3   | 3:J:274:ASN:OD1   | 2.08                     | 0.54              |
| 3:J:85:CYS:SG    | 3:J:86:GLU:N      | 2.81                     | 0.54              |
| 3:J:1241:TYR:CD2 | 3:J:1248:ILE:HD12 | 2.43                     | 0.54              |
| 4:K:50:ALA:O     | 4:K:54:ILE:HG12   | 2.08                     | 0.54              |
| 5:L:164:GLY:O    | 5:L:260:ARG:HB3   | 2.08                     | 0.54              |
| 5:L:276:MET:SD   | 5:L:347:ILE:HG23  | 2.47                     | 0.54              |
| 2:I:224:PHE:CG   | 2:I:347:ILE:HG13  | 2.43                     | 0.54              |
| 2:I:1223:ARG:NH1 | 3:J:724:MET:HE1   | 2.23                     | 0.54              |
| 5:L:489:MET:SD   | 5:L:493:LYS:HD2   | 2.48                     | 0.54              |
| 7:Q:78:DG:H1'    | 7:Q:79:DT:H5'     | 1.88                     | 0.54              |
| 2:I:136:PHE:CE2  | 2:I:145:ILE:HD13  | 2.43                     | 0.54              |
| 8:I:1401:1N7:C3  | 8:I:1401:1N7:C2   | 2.74                     | 0.54              |
| 3:J:1079:LYS:HD2 | 3:J:1096:PRO:HB3  | 1.90                     | 0.54              |
| 3:J:1146:GLU:OE1 | 3:J:1148:ARG:NH2  | 2.41                     | 0.54              |
| 5:L:148:TYR:HA   | 5:L:161:LEU:CD2   | 2.38                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:54:CYS:SG     | 1:G:148:ARG:HG3   | 2.47                     | 0.54              |
| 1:G:192:VAL:CG1   | 1:G:198:LEU:HD12  | 2.37                     | 0.54              |
| 2:I:215:TYR:OH    | 2:I:422:LYS:HD2   | 2.08                     | 0.54              |
| 2:I:693:LEU:HB2   | 2:I:829:THR:O     | 2.07                     | 0.54              |
| 3:J:925:GLU:HG3   | 3:J:926:PRO:HD3   | 1.88                     | 0.54              |
| 3:J:1169:THR:HG22 | 3:J:1170:LYS:N    | 2.23                     | 0.54              |
| 5:L:134:VAL:HG13  | 5:L:273:MET:HE1   | 1.90                     | 0.54              |
| 1:H:86:LYS:HD3    | 1:H:174:ASP:HB2   | 1.90                     | 0.53              |
| 5:L:250:LEU:O     | 5:L:254:GLU:HG2   | 2.08                     | 0.53              |
| 7:Q:76:DT:H2''    | 7:Q:77:DT:H71     | 1.90                     | 0.53              |
| 1:H:205:MET:HE3   | 1:H:213:PRO:CA    | 2.36                     | 0.53              |
| 1:H:205:MET:CE    | 1:H:217:ILE:HG13  | 2.34                     | 0.53              |
| 2:I:673:HIS:HB3   | 2:I:1109:ILE:HG22 | 1.89                     | 0.53              |
| 3:J:1027:VAL:HG23 | 3:J:1122:ALA:O    | 2.07                     | 0.53              |
| 1:G:104:LYS:O     | 1:G:139:SER:OG    | 2.17                     | 0.53              |
| 2:I:1138:VAL:HG12 | 2:I:1170:MET:SD   | 2.48                     | 0.53              |
| 3:J:393:THR:HG23  | 3:J:396:ALA:H     | 1.71                     | 0.53              |
| 3:J:482:ALA:O     | 3:J:488:ASN:ND2   | 2.42                     | 0.53              |
| 3:J:1061:VAL:HG13 | 3:J:1076:PRO:HG3  | 1.90                     | 0.53              |
| 7:Q:73:DG:H2''    | 7:Q:74:DA:C8      | 2.44                     | 0.53              |
| 2:I:1104:PRO:HG2  | 3:J:725:MET:HE3   | 1.91                     | 0.53              |
| 3:J:368:LEU:HD21  | 3:J:373:ALA:HB2   | 1.89                     | 0.53              |
| 3:J:1003:LEU:HD23 | 3:J:1018:ALA:HA   | 1.89                     | 0.53              |
| 3:J:1169:THR:HG21 | 3:J:1172:LYS:CB   | 2.38                     | 0.53              |
| 2:I:133:ASN:HB3   | 2:I:527:LYS:NZ    | 2.23                     | 0.53              |
| 2:I:671:LEU:HB3   | 2:I:1186:VAL:CG1  | 2.38                     | 0.53              |
| 2:I:1101:LEU:HB3  | 3:J:731:ARG:HG3   | 1.90                     | 0.53              |
| 3:J:668:PHE:HD1   | 3:J:673:VAL:HG23  | 1.73                     | 0.53              |
| 3:J:712:GLN:HG2   | 3:J:713:GLU:N     | 2.24                     | 0.53              |
| 3:J:858:VAL:HG12  | 3:J:868:TRP:CZ3   | 2.43                     | 0.53              |
| 5:L:602:SER:HB3   | 1:R:259:ASP:OD1   | 2.09                     | 0.53              |
| 1:H:68:TYR:O      | 1:H:69:SER:OG     | 2.26                     | 0.53              |
| 2:I:245:ARG:HB3   | 2:I:337:PHE:CE1   | 2.44                     | 0.53              |
| 2:I:264:GLU:HB2   | 2:I:267:ARG:HG3   | 1.91                     | 0.53              |
| 6:P:28:DG:H2''    | 6:P:29:DA:C5'     | 2.39                     | 0.53              |
| 1:R:269:CYS:CB    | 1:R:295:LEU:HD12  | 2.35                     | 0.53              |
| 2:I:1103:VAL:HB   | 2:I:1104:PRO:HD3  | 1.91                     | 0.53              |
| 2:I:1287:LEU:HD13 | 3:J:1357:ILE:CD1  | 2.38                     | 0.53              |
| 5:L:511:ILE:O     | 5:L:513:ASP:HB2   | 2.09                     | 0.53              |
| 1:H:33:ARG:HH12   | 2:I:1081:PRO:HG3  | 1.72                     | 0.53              |
| 1:H:100:LEU:HD23  | 1:H:115:ILE:CG2   | 2.38                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:746:ALA:HB2   | 2:I:970:GLY:N     | 2.23                     | 0.53              |
| 2:I:1325:VAL:HG22 | 3:J:249:LEU:HD22  | 1.91                     | 0.53              |
| 3:J:1169:THR:HG22 | 3:J:1171:GLY:H    | 1.73                     | 0.53              |
| 3:J:1291:GLU:O    | 3:J:1294:ALA:HB3  | 2.08                     | 0.53              |
| 5:L:399:LEU:HD23  | 5:L:404:LEU:CD2   | 2.38                     | 0.53              |
| 1:G:211:ILE:CG2   | 1:G:216:ALA:HB2   | 2.36                     | 0.53              |
| 5:L:232:ARG:O     | 5:L:235:ILE:HG12  | 2.08                     | 0.53              |
| 2:I:1268:GLN:NE2  | 3:J:352:ARG:HD2   | 2.23                     | 0.53              |
| 3:J:745:GLY:O     | 3:J:758:PRO:HB3   | 2.09                     | 0.53              |
| 3:J:759:ILE:CG2   | 3:J:771:GLN:HB3   | 2.37                     | 0.53              |
| 3:J:955:LYS:HE2   | 3:J:1010:GLN:NE2  | 2.24                     | 0.53              |
| 3:J:960:LEU:HD23  | 3:J:963:VAL:CG2   | 2.33                     | 0.53              |
| 3:J:1011:VAL:HB   | 3:J:1015:GLU:OE1  | 2.09                     | 0.53              |
| 5:L:319:ALA:HB1   | 5:L:326:TRP:CZ3   | 2.44                     | 0.53              |
| 5:L:374:ARG:O     | 5:L:378:GLU:HG3   | 2.08                     | 0.53              |
| 5:L:561:MET:HA    | 5:L:567:MET:HE1   | 1.90                     | 0.53              |
| 6:P:63:DT:C2'     | 6:P:64:DT:H71     | 2.39                     | 0.53              |
| 2:I:396:ASP:HA    | 2:I:418:GLY:O     | 2.09                     | 0.52              |
| 2:I:432:LEU:HA    | 2:I:435:ILE:HG22  | 1.89                     | 0.52              |
| 2:I:1115:THR:HG23 | 2:I:1228:GLY:HA3  | 1.92                     | 0.52              |
| 3:J:580:TRP:CZ3   | 3:J:589:TYR:HA    | 2.43                     | 0.52              |
| 3:J:1048:ARG:CZ   | 3:J:1057:SER:HB2  | 2.39                     | 0.52              |
| 5:L:295:CYS:SG    | 5:L:330:LEU:HA    | 2.49                     | 0.52              |
| 6:P:37:DA:H2'     | 6:P:37:DA:OP2     | 2.09                     | 0.52              |
| 1:H:158:ARG:HB2   | 1:H:172:LEU:HD23  | 1.92                     | 0.52              |
| 2:I:103:VAL:CG1   | 2:I:117:ILE:HG22  | 2.36                     | 0.52              |
| 2:I:987:GLU:HG2   | 2:I:991:LYS:HE3   | 1.91                     | 0.52              |
| 3:J:382:TYR:HB3   | 3:J:394:ILE:HD11  | 1.91                     | 0.52              |
| 3:J:574:VAL:O     | 3:J:578:ILE:HG13  | 2.09                     | 0.52              |
| 5:L:571:TYR:CD1   | 5:L:575:GLU:HG2   | 2.45                     | 0.52              |
| 2:I:558:VAL:CG1   | 2:I:573:ASN:HB3   | 2.39                     | 0.52              |
| 2:I:1131:MET:CE   | 2:I:1141:LEU:HA   | 2.40                     | 0.52              |
| 2:I:1141:LEU:O    | 2:I:1145:ILE:HD12 | 2.10                     | 0.52              |
| 2:I:1268:GLN:HE22 | 3:J:352:ARG:HD2   | 1.74                     | 0.52              |
| 3:J:384:LYS:HG2   | 3:J:411:ILE:HG23  | 1.90                     | 0.52              |
| 3:J:514:THR:HG21  | 3:J:596:LEU:CB    | 2.36                     | 0.52              |
| 3:J:621:ALA:O     | 3:J:624:ILE:HG22  | 2.09                     | 0.52              |
| 3:J:1149:ARG:HH22 | 3:J:1153:PRO:HG3  | 1.75                     | 0.52              |
| 5:L:512:GLY:HA3   | 5:L:513:ASP:CB    | 2.39                     | 0.52              |
| 1:R:299:SER:O     | 1:R:303:ILE:HG13  | 2.10                     | 0.52              |
| 1:G:68:TYR:HA     | 2:I:756:TYR:HE2   | 1.74                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:39:ILE:O      | 2:I:39:ILE:HG23   | 2.09                     | 0.52              |
| 2:I:699:LEU:HD13  | 2:I:699:LEU:O     | 2.09                     | 0.52              |
| 2:I:1281:TYR:CD2  | 3:J:484:MET:HG2   | 2.44                     | 0.52              |
| 5:L:138:PRO:O     | 5:L:142:THR:HG23  | 2.10                     | 0.52              |
| 5:L:315:TRP:CZ2   | 5:L:341:LEU:HD21  | 2.44                     | 0.52              |
| 5:L:339:ARG:HA    | 5:L:342:GLN:HG2   | 1.90                     | 0.52              |
| 6:P:75:DA:H2"     | 6:P:76:DT:OP2     | 2.09                     | 0.52              |
| 1:H:88:LEU:O      | 1:H:90:VAL:HG23   | 2.10                     | 0.52              |
| 2:I:93:SER:OG     | 2:I:126:GLU:OE1   | 2.15                     | 0.52              |
| 2:I:765:ILE:HG13  | 2:I:787:PRO:HG3   | 1.91                     | 0.52              |
| 3:J:129:ASP:HB2   | 3:J:220:ARG:NE    | 2.24                     | 0.52              |
| 3:J:516:ASP:HB3   | 3:J:573:THR:HG21  | 1.90                     | 0.52              |
| 5:L:215:GLU:HG2   | 5:L:218:ARG:NH2   | 2.20                     | 0.52              |
| 1:H:79:LEU:HD23   | 1:H:79:LEU:H      | 1.75                     | 0.52              |
| 2:I:1043:ALA:O    | 2:I:1046:VAL:HG12 | 2.10                     | 0.52              |
| 5:L:145:LEU:HD21  | 5:L:224:LEU:HG    | 1.90                     | 0.52              |
| 5:L:285:ARG:HD3   | 5:L:288:MET:HE2   | 1.92                     | 0.52              |
| 5:L:407:GLU:OE1   | 5:L:442:SER:OG    | 2.08                     | 0.52              |
| 1:R:280:ASP:OD1   | 1:R:283:GLN:NE2   | 2.43                     | 0.52              |
| 1:R:287:VAL:O     | 1:R:291:LYS:HG3   | 2.10                     | 0.52              |
| 1:G:183:ILE:O     | 2:I:1091:GLY:HA3  | 2.10                     | 0.52              |
| 1:G:214:GLU:O     | 1:G:218:ARG:HG2   | 2.10                     | 0.52              |
| 1:H:173:VAL:HG12  | 1:H:174:ASP:O     | 2.10                     | 0.52              |
| 2:I:714:VAL:O     | 2:I:767:GLN:NE2   | 2.42                     | 0.52              |
| 2:I:739:ASP:OD1   | 2:I:740:GLU:N     | 2.43                     | 0.52              |
| 2:I:1279:GLU:HG2  | 3:J:1357:ILE:CD1  | 2.37                     | 0.52              |
| 3:J:712:GLN:HG2   | 3:J:713:GLU:H     | 1.74                     | 0.52              |
| 8:J:1504:1N7:H9   | 5:L:511:ILE:HD13  | 1.92                     | 0.52              |
| 1:H:85:LEU:HD22   | 1:H:144:ILE:HD11  | 1.91                     | 0.52              |
| 2:I:398:SER:O     | 2:I:401:GLY:N     | 2.42                     | 0.52              |
| 2:I:1109:ILE:HD11 | 3:J:644:MET:CE    | 2.40                     | 0.52              |
| 2:I:1113:LEU:CD1  | 3:J:641:ILE:HD13  | 2.40                     | 0.52              |
| 8:I:1401:1N7:H31  | 8:I:1401:1N7:H5   | 1.90                     | 0.52              |
| 3:J:902:ASP:HB2   | 3:J:903:LEU:O     | 2.09                     | 0.52              |
| 3:J:1136:GLY:HA2  | 3:J:1140:ARG:HB2  | 1.92                     | 0.52              |
| 3:J:1267:VAL:HB   | 3:J:1301:THR:OG1  | 2.09                     | 0.52              |
| 5:L:562:ARG:HG2   | 5:L:591:GLU:CD    | 2.35                     | 0.52              |
| 2:I:617:ALA:HB3   | 2:I:653:MET:HG3   | 1.92                     | 0.52              |
| 2:I:1131:MET:HE1  | 2:I:1141:LEU:HA   | 1.92                     | 0.52              |
| 2:I:1268:GLN:HE22 | 3:J:352:ARG:HH11  | 1.58                     | 0.52              |
| 3:J:424:ASN:OD1   | 3:J:425:ARG:N     | 2.43                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:J:716:GLN:HG2  | 3:J:717:VAL:O     | 2.10                     | 0.52              |
| 3:J:982:LEU:HB2  | 3:J:997:VAL:CG2   | 2.39                     | 0.52              |
| 6:P:38:DG:H2"    | 6:P:39:DG:C8      | 2.44                     | 0.52              |
| 1:G:192:VAL:HG13 | 1:G:195:ARG:HB3   | 1.92                     | 0.52              |
| 1:H:104:LYS:H    | 1:H:140:ILE:CG2   | 2.23                     | 0.52              |
| 2:I:731:ARG:NH1  | 2:I:962:GLU:OE1   | 2.34                     | 0.52              |
| 3:J:848:VAL:HB   | 3:J:858:VAL:HG22  | 1.91                     | 0.52              |
| 3:J:870:ASP:O    | 3:J:874:GLU:HG2   | 2.09                     | 0.52              |
| 3:J:968:ASN:HD21 | 3:J:972:LYS:HB2   | 1.74                     | 0.52              |
| 4:K:39:VAL:HG23  | 4:K:40:PRO:HD2    | 1.92                     | 0.52              |
| 1:H:41:ASN:ND2   | 2:I:1217:THR:HA   | 2.25                     | 0.51              |
| 2:I:4:SER:HB2    | 2:I:7:GLU:CB      | 2.39                     | 0.51              |
| 2:I:521:LEU:HD23 | 2:I:708:VAL:HG11  | 1.92                     | 0.51              |
| 2:I:564:PRO:HG3  | 2:I:572:ILE:HB    | 1.92                     | 0.51              |
| 2:I:1136:GLN:HG2 | 2:I:1137:GLU:H    | 1.74                     | 0.51              |
| 3:J:429:LEU:HB3  | 3:J:925:GLU:CB    | 2.38                     | 0.51              |
| 3:J:664:ILE:HD12 | 3:J:681:LYS:HG2   | 1.92                     | 0.51              |
| 3:J:1034:PHE:CD1 | 3:J:1114:GLN:HB2  | 2.45                     | 0.51              |
| 3:J:45:ASN:O     | 3:J:47:ARG:N      | 2.42                     | 0.51              |
| 5:L:291:CYS:O    | 5:L:295:CYS:HB2   | 2.10                     | 0.51              |
| 5:L:389:SER:HA   | 5:L:392:LYS:HE2   | 1.92                     | 0.51              |
| 6:P:69:DT:H1'    | 6:P:70:DT:H5'     | 1.92                     | 0.51              |
| 7:Q:19:DT:H2"    | 7:Q:20:DA:O5'     | 2.10                     | 0.51              |
| 1:R:290:LEU:HA   | 1:R:295:LEU:CD2   | 2.40                     | 0.51              |
| 2:I:384:LEU:O    | 2:I:388:LEU:HG    | 2.10                     | 0.51              |
| 2:I:1119:MET:HE3 | 2:I:1210:ILE:HD11 | 1.92                     | 0.51              |
| 2:I:1311:GLY:O   | 4:K:31:GLN:NE2    | 2.38                     | 0.51              |
| 3:J:126:LEU:HD11 | 3:J:223:LEU:HD22  | 1.92                     | 0.51              |
| 3:J:287:ALA:HB1  | 3:J:288:PRO:HD2   | 1.91                     | 0.51              |
| 3:J:294:ASN:ND2  | 5:L:406:GLN:HE21  | 2.08                     | 0.51              |
| 3:J:660:GLU:HB3  | 3:J:685:ILE:HD11  | 1.93                     | 0.51              |
| 3:J:807:LEU:HD23 | 3:J:1255:VAL:CG2  | 2.39                     | 0.51              |
| 3:J:961:SER:O    | 3:J:980:THR:HA    | 2.10                     | 0.51              |
| 5:L:471:LEU:HA   | 5:L:476:ARG:O     | 2.10                     | 0.51              |
| 1:R:256:PRO:HA   | 1:R:276:HIS:O     | 2.11                     | 0.51              |
| 1:H:74:VAL:HG13  | 1:H:132:HIS:O     | 2.09                     | 0.51              |
| 1:H:76:GLU:OE2   | 1:H:132:HIS:HB2   | 2.10                     | 0.51              |
| 2:I:118:LYS:CE   | 2:I:488:MET:HA    | 2.41                     | 0.51              |
| 2:I:171:LEU:HD22 | 2:I:188:PHE:O     | 2.10                     | 0.51              |
| 3:J:482:ALA:HA   | 4:K:6:VAL:HG21    | 1.93                     | 0.51              |
| 3:J:526:VAL:HG12 | 3:J:549:LYS:HB2   | 1.91                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:733:SER:O     | 3:J:737:ILE:HG12  | 2.10                     | 0.51              |
| 3:J:785:ASP:O     | 3:J:788:LEU:N     | 2.39                     | 0.51              |
| 3:J:1267:VAL:HG22 | 3:J:1303:SER:HB2  | 1.91                     | 0.51              |
| 5:L:234:THR:O     | 5:L:245:ALA:HB2   | 2.11                     | 0.51              |
| 5:L:429:THR:HA    | 6:P:53:DT:C7      | 2.40                     | 0.51              |
| 5:L:452:ILE:HG13  | 5:L:457:ILE:HG13  | 1.92                     | 0.51              |
| 1:R:307:LEU:HA    | 1:R:312:LEU:HB2   | 1.91                     | 0.51              |
| 3:J:1037:PHE:CE2  | 3:J:1059:LEU:HD12 | 2.46                     | 0.51              |
| 5:L:122:ARG:NH1   | 5:L:378:GLU:OE1   | 2.44                     | 0.51              |
| 5:L:151:VAL:CG2   | 5:L:161:LEU:HD22  | 2.40                     | 0.51              |
| 5:L:388:ILE:O     | 5:L:392:LYS:HG3   | 2.10                     | 0.51              |
| 1:G:50:SER:HB3    | 1:H:8:PHE:HZ      | 1.76                     | 0.51              |
| 1:H:100:LEU:HG    | 1:H:118:ASP:OD2   | 2.11                     | 0.51              |
| 2:I:75:LEU:HD11   | 2:I:127:ILE:CD1   | 2.29                     | 0.51              |
| 2:I:689:ALA:HB2   | 2:I:1233:LEU:HD12 | 1.93                     | 0.51              |
| 2:I:901:LEU:HD22  | 5:L:565:ILE:CD1   | 2.41                     | 0.51              |
| 3:J:79:LYS:HG2    | 5:L:569:THR:HA    | 1.92                     | 0.51              |
| 3:J:291:ILE:HD13  | 5:L:409:ASN:HB3   | 1.93                     | 0.51              |
| 3:J:416:ILE:HG21  | 3:J:441:LEU:CD2   | 2.41                     | 0.51              |
| 3:J:902:ASP:HA    | 3:J:903:LEU:CD2   | 2.40                     | 0.51              |
| 5:L:98:VAL:HG22   | 5:L:402:LEU:CD1   | 2.30                     | 0.51              |
| 6:P:75:DA:H1'     | 6:P:76:DT:H5'     | 1.93                     | 0.51              |
| 1:H:185:TYR:HB2   | 1:H:201:LEU:CD1   | 2.41                     | 0.51              |
| 2:I:135:THR:OG1   | 2:I:142:GLU:OE2   | 2.11                     | 0.51              |
| 2:I:1153:ALA:HB3  | 2:I:1194:GLU:OE2  | 2.11                     | 0.51              |
| 3:J:54:ASP:OD1    | 3:J:54:ASP:N      | 2.42                     | 0.51              |
| 3:J:139:LEU:HA    | 3:J:181:GLY:HA2   | 1.93                     | 0.51              |
| 3:J:360:TYR:OH    | 3:J:448:GLN:OE1   | 2.12                     | 0.51              |
| 3:J:369:PRO:HA    | 3:J:442:ILE:O     | 2.11                     | 0.51              |
| 3:J:423:LEU:HB3   | 3:J:466:MET:HE1   | 1.93                     | 0.51              |
| 3:J:978:ARG:NH1   | 3:J:999:TYR:H     | 2.07                     | 0.51              |
| 5:L:276:MET:O     | 5:L:280:VAL:HG23  | 2.11                     | 0.51              |
| 1:G:57:THR:HG21   | 1:G:147:GLN:NE2   | 2.26                     | 0.51              |
| 1:G:234:LEU:HD22  | 1:H:13:LEU:CD2    | 2.40                     | 0.51              |
| 1:H:115:ILE:HG22  | 1:H:116:THR:O     | 2.10                     | 0.51              |
| 1:H:196:THR:HG21  | 3:J:443:GLU:CG    | 2.39                     | 0.51              |
| 2:I:699:LEU:HB2   | 2:I:799:ASN:HD22  | 1.75                     | 0.51              |
| 2:I:1136:GLN:HG2  | 2:I:1137:GLU:N    | 2.26                     | 0.51              |
| 3:J:140:TYR:O     | 3:J:297:ARG:HD3   | 2.11                     | 0.51              |
| 3:J:670:SER:O     | 3:J:672:LEU:HD12  | 2.10                     | 0.51              |
| 3:J:788:LEU:O     | 3:J:788:LEU:HD23  | 2.11                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:K:38:LEU:CD2    | 4:K:58:LEU:HD13   | 2.41                     | 0.51              |
| 5:L:320:ILE:HG12  | 5:L:327:SER:O     | 2.11                     | 0.51              |
| 5:L:551:LEU:CD2   | 5:L:597:LYS:HD2   | 2.40                     | 0.51              |
| 6:P:40:DC:H2''    | 6:P:41:DT:C6      | 2.46                     | 0.51              |
| 1:H:214:GLU:HG2   | 1:H:218:ARG:NH1   | 2.21                     | 0.51              |
| 2:I:877:VAL:HG11  | 2:I:883:LEU:HD21  | 1.91                     | 0.51              |
| 3:J:153:ASN:O     | 3:J:154:LEU:HD12  | 2.10                     | 0.51              |
| 3:J:282:LEU:HD13  | 3:J:291:ILE:HG22  | 1.91                     | 0.51              |
| 3:J:876:SER:HA    | 3:J:990:ARG:HH21  | 1.75                     | 0.51              |
| 3:J:968:ASN:ND2   | 3:J:972:LYS:HB2   | 2.26                     | 0.51              |
| 3:J:1271:SER:OG   | 3:J:1297:LYS:HD3  | 2.10                     | 0.51              |
| 3:J:1287:ILE:HD12 | 3:J:1288:ALA:N    | 2.26                     | 0.51              |
| 2:I:94:ALA:HB2    | 2:I:129:LEU:HD11  | 1.93                     | 0.51              |
| 2:I:856:ASN:HA    | 5:L:613:ASP:HB2   | 1.93                     | 0.51              |
| 2:I:1267:GLY:HA3  | 3:J:347:VAL:O     | 2.10                     | 0.51              |
| 3:J:1350:ASN:HD22 | 3:J:1358:PRO:HD3  | 1.76                     | 0.51              |
| 5:L:225:ARG:O     | 5:L:229:VAL:HG22  | 2.11                     | 0.51              |
| 6:P:78:DT:H2''    | 6:P:79:DA:C8      | 2.46                     | 0.51              |
| 6:P:80:DG:H2''    | 6:P:81:DA:C8      | 2.45                     | 0.51              |
| 1:G:228:LEU:HD21  | 1:H:221:ALA:O     | 2.10                     | 0.50              |
| 1:G:231:PHE:HZ    | 1:H:201:LEU:HD23  | 1.75                     | 0.50              |
| 2:I:452:ARG:NH2   | 2:I:458:GLU:OE1   | 2.43                     | 0.50              |
| 2:I:809:GLY:O     | 3:J:357:VAL:HG11  | 2.10                     | 0.50              |
| 3:J:412:LEU:HD23  | 3:J:416:ILE:HG13  | 1.93                     | 0.50              |
| 3:J:611:ILE:HG22  | 3:J:612:LEU:HD12  | 1.92                     | 0.50              |
| 3:J:707:ILE:HD11  | 3:J:714:GLU:HB3   | 1.93                     | 0.50              |
| 1:R:270:LEU:HD21  | 1:R:281:LEU:HD13  | 1.94                     | 0.50              |
| 1:G:25:LYS:HG2    | 1:G:204:GLU:HB3   | 1.93                     | 0.50              |
| 1:H:155:ALA:N     | 1:H:174:ASP:OD1   | 2.44                     | 0.50              |
| 2:I:297:VAL:HG12  | 2:I:315:MET:O     | 2.12                     | 0.50              |
| 2:I:964:LEU:HD22  | 2:I:1025:PHE:CD2  | 2.45                     | 0.50              |
| 2:I:1245:ALA:HB3  | 3:J:375:GLU:HG2   | 1.93                     | 0.50              |
| 3:J:144:TYR:N     | 3:J:160:LEU:O     | 2.44                     | 0.50              |
| 3:J:658:GLU:O     | 3:J:661:VAL:HG22  | 2.11                     | 0.50              |
| 3:J:807:LEU:CD2   | 3:J:1255:VAL:HG23 | 2.41                     | 0.50              |
| 1:G:54:CYS:SG     | 1:G:92:VAL:HG22   | 2.51                     | 0.50              |
| 2:I:71:VAL:HB     | 2:I:99:LYS:O      | 2.10                     | 0.50              |
| 2:I:636:CYS:HB2   | 2:I:645:PHE:HD2   | 1.75                     | 0.50              |
| 2:I:1101:LEU:HD23 | 3:J:725:MET:SD    | 2.52                     | 0.50              |
| 3:J:103:GLY:C     | 3:J:244:VAL:HG22  | 2.36                     | 0.50              |
| 3:J:391:ALA:HB2   | 3:J:400:MET:SD    | 2.51                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:679:TYR:OH    | 3:J:754:ILE:O     | 2.27                     | 0.50              |
| 3:J:707:ILE:CD1   | 3:J:714:GLU:HB3   | 2.41                     | 0.50              |
| 3:J:1169:THR:CG2  | 3:J:1171:GLY:H    | 2.24                     | 0.50              |
| 1:R:300:LEU:HA    | 1:R:303:ILE:CD1   | 2.33                     | 0.50              |
| 1:R:321:TRP:CD2   | 1:R:322:PRO:HA    | 2.46                     | 0.50              |
| 1:H:158:ARG:HB3   | 1:H:172:LEU:HD23  | 1.93                     | 0.50              |
| 1:H:197:ASP:C     | 1:H:198:LEU:HD22  | 2.37                     | 0.50              |
| 2:I:934:PHE:O     | 2:I:1048:LYS:HA   | 2.11                     | 0.50              |
| 3:J:1319:PHE:CD1  | 3:J:1342:ASP:HB2  | 2.47                     | 0.50              |
| 1:G:124:VAL:O     | 1:G:126:PRO:HD3   | 2.11                     | 0.50              |
| 1:G:182:ARG:HB3   | 1:G:206:GLU:HB3   | 1.94                     | 0.50              |
| 1:H:59:VAL:HG21   | 1:H:85:LEU:CD1    | 2.41                     | 0.50              |
| 2:I:39:ILE:HD12   | 2:I:127:ILE:CD1   | 2.41                     | 0.50              |
| 2:I:192:ASP:HB3   | 2:I:346:TYR:CD1   | 2.47                     | 0.50              |
| 3:J:298:MET:SD    | 5:L:402:LEU:HB3   | 2.52                     | 0.50              |
| 3:J:701:LEU:HD11  | 3:J:723:TYR:HB2   | 1.93                     | 0.50              |
| 5:L:347:ILE:O     | 5:L:351:THR:HG23  | 2.11                     | 0.50              |
| 7:Q:75:DT:C6      | 7:Q:76:DT:H72     | 2.46                     | 0.50              |
| 1:R:253:LEU:HD22  | 1:R:279:GLY:HA2   | 1.94                     | 0.50              |
| 1:H:16:ILE:HG13   | 1:H:26:VAL:HG22   | 1.93                     | 0.50              |
| 2:I:269:ILE:HG22  | 2:I:274:ILE:HG13  | 1.94                     | 0.50              |
| 2:I:978:VAL:HG11  | 2:I:1010:GLN:OE1  | 2.11                     | 0.50              |
| 2:I:1109:ILE:HG21 | 3:J:763:PHE:O     | 2.12                     | 0.50              |
| 3:J:481:ARG:O     | 3:J:485:MET:HB2   | 2.12                     | 0.50              |
| 3:J:1163:VAL:HG13 | 3:J:1200:GLU:O    | 2.12                     | 0.50              |
| 1:H:99:ILE:HG13   | 1:H:144:ILE:O     | 2.10                     | 0.50              |
| 2:I:812:PHE:CD2   | 2:I:813:GLU:HG2   | 2.47                     | 0.50              |
| 2:I:1101:LEU:O    | 3:J:731:ARG:HG3   | 2.11                     | 0.50              |
| 2:I:1308:ILE:HG21 | 3:J:379:PRO:HB2   | 1.92                     | 0.50              |
| 3:J:126:LEU:HD22  | 3:J:219:LYS:HE2   | 1.92                     | 0.50              |
| 3:J:1141:VAL:HG22 | 3:J:1237:VAL:HG23 | 1.93                     | 0.50              |
| 2:I:159:SER:OG    | 2:I:161:LYS:HB3   | 2.12                     | 0.50              |
| 2:I:1212:LEU:HD11 | 2:I:1227:VAL:CG1  | 2.41                     | 0.50              |
| 3:J:62:PHE:O      | 3:J:98:ARG:HA     | 2.11                     | 0.50              |
| 3:J:320:ASN:O     | 3:J:321:LYS:HG2   | 2.11                     | 0.50              |
| 3:J:364:HIS:HB2   | 3:J:485:MET:HE2   | 1.94                     | 0.50              |
| 3:J:657:ALA:O     | 3:J:661:VAL:HG13  | 2.12                     | 0.50              |
| 3:J:958:ILE:HD13  | 3:J:984:LEU:CD1   | 2.42                     | 0.50              |
| 5:L:230:VAL:O     | 5:L:234:THR:HG23  | 2.12                     | 0.50              |
| 5:L:296:LYS:HE2   | 5:L:296:LYS:HA    | 1.94                     | 0.50              |
| 1:G:16:ILE:CD1    | 1:G:214:GLU:HB2   | 2.38                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:1022:LYS:O    | 2:I:1026:GLU:HG2  | 2.11                     | 0.50              |
| 2:I:1122:LYS:HG2  | 2:I:1229:TYR:CE2  | 2.46                     | 0.50              |
| 3:J:38:VAL:CG1    | 3:J:56:LEU:HD12   | 2.41                     | 0.50              |
| 3:J:487:THR:O     | 3:J:614:LEU:HD21  | 2.12                     | 0.50              |
| 3:J:547:ARG:CA    | 3:J:573:THR:HG22  | 2.33                     | 0.50              |
| 2:I:520:PRO:HG3   | 2:I:714:VAL:HG21  | 1.94                     | 0.49              |
| 2:I:967:LEU:CD2   | 2:I:1021:LEU:HD22 | 2.42                     | 0.49              |
| 3:J:128:LEU:HD23  | 3:J:192:MET:CE    | 2.42                     | 0.49              |
| 5:L:124:GLU:O     | 5:L:127:ILE:HG13  | 2.11                     | 0.49              |
| 5:L:399:LEU:HD23  | 5:L:404:LEU:HD23  | 1.94                     | 0.49              |
| 2:I:817:LEU:O     | 2:I:817:LEU:HD13  | 2.12                     | 0.49              |
| 2:I:1010:GLN:HA   | 2:I:1013:GLN:CG   | 2.43                     | 0.49              |
| 2:I:1024:GLU:O    | 2:I:1027:LYS:HG2  | 2.11                     | 0.49              |
| 2:I:1253:LEU:HD23 | 5:L:525:ASP:HA    | 1.94                     | 0.49              |
| 3:J:80:HIS:HB3    | 3:J:83:VAL:CG1    | 2.41                     | 0.49              |
| 3:J:268:LEU:O     | 3:J:272:VAL:HG23  | 2.11                     | 0.49              |
| 3:J:1111:ASP:OD1  | 3:J:1112:GLY:N    | 2.44                     | 0.49              |
| 3:J:1171:GLY:HA3  | 3:J:1172:LYS:CB   | 2.41                     | 0.49              |
| 4:K:38:LEU:HD22   | 4:K:58:LEU:CD1    | 2.42                     | 0.49              |
| 6:P:25:DA:H2'     | 6:P:26:DT:H72     | 1.95                     | 0.49              |
| 1:G:50:SER:HB3    | 1:H:8:PHE:CZ      | 2.48                     | 0.49              |
| 1:H:103:ASN:HB3   | 1:H:141:SER:CA    | 2.33                     | 0.49              |
| 2:I:866:ASP:HB3   | 2:I:872:TYR:CZ    | 2.47                     | 0.49              |
| 2:I:976:ARG:HB2   | 2:I:997:TRP:HZ2   | 1.78                     | 0.49              |
| 2:I:1307:ASN:HB3  | 2:I:1312:ASN:O    | 2.12                     | 0.49              |
| 2:I:1339:LEU:HD23 | 3:J:17:PHE:CG     | 2.47                     | 0.49              |
| 3:J:79:LYS:CG     | 5:L:569:THR:HG22  | 2.41                     | 0.49              |
| 3:J:978:ARG:HE    | 3:J:1197:ASN:HD21 | 1.59                     | 0.49              |
| 6:P:27:DT:C1'     | 6:P:28:DG:H5'     | 2.42                     | 0.49              |
| 2:I:149:LEU:HG    | 2:I:451:ARG:HG2   | 1.94                     | 0.49              |
| 2:I:240:GLU:HG2   | 2:I:284:LEU:HD13  | 1.93                     | 0.49              |
| 2:I:1108:ASN:OD1  | 2:I:1111:GLN:NE2  | 2.45                     | 0.49              |
| 2:I:1111:GLN:HB2  | 2:I:1230:MET:CE   | 2.42                     | 0.49              |
| 2:I:1276:TRP:CE2  | 3:J:801:VAL:HG21  | 2.47                     | 0.49              |
| 3:J:78:LEU:HD12   | 3:J:81:ARG:HB2    | 1.94                     | 0.49              |
| 3:J:279:LEU:HD11  | 3:J:296:LYS:CG    | 2.41                     | 0.49              |
| 3:J:1028:ILE:HG22 | 3:J:1120:THR:CA   | 2.41                     | 0.49              |
| 1:G:133:LEU:HD21  | 1:G:140:ILE:HG12  | 1.94                     | 0.49              |
| 1:H:214:GLU:O     | 1:H:218:ARG:NH1   | 2.46                     | 0.49              |
| 2:I:81:ASP:N      | 2:I:81:ASP:OD1    | 2.43                     | 0.49              |
| 2:I:577:VAL:HG23  | 2:I:661:VAL:O     | 2.12                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:I:594:VAL:HG13 | 2:I:598:VAL:O     | 2.12                     | 0.49              |
| 2:I:978:VAL:O    | 2:I:1007:LYS:HE2  | 2.13                     | 0.49              |
| 3:J:357:VAL:HG22 | 3:J:461:PHE:HD2   | 1.74                     | 0.49              |
| 3:J:442:ILE:HG22 | 3:J:443:GLU:O     | 2.13                     | 0.49              |
| 3:J:796:LEU:O    | 3:J:800:LEU:HD13  | 2.12                     | 0.49              |
| 3:J:822:MET:CB   | 3:J:839:VAL:HG22  | 2.42                     | 0.49              |
| 3:J:1272:SER:CB  | 3:J:1273:ASP:HB3  | 2.38                     | 0.49              |
| 1:R:260:LEU:CD1  | 1:R:281:LEU:HD22  | 2.43                     | 0.49              |
| 1:R:265:ARG:HE   | 1:R:294:ASN:HB3   | 1.77                     | 0.49              |
| 1:H:85:LEU:HD22  | 1:H:144:ILE:CD1   | 2.43                     | 0.49              |
| 2:I:145:ILE:HG22 | 2:I:456:VAL:HG22  | 1.95                     | 0.49              |
| 2:I:155:VAL:HA   | 2:I:175:ARG:O     | 2.12                     | 0.49              |
| 2:I:252:SER:C    | 2:I:265:LYS:HG3   | 2.37                     | 0.49              |
| 2:I:447:HIS:CE1  | 2:I:609:ILE:HG22  | 2.48                     | 0.49              |
| 2:I:521:LEU:HB2  | 2:I:794:LEU:HD21  | 1.95                     | 0.49              |
| 2:I:680:LEU:O    | 2:I:684:ASN:HB2   | 2.13                     | 0.49              |
| 2:I:808:ASN:OD1  | 2:I:1216:ARG:NH2  | 2.45                     | 0.49              |
| 2:I:971:LEU:CD2  | 2:I:975:ILE:HD11  | 2.43                     | 0.49              |
| 2:I:982:GLY:O    | 2:I:1007:LYS:NZ   | 2.36                     | 0.49              |
| 2:I:1250:SER:OG  | 5:L:524:GLU:OE1   | 2.23                     | 0.49              |
| 3:J:537:TYR:CE1  | 3:J:544:LEU:HB2   | 2.48                     | 0.49              |
| 3:J:836:ARG:O    | 3:J:840:LEU:HB2   | 2.13                     | 0.49              |
| 5:L:315:TRP:O    | 5:L:319:ALA:HB2   | 2.11                     | 0.49              |
| 1:R:303:ILE:O    | 1:R:307:LEU:HG    | 2.13                     | 0.49              |
| 1:G:195:ARG:HG2  | 1:G:198:LEU:HG    | 1.94                     | 0.49              |
| 2:I:270:THR:H    | 2:I:273:HIS:HD2   | 1.59                     | 0.49              |
| 2:I:375:PRO:HD3  | 5:L:103:ARG:HG2   | 1.95                     | 0.49              |
| 3:J:154:LEU:HD22 | 3:J:176:PHE:HE1   | 1.77                     | 0.49              |
| 3:J:252:LEU:O    | 3:J:252:LEU:HD23  | 2.13                     | 0.49              |
| 3:J:514:THR:HG23 | 3:J:595:ALA:O     | 2.13                     | 0.49              |
| 5:L:125:ASP:O    | 5:L:129:GLN:HG3   | 2.11                     | 0.49              |
| 1:G:67:GLU:HB3   | 1:G:171:LEU:CD1   | 2.43                     | 0.49              |
| 1:H:183:ILE:HD12 | 1:H:183:ILE:O     | 2.12                     | 0.49              |
| 2:I:14:ASP:HA    | 2:I:1183:ALA:HB3  | 1.94                     | 0.49              |
| 2:I:1331:ARG:HG3 | 3:J:33:TRP:CH2    | 2.48                     | 0.49              |
| 3:J:809:VAL:HG21 | 3:J:909:ILE:HG12  | 1.95                     | 0.49              |
| 1:G:45:ARG:HD3   | 2:I:1083:GLU:HB3  | 1.95                     | 0.49              |
| 2:I:74:ARG:NH2   | 2:I:97:ARG:HG3    | 2.28                     | 0.49              |
| 2:I:1120:ALA:HA  | 2:I:1199:LEU:HD23 | 1.95                     | 0.49              |
| 2:I:1304:MET:O   | 2:I:1308:ILE:HG12 | 2.12                     | 0.49              |
| 3:J:34:SER:OG    | 3:J:103:GLY:HA2   | 2.13                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:468:VAL:HG23  | 3:J:468:VAL:O     | 2.13                     | 0.49              |
| 3:J:1184:ASP:N    | 3:J:1185:PRO:HD3  | 2.27                     | 0.49              |
| 1:R:307:LEU:O     | 1:R:312:LEU:N     | 2.26                     | 0.49              |
| 1:G:36:GLY:HA3    | 1:G:187:VAL:HG11  | 1.95                     | 0.49              |
| 2:I:455:SER:O     | 2:I:459:MET:HE2   | 2.13                     | 0.49              |
| 2:I:636:CYS:SG    | 2:I:650:VAL:HG12  | 2.52                     | 0.49              |
| 2:I:1293:VAL:CG2  | 2:I:1315:MET:HE3  | 2.43                     | 0.49              |
| 3:J:950:ILE:O     | 3:J:1016:THR:HG23 | 2.12                     | 0.49              |
| 3:J:1035:VAL:HG21 | 3:J:1115:ILE:HG23 | 1.95                     | 0.49              |
| 5:L:165:PHE:HE2   | 5:L:217:ALA:HB1   | 1.78                     | 0.49              |
| 5:L:286:LEU:O     | 5:L:290:LEU:HG    | 2.13                     | 0.49              |
| 5:L:402:LEU:HG    | 5:L:405:ILE:HD11  | 1.95                     | 0.49              |
| 1:R:250:ASP:HB2   | 1:R:253:LEU:HD12  | 1.95                     | 0.49              |
| 1:G:190:ALA:HB2   | 1:G:200:LYS:HB2   | 1.95                     | 0.48              |
| 2:I:299:LYS:HG3   | 2:I:334:GLU:OE2   | 2.13                     | 0.48              |
| 2:I:1030:GLU:O    | 2:I:1034:ARG:HG2  | 2.13                     | 0.48              |
| 3:J:105:ILE:HD13  | 3:J:273:ILE:HG12  | 1.95                     | 0.48              |
| 3:J:1071:GLY:HA2  | 3:J:1074:LEU:HD12 | 1.95                     | 0.48              |
| 3:J:1270:GLY:C    | 3:J:1298:VAL:HG13 | 2.38                     | 0.48              |
| 3:J:1328:THR:HG22 | 3:J:1332:LEU:HD23 | 1.94                     | 0.48              |
| 5:L:142:THR:O     | 5:L:146:GLU:HG3   | 2.13                     | 0.48              |
| 7:Q:49:DC:H2''    | 7:Q:50:DC:C5'     | 2.43                     | 0.48              |
| 2:I:839:VAL:HG21  | 2:I:841:ARG:HH12  | 1.78                     | 0.48              |
| 3:J:536:LEU:HD13  | 3:J:541:LEU:HB2   | 1.95                     | 0.48              |
| 1:H:47:LEU:CD2    | 1:H:220:ALA:HB2   | 2.43                     | 0.48              |
| 2:I:251:ALA:HB3   | 2:I:263:VAL:HG11  | 1.95                     | 0.48              |
| 2:I:1010:GLN:HA   | 2:I:1013:GLN:HG2  | 1.95                     | 0.48              |
| 2:I:1289:GLU:OE1  | 3:J:473:THR:HG22  | 2.13                     | 0.48              |
| 3:J:647:PRO:HG3   | 3:J:697:MET:HA    | 1.94                     | 0.48              |
| 3:J:800:LEU:O     | 3:J:803:VAL:HG12  | 2.13                     | 0.48              |
| 5:L:363:ARG:O     | 5:L:367:ILE:HG13  | 2.13                     | 0.48              |
| 1:R:300:LEU:HD13  | 1:R:304:LYS:HE2   | 1.94                     | 0.48              |
| 1:R:307:LEU:CA    | 1:R:312:LEU:HB2   | 2.44                     | 0.48              |
| 1:H:98:VAL:HG22   | 1:H:100:LEU:HD11  | 1.94                     | 0.48              |
| 1:H:101:THR:HG22  | 1:H:116:THR:CG2   | 2.43                     | 0.48              |
| 2:I:179:TYR:OH    | 2:I:458:GLU:OE2   | 2.24                     | 0.48              |
| 2:I:251:ALA:CB    | 2:I:263:VAL:HG11  | 2.43                     | 0.48              |
| 2:I:360:LEU:HD22  | 2:I:378:ARG:NH2   | 2.28                     | 0.48              |
| 2:I:624:ASP:OD1   | 2:I:625:GLU:HG2   | 2.12                     | 0.48              |
| 5:L:311:THR:C     | 5:L:341:LEU:HD23  | 2.38                     | 0.48              |
| 5:L:470:MET:HB2   | 5:L:478:PRO:HG3   | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:R:257:VAL:HA    | 1:R:260:LEU:HG    | 1.95                     | 0.48              |
| 1:H:98:VAL:HG22   | 1:H:100:LEU:CD1   | 2.44                     | 0.48              |
| 2:I:557:ARG:NH2   | 2:I:611:GLU:OE1   | 2.46                     | 0.48              |
| 2:I:646:SER:HB3   | 2:I:649:GLN:CG    | 2.43                     | 0.48              |
| 2:I:1149:TYR:CE1  | 2:I:1180:MET:HE3  | 2.49                     | 0.48              |
| 3:J:401:VAL:HG12  | 3:J:408:VAL:CG1   | 2.44                     | 0.48              |
| 3:J:742:GLY:O     | 3:J:762:ASN:HB3   | 2.12                     | 0.48              |
| 3:J:850:LYS:CG    | 3:J:851:PRO:HD2   | 2.44                     | 0.48              |
| 5:L:139:GLU:HA    | 5:L:142:THR:OG1   | 2.13                     | 0.48              |
| 5:L:287:ILE:CD1   | 5:L:341:LEU:HD12  | 2.41                     | 0.48              |
| 5:L:425:TYR:CE1   | 6:P:51:DT:H5''    | 2.49                     | 0.48              |
| 8:L:701:1N7:H31   | 8:L:701:1N7:H14   | 1.96                     | 0.48              |
| 2:I:148:GLN:O     | 2:I:453:ILE:HA    | 2.13                     | 0.48              |
| 2:I:560:PRO:CB    | 3:J:776:THR:HG21  | 2.42                     | 0.48              |
| 3:J:960:LEU:HD23  | 3:J:963:VAL:HG11  | 1.95                     | 0.48              |
| 3:J:1108:GLN:HG3  | 3:J:1109:LEU:CD1  | 2.42                     | 0.48              |
| 3:J:1155:ILE:HG13 | 3:J:1211:SER:OG   | 2.12                     | 0.48              |
| 5:L:127:ILE:HD12  | 5:L:128:ASN:N     | 2.28                     | 0.48              |
| 7:Q:32:DA:H2''    | 7:Q:33:DA:O5'     | 2.14                     | 0.48              |
| 1:G:43:LEU:HD13   | 1:G:217:ILE:HD11  | 1.96                     | 0.48              |
| 1:G:104:LYS:HG2   | 1:G:110:VAL:HG22  | 1.94                     | 0.48              |
| 2:I:56:VAL:HG13   | 2:I:57:PHE:CD2    | 2.48                     | 0.48              |
| 2:I:689:ALA:HB1   | 2:I:1233:LEU:HD12 | 1.96                     | 0.48              |
| 2:I:1003:THR:O    | 2:I:1008:GLN:HB2  | 2.14                     | 0.48              |
| 2:I:1250:SER:OG   | 5:L:524:GLU:HB2   | 2.14                     | 0.48              |
| 3:J:66:LYS:HE2    | 3:J:69:GLU:OE1    | 2.12                     | 0.48              |
| 3:J:518:VAL:HG11  | 3:J:707:ILE:CG1   | 2.44                     | 0.48              |
| 3:J:770:LEU:HD22  | 3:J:770:LEU:HA    | 1.56                     | 0.48              |
| 3:J:950:ILE:HG13  | 3:J:1020:TRP:CH2  | 2.49                     | 0.48              |
| 5:L:555:GLU:O     | 5:L:558:VAL:HG12  | 2.13                     | 0.48              |
| 1:R:252:ILE:HG12  | 1:R:278:ILE:CD1   | 2.44                     | 0.48              |
| 1:G:90:VAL:CG1    | 1:G:146:VAL:HG11  | 2.42                     | 0.48              |
| 2:I:242:VAL:HG12  | 2:I:244:GLU:OE1   | 2.14                     | 0.48              |
| 2:I:274:ILE:O     | 2:I:278:GLU:HG3   | 2.14                     | 0.48              |
| 2:I:303:ASP:OD1   | 2:I:328:SER:HB2   | 2.13                     | 0.48              |
| 2:I:431:LYS:O     | 2:I:435:ILE:HG22  | 2.13                     | 0.48              |
| 2:I:757:THR:HG23  | 2:I:765:ILE:HG23  | 1.95                     | 0.48              |
| 2:I:975:ILE:HG12  | 2:I:1014:LEU:CG   | 2.43                     | 0.48              |
| 2:I:1184:THR:HG23 | 2:I:1189:GLY:CA   | 2.44                     | 0.48              |
| 2:I:1230:MET:HB2  | 2:I:1230:MET:HE3  | 1.61                     | 0.48              |
| 2:I:1259:LEU:HD23 | 2:I:1264:GLN:HG2  | 1.96                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:103:GLY:O     | 3:J:244:VAL:HG22  | 2.14                     | 0.48              |
| 3:J:262:THR:HG23  | 3:J:263:SER:O     | 2.14                     | 0.48              |
| 3:J:668:PHE:HA    | 3:J:673:VAL:HG22  | 1.95                     | 0.48              |
| 6:P:66:DG:H2''    | 6:P:67:DA:H5'     | 1.94                     | 0.48              |
| 7:Q:20:DA:H2''    | 7:Q:21:DT:O5'     | 2.14                     | 0.48              |
| 1:G:184:ALA:HB2   | 2:I:1090:ASN:O    | 2.14                     | 0.48              |
| 2:I:232:ILE:HG12  | 2:I:237:LEU:HD22  | 1.95                     | 0.48              |
| 3:J:80:HIS:HB3    | 3:J:83:VAL:HG11   | 1.96                     | 0.48              |
| 3:J:925:GLU:HG3   | 3:J:926:PRO:CD    | 2.44                     | 0.48              |
| 6:P:17:DA:H2''    | 6:P:18:DC:C6      | 2.49                     | 0.48              |
| 2:I:141:THR:O     | 2:I:143:ARG:HG3   | 2.13                     | 0.48              |
| 2:I:322:LEU:HA    | 2:I:325:LEU:HD21  | 1.95                     | 0.48              |
| 2:I:636:CYS:HB2   | 2:I:645:PHE:CD2   | 2.49                     | 0.48              |
| 2:I:1212:LEU:HD22 | 2:I:1225:VAL:CG2  | 2.31                     | 0.48              |
| 4:K:44:ASP:HB2    | 4:K:49:ILE:HG13   | 1.96                     | 0.48              |
| 5:L:151:VAL:CG2   | 5:L:156:ALA:HB3   | 2.35                     | 0.48              |
| 5:L:227:GLN:HA    | 5:L:230:VAL:CG1   | 2.42                     | 0.48              |
| 5:L:244:THR:HA    | 5:L:247:GLU:OE1   | 2.14                     | 0.48              |
| 5:L:281:ARG:HA    | 5:L:284:GLU:CD    | 2.38                     | 0.48              |
| 7:Q:70:DA:H2'     | 7:Q:71:DT:H72     | 1.95                     | 0.48              |
| 1:H:74:VAL:HG12   | 1:H:76:GLU:N      | 2.14                     | 0.47              |
| 1:H:188:GLU:O     | 1:H:200:LYS:HB3   | 2.14                     | 0.47              |
| 2:I:53:PHE:O      | 2:I:57:PHE:HB2    | 2.14                     | 0.47              |
| 2:I:463:GLN:HG3   | 2:I:505:PHE:HB2   | 1.96                     | 0.47              |
| 2:I:854:ILE:HG23  | 2:I:855:PRO:HD2   | 1.95                     | 0.47              |
| 2:I:1342:GLU:HG3  | 3:J:18:ASP:OD2    | 2.14                     | 0.47              |
| 3:J:513:MET:CE    | 3:J:579:LEU:HB2   | 2.43                     | 0.47              |
| 3:J:606:ASN:O     | 3:J:610:ARG:HG2   | 2.14                     | 0.47              |
| 3:J:680:ASN:HA    | 3:J:683:ILE:CG2   | 2.41                     | 0.47              |
| 3:J:839:VAL:HG12  | 3:J:864:LEU:CD1   | 2.43                     | 0.47              |
| 3:J:955:LYS:HE2   | 3:J:1010:GLN:HE22 | 1.79                     | 0.47              |
| 3:J:1163:VAL:HA   | 3:J:1176:VAL:O    | 2.14                     | 0.47              |
| 5:L:105:MET:HE3   | 5:L:388:ILE:CD1   | 2.37                     | 0.47              |
| 5:L:133:SER:CB    | 5:L:365:MET:HB2   | 2.44                     | 0.47              |
| 5:L:318:ALA:O     | 5:L:322:MET:HG3   | 2.14                     | 0.47              |
| 5:L:385:ARG:HH22  | 6:P:55:DC:N4      | 2.12                     | 0.47              |
| 5:L:561:MET:HG3   | 5:L:571:TYR:CD2   | 2.48                     | 0.47              |
| 1:H:9:LEU:HD23    | 1:H:9:LEU:H       | 1.79                     | 0.47              |
| 2:I:257:ALA:HB3   | 2:I:262:TYR:CE2   | 2.38                     | 0.47              |
| 2:I:396:ASP:OD2   | 2:I:398:SER:HB3   | 2.13                     | 0.47              |
| 2:I:599:VAL:HG21  | 2:I:623:LEU:HD22  | 1.97                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:669:PRO:HG3   | 2:I:1069:ARG:NH2  | 2.30                     | 0.47              |
| 2:I:757:THR:CG2   | 2:I:765:ILE:HG23  | 2.43                     | 0.47              |
| 3:J:46:TYR:CE1    | 5:L:453:PRO:HD3   | 2.49                     | 0.47              |
| 3:J:83:VAL:O      | 3:J:92:VAL:HG12   | 2.13                     | 0.47              |
| 3:J:325:LYS:HG2   | 3:J:330:MET:HE2   | 1.95                     | 0.47              |
| 3:J:1328:THR:CG2  | 3:J:1332:LEU:HD23 | 2.44                     | 0.47              |
| 4:K:3:ARG:HD3     | 4:K:4:VAL:N       | 2.29                     | 0.47              |
| 5:L:130:VAL:O     | 5:L:134:VAL:HG23  | 2.13                     | 0.47              |
| 5:L:227:GLN:HG3   | 5:L:252:LEU:HD13  | 1.96                     | 0.47              |
| 5:L:287:ILE:HD13  | 5:L:341:LEU:CD1   | 2.42                     | 0.47              |
| 5:L:437:GLN:HB2   | 6:P:49:DC:H41     | 1.80                     | 0.47              |
| 1:H:79:LEU:HD12   | 3:J:526:VAL:HG11  | 1.95                     | 0.47              |
| 2:I:84:GLU:OE1    | 2:I:84:GLU:N      | 2.36                     | 0.47              |
| 2:I:91:THR:HG21   | 2:I:503:LYS:NZ    | 2.29                     | 0.47              |
| 2:I:445:ILE:HG12  | 2:I:451:ARG:HH21  | 1.78                     | 0.47              |
| 3:J:53:ARG:O      | 3:J:53:ARG:HD3    | 2.15                     | 0.47              |
| 3:J:351:GLY:O     | 3:J:467:ALA:HA    | 2.15                     | 0.47              |
| 3:J:683:ILE:HD11  | 3:J:754:ILE:HG21  | 1.96                     | 0.47              |
| 3:J:968:ASN:OD1   | 3:J:972:LYS:N     | 2.43                     | 0.47              |
| 5:L:281:ARG:HA    | 5:L:284:GLU:HB2   | 1.95                     | 0.47              |
| 5:L:586:ARG:HD3   | 6:P:25:DA:OP2     | 2.13                     | 0.47              |
| 1:G:31:LEU:HB2    | 1:G:199:ASP:O     | 2.13                     | 0.47              |
| 2:I:599:VAL:HG21  | 2:I:623:LEU:CD2   | 2.45                     | 0.47              |
| 2:I:623:LEU:HB2   | 2:I:628:HIS:O     | 2.15                     | 0.47              |
| 2:I:718:ALA:HB2   | 2:I:783:LEU:CD2   | 2.32                     | 0.47              |
| 2:I:737:ASN:O     | 2:I:741:MET:HB2   | 2.14                     | 0.47              |
| 2:I:817:LEU:HD23  | 2:I:1078:LYS:HB3  | 1.96                     | 0.47              |
| 2:I:1140:LYS:O    | 2:I:1143:GLU:HG3  | 2.14                     | 0.47              |
| 2:I:1275:VAL:HG13 | 2:I:1287:LEU:HD11 | 1.95                     | 0.47              |
| 3:J:482:ALA:CB    | 4:K:6:VAL:HG21    | 2.45                     | 0.47              |
| 3:J:744:ARG:HD3   | 3:J:759:ILE:HB    | 1.95                     | 0.47              |
| 3:J:1077:ALA:HB2  | 3:J:1100:PHE:CD1  | 2.49                     | 0.47              |
| 4:K:6:VAL:O       | 4:K:10:VAL:HG23   | 2.14                     | 0.47              |
| 5:L:161:LEU:HD12  | 5:L:265:GLN:NE2   | 2.29                     | 0.47              |
| 5:L:286:LEU:HD23  | 5:L:340:ALA:CB    | 2.44                     | 0.47              |
| 6:P:77:DA:H2"     | 6:P:78:DT:OP2     | 2.14                     | 0.47              |
| 1:G:68:TYR:HB3    | 2:I:756:TYR:CD2   | 2.48                     | 0.47              |
| 2:I:250:THR:HA    | 2:I:268:ARG:HA    | 1.96                     | 0.47              |
| 2:I:660:VAL:HG11  | 3:J:769:VAL:HG13  | 1.97                     | 0.47              |
| 2:I:820:GLU:HB2   | 2:I:1080:ASN:O    | 2.15                     | 0.47              |
| 2:I:1002:LEU:HD23 | 2:I:1003:THR:N    | 2.29                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:1067:ALA:CB   | 2:I:1235:LEU:HD11 | 2.45                     | 0.47              |
| 3:J:134:ASP:CG    | 3:J:159:ILE:HD12  | 2.40                     | 0.47              |
| 3:J:720:ASN:HB3   | 3:J:723:TYR:HB3   | 1.95                     | 0.47              |
| 3:J:1101:LEU:HB3  | 3:J:1105:ALA:CB   | 2.43                     | 0.47              |
| 5:L:141:ILE:O     | 5:L:145:LEU:HG    | 2.14                     | 0.47              |
| 6:P:27:DT:H1'     | 6:P:28:DG:O4'     | 2.14                     | 0.47              |
| 1:H:89:ALA:HB3    | 1:H:124:VAL:CG1   | 2.45                     | 0.47              |
| 2:I:322:LEU:HA    | 2:I:325:LEU:CD2   | 2.45                     | 0.47              |
| 2:I:615:VAL:HG21  | 2:I:645:PHE:CD2   | 2.50                     | 0.47              |
| 2:I:1251:TYR:HB2  | 5:L:528:LEU:HD11  | 1.97                     | 0.47              |
| 3:J:872:LEU:O     | 3:J:877:VAL:HG23  | 2.15                     | 0.47              |
| 3:J:1005:LYS:HA   | 3:J:1009:GLU:OE1  | 2.15                     | 0.47              |
| 3:J:1037:PHE:HE2  | 3:J:1059:LEU:HD12 | 1.79                     | 0.47              |
| 5:L:119:ILE:CG2   | 5:L:379:MET:HE3   | 2.45                     | 0.47              |
| 5:L:387:VAL:HG22  | 5:L:435:ILE:CD1   | 2.42                     | 0.47              |
| 7:Q:20:DA:H2''    | 7:Q:21:DT:C5'     | 2.44                     | 0.47              |
| 2:I:39:ILE:HD11   | 2:I:75:LEU:CD1    | 2.44                     | 0.47              |
| 2:I:101:ARG:HG3   | 2:I:118:LYS:O     | 2.14                     | 0.47              |
| 2:I:322:LEU:HD23  | 2:I:325:LEU:HD21  | 1.97                     | 0.47              |
| 2:I:1283:ALA:HA   | 3:J:479:GLU:OE1   | 2.15                     | 0.47              |
| 3:J:45:ASN:O      | 3:J:45:ASN:ND2    | 2.47                     | 0.47              |
| 3:J:48:THR:O      | 3:J:50:LYS:N      | 2.47                     | 0.47              |
| 3:J:147:ILE:HG22  | 3:J:188:LEU:CD2   | 2.44                     | 0.47              |
| 3:J:518:VAL:HG23  | 3:J:547:ARG:HH12  | 1.79                     | 0.47              |
| 3:J:603:LYS:O     | 3:J:607:THR:HG23  | 2.14                     | 0.47              |
| 3:J:950:ILE:HG13  | 3:J:1020:TRP:HH2  | 1.80                     | 0.47              |
| 3:J:952:VAL:CG2   | 3:J:984:LEU:HD22  | 2.44                     | 0.47              |
| 3:J:1041:ILE:O    | 3:J:1046:ILE:HG12 | 2.14                     | 0.47              |
| 3:J:1178:THR:HG23 | 3:J:1184:ASP:OD2  | 2.14                     | 0.47              |
| 5:L:341:LEU:O     | 5:L:345:GLN:HG3   | 2.14                     | 0.47              |
| 6:P:36:DA:H2''    | 6:P:37:DA:C8      | 2.50                     | 0.47              |
| 2:I:398:SER:O     | 2:I:400:VAL:N     | 2.48                     | 0.47              |
| 2:I:484:LEU:HD12  | 2:I:485:ASP:N     | 2.30                     | 0.47              |
| 2:I:551:HIS:CE1   | 2:I:553:THR:HG23  | 2.50                     | 0.47              |
| 2:I:1212:LEU:HD13 | 2:I:1225:VAL:HG22 | 1.96                     | 0.47              |
| 3:J:647:PRO:HG3   | 3:J:697:MET:CA    | 2.44                     | 0.47              |
| 3:J:665:GLN:O     | 3:J:669:GLN:HG3   | 2.15                     | 0.47              |
| 3:J:1237:VAL:HG13 | 3:J:1253:ILE:HD13 | 1.96                     | 0.47              |
| 6:P:28:DG:H2''    | 6:P:29:DA:O5'     | 2.15                     | 0.47              |
| 6:P:51:DT:H2''    | 6:P:52:DA:OP1     | 2.15                     | 0.47              |
| 2:I:161:LYS:O     | 2:I:161:LYS:HG2   | 2.15                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:766:ASN:OD1   | 2:I:767:GLN:N     | 2.47                     | 0.47              |
| 2:I:802:VAL:CG2   | 2:I:1098:LEU:HD13 | 2.45                     | 0.47              |
| 2:I:1250:SER:HG   | 5:L:524:GLU:HB2   | 1.79                     | 0.47              |
| 3:J:203:GLU:O     | 3:J:206:ASN:HB3   | 2.14                     | 0.47              |
| 3:J:473:THR:OG1   | 3:J:474:LEU:N     | 2.44                     | 0.47              |
| 3:J:490:ILE:O     | 3:J:491:LEU:HD12  | 2.14                     | 0.47              |
| 3:J:825:VAL:O     | 3:J:831:VAL:HG23  | 2.14                     | 0.47              |
| 3:J:1047:THR:HG22 | 3:J:1060:VAL:HB   | 1.97                     | 0.47              |
| 7:Q:27:DA:H2'     | 7:Q:28:DT:H72     | 1.96                     | 0.47              |
| 1:G:25:LYS:HG2    | 1:G:204:GLU:CB    | 2.45                     | 0.47              |
| 2:I:145:ILE:HB    | 2:I:456:VAL:HG22  | 1.97                     | 0.47              |
| 2:I:975:ILE:CD1   | 2:I:1014:LEU:HG   | 2.45                     | 0.47              |
| 2:I:1243:MET:HG3  | 3:J:372:MET:SD    | 2.55                     | 0.47              |
| 3:J:491:LEU:O     | 3:J:904:ALA:HB2   | 2.15                     | 0.47              |
| 3:J:700:ASN:O     | 3:J:704:GLU:HB2   | 2.14                     | 0.47              |
| 3:J:1026:PRO:HB2  | 3:J:1028:ILE:HG23 | 1.96                     | 0.47              |
| 3:J:1163:VAL:HG23 | 3:J:1175:LEU:CD1  | 2.45                     | 0.47              |
| 3:J:1163:VAL:HG23 | 3:J:1175:LEU:HD11 | 1.97                     | 0.47              |
| 3:J:1190:ILE:HG22 | 3:J:1191:PRO:O    | 2.15                     | 0.47              |
| 3:J:1327:GLU:HG2  | 3:J:1327:GLU:O    | 2.15                     | 0.47              |
| 5:L:111:LEU:HD13  | 5:L:116:GLU:HG2   | 1.97                     | 0.47              |
| 6:P:25:DA:H2'     | 6:P:26:DT:C7      | 2.45                     | 0.47              |
| 1:R:269:CYS:SG    | 1:R:295:LEU:HD12  | 2.55                     | 0.47              |
| 1:R:286:GLU:HG2   | 1:R:290:LEU:HD11  | 1.96                     | 0.47              |
| 1:H:65:LEU:O      | 1:H:65:LEU:HD13   | 2.16                     | 0.46              |
| 1:H:195:ARG:HB3   | 1:H:198:LEU:HD21  | 1.97                     | 0.46              |
| 2:I:16:GLY:HA3    | 2:I:1156:ARG:NH1  | 2.30                     | 0.46              |
| 2:I:453:ILE:HD11  | 2:I:587:LEU:CD1   | 2.44                     | 0.46              |
| 2:I:691:PRO:HA    | 2:I:788:SER:OG    | 2.15                     | 0.46              |
| 2:I:956:ALA:HB1   | 2:I:1032:LYS:HG2  | 1.97                     | 0.46              |
| 3:J:51:PRO:HG2    | 3:J:65:VAL:CG2    | 2.45                     | 0.46              |
| 3:J:127:LEU:HD23  | 3:J:189:LEU:HD22  | 1.97                     | 0.46              |
| 3:J:479:GLU:CG    | 4:K:20:VAL:HG11   | 2.45                     | 0.46              |
| 3:J:709:ARG:HD3   | 3:J:710:ASP:CG    | 2.40                     | 0.46              |
| 5:L:346:GLN:O     | 5:L:350:GLU:HG3   | 2.15                     | 0.46              |
| 5:L:511:ILE:O     | 5:L:511:ILE:HG23  | 2.14                     | 0.46              |
| 1:R:287:VAL:CG1   | 1:R:291:LYS:HE3   | 2.36                     | 0.46              |
| 1:R:307:LEU:HD22  | 1:R:312:LEU:HB3   | 1.97                     | 0.46              |
| 2:I:633:LEU:O     | 2:I:633:LEU:HD12  | 2.14                     | 0.46              |
| 3:J:141:PHE:CD1   | 3:J:180:MET:HG3   | 2.50                     | 0.46              |
| 3:J:306:LEU:O     | 3:J:326:SER:HB2   | 2.15                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:J:680:ASN:O    | 3:J:683:ILE:HG22  | 2.15                     | 0.46              |
| 5:L:290:LEU:HD13 | 5:L:333:VAL:HG22  | 1.96                     | 0.46              |
| 5:L:420:GLU:OE1  | 5:L:423:ARG:NH1   | 2.45                     | 0.46              |
| 5:L:452:ILE:CG1  | 5:L:457:ILE:HG13  | 2.45                     | 0.46              |
| 7:Q:77:DT:OP1    | 1:R:298:LYS:HD3   | 2.14                     | 0.46              |
| 1:G:229:GLU:HA   | 1:G:232:VAL:HG12  | 1.96                     | 0.46              |
| 2:I:26:TYR:HE2   | 2:I:32:LEU:HD12   | 1.79                     | 0.46              |
| 2:I:148:GLN:OE1  | 2:I:454:ARG:HD2   | 2.15                     | 0.46              |
| 2:I:148:GLN:HB3  | 2:I:454:ARG:HB2   | 1.97                     | 0.46              |
| 2:I:1109:ILE:HA  | 2:I:1109:ILE:HD12 | 1.66                     | 0.46              |
| 3:J:17:PHE:HZ    | 3:J:1353:VAL:HG21 | 1.79                     | 0.46              |
| 3:J:189:LEU:HB3  | 3:J:234:PRO:HB2   | 1.97                     | 0.46              |
| 3:J:813:ASP:OD1  | 3:J:814:CYS:N     | 2.48                     | 0.46              |
| 3:J:960:LEU:HD13 | 3:J:1007:ASP:CA   | 2.45                     | 0.46              |
| 5:L:236:LYS:O    | 5:L:243:ALA:N     | 2.49                     | 0.46              |
| 7:Q:48:DC:H2"    | 7:Q:49:DC:C6      | 2.51                     | 0.46              |
| 1:G:160:HIS:HA   | 1:G:161:SER:HA    | 1.71                     | 0.46              |
| 1:H:67:GLU:OE2   | 1:H:79:LEU:HB3    | 2.15                     | 0.46              |
| 3:J:62:PHE:HZ    | 3:J:244:VAL:HG21  | 1.79                     | 0.46              |
| 3:J:129:ASP:HB2  | 3:J:220:ARG:CZ    | 2.46                     | 0.46              |
| 3:J:479:GLU:HG3  | 4:K:20:VAL:HG11   | 1.96                     | 0.46              |
| 3:J:509:GLY:CA   | 3:J:632:ALA:HB2   | 2.46                     | 0.46              |
| 3:J:843:VAL:C    | 3:J:882:VAL:HG23  | 2.39                     | 0.46              |
| 5:L:576:VAL:HB   | 5:L:587:ILE:CD1   | 2.46                     | 0.46              |
| 1:G:135:ASP:OD1  | 1:G:136:GLU:N     | 2.49                     | 0.46              |
| 1:H:100:LEU:HD11 | 1:H:121:VAL:HG21  | 1.96                     | 0.46              |
| 1:H:112:ALA:CB   | 1:H:126:PRO:HA    | 2.40                     | 0.46              |
| 1:H:179:PRO:HA   | 1:H:208:ASN:ND2   | 2.31                     | 0.46              |
| 2:I:56:VAL:HG11  | 2:I:468:LEU:HD13  | 1.98                     | 0.46              |
| 2:I:338:THR:HG21 | 2:I:345:PRO:HB3   | 1.97                     | 0.46              |
| 3:J:807:LEU:HB2  | 3:J:1259:GLN:NE2  | 2.31                     | 0.46              |
| 3:J:1175:LEU:HB2 | 3:J:1190:ILE:CD1  | 2.44                     | 0.46              |
| 1:H:185:TYR:HB2  | 1:H:201:LEU:HD12  | 1.98                     | 0.46              |
| 2:I:678:ARG:HA   | 2:I:678:ARG:HD3   | 1.72                     | 0.46              |
| 2:I:1132:LEU:CD2 | 2:I:1141:LEU:HD21 | 2.45                     | 0.46              |
| 3:J:327:LEU:O    | 3:J:330:MET:HB2   | 2.15                     | 0.46              |
| 3:J:654:ILE:HG12 | 3:J:743:MET:HE1   | 1.97                     | 0.46              |
| 5:L:479:THR:OG1  | 5:L:480:PRO:HD2   | 2.16                     | 0.46              |
| 1:H:76:GLU:N     | 1:H:76:GLU:OE1    | 2.48                     | 0.46              |
| 2:I:204:LEU:HD13 | 2:I:208:ILE:HD13  | 1.96                     | 0.46              |
| 2:I:960:LEU:HB3  | 2:I:1025:PHE:CZ   | 2.50                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:141:PHE:HE1   | 3:J:181:GLY:HA3   | 1.77                     | 0.46              |
| 3:J:370:LYS:HA    | 3:J:441:LEU:HD12  | 1.98                     | 0.46              |
| 3:J:829:GLY:HA2   | 3:J:993:GLU:OE1   | 2.16                     | 0.46              |
| 3:J:1048:ARG:NE   | 3:J:1048:ARG:HA   | 2.31                     | 0.46              |
| 3:J:1071:GLY:CA   | 3:J:1074:LEU:HB2  | 2.44                     | 0.46              |
| 4:K:38:LEU:HB2    | 4:K:53:GLU:CD     | 2.41                     | 0.46              |
| 1:H:59:VAL:HG21   | 1:H:85:LEU:HD13   | 1.98                     | 0.46              |
| 2:I:1080:ASN:CB   | 2:I:1085:MET:HE3  | 2.44                     | 0.46              |
| 2:I:1253:LEU:HD12 | 3:J:251:PRO:HG3   | 1.98                     | 0.46              |
| 3:J:646:ILE:CD1   | 3:J:762:ASN:HD21  | 2.27                     | 0.46              |
| 3:J:806:ASP:O     | 3:J:808:VAL:HG23  | 2.15                     | 0.46              |
| 3:J:1061:VAL:HB   | 3:J:1105:ALA:HB3  | 1.98                     | 0.46              |
| 5:L:420:GLU:HG3   | 5:L:422:ARG:NH2   | 2.30                     | 0.46              |
| 5:L:511:ILE:HG22  | 5:L:517:SER:O     | 2.16                     | 0.46              |
| 1:R:278:ILE:O     | 1:R:282:VAL:HG13  | 2.16                     | 0.46              |
| 1:G:97:GLU:HA     | 1:G:147:GLN:HA    | 1.97                     | 0.46              |
| 2:I:103:VAL:HA    | 2:I:116:ASP:O     | 2.16                     | 0.46              |
| 2:I:192:ASP:HB3   | 2:I:346:TYR:CE1   | 2.51                     | 0.46              |
| 2:I:1105:SER:HB2  | 3:J:731:ARG:HB3   | 1.98                     | 0.46              |
| 3:J:291:ILE:CD1   | 5:L:409:ASN:HB3   | 2.46                     | 0.46              |
| 3:J:491:LEU:HD23  | 3:J:496:GLY:O     | 2.16                     | 0.46              |
| 3:J:712:GLN:N     | 3:J:712:GLN:OE1   | 2.48                     | 0.46              |
| 3:J:844:THR:CG2   | 3:J:864:LEU:HD11  | 2.46                     | 0.46              |
| 6:P:21:DA:C8      | 6:P:22:DT:H72     | 2.50                     | 0.46              |
| 6:P:64:DT:H2''    | 6:P:65:DT:H71     | 1.98                     | 0.46              |
| 6:P:79:DA:H2''    | 6:P:80:DG:C8      | 2.51                     | 0.46              |
| 1:G:47:LEU:O      | 1:G:180:VAL:HG21  | 2.16                     | 0.46              |
| 1:G:67:GLU:HB3    | 1:G:171:LEU:HD12  | 1.98                     | 0.46              |
| 1:G:83:LEU:HD21   | 2:I:693:LEU:CD2   | 2.44                     | 0.46              |
| 2:I:815:SER:HB3   | 2:I:1077:SER:HB3  | 1.98                     | 0.46              |
| 2:I:980:VAL:HG22  | 2:I:984:VAL:CG2   | 2.41                     | 0.46              |
| 2:I:1304:MET:CE   | 2:I:1308:ILE:HD11 | 2.42                     | 0.46              |
| 3:J:735:ALA:O     | 3:J:738:ARG:HB3   | 2.16                     | 0.46              |
| 3:J:1078:LEU:CD1  | 3:J:1101:LEU:HD11 | 2.40                     | 0.46              |
| 5:L:261:LEU:HD23  | 5:L:265:GLN:CB    | 2.45                     | 0.46              |
| 5:L:290:LEU:HD12  | 5:L:337:VAL:HG22  | 1.98                     | 0.46              |
| 6:P:32:DA:H1'     | 6:P:33:DA:H5'     | 1.98                     | 0.46              |
| 1:G:79:LEU:HD13   | 1:G:83:LEU:HD13   | 1.98                     | 0.45              |
| 1:H:13:LEU:HA     | 1:H:28:LEU:CD2    | 2.43                     | 0.45              |
| 1:H:13:LEU:O      | 1:H:13:LEU:HG     | 2.16                     | 0.45              |
| 2:I:133:ASN:HB3   | 2:I:527:LYS:HZ1   | 1.80                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:292:ILE:O     | 2:I:292:ILE:HG22  | 2.16                     | 0.45              |
| 2:I:666:SER:O     | 2:I:702:THR:OG1   | 2.29                     | 0.45              |
| 2:I:830:THR:OG1   | 2:I:831:ILE:N     | 2.48                     | 0.45              |
| 2:I:886:LYS:HE3   | 2:I:916:SER:O     | 2.16                     | 0.45              |
| 4:K:39:VAL:CG2    | 4:K:40:PRO:HD2    | 2.46                     | 0.45              |
| 5:L:285:ARG:HD3   | 5:L:288:MET:CE    | 2.46                     | 0.45              |
| 5:L:287:ILE:HG23  | 5:L:337:VAL:CG1   | 2.45                     | 0.45              |
| 1:H:107:ILE:HG12  | 1:H:136:GLU:H     | 1.81                     | 0.45              |
| 2:I:1066:MET:HE2  | 2:I:1076:ILE:HD11 | 1.97                     | 0.45              |
| 3:J:526:VAL:HA    | 3:J:549:LYS:O     | 2.16                     | 0.45              |
| 3:J:1158:GLU:HG3  | 3:J:1186:TYR:CE1  | 2.51                     | 0.45              |
| 6:P:74:DC:H5'     | 6:P:74:DC:C6      | 2.51                     | 0.45              |
| 1:R:321:TRP:CE3   | 1:R:322:PRO:HA    | 2.50                     | 0.45              |
| 1:H:31:LEU:O      | 1:H:198:LEU:HD12  | 2.16                     | 0.45              |
| 1:H:99:ILE:C      | 1:H:100:LEU:HD12  | 2.41                     | 0.45              |
| 2:I:364:VAL:HG13  | 2:I:376:PRO:CG    | 2.46                     | 0.45              |
| 2:I:905:ILE:HG22  | 2:I:906:PHE:CE1   | 2.52                     | 0.45              |
| 2:I:1087:TYR:HD2  | 2:I:1091:GLY:HA2  | 1.80                     | 0.45              |
| 2:I:1091:GLY:O    | 2:I:1093:PRO:HD3  | 2.16                     | 0.45              |
| 3:J:592:VAL:HG12  | 3:J:604:MET:HE2   | 1.98                     | 0.45              |
| 3:J:807:LEU:HD22  | 3:J:1259:GLN:HE21 | 1.81                     | 0.45              |
| 3:J:1115:ILE:HD12 | 3:J:1115:ILE:O    | 2.17                     | 0.45              |
| 5:L:137:TYR:HB3   | 5:L:273:MET:HE2   | 1.97                     | 0.45              |
| 5:L:254:GLU:OE1   | 5:L:257:LYS:HD3   | 2.17                     | 0.45              |
| 5:L:316:PHE:CZ    | 5:L:334:SER:HB3   | 2.50                     | 0.45              |
| 5:L:411:GLY:O     | 5:L:414:LYS:HB3   | 2.16                     | 0.45              |
| 3:J:161:THR:HG22  | 3:J:164:GLN:HG3   | 1.99                     | 0.45              |
| 3:J:355:ILE:HG21  | 3:J:466:MET:SD    | 2.57                     | 0.45              |
| 3:J:372:MET:HE1   | 3:J:447:ILE:HD11  | 1.98                     | 0.45              |
| 3:J:516:ASP:N     | 3:J:516:ASP:OD1   | 2.48                     | 0.45              |
| 3:J:955:LYS:HD3   | 3:J:956:GLY:N     | 2.31                     | 0.45              |
| 3:J:1329:THR:O    | 3:J:1333:THR:HG22 | 2.16                     | 0.45              |
| 5:L:137:TYR:CB    | 5:L:273:MET:HE2   | 2.46                     | 0.45              |
| 5:L:151:VAL:HG21  | 5:L:161:LEU:CB    | 2.44                     | 0.45              |
| 5:L:162:ILE:HD13  | 5:L:221:PHE:CZ    | 2.46                     | 0.45              |
| 5:L:456:MET:HE3   | 5:L:497:VAL:HG22  | 1.96                     | 0.45              |
| 6:P:31:DA:H2''    | 6:P:32:DA:C8      | 2.51                     | 0.45              |
| 7:Q:28:DT:H2''    | 7:Q:29:DT:H71     | 1.98                     | 0.45              |
| 7:Q:78:DG:H1'     | 7:Q:79:DT:C5'     | 2.47                     | 0.45              |
| 1:R:250:ASP:OD2   | 1:R:252:ILE:HG22  | 2.17                     | 0.45              |
| 1:H:33:ARG:HD3    | 1:H:197:ASP:CG    | 2.42                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:H:73:GLY:O     | 1:H:133:LEU:HD12  | 2.16                     | 0.45              |
| 1:H:107:ILE:HG23 | 1:H:134:THR:C     | 2.42                     | 0.45              |
| 2:I:702:THR:HG22 | 2:I:1184:THR:O    | 2.16                     | 0.45              |
| 2:I:889:PRO:HA   | 2:I:913:VAL:HG23  | 1.98                     | 0.45              |
| 2:I:971:LEU:HD11 | 2:I:1017:GLN:HB3  | 1.97                     | 0.45              |
| 2:I:1281:TYR:CE2 | 3:J:484:MET:HG2   | 2.52                     | 0.45              |
| 3:J:868:TRP:CE3  | 3:J:871:LEU:HD12  | 2.51                     | 0.45              |
| 5:L:380:VAL:O    | 5:L:384:LEU:HG    | 2.17                     | 0.45              |
| 1:G:43:LEU:O     | 1:G:47:LEU:HG     | 2.17                     | 0.45              |
| 1:H:92:VAL:HG12  | 1:H:93:GLN:O      | 2.17                     | 0.45              |
| 2:I:239:MET:C    | 2:I:284:LEU:HD12  | 2.42                     | 0.45              |
| 2:I:287:VAL:HG13 | 2:I:288:PRO:HD2   | 1.99                     | 0.45              |
| 2:I:301:TYR:HB2  | 2:I:311:CYS:SG    | 2.57                     | 0.45              |
| 2:I:483:ASP:OD2  | 2:I:486:THR:HG21  | 2.17                     | 0.45              |
| 2:I:543:ALA:HA   | 2:I:544:GLY:HA3   | 1.60                     | 0.45              |
| 2:I:898:GLU:HG2  | 5:L:544:THR:OG1   | 2.17                     | 0.45              |
| 3:J:485:MET:HG3  | 3:J:486:SER:H     | 1.80                     | 0.45              |
| 3:J:579:LEU:HD12 | 3:J:579:LEU:O     | 2.17                     | 0.45              |
| 3:J:653:ILE:HG21 | 3:J:693:VAL:HG23  | 1.99                     | 0.45              |
| 3:J:956:GLY:C    | 3:J:984:LEU:HD11  | 2.41                     | 0.45              |
| 3:J:1027:VAL:O   | 3:J:1027:VAL:HG12 | 2.16                     | 0.45              |
| 3:J:1029:THR:CG2 | 3:J:1121:LEU:HD11 | 2.47                     | 0.45              |
| 5:L:533:ASP:HA   | 5:L:536:THR:CG2   | 2.44                     | 0.45              |
| 2:I:876:GLU:HA   | 2:I:926:GLY:O     | 2.16                     | 0.45              |
| 2:I:975:ILE:CG1  | 2:I:1014:LEU:HG   | 2.43                     | 0.45              |
| 2:I:1119:MET:HE1 | 2:I:1210:ILE:HD11 | 1.98                     | 0.45              |
| 2:I:1120:ALA:HB2 | 2:I:1199:LEU:CD2  | 2.47                     | 0.45              |
| 3:J:140:TYR:O    | 3:J:141:PHE:HB2   | 2.16                     | 0.45              |
| 3:J:352:ARG:HA   | 3:J:466:MET:O     | 2.17                     | 0.45              |
| 5:L:280:VAL:HG22 | 5:L:347:ILE:HG21  | 1.99                     | 0.45              |
| 1:R:257:VAL:HG12 | 1:R:260:LEU:CD1   | 2.46                     | 0.45              |
| 1:R:280:ASP:HA   | 1:R:283:GLN:HG3   | 1.98                     | 0.45              |
| 1:G:92:VAL:HG12  | 1:G:121:VAL:HG22  | 1.99                     | 0.45              |
| 1:H:39:LEU:HA    | 1:H:39:LEU:HD23   | 1.69                     | 0.45              |
| 1:H:98:VAL:HG11  | 1:H:121:VAL:CG2   | 2.46                     | 0.45              |
| 1:H:105:SER:CA   | 1:H:138:ALA:HB2   | 2.31                     | 0.45              |
| 2:I:24:VAL:HA    | 2:I:578:TYR:HE1   | 1.81                     | 0.45              |
| 2:I:303:ASP:CB   | 2:I:310:ILE:HD11  | 2.45                     | 0.45              |
| 2:I:468:LEU:HA   | 2:I:471:VAL:HG12  | 1.98                     | 0.45              |
| 2:I:623:LEU:HD12 | 2:I:623:LEU:O     | 2.16                     | 0.45              |
| 2:I:672:GLU:OE1  | 2:I:672:GLU:N     | 2.32                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:I:960:LEU:HB3   | 2:I:1025:PHE:HE1 | 1.79                     | 0.45              |
| 3:J:298:MET:SD    | 5:L:406:GLN:HG3  | 2.56                     | 0.45              |
| 3:J:816:THR:HG22  | 3:J:889:ASP:OD2  | 2.17                     | 0.45              |
| 3:J:820:ILE:O     | 3:J:881:LYS:HA   | 2.16                     | 0.45              |
| 3:J:884:SER:OG    | 3:J:1254:GLU:OE1 | 2.26                     | 0.45              |
| 3:J:1061:VAL:HG13 | 3:J:1076:PRO:HG2 | 1.99                     | 0.45              |
| 3:J:1208:ASP:OD1  | 3:J:1209:VAL:N   | 2.50                     | 0.45              |
| 4:K:13:ILE:HD12   | 4:K:54:ILE:CG2   | 2.46                     | 0.45              |
| 5:L:218:ARG:HA    | 5:L:221:PHE:CD2  | 2.36                     | 0.45              |
| 5:L:297:MET:HE2   | 5:L:302:PHE:CA   | 2.46                     | 0.45              |
| 6:P:63:DT:H2'     | 6:P:64:DT:H71    | 1.99                     | 0.45              |
| 1:H:182:ARG:NH1   | 3:J:581:MET:HE1  | 2.31                     | 0.45              |
| 2:I:669:PRO:HD3   | 2:I:1069:ARG:NH1 | 2.31                     | 0.45              |
| 2:I:1288:GLN:NE2  | 2:I:1317:PRO:HB3 | 2.31                     | 0.45              |
| 3:J:125:GLY:HA2   | 3:J:135:ILE:CD1  | 2.47                     | 0.45              |
| 3:J:623:GLN:O     | 3:J:627:THR:HG22 | 2.16                     | 0.45              |
| 3:J:876:SER:HA    | 3:J:990:ARG:NH2  | 2.31                     | 0.45              |
| 6:P:50:DA:OP2     | 6:P:50:DA:H2'    | 2.17                     | 0.45              |
| 1:R:252:ILE:HG12  | 1:R:278:ILE:HD12 | 1.99                     | 0.45              |
| 1:H:112:ALA:HB3   | 1:H:126:PRO:C    | 2.42                     | 0.45              |
| 2:I:15:PHE:CD2    | 2:I:1190:ALA:HB2 | 2.52                     | 0.45              |
| 2:I:98:VAL:CB     | 2:I:124:MET:HE3  | 2.47                     | 0.45              |
| 2:I:364:VAL:HG13  | 2:I:376:PRO:HG3  | 1.98                     | 0.45              |
| 2:I:818:VAL:O     | 2:I:1079:ILE:HA  | 2.17                     | 0.45              |
| 2:I:1080:ASN:HD22 | 2:I:1085:MET:CE  | 2.29                     | 0.45              |
| 3:J:198:CYS:SG    | 3:J:221:ILE:HD11 | 2.57                     | 0.45              |
| 3:J:657:ALA:HB2   | 3:J:689:ALA:HB2  | 1.98                     | 0.45              |
| 3:J:961:SER:O     | 3:J:980:THR:HG23 | 2.16                     | 0.45              |
| 3:J:1344:LEU:CD2  | 3:J:1349:GLU:HB3 | 2.41                     | 0.45              |
| 5:L:489:MET:HG3   | 5:L:494:ILE:HD11 | 1.99                     | 0.45              |
| 7:Q:49:DC:H2''    | 7:Q:50:DC:O5'    | 2.16                     | 0.45              |
| 1:G:47:LEU:CD2    | 1:G:220:ALA:HB2  | 2.47                     | 0.44              |
| 1:G:52:PRO:HA     | 1:G:149:GLY:O    | 2.16                     | 0.44              |
| 1:H:69:SER:HB2    | 1:H:78:ILE:HD11  | 1.98                     | 0.44              |
| 2:I:812:PHE:O     | 3:J:504:GLN:NE2  | 2.46                     | 0.44              |
| 2:I:980:VAL:CA    | 2:I:984:VAL:HB   | 2.43                     | 0.44              |
| 3:J:708:ASN:N     | 3:J:708:ASN:OD1  | 2.48                     | 0.44              |
| 3:J:1346:GLY:O    | 3:J:1350:ASN:ND2 | 2.49                     | 0.44              |
| 1:H:57:THR:O      | 1:H:173:VAL:HB   | 2.16                     | 0.44              |
| 1:H:102:LEU:HD12  | 1:H:114:ASP:O    | 2.17                     | 0.44              |
| 1:H:192:VAL:HG12  | 1:H:193:GLU:H    | 1.82                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:560:PRO:HG3   | 3:J:773:PHE:HE1   | 1.82                     | 0.44              |
| 2:I:893:THR:OG1   | 2:I:894:GLN:N     | 2.50                     | 0.44              |
| 2:I:1043:ALA:HB1  | 2:I:1044:PRO:HD2  | 2.00                     | 0.44              |
| 2:I:1125:GLY:HA3  | 2:I:1179:GLY:HA2  | 1.99                     | 0.44              |
| 2:I:1326:LEU:HD12 | 2:I:1326:LEU:HA   | 1.73                     | 0.44              |
| 3:J:325:LYS:CD    | 3:J:330:MET:HE2   | 2.47                     | 0.44              |
| 3:J:478:LEU:HD23  | 3:J:478:LEU:HA    | 1.78                     | 0.44              |
| 3:J:485:MET:HB3   | 3:J:488:ASN:ND2   | 2.32                     | 0.44              |
| 3:J:812:ASP:HB2   | 3:J:911:LYS:HE2   | 1.99                     | 0.44              |
| 5:L:286:LEU:HG    | 5:L:290:LEU:HD11  | 1.99                     | 0.44              |
| 1:H:104:LYS:H     | 1:H:140:ILE:HG23  | 1.82                     | 0.44              |
| 2:I:62:TYR:CE1    | 2:I:476:LYS:HE3   | 2.51                     | 0.44              |
| 2:I:1075:VAL:HB   | 3:J:461:PHE:O     | 2.17                     | 0.44              |
| 2:I:1113:LEU:HD11 | 3:J:641:ILE:CD1   | 2.47                     | 0.44              |
| 2:I:1204:LEU:HB3  | 2:I:1205:PRO:HD2  | 2.00                     | 0.44              |
| 3:J:506:VAL:HG23  | 3:J:628:GLY:HA3   | 1.99                     | 0.44              |
| 3:J:965:SER:OG    | 3:J:973:LEU:HD11  | 2.17                     | 0.44              |
| 3:J:1265:THR:OG1  | 3:J:1303:SER:HB3  | 2.17                     | 0.44              |
| 5:L:275:VAL:O     | 5:L:279:ARG:HG3   | 2.16                     | 0.44              |
| 6:P:39:DG:OP2     | 6:P:39:DG:H2'     | 2.17                     | 0.44              |
| 1:G:102:LEU:HD11  | 1:G:110:VAL:HG11  | 2.00                     | 0.44              |
| 1:H:107:ILE:CG2   | 1:H:135:ASP:HA    | 2.48                     | 0.44              |
| 2:I:469:VAL:HA    | 2:I:472:GLU:HG2   | 2.00                     | 0.44              |
| 2:I:685:MET:HE3   | 2:I:685:MET:HB2   | 1.86                     | 0.44              |
| 2:I:980:VAL:HG13  | 2:I:984:VAL:HG21  | 1.98                     | 0.44              |
| 2:I:1115:THR:CG2  | 2:I:1228:GLY:HA3  | 2.48                     | 0.44              |
| 2:I:1319:MET:HE3  | 2:I:1319:MET:HB3  | 1.83                     | 0.44              |
| 3:J:218:THR:HA    | 3:J:221:ILE:CG2   | 2.47                     | 0.44              |
| 3:J:930:LEU:HD23  | 3:J:1244:GLN:HG2  | 1.98                     | 0.44              |
| 3:J:1353:VAL:O    | 3:J:1353:VAL:HG22 | 2.17                     | 0.44              |
| 5:L:286:LEU:HG    | 5:L:290:LEU:CD1   | 2.47                     | 0.44              |
| 6:P:29:DA:H2''    | 6:P:30:DC:O5'     | 2.17                     | 0.44              |
| 7:Q:20:DA:H2''    | 7:Q:21:DT:H5'     | 1.98                     | 0.44              |
| 1:G:52:PRO:HB3    | 1:H:5:VAL:HG11    | 2.00                     | 0.44              |
| 1:G:207:THR:HG21  | 1:G:211:ILE:HB    | 1.99                     | 0.44              |
| 1:H:26:VAL:O      | 1:H:203:ILE:N     | 2.51                     | 0.44              |
| 1:H:103:ASN:CB    | 1:H:141:SER:HA    | 2.35                     | 0.44              |
| 3:J:93:THR:HG22   | 3:J:94:GLN:N      | 2.33                     | 0.44              |
| 3:J:902:ASP:N     | 3:J:902:ASP:OD1   | 2.47                     | 0.44              |
| 3:J:1273:ASP:OD1  | 3:J:1273:ASP:N    | 2.51                     | 0.44              |
| 5:L:141:ILE:HG23  | 5:L:224:LEU:HD11  | 2.00                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:L:419:PHE:CE1  | 5:L:427:PHE:HA    | 2.52                     | 0.44              |
| 6:P:37:DA:H2''   | 6:P:38:DG:C8      | 2.53                     | 0.44              |
| 2:I:303:ASP:OD1  | 2:I:304:GLU:N     | 2.50                     | 0.44              |
| 2:I:558:VAL:HG13 | 2:I:573:ASN:HB3   | 2.00                     | 0.44              |
| 2:I:890:LYS:HB2  | 2:I:914:LYS:HB2   | 2.00                     | 0.44              |
| 2:I:989:LEU:HD13 | 2:I:1000:LEU:CD1  | 2.48                     | 0.44              |
| 2:I:1236:ASN:HA  | 2:I:1238:LEU:CD1  | 2.48                     | 0.44              |
| 2:I:1274:GLU:HG2 | 3:J:424:ASN:ND2   | 2.33                     | 0.44              |
| 3:J:165:TYR:OH   | 3:J:169:LEU:HD12  | 2.17                     | 0.44              |
| 3:J:1005:LYS:HE3 | 3:J:1015:GLU:OE2  | 2.18                     | 0.44              |
| 6:P:77:DA:H2''   | 6:P:78:DT:C6      | 2.53                     | 0.44              |
| 2:I:39:ILE:HD13  | 2:I:129:LEU:HD21  | 2.00                     | 0.44              |
| 2:I:118:LYS:NZ   | 2:I:488:MET:HA    | 2.32                     | 0.44              |
| 2:I:244:GLU:OE1  | 2:I:244:GLU:N     | 2.36                     | 0.44              |
| 2:I:551:HIS:HB3  | 2:I:554:HIS:HE1   | 1.82                     | 0.44              |
| 2:I:572:ILE:O    | 2:I:572:ILE:HG22  | 2.17                     | 0.44              |
| 2:I:1305:TYR:O   | 2:I:1309:VAL:HG22 | 2.18                     | 0.44              |
| 3:J:490:ILE:HG13 | 3:J:491:LEU:CD1   | 2.47                     | 0.44              |
| 3:J:534:GLU:OE1  | 3:J:581:MET:HE1   | 2.17                     | 0.44              |
| 3:J:747:MET:O    | 3:J:755:ILE:HD12  | 2.18                     | 0.44              |
| 4:K:39:VAL:HG22  | 4:K:52:ARG:HH21   | 1.83                     | 0.44              |
| 2:I:69:GLN:NE2   | 2:I:101:ARG:HH21  | 2.15                     | 0.44              |
| 2:I:468:LEU:HA   | 2:I:468:LEU:HD23  | 1.60                     | 0.44              |
| 2:I:621:SER:HB2  | 2:I:653:MET:CE    | 2.46                     | 0.44              |
| 2:I:757:THR:O    | 2:I:765:ILE:HG22  | 2.17                     | 0.44              |
| 2:I:969:ALA:HB1  | 8:I:1401:1N7:C24  | 2.47                     | 0.44              |
| 3:J:56:LEU:HD11  | 3:J:273:ILE:CD1   | 2.40                     | 0.44              |
| 3:J:275:ARG:HD3  | 3:J:298:MET:HB3   | 2.00                     | 0.44              |
| 3:J:325:LYS:HG3  | 3:J:329:ASP:HB3   | 2.00                     | 0.44              |
| 3:J:664:ILE:HD11 | 3:J:681:LYS:HE3   | 2.00                     | 0.44              |
| 3:J:842:ARG:HB2  | 3:J:882:VAL:HG21  | 1.99                     | 0.44              |
| 3:J:1028:ILE:CG2 | 3:J:1120:THR:HG22 | 2.48                     | 0.44              |
| 7:Q:19:DT:H3'    | 7:Q:19:DT:P       | 2.57                     | 0.44              |
| 7:Q:72:DG:H2'    | 7:Q:73:DG:C8      | 2.52                     | 0.44              |
| 2:I:131:THR:HG22 | 2:I:132:ASP:N     | 2.30                     | 0.44              |
| 2:I:794:LEU:HG   | 2:I:796:LEU:CD1   | 2.46                     | 0.44              |
| 3:J:83:VAL:O     | 3:J:83:VAL:HG13   | 2.18                     | 0.44              |
| 3:J:432:LEU:CD1  | 3:J:499:ILE:HG21  | 2.48                     | 0.44              |
| 3:J:1162:ILE:O   | 3:J:1177:ILE:HA   | 2.18                     | 0.44              |
| 3:J:1261:LEU:O   | 3:J:1261:LEU:HD12 | 2.18                     | 0.44              |
| 3:J:1368:ASP:O   | 3:J:1371:ARG:HG2  | 2.18                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:L:133:SER:HB3  | 5:L:365:MET:HB2   | 2.00                     | 0.44              |
| 5:L:404:LEU:HD22 | 5:L:439:ILE:HG23  | 2.00                     | 0.44              |
| 1:G:192:VAL:CG1  | 1:G:195:ARG:HB3   | 2.48                     | 0.43              |
| 2:I:151:ARG:HD2  | 2:I:445:ILE:HD12  | 1.99                     | 0.43              |
| 2:I:572:ILE:HD12 | 2:I:572:ILE:HG23  | 1.78                     | 0.43              |
| 2:I:1136:GLN:OE1 | 2:I:1136:GLN:N    | 2.38                     | 0.43              |
| 8:I:1401:1N7:H17 | 8:I:1401:1N7:H4   | 2.00                     | 0.43              |
| 3:J:67:ASP:OD1   | 3:J:95:THR:N      | 2.33                     | 0.43              |
| 3:J:120:LEU:HB3  | 3:J:121:PRO:HD3   | 1.99                     | 0.43              |
| 3:J:123:ARG:HG2  | 3:J:1337:VAL:HG11 | 1.99                     | 0.43              |
| 3:J:858:VAL:HA   | 3:J:859:PRO:HD3   | 1.89                     | 0.43              |
| 3:J:963:VAL:HG13 | 3:J:963:VAL:O     | 2.18                     | 0.43              |
| 3:J:1104:LYS:HB3 | 3:J:1125:PRO:CD   | 2.48                     | 0.43              |
| 3:J:1270:GLY:H   | 3:J:1300:ALA:HA   | 1.83                     | 0.43              |
| 7:Q:59:DT:C2'    | 7:Q:60:DT:H71     | 2.48                     | 0.43              |
| 7:Q:69:DA:H2''   | 7:Q:70:DA:O5'     | 2.18                     | 0.43              |
| 1:H:57:THR:OG1   | 1:H:147:GLN:HB3   | 2.18                     | 0.43              |
| 2:I:257:ALA:O    | 2:I:260:LYS:HB3   | 2.19                     | 0.43              |
| 3:J:287:ALA:HA   | 5:L:413:MET:CE    | 2.48                     | 0.43              |
| 3:J:876:SER:CB   | 3:J:990:ARG:HH21  | 2.31                     | 0.43              |
| 3:J:1105:ALA:HA  | 3:J:1123:ARG:O    | 2.18                     | 0.43              |
| 5:L:105:MET:HE1  | 5:L:385:ARG:HG2   | 2.01                     | 0.43              |
| 6:P:31:DA:H2''   | 6:P:32:DA:H8      | 1.83                     | 0.43              |
| 7:Q:49:DC:OP2    | 7:Q:49:DC:H6      | 2.01                     | 0.43              |
| 7:Q:70:DA:H2'    | 7:Q:71:DT:C7      | 2.49                     | 0.43              |
| 1:R:279:GLY:HA2  | 1:R:282:VAL:HG22  | 2.00                     | 0.43              |
| 1:R:282:VAL:HB   | 1:R:316:MET:SD    | 2.59                     | 0.43              |
| 1:G:11:PRO:HB3   | 1:G:31:LEU:CD2    | 2.48                     | 0.43              |
| 2:I:734:ILE:HD12 | 2:I:734:ILE:HG23  | 1.71                     | 0.43              |
| 3:J:153:ASN:C    | 3:J:154:LEU:HD12  | 2.43                     | 0.43              |
| 3:J:401:VAL:HG12 | 3:J:408:VAL:HG12  | 1.98                     | 0.43              |
| 3:J:582:ILE:HG22 | 3:J:620:PHE:CD1   | 2.53                     | 0.43              |
| 3:J:1078:LEU:O   | 3:J:1099:TYR:N    | 2.46                     | 0.43              |
| 1:H:73:GLY:HA2   | 1:H:134:THR:HB    | 2.01                     | 0.43              |
| 1:H:74:VAL:HG22  | 1:H:133:LEU:HD12  | 2.00                     | 0.43              |
| 2:I:21:VAL:CG1   | 2:I:655:VAL:HG13  | 2.49                     | 0.43              |
| 2:I:186:PHE:HZ   | 2:I:425:ILE:HG23  | 1.82                     | 0.43              |
| 2:I:316:GLU:O    | 2:I:316:GLU:HG2   | 2.18                     | 0.43              |
| 3:J:68:TYR:C     | 3:J:92:VAL:HG23   | 2.44                     | 0.43              |
| 3:J:142:GLU:HB3  | 5:L:91:ILE:CG2    | 2.49                     | 0.43              |
| 3:J:430:HIS:CD2  | 3:J:432:LEU:HB2   | 2.53                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:K:13:ILE:HD12  | 4:K:54:ILE:HG23   | 2.00                     | 0.43              |
| 4:K:38:LEU:HD13  | 4:K:53:GLU:OE1    | 2.18                     | 0.43              |
| 5:L:291:CYS:HA   | 5:L:295:CYS:HB2   | 2.00                     | 0.43              |
| 1:G:90:VAL:HG11  | 1:G:146:VAL:CG1   | 2.45                     | 0.43              |
| 1:G:182:ARG:O    | 1:G:183:ILE:HD13  | 2.19                     | 0.43              |
| 1:G:196:THR:OG1  | 1:G:197:ASP:N     | 2.52                     | 0.43              |
| 1:H:89:ALA:HB3   | 1:H:124:VAL:HG12  | 2.00                     | 0.43              |
| 2:I:22:LEU:HD13  | 2:I:603:ILE:CD1   | 2.45                     | 0.43              |
| 2:I:27:LEU:HD22  | 2:I:663:VAL:HG11  | 2.00                     | 0.43              |
| 2:I:218:GLU:HG2  | 2:I:299:LYS:HA    | 1.99                     | 0.43              |
| 2:I:969:ALA:HB2  | 8:I:1401:1N7:H34  | 2.00                     | 0.43              |
| 2:I:976:ARG:HB2  | 2:I:997:TRP:CZ2   | 2.53                     | 0.43              |
| 3:J:194:LEU:HD22 | 3:J:224:LEU:HD22  | 2.00                     | 0.43              |
| 3:J:923:ILE:HD11 | 3:J:1252:HIS:C    | 2.42                     | 0.43              |
| 3:J:930:LEU:HA   | 3:J:1244:GLN:HG2  | 1.99                     | 0.43              |
| 3:J:1279:GLN:NE2 | 3:J:1305:ASP:OD2  | 2.51                     | 0.43              |
| 5:L:313:ASP:HA   | 5:L:316:PHE:CB    | 2.42                     | 0.43              |
| 5:L:390:ILE:CD1  | 5:L:432:THR:HG23  | 2.48                     | 0.43              |
| 1:G:27:THR:C     | 1:G:28:LEU:HD12   | 2.43                     | 0.43              |
| 2:I:312:ALA:H    | 2:I:315:MET:CE    | 2.31                     | 0.43              |
| 2:I:566:GLY:O    | 2:I:569:ILE:HG13  | 2.17                     | 0.43              |
| 3:J:53:ARG:HA    | 3:J:54:ASP:HA     | 1.56                     | 0.43              |
| 3:J:960:LEU:CD2  | 3:J:963:VAL:HG11  | 2.49                     | 0.43              |
| 4:K:4:VAL:HG22   | 4:K:5:THR:HG23    | 2.01                     | 0.43              |
| 5:L:124:GLU:HA   | 5:L:127:ILE:CG1   | 2.48                     | 0.43              |
| 5:L:150:ARG:O    | 5:L:155:GLU:HB2   | 2.18                     | 0.43              |
| 6:P:68:DA:H1'    | 6:P:69:DT:H5'     | 1.99                     | 0.43              |
| 1:G:105:SER:CB   | 1:G:139:SER:HB2   | 2.49                     | 0.43              |
| 2:I:281:ASP:OD1  | 2:I:283:LYS:HE3   | 2.19                     | 0.43              |
| 2:I:971:LEU:O    | 2:I:975:ILE:HG13  | 2.18                     | 0.43              |
| 2:I:1120:ALA:CA  | 2:I:1199:LEU:HD23 | 2.49                     | 0.43              |
| 2:I:1196:LYS:HD2 | 2:I:1206:THR:HG23 | 2.00                     | 0.43              |
| 3:J:166:LEU:HD12 | 3:J:166:LEU:HA    | 1.86                     | 0.43              |
| 3:J:268:LEU:HB2  | 3:J:306:LEU:HD23  | 2.01                     | 0.43              |
| 3:J:537:TYR:HE2  | 3:J:634:ARG:HH12  | 1.65                     | 0.43              |
| 3:J:902:ASP:HA   | 3:J:903:LEU:HD23  | 1.98                     | 0.43              |
| 5:L:452:ILE:HD11 | 5:L:457:ILE:CG1   | 2.48                     | 0.43              |
| 5:L:481:GLU:O    | 5:L:484:ALA:HB3   | 2.18                     | 0.43              |
| 1:G:74:VAL:HG13  | 1:G:74:VAL:O      | 2.19                     | 0.43              |
| 2:I:12:ARG:HH21  | 2:I:793:GLU:CD    | 2.24                     | 0.43              |
| 2:I:221:LEU:HD11 | 2:I:314:ASN:HB2   | 2.00                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:I:716:ALA:HB3   | 2:I:784:ALA:HB3  | 2.01                     | 0.43              |
| 2:I:922:ASN:HD22  | 2:I:923:GLY:H    | 1.66                     | 0.43              |
| 3:J:394:ILE:HG13  | 5:L:532:LEU:HD11 | 2.01                     | 0.43              |
| 3:J:718:SER:OG    | 3:J:719:PHE:N    | 2.51                     | 0.43              |
| 3:J:741:ALA:C     | 3:J:762:ASN:HD22 | 2.25                     | 0.43              |
| 3:J:1370:MET:HE3  | 3:J:1370:MET:HB2 | 1.88                     | 0.43              |
| 5:L:456:MET:HE2   | 5:L:500:ILE:CD1  | 2.49                     | 0.43              |
| 5:L:533:ASP:CA    | 5:L:536:THR:HG22 | 2.45                     | 0.43              |
| 1:H:56:VAL:HA     | 1:H:146:VAL:HA   | 2.00                     | 0.43              |
| 2:I:18:ARG:NH1    | 2:I:620:ASN:HA   | 2.34                     | 0.43              |
| 2:I:230:PHE:HB3   | 2:I:237:LEU:HD12 | 2.01                     | 0.43              |
| 2:I:237:LEU:HD11  | 2:I:333:ILE:HD13 | 2.00                     | 0.43              |
| 2:I:582:ASN:OD1   | 2:I:583:GLU:N    | 2.49                     | 0.43              |
| 3:J:79:LYS:CB     | 5:L:569:THR:HG22 | 2.49                     | 0.43              |
| 3:J:213:LYS:O     | 3:J:217:LEU:HG   | 2.19                     | 0.43              |
| 3:J:841:GLY:O     | 3:J:863:LEU:HD11 | 2.18                     | 0.43              |
| 3:J:1046:ILE:HD12 | 3:J:1059:LEU:CD1 | 2.44                     | 0.43              |
| 3:J:1164:SER:HA   | 3:J:1200:GLU:OE2 | 2.19                     | 0.43              |
| 3:J:1332:LEU:HD13 | 3:J:1332:LEU:HA  | 1.83                     | 0.43              |
| 5:L:386:LEU:O     | 5:L:389:SER:OG   | 2.27                     | 0.43              |
| 7:Q:28:DT:H2'     | 7:Q:29:DT:H71    | 2.01                     | 0.43              |
| 1:R:300:LEU:CA    | 1:R:303:ILE:HD12 | 2.34                     | 0.43              |
| 1:G:57:THR:C      | 1:G:173:VAL:HG22 | 2.44                     | 0.43              |
| 2:I:300:ASP:HB2   | 2:I:309:LEU:HD11 | 2.00                     | 0.43              |
| 2:I:344:GLY:HA3   | 2:I:346:TYR:CE2  | 2.54                     | 0.43              |
| 2:I:612:GLY:O     | 2:I:639:LYS:HG2  | 2.19                     | 0.43              |
| 2:I:1225:VAL:HA   | 3:J:638:SER:HB3  | 2.01                     | 0.43              |
| 3:J:84:ILE:O      | 3:J:84:ILE:HG13  | 2.18                     | 0.43              |
| 3:J:422:LEU:CD1   | 3:J:471:PRO:HG3  | 2.49                     | 0.43              |
| 3:J:511:TYR:HE2   | 3:J:724:MET:HG2  | 1.83                     | 0.43              |
| 3:J:1046:ILE:HD12 | 3:J:1059:LEU:HB3 | 2.00                     | 0.43              |
| 3:J:1062:LEU:HD13 | 3:J:1066:GLU:CD  | 2.44                     | 0.43              |
| 5:L:143:TYR:O     | 5:L:147:GLN:HG2  | 2.19                     | 0.43              |
| 7:Q:78:DG:H2''    | 7:Q:79:DT:OP2    | 2.19                     | 0.43              |
| 1:R:265:ARG:NE    | 1:R:294:ASN:O    | 2.49                     | 0.43              |
| 1:G:56:VAL:HA     | 1:G:146:VAL:HA   | 2.01                     | 0.42              |
| 1:H:107:ILE:HA    | 1:H:134:THR:O    | 2.19                     | 0.42              |
| 2:I:39:ILE:HD12   | 2:I:127:ILE:HD12 | 2.01                     | 0.42              |
| 2:I:127:ILE:HG13  | 2:I:127:ILE:O    | 2.19                     | 0.42              |
| 2:I:432:LEU:HA    | 2:I:435:ILE:CG2  | 2.49                     | 0.42              |
| 2:I:542:ARG:O     | 6:P:63:DT:H5''   | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:1247:SER:HB3  | 3:J:375:GLU:O     | 2.19                     | 0.42              |
| 3:J:111:THR:HG21  | 3:J:303:VAL:HB    | 2.01                     | 0.42              |
| 3:J:596:LEU:HD11  | 3:J:604:MET:CE    | 2.49                     | 0.42              |
| 3:J:793:SER:OG    | 3:J:927:GLY:HA3   | 2.19                     | 0.42              |
| 3:J:807:LEU:HA    | 3:J:807:LEU:HD12  | 1.54                     | 0.42              |
| 3:J:842:ARG:CB    | 3:J:882:VAL:HG21  | 2.49                     | 0.42              |
| 3:J:1251:LYS:O    | 3:J:1255:VAL:HG12 | 2.19                     | 0.42              |
| 5:L:101:TYR:CD2   | 5:L:405:ILE:HD12  | 2.54                     | 0.42              |
| 5:L:318:ALA:CA    | 5:L:321:ALA:HB3   | 2.40                     | 0.42              |
| 2:I:228:VAL:CG1   | 2:I:239:MET:HE3   | 2.50                     | 0.42              |
| 2:I:367:TYR:CD2   | 2:I:376:PRO:HB3   | 2.53                     | 0.42              |
| 2:I:496:LYS:O     | 2:I:500:ALA:CB    | 2.67                     | 0.42              |
| 2:I:717:VAL:HA    | 2:I:781:ASP:O     | 2.19                     | 0.42              |
| 2:I:1288:GLN:O    | 2:I:1292:THR:HB   | 2.19                     | 0.42              |
| 3:J:266:ASN:O     | 3:J:270:ARG:HB2   | 2.19                     | 0.42              |
| 3:J:500:ILE:HG22  | 3:J:500:ILE:O     | 2.19                     | 0.42              |
| 3:J:530:PRO:HB3   | 3:J:581:MET:HG3   | 2.00                     | 0.42              |
| 3:J:966:VAL:N     | 3:J:974:VAL:O     | 2.51                     | 0.42              |
| 3:J:1096:PRO:HB2  | 3:J:1098:GLN:OE1  | 2.19                     | 0.42              |
| 3:J:1261:LEU:HD13 | 3:J:1304:ARG:NH1  | 2.33                     | 0.42              |
| 3:J:1266:ILE:CD1  | 3:J:1285:VAL:HG21 | 2.49                     | 0.42              |
| 5:L:142:THR:HG22  | 5:L:228:TYR:OH    | 2.19                     | 0.42              |
| 5:L:165:PHE:CE2   | 5:L:217:ALA:HB1   | 2.54                     | 0.42              |
| 5:L:585:GLU:OE1   | 7:Q:68:DC:N4      | 2.49                     | 0.42              |
| 1:G:48:LEU:HD23   | 1:G:48:LEU:HA     | 1.62                     | 0.42              |
| 1:G:228:LEU:CD1   | 1:H:224:LEU:HD23  | 2.48                     | 0.42              |
| 2:I:706:ARG:HD3   | 2:I:792:GLY:O     | 2.19                     | 0.42              |
| 2:I:1304:MET:HE2  | 3:J:472:LEU:HB3   | 2.01                     | 0.42              |
| 2:I:1312:ASN:HD21 | 2:I:1314:GLN:NE2  | 2.17                     | 0.42              |
| 3:J:680:ASN:CA    | 3:J:683:ILE:HG22  | 2.46                     | 0.42              |
| 5:L:214:PRO:O     | 5:L:218:ARG:HG3   | 2.18                     | 0.42              |
| 5:L:262:VAL:HG13  | 5:L:263:PRO:HD2   | 2.01                     | 0.42              |
| 5:L:560:ARG:O     | 5:L:567:MET:HE2   | 2.19                     | 0.42              |
| 2:I:151:ARG:HD2   | 2:I:445:ILE:CD1   | 2.50                     | 0.42              |
| 2:I:561:ILE:HG21  | 3:J:772:TYR:HE2   | 1.85                     | 0.42              |
| 2:I:561:ILE:CD1   | 2:I:671:LEU:HD21  | 2.50                     | 0.42              |
| 2:I:971:LEU:HD11  | 2:I:1017:GLN:CB   | 2.49                     | 0.42              |
| 3:J:1064:SER:HB3  | 3:J:1192:LYS:NZ   | 2.34                     | 0.42              |
| 3:J:1098:GLN:HG2  | 3:J:1098:GLN:O    | 2.18                     | 0.42              |
| 3:J:1172:LYS:O    | 3:J:1192:LYS:HE2  | 2.19                     | 0.42              |
| 5:L:137:TYR:O     | 5:L:140:ALA:HB3   | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:L:252:LEU:O     | 5:L:255:VAL:HG22  | 2.20                     | 0.42              |
| 5:L:606:VAL:HG13  | 5:L:607:LEU:HD22  | 2.00                     | 0.42              |
| 6:P:66:DG:H1'     | 6:P:67:DA:H5'     | 2.00                     | 0.42              |
| 1:H:75:GLN:OE1    | 1:H:75:GLN:N      | 2.40                     | 0.42              |
| 1:H:112:ALA:HB3   | 1:H:126:PRO:O     | 2.19                     | 0.42              |
| 2:I:118:LYS:HE2   | 2:I:488:MET:HG2   | 2.00                     | 0.42              |
| 2:I:1099:ASN:OD1  | 2:I:1100:PRO:HD2  | 2.19                     | 0.42              |
| 2:I:1240:ASP:OD1  | 2:I:1240:ASP:N    | 2.49                     | 0.42              |
| 3:J:218:THR:CA    | 3:J:221:ILE:HG22  | 2.48                     | 0.42              |
| 3:J:262:THR:H     | 5:L:504:PRO:HB2   | 1.84                     | 0.42              |
| 3:J:612:LEU:HB3   | 3:J:616:PRO:HG2   | 2.02                     | 0.42              |
| 3:J:1172:LYS:O    | 3:J:1192:LYS:HB3  | 2.19                     | 0.42              |
| 1:H:97:GLU:HG2    | 1:H:147:GLN:HG3   | 2.01                     | 0.42              |
| 2:I:14:ASP:HB3    | 2:I:1157:GLN:HB2  | 2.01                     | 0.42              |
| 2:I:157:PHE:O     | 2:I:442:VAL:HB    | 2.20                     | 0.42              |
| 2:I:788:SER:HB3   | 2:I:795:ALA:O     | 2.19                     | 0.42              |
| 2:I:970:GLY:O     | 2:I:973:SER:OG    | 2.22                     | 0.42              |
| 2:I:1006:GLU:O    | 2:I:1009:ASN:O    | 2.37                     | 0.42              |
| 2:I:1270:PHE:CE2  | 2:I:1290:MET:HG2  | 2.54                     | 0.42              |
| 3:J:426:ALA:HB3   | 3:J:427:PRO:CD    | 2.50                     | 0.42              |
| 3:J:845:ALA:HB2   | 3:J:883:ARG:HG3   | 2.01                     | 0.42              |
| 3:J:982:LEU:HD12  | 3:J:982:LEU:HA    | 1.93                     | 0.42              |
| 1:R:289:LEU:O     | 1:R:295:LEU:HD22  | 2.20                     | 0.42              |
| 1:G:228:LEU:HD11  | 1:H:224:LEU:HB3   | 2.02                     | 0.42              |
| 2:I:128:PRO:HG2   | 2:I:506:PHE:CD2   | 2.55                     | 0.42              |
| 2:I:615:VAL:HG13  | 2:I:615:VAL:O     | 2.18                     | 0.42              |
| 2:I:850:ILE:O     | 2:I:850:ILE:HG22  | 2.20                     | 0.42              |
| 2:I:851:THR:HG22  | 2:I:887:VAL:HG12  | 2.01                     | 0.42              |
| 2:I:888:THR:HG23  | 2:I:916:SER:CB    | 2.50                     | 0.42              |
| 2:I:898:GLU:HB3   | 5:L:540:LEU:CD2   | 2.50                     | 0.42              |
| 2:I:1096:ILE:HD13 | 2:I:1096:ILE:HG21 | 1.81                     | 0.42              |
| 2:I:1276:TRP:CD2  | 3:J:801:VAL:HG21  | 2.54                     | 0.42              |
| 3:J:1037:PHE:HA   | 3:J:1040:MET:SD   | 2.60                     | 0.42              |
| 3:J:1097:ALA:HB1  | 3:J:1099:TYR:CZ   | 2.55                     | 0.42              |
| 6:P:63:DT:H2'     | 6:P:63:DT:H6      | 1.72                     | 0.42              |
| 2:I:339:ASN:N     | 2:I:343:HIS:O     | 2.43                     | 0.42              |
| 2:I:817:LEU:HD21  | 2:I:1080:ASN:ND2  | 2.34                     | 0.42              |
| 2:I:975:ILE:CG2   | 2:I:997:TRP:HE1   | 2.32                     | 0.42              |
| 3:J:68:TYR:CA     | 3:J:92:VAL:HG23   | 2.50                     | 0.42              |
| 3:J:716:GLN:OE1   | 3:J:716:GLN:N     | 2.53                     | 0.42              |
| 3:J:812:ASP:HB2   | 3:J:911:LYS:CE    | 2.49                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:886:VAL:O     | 3:J:886:VAL:HG22  | 2.19                     | 0.42              |
| 3:J:1035:VAL:CG2  | 3:J:1115:ILE:HG23 | 2.49                     | 0.42              |
| 3:J:1040:MET:HA   | 3:J:1045:THR:HG21 | 2.02                     | 0.42              |
| 3:J:1145:PHE:HB3  | 3:J:1309:ILE:HD13 | 2.01                     | 0.42              |
| 3:J:1256:ILE:HD13 | 3:J:1256:ILE:HA   | 1.84                     | 0.42              |
| 5:L:105:MET:HE1   | 5:L:385:ARG:HA    | 2.02                     | 0.42              |
| 5:L:330:LEU:O     | 5:L:334:SER:N     | 2.53                     | 0.42              |
| 5:L:423:ARG:HG2   | 5:L:425:TYR:CD2   | 2.54                     | 0.42              |
| 6:P:22:DT:H5'     | 6:P:22:DT:H6      | 1.83                     | 0.42              |
| 6:P:25:DA:H2'     | 6:P:26:DT:C6      | 2.55                     | 0.42              |
| 1:G:66:HIS:HB2    | 2:I:927:THR:HG21  | 2.01                     | 0.42              |
| 1:H:98:VAL:O      | 1:H:146:VAL:HG22  | 2.20                     | 0.42              |
| 2:I:237:LEU:HD13  | 2:I:237:LEU:HA    | 1.86                     | 0.42              |
| 2:I:359:ARG:O     | 2:I:363:LEU:HG    | 2.20                     | 0.42              |
| 2:I:452:ARG:HH21  | 2:I:458:GLU:CD    | 2.27                     | 0.42              |
| 2:I:453:ILE:HG21  | 2:I:453:ILE:HD13  | 1.75                     | 0.42              |
| 2:I:593:LYS:O     | 2:I:600:THR:HB    | 2.19                     | 0.42              |
| 2:I:620:ASN:HD21  | 3:J:768:ASN:HB2   | 1.84                     | 0.42              |
| 2:I:971:LEU:HD23  | 2:I:975:ILE:CD1   | 2.48                     | 0.42              |
| 2:I:1282:GLY:O    | 2:I:1284:ALA:N    | 2.52                     | 0.42              |
| 3:J:294:ASN:HD22  | 5:L:406:GLN:HE21  | 1.67                     | 0.42              |
| 3:J:363:LEU:HB3   | 3:J:450:HIS:CE1   | 2.55                     | 0.42              |
| 3:J:849:LEU:HA    | 3:J:849:LEU:HD13  | 1.80                     | 0.42              |
| 3:J:1037:PHE:HB3  | 3:J:1040:MET:HB2  | 2.02                     | 0.42              |
| 3:J:1051:ASP:HB2  | 3:J:1054:THR:OG1  | 2.20                     | 0.42              |
| 3:J:1231:ARG:HG2  | 3:J:1235:ASN:OD1  | 2.19                     | 0.42              |
| 3:J:1284:ARG:O    | 3:J:1287:ILE:HG13 | 2.20                     | 0.42              |
| 5:L:119:ILE:HG21  | 5:L:379:MET:HE3   | 2.01                     | 0.42              |
| 5:L:313:ASP:HB3   | 5:L:317:ASN:OD1   | 2.19                     | 0.42              |
| 5:L:313:ASP:O     | 5:L:317:ASN:N     | 2.51                     | 0.42              |
| 5:L:376:LYS:O     | 5:L:380:VAL:HG23  | 2.20                     | 0.42              |
| 5:L:390:ILE:HD13  | 5:L:432:THR:HG23  | 2.01                     | 0.42              |
| 5:L:453:PRO:HG2   | 6:P:44:DA:OP2     | 2.19                     | 0.42              |
| 6:P:41:DT:H2''    | 6:P:42:DA:C8      | 2.55                     | 0.42              |
| 1:R:250:ASP:CB    | 1:R:253:LEU:HD12  | 2.50                     | 0.42              |
| 1:R:264:VAL:HA    | 1:R:267:ALA:HB3   | 2.01                     | 0.42              |
| 2:I:311:CYS:HB2   | 2:I:315:MET:SD    | 2.59                     | 0.42              |
| 2:I:325:LEU:HD12  | 2:I:326:SER:N     | 2.34                     | 0.42              |
| 2:I:444:ASP:OD1   | 2:I:444:ASP:N     | 2.47                     | 0.42              |
| 2:I:633:LEU:CD1   | 2:I:644:LEU:HD12  | 2.50                     | 0.42              |
| 2:I:867:GLU:OE2   | 2:I:943:LYS:HG3   | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:1277:ALA:HB3  | 3:J:434:ILE:CD1   | 2.48                     | 0.42              |
| 3:J:142:GLU:OE1   | 5:L:91:ILE:HG23   | 2.19                     | 0.42              |
| 3:J:316:ILE:HD13  | 3:J:316:ILE:HG21  | 1.82                     | 0.42              |
| 3:J:420:PRO:O     | 3:J:471:PRO:HD2   | 2.20                     | 0.42              |
| 3:J:422:LEU:HG    | 3:J:484:MET:HE1   | 2.02                     | 0.42              |
| 3:J:963:VAL:HG23  | 3:J:975:ILE:CG1   | 2.48                     | 0.42              |
| 3:J:1035:VAL:HG22 | 3:J:1115:ILE:HG12 | 2.00                     | 0.42              |
| 5:L:105:MET:CE    | 5:L:388:ILE:HD12  | 2.42                     | 0.42              |
| 5:L:311:THR:HG22  | 5:L:344:LEU:CD2   | 2.49                     | 0.42              |
| 6:P:56:DC:H2'     | 6:P:57:DT:C7      | 2.50                     | 0.42              |
| 1:G:75:GLN:C      | 2:I:729:ALA:HB2   | 2.45                     | 0.41              |
| 1:H:192:VAL:HG12  | 1:H:193:GLU:N     | 2.35                     | 0.41              |
| 2:I:90:VAL:HG12   | 2:I:91:THR:N      | 2.35                     | 0.41              |
| 2:I:484:LEU:HD12  | 2:I:485:ASP:CB    | 2.48                     | 0.41              |
| 2:I:558:VAL:HG11  | 2:I:573:ASN:HB3   | 2.02                     | 0.41              |
| 2:I:800:MET:HB3   | 2:I:800:MET:HE2   | 1.46                     | 0.41              |
| 2:I:1103:VAL:HG11 | 2:I:1112:ILE:HD12 | 2.02                     | 0.41              |
| 3:J:550:VAL:O     | 3:J:569:LEU:HA    | 2.20                     | 0.41              |
| 3:J:584:PRO:O     | 3:J:586:GLY:N     | 2.53                     | 0.41              |
| 3:J:1158:GLU:HG3  | 3:J:1186:TYR:OH   | 2.20                     | 0.41              |
| 5:L:149:ASP:O     | 5:L:153:ALA:N     | 2.52                     | 0.41              |
| 1:G:49:SER:HB3    | 2:I:1083:GLU:OE2  | 2.20                     | 0.41              |
| 1:G:160:HIS:NE2   | 1:G:161:SER:HB2   | 2.35                     | 0.41              |
| 1:H:48:LEU:HD13   | 1:H:183:ILE:HD11  | 2.01                     | 0.41              |
| 1:H:100:LEU:HB2   | 1:H:144:ILE:CG2   | 2.49                     | 0.41              |
| 2:I:195:PHE:HA    | 2:I:204:LEU:O     | 2.20                     | 0.41              |
| 2:I:666:SER:HA    | 2:I:1186:VAL:HG21 | 2.00                     | 0.41              |
| 2:I:1291:LEU:HB2  | 3:J:345:LYS:HD2   | 2.02                     | 0.41              |
| 3:J:114:ILE:HD11  | 3:J:311:ARG:CG    | 2.50                     | 0.41              |
| 3:J:551:ARG:O     | 3:J:551:ARG:HG2   | 2.20                     | 0.41              |
| 3:J:668:PHE:HB2   | 3:J:678:ARG:HG3   | 2.02                     | 0.41              |
| 3:J:830:ASP:OD2   | 3:J:953:LYS:NZ    | 2.51                     | 0.41              |
| 1:G:150:ARG:HD2   | 1:H:8:PHE:CZ      | 2.54                     | 0.41              |
| 1:G:214:GLU:O     | 1:G:217:ILE:HG22  | 2.21                     | 0.41              |
| 2:I:149:LEU:HG    | 2:I:451:ARG:CG    | 2.51                     | 0.41              |
| 2:I:561:ILE:HG21  | 2:I:561:ILE:HD13  | 1.75                     | 0.41              |
| 2:I:976:ARG:HG2   | 2:I:980:VAL:CG2   | 2.50                     | 0.41              |
| 3:J:35:PHE:CE2    | 3:J:101:ARG:HG2   | 2.55                     | 0.41              |
| 3:J:605:LEU:HD23  | 3:J:605:LEU:HA    | 1.79                     | 0.41              |
| 5:L:90:GLU:O      | 5:L:90:GLU:HG2    | 2.20                     | 0.41              |
| 5:L:600:HIS:O     | 5:L:603:ARG:HB3   | 2.20                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:P:23:DC:H6     | 6:P:23:DC:O5'     | 2.03                     | 0.41              |
| 6:P:39:DG:C1'    | 6:P:40:DC:H5'     | 2.49                     | 0.41              |
| 1:H:42:ALA:HB1   | 1:H:224:LEU:CD2   | 2.50                     | 0.41              |
| 1:H:100:LEU:HD23 | 1:H:115:ILE:HG21  | 2.03                     | 0.41              |
| 2:I:113:THR:HG22 | 2:I:114:VAL:N     | 2.35                     | 0.41              |
| 2:I:114:VAL:HG23 | 2:I:114:VAL:O     | 2.20                     | 0.41              |
| 2:I:228:VAL:HG13 | 2:I:239:MET:HE3   | 2.01                     | 0.41              |
| 2:I:413:GLU:OE1  | 2:I:413:GLU:N     | 2.53                     | 0.41              |
| 2:I:757:THR:HG23 | 2:I:765:ILE:CG2   | 2.50                     | 0.41              |
| 2:I:839:VAL:HG12 | 2:I:1049:ILE:HG12 | 2.01                     | 0.41              |
| 2:I:1107:MET:HG2 | 3:J:740:LEU:HD11  | 2.02                     | 0.41              |
| 3:J:113:HIS:CE1  | 3:J:115:TRP:HB2   | 2.56                     | 0.41              |
| 3:J:246:PRO:O    | 3:J:250:ARG:NE    | 2.53                     | 0.41              |
| 3:J:283:LEU:HD23 | 3:J:283:LEU:HA    | 1.86                     | 0.41              |
| 3:J:343:LEU:HD23 | 3:J:343:LEU:HA    | 1.79                     | 0.41              |
| 3:J:480:ALA:HA   | 3:J:484:MET:HB2   | 2.02                     | 0.41              |
| 5:L:139:GLU:OE1  | 5:L:142:THR:OG1   | 2.28                     | 0.41              |
| 7:Q:52:DT:H2'    | 7:Q:53:DT:H72     | 2.01                     | 0.41              |
| 1:R:300:LEU:O    | 1:R:303:ILE:HB    | 2.19                     | 0.41              |
| 1:H:95:LYS:HB2   | 1:H:120:ASP:OD2   | 2.21                     | 0.41              |
| 1:H:99:ILE:HD11  | 1:H:143:ARG:HB3   | 2.03                     | 0.41              |
| 1:H:149:GLY:HA3  | 1:H:177:TYR:CE1   | 2.56                     | 0.41              |
| 2:I:98:VAL:HG21  | 2:I:124:MET:HE3   | 2.03                     | 0.41              |
| 2:I:98:VAL:CG2   | 2:I:124:MET:HE3   | 2.50                     | 0.41              |
| 2:I:124:MET:O    | 2:I:124:MET:HG3   | 2.21                     | 0.41              |
| 2:I:594:VAL:HG12 | 2:I:595:THR:O     | 2.20                     | 0.41              |
| 2:I:873:ILE:HG13 | 2:I:944:ARG:NH2   | 2.35                     | 0.41              |
| 2:I:976:ARG:HG2  | 2:I:980:VAL:HG23  | 2.02                     | 0.41              |
| 3:J:322:ARG:NH1  | 5:L:510:PRO:HG3   | 2.34                     | 0.41              |
| 3:J:419:HIS:O    | 3:J:439:PRO:HD3   | 2.21                     | 0.41              |
| 3:J:495:ASN:OD1  | 3:J:495:ASN:N     | 2.53                     | 0.41              |
| 3:J:1047:THR:O   | 3:J:1059:LEU:HD23 | 2.20                     | 0.41              |
| 5:L:489:MET:HG3  | 5:L:494:ILE:CG1   | 2.51                     | 0.41              |
| 6:P:68:DA:C8     | 6:P:69:DT:H72     | 2.56                     | 0.41              |
| 7:Q:29:DT:H2''   | 7:Q:30:DC:C6      | 2.55                     | 0.41              |
| 1:G:16:ILE:HG23  | 1:G:26:VAL:HG12   | 2.03                     | 0.41              |
| 2:I:303:ASP:O    | 2:I:307:GLY:HA2   | 2.20                     | 0.41              |
| 2:I:471:VAL:CG2  | 2:I:493:ILE:HG13  | 2.48                     | 0.41              |
| 2:I:471:VAL:HB   | 2:I:498:ILE:HD11  | 2.03                     | 0.41              |
| 3:J:364:HIS:CD2  | 4:K:4:VAL:HG23    | 2.55                     | 0.41              |
| 3:J:822:MET:HB3  | 3:J:839:VAL:HG22  | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:961:SER:HB2   | 3:J:981:GLU:O     | 2.21                     | 0.41              |
| 3:J:1048:ARG:NH1  | 3:J:1050:THR:OG1  | 2.49                     | 0.41              |
| 3:J:1316:THR:HG22 | 3:J:1317:GLU:N    | 2.36                     | 0.41              |
| 4:K:2:ALA:HA      | 4:K:3:ARG:HA      | 1.82                     | 0.41              |
| 5:L:127:ILE:HA    | 5:L:130:VAL:HG22  | 2.02                     | 0.41              |
| 5:L:432:THR:HG21  | 6:P:53:DT:C4      | 2.56                     | 0.41              |
| 5:L:470:MET:HE3   | 5:L:470:MET:HB3   | 1.87                     | 0.41              |
| 6:P:63:DT:H3'     | 6:P:63:DT:OP2     | 2.20                     | 0.41              |
| 1:R:255:ARG:HG2   | 1:R:259:ASP:OD2   | 2.21                     | 0.41              |
| 1:R:265:ARG:HH21  | 1:R:294:ASN:HA    | 1.86                     | 0.41              |
| 1:H:197:ASP:OD1   | 1:H:197:ASP:N     | 2.54                     | 0.41              |
| 2:I:545:PHE:HE1   | 3:J:784:ALA:HB3   | 1.84                     | 0.41              |
| 2:I:1323:PHE:O    | 2:I:1326:LEU:HB3  | 2.20                     | 0.41              |
| 3:J:141:PHE:CE2   | 3:J:296:LYS:HB2   | 2.42                     | 0.41              |
| 5:L:348:GLU:OE2   | 5:L:355:ILE:HG12  | 2.20                     | 0.41              |
| 5:L:555:GLU:CG    | 5:L:594:ALA:HB2   | 2.51                     | 0.41              |
| 6:P:26:DT:H2''    | 6:P:27:DT:C5'     | 2.51                     | 0.41              |
| 2:I:165:HIS:CD2   | 2:I:167:SER:H     | 2.38                     | 0.41              |
| 2:I:520:PRO:HB2   | 2:I:794:LEU:CD1   | 2.51                     | 0.41              |
| 2:I:883:LEU:HD13  | 2:I:1052:VAL:HG11 | 2.02                     | 0.41              |
| 3:J:514:THR:HG23  | 3:J:514:THR:O     | 2.21                     | 0.41              |
| 3:J:527:LEU:HD13  | 3:J:548:VAL:HG13  | 1.98                     | 0.41              |
| 3:J:850:LYS:HG2   | 3:J:851:PRO:HD2   | 2.01                     | 0.41              |
| 3:J:903:LEU:HA    | 3:J:904:ALA:HA    | 1.87                     | 0.41              |
| 6:P:48:DG:H2''    | 6:P:49:DC:O5'     | 2.20                     | 0.41              |
| 1:G:45:ARG:CD     | 2:I:1083:GLU:HB3  | 2.50                     | 0.41              |
| 1:G:183:ILE:HG23  | 1:G:183:ILE:HD12  | 1.71                     | 0.41              |
| 2:I:60:GLN:HA     | 2:I:67:GLU:CB     | 2.51                     | 0.41              |
| 2:I:251:ALA:HB2   | 2:I:269:ILE:CD1   | 2.40                     | 0.41              |
| 2:I:471:VAL:O     | 2:I:475:VAL:HG23  | 2.21                     | 0.41              |
| 2:I:481:LEU:O     | 2:I:481:LEU:HD12  | 2.21                     | 0.41              |
| 2:I:550:VAL:O     | 2:I:550:VAL:HG13  | 2.21                     | 0.41              |
| 2:I:576:SER:HA    | 2:I:662:SER:HA    | 2.02                     | 0.41              |
| 2:I:599:VAL:N     | 2:I:627:GLY:O     | 2.50                     | 0.41              |
| 2:I:742:TYR:HB3   | 2:I:743:PRO:CD    | 2.44                     | 0.41              |
| 2:I:981:ALA:O     | 2:I:1007:LYS:NZ   | 2.45                     | 0.41              |
| 2:I:1119:MET:HB2  | 2:I:1228:GLY:HA2  | 2.02                     | 0.41              |
| 2:I:1244:HIS:CD2  | 2:I:1262:LYS:HA   | 2.55                     | 0.41              |
| 2:I:1246:ARG:HH11 | 2:I:1267:GLY:N    | 2.19                     | 0.41              |
| 2:I:1315:MET:HE3  | 2:I:1315:MET:HB2  | 1.91                     | 0.41              |
| 3:J:97:VAL:CG1    | 3:J:101:ARG:HE    | 2.33                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:145:VAL:O     | 3:J:178:ALA:HA    | 2.21                     | 0.41              |
| 3:J:179:LYS:HB2   | 3:J:184:ALA:HA    | 2.03                     | 0.41              |
| 3:J:466:MET:HE2   | 3:J:466:MET:HB3   | 1.95                     | 0.41              |
| 3:J:868:TRP:CZ3   | 3:J:871:LEU:HD12  | 2.56                     | 0.41              |
| 3:J:963:VAL:CG2   | 3:J:975:ILE:HG12  | 2.46                     | 0.41              |
| 3:J:1162:ILE:HG22 | 3:J:1178:THR:HB   | 2.02                     | 0.41              |
| 5:L:139:GLU:HA    | 5:L:142:THR:HG23  | 2.03                     | 0.41              |
| 5:L:150:ARG:NE    | 5:L:155:GLU:OE1   | 2.40                     | 0.41              |
| 5:L:227:GLN:CA    | 5:L:230:VAL:HG12  | 2.48                     | 0.41              |
| 5:L:586:ARG:O     | 5:L:590:ILE:HG13  | 2.20                     | 0.41              |
| 7:Q:51:DT:C2'     | 7:Q:52:DT:H71     | 2.51                     | 0.41              |
| 7:Q:57:DC:H2''    | 7:Q:58:DC:C6      | 2.56                     | 0.41              |
| 1:R:290:LEU:HD21  | 1:R:300:LEU:HB3   | 2.03                     | 0.41              |
| 1:G:194:GLN:O     | 1:G:195:ARG:HB2   | 2.21                     | 0.41              |
| 1:H:6:THR:HG22    | 1:H:6:THR:O       | 2.21                     | 0.41              |
| 2:I:606:LEU:HD11  | 2:I:652:TYR:HE2   | 1.86                     | 0.41              |
| 2:I:724:VAL:HG11  | 2:I:727:VAL:CG2   | 2.51                     | 0.41              |
| 2:I:787:PRO:O     | 2:I:788:SER:HB2   | 2.21                     | 0.41              |
| 2:I:1274:GLU:HG2  | 3:J:424:ASN:HD21  | 1.85                     | 0.41              |
| 3:J:361:LEU:HB2   | 3:J:450:HIS:HD2   | 1.85                     | 0.41              |
| 3:J:528:THR:HG22  | 3:J:532:GLU:HG2   | 2.02                     | 0.41              |
| 3:J:586:GLY:HA3   | 3:J:612:LEU:HD11  | 2.02                     | 0.41              |
| 3:J:792:ASN:O     | 3:J:795:TYR:N     | 2.44                     | 0.41              |
| 3:J:1220:ILE:HG23 | 3:J:1224:ARG:HH21 | 1.85                     | 0.41              |
| 1:H:22:THR:O      | 1:H:206:GLU:HA    | 2.20                     | 0.40              |
| 1:H:73:GLY:O      | 1:H:134:THR:N     | 2.54                     | 0.40              |
| 2:I:102:LEU:HD12  | 2:I:103:VAL:H     | 1.84                     | 0.40              |
| 2:I:189:ASP:O     | 2:I:192:ASP:N     | 2.37                     | 0.40              |
| 2:I:273:HIS:O     | 2:I:277:LEU:HG    | 2.21                     | 0.40              |
| 2:I:782:VAL:C     | 2:I:783:LEU:HD22  | 2.46                     | 0.40              |
| 2:I:1066:MET:HE2  | 2:I:1076:ILE:CD1  | 2.50                     | 0.40              |
| 2:I:1184:THR:O    | 2:I:1184:THR:HG22 | 2.20                     | 0.40              |
| 2:I:1287:LEU:HD22 | 3:J:1357:ILE:CD1  | 2.51                     | 0.40              |
| 3:J:442:ILE:HD13  | 3:J:442:ILE:HA    | 1.90                     | 0.40              |
| 5:L:297:MET:HE3   | 5:L:326:TRP:CH2   | 2.55                     | 0.40              |
| 1:R:286:GLU:HG2   | 1:R:290:LEU:CD1   | 2.51                     | 0.40              |
| 2:I:149:LEU:HB2   | 2:I:530:ILE:CG2   | 2.50                     | 0.40              |
| 2:I:208:ILE:HD11  | 2:I:365:GLU:CG    | 2.52                     | 0.40              |
| 2:I:802:VAL:HG13  | 2:I:803:ALA:N     | 2.35                     | 0.40              |
| 2:I:836:LEU:O     | 2:I:1051:LYS:HA   | 2.21                     | 0.40              |
| 2:I:1103:VAL:HG11 | 2:I:1112:ILE:CD1  | 2.51                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:423:LEU:CD1   | 3:J:468:VAL:HG12  | 2.51                     | 0.40              |
| 3:J:473:THR:O     | 3:J:477:GLN:HG3   | 2.22                     | 0.40              |
| 3:J:497:GLU:OE2   | 3:J:1247:LYS:HE2  | 2.22                     | 0.40              |
| 3:J:573:THR:HG23  | 3:J:576:ARG:NH1   | 2.36                     | 0.40              |
| 3:J:797:THR:HG22  | 3:J:924:GLY:CA    | 2.38                     | 0.40              |
| 3:J:842:ARG:NH1   | 3:J:1251:LYS:HG2  | 2.36                     | 0.40              |
| 5:L:489:MET:HG3   | 5:L:494:ILE:HG13  | 2.04                     | 0.40              |
| 5:L:562:ARG:NH2   | 7:Q:66:DG:H5"     | 2.36                     | 0.40              |
| 1:R:282:VAL:O     | 1:R:316:MET:HB2   | 2.22                     | 0.40              |
| 1:R:321:TRP:HA    | 1:R:322:PRO:C     | 2.46                     | 0.40              |
| 1:H:23:HIS:ND1    | 1:H:206:GLU:OE2   | 2.49                     | 0.40              |
| 2:I:896:THR:O     | 2:I:899:GLU:HB2   | 2.21                     | 0.40              |
| 2:I:932:GLN:O     | 2:I:1050:VAL:HA   | 2.21                     | 0.40              |
| 2:I:1246:ARG:HH12 | 2:I:1266:GLY:HA2  | 1.86                     | 0.40              |
| 2:I:1339:LEU:HD23 | 3:J:17:PHE:CD1    | 2.57                     | 0.40              |
| 3:J:694:SER:OG    | 3:J:738:ARG:NE    | 2.55                     | 0.40              |
| 3:J:827:GLU:HB3   | 3:J:832:LYS:HD2   | 2.02                     | 0.40              |
| 3:J:1061:VAL:HG11 | 3:J:1101:LEU:CB   | 2.42                     | 0.40              |
| 3:J:1272:SER:HB3  | 3:J:1273:ASP:CB   | 2.39                     | 0.40              |
| 3:J:1355:ARG:NH1  | 3:J:1369:ARG:HH12 | 2.19                     | 0.40              |
| 4:K:49:ILE:O      | 4:K:53:GLU:HG2    | 2.22                     | 0.40              |
| 5:L:290:LEU:CB    | 5:L:333:VAL:HG21  | 2.39                     | 0.40              |
| 5:L:420:GLU:HG3   | 5:L:422:ARG:NE    | 2.33                     | 0.40              |
| 5:L:476:ARG:HD2   | 5:L:477:GLU:N     | 2.36                     | 0.40              |
| 7:Q:71:DT:H2"     | 7:Q:72:DG:C8      | 2.55                     | 0.40              |
| 1:R:265:ARG:HH21  | 1:R:294:ASN:CA    | 2.35                     | 0.40              |
| 1:G:20:SER:OG     | 1:G:21:SER:N      | 2.54                     | 0.40              |
| 1:H:203:ILE:HG23  | 1:H:203:ILE:HD12  | 1.68                     | 0.40              |
| 2:I:232:ILE:HG12  | 2:I:237:LEU:HD21  | 2.03                     | 0.40              |
| 3:J:306:LEU:C     | 3:J:306:LEU:HD22  | 2.47                     | 0.40              |
| 3:J:382:TYR:HB3   | 3:J:394:ILE:CD1   | 2.51                     | 0.40              |
| 3:J:450:HIS:HA    | 3:J:451:PRO:HD3   | 1.93                     | 0.40              |
| 3:J:1034:PHE:HA   | 3:J:1114:GLN:HA   | 2.03                     | 0.40              |
| 3:J:1058:SER:CB   | 3:J:1106:ILE:HG23 | 2.49                     | 0.40              |
| 3:J:1154:ALA:HB2  | 3:J:1213:GLY:O    | 2.22                     | 0.40              |
| 5:L:379:MET:O     | 5:L:382:ALA:HB3   | 2.21                     | 0.40              |
| 6:P:74:DC:H5'     | 6:P:74:DC:H6      | 1.86                     | 0.40              |
| 7:Q:18:DA:H2"     | 7:Q:19:DT:C6      | 2.56                     | 0.40              |
| 1:R:250:ASP:OD2   | 1:R:252:ILE:N     | 2.55                     | 0.40              |
| 1:G:45:ARG:HD3    | 1:G:45:ARG:HA     | 1.86                     | 0.40              |
| 1:G:56:VAL:H      | 1:G:56:VAL:HG12   | 1.67                     | 0.40              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:I:453:ILE:HD13  | 2:I:530:ILE:CD1  | 2.51                     | 0.40              |
| 2:I:799:ASN:OD1   | 2:I:799:ASN:N    | 2.35                     | 0.40              |
| 2:I:1132:LEU:HD21 | 2:I:1141:LEU:CD2 | 2.50                     | 0.40              |
| 2:I:1325:VAL:HG22 | 3:J:249:LEU:CD2  | 2.51                     | 0.40              |
| 3:J:755:ILE:HG22  | 3:J:757:THR:H    | 1.86                     | 0.40              |
| 3:J:1041:ILE:H    | 3:J:1045:THR:HG1 | 1.59                     | 0.40              |
| 5:L:555:GLU:HG2   | 5:L:594:ALA:HB2  | 2.04                     | 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   | G     | 229/329 (70%)    | 194 (85%)  | 35 (15%)  | 0        | 100         | 100 |
| 1   | H     | 215/329 (65%)    | 185 (86%)  | 30 (14%)  | 0        | 100         | 100 |
| 1   | R     | 71/329 (22%)     | 62 (87%)   | 9 (13%)   | 0        | 100         | 100 |
| 2   | I     | 1339/1342 (100%) | 1161 (87%) | 175 (13%) | 3 (0%)   | 43          | 71  |
| 3   | J     | 1331/1430 (93%)  | 1167 (88%) | 157 (12%) | 7 (0%)   | 24          | 54  |
| 4   | K     | 77/91 (85%)      | 67 (87%)   | 10 (13%)  | 0        | 100         | 100 |
| 5   | L     | 465/616 (76%)    | 428 (92%)  | 37 (8%)   | 0        | 100         | 100 |
| All | All   | 3727/4466 (84%)  | 3264 (88%) | 453 (12%) | 10 (0%)  | 37          | 65  |

All (10) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | J     | 854  | ALA  |
| 3   | J     | 1169 | THR  |
| 2   | I     | 399  | ALA  |
| 3   | J     | 320  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | J     | 1172 | LYS  |
| 3   | J     | 46   | TYR  |
| 2   | I     | 1224 | PRO  |
| 3   | J     | 906  | GLY  |
| 3   | J     | 1138 | LEU  |
| 2   | I     | 697  | LYS  |

### 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   | G     | 196/286 (68%)    | 194 (99%)   | 2 (1%)   | 68          | 75  |
| 1   | H     | 186/286 (65%)    | 185 (100%)  | 1 (0%)   | 81          | 81  |
| 1   | R     | 65/286 (23%)     | 65 (100%)   | 0        | 100         | 100 |
| 2   | I     | 1155/1157 (100%) | 1151 (100%) | 4 (0%)   | 86          | 84  |
| 3   | J     | 1118/1189 (94%)  | 1115 (100%) | 3 (0%)   | 86          | 84  |
| 4   | K     | 67/75 (89%)      | 67 (100%)   | 0        | 100         | 100 |
| 5   | L     | 415/543 (76%)    | 415 (100%)  | 0        | 100         | 100 |
| All | All   | 3202/3822 (84%)  | 3192 (100%) | 10 (0%)  | 84          | 84  |

All (10) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | G     | 56   | VAL  |
| 1   | G     | 130  | ILE  |
| 1   | H     | 183  | ILE  |
| 2   | I     | 91   | THR  |
| 2   | I     | 138  | ILE  |
| 2   | I     | 684  | ASN  |
| 2   | I     | 802  | VAL  |
| 3   | J     | 770  | LEU  |
| 3   | J     | 1155 | ILE  |
| 3   | J     | 1255 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | G     | 23   | HIS  |
| 1   | G     | 93   | GLN  |
| 1   | G     | 132  | HIS  |
| 1   | H     | 84   | ASN  |
| 1   | H     | 117  | HIS  |
| 1   | H     | 208  | ASN  |
| 2   | I     | 31   | GLN  |
| 2   | I     | 69   | GLN  |
| 2   | I     | 165  | HIS  |
| 2   | I     | 273  | HIS  |
| 2   | I     | 276  | GLN  |
| 2   | I     | 330  | HIS  |
| 2   | I     | 447  | HIS  |
| 2   | I     | 519  | ASN  |
| 2   | I     | 618  | GLN  |
| 2   | I     | 684  | ASN  |
| 2   | I     | 767  | GLN  |
| 2   | I     | 832  | HIS  |
| 2   | I     | 922  | ASN  |
| 2   | I     | 1080 | ASN  |
| 2   | I     | 1116 | HIS  |
| 2   | I     | 1134 | GLN  |
| 2   | I     | 1237 | HIS  |
| 2   | I     | 1268 | GLN  |
| 2   | I     | 1314 | GLN  |
| 3   | J     | 45   | ASN  |
| 3   | J     | 294  | ASN  |
| 3   | J     | 320  | ASN  |
| 3   | J     | 450  | HIS  |
| 3   | J     | 477  | GLN  |
| 3   | J     | 488  | ASN  |
| 3   | J     | 817  | HIS  |
| 3   | J     | 1114 | GLN  |
| 3   | J     | 1197 | ASN  |
| 3   | J     | 1227 | HIS  |
| 3   | J     | 1326 | GLN  |
| 3   | J     | 1350 | ASN  |
| 3   | J     | 1366 | HIS  |
| 3   | J     | 1367 | GLN  |
| 5   | L     | 265  | GLN  |
| 5   | L     | 309  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | L     | 331 | HIS  |
| 5   | L     | 338 | HIS  |
| 5   | L     | 342 | GLN  |
| 5   | L     | 469 | GLN  |
| 5   | L     | 600 | HIS  |
| 1   | R     | 283 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 3 are 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$ |
| 8   | 1N7  | L     | 701  | -    | 30,30,46     | 5.17 | 15 (50%)    | 47,48,72    | 2.68 | 16 (34%)    |
| 8   | 1N7  | I     | 1401 | -    | 30,30,46     | 5.17 | 16 (53%)    | 47,48,72    | 2.60 | 18 (38%)    |
| 8   | 1N7  | J     | 1504 | -    | 30,30,46     | 5.26 | 15 (50%)    | 47,48,72    | 2.85 | 25 (53%)    |

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   |
|-----|------|-------|------|------|---------|-----------|---------|
| 8   | 1N7  | L     | 701  | -    | -       | 0/7/72/92 | 0/4/4/4 |
| 8   | 1N7  | I     | 1401 | -    | -       | 1/7/72/92 | 0/4/4/4 |
| 8   | 1N7  | J     | 1504 | -    | -       | 7/7/72/92 | 0/4/4/4 |

All (46) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 8   | J     | 1504 | 1N7  | C3-C19  | 19.03 | 1.84        | 1.53     |
| 8   | L     | 701  | 1N7  | C3-C19  | 19.00 | 1.84        | 1.53     |
| 8   | I     | 1401 | 1N7  | C3-C19  | 18.48 | 1.83        | 1.53     |
| 8   | I     | 1401 | 1N7  | C3-C4   | 12.66 | 1.73        | 1.53     |
| 8   | L     | 701  | 1N7  | C3-C4   | 12.08 | 1.73        | 1.53     |
| 8   | J     | 1504 | 1N7  | C3-C4   | 11.54 | 1.72        | 1.53     |
| 8   | J     | 1504 | 1N7  | C5-C4   | -9.53 | 1.39        | 1.54     |
| 8   | I     | 1401 | 1N7  | C5-C4   | -8.80 | 1.41        | 1.54     |
| 8   | L     | 701  | 1N7  | C5-C4   | -8.68 | 1.41        | 1.54     |
| 8   | L     | 701  | 1N7  | C2-C19  | -7.89 | 1.42        | 1.56     |
| 8   | I     | 1401 | 1N7  | C2-C19  | -7.18 | 1.43        | 1.56     |
| 8   | J     | 1504 | 1N7  | C2-C19  | -6.75 | 1.44        | 1.56     |
| 8   | J     | 1504 | 1N7  | C8-C7   | 6.08  | 1.70        | 1.54     |
| 8   | L     | 701  | 1N7  | C8-C7   | 5.81  | 1.69        | 1.54     |
| 8   | I     | 1401 | 1N7  | C8-C7   | 5.75  | 1.69        | 1.54     |
| 8   | J     | 1504 | 1N7  | C2-C15  | 5.13  | 1.63        | 1.55     |
| 8   | I     | 1401 | 1N7  | C2-C15  | 5.02  | 1.63        | 1.55     |
| 8   | J     | 1504 | 1N7  | O4-C4   | -4.55 | 1.36        | 1.43     |
| 8   | L     | 701  | 1N7  | C5-C9   | 4.40  | 1.62        | 1.55     |
| 8   | I     | 1401 | 1N7  | O4-C4   | -4.32 | 1.36        | 1.43     |
| 8   | I     | 1401 | 1N7  | C5-C9   | 4.09  | 1.62        | 1.55     |
| 8   | J     | 1504 | 1N7  | C5-C6   | -3.95 | 1.48        | 1.55     |
| 8   | L     | 701  | 1N7  | C14-C15 | -3.87 | 1.47        | 1.53     |
| 8   | L     | 701  | 1N7  | O4-C4   | -3.63 | 1.37        | 1.43     |
| 8   | L     | 701  | 1N7  | C18-C6  | -3.55 | 1.47        | 1.53     |
| 8   | L     | 701  | 1N7  | C2-C15  | 3.52  | 1.60        | 1.55     |
| 8   | J     | 1504 | 1N7  | C14-C15 | -3.51 | 1.48        | 1.53     |
| 8   | J     | 1504 | 1N7  | C18-C6  | -3.50 | 1.47        | 1.53     |
| 8   | J     | 1504 | 1N7  | C1-C2   | 3.38  | 1.60        | 1.54     |
| 8   | J     | 1504 | 1N7  | C10-C5  | 3.26  | 1.59        | 1.54     |
| 8   | I     | 1401 | 1N7  | C14-C15 | -3.20 | 1.48        | 1.53     |
| 8   | J     | 1504 | 1N7  | C5-C9   | 3.19  | 1.60        | 1.55     |
| 8   | J     | 1504 | 1N7  | C7-C6   | 3.13  | 1.60        | 1.54     |
| 8   | I     | 1401 | 1N7  | C7-C6   | 2.99  | 1.60        | 1.54     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 8   | L     | 701  | 1N7  | C1-C2   | 2.94  | 1.59        | 1.54     |
| 8   | L     | 701  | 1N7  | C5-C6   | -2.92 | 1.50        | 1.55     |
| 8   | I     | 1401 | 1N7  | C1-C2   | 2.87  | 1.59        | 1.54     |
| 8   | L     | 701  | 1N7  | C7-C6   | 2.82  | 1.60        | 1.54     |
| 8   | I     | 1401 | 1N7  | C5-C6   | -2.77 | 1.50        | 1.55     |
| 8   | I     | 1401 | 1N7  | C18-C6  | -2.70 | 1.48        | 1.53     |
| 8   | L     | 701  | 1N7  | O2-C13  | -2.62 | 1.35        | 1.43     |
| 8   | I     | 1401 | 1N7  | C10-C5  | 2.59  | 1.58        | 1.54     |
| 8   | I     | 1401 | 1N7  | O2-C13  | -2.51 | 1.36        | 1.43     |
| 8   | J     | 1504 | 1N7  | O2-C13  | -2.40 | 1.36        | 1.43     |
| 8   | I     | 1401 | 1N7  | C16-C15 | 2.33  | 1.57        | 1.53     |
| 8   | L     | 701  | 1N7  | C10-C5  | 2.06  | 1.57        | 1.54     |

All (59) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 8   | J     | 1504 | 1N7  | C9-C5-C4    | -8.69 | 109.84      | 117.67   |
| 8   | L     | 701  | 1N7  | C7-C6-C18   | -7.26 | 108.40      | 118.36   |
| 8   | L     | 701  | 1N7  | C9-C5-C6    | 6.83  | 106.97      | 100.11   |
| 8   | I     | 1401 | 1N7  | C9-C5-C6    | 6.45  | 106.59      | 100.11   |
| 8   | L     | 701  | 1N7  | C9-C5-C4    | -6.24 | 112.05      | 117.67   |
| 8   | I     | 1401 | 1N7  | C16-C15-C14 | -6.21 | 104.13      | 111.23   |
| 8   | I     | 1401 | 1N7  | C11-C2-C1   | -5.25 | 99.96       | 108.31   |
| 8   | J     | 1504 | 1N7  | C16-C17-C18 | -5.24 | 105.77      | 111.50   |
| 8   | I     | 1401 | 1N7  | C9-C5-C4    | -5.23 | 112.96      | 117.67   |
| 8   | J     | 1504 | 1N7  | C1-C2-C15   | 4.99  | 114.91      | 107.75   |
| 8   | I     | 1401 | 1N7  | C7-C6-C18   | -4.88 | 111.66      | 118.36   |
| 8   | I     | 1401 | 1N7  | C16-C17-C18 | -4.87 | 106.18      | 111.50   |
| 8   | J     | 1504 | 1N7  | C14-C13-C12 | -4.66 | 104.93      | 110.62   |
| 8   | L     | 701  | 1N7  | C19-C18-C17 | -4.66 | 106.00      | 111.86   |
| 8   | J     | 1504 | 1N7  | C7-C6-C18   | -4.49 | 112.20      | 118.36   |
| 8   | L     | 701  | 1N7  | C16-C17-C18 | -4.33 | 106.77      | 111.50   |
| 8   | L     | 701  | 1N7  | C11-C2-C15  | -4.29 | 103.26      | 110.44   |
| 8   | I     | 1401 | 1N7  | C14-C13-C12 | -4.19 | 105.50      | 110.62   |
| 8   | L     | 701  | 1N7  | C16-C15-C14 | -4.04 | 106.61      | 111.23   |
| 8   | J     | 1504 | 1N7  | C15-C14-C13 | -3.98 | 106.71      | 112.71   |
| 8   | L     | 701  | 1N7  | C14-C13-C12 | -3.94 | 105.81      | 110.62   |
| 8   | L     | 701  | 1N7  | C6-C5-C4    | 3.92  | 111.00      | 107.42   |
| 8   | J     | 1504 | 1N7  | C11-C2-C15  | -3.89 | 103.93      | 110.44   |
| 8   | I     | 1401 | 1N7  | C21-C20-C22 | -3.88 | 104.34      | 110.34   |
| 8   | J     | 1504 | 1N7  | C16-C15-C14 | -3.82 | 106.86      | 111.23   |
| 8   | L     | 701  | 1N7  | C5-C6-C18   | 3.82  | 119.55      | 114.72   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 8   | L     | 701  | 1N7  | C21-C20-C22 | -3.75 | 104.53      | 110.34   |
| 8   | J     | 1504 | 1N7  | C21-C20-C9  | -3.74 | 107.27      | 112.88   |
| 8   | J     | 1504 | 1N7  | C19-C18-C17 | -3.69 | 107.21      | 111.86   |
| 8   | I     | 1401 | 1N7  | C19-C18-C17 | -3.59 | 107.34      | 111.86   |
| 8   | J     | 1504 | 1N7  | C5-C9-C20   | -3.42 | 115.34      | 119.48   |
| 8   | J     | 1504 | 1N7  | C9-C5-C6    | 3.42  | 103.54      | 100.11   |
| 8   | J     | 1504 | 1N7  | C22-C20-C9  | 3.19  | 116.94      | 110.33   |
| 8   | J     | 1504 | 1N7  | C6-C5-C4    | 3.15  | 110.29      | 107.42   |
| 8   | J     | 1504 | 1N7  | C11-C2-C1   | -3.11 | 103.36      | 108.31   |
| 8   | L     | 701  | 1N7  | C10-C5-C9   | -3.07 | 106.39      | 111.20   |
| 8   | J     | 1504 | 1N7  | C8-C9-C20   | 3.03  | 116.76      | 112.18   |
| 8   | I     | 1401 | 1N7  | C16-C15-C2  | 2.93  | 115.78      | 112.66   |
| 8   | J     | 1504 | 1N7  | C11-C2-C19  | 2.93  | 115.11      | 111.18   |
| 8   | I     | 1401 | 1N7  | C10-C5-C9   | -2.89 | 106.67      | 111.20   |
| 8   | L     | 701  | 1N7  | C6-C18-C17  | 2.85  | 115.63      | 111.85   |
| 8   | L     | 701  | 1N7  | C1-C12-C13  | -2.85 | 106.71      | 110.48   |
| 8   | I     | 1401 | 1N7  | C6-C18-C17  | 2.69  | 115.42      | 111.85   |
| 8   | J     | 1504 | 1N7  | C19-C2-C15  | 2.68  | 112.23      | 108.51   |
| 8   | J     | 1504 | 1N7  | C1-C2-C19   | -2.68 | 107.19      | 111.34   |
| 8   | J     | 1504 | 1N7  | C16-C15-C2  | 2.65  | 115.48      | 112.66   |
| 8   | J     | 1504 | 1N7  | C2-C19-C18  | 2.59  | 114.73      | 111.84   |
| 8   | I     | 1401 | 1N7  | C8-C9-C20   | -2.44 | 108.48      | 112.18   |
| 8   | L     | 701  | 1N7  | C8-C9-C20   | -2.44 | 108.48      | 112.18   |
| 8   | J     | 1504 | 1N7  | C12-C1-C2   | 2.42  | 116.83      | 112.74   |
| 8   | J     | 1504 | 1N7  | O4-C4-C3    | -2.38 | 104.28      | 109.12   |
| 8   | I     | 1401 | 1N7  | C5-C6-C18   | 2.38  | 117.73      | 114.72   |
| 8   | I     | 1401 | 1N7  | C7-C6-C5    | 2.35  | 105.82      | 103.54   |
| 8   | I     | 1401 | 1N7  | C12-C1-C2   | 2.34  | 116.69      | 112.74   |
| 8   | J     | 1504 | 1N7  | C5-C6-C18   | 2.16  | 117.46      | 114.72   |
| 8   | J     | 1504 | 1N7  | C21-C20-C22 | -2.12 | 107.06      | 110.34   |
| 8   | I     | 1401 | 1N7  | C1-C2-C15   | 2.07  | 110.72      | 107.75   |
| 8   | L     | 701  | 1N7  | C19-C2-C15  | 2.06  | 111.38      | 108.51   |
| 8   | I     | 1401 | 1N7  | C3-C4-C5    | 2.05  | 113.35      | 111.26   |

There are no chirality outliers.

All (8) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms         |
|-----|-------|------|------|---------------|
| 8   | J     | 1504 | 1N7  | C21-C20-C9-C5 |
| 8   | J     | 1504 | 1N7  | C21-C20-C9-C8 |
| 8   | J     | 1504 | 1N7  | C22-C20-C9-C5 |
| 8   | J     | 1504 | 1N7  | C22-C20-C9-C8 |

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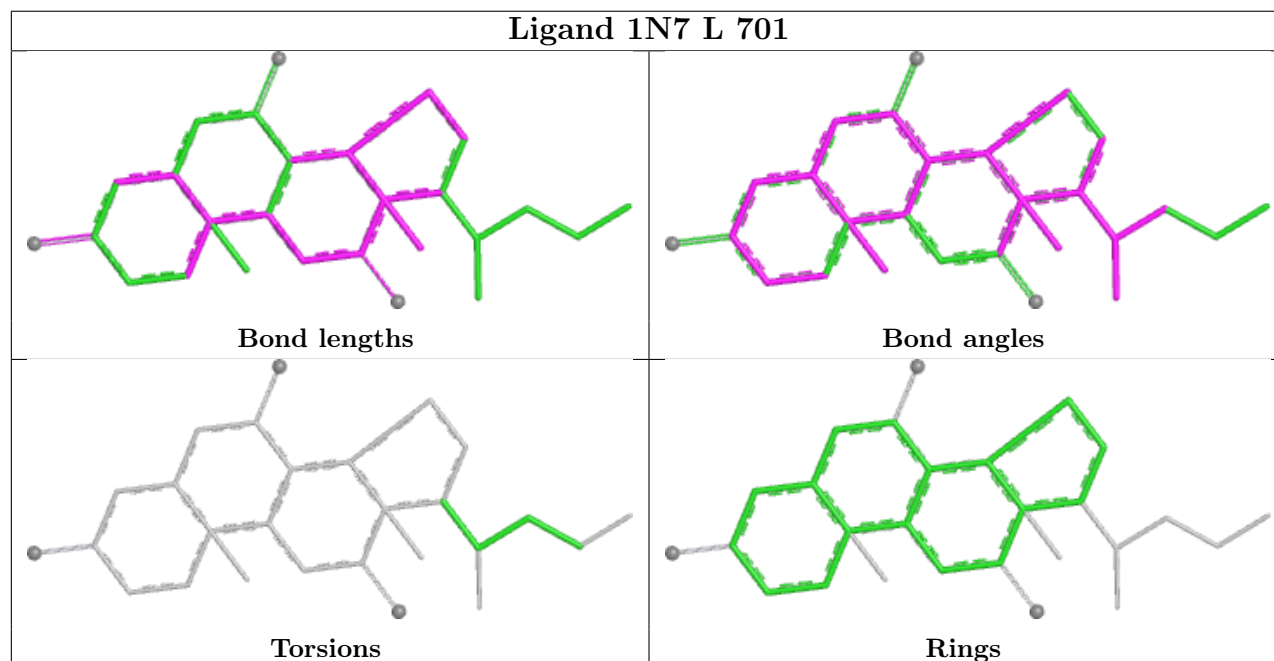
| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 8   | J     | 1504 | 1N7  | C9-C20-C22-C23  |
| 8   | J     | 1504 | 1N7  | C21-C20-C22-C23 |
| 8   | J     | 1504 | 1N7  | C20-C22-C23-C24 |
| 8   | I     | 1401 | 1N7  | C20-C22-C23-C24 |

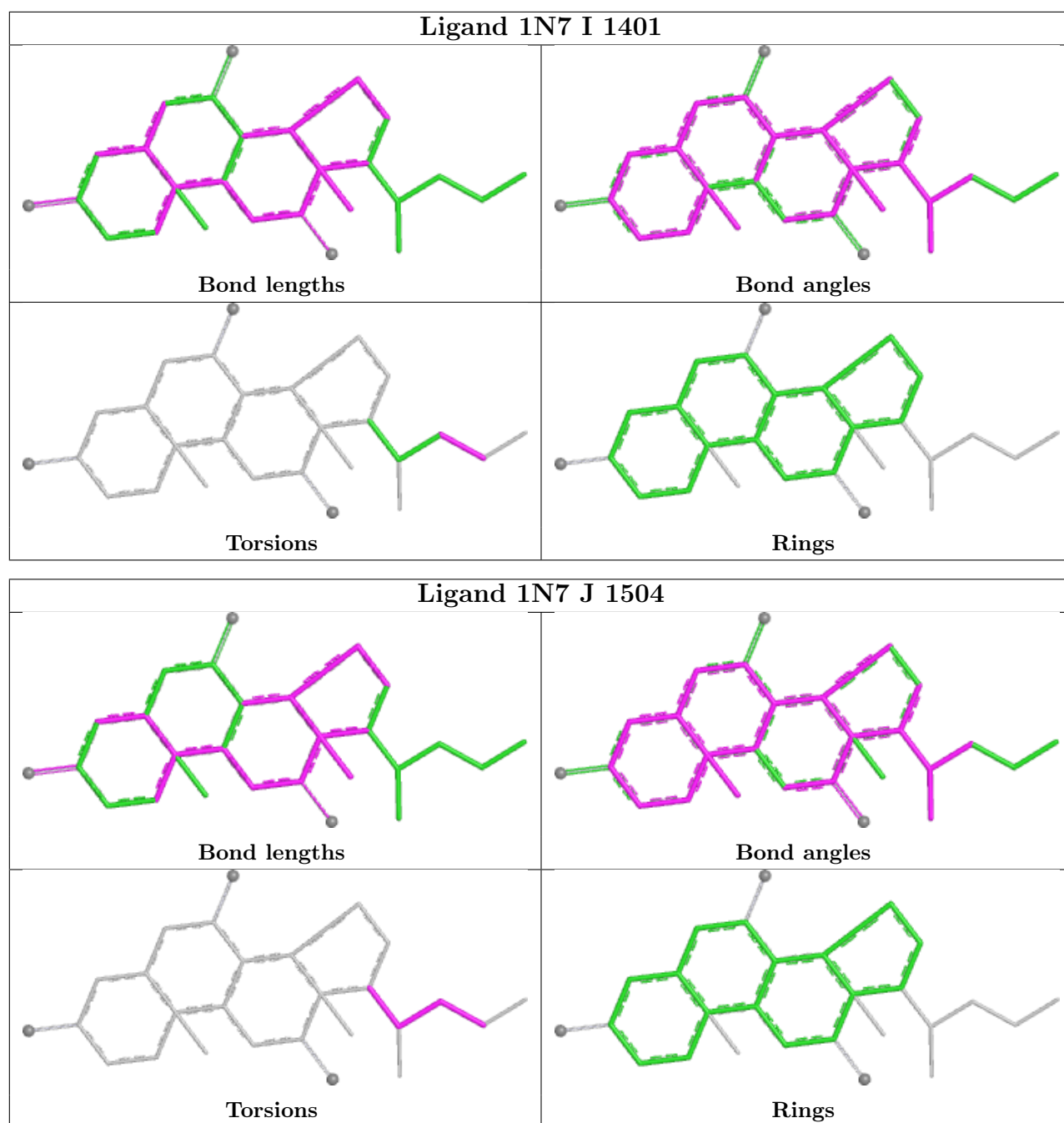
There are no ring outliers.

3 monomers are involved in 14 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 8   | L     | 701  | 1N7  | 4       | 0            |
| 8   | I     | 1401 | 1N7  | 6       | 0            |
| 8   | J     | 1504 | 1N7  | 4       | 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.

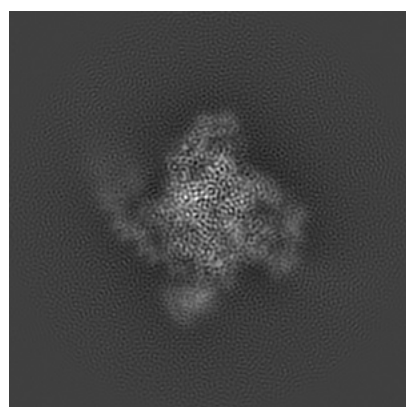
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20203. These allow visual inspection of the internal detail of the map and identification of artifacts.

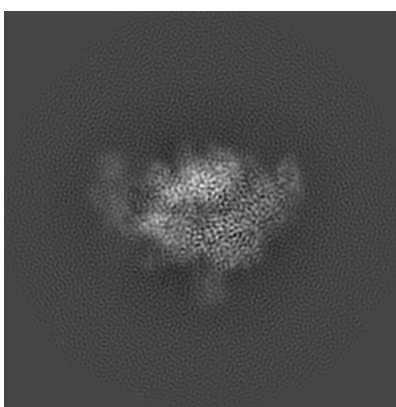
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

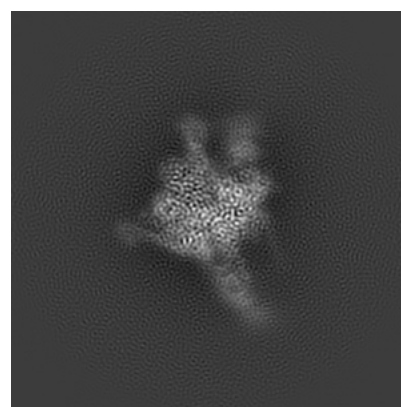
#### 6.1.1 Primary map



X



Y

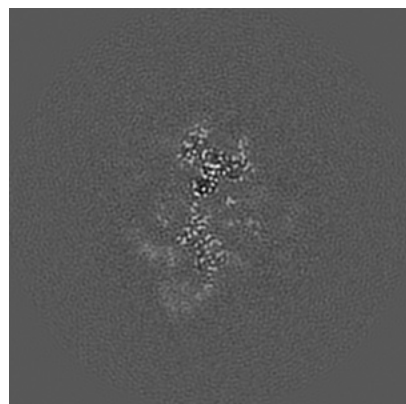


Z

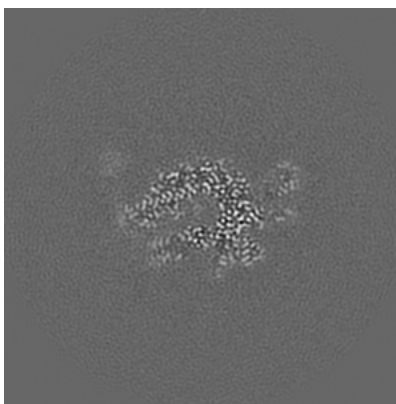
The images above show the map projected in three orthogonal directions.

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

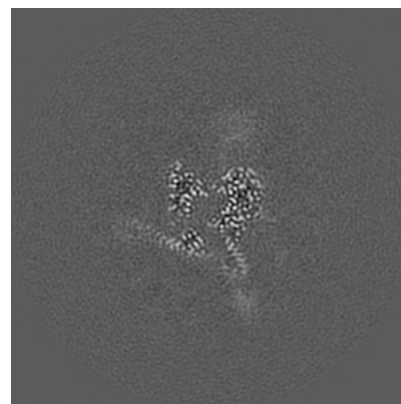
#### 6.2.1 Primary map



X Index: 128



Y Index: 128

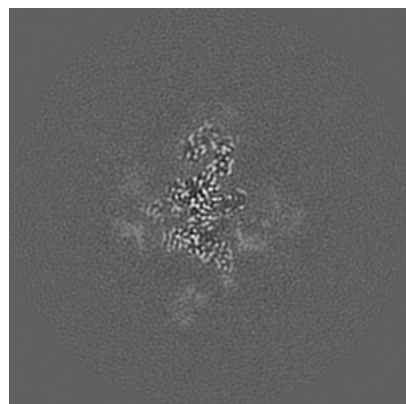


Z Index: 128

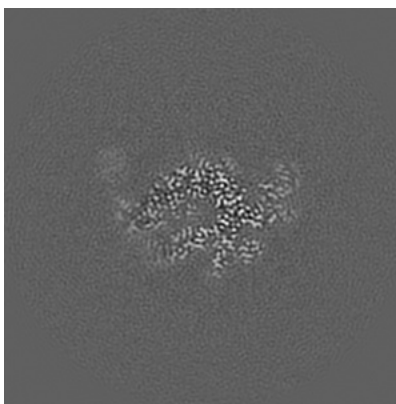
The images above show central slices of the map in three orthogonal directions.

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

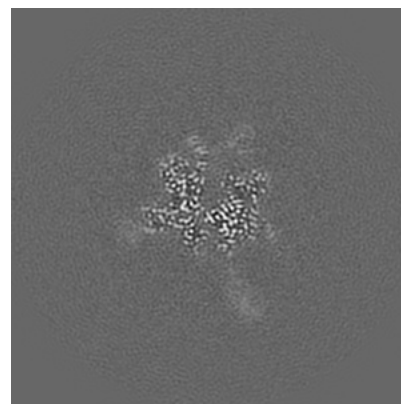
### 6.3.1 Primary map



X Index: 138



Y Index: 126

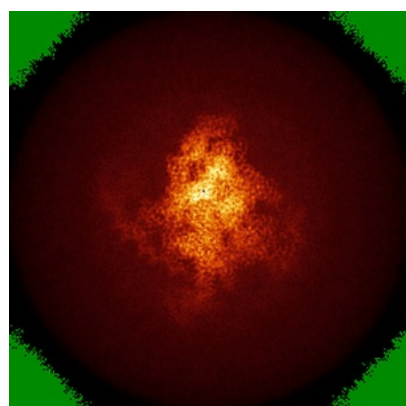


Z Index: 136

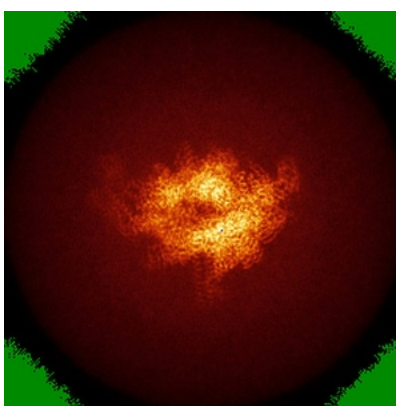
The images above show the largest variance slices of the map in three orthogonal directions.

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

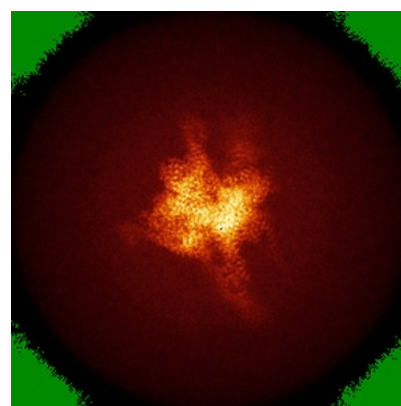
### 6.4.1 Primary map



X



Y

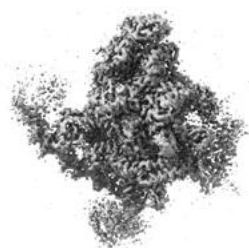


Z

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

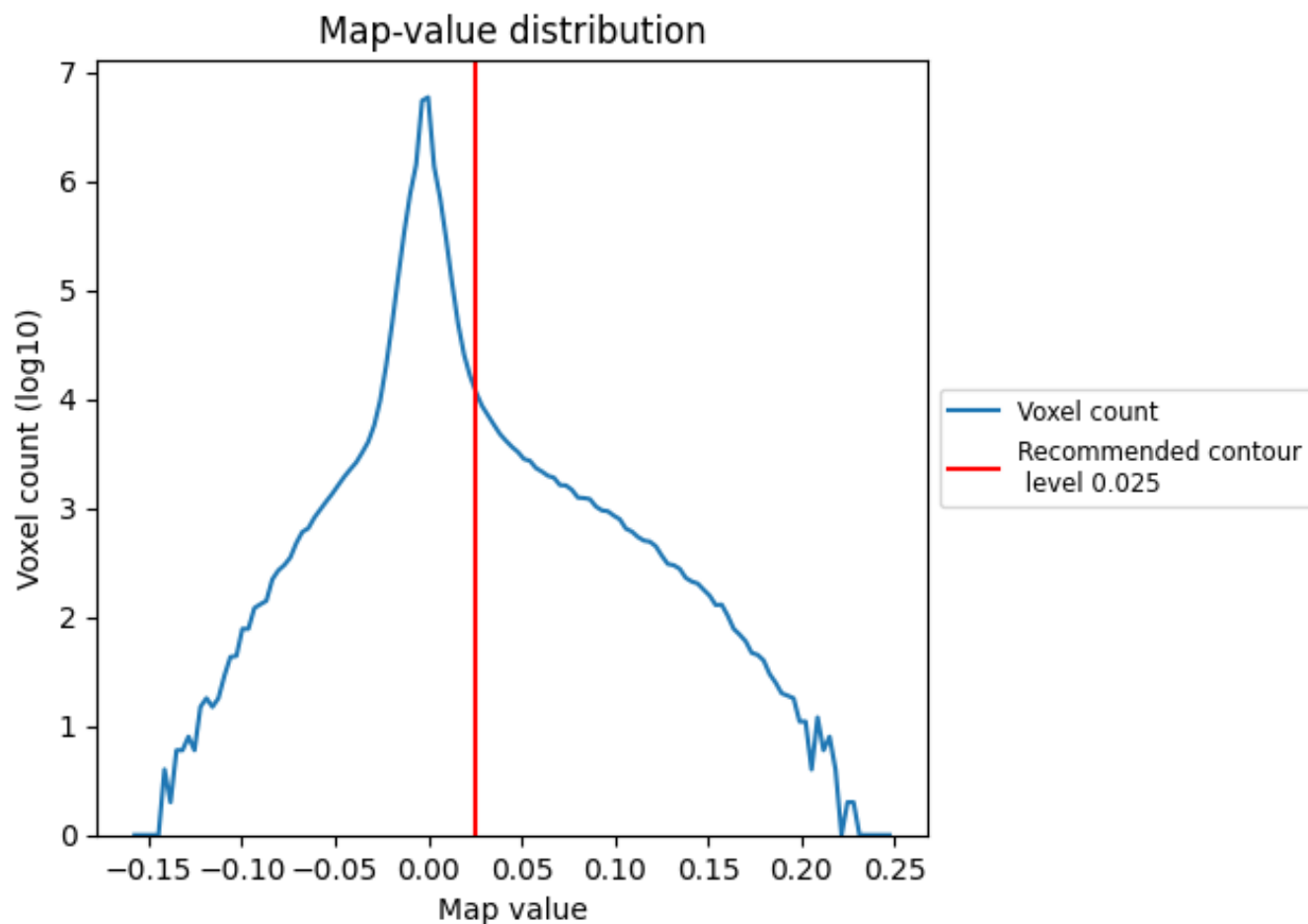
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

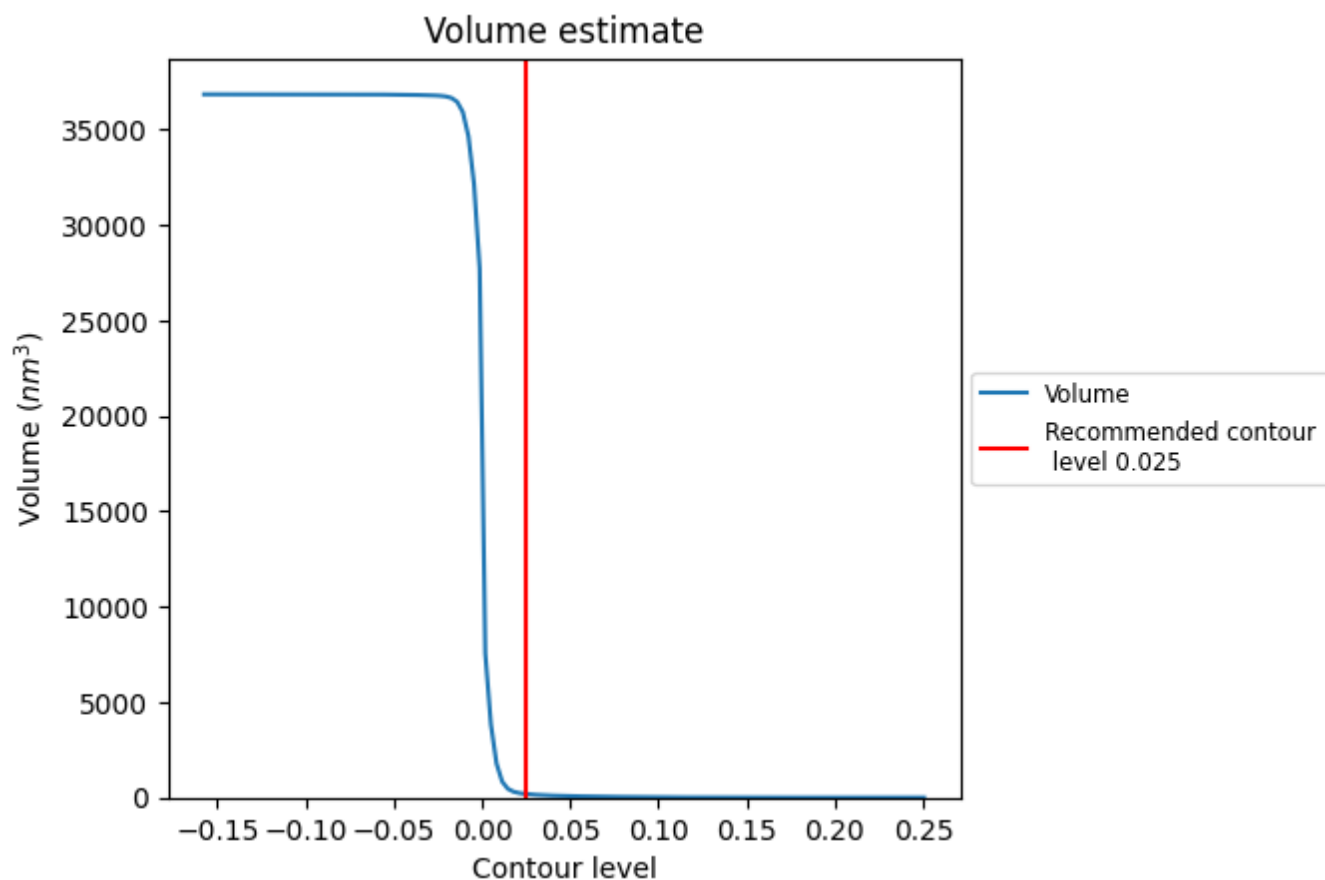
This section contains the results of statistical analysis of the map.

### 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.

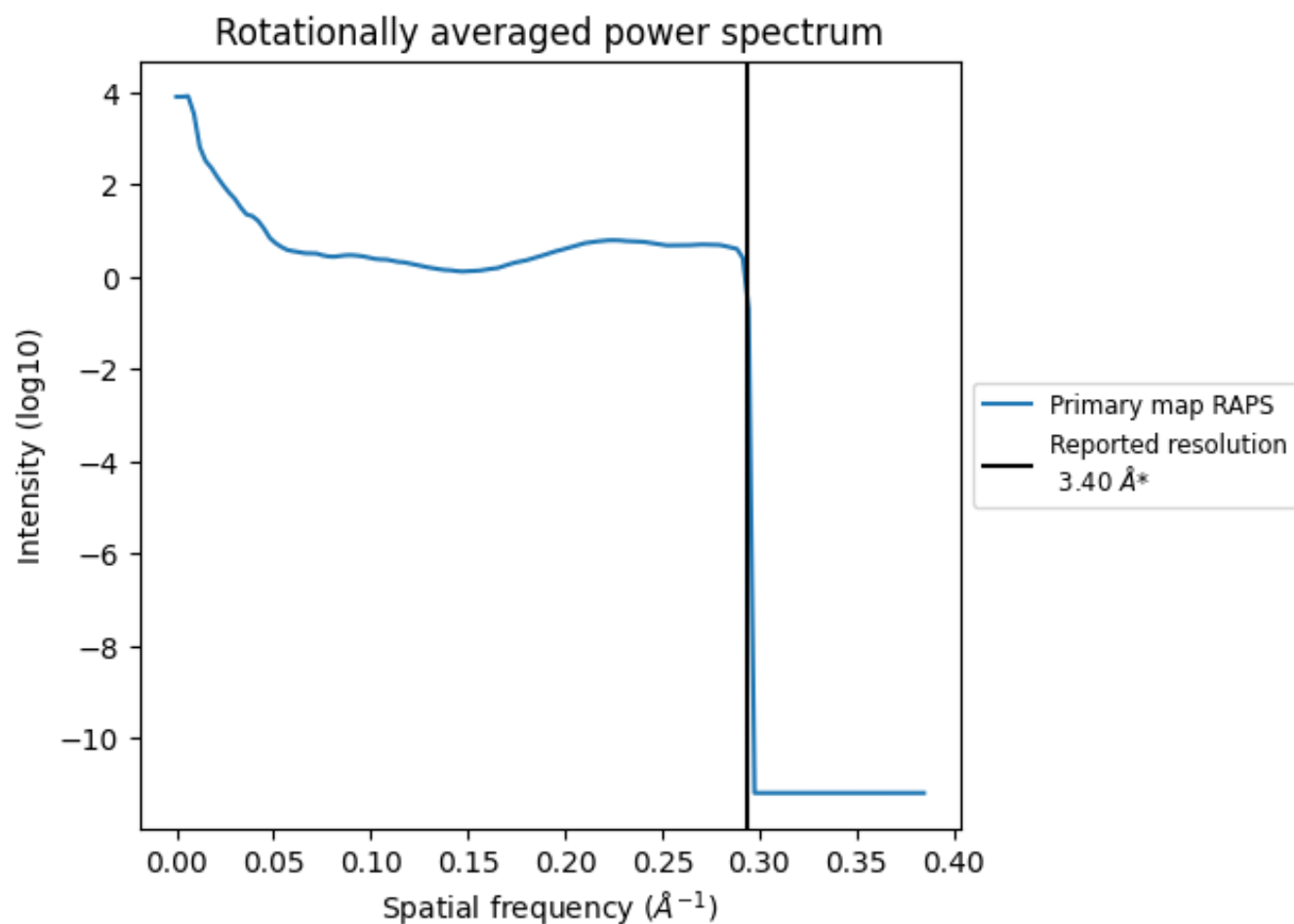
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 187 nm<sup>3</sup>; this corresponds to an approximate mass of 169 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

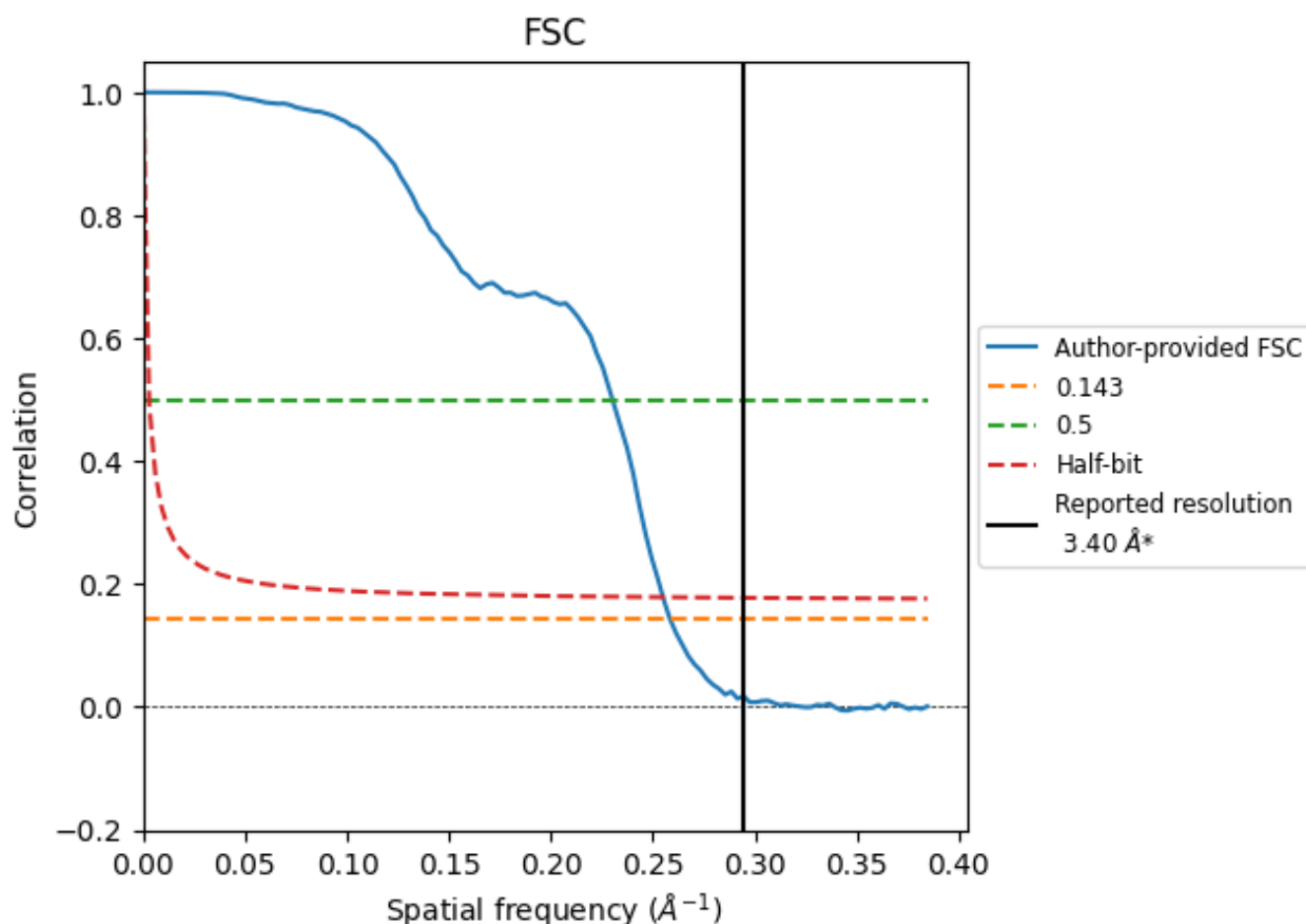


\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

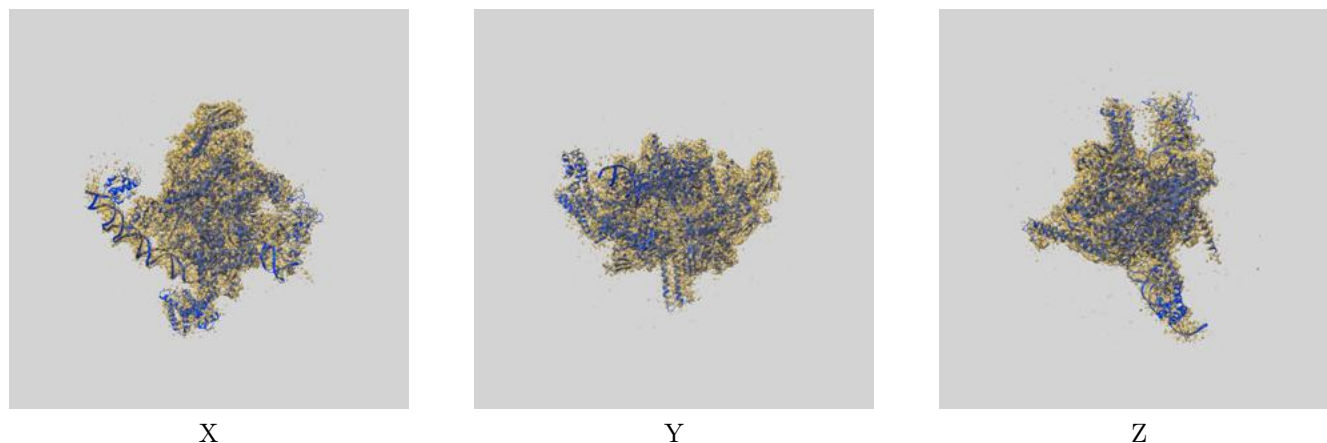
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.40                               | -    | -        |
| Author-provided FSC curve | 3.87                               | 4.34 | 3.92     |
| Unmasked-calculated*      | -                                  | -    | -        |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.87 differs from the reported value 3.4 by more than 10 %

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

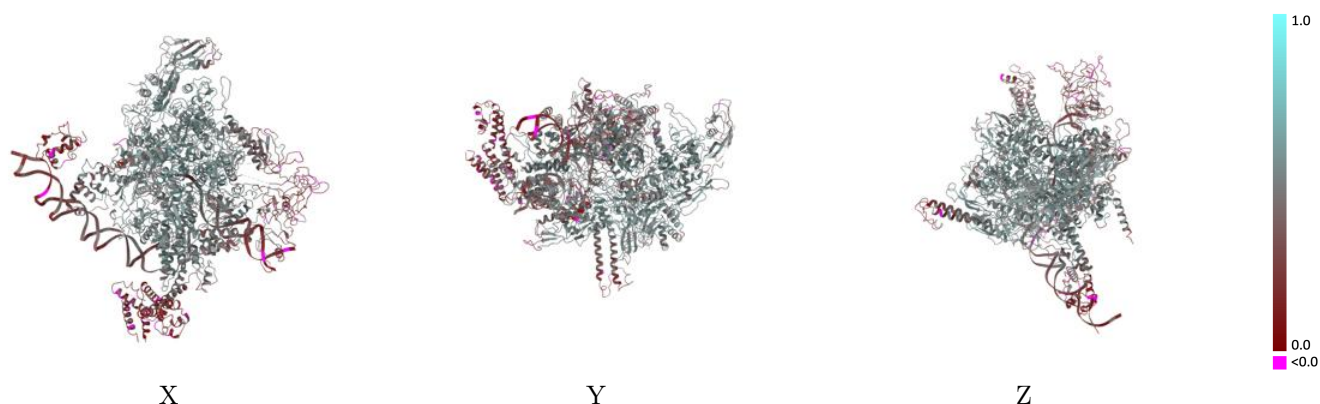
This section contains information regarding the fit between EMDB map EMD-20203 and PDB model 6OUL. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

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



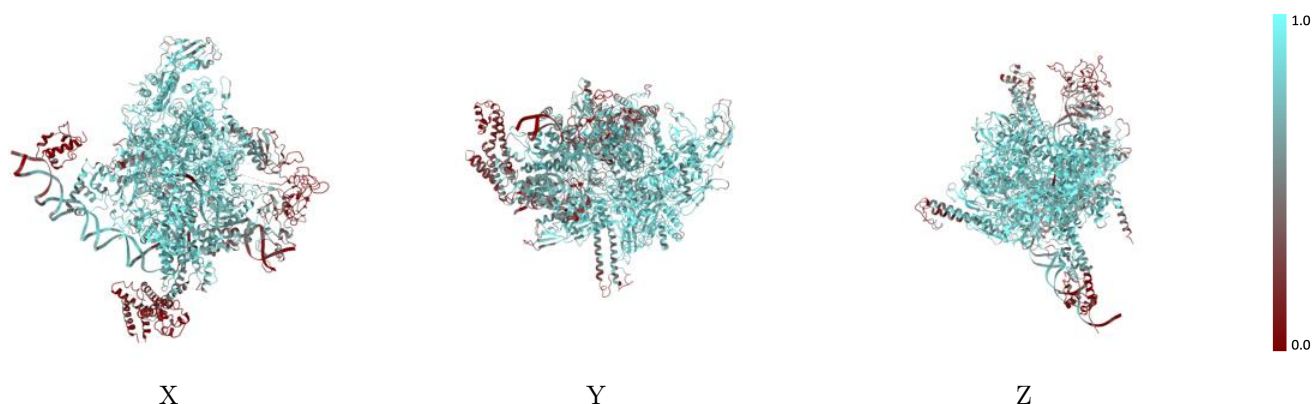
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



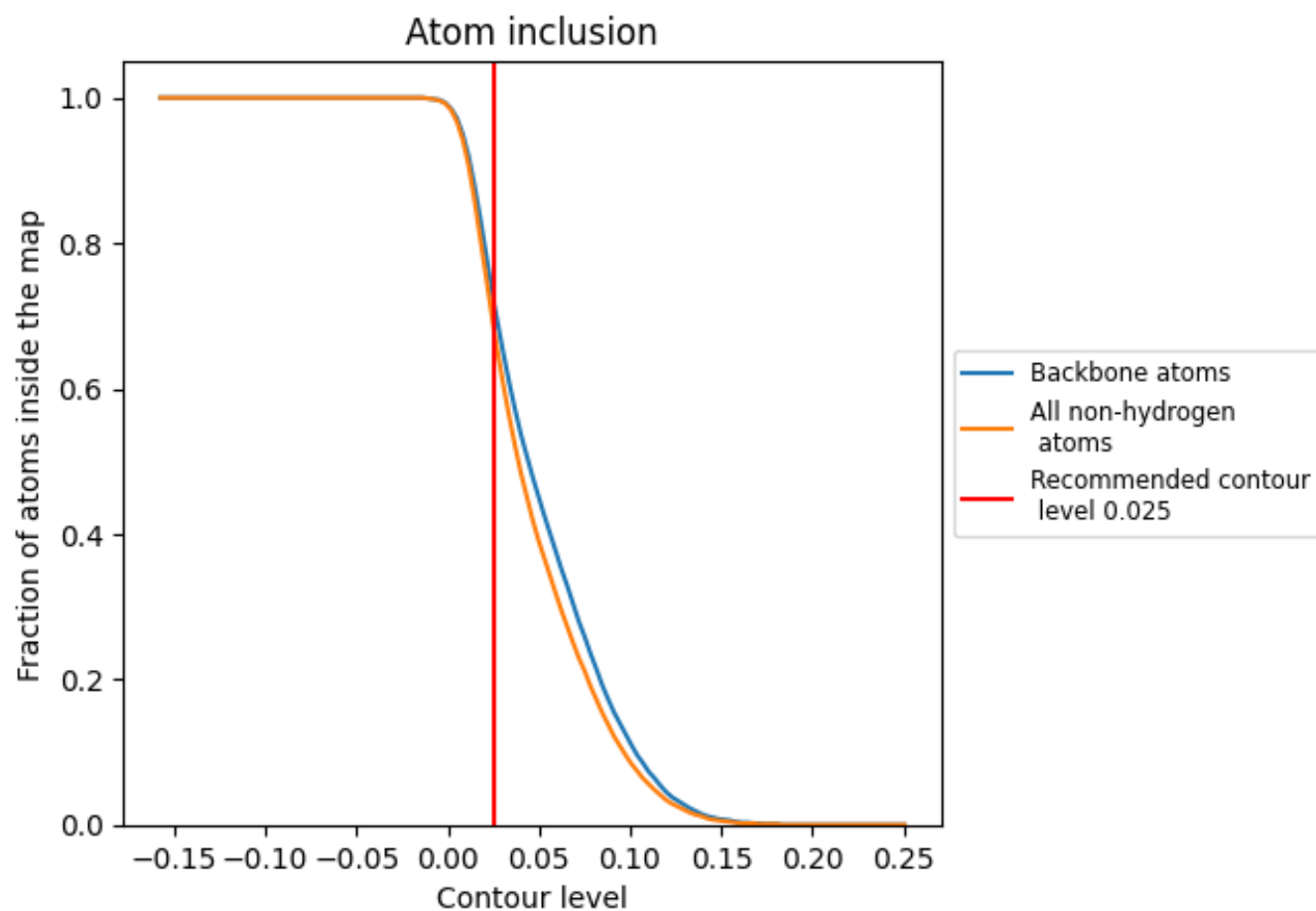
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| All   |  0.6860 |  0.4600 |
| G     |  0.7840 |  0.5150 |
| H     |  0.7480 |  0.4900 |
| I     |  0.7640 |  0.4990 |
| J     |  0.7240 |  0.4850 |
| K     |  0.6790 |  0.4830 |
| L     |  0.5050 |  0.3730 |
| P     |  0.5540 |  0.3180 |
| Q     |  0.5380 |  0.2950 |
| R     |  0.0770 |  0.2020 |

