



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:55 am GMT

PDB ID : 4A0K  
Title : STRUCTURE OF DDB1-DDB2-CUL4A-RBX1 BOUND TO A 12 BP ABA-SIC SITE CONTAINING DNA-DUPLEX  
Authors : Fischer, E.S.; Scrima, A.; Gut, H.; Thoma, N.H.  
Deposited on : 2011-09-09  
Resolution : 5.93 Å(reported)

This is a Full wwPDB X-ray Structure 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

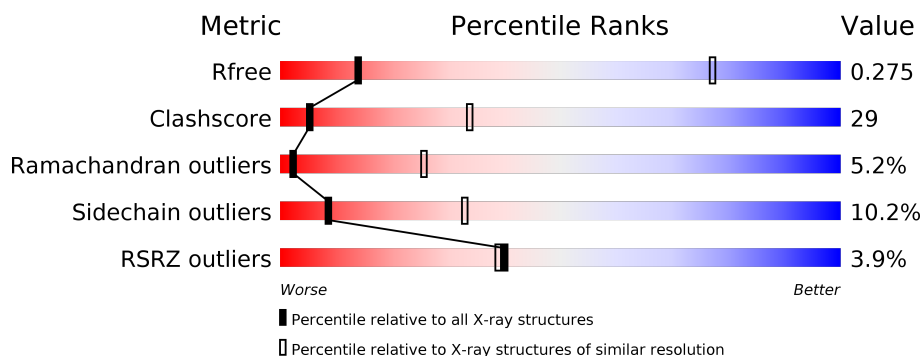
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 5.93 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) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 100719                      | 1083 (8.00-3.70)                                      |
| Clashscore            | 112137                      | 1016 (8.00-3.80)                                      |
| Ramachandran outliers | 110173                      | 1000 (8.00-3.72)                                      |
| Sidechain outliers    | 110143                      | 1083 (8.00-3.70)                                      |
| RSRZ outliers         | 101464                      | 1092 (8.00-3.70)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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 electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | A     | 742    | <div> <div>4%</div> <div> <div>35%</div> <div>47%</div> <div>13%</div> <div>• •</div> </div> </div> |
| 2   | B     | 117    | <div> <div>3%</div> <div> <div>7%</div> <div>6%</div> <div>• •</div> </div> <div>82%</div> </div>   |
| 3   | C     | 1159   | <div> <div>3%</div> <div> <div>64%</div> <div>25%</div> <div>6%</div> <div>• 5%</div> </div> </div> |
| 4   | D     | 382    | <div> <div>2%</div> <div> <div>75%</div> <div>15%</div> <div>• • 7%</div> </div> </div>             |
| 5   | E     | 12     | <div> <div>25%</div> <div> <div>75%</div> <div>25%</div> </div> </div>                              |
| 6   | F     | 12     | <div> <div>8%</div> <div> <div>50%</div> <div>50%</div> </div> </div>                               |

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17885 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 CULLIN-4A.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
|     |       |          | Total | C    | N    | O    | S  |         |         |       |
| 1   | A     | 719      | 5809  | 3692 | 1007 | 1076 | 34 | 0       | 0       | 0     |

There are 20 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 18      | MET      | -      | EXPRESSION TAG | UNP Q13619 |
| A     | 19      | HIS      | -      | EXPRESSION TAG | UNP Q13619 |
| A     | 20      | HIS      | -      | EXPRESSION TAG | UNP Q13619 |
| A     | 21      | HIS      | -      | EXPRESSION TAG | UNP Q13619 |
| A     | 22      | HIS      | -      | EXPRESSION TAG | UNP Q13619 |
| A     | 23      | HIS      | -      | EXPRESSION TAG | UNP Q13619 |
| A     | 24      | HIS      | -      | EXPRESSION TAG | UNP Q13619 |
| A     | 25      | VAL      | -      | EXPRESSION TAG | UNP Q13619 |
| A     | 26      | ASP      | -      | EXPRESSION TAG | UNP Q13619 |
| A     | 27      | GLU      | -      | EXPRESSION TAG | UNP Q13619 |
| A     | 28      | GLU      | -      | EXPRESSION TAG | UNP Q13619 |
| A     | 29      | ASN      | -      | EXPRESSION TAG | UNP Q13619 |
| A     | 30      | LEU      | -      | EXPRESSION TAG | UNP Q13619 |
| A     | 31      | TYR      | -      | EXPRESSION TAG | UNP Q13619 |
| A     | 32      | PHE      | -      | EXPRESSION TAG | UNP Q13619 |
| A     | 33      | GLN      | -      | EXPRESSION TAG | UNP Q13619 |
| A     | 34      | GLY      | -      | EXPRESSION TAG | UNP Q13619 |
| A     | 35      | GLY      | -      | EXPRESSION TAG | UNP Q13619 |
| A     | 36      | GLY      | -      | EXPRESSION TAG | UNP Q13619 |
| A     | 37      | ARG      | -      | EXPRESSION TAG | UNP Q13619 |

- Molecule 2 is a protein called E3 UBIQUITIN-PROTEIN LIGASE RBX1.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
|     |       |          | Total | C   | N  | O  |         |         |       |
| 2   | B     | 21       | 184   | 126 | 32 | 26 | 0       | 0       | 0     |

There are 20 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | -8      | MET      | -      | EXPRESSION TAG | UNP P62877 |
| B     | -7      | HIS      | -      | EXPRESSION TAG | UNP P62877 |
| B     | -6      | HIS      | -      | EXPRESSION TAG | UNP P62877 |
| B     | -5      | HIS      | -      | EXPRESSION TAG | UNP P62877 |
| B     | -4      | HIS      | -      | EXPRESSION TAG | UNP P62877 |
| B     | -3      | HIS      | -      | EXPRESSION TAG | UNP P62877 |
| B     | -2      | HIS      | -      | EXPRESSION TAG | UNP P62877 |
| B     | -1      | VAL      | -      | EXPRESSION TAG | UNP P62877 |
| B     | 0       | ASP      | -      | EXPRESSION TAG | UNP P62877 |
| B     | 1       | GLU      | -      | EXPRESSION TAG | UNP P62877 |
| B     | 2       | GLU      | -      | EXPRESSION TAG | UNP P62877 |
| B     | 3       | ASN      | -      | EXPRESSION TAG | UNP P62877 |
| B     | 4       | LEU      | -      | EXPRESSION TAG | UNP P62877 |
| B     | 5       | TYR      | -      | EXPRESSION TAG | UNP P62877 |
| B     | 6       | PHE      | -      | EXPRESSION TAG | UNP P62877 |
| B     | 7       | GLN      | -      | EXPRESSION TAG | UNP P62877 |
| B     | 8       | GLY      | -      | EXPRESSION TAG | UNP P62877 |
| B     | 9       | GLY      | -      | EXPRESSION TAG | UNP P62877 |
| B     | 10      | GLY      | -      | EXPRESSION TAG | UNP P62877 |
| B     | 11      | ARG      | -      | EXPRESSION TAG | UNP P62877 |

- Molecule 3 is a protein called DNA DAMAGE-BINDING PROTEIN 1.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 3   | C     | 1105     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 8605  | 5460 | 1442 | 1657 | 46 |         |         |       |

There are 19 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | -18     | MET      | -      | EXPRESSION TAG | UNP Q16531 |
| C     | -17     | HIS      | -      | EXPRESSION TAG | UNP Q16531 |
| C     | -16     | HIS      | -      | EXPRESSION TAG | UNP Q16531 |
| C     | -15     | HIS      | -      | EXPRESSION TAG | UNP Q16531 |
| C     | -14     | HIS      | -      | EXPRESSION TAG | UNP Q16531 |
| C     | -13     | HIS      | -      | EXPRESSION TAG | UNP Q16531 |
| C     | -12     | HIS      | -      | EXPRESSION TAG | UNP Q16531 |
| C     | -11     | VAL      | -      | EXPRESSION TAG | UNP Q16531 |
| C     | -10     | ASP      | -      | EXPRESSION TAG | UNP Q16531 |
| C     | -9      | GLU      | -      | EXPRESSION TAG | UNP Q16531 |
| C     | -8      | ASN      | -      | EXPRESSION TAG | UNP Q16531 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | -7      | LEU      | -      | EXPRESSION TAG | UNP Q16531 |
| C     | -6      | TYR      | -      | EXPRESSION TAG | UNP Q16531 |
| C     | -5      | PHE      | -      | EXPRESSION TAG | UNP Q16531 |
| C     | -4      | GLN      | -      | EXPRESSION TAG | UNP Q16531 |
| C     | -3      | GLY      | -      | EXPRESSION TAG | UNP Q16531 |
| C     | -2      | GLY      | -      | EXPRESSION TAG | UNP Q16531 |
| C     | -1      | GLY      | -      | EXPRESSION TAG | UNP Q16531 |
| C     | 0       | ARG      | -      | EXPRESSION TAG | UNP Q16531 |

- Molecule 4 is a protein called DNA DAMAGE-BINDING PROTEIN 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4   | D     | 355      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2804  | 1781 | 491 | 521 | 11 |         |         |       |

There are 20 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| D     | 76      | MET      | -      | EXPRESSION TAG | UNP Q2YDS1 |
| D     | 77      | HIS      | -      | EXPRESSION TAG | UNP Q2YDS1 |
| D     | 78      | HIS      | -      | EXPRESSION TAG | UNP Q2YDS1 |
| D     | 79      | HIS      | -      | EXPRESSION TAG | UNP Q2YDS1 |
| D     | 80      | HIS      | -      | EXPRESSION TAG | UNP Q2YDS1 |
| D     | 81      | HIS      | -      | EXPRESSION TAG | UNP Q2YDS1 |
| D     | 82      | HIS      | -      | EXPRESSION TAG | UNP Q2YDS1 |
| D     | 83      | ARG      | -      | EXPRESSION TAG | UNP Q2YDS1 |
| D     | 84      | ARG      | -      | EXPRESSION TAG | UNP Q2YDS1 |
| D     | 85      | LEU      | -      | EXPRESSION TAG | UNP Q2YDS1 |
| D     | 86      | VAL      | -      | EXPRESSION TAG | UNP Q2YDS1 |
| D     | 87      | PRO      | -      | EXPRESSION TAG | UNP Q2YDS1 |
| D     | 88      | ARG      | -      | EXPRESSION TAG | UNP Q2YDS1 |
| D     | 89      | GLY      | -      | EXPRESSION TAG | UNP Q2YDS1 |
| D     | 90      | SER      | -      | EXPRESSION TAG | UNP Q2YDS1 |
| D     | 91      | GLY      | -      | EXPRESSION TAG | UNP Q2YDS1 |
| D     | 92      | GLY      | -      | EXPRESSION TAG | UNP Q2YDS1 |
| D     | 93      | ARG      | -      | EXPRESSION TAG | UNP Q2YDS1 |
| D     | 180     | GLN      | LEU    | VARIANT        | UNP Q2YDS1 |
| D     | 214     | ARG      | TRP    | VARIANT        | UNP Q2YDS1 |

- Molecule 5 is a DNA chain called 12 BP THF CONTAINING DNA.

| Mol | Chain | Residues | Atoms        |          |         |         |         | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|---------|---------|---------|-------|
| 5   | E     | 12       | Total<br>234 | C<br>111 | N<br>41 | O<br>70 | P<br>12 | 0       | 0       | 0     |

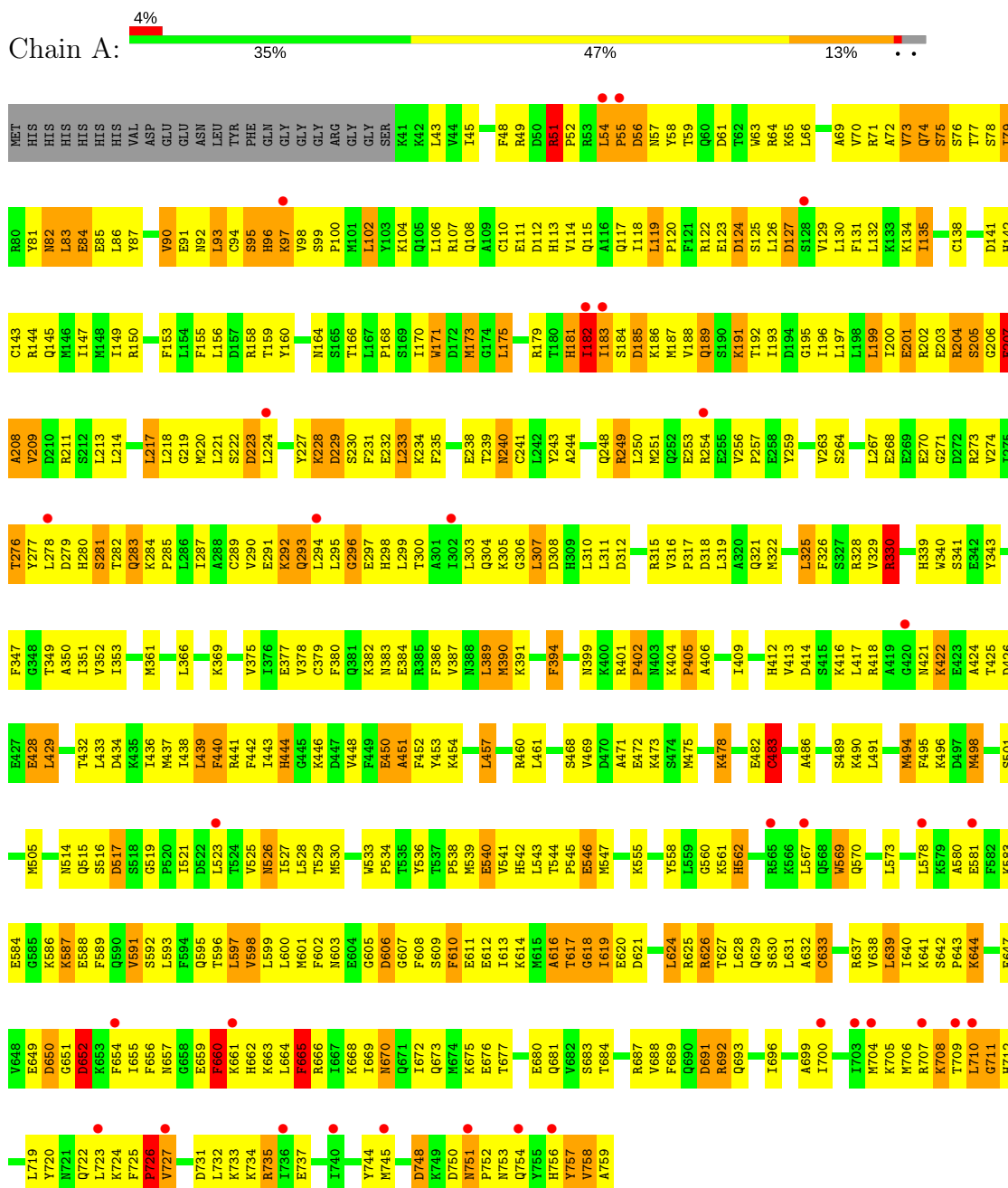
- Molecule 6 is a DNA chain called 12 BP DNA.

| Mol | Chain | Residues | Atoms        |          |         |         |         | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|---------|---------|---------|-------|
| 6   | F     | 12       | Total<br>249 | C<br>118 | N<br>47 | O<br>72 | P<br>12 | 0       | 0       | 0     |

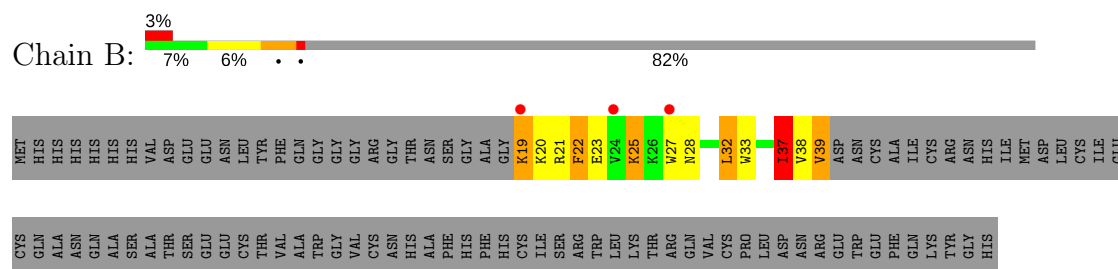
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

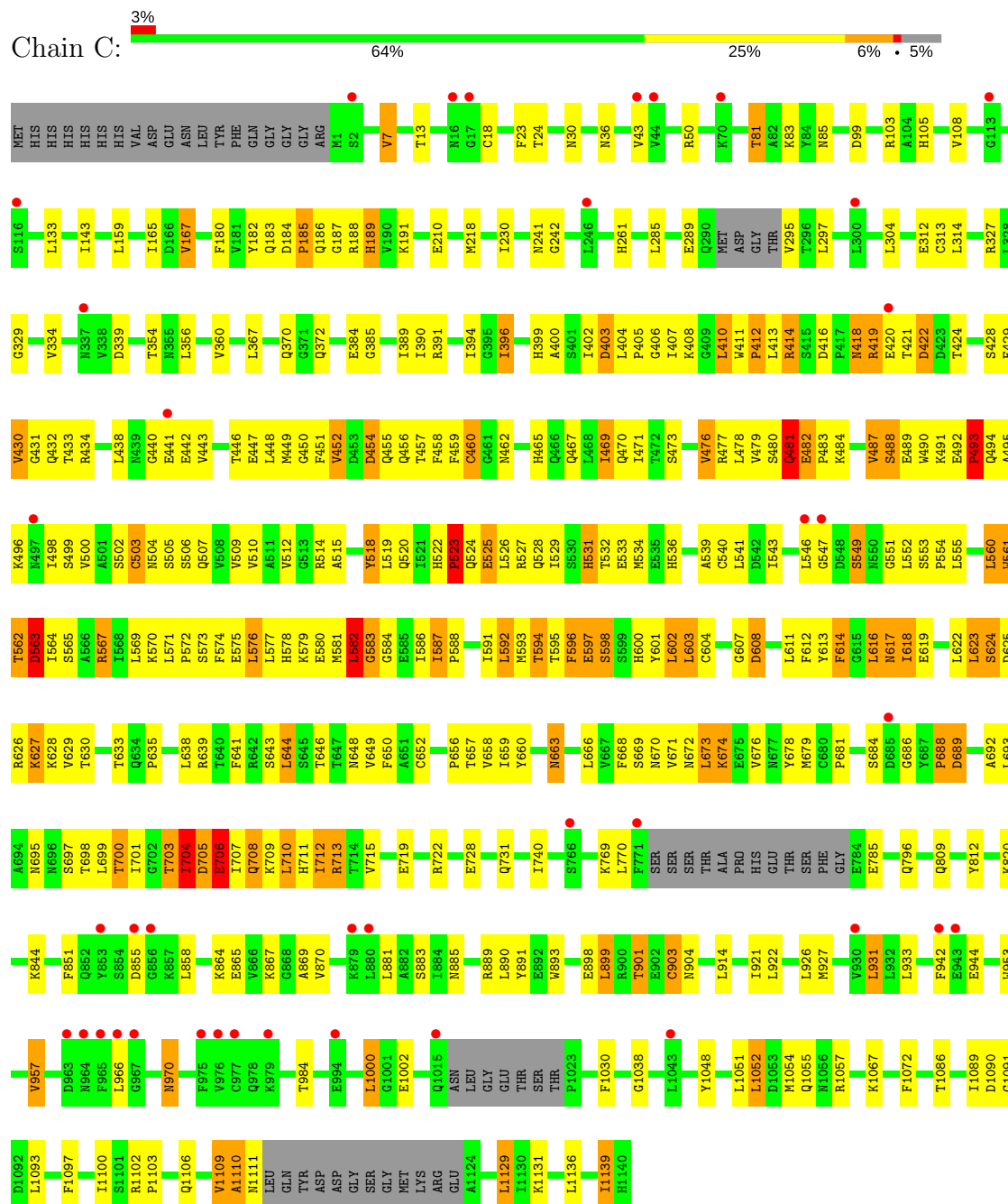
#### • Molecule 1: CULLIN-4A



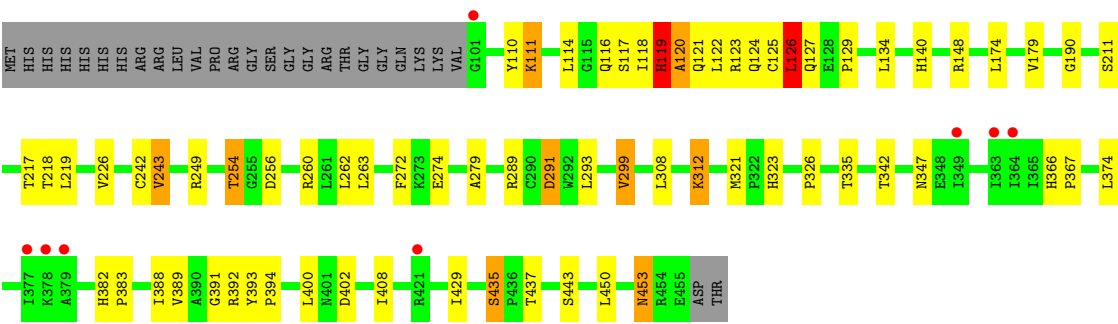
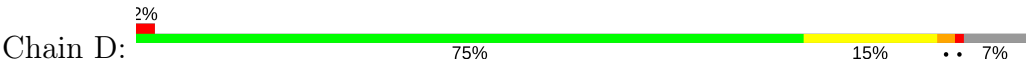
• Molecule 2: E3 UBIQUITIN-PROTEIN LIGASE RBX1



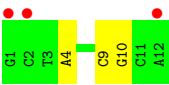
• Molecule 3: DNA DAMAGE-BINDING PROTEIN 1



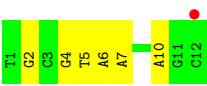




• Molecule 5: 12 BP THF CONTAINING DNA



• Molecule 6: 12 BP DNA



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | C 1 2 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 210.65Å 78.02Å 276.62Å<br>90.00° 108.50° 90.00°             | Depositor        |
| Resolution (Å)  | 19.98 – 5.93<br>47.64 – 5.93                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.3 (19.98-5.93)<br>98.9 (47.64-5.93)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.14  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.08 (at 6.15Å)   | Xtriage          |
| Refinement program  | PHENIX (PHENIX.REFINE)                                      | Depositor        |
| R, $R_{free}$   | 0.269 , 0.270<br>0.279 , 0.275                              | Depositor<br>DCC |
| $R_{free}$ test set   | 564 reflections (5.01%)                                     | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 261.2   | Xtriage          |
| Anisotropy  | 0.597   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 330.1  | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.86  | EDS              |
| Total number of atoms   | 17885   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 326.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: 3DR

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

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5         |
| 1   | A     | 0.44         | 0/5915         | 0.74        | 11/7954 (0.1%)  |
| 2   | B     | 0.40         | 0/190          | 0.48        | 0/257           |
| 3   | C     | 0.46         | 5/8762 (0.1%)  | 0.67        | 9/11875 (0.1%)  |
| 4   | D     | 0.37         | 0/2877         | 0.58        | 0/3912          |
| 5   | E     | 0.93         | 1/248 (0.4%)   | 1.12        | 0/377           |
| 6   | F     | 0.89         | 0/279          | 1.36        | 1/429 (0.2%)    |
| All | All   | 0.46         | 6/18271 (0.0%) | 0.70        | 21/24804 (0.1%) |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 3   | C     | 354 | THR  | C-N    | -11.77 | 1.06        | 1.34     |
| 3   | C     | 582 | LEU  | C-N    | 6.64   | 1.45        | 1.33     |
| 3   | C     | 13  | THR  | C-N    | 6.59   | 1.49        | 1.34     |
| 3   | C     | 706 | GLU  | C-N    | -5.68  | 1.21        | 1.34     |
| 5   | E     | 9   | DC   | C1'-N1 | 5.59   | 1.56        | 1.49     |
| 3   | C     | 903 | CYS  | CB-SG  | -5.18  | 1.73        | 1.81     |

All (21) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | A     | 298 | HIS  | CB-CA-C    | -10.74 | 88.92       | 110.40   |
| 1   | A     | 182 | ILE  | N-CA-C     | 9.33   | 136.18      | 111.00   |
| 1   | A     | 181 | HIS  | CB-CA-C    | 7.11   | 124.62      | 110.40   |
| 3   | C     | 624 | SER  | N-CA-C     | 7.02   | 129.96      | 111.00   |
| 1   | A     | 48  | PHE  | N-CA-C     | -6.88  | 92.43       | 111.00   |
| 3   | C     | 688 | PRO  | N-CA-C     | 6.59   | 129.22      | 112.10   |
| 3   | C     | 689 | ASP  | N-CA-C     | -6.45  | 93.58       | 111.00   |
| 6   | F     | 2   | DG   | O4'-C1'-N9 | 6.33   | 112.43      | 108.00   |
| 1   | A     | 182 | ILE  | N-CA-CB    | -5.97  | 97.07       | 110.80   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | A     | 51   | ARG  | CB-CA-C   | -5.95 | 98.51       | 110.40   |
| 3   | C     | 688  | PRO  | CA-N-CD   | -5.90 | 103.24      | 111.50   |
| 3   | C     | 624  | SER  | CB-CA-C   | -5.85 | 98.99       | 110.10   |
| 3   | C     | 1139 | ILE  | N-CA-CB   | 5.58  | 123.64      | 110.80   |
| 3   | C     | 354  | THR  | O-C-N     | 5.52  | 131.53      | 122.70   |
| 1   | A     | 637  | ARG  | N-CA-C    | 5.46  | 125.74      | 111.00   |
| 1   | A     | 296  | GLY  | N-CA-C    | -5.43 | 99.52       | 113.10   |
| 1   | A     | 665  | PHE  | N-CA-C    | -5.37 | 96.50       | 111.00   |
| 1   | A     | 74   | GLN  | N-CA-C    | -5.36 | 96.53       | 111.00   |
| 1   | A     | 73   | VAL  | N-CA-C    | -5.28 | 96.75       | 111.00   |
| 3   | C     | 523  | PRO  | CA-N-CD   | -5.25 | 104.14      | 111.50   |
| 3   | C     | 422  | ASP  | CB-CG-OD2 | 5.17  | 122.95      | 118.30   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 5809  | 0        | 5796     | 617     | 0            |
| 2   | B     | 184   | 0        | 192      | 29      | 0            |
| 3   | C     | 8605  | 0        | 8542     | 369     | 1            |
| 4   | D     | 2804  | 0        | 2720     | 45      | 0            |
| 5   | E     | 234   | 0        | 132      | 3       | 0            |
| 6   | F     | 249   | 0        | 136      | 7       | 0            |
| All | All   | 17885 | 0        | 17518    | 1034    | 1            |

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 29.

All (1034) 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) |
|-----------------|----------------|--------------------------|-------------------|
| 1:A:131:PHE:CZ  | 1:A:188:VAL:HA | 1.63                     | 1.33              |
| 1:A:696:ILE:CD1 | 1:A:723:LEU:HG | 1.57                     | 1.33              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:118:ILE:CD1  | 1:A:181:HIS:HB3  | 1.60                     | 1.29              |
| 1:A:135:ILE:HD11 | 1:A:188:VAL:CG1  | 1.63                     | 1.26              |
| 1:A:696:ILE:HD13 | 1:A:723:LEU:CD1  | 1.69                     | 1.21              |
| 1:A:696:ILE:HD13 | 1:A:723:LEU:CG   | 1.71                     | 1.20              |
| 1:A:135:ILE:CD1  | 1:A:188:VAL:CG1  | 2.21                     | 1.19              |
| 1:A:118:ILE:HD11 | 1:A:181:HIS:CB   | 1.73                     | 1.16              |
| 1:A:131:PHE:CZ   | 1:A:188:VAL:HG13 | 1.79                     | 1.15              |
| 1:A:118:ILE:HD11 | 1:A:181:HIS:HB3  | 1.20                     | 1.15              |
| 1:A:699:ALA:HB1  | 1:A:722:GLN:NE2  | 1.63                     | 1.13              |
| 1:A:692:ARG:CB   | 1:A:725:PHE:CE2  | 2.32                     | 1.12              |
| 1:A:118:ILE:HD11 | 1:A:181:HIS:CG   | 1.84                     | 1.12              |
| 1:A:183:ILE:HD11 | 1:A:220:MET:CE   | 1.83                     | 1.08              |
| 1:A:43:LEU:HD11  | 3:C:400:ALA:HB1  | 1.17                     | 1.08              |
| 1:A:131:PHE:HZ   | 1:A:188:VAL:CA   | 1.67                     | 1.07              |
| 1:A:69:ALA:HA    | 1:A:79:ILE:HG21  | 1.33                     | 1.07              |
| 2:B:37:ILE:HD13  | 2:B:38:VAL:N     | 1.69                     | 1.07              |
| 2:B:25:LYS:HE3   | 2:B:25:LYS:HA    | 1.30                     | 1.07              |
| 1:A:692:ARG:HB3  | 1:A:725:PHE:CE2  | 1.89                     | 1.06              |
| 1:A:692:ARG:HB2  | 1:A:725:PHE:CZ   | 1.90                     | 1.05              |
| 1:A:107:ARG:NH1  | 1:A:173:MET:HG3  | 1.70                     | 1.05              |
| 1:A:129:VAL:HG13 | 1:A:130:LEU:N    | 1.71                     | 1.04              |
| 2:B:37:ILE:HG12  | 2:B:38:VAL:H     | 1.20                     | 1.04              |
| 1:A:700:ILE:HD13 | 1:A:719:LEU:HD21 | 1.38                     | 1.04              |
| 1:A:129:VAL:CG1  | 1:A:130:LEU:H    | 1.72                     | 1.03              |
| 1:A:135:ILE:HD11 | 1:A:188:VAL:HG11 | 1.04                     | 1.03              |
| 3:C:539:ALA:HB2  | 3:C:561:TRP:CD1  | 1.94                     | 1.02              |
| 2:B:37:ILE:CG1   | 2:B:38:VAL:H     | 1.71                     | 1.02              |
| 3:C:562:THR:O    | 3:C:564:ILE:HG13 | 1.61                     | 1.01              |
| 2:B:37:ILE:HD13  | 2:B:37:ILE:C     | 1.80                     | 1.01              |
| 3:C:185:PRO:HD3  | 4:D:289:ARG:HB3  | 1.40                     | 1.01              |
| 1:A:131:PHE:CZ   | 1:A:188:VAL:CA   | 2.44                     | 1.00              |
| 1:A:626:ARG:HA   | 1:A:629:GLN:HB2  | 1.41                     | 0.99              |
| 1:A:692:ARG:HB2  | 1:A:725:PHE:CE2  | 1.94                     | 0.99              |
| 3:C:539:ALA:HB2  | 3:C:561:TRP:HD1  | 1.26                     | 0.99              |
| 1:A:705:LYS:HB2  | 1:A:757:TYR:CE2  | 1.98                     | 0.99              |
| 3:C:185:PRO:CD   | 4:D:289:ARG:HB3  | 1.93                     | 0.99              |
| 1:A:422:LYS:HB3  | 1:A:422:LYS:NZ   | 1.77                     | 0.98              |
| 1:A:700:ILE:CD1  | 1:A:719:LEU:HD21 | 1.93                     | 0.98              |
| 1:A:642:SER:HB2  | 1:A:643:PRO:HD3  | 1.46                     | 0.97              |
| 1:A:696:ILE:HD13 | 1:A:723:LEU:HD11 | 1.44                     | 0.97              |
| 1:A:657:ASN:HD21 | 1:A:659:GLU:HB2  | 1.28                     | 0.96              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:696:ILE:HD13 | 1:A:723:LEU:HG   | 1.32                     | 0.96              |
| 1:A:74:GLN:HE22  | 1:A:110:CYS:HA   | 1.31                     | 0.96              |
| 1:A:197:LEU:CD2  | 1:A:235:PHE:HA   | 1.96                     | 0.96              |
| 1:A:491:LEU:HA   | 1:A:494:MET:HG3  | 1.48                     | 0.96              |
| 1:A:705:LYS:HA   | 1:A:757:TYR:CD2  | 2.01                     | 0.95              |
| 1:A:638:VAL:HG12 | 1:A:639:LEU:HD23 | 1.48                     | 0.95              |
| 3:C:465:HIS:ND1  | 3:C:523:PRO:HD3  | 1.82                     | 0.95              |
| 3:C:329:GLY:HA3  | 3:C:384:GLU:HG2  | 1.45                     | 0.95              |
| 2:B:37:ILE:CD1   | 2:B:38:VAL:N     | 2.30                     | 0.94              |
| 1:A:131:PHE:HZ   | 1:A:188:VAL:HA   | 1.13                     | 0.94              |
| 1:A:183:ILE:HD11 | 1:A:220:MET:HE3  | 1.49                     | 0.93              |
| 1:A:131:PHE:CE1  | 1:A:191:LYS:HD3  | 2.04                     | 0.93              |
| 1:A:118:ILE:CG1  | 1:A:181:HIS:HB3  | 1.98                     | 0.93              |
| 1:A:183:ILE:HD11 | 1:A:220:MET:SD   | 2.09                     | 0.93              |
| 2:B:37:ILE:CG1   | 2:B:38:VAL:N     | 2.30                     | 0.92              |
| 1:A:122:ARG:HD2  | 1:A:186:LYS:HZ2  | 1.34                     | 0.91              |
| 1:A:696:ILE:HD11 | 1:A:723:LEU:HG   | 1.51                     | 0.91              |
| 1:A:197:LEU:HD22 | 1:A:235:PHE:HA   | 1.50                     | 0.91              |
| 1:A:131:PHE:HZ   | 1:A:188:VAL:CB   | 1.84                     | 0.91              |
| 3:C:507:GLN:NE2  | 3:C:552:LEU:HA   | 1.85                     | 0.91              |
| 2:B:19:LYS:HA    | 2:B:19:LYS:HE3   | 1.53                     | 0.91              |
| 1:A:82:ASN:OD1   | 1:A:85:GLU:HG3   | 1.69                     | 0.90              |
| 1:A:51:ARG:O     | 1:A:51:ARG:HG2   | 1.72                     | 0.90              |
| 1:A:63:TRP:CZ3   | 1:A:102:LEU:HA   | 2.07                     | 0.90              |
| 1:A:196:ILE:HD13 | 1:A:218:LEU:HD21 | 1.53                     | 0.90              |
| 1:A:129:VAL:CG1  | 1:A:130:LEU:N    | 2.30                     | 0.90              |
| 3:C:356:LEU:HD21 | 3:C:712:ILE:HD13 | 1.52                     | 0.90              |
| 3:C:465:HIS:CE1  | 3:C:523:PRO:HD3  | 2.07                     | 0.90              |
| 3:C:18:CYS:HB2   | 3:C:313:CYS:SG   | 2.12                     | 0.90              |
| 1:A:131:PHE:CZ   | 1:A:188:VAL:CG1  | 2.54                     | 0.89              |
| 1:A:745:MET:HA   | 1:A:757:TYR:O    | 1.71                     | 0.89              |
| 1:A:43:LEU:CD1   | 3:C:400:ALA:HB1  | 2.03                     | 0.89              |
| 1:A:99:SER:HB2   | 1:A:100:PRO:HD3  | 1.53                     | 0.88              |
| 1:A:696:ILE:CD1  | 1:A:723:LEU:CG   | 2.35                     | 0.88              |
| 1:A:106:LEU:HD22 | 1:A:153:PHE:CE2  | 2.09                     | 0.87              |
| 3:C:578:HIS:CD2  | 3:C:623:LEU:HD12 | 2.09                     | 0.87              |
| 4:D:323:HIS:NE2  | 4:D:342:THR:HG21 | 1.88                     | 0.87              |
| 1:A:538:PRO:HA   | 1:A:570:GLN:HE22 | 1.40                     | 0.87              |
| 1:A:70:VAL:HG21  | 1:A:106:LEU:CD1  | 2.05                     | 0.87              |
| 3:C:649:VAL:HG12 | 3:C:650:PHE:H    | 1.39                     | 0.86              |
| 1:A:196:ILE:HD13 | 1:A:218:LEU:CD2  | 2.06                     | 0.86              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:274:VAL:HA   | 1:A:278:LEU:HB2  | 1.57                     | 0.86              |
| 1:A:605:GLY:O    | 1:A:606:ASP:HB2  | 1.75                     | 0.86              |
| 1:A:131:PHE:CD1  | 1:A:191:LYS:HD3  | 2.11                     | 0.86              |
| 1:A:144:ARG:HA   | 1:A:147:ILE:HD12 | 1.58                     | 0.86              |
| 1:A:63:TRP:CH2   | 1:A:102:LEU:HA   | 2.11                     | 0.85              |
| 3:C:711:HIS:CG   | 3:C:712:ILE:N    | 2.43                     | 0.85              |
| 3:C:23:PHE:H     | 3:C:30:ASN:HD22  | 1.21                     | 0.85              |
| 1:A:122:ARG:NE   | 1:A:186:LYS:HZ3  | 1.74                     | 0.85              |
| 1:A:199:LEU:HD12 | 1:A:214:LEU:HD11 | 1.59                     | 0.85              |
| 3:C:165:ILE:HD11 | 3:C:188:ARG:NH2  | 1.92                     | 0.85              |
| 1:A:213:LEU:O    | 1:A:217:LEU:HD12 | 1.76                     | 0.85              |
| 3:C:81:THR:HG21  | 3:C:85:ASN:HD22  | 1.41                     | 0.84              |
| 1:A:422:LYS:HB3  | 1:A:422:LYS:HZ2  | 1.38                     | 0.84              |
| 1:A:115:GLN:HG2  | 1:A:181:HIS:CE1  | 2.14                     | 0.83              |
| 1:A:696:ILE:HA   | 1:A:723:LEU:HD11 | 1.60                     | 0.83              |
| 3:C:707:ILE:HG23 | 3:C:708:GLN:N    | 1.92                     | 0.83              |
| 1:A:119:LEU:HB2  | 1:A:120:PRO:HD3  | 1.60                     | 0.83              |
| 3:C:446:THR:HG22 | 3:C:447:GLU:H    | 1.43                     | 0.83              |
| 3:C:520:GLN:HG3  | 3:C:529:ILE:HG13 | 1.60                     | 0.82              |
| 1:A:135:ILE:CD1  | 1:A:188:VAL:HG13 | 2.06                     | 0.82              |
| 1:A:581:GLU:HB2  | 2:B:21:ARG:HA    | 1.62                     | 0.82              |
| 3:C:482:GLU:CD   | 3:C:483:PRO:HD3  | 2.00                     | 0.81              |
| 1:A:705:LYS:HB2  | 1:A:757:TYR:HE2  | 1.45                     | 0.81              |
| 1:A:93:LEU:O     | 1:A:93:LEU:HD22  | 1.79                     | 0.81              |
| 1:A:699:ALA:CB   | 1:A:722:GLN:NE2  | 2.43                     | 0.81              |
| 2:B:38:VAL:O     | 2:B:38:VAL:HG12  | 1.80                     | 0.81              |
| 3:C:413:LEU:HB2  | 3:C:424:THR:HB   | 1.62                     | 0.81              |
| 3:C:507:GLN:HE22 | 3:C:553:SER:H    | 1.25                     | 0.81              |
| 1:A:757:TYR:HE1  | 1:A:759:ALA:HA   | 1.47                     | 0.80              |
| 3:C:708:GLN:NE2  | 3:C:708:GLN:HA   | 1.94                     | 0.80              |
| 1:A:284:LYS:HB3  | 1:A:285:PRO:HD3  | 1.61                     | 0.80              |
| 1:A:131:PHE:HZ   | 1:A:188:VAL:CG1  | 1.93                     | 0.80              |
| 1:A:366:LEU:HD23 | 1:A:439:LEU:HD12 | 1.62                     | 0.80              |
| 1:A:131:PHE:CE2  | 1:A:188:VAL:HG13 | 2.16                     | 0.80              |
| 1:A:680:GLU:O    | 1:A:684:THR:HG22 | 1.81                     | 0.80              |
| 3:C:534:MET:HE2  | 3:C:569:LEU:HD11 | 1.62                     | 0.80              |
| 1:A:296:GLY:O    | 1:A:297:GLU:HB2  | 1.82                     | 0.79              |
| 3:C:509:VAL:HG23 | 3:C:543:ILE:HD13 | 1.62                     | 0.79              |
| 1:A:705:LYS:CA   | 1:A:757:TYR:CD2  | 2.65                     | 0.79              |
| 1:A:93:LEU:CD2   | 1:A:93:LEU:O     | 2.30                     | 0.79              |
| 1:A:122:ARG:NE   | 1:A:186:LYS:NZ   | 2.30                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:599:LEU:HD21 | 1:A:631:LEU:HD12 | 1.64                     | 0.79              |
| 1:A:211:ARG:HD2  | 1:A:276:THR:HG21 | 1.64                     | 0.79              |
| 3:C:182:TYR:O    | 3:C:188:ARG:CB   | 2.30                     | 0.79              |
| 1:A:696:ILE:HD11 | 1:A:725:PHE:CZ   | 2.18                     | 0.78              |
| 1:A:204:ARG:HH21 | 1:A:270:GLU:CD   | 1.86                     | 0.78              |
| 3:C:412:PRO:HB2  | 3:C:422:ASP:OD2  | 1.83                     | 0.78              |
| 3:C:185:PRO:CG   | 4:D:289:ARG:CB   | 2.62                     | 0.78              |
| 1:A:692:ARG:O    | 1:A:696:ILE:HG12 | 1.84                     | 0.78              |
| 1:A:138:CYS:SG   | 1:A:182:ILE:CD1  | 2.71                     | 0.77              |
| 1:A:175:LEU:HD12 | 1:A:223:ASP:O    | 1.85                     | 0.77              |
| 1:A:461:LEU:HB3  | 1:A:498:MET:HE2  | 1.65                     | 0.77              |
| 1:A:704:MET:C    | 1:A:757:TYR:HD2  | 1.86                     | 0.77              |
| 3:C:649:VAL:HG12 | 3:C:650:PHE:N    | 2.00                     | 0.77              |
| 1:A:527:ILE:HD11 | 1:A:567:LEU:HD22 | 1.65                     | 0.77              |
| 1:A:274:VAL:HG11 | 1:A:283:GLN:HE21 | 1.49                     | 0.77              |
| 3:C:185:PRO:HG3  | 4:D:289:ARG:HB2  | 1.65                     | 0.77              |
| 1:A:129:VAL:HG13 | 1:A:130:LEU:H    | 1.32                     | 0.77              |
| 3:C:578:HIS:NE2  | 3:C:623:LEU:HD12 | 1.99                     | 0.77              |
| 3:C:602:LEU:C    | 3:C:603:LEU:HD23 | 2.04                     | 0.76              |
| 1:A:186:LYS:HB3  | 1:A:188:VAL:HG23 | 1.67                     | 0.76              |
| 1:A:603:ASN:OD1  | 2:B:22:PHE:HB2   | 1.86                     | 0.76              |
| 3:C:23:PHE:H     | 3:C:30:ASN:ND2   | 1.83                     | 0.76              |
| 3:C:452:VAL:HG12 | 3:C:454:ASP:OD1  | 1.86                     | 0.75              |
| 1:A:329:VAL:HG12 | 1:A:330:ARG:H    | 1.49                     | 0.75              |
| 1:A:601:MET:HE1  | 1:A:616:ALA:CB   | 2.17                     | 0.75              |
| 1:A:597:LEU:HB3  | 1:A:617:THR:HG21 | 1.68                     | 0.75              |
| 1:A:276:THR:HG22 | 1:A:277:TYR:N    | 2.02                     | 0.75              |
| 1:A:578:LEU:HD11 | 1:A:596:THR:HG23 | 1.67                     | 0.75              |
| 3:C:450:GLY:HA3  | 3:C:479:VAL:CG2  | 2.17                     | 0.75              |
| 3:C:448:LEU:HB3  | 3:C:451:PHE:HD2  | 1.52                     | 0.74              |
| 3:C:469:ILE:HD11 | 3:C:476:VAL:HG23 | 1.69                     | 0.74              |
| 3:C:507:GLN:HE22 | 3:C:552:LEU:HA   | 1.49                     | 0.74              |
| 3:C:389:ILE:HD13 | 3:C:713:ARG:HG2  | 1.68                     | 0.74              |
| 1:A:279:ASP:OD1  | 1:A:281:SER:HB3  | 1.87                     | 0.74              |
| 1:A:705:LYS:O    | 1:A:708:LYS:NZ   | 2.21                     | 0.74              |
| 3:C:185:PRO:CG   | 4:D:289:ARG:HB2  | 2.17                     | 0.74              |
| 1:A:595:GLN:HE22 | 1:A:669:ILE:HG22 | 1.53                     | 0.74              |
| 1:A:316:VAL:HB   | 1:A:317:PRO:HD3  | 1.70                     | 0.74              |
| 1:A:688:VAL:O    | 1:A:692:ARG:HG3  | 1.88                     | 0.73              |
| 1:A:696:ILE:O    | 1:A:700:ILE:HG12 | 1.88                     | 0.73              |
| 1:A:106:LEU:HD22 | 1:A:153:PHE:CZ   | 2.22                     | 0.73              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:122:ARG:CD    | 1:A:186:LYS:NZ   | 2.51                     | 0.73              |
| 3:C:451:PHE:CD1   | 3:C:470:GLN:HB2  | 2.24                     | 0.73              |
| 1:A:294:LEU:O     | 1:A:295:LEU:HD23 | 1.86                     | 0.73              |
| 1:A:630:SER:HB3   | 1:A:672:ILE:HD11 | 1.70                     | 0.73              |
| 3:C:578:HIS:CD2   | 3:C:623:LEU:H    | 2.06                     | 0.73              |
| 1:A:609:SER:O     | 1:A:612:GLU:HG2  | 1.87                     | 0.73              |
| 1:A:77:THR:HG22   | 1:A:78:SER:H     | 1.53                     | 0.73              |
| 3:C:1055:GLN:HE22 | 3:C:1090:ASP:H   | 1.37                     | 0.73              |
| 1:A:118:ILE:HG12  | 1:A:181:HIS:HB3  | 1.71                     | 0.73              |
| 3:C:465:HIS:O     | 3:C:467:GLN:HG3  | 1.89                     | 0.72              |
| 1:A:138:CYS:SG    | 1:A:182:ILE:HD13 | 2.29                     | 0.72              |
| 1:A:135:ILE:HD12  | 1:A:188:VAL:HG13 | 1.70                     | 0.72              |
| 3:C:184:ASP:HB2   | 3:C:185:PRO:HD2  | 1.70                     | 0.72              |
| 1:A:529:THR:HA    | 2:B:33:TRP:NE1   | 2.03                     | 0.72              |
| 3:C:657:THR:HG22  | 3:C:658:VAL:H    | 1.54                     | 0.72              |
| 1:A:240:ASN:OD1   | 1:A:289:CYS:HB3  | 1.90                     | 0.72              |
| 1:A:340:TRP:CH2   | 1:A:390:MET:HB2  | 2.25                     | 0.72              |
| 1:A:208:ALA:O     | 1:A:209:VAL:CB   | 2.38                     | 0.72              |
| 1:A:49:ARG:HD2    | 1:A:51:ARG:NH2   | 2.05                     | 0.72              |
| 3:C:465:HIS:HB2   | 3:C:467:GLN:HE21 | 1.55                     | 0.72              |
| 3:C:469:ILE:HD13  | 3:C:470:GLN:N    | 2.05                     | 0.72              |
| 1:A:601:MET:HE1   | 1:A:616:ALA:HB3  | 1.72                     | 0.71              |
| 1:A:239:THR:C     | 1:A:241:CYS:H    | 1.91                     | 0.71              |
| 3:C:182:TYR:O     | 3:C:188:ARG:HB2  | 1.89                     | 0.71              |
| 4:D:263:LEU:HB2   | 4:D:272:PHE:HB3  | 1.73                     | 0.71              |
| 1:A:660:PHE:O     | 1:A:662:HIS:N    | 2.23                     | 0.71              |
| 3:C:329:GLY:HA3   | 3:C:384:GLU:CG   | 2.20                     | 0.71              |
| 1:A:601:MET:CE    | 1:A:616:ALA:CB   | 2.68                     | 0.71              |
| 3:C:889:ARG:HD3   | 3:C:901:THR:HB   | 1.73                     | 0.71              |
| 1:A:118:ILE:HD11  | 1:A:181:HIS:ND1  | 2.06                     | 0.71              |
| 1:A:432:THR:O     | 1:A:436:ILE:HG13 | 1.91                     | 0.71              |
| 3:C:185:PRO:CG    | 4:D:289:ARG:HB3  | 2.21                     | 0.71              |
| 1:A:602:PHE:HD2   | 1:A:656:PHE:HB2  | 1.54                     | 0.70              |
| 3:C:561:TRP:O     | 3:C:587:ILE:CG2  | 2.40                     | 0.70              |
| 1:A:643:PRO:CD    | 1:A:652:ASP:HA   | 2.21                     | 0.70              |
| 3:C:704:ILE:O     | 3:C:705:ASP:HB2  | 1.91                     | 0.70              |
| 3:C:396:ILE:HA    | 3:C:704:ILE:O    | 1.90                     | 0.70              |
| 3:C:451:PHE:CE1   | 3:C:470:GLN:HB2  | 2.25                     | 0.70              |
| 3:C:592:LEU:HD23  | 3:C:593:MET:O    | 1.92                     | 0.70              |
| 1:A:204:ARG:NH2   | 1:A:270:GLU:OE1  | 2.23                     | 0.70              |
| 1:A:578:LEU:HD13  | 1:A:591:VAL:CG2  | 2.21                     | 0.70              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:129:VAL:HG12 | 1:A:130:LEU:H     | 1.55                     | 0.70              |
| 1:A:122:ARG:HD2  | 1:A:186:LYS:NZ    | 2.06                     | 0.70              |
| 1:A:705:LYS:CB   | 1:A:757:TYR:CE2   | 2.73                     | 0.70              |
| 1:A:587:LYS:HD2  | 1:A:587:LYS:H     | 1.57                     | 0.69              |
| 3:C:399:HIS:NE2  | 3:C:703:THR:HG22  | 2.07                     | 0.69              |
| 1:A:692:ARG:O    | 1:A:725:PHE:HZ    | 1.76                     | 0.69              |
| 3:C:652:CYS:HB3  | 3:C:676:VAL:O     | 1.91                     | 0.69              |
| 3:C:706:GLU:OE1  | 3:C:706:GLU:HA    | 1.90                     | 0.69              |
| 1:A:329:VAL:HG12 | 1:A:330:ARG:N     | 2.08                     | 0.69              |
| 3:C:480:SER:O    | 3:C:484:LYS:HA    | 1.92                     | 0.69              |
| 3:C:532:THR:HG22 | 3:C:533:GLU:N     | 2.06                     | 0.69              |
| 1:A:619:ILE:HG22 | 1:A:620:GLU:H     | 1.56                     | 0.69              |
| 3:C:618:ILE:HG13 | 3:C:619:GLU:N     | 2.08                     | 0.68              |
| 3:C:452:VAL:HG23 | 3:C:470:GLN:OE1   | 1.93                     | 0.68              |
| 1:A:560:GLY:O    | 1:A:561:LYS:HB2   | 1.93                     | 0.68              |
| 1:A:751:ASN:O    | 1:A:753:ASN:N     | 2.27                     | 0.68              |
| 3:C:536:HIS:CD2  | 3:C:563:ASP:HB3   | 2.29                     | 0.68              |
| 3:C:722:ARG:NH2  | 3:C:812:TYR:OH    | 2.26                     | 0.68              |
| 1:A:204:ARG:CZ   | 1:A:243:TYR:HE2   | 2.07                     | 0.68              |
| 3:C:450:GLY:HA3  | 3:C:479:VAL:HG21  | 1.74                     | 0.68              |
| 3:C:1051:LEU:HB2 | 3:C:1089:ILE:HD13 | 1.76                     | 0.68              |
| 3:C:440:GLY:O    | 3:C:686:GLY:HA3   | 1.94                     | 0.68              |
| 1:A:122:ARG:CD   | 1:A:186:LYS:HZ2   | 2.06                     | 0.68              |
| 1:A:555:LYS:HD2  | 1:A:569:TRP:HZ3   | 1.58                     | 0.67              |
| 1:A:70:VAL:HG21  | 1:A:106:LEU:HD11  | 1.77                     | 0.67              |
| 1:A:630:SER:CB   | 1:A:672:ILE:HD11  | 2.24                     | 0.67              |
| 3:C:596:PHE:HE1  | 3:C:648:ASN:HA    | 1.58                     | 0.67              |
| 1:A:249:ARG:O    | 1:A:253:GLU:HB2   | 1.95                     | 0.67              |
| 3:C:711:HIS:CG   | 3:C:712:ILE:H     | 2.08                     | 0.67              |
| 1:A:630:SER:O    | 1:A:631:LEU:HB2   | 1.94                     | 0.67              |
| 1:A:63:TRP:CH2   | 1:A:102:LEU:CA    | 2.77                     | 0.67              |
| 1:A:82:ASN:O     | 1:A:83:LEU:C      | 2.33                     | 0.67              |
| 3:C:165:ILE:CD1  | 3:C:188:ARG:NH2   | 2.58                     | 0.67              |
| 1:A:274:VAL:HG11 | 1:A:283:GLN:HB2   | 1.76                     | 0.66              |
| 1:A:593:LEU:HD21 | 2:B:27:TRP:HE1    | 1.60                     | 0.66              |
| 1:A:63:TRP:NE1   | 1:A:93:LEU:HD11   | 2.10                     | 0.66              |
| 3:C:460:CYS:HA   | 3:C:469:ILE:O     | 1.95                     | 0.66              |
| 1:A:183:ILE:CD1  | 1:A:220:MET:SD    | 2.84                     | 0.66              |
| 1:A:49:ARG:HD2   | 1:A:51:ARG:HH21   | 1.60                     | 0.66              |
| 1:A:409:ILE:HG13 | 1:A:443:ILE:CD1   | 2.26                     | 0.66              |
| 1:A:538:PRO:CA   | 1:A:570:GLN:HE22  | 2.08                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:705:LYS:N    | 1:A:757:TYR:HD2  | 1.94                     | 0.66              |
| 1:A:79:ILE:H     | 1:A:79:ILE:HD12  | 1.59                     | 0.66              |
| 3:C:189:HIS:HB3  | 3:C:210:GLU:O    | 1.95                     | 0.66              |
| 1:A:696:ILE:HD11 | 1:A:725:PHE:CE1  | 2.31                     | 0.66              |
| 3:C:582:LEU:O    | 3:C:583:GLY:O    | 2.14                     | 0.66              |
| 1:A:118:ILE:CG2  | 1:A:186:LYS:HE3  | 2.25                     | 0.66              |
| 3:C:711:HIS:O    | 3:C:712:ILE:HG13 | 1.95                     | 0.66              |
| 3:C:507:GLN:HE22 | 3:C:553:SER:N    | 1.94                     | 0.66              |
| 1:A:366:LEU:CD2  | 1:A:439:LEU:HD12 | 2.25                     | 0.65              |
| 4:D:443:SER:HB2  | 4:D:450:LEU:HB2  | 1.77                     | 0.65              |
| 1:A:709:THR:O    | 1:A:710:LEU:HB2  | 1.95                     | 0.65              |
| 1:A:74:GLN:HE22  | 1:A:110:CYS:CA   | 2.07                     | 0.65              |
| 1:A:83:LEU:O     | 1:A:84:GLU:C     | 2.35                     | 0.65              |
| 1:A:688:VAL:O    | 1:A:692:ARG:CG   | 2.45                     | 0.65              |
| 3:C:520:GLN:HG3  | 3:C:529:ILE:CG1  | 2.27                     | 0.65              |
| 3:C:184:ASP:O    | 3:C:187:GLY:N    | 2.30                     | 0.65              |
| 1:A:251:MET:HA   | 1:A:251:MET:CE   | 2.27                     | 0.65              |
| 1:A:96:HIS:O     | 1:A:97:LYS:CB    | 2.44                     | 0.65              |
| 1:A:69:ALA:O     | 1:A:73:VAL:HG23  | 1.97                     | 0.65              |
| 1:A:734:LYS:HA   | 1:A:737:GLU:CD   | 2.18                     | 0.65              |
| 3:C:188:ARG:C    | 3:C:189:HIS:CG   | 2.71                     | 0.65              |
| 3:C:562:THR:O    | 3:C:564:ILE:N    | 2.30                     | 0.65              |
| 1:A:84:GLU:O     | 1:A:87:TYR:N     | 2.29                     | 0.64              |
| 1:A:312:ASP:HB3  | 1:A:343:TYR:OH   | 1.97                     | 0.64              |
| 1:A:54:LEU:CB    | 1:A:55:PRO:HD3   | 2.27                     | 0.64              |
| 3:C:601:TYR:CE2  | 3:C:666:LEU:HD21 | 2.32                     | 0.64              |
| 4:D:119:HIS:O    | 4:D:122:LEU:N    | 2.30                     | 0.64              |
| 3:C:188:ARG:C    | 3:C:189:HIS:CD2  | 2.71                     | 0.64              |
| 1:A:183:ILE:HG21 | 1:A:221:LEU:HD23 | 1.78                     | 0.64              |
| 1:A:249:ARG:HH11 | 1:A:249:ARG:HB3  | 1.62                     | 0.64              |
| 1:A:630:SER:C    | 1:A:632:ALA:H    | 2.01                     | 0.64              |
| 3:C:507:GLN:NE2  | 3:C:553:SER:H    | 1.94                     | 0.64              |
| 1:A:642:SER:CB   | 1:A:643:PRO:HD3  | 2.24                     | 0.64              |
| 2:B:25:LYS:CE    | 2:B:25:LYS:HA    | 2.15                     | 0.64              |
| 1:A:94:CYS:SG    | 1:A:156:LEU:HD13 | 2.37                     | 0.64              |
| 4:D:125:CYS:O    | 4:D:127:GLN:N    | 2.30                     | 0.64              |
| 3:C:926:LEU:CD2  | 4:D:129:PRO:HG3  | 2.28                     | 0.64              |
| 1:A:707:ARG:CD   | 1:A:710:LEU:HD22 | 2.28                     | 0.64              |
| 3:C:184:ASP:O    | 3:C:186:GLN:N    | 2.31                     | 0.63              |
| 4:D:124:GLN:O    | 4:D:124:GLN:CG   | 2.45                     | 0.63              |
| 1:A:197:LEU:HD21 | 1:A:235:PHE:HA   | 1.78                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:119:HIS:O    | 4:D:120:ALA:C    | 2.36                     | 0.63              |
| 1:A:422:LYS:HB3  | 1:A:422:LYS:HZ3  | 1.63                     | 0.63              |
| 1:A:705:LYS:N    | 1:A:757:TYR:CD2  | 2.67                     | 0.63              |
| 1:A:705:LYS:CA   | 1:A:757:TYR:CE2  | 2.82                     | 0.63              |
| 1:A:292:LYS:HD2  | 1:A:292:LYS:O    | 1.99                     | 0.63              |
| 1:A:183:ILE:HG21 | 1:A:221:LEU:CD2  | 2.28                     | 0.63              |
| 1:A:404:LYS:N    | 1:A:405:PRO:HD2  | 2.14                     | 0.63              |
| 3:C:414:ARG:CB   | 3:C:462:ASN:HD21 | 2.12                     | 0.63              |
| 4:D:249:ARG:HE   | 4:D:291:ASP:HB3  | 1.64                     | 0.63              |
| 1:A:108:GLN:HA   | 1:A:111:GLU:HB3  | 1.81                     | 0.63              |
| 2:B:37:ILE:C     | 2:B:37:ILE:CD1   | 2.54                     | 0.63              |
| 1:A:122:ARG:CZ   | 1:A:186:LYS:NZ   | 2.61                     | 0.63              |
| 1:A:118:ILE:HG23 | 1:A:186:LYS:HE3  | 1.80                     | 0.62              |
| 1:A:523:LEU:HD11 | 1:A:525:VAL:HG22 | 1.81                     | 0.62              |
| 1:A:700:ILE:HD13 | 1:A:719:LEU:CD2  | 2.23                     | 0.62              |
| 3:C:482:GLU:OE1  | 3:C:483:PRO:HD3  | 2.00                     | 0.62              |
| 3:C:518:TYR:HD1  | 3:C:519:LEU:N    | 1.95                     | 0.62              |
| 1:A:77:THR:HG22  | 1:A:78:SER:N     | 2.13                     | 0.62              |
| 1:A:757:TYR:O    | 1:A:758:VAL:HB   | 1.99                     | 0.62              |
| 3:C:446:THR:CG2  | 3:C:447:GLU:H    | 2.06                     | 0.62              |
| 3:C:591:ILE:O    | 3:C:592:LEU:HB2  | 2.00                     | 0.62              |
| 1:A:369:LYS:HE2  | 1:A:390:MET:HE3  | 1.82                     | 0.62              |
| 3:C:657:THR:HG21 | 3:C:668:PHE:HB3  | 1.82                     | 0.62              |
| 1:A:726:PRO:O    | 1:A:727:VAL:HB   | 2.00                     | 0.62              |
| 3:C:399:HIS:CE1  | 3:C:703:THR:HG22 | 2.34                     | 0.62              |
| 1:A:609:SER:H    | 1:A:612:GLU:CD   | 2.03                     | 0.62              |
| 3:C:476:VAL:HG13 | 3:C:490:TRP:HB3  | 1.81                     | 0.61              |
| 1:A:126:LEU:O    | 1:A:127:ASP:CG   | 2.38                     | 0.61              |
| 1:A:692:ARG:O    | 1:A:725:PHE:CZ   | 2.52                     | 0.61              |
| 1:A:66:LEU:HD23  | 1:A:86:LEU:HD22  | 1.81                     | 0.61              |
| 1:A:310:LEU:HD22 | 1:A:315:ARG:HB2  | 1.81                     | 0.61              |
| 1:A:57:ASN:O     | 1:A:59:THR:N     | 2.27                     | 0.61              |
| 5:E:10:DG:N2     | 6:F:4:DG:C2      | 2.69                     | 0.61              |
| 1:A:228:LYS:HD3  | 1:A:232:GLU:HG2  | 1.81                     | 0.61              |
| 3:C:562:THR:HG22 | 3:C:563:ASP:N    | 2.16                     | 0.61              |
| 1:A:132:LEU:HD21 | 1:A:192:THR:HA   | 1.83                     | 0.61              |
| 1:A:203:GLU:C    | 1:A:205:SER:H    | 2.03                     | 0.61              |
| 1:A:409:ILE:O    | 1:A:413:VAL:HG23 | 2.00                     | 0.61              |
| 3:C:7:VAL:HG13   | 3:C:1091:GLY:HA3 | 1.81                     | 0.61              |
| 4:D:127:GLN:O    | 4:D:127:GLN:HG2  | 2.00                     | 0.61              |
| 1:A:183:ILE:HD13 | 1:A:221:LEU:HD23 | 1.81                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:624:LEU:CD2  | 1:A:628:LEU:HG   | 2.30                     | 0.61              |
| 1:A:696:ILE:CD1  | 1:A:723:LEU:CD1  | 2.63                     | 0.61              |
| 1:A:570:GLN:HG2  | 2:B:32:LEU:HD11  | 1.81                     | 0.61              |
| 3:C:582:LEU:HD13 | 3:C:583:GLY:H    | 1.65                     | 0.61              |
| 3:C:617:ASN:HD21 | 3:C:619:GLU:HB2  | 1.64                     | 0.61              |
| 1:A:131:PHE:CD1  | 1:A:191:LYS:CD   | 2.84                     | 0.61              |
| 1:A:689:PHE:O    | 1:A:693:GLN:NE2  | 2.33                     | 0.61              |
| 1:A:640:ILE:O    | 1:A:654:PHE:HA   | 2.01                     | 0.61              |
| 3:C:492:GLU:HG3  | 3:C:496:LYS:HB2  | 1.83                     | 0.61              |
| 3:C:927:MET:SD   | 4:D:129:PRO:HB2  | 2.41                     | 0.61              |
| 1:A:83:LEU:O     | 1:A:86:LEU:N     | 2.30                     | 0.60              |
| 1:A:276:THR:HG22 | 1:A:277:TYR:H    | 1.67                     | 0.60              |
| 1:A:340:TRP:HH2  | 1:A:390:MET:HB2  | 1.65                     | 0.60              |
| 1:A:724:LYS:HE2  | 1:A:724:LYS:HA   | 1.82                     | 0.60              |
| 1:A:486:ALA:HA   | 1:A:489:SER:HB2  | 1.83                     | 0.60              |
| 3:C:446:THR:HG22 | 3:C:447:GLU:N    | 2.16                     | 0.60              |
| 1:A:73:VAL:HG12  | 1:A:145:GLN:HB2  | 1.84                     | 0.60              |
| 1:A:538:PRO:HA   | 1:A:570:GLN:NE2  | 2.12                     | 0.60              |
| 1:A:707:ARG:HD2  | 1:A:710:LEU:HD22 | 1.84                     | 0.60              |
| 3:C:889:ARG:HG3  | 3:C:904:ASN:ND2  | 2.16                     | 0.60              |
| 3:C:167:VAL:HG13 | 3:C:180:PHE:HB3  | 1.84                     | 0.60              |
| 1:A:527:ILE:HD11 | 1:A:567:LEU:CD2  | 2.31                     | 0.60              |
| 1:A:587:LYS:CD   | 1:A:587:LYS:H    | 2.15                     | 0.60              |
| 3:C:396:ILE:H    | 3:C:396:ILE:HD13 | 1.66                     | 0.60              |
| 1:A:183:ILE:CG2  | 1:A:221:LEU:CD2  | 2.79                     | 0.60              |
| 1:A:602:PHE:CD2  | 1:A:656:PHE:HB2  | 2.35                     | 0.60              |
| 3:C:573:SER:OG   | 3:C:575:GLU:HB2  | 2.01                     | 0.60              |
| 1:A:51:ARG:H     | 1:A:52:PRO:HD2   | 1.67                     | 0.60              |
| 1:A:589:PHE:CD1  | 1:A:669:ILE:HD11 | 2.37                     | 0.60              |
| 1:A:700:ILE:CD1  | 1:A:719:LEU:CD2  | 2.74                     | 0.60              |
| 1:A:233:LEU:O    | 1:A:234:LYS:C    | 2.39                     | 0.59              |
| 3:C:407:ILE:HG21 | 3:C:410:LEU:HD23 | 1.84                     | 0.59              |
| 3:C:889:ARG:HG3  | 3:C:904:ASN:HD21 | 1.67                     | 0.59              |
| 1:A:707:ARG:O    | 1:A:708:LYS:C    | 2.40                     | 0.59              |
| 1:A:751:ASN:HD22 | 1:A:751:ASN:N    | 2.00                     | 0.59              |
| 3:C:498:ILE:N    | 3:C:498:ILE:HD12 | 2.17                     | 0.59              |
| 1:A:138:CYS:SG   | 1:A:182:ILE:HD11 | 2.42                     | 0.59              |
| 1:A:725:PHE:HB2  | 1:A:726:PRO:HD2  | 1.84                     | 0.59              |
| 3:C:441:GLU:O    | 3:C:441:GLU:HG2  | 2.02                     | 0.59              |
| 1:A:192:THR:O    | 1:A:196:ILE:HG13 | 2.02                     | 0.59              |
| 1:A:417:LEU:HD23 | 1:A:460:ARG:HH12 | 1.66                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:521:ILE:HD12 | 1:A:521:ILE:N    | 2.18                     | 0.59              |
| 3:C:922:LEU:HD23 | 3:C:957:VAL:HG13 | 1.85                     | 0.59              |
| 4:D:110:TYR:CZ   | 4:D:114:LEU:HD11 | 2.37                     | 0.59              |
| 1:A:118:ILE:CD1  | 1:A:181:HIS:CB   | 2.44                     | 0.59              |
| 1:A:454:LYS:HD2  | 1:A:534:PRO:HG3  | 1.83                     | 0.59              |
| 3:C:414:ARG:HB3  | 3:C:462:ASN:HD21 | 1.68                     | 0.59              |
| 3:C:673:LEU:HD23 | 3:C:674:LYS:H    | 1.68                     | 0.59              |
| 1:A:282:THR:O    | 1:A:285:PRO:HD2  | 2.01                     | 0.59              |
| 1:A:405:PRO:O    | 1:A:409:ILE:HG12 | 2.02                     | 0.59              |
| 1:A:699:ALA:HB1  | 1:A:722:GLN:HE22 | 1.64                     | 0.59              |
| 1:A:296:GLY:O    | 1:A:297:GLU:CB   | 2.50                     | 0.59              |
| 3:C:692:ALA:C    | 3:C:693:LEU:HD23 | 2.23                     | 0.59              |
| 1:A:305:LYS:O    | 1:A:305:LYS:HG3  | 2.02                     | 0.58              |
| 1:A:621:ASP:O    | 1:A:625:ARG:HG2  | 2.03                     | 0.58              |
| 3:C:705:ASP:O    | 3:C:706:GLU:CB   | 2.51                     | 0.58              |
| 3:C:851:PHE:HB3  | 3:C:858:LEU:HD22 | 1.85                     | 0.58              |
| 1:A:228:LYS:HA   | 1:A:232:GLU:HB2  | 1.84                     | 0.58              |
| 1:A:665:PHE:O    | 1:A:666:ARG:HB2  | 2.03                     | 0.58              |
| 1:A:692:ARG:HB3  | 1:A:725:PHE:CD2  | 2.38                     | 0.58              |
| 3:C:588:PRO:HB3  | 3:C:604:CYS:SG   | 2.43                     | 0.58              |
| 1:A:228:LYS:CE   | 1:A:232:GLU:HG2  | 2.34                     | 0.58              |
| 3:C:695:ASN:OD1  | 3:C:697:SER:N    | 2.30                     | 0.58              |
| 1:A:601:MET:HB3  | 1:A:608:PHE:HE2  | 1.69                     | 0.58              |
| 1:A:643:PRO:HD2  | 1:A:652:ASP:HA   | 1.86                     | 0.58              |
| 1:A:239:THR:O    | 1:A:241:CYS:N    | 2.36                     | 0.58              |
| 1:A:705:LYS:O    | 1:A:708:LYS:CE   | 2.51                     | 0.58              |
| 3:C:553:SER:O    | 3:C:571:LEU:HD12 | 2.03                     | 0.58              |
| 6:F:5:DT:H73     | 6:F:6:DA:C6      | 2.39                     | 0.58              |
| 1:A:244:ALA:HA   | 1:A:293:GLN:OE1  | 2.03                     | 0.58              |
| 3:C:903:CYS:HB3  | 3:C:942:PHE:CE2  | 2.39                     | 0.58              |
| 1:A:369:LYS:HE2  | 1:A:390:MET:CE   | 2.33                     | 0.58              |
| 1:A:43:LEU:HD12  | 3:C:402:ILE:HD13 | 1.85                     | 0.58              |
| 1:A:708:LYS:HD3  | 1:A:708:LYS:N    | 2.19                     | 0.58              |
| 3:C:704:ILE:H    | 3:C:704:ILE:HD12 | 1.68                     | 0.58              |
| 1:A:228:LYS:HE2  | 1:A:232:GLU:OE2  | 2.03                     | 0.58              |
| 3:C:429:PHE:O    | 3:C:430:VAL:O    | 2.22                     | 0.58              |
| 1:A:240:ASN:ND2  | 1:A:289:CYS:SG   | 2.77                     | 0.57              |
| 1:A:95:SER:O     | 1:A:96:HIS:C     | 2.42                     | 0.57              |
| 1:A:540:GLU:CD   | 1:A:540:GLU:H    | 2.08                     | 0.57              |
| 1:A:249:ARG:CB   | 1:A:249:ARG:HH11 | 2.16                     | 0.57              |
| 3:C:712:ILE:O    | 3:C:712:ILE:HG22 | 2.03                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:429:LEU:O    | 1:A:433:LEU:HB2  | 2.03                     | 0.57              |
| 1:A:528:LEU:HD22 | 1:A:533:TRP:CZ2  | 2.40                     | 0.57              |
| 1:A:657:ASN:HD21 | 1:A:659:GLU:CB   | 2.10                     | 0.57              |
| 3:C:432:GLN:HA   | 3:C:455:GLN:O    | 2.04                     | 0.57              |
| 3:C:669:SER:O    | 3:C:670:ASN:C    | 2.43                     | 0.57              |
| 1:A:468:SER:HB3  | 1:A:471:ALA:HB2  | 1.86                     | 0.57              |
| 3:C:188:ARG:O    | 3:C:189:HIS:CG   | 2.58                     | 0.57              |
| 3:C:414:ARG:HH11 | 3:C:414:ARG:HG2  | 1.69                     | 0.57              |
| 3:C:600:HIS:HB2  | 3:C:616:LEU:O    | 2.04                     | 0.57              |
| 1:A:159:THR:HG22 | 1:A:160:TYR:N    | 2.19                     | 0.57              |
| 4:D:242:CYS:O    | 4:D:254:THR:HG23 | 2.05                     | 0.57              |
| 3:C:536:HIS:HB2  | 3:C:560:LEU:HD13 | 1.87                     | 0.57              |
| 1:A:541:VAL:HG12 | 1:A:618:GLY:O    | 2.05                     | 0.57              |
| 3:C:493:PRO:HB2  | 3:C:494:GLN:HE22 | 1.70                     | 0.57              |
| 3:C:711:HIS:NE2  | 3:C:713:ARG:N    | 2.53                     | 0.57              |
| 1:A:601:MET:CE   | 1:A:616:ALA:HB2  | 2.34                     | 0.57              |
| 3:C:890:LEU:HB3  | 3:C:903:CYS:HB2  | 1.84                     | 0.57              |
| 1:A:197:LEU:HB3  | 1:A:238:GLU:OE1  | 2.04                     | 0.57              |
| 3:C:477:ARG:HG2  | 3:C:489:GLU:HG3  | 1.86                     | 0.56              |
| 3:C:578:HIS:CE1  | 3:C:623:LEU:HD12 | 2.39                     | 0.56              |
| 3:C:185:PRO:HG3  | 4:D:289:ARG:CB   | 2.30                     | 0.56              |
| 1:A:390:MET:O    | 1:A:390:MET:HE2  | 2.05                     | 0.56              |
| 1:A:390:MET:O    | 1:A:394:PHE:HB2  | 2.06                     | 0.56              |
| 1:A:422:LYS:NZ   | 1:A:422:LYS:CB   | 2.59                     | 0.56              |
| 1:A:199:LEU:HD13 | 1:A:209:VAL:CB   | 2.35                     | 0.56              |
| 3:C:454:ASP:N    | 3:C:454:ASP:OD1  | 2.28                     | 0.56              |
| 3:C:562:THR:C    | 3:C:564:ILE:H    | 2.08                     | 0.56              |
| 3:C:433:THR:HG22 | 3:C:434:ARG:H    | 1.68                     | 0.56              |
| 1:A:84:GLU:HG2   | 3:C:499:SER:HB3  | 1.87                     | 0.56              |
| 1:A:49:ARG:CD    | 1:A:51:ARG:HH21  | 2.18                     | 0.56              |
| 3:C:165:ILE:CD1  | 3:C:188:ARG:HH22 | 2.19                     | 0.56              |
| 3:C:389:ILE:HB   | 3:C:713:ARG:HB3  | 1.87                     | 0.56              |
| 3:C:502:SER:O    | 3:C:503:CYS:HB2  | 2.04                     | 0.56              |
| 1:A:129:VAL:CG1  | 1:A:130:LEU:HG   | 2.35                     | 0.56              |
| 3:C:503:CYS:SG   | 3:C:504:ASN:N    | 2.78                     | 0.56              |
| 3:C:430:VAL:HG12 | 3:C:431:GLY:N    | 2.19                     | 0.56              |
| 1:A:676:GLU:HA   | 1:A:680:GLU:OE1  | 2.06                     | 0.56              |
| 3:C:403:ASP:HA   | 3:C:698:THR:HG22 | 1.88                     | 0.56              |
| 1:A:166:THR:O    | 1:A:168:PRO:HD3  | 2.06                     | 0.56              |
| 1:A:751:ASN:C    | 1:A:753:ASN:H    | 2.10                     | 0.56              |
| 3:C:644:LEU:HD12 | 3:C:706:GLU:OE2  | 2.06                     | 0.56              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:D:140:HIS:HB2   | 4:D:453:ASN:HB2  | 1.88                     | 0.55              |
| 1:A:155:PHE:O     | 1:A:159:THR:HB   | 2.06                     | 0.55              |
| 1:A:183:ILE:HG23  | 1:A:221:LEU:HD21 | 1.88                     | 0.55              |
| 1:A:643:PRO:HG2   | 1:A:652:ASP:HA   | 1.88                     | 0.55              |
| 1:A:601:MET:HE3   | 1:A:616:ALA:CB   | 2.36                     | 0.55              |
| 1:A:93:LEU:HD23   | 1:A:93:LEU:O     | 2.05                     | 0.55              |
| 3:C:522:HIS:HB3   | 3:C:523:PRO:HD2  | 1.88                     | 0.55              |
| 3:C:525:GLU:OE2   | 3:C:527:ARG:NH2  | 2.39                     | 0.55              |
| 3:C:433:THR:HG22  | 3:C:434:ARG:N    | 2.22                     | 0.55              |
| 3:C:479:VAL:HG12  | 3:C:480:SER:N    | 2.22                     | 0.55              |
| 1:A:197:LEU:HD21  | 1:A:235:PHE:CA   | 2.37                     | 0.55              |
| 3:C:493:PRO:HB2   | 3:C:494:GLN:NE2  | 2.21                     | 0.55              |
| 1:A:129:VAL:HG13  | 1:A:130:LEU:HG   | 1.89                     | 0.55              |
| 1:A:72:ALA:HB3    | 1:A:79:ILE:HG23  | 1.88                     | 0.55              |
| 3:C:481:GLN:HA    | 3:C:484:LYS:HZ3  | 1.71                     | 0.55              |
| 1:A:227:TYR:HD1   | 1:A:228:LYS:N    | 2.04                     | 0.55              |
| 1:A:292:LYS:HG3   | 1:A:330:ARG:NH2  | 2.22                     | 0.55              |
| 1:A:421:ASN:O     | 1:A:424:ALA:HB2  | 2.07                     | 0.55              |
| 1:A:570:GLN:CG    | 2:B:32:LEU:HD11  | 2.37                     | 0.55              |
| 3:C:502:SER:OG    | 3:C:543:ILE:HG12 | 2.07                     | 0.55              |
| 3:C:659:ILE:HG22  | 3:C:660:TYR:N    | 2.22                     | 0.55              |
| 1:A:267:LEU:HD23  | 1:A:290:VAL:HG11 | 1.87                     | 0.55              |
| 3:C:582:LEU:CD1   | 3:C:583:GLY:H    | 2.19                     | 0.55              |
| 1:A:448:VAL:O     | 1:A:452:PHE:HD1  | 1.90                     | 0.55              |
| 3:C:1000:LEU:HD13 | 3:C:1002:GLU:HB2 | 1.88                     | 0.55              |
| 1:A:472:GLU:HG2   | 1:A:495:PHE:HZ   | 1.72                     | 0.54              |
| 3:C:431:GLY:O     | 3:C:432:GLN:HB3  | 2.07                     | 0.54              |
| 3:C:649:VAL:CG1   | 3:C:650:PHE:H    | 2.17                     | 0.54              |
| 3:C:671:VAL:O     | 3:C:673:LEU:N    | 2.38                     | 0.54              |
| 3:C:644:LEU:CD1   | 3:C:706:GLU:OE2  | 2.55                     | 0.54              |
| 1:A:171:TRP:CZ3   | 1:A:175:LEU:HD11 | 2.42                     | 0.54              |
| 1:A:699:ALA:CB    | 1:A:722:GLN:HE21 | 2.17                     | 0.54              |
| 1:A:733:LYS:O     | 1:A:737:GLU:HG3  | 2.07                     | 0.54              |
| 3:C:448:LEU:HD23  | 3:C:451:PHE:CE2  | 2.42                     | 0.54              |
| 3:C:532:THR:OG1   | 3:C:574:PHE:HD2  | 1.91                     | 0.54              |
| 1:A:107:ARG:HH12  | 1:A:173:MET:HG3  | 1.63                     | 0.54              |
| 1:A:597:LEU:O     | 1:A:598:VAL:C    | 2.45                     | 0.54              |
| 1:A:81:TYR:O      | 1:A:82:ASN:ND2   | 2.41                     | 0.54              |
| 3:C:83:LYS:HB3    | 3:C:1072:PHE:CE2 | 2.42                     | 0.54              |
| 3:C:285:LEU:HB3   | 3:C:297:LEU:HD11 | 1.89                     | 0.54              |
| 3:C:596:PHE:CZ    | 3:C:649:VAL:HG23 | 2.43                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:708:LYS:HD3  | 1:A:708:LYS:H    | 1.72                     | 0.54              |
| 3:C:579:LYS:HG2  | 3:C:581:MET:HE3  | 1.89                     | 0.54              |
| 3:C:602:LEU:O    | 3:C:603:LEU:HD23 | 2.07                     | 0.54              |
| 1:A:630:SER:OG   | 1:A:672:ILE:HD11 | 2.07                     | 0.54              |
| 3:C:518:TYR:CD1  | 3:C:518:TYR:C    | 2.79                     | 0.54              |
| 3:C:532:THR:CG2  | 3:C:533:GLU:N    | 2.69                     | 0.54              |
| 1:A:655:ILE:HD12 | 1:A:655:ILE:N    | 2.23                     | 0.54              |
| 3:C:518:TYR:CD1  | 3:C:519:LEU:N    | 2.75                     | 0.54              |
| 3:C:931:LEU:HD21 | 3:C:944:GLU:HG3  | 1.90                     | 0.54              |
| 1:A:287:ILE:O    | 1:A:291:GLU:HG3  | 2.07                     | 0.53              |
| 1:A:628:LEU:O    | 1:A:630:SER:O    | 2.26                     | 0.53              |
| 1:A:65:LYS:HD2   | 1:A:81:TYR:CD2   | 2.43                     | 0.53              |
| 1:A:84:GLU:O     | 1:A:87:TYR:HB3   | 2.08                     | 0.53              |
| 4:D:124:GLN:HG3  | 4:D:124:GLN:O    | 2.08                     | 0.53              |
| 1:A:316:VAL:CB   | 1:A:317:PRO:HD3  | 2.38                     | 0.53              |
| 3:C:562:THR:C    | 3:C:564:ILE:N    | 2.60                     | 0.53              |
| 1:A:182:ILE:HG22 | 1:A:183:ILE:HG13 | 1.89                     | 0.53              |
| 3:C:184:ASP:HB2  | 3:C:185:PRO:CD   | 2.38                     | 0.53              |
| 1:A:347:PHE:CE1  | 1:A:351:ILE:HD11 | 2.43                     | 0.53              |
| 1:A:267:LEU:HD13 | 1:A:328:ARG:NH1  | 2.22                     | 0.53              |
| 3:C:614:PHE:N    | 3:C:614:PHE:CD1  | 2.75                     | 0.53              |
| 1:A:82:ASN:HD21  | 1:A:85:GLU:CD    | 2.12                     | 0.53              |
| 4:D:299:VAL:HA   | 4:D:326:PRO:HB3  | 1.89                     | 0.53              |
| 6:F:5:DT:H73     | 6:F:6:DA:N6      | 2.24                     | 0.53              |
| 1:A:406:ALA:HB2  | 1:A:443:ILE:HG21 | 1.91                     | 0.53              |
| 1:A:468:SER:HB3  | 1:A:471:ALA:CB   | 2.39                     | 0.53              |
| 1:A:100:PRO:O    | 1:A:104:LYS:HG3  | 2.09                     | 0.53              |
| 1:A:228:LYS:NZ   | 1:A:232:GLU:HG2  | 2.24                     | 0.53              |
| 1:A:731:ASP:O    | 1:A:734:LYS:HB3  | 2.09                     | 0.53              |
| 1:A:676:GLU:O    | 1:A:676:GLU:HG3  | 2.09                     | 0.52              |
| 1:A:239:THR:C    | 1:A:241:CYS:N    | 2.60                     | 0.52              |
| 1:A:227:TYR:O    | 1:A:229:ASP:N    | 2.37                     | 0.52              |
| 1:A:732:LEU:O    | 1:A:733:LYS:C    | 2.45                     | 0.52              |
| 3:C:289:GLU:HA   | 3:C:295:VAL:HA   | 1.89                     | 0.52              |
| 3:C:622:LEU:C    | 3:C:622:LEU:HD12 | 2.29                     | 0.52              |
| 1:A:204:ARG:CZ   | 1:A:243:TYR:CE2  | 2.91                     | 0.52              |
| 1:A:43:LEU:HD11  | 3:C:400:ALA:CB   | 2.12                     | 0.52              |
| 1:A:544:THR:O    | 1:A:547:MET:HB2  | 2.08                     | 0.52              |
| 1:A:642:SER:C    | 1:A:644:LYS:H    | 2.11                     | 0.52              |
| 1:A:227:TYR:C    | 1:A:227:TYR:CD1  | 2.83                     | 0.52              |
| 2:B:37:ILE:HG12  | 2:B:38:VAL:N     | 2.00                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:525:GLU:OE2  | 3:C:527:ARG:NE   | 2.41                     | 0.52              |
| 1:A:587:LYS:HE3  | 1:A:664:LEU:O    | 2.10                     | 0.52              |
| 1:A:709:THR:HG22 | 1:A:710:LEU:N    | 2.25                     | 0.52              |
| 1:A:735:ARG:NE   | 1:A:735:ARG:HA   | 2.24                     | 0.52              |
| 3:C:649:VAL:CG1  | 3:C:650:PHE:N    | 2.71                     | 0.52              |
| 3:C:658:VAL:HG12 | 3:C:658:VAL:O    | 2.09                     | 0.52              |
| 4:D:119:HIS:O    | 4:D:121:GLN:N    | 2.43                     | 0.52              |
| 1:A:352:VAL:HG12 | 1:A:361:MET:SD   | 2.50                     | 0.52              |
| 1:A:120:PRO:O    | 1:A:123:GLU:HG3  | 2.10                     | 0.52              |
| 1:A:625:ARG:O    | 1:A:629:GLN:N    | 2.43                     | 0.52              |
| 1:A:660:PHE:C    | 1:A:662:HIS:H    | 2.14                     | 0.52              |
| 1:A:99:SER:HB2   | 1:A:100:PRO:CD   | 2.35                     | 0.52              |
| 3:C:450:GLY:HA3  | 3:C:479:VAL:HG22 | 1.91                     | 0.52              |
| 3:C:487:VAL:O    | 3:C:488:SER:HB2  | 2.09                     | 0.52              |
| 3:C:659:ILE:HD12 | 3:C:659:ILE:H    | 1.75                     | 0.52              |
| 1:A:643:PRO:CG   | 1:A:652:ASP:HA   | 2.39                     | 0.52              |
| 3:C:218:MET:CE   | 3:C:261:HIS:HD2  | 2.22                     | 0.52              |
| 3:C:402:ILE:O    | 3:C:698:THR:HB   | 2.10                     | 0.52              |
| 1:A:43:LEU:CD1   | 3:C:402:ILE:HD13 | 2.40                     | 0.52              |
| 1:A:657:ASN:ND2  | 1:A:659:GLU:HB2  | 2.11                     | 0.52              |
| 1:A:699:ALA:HB1  | 1:A:722:GLN:HE21 | 1.61                     | 0.52              |
| 1:A:257:PRO:HB3  | 1:A:318:ASP:OD1  | 2.10                     | 0.51              |
| 1:A:299:LEU:HD23 | 1:A:326:PHE:CE2  | 2.45                     | 0.51              |
| 3:C:448:LEU:HD23 | 3:C:451:PHE:HE2  | 1.75                     | 0.51              |
| 3:C:573:SER:O    | 3:C:574:PHE:HB2  | 2.10                     | 0.51              |
| 1:A:609:SER:H    | 1:A:612:GLU:CG   | 2.24                     | 0.51              |
| 3:C:578:HIS:CE1  | 3:C:623:LEU:CD1  | 2.94                     | 0.51              |
| 4:D:217:THR:OG1  | 4:D:254:THR:HG21 | 2.09                     | 0.51              |
| 1:A:516:SER:O    | 1:A:517:ASP:O    | 2.29                     | 0.51              |
| 3:C:408:LYS:HA   | 3:C:678:TYR:CE1  | 2.46                     | 0.51              |
| 3:C:594:THR:CG2  | 3:C:595:THR:N    | 2.73                     | 0.51              |
| 1:A:158:ARG:NH1  | 3:C:633:THR:O    | 2.44                     | 0.51              |
| 1:A:404:LYS:O    | 1:A:405:PRO:C    | 2.49                     | 0.51              |
| 1:A:539:MET:HE3  | 1:A:619:ILE:HA   | 1.91                     | 0.51              |
| 1:A:55:PRO:O     | 1:A:56:ASP:HB2   | 2.11                     | 0.51              |
| 1:A:583:LYS:O    | 1:A:584:GLU:HB2  | 2.10                     | 0.51              |
| 3:C:416:ASP:OD1  | 3:C:418:ASN:HB2  | 2.11                     | 0.51              |
| 3:C:490:TRP:CG   | 3:C:491:LYS:N    | 2.79                     | 0.51              |
| 3:C:711:HIS:CE1  | 3:C:712:ILE:C    | 2.84                     | 0.51              |
| 1:A:107:ARG:HH11 | 1:A:173:MET:HG3  | 1.72                     | 0.51              |
| 1:A:439:LEU:O    | 1:A:440:PHE:C    | 2.49                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:757:TYR:HD1  | 1:A:758:VAL:N     | 2.09                     | 0.51              |
| 3:C:471:ILE:HA   | 3:C:476:VAL:HA    | 1.92                     | 0.51              |
| 1:A:183:ILE:HD13 | 1:A:221:LEU:CD2   | 2.41                     | 0.51              |
| 1:A:501:SER:O    | 1:A:505:MET:HB2   | 2.11                     | 0.51              |
| 3:C:105:HIS:CD2  | 3:C:1067:LYS:HB2  | 2.46                     | 0.51              |
| 3:C:459:PHE:CD2  | 3:C:460:CYS:N     | 2.79                     | 0.51              |
| 3:C:561:TRP:HA   | 3:C:587:ILE:HG21  | 1.92                     | 0.50              |
| 1:A:119:LEU:HB2  | 1:A:120:PRO:CD    | 2.37                     | 0.50              |
| 1:A:228:LYS:CD   | 1:A:232:GLU:HG2   | 2.41                     | 0.50              |
| 1:A:417:LEU:HD23 | 1:A:460:ARG:NH1   | 2.26                     | 0.50              |
| 3:C:184:ASP:OD1  | 3:C:184:ASP:C     | 2.48                     | 0.50              |
| 1:A:131:PHE:CD1  | 1:A:191:LYS:CE    | 2.95                     | 0.50              |
| 1:A:602:PHE:N    | 1:A:602:PHE:CD1   | 2.79                     | 0.50              |
| 3:C:512:VAL:HB   | 3:C:515:ALA:HB3   | 1.94                     | 0.50              |
| 1:A:186:LYS:CB   | 1:A:188:VAL:HG23  | 2.40                     | 0.50              |
| 1:A:45:ILE:HD11  | 3:C:404:LEU:HD21  | 1.92                     | 0.50              |
| 3:C:570:LYS:O    | 3:C:574:PHE:N     | 2.41                     | 0.50              |
| 3:C:613:TYR:CE1  | 3:C:627:LYS:HB2   | 2.47                     | 0.50              |
| 1:A:207:GLU:O    | 1:A:208:ALA:O     | 2.30                     | 0.50              |
| 1:A:96:HIS:O     | 1:A:97:LYS:HB2    | 2.11                     | 0.50              |
| 1:A:380:PHE:CD2  | 1:A:386:PHE:CD2   | 3.00                     | 0.50              |
| 3:C:183:GLN:HA   | 3:C:188:ARG:HA    | 1.94                     | 0.50              |
| 3:C:663:ASN:HD21 | 3:C:1131:LYS:HB3  | 1.76                     | 0.50              |
| 1:A:705:LYS:HA   | 1:A:757:TYR:CE2   | 2.43                     | 0.50              |
| 1:A:135:ILE:CD1  | 1:A:188:VAL:HG12  | 2.30                     | 0.50              |
| 1:A:182:ILE:O    | 1:A:188:VAL:HG11  | 2.12                     | 0.50              |
| 1:A:587:LYS:HD2  | 1:A:587:LYS:N     | 2.25                     | 0.50              |
| 3:C:451:PHE:HD1  | 3:C:470:GLN:HB2   | 1.74                     | 0.50              |
| 1:A:141:ASP:C    | 1:A:143:CYS:N     | 2.64                     | 0.49              |
| 1:A:173:MET:HG2  | 1:A:173:MET:O     | 2.11                     | 0.49              |
| 3:C:492:GLU:CG   | 3:C:496:LYS:HB2   | 2.42                     | 0.49              |
| 1:A:206:GLY:O    | 1:A:207:GLU:O     | 2.30                     | 0.49              |
| 1:A:74:GLN:O     | 1:A:75:SER:C      | 2.49                     | 0.49              |
| 1:A:382:LYS:O    | 1:A:383:ASN:C     | 2.50                     | 0.49              |
| 1:A:601:MET:HE1  | 1:A:616:ALA:HB2   | 1.91                     | 0.49              |
| 1:A:757:TYR:CE1  | 1:A:759:ALA:HA    | 2.37                     | 0.49              |
| 3:C:893:TRP:HE3  | 3:C:899:LEU:HD13  | 1.77                     | 0.49              |
| 1:A:707:ARG:O    | 1:A:709:THR:O     | 2.30                     | 0.49              |
| 1:A:710:LEU:O    | 1:A:711:GLY:O     | 2.30                     | 0.49              |
| 3:C:1054:MET:SD  | 3:C:1129:LEU:HD11 | 2.52                     | 0.49              |
| 3:C:514:ARG:HG3  | 3:C:514:ARG:HH11  | 1.78                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:612:PHE:CE2  | 3:C:628:LYS:HD2  | 2.47                     | 0.49              |
| 3:C:668:PHE:CD1  | 3:C:668:PHE:N    | 2.80                     | 0.49              |
| 3:C:715:VAL:O    | 3:C:715:VAL:HG12 | 2.12                     | 0.49              |
| 4:D:211:SER:HB3  | 4:D:243:VAL:HG13 | 1.94                     | 0.49              |
| 1:A:330:ARG:H    | 1:A:330:ARG:CD   | 2.26                     | 0.49              |
| 1:A:412:HIS:HE1  | 1:A:416:LYS:HE3  | 1.77                     | 0.49              |
| 1:A:82:ASN:OD1   | 1:A:82:ASN:O     | 2.30                     | 0.49              |
| 3:C:704:ILE:O    | 3:C:705:ASP:CB   | 2.57                     | 0.49              |
| 1:A:347:PHE:O    | 1:A:351:ILE:HG13 | 2.12                     | 0.49              |
| 3:C:596:PHE:CE2  | 3:C:659:ILE:HG22 | 2.48                     | 0.49              |
| 3:C:709:LYS:O    | 3:C:710:LEU:O    | 2.30                     | 0.49              |
| 4:D:256:ASP:OD2  | 4:D:260:ARG:HB2  | 2.13                     | 0.49              |
| 1:A:457:LEU:HD22 | 1:A:461:LEU:HD12 | 1.94                     | 0.49              |
| 3:C:594:THR:HG23 | 3:C:595:THR:N    | 2.28                     | 0.49              |
| 3:C:596:PHE:HZ   | 3:C:649:VAL:HG23 | 1.78                     | 0.49              |
| 4:D:111:LYS:HE2  | 4:D:118:ILE:CB   | 2.43                     | 0.49              |
| 1:A:203:GLU:O    | 1:A:205:SER:N    | 2.45                     | 0.49              |
| 1:A:469:VAL:HG12 | 1:A:473:LYS:HE3  | 1.94                     | 0.49              |
| 1:A:696:ILE:CD1  | 1:A:725:PHE:CZ   | 2.93                     | 0.49              |
| 3:C:490:TRP:CD2  | 3:C:491:LYS:N    | 2.81                     | 0.49              |
| 1:A:197:LEU:CD2  | 1:A:235:PHE:CA   | 2.80                     | 0.49              |
| 1:A:440:PHE:CE2  | 1:A:446:LYS:HD3  | 2.47                     | 0.49              |
| 2:B:21:ARG:O     | 2:B:22:PHE:CD1   | 2.66                     | 0.49              |
| 3:C:578:HIS:HD2  | 3:C:623:LEU:H    | 1.55                     | 0.49              |
| 1:A:124:ASP:N    | 1:A:124:ASP:OD1  | 2.46                     | 0.49              |
| 1:A:49:ARG:CD    | 1:A:51:ARG:NH2   | 2.75                     | 0.49              |
| 1:A:726:PRO:O    | 1:A:727:VAL:CB   | 2.60                     | 0.49              |
| 1:A:649:GLU:HB2  | 1:A:652:ASP:OD2  | 2.13                     | 0.48              |
| 3:C:731:GLN:HA   | 3:C:796:GLN:HE21 | 1.78                     | 0.48              |
| 1:A:300:THR:O    | 1:A:304:GLN:HB2  | 2.13                     | 0.48              |
| 1:A:57:ASN:C     | 1:A:59:THR:H     | 2.14                     | 0.48              |
| 1:A:601:MET:HE1  | 1:A:613:ILE:HA   | 1.95                     | 0.48              |
| 1:A:751:ASN:ND2  | 1:A:751:ASN:O    | 2.46                     | 0.48              |
| 3:C:587:ILE:HD12 | 3:C:587:ILE:H    | 1.78                     | 0.48              |
| 3:C:770:LEU:HD13 | 3:C:865:GLU:HB2  | 1.96                     | 0.48              |
| 4:D:272:PHE:HE2  | 4:D:312:LYS:HA   | 1.78                     | 0.48              |
| 1:A:63:TRP:HH2   | 1:A:102:LEU:CA   | 2.25                     | 0.48              |
| 1:A:92:ASN:ND2   | 3:C:408:LYS:NZ   | 2.61                     | 0.48              |
| 3:C:182:TYR:O    | 3:C:188:ARG:CA   | 2.61                     | 0.48              |
| 3:C:571:LEU:O    | 3:C:572:PRO:C    | 2.50                     | 0.48              |
| 3:C:641:PHE:CE2  | 3:C:650:PHE:HB2  | 2.48                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:131:PHE:CE2  | 1:A:188:VAL:CG1   | 2.91                     | 0.48              |
| 1:A:197:LEU:HD11 | 1:A:234:LYS:HB3   | 1.94                     | 0.48              |
| 1:A:457:LEU:O    | 1:A:460:ARG:N     | 2.47                     | 0.48              |
| 1:A:82:ASN:O     | 1:A:83:LEU:O      | 2.31                     | 0.48              |
| 2:B:38:VAL:O     | 2:B:39:VAL:O      | 2.30                     | 0.48              |
| 1:A:206:GLY:O    | 1:A:207:GLU:C     | 2.51                     | 0.48              |
| 3:C:1136:LEU:O   | 3:C:1139:ILE:HG12 | 2.13                     | 0.48              |
| 3:C:565:SER:OG   | 3:C:567:ARG:NH1   | 2.46                     | 0.48              |
| 3:C:602:LEU:HD13 | 3:C:602:LEU:C     | 2.33                     | 0.48              |
| 3:C:641:PHE:HB2  | 3:C:681:PRO:HG3   | 1.94                     | 0.48              |
| 3:C:659:ILE:O    | 3:C:660:TYR:HB3   | 2.14                     | 0.48              |
| 1:A:515:GLN:O    | 1:A:515:GLN:HG2   | 2.14                     | 0.48              |
| 1:A:541:VAL:HG23 | 1:A:543:LEU:CD2   | 2.43                     | 0.48              |
| 3:C:443:VAL:HG12 | 3:C:443:VAL:O     | 2.13                     | 0.48              |
| 1:A:315:ARG:O    | 1:A:319:LEU:HG    | 2.14                     | 0.48              |
| 3:C:1109:VAL:O   | 3:C:1111:ASN:N    | 2.42                     | 0.48              |
| 1:A:624:LEU:HD22 | 1:A:628:LEU:CD1   | 2.44                     | 0.48              |
| 1:A:751:ASN:ND2  | 1:A:751:ASN:N     | 2.61                     | 0.48              |
| 3:C:218:MET:HE2  | 3:C:261:HIS:HD2   | 1.79                     | 0.48              |
| 3:C:457:THR:HG22 | 3:C:458:PHE:N     | 2.29                     | 0.48              |
| 1:A:401:ARG:NH2  | 1:A:404:LYS:HG3   | 2.29                     | 0.48              |
| 1:A:448:VAL:O    | 1:A:451:ALA:HB3   | 2.14                     | 0.48              |
| 1:A:692:ARG:HB3  | 1:A:725:PHE:HE2   | 1.69                     | 0.48              |
| 1:A:719:LEU:HD22 | 1:A:723:LEU:HD21  | 1.96                     | 0.48              |
| 1:A:82:ASN:O     | 1:A:82:ASN:CG     | 2.53                     | 0.48              |
| 1:A:106:LEU:HD22 | 1:A:153:PHE:CD2   | 2.49                     | 0.47              |
| 1:A:529:THR:HA   | 2:B:33:TRP:CD1    | 2.49                     | 0.47              |
| 1:A:629:GLN:O    | 1:A:633:CYS:HB2   | 2.14                     | 0.47              |
| 1:A:450:GLU:OE2  | 1:A:454:LYS:HE3   | 2.14                     | 0.47              |
| 1:A:544:THR:HG23 | 1:A:545:PRO:HD2   | 1.96                     | 0.47              |
| 3:C:184:ASP:O    | 3:C:185:PRO:C     | 2.50                     | 0.47              |
| 3:C:459:PHE:O    | 3:C:460:CYS:HB3   | 2.13                     | 0.47              |
| 3:C:479:VAL:CG1  | 3:C:480:SER:N     | 2.77                     | 0.47              |
| 4:D:394:PRO:HB3  | 4:D:402:ASP:HB3   | 1.96                     | 0.47              |
| 1:A:248:GLN:O    | 1:A:249:ARG:C     | 2.52                     | 0.47              |
| 1:A:70:VAL:HG21  | 1:A:106:LEU:HD13  | 1.95                     | 0.47              |
| 1:A:73:VAL:C     | 1:A:74:GLN:O      | 2.45                     | 0.47              |
| 1:A:748:ASP:C    | 1:A:750:ASP:H     | 2.17                     | 0.47              |
| 3:C:459:PHE:CG   | 3:C:460:CYS:N     | 2.82                     | 0.47              |
| 1:A:251:MET:HE3  | 1:A:251:MET:HA    | 1.97                     | 0.47              |
| 1:A:417:LEU:CD2  | 1:A:460:ARG:HH12  | 2.27                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:587:ILE:HD12 | 3:C:587:ILE:N    | 2.29                     | 0.47              |
| 1:A:341:SER:HB3  | 1:A:389:LEU:HD12 | 1.97                     | 0.47              |
| 1:A:588:GLU:O    | 1:A:666:ARG:HA   | 2.15                     | 0.47              |
| 3:C:1048:TYR:O   | 3:C:1052:LEU:HB2 | 2.15                     | 0.47              |
| 3:C:450:GLY:O    | 3:C:477:ARG:NH2  | 2.46                     | 0.47              |
| 3:C:679:MET:SD   | 3:C:679:MET:C    | 2.93                     | 0.47              |
| 1:A:170:ILE:O    | 1:A:173:MET:HB3  | 2.14                     | 0.47              |
| 1:A:196:ILE:HG21 | 1:A:231:PHE:CE1  | 2.50                     | 0.47              |
| 1:A:241:CYS:O    | 1:A:244:ALA:HB3  | 2.15                     | 0.47              |
| 1:A:308:ASP:OD1  | 1:A:343:TYR:HD2  | 1.97                     | 0.47              |
| 3:C:189:HIS:CD2  | 3:C:189:HIS:N    | 2.83                     | 0.47              |
| 3:C:433:THR:O    | 3:C:434:ARG:HG3  | 2.14                     | 0.47              |
| 3:C:657:THR:HG22 | 3:C:658:VAL:N    | 2.25                     | 0.47              |
| 3:C:663:ASN:HD21 | 3:C:1131:LYS:CB  | 2.27                     | 0.47              |
| 1:A:627:THR:O    | 1:A:631:LEU:HD23 | 2.14                     | 0.47              |
| 1:A:641:LYS:HE2  | 1:A:647:GLU:O    | 2.14                     | 0.47              |
| 1:A:74:GLN:HA    | 1:A:145:GLN:NE2  | 2.30                     | 0.47              |
| 1:A:437:MET:HE3  | 1:A:478:LYS:HD2  | 1.96                     | 0.47              |
| 1:A:482:GLU:O    | 1:A:483:CYS:HB2  | 2.14                     | 0.47              |
| 1:A:707:ARG:HD3  | 1:A:710:LEU:HD13 | 1.96                     | 0.47              |
| 1:A:638:VAL:HG12 | 1:A:639:LEU:CD2  | 2.31                     | 0.47              |
| 1:A:660:PHE:C    | 1:A:662:HIS:N    | 2.67                     | 0.47              |
| 1:A:95:SER:O     | 1:A:96:HIS:O     | 2.33                     | 0.47              |
| 3:C:579:LYS:HE3  | 3:C:581:MET:CE   | 2.45                     | 0.47              |
| 3:C:385:GLY:HA3  | 3:C:719:GLU:O    | 2.14                     | 0.47              |
| 1:A:757:TYR:CD1  | 1:A:758:VAL:N    | 2.82                     | 0.47              |
| 3:C:403:ASP:O    | 3:C:405:PRO:HD3  | 2.15                     | 0.47              |
| 3:C:43:VAL:HG21  | 3:C:50:ARG:CZ    | 2.45                     | 0.47              |
| 1:A:263:VAL:HG11 | 1:A:295:LEU:HD21 | 1.97                     | 0.46              |
| 3:C:638:LEU:O    | 3:C:639:ARG:HG2  | 2.15                     | 0.46              |
| 3:C:643:SER:OG   | 3:C:644:LEU:N    | 2.47                     | 0.46              |
| 3:C:438:LEU:CD1  | 3:C:684:SER:HB2  | 2.46                     | 0.46              |
| 1:A:592:SER:HB2  | 1:A:673:GLN:NE2  | 2.29                     | 0.46              |
| 1:A:696:ILE:CG1  | 1:A:725:PHE:HZ   | 2.28                     | 0.46              |
| 1:A:732:LEU:O    | 1:A:735:ARG:N    | 2.45                     | 0.46              |
| 3:C:1055:GLN:NE2 | 3:C:1090:ASP:H   | 2.09                     | 0.46              |
| 3:C:407:ILE:CD1  | 3:C:699:LEU:HB2  | 2.44                     | 0.46              |
| 3:C:531:HIS:ND1  | 3:C:532:THR:N    | 2.63                     | 0.46              |
| 3:C:704:ILE:N    | 3:C:704:ILE:HD12 | 2.30                     | 0.46              |
| 1:A:196:ILE:HD13 | 1:A:218:LEU:HD23 | 1.93                     | 0.46              |
| 1:A:204:ARG:NE   | 1:A:243:TYR:OH   | 2.48                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:396:ILE:O    | 3:C:396:ILE:HD13 | 2.15                     | 0.46              |
| 3:C:596:PHE:CZ   | 3:C:659:ILE:HG22 | 2.50                     | 0.46              |
| 1:A:321:GLN:O    | 1:A:325:LEU:HD12 | 2.16                     | 0.46              |
| 1:A:630:SER:C    | 1:A:632:ALA:N    | 2.67                     | 0.46              |
| 3:C:402:ILE:HG22 | 3:C:403:ASP:H    | 1.80                     | 0.46              |
| 3:C:656:PRO:HG2  | 3:C:676:VAL:HG23 | 1.97                     | 0.46              |
| 1:A:83:LEU:O     | 1:A:85:GLU:N     | 2.49                     | 0.46              |
| 1:A:200:ILE:O    | 1:A:203:GLU:N    | 2.25                     | 0.46              |
| 1:A:303:LEU:HD23 | 1:A:322:MET:CE   | 2.46                     | 0.46              |
| 1:A:440:PHE:CZ   | 1:A:446:LYS:HD3  | 2.51                     | 0.46              |
| 1:A:705:LYS:HD3  | 1:A:705:LYS:C    | 2.35                     | 0.46              |
| 3:C:312:GLU:HG3  | 3:C:327:ARG:HD2  | 1.98                     | 0.46              |
| 3:C:414:ARG:HB3  | 3:C:462:ASN:ND2  | 2.29                     | 0.46              |
| 3:C:695:ASN:OD1  | 3:C:698:THR:N    | 2.41                     | 0.46              |
| 1:A:113:HIS:O    | 1:A:117:GLN:HG2  | 2.16                     | 0.46              |
| 1:A:534:PRO:HB2  | 1:A:536:TYR:CE1  | 2.51                     | 0.46              |
| 3:C:23:PHE:N     | 3:C:30:ASN:ND2   | 2.59                     | 0.46              |
| 3:C:953:TRP:HB2  | 3:C:970:ASN:HB2  | 1.98                     | 0.46              |
| 1:A:130:LEU:O    | 1:A:131:PHE:C    | 2.54                     | 0.46              |
| 1:A:131:PHE:CZ   | 1:A:188:VAL:HG22 | 2.51                     | 0.46              |
| 1:A:375:VAL:HG13 | 1:A:379:CYS:HB2  | 1.98                     | 0.46              |
| 1:A:587:LYS:HD3  | 1:A:660:PHE:CE2  | 2.51                     | 0.46              |
| 3:C:442:GLU:HG3  | 3:C:443:VAL:H    | 1.81                     | 0.46              |
| 3:C:512:VAL:O    | 3:C:515:ALA:HB3  | 2.15                     | 0.46              |
| 3:C:407:ILE:HD11 | 3:C:699:LEU:HB2  | 1.98                     | 0.46              |
| 3:C:889:ARG:HD2  | 3:C:891:TYR:CZ   | 2.51                     | 0.46              |
| 1:A:193:ILE:C    | 1:A:195:GLY:N    | 2.68                     | 0.45              |
| 1:A:491:LEU:HA   | 1:A:494:MET:CG   | 2.33                     | 0.45              |
| 1:A:92:ASN:ND2   | 3:C:408:LYS:HZ1  | 2.14                     | 0.45              |
| 6:F:5:DT:C7      | 6:F:6:DA:C6      | 2.99                     | 0.45              |
| 1:A:267:LEU:CD2  | 1:A:290:VAL:HG11 | 2.46                     | 0.45              |
| 1:A:587:LYS:HB2  | 1:A:660:PHE:CE2  | 2.51                     | 0.45              |
| 1:A:632:ALA:O    | 1:A:633:CYS:C    | 2.55                     | 0.45              |
| 3:C:490:TRP:O    | 3:C:491:LYS:HB2  | 2.15                     | 0.45              |
| 3:C:705:ASP:O    | 3:C:706:GLU:HB3  | 2.16                     | 0.45              |
| 3:C:869:ALA:H    | 3:C:885:ASN:ND2  | 2.14                     | 0.45              |
| 1:A:179:ARG:O    | 1:A:184:SER:HB3  | 2.16                     | 0.45              |
| 1:A:202:ARG:HH21 | 1:A:207:GLU:CD   | 2.19                     | 0.45              |
| 1:A:341:SER:CB   | 1:A:389:LEU:HD12 | 2.46                     | 0.45              |
| 1:A:433:LEU:HD23 | 1:A:478:LYS:HE3  | 1.97                     | 0.45              |
| 1:A:601:MET:CE   | 1:A:616:ALA:HB3  | 2.40                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:396:ILE:CD1  | 3:C:396:ILE:N    | 2.79                     | 0.45              |
| 3:C:411:TRP:HB2  | 3:C:460:CYS:SG   | 2.56                     | 0.45              |
| 1:A:303:LEU:HD13 | 1:A:339:HIS:CD2  | 2.52                     | 0.45              |
| 1:A:527:ILE:CG2  | 1:A:527:ILE:O    | 2.65                     | 0.45              |
| 1:A:55:PRO:O     | 1:A:56:ASP:CB    | 2.64                     | 0.45              |
| 2:B:20:LYS:HB2   | 2:B:20:LYS:HE3   | 1.72                     | 0.45              |
| 4:D:122:LEU:O    | 4:D:123:ARG:C    | 2.54                     | 0.45              |
| 1:A:100:PRO:HG3  | 1:A:160:TYR:CZ   | 2.51                     | 0.45              |
| 1:A:704:MET:O    | 1:A:757:TYR:HD2  | 2.00                     | 0.45              |
| 2:B:38:VAL:O     | 2:B:39:VAL:C     | 2.55                     | 0.45              |
| 1:A:196:ILE:HG21 | 1:A:218:LEU:HD21 | 1.99                     | 0.45              |
| 3:C:312:GLU:HG3  | 3:C:327:ARG:CD   | 2.47                     | 0.45              |
| 1:A:271:GLY:C    | 1:A:273:ARG:H    | 2.20                     | 0.45              |
| 1:A:292:LYS:O    | 1:A:293:GLN:HG2  | 2.17                     | 0.45              |
| 1:A:295:LEU:HD11 | 1:A:325:LEU:HD22 | 1.99                     | 0.45              |
| 2:B:37:ILE:H     | 2:B:37:ILE:HD12  | 1.82                     | 0.45              |
| 3:C:659:ILE:CG2  | 3:C:660:TYR:N    | 2.80                     | 0.45              |
| 3:C:921:ILE:HB   | 3:C:933:LEU:HB2  | 1.99                     | 0.45              |
| 4:D:123:ARG:HA   | 4:D:126:LEU:HD12 | 1.97                     | 0.45              |
| 3:C:663:ASN:HD21 | 3:C:1131:LYS:HG2 | 1.81                     | 0.45              |
| 1:A:114:VAL:O    | 1:A:117:GLN:N    | 2.50                     | 0.45              |
| 1:A:141:ASP:OD2  | 1:A:144:ARG:NH2  | 2.46                     | 0.45              |
| 1:A:200:ILE:O    | 1:A:202:ARG:N    | 2.50                     | 0.45              |
| 1:A:203:GLU:C    | 1:A:205:SER:N    | 2.70                     | 0.45              |
| 1:A:460:ARG:NH1  | 1:A:472:GLU:OE2  | 2.49                     | 0.45              |
| 1:A:539:MET:HE1  | 1:A:619:ILE:HG23 | 1.99                     | 0.45              |
| 1:A:580:ALA:HB2  | 2:B:22:PHE:HE1   | 1.82                     | 0.45              |
| 3:C:478:LEU:HB3  | 3:C:488:SER:HB3  | 1.99                     | 0.45              |
| 3:C:926:LEU:HD21 | 4:D:129:PRO:HG3  | 1.99                     | 0.45              |
| 1:A:264:SER:O    | 1:A:268:GLU:HG2  | 2.17                     | 0.45              |
| 1:A:329:VAL:CG1  | 1:A:330:ARG:H    | 2.23                     | 0.45              |
| 1:A:437:MET:HE2  | 1:A:475:MET:HE1  | 1.99                     | 0.45              |
| 2:B:19:LYS:CE    | 2:B:19:LYS:HA    | 2.35                     | 0.45              |
| 3:C:390:ILE:HG22 | 3:C:391:ARG:N    | 2.32                     | 0.45              |
| 3:C:597:GLU:O    | 3:C:598:SER:HB3  | 2.16                     | 0.45              |
| 3:C:607:GLY:HA2  | 3:C:635:PRO:HB3  | 1.99                     | 0.45              |
| 1:A:434:ASP:O    | 1:A:438:ILE:HG13 | 2.18                     | 0.44              |
| 1:A:601:MET:HB3  | 1:A:608:PHE:CE2  | 2.49                     | 0.44              |
| 1:A:61:ASP:O     | 1:A:65:LYS:HG3   | 2.17                     | 0.44              |
| 1:A:668:LYS:NZ   | 1:A:670:ASN:HB3  | 2.32                     | 0.44              |
| 1:A:710:LEU:O    | 1:A:711:GLY:C    | 2.55                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:93:LEU:CD2    | 1:A:93:LEU:C     | 2.82                     | 0.44              |
| 4:D:388:ILE:O     | 4:D:408:ILE:HA   | 2.17                     | 0.44              |
| 1:A:227:TYR:CD1   | 1:A:228:LYS:N    | 2.83                     | 0.44              |
| 1:A:526:ASN:HD22  | 1:A:526:ASN:HA   | 1.61                     | 0.44              |
| 1:A:70:VAL:O      | 1:A:72:ALA:N     | 2.50                     | 0.44              |
| 3:C:707:ILE:HG23  | 3:C:708:GLN:H    | 1.80                     | 0.44              |
| 1:A:183:ILE:CD1   | 1:A:220:MET:CE   | 2.75                     | 0.44              |
| 1:A:274:VAL:CG1   | 1:A:283:GLN:HE21 | 2.23                     | 0.44              |
| 3:C:1057:ARG:HH12 | 3:C:1110:ALA:HB3 | 1.83                     | 0.44              |
| 3:C:476:VAL:HG22  | 3:C:526:LEU:CD1  | 2.47                     | 0.44              |
| 3:C:580:GLU:OE2   | 3:C:626:ARG:HD2  | 2.17                     | 0.44              |
| 3:C:740:ILE:HG23  | 3:C:785:GLU:HG3  | 1.99                     | 0.44              |
| 1:A:256:VAL:O     | 1:A:257:PRO:C    | 2.56                     | 0.44              |
| 1:A:349:THR:C     | 1:A:351:ILE:H    | 2.21                     | 0.44              |
| 1:A:610:PHE:CE1   | 1:A:614:LYS:HE3  | 2.52                     | 0.44              |
| 3:C:451:PHE:HE1   | 3:C:470:GLN:HB2  | 1.79                     | 0.44              |
| 3:C:528:GLN:HG2   | 3:C:528:GLN:O    | 2.16                     | 0.44              |
| 3:C:546:LEU:O     | 3:C:549:SER:HB3  | 2.17                     | 0.44              |
| 1:A:696:ILE:HG12  | 1:A:725:PHE:HZ   | 1.81                     | 0.44              |
| 3:C:629:VAL:HG23  | 3:C:630:THR:N    | 2.31                     | 0.44              |
| 1:A:453:TYR:C     | 1:A:453:TYR:CD1  | 2.91                     | 0.44              |
| 3:C:165:ILE:HG13  | 3:C:188:ARG:NH1  | 2.33                     | 0.44              |
| 3:C:447:GLU:O     | 3:C:448:LEU:HD12 | 2.18                     | 0.44              |
| 3:C:586:ILE:HG22  | 3:C:607:GLY:H    | 1.83                     | 0.44              |
| 3:C:692:ALA:O     | 3:C:693:LEU:HD23 | 2.18                     | 0.44              |
| 3:C:81:THR:HG21   | 3:C:85:ASN:ND2   | 2.22                     | 0.44              |
| 1:A:184:SER:O     | 1:A:186:LYS:N    | 2.50                     | 0.44              |
| 1:A:758:VAL:O     | 1:A:758:VAL:HG12 | 2.17                     | 0.44              |
| 1:A:90:VAL:O      | 1:A:92:ASN:N     | 2.51                     | 0.44              |
| 1:A:143:CYS:O     | 1:A:147:ILE:HG13 | 2.17                     | 0.44              |
| 1:A:222:SER:O     | 1:A:224:LEU:N    | 2.51                     | 0.44              |
| 1:A:251:MET:HE3   | 1:A:259:TYR:CE1  | 2.53                     | 0.44              |
| 3:C:396:ILE:N     | 3:C:396:ILE:HD13 | 2.29                     | 0.44              |
| 3:C:641:PHE:HB3   | 3:C:679:MET:HE1  | 1.99                     | 0.44              |
| 1:A:70:VAL:CG2    | 1:A:106:LEU:HD11 | 2.47                     | 0.43              |
| 1:A:65:LYS:HD2    | 1:A:81:TYR:HD2   | 1.82                     | 0.43              |
| 4:D:382:HIS:CG    | 4:D:383:PRO:HD2  | 2.53                     | 0.43              |
| 1:A:307:LEU:O     | 1:A:308:ASP:C    | 2.56                     | 0.43              |
| 1:A:704:MET:HG3   | 1:A:745:MET:CE   | 2.48                     | 0.43              |
| 1:A:412:HIS:CE1   | 1:A:416:LYS:HE3  | 2.53                     | 0.43              |
| 1:A:693:GLN:O     | 1:A:696:ILE:HB   | 2.18                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:430:VAL:O    | 3:C:456:GLN:HB2   | 2.18                     | 0.43              |
| 3:C:532:THR:CG2  | 3:C:533:GLU:H     | 2.31                     | 0.43              |
| 1:A:725:PHE:HB2  | 1:A:726:PRO:CD    | 2.47                     | 0.43              |
| 1:A:90:VAL:O     | 1:A:94:CYS:N      | 2.42                     | 0.43              |
| 3:C:419:ARG:HD3  | 3:C:421:THR:O     | 2.18                     | 0.43              |
| 3:C:429:PHE:O    | 3:C:456:GLN:HG3   | 2.18                     | 0.43              |
| 3:C:582:LEU:CD1  | 3:C:583:GLY:N     | 2.81                     | 0.43              |
| 3:C:663:ASN:HD21 | 3:C:1131:LYS:CG   | 2.30                     | 0.43              |
| 3:C:893:TRP:CE3  | 3:C:899:LEU:HD13  | 2.54                     | 0.43              |
| 1:A:617:THR:OG1  | 1:A:618:GLY:N     | 2.50                     | 0.43              |
| 1:A:704:MET:O    | 1:A:757:TYR:HB2   | 2.18                     | 0.43              |
| 1:A:712:HIS:C    | 1:A:712:HIS:CD2   | 2.90                     | 0.43              |
| 3:C:185:PRO:HB2  | 3:C:186:GLN:NE2   | 2.33                     | 0.43              |
| 1:A:149:ILE:O    | 1:A:150:ARG:C     | 2.56                     | 0.43              |
| 1:A:193:ILE:C    | 1:A:195:GLY:H     | 2.22                     | 0.43              |
| 1:A:183:ILE:CG2  | 1:A:221:LEU:HD21  | 2.48                     | 0.43              |
| 1:A:428:GLU:O    | 1:A:432:THR:HG23  | 2.18                     | 0.43              |
| 1:A:545:PRO:O    | 1:A:546:GLU:C     | 2.56                     | 0.43              |
| 3:C:184:ASP:C    | 3:C:186:GLN:N     | 2.72                     | 0.43              |
| 3:C:428:SER:OG   | 3:C:456:GLN:HG2   | 2.18                     | 0.43              |
| 3:C:586:ILE:HG21 | 3:C:608:ASP:N     | 2.34                     | 0.43              |
| 5:E:10:DG:C2     | 6:F:4:DG:C2       | 3.06                     | 0.43              |
| 1:A:390:MET:HE2  | 1:A:390:MET:C     | 2.38                     | 0.43              |
| 1:A:523:LEU:HD11 | 1:A:525:VAL:CG2   | 2.49                     | 0.43              |
| 1:A:63:TRP:CH2   | 1:A:102:LEU:HG    | 2.53                     | 0.43              |
| 3:C:532:THR:HG22 | 3:C:533:GLU:H     | 1.80                     | 0.43              |
| 4:D:279:ALA:HB1  | 4:D:299:VAL:HG22  | 2.01                     | 0.43              |
| 1:A:440:PHE:O    | 1:A:442:PHE:N     | 2.51                     | 0.43              |
| 1:A:450:GLU:HG3  | 1:A:451:ALA:N     | 2.34                     | 0.43              |
| 4:D:383:PRO:HG3  | 4:D:435:SER:O     | 2.18                     | 0.43              |
| 1:A:279:ASP:O    | 1:A:281:SER:N     | 2.52                     | 0.43              |
| 1:A:311:LEU:HD11 | 1:A:340:TRP:HD1   | 1.84                     | 0.43              |
| 3:C:1097:PHE:O   | 3:C:1100:ILE:HG12 | 2.19                     | 0.43              |
| 3:C:889:ARG:CD   | 3:C:901:THR:HB    | 2.45                     | 0.43              |
| 1:A:555:LYS:HD2  | 1:A:569:TRP:CZ3   | 2.47                     | 0.42              |
| 1:A:583:LYS:O    | 1:A:584:GLU:CB    | 2.66                     | 0.42              |
| 1:A:84:GLU:O     | 1:A:85:GLU:C      | 2.57                     | 0.42              |
| 3:C:407:ILE:HD13 | 3:C:699:LEU:HD23  | 2.01                     | 0.42              |
| 1:A:131:PHE:CZ   | 1:A:188:VAL:CB    | 2.75                     | 0.42              |
| 3:C:494:GLN:O    | 3:C:495:ALA:HB3   | 2.19                     | 0.42              |
| 3:C:505:SER:OG   | 3:C:506:SER:N     | 2.51                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:565:SER:HB2  | 3:C:581:MET:HE2  | 2.01                     | 0.42              |
| 3:C:657:THR:CG2  | 3:C:668:PHE:HB3  | 2.48                     | 0.42              |
| 4:D:367:PRO:HG2  | 4:D:392:ARG:HG3  | 2.01                     | 0.42              |
| 1:A:437:MET:O    | 1:A:440:PHE:HB3  | 2.19                     | 0.42              |
| 1:A:592:SER:OG   | 1:A:595:GLN:HG3  | 2.19                     | 0.42              |
| 1:A:609:SER:O    | 1:A:610:PHE:C    | 2.57                     | 0.42              |
| 1:A:542:HIS:HB2  | 1:A:617:THR:HA   | 2.00                     | 0.42              |
| 1:A:696:ILE:CG1  | 1:A:725:PHE:CZ   | 3.01                     | 0.42              |
| 3:C:500:VAL:HG12 | 3:C:541:LEU:HD12 | 2.01                     | 0.42              |
| 3:C:603:LEU:HD23 | 3:C:603:LEU:N    | 2.33                     | 0.42              |
| 1:A:141:ASP:O    | 1:A:145:GLN:HG2  | 2.19                     | 0.42              |
| 1:A:399:ASN:ND2  | 1:A:444:HIS:CE1  | 2.87                     | 0.42              |
| 1:A:541:VAL:HG23 | 1:A:543:LEU:HD21 | 2.02                     | 0.42              |
| 3:C:611:LEU:HD23 | 3:C:611:LEU:C    | 2.40                     | 0.42              |
| 4:D:323:HIS:CD2  | 4:D:342:THR:HG21 | 2.53                     | 0.42              |
| 4:D:391:GLY:HA3  | 4:D:429:ILE:O    | 2.19                     | 0.42              |
| 1:A:122:ARG:CZ   | 1:A:186:LYS:HZ1  | 2.30                     | 0.42              |
| 1:A:496:LYS:HA   | 1:A:496:LYS:HD3  | 1.84                     | 0.42              |
| 3:C:1030:PHE:CZ  | 3:C:1038:GLY:HA3 | 2.55                     | 0.42              |
| 5:E:4:DA:C2      | 6:F:10:DA:C2     | 3.07                     | 0.42              |
| 1:A:110:CYS:O    | 1:A:111:GLU:C    | 2.58                     | 0.42              |
| 1:A:425:THR:HG22 | 1:A:426:ASP:N    | 2.35                     | 0.42              |
| 1:A:555:LYS:HB2  | 1:A:569:TRP:HH2  | 1.84                     | 0.42              |
| 1:A:578:LEU:HD13 | 1:A:591:VAL:HG21 | 1.99                     | 0.42              |
| 1:A:59:THR:O     | 1:A:63:TRP:HD1   | 2.02                     | 0.42              |
| 1:A:530:MET:HB2  | 2:B:33:TRP:O     | 2.19                     | 0.42              |
| 3:C:1102:ARG:N   | 3:C:1103:PRO:HD2 | 2.35                     | 0.42              |
| 3:C:356:LEU:CD2  | 3:C:712:ILE:HG21 | 2.49                     | 0.42              |
| 1:A:118:ILE:CG1  | 1:A:181:HIS:CB   | 2.86                     | 0.42              |
| 1:A:182:ILE:CG2  | 1:A:183:ILE:HG13 | 2.50                     | 0.42              |
| 1:A:72:ALA:HB1   | 1:A:77:THR:HB    | 2.01                     | 0.42              |
| 3:C:230:ILE:HD11 | 3:C:285:LEU:HD21 | 2.02                     | 0.42              |
| 1:A:200:ILE:O    | 1:A:201:GLU:C    | 2.58                     | 0.42              |
| 1:A:218:LEU:HD12 | 1:A:277:TYR:HB2  | 2.00                     | 0.42              |
| 1:A:437:MET:HE1  | 1:A:475:MET:HE3  | 2.02                     | 0.42              |
| 1:A:75:SER:O     | 1:A:77:THR:N     | 2.53                     | 0.42              |
| 1:A:707:ARG:HD3  | 1:A:710:LEU:HD22 | 2.02                     | 0.42              |
| 3:C:404:LEU:HD12 | 3:C:429:PHE:CZ   | 2.55                     | 0.42              |
| 3:C:576:LEU:C    | 3:C:577:LEU:HD23 | 2.41                     | 0.42              |
| 3:C:578:HIS:CG   | 3:C:623:LEU:HD12 | 2.54                     | 0.42              |
| 4:D:289:ARG:NH2  | 4:D:335:THR:O    | 2.53                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:640:ILE:O    | 1:A:655:ILE:HD12 | 2.20                     | 0.42              |
| 3:C:563:ASP:OD2  | 3:C:565:SER:HB3  | 2.20                     | 0.42              |
| 1:A:536:TYR:CD2  | 1:A:573:LEU:HD11 | 2.54                     | 0.41              |
| 3:C:185:PRO:HD3  | 4:D:289:ARG:CB   | 2.28                     | 0.41              |
| 1:A:221:LEU:HA   | 1:A:221:LEU:HD23 | 1.91                     | 0.41              |
| 1:A:597:LEU:HA   | 1:A:600:LEU:HD12 | 2.01                     | 0.41              |
| 3:C:404:LEU:HD13 | 3:C:404:LEU:HA   | 1.89                     | 0.41              |
| 3:C:571:LEU:HA   | 3:C:571:LEU:HD23 | 1.87                     | 0.41              |
| 3:C:708:GLN:HB3  | 3:C:709:LYS:H    | 1.60                     | 0.41              |
| 1:A:189:GLN:CD   | 1:A:230:SER:HB3  | 2.41                     | 0.41              |
| 1:A:267:LEU:HD21 | 1:A:290:VAL:HG12 | 2.03                     | 0.41              |
| 1:A:390:MET:HE2  | 1:A:394:PHE:HB2  | 2.02                     | 0.41              |
| 3:C:184:ASP:CB   | 3:C:185:PRO:CD   | 2.97                     | 0.41              |
| 3:C:185:PRO:CD   | 4:D:289:ARG:CB   | 2.78                     | 0.41              |
| 3:C:24:THR:H     | 3:C:30:ASN:ND2   | 2.18                     | 0.41              |
| 3:C:523:PRO:HB3  | 3:C:524:GLN:NE2  | 2.35                     | 0.41              |
| 1:A:74:GLN:NE2   | 1:A:110:CYS:HA   | 2.15                     | 0.41              |
| 1:A:232:GLU:O    | 1:A:235:PHE:HB3  | 2.20                     | 0.41              |
| 1:A:49:ARG:NE    | 1:A:49:ARG:HA    | 2.35                     | 0.41              |
| 1:A:651:GLY:O    | 1:A:652:ASP:C    | 2.57                     | 0.41              |
| 1:A:744:TYR:O    | 1:A:757:TYR:O    | 2.38                     | 0.41              |
| 3:C:602:LEU:HD22 | 3:C:603:LEU:N    | 2.34                     | 0.41              |
| 3:C:673:LEU:HD23 | 3:C:674:LYS:N    | 2.33                     | 0.41              |
| 4:D:347:ASN:HA   | 4:D:366:HIS:O    | 2.21                     | 0.41              |
| 1:A:123:GLU:HB3  | 1:A:124:ASP:H    | 1.61                     | 0.41              |
| 1:A:131:PHE:O    | 1:A:134:LYS:HB2  | 2.21                     | 0.41              |
| 1:A:250:LEU:HD22 | 1:A:254:ARG:HD3  | 2.01                     | 0.41              |
| 1:A:79:ILE:CD1   | 1:A:79:ILE:H     | 2.23                     | 0.41              |
| 3:C:567:ARG:HB3  | 3:C:579:LYS:HA   | 2.01                     | 0.41              |
| 3:C:711:HIS:CE1  | 3:C:713:ARG:N    | 2.88                     | 0.41              |
| 1:A:63:TRP:HZ3   | 1:A:102:LEU:HA   | 1.75                     | 0.41              |
| 3:C:182:TYR:O    | 3:C:188:ARG:HA   | 2.20                     | 0.41              |
| 3:C:641:PHE:CD1  | 3:C:641:PHE:C    | 2.93                     | 0.41              |
| 1:A:184:SER:O    | 1:A:185:ASP:C    | 2.58                     | 0.41              |
| 1:A:219:GLY:O    | 1:A:220:MET:C    | 2.57                     | 0.41              |
| 1:A:543:LEU:HD22 | 1:A:543:LEU:N    | 2.36                     | 0.41              |
| 1:A:581:GLU:HB2  | 2:B:21:ARG:CA    | 2.43                     | 0.41              |
| 1:A:734:LYS:HD3  | 1:A:737:GLU:OE1  | 2.21                     | 0.41              |
| 1:A:751:ASN:HD21 | 1:A:754:GLN:HB2  | 1.86                     | 0.41              |
| 1:A:757:TYR:O    | 1:A:758:VAL:CB   | 2.65                     | 0.41              |
| 3:C:699:LEU:HD13 | 3:C:700:THR:N    | 2.35                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:6:DA:C2      | 6:F:7:DA:N6      | 2.88                     | 0.41              |
| 1:A:74:GLN:HB3   | 1:A:113:HIS:CE1  | 2.55                     | 0.41              |
| 1:A:578:LEU:HD13 | 1:A:591:VAL:HG23 | 1.99                     | 0.41              |
| 1:A:650:ASP:OD1  | 1:A:650:ASP:N    | 2.53                     | 0.41              |
| 3:C:389:ILE:HD13 | 3:C:713:ARG:CG   | 2.45                     | 0.41              |
| 1:A:734:LYS:HA   | 1:A:737:GLU:OE2  | 2.20                     | 0.41              |
| 1:A:735:ARG:HA   | 1:A:735:ARG:HE   | 1.84                     | 0.41              |
| 1:A:578:LEU:HA   | 2:B:23:GLU:O     | 2.20                     | 0.41              |
| 3:C:413:LEU:HB3  | 3:C:414:ARG:H    | 1.69                     | 0.41              |
| 1:A:414:ASP:O    | 1:A:418:ARG:HG3  | 2.21                     | 0.41              |
| 1:A:428:GLU:HG3  | 1:A:428:GLU:H    | 1.63                     | 0.41              |
| 1:A:454:LYS:HE2  | 1:A:490:LYS:HD2  | 2.02                     | 0.41              |
| 1:A:51:ARG:N     | 1:A:52:PRO:HD2   | 2.33                     | 0.41              |
| 1:A:587:LYS:HB2  | 1:A:660:PHE:CZ   | 2.55                     | 0.41              |
| 3:C:457:THR:CG2  | 3:C:459:PHE:O    | 2.69                     | 0.41              |
| 3:C:502:SER:O    | 3:C:503:CYS:CB   | 2.68                     | 0.41              |
| 1:A:131:PHE:HZ   | 1:A:188:VAL:CG2  | 2.31                     | 0.41              |
| 1:A:141:ASP:O    | 1:A:142:HIS:C    | 2.58                     | 0.41              |
| 1:A:558:TYR:O    | 1:A:562:HIS:HB2  | 2.21                     | 0.41              |
| 1:A:602:PHE:N    | 1:A:602:PHE:HD1  | 2.19                     | 0.41              |
| 3:C:498:ILE:N    | 3:C:498:ILE:CD1  | 2.84                     | 0.41              |
| 3:C:553:SER:HA   | 3:C:554:PRO:HD3  | 1.80                     | 0.41              |
| 3:C:394:ILE:HD13 | 3:C:708:GLN:HE22 | 1.85                     | 0.41              |
| 3:C:870:VAL:HA   | 3:C:883:SER:O    | 2.21                     | 0.41              |
| 1:A:187:MET:O    | 1:A:191:LYS:HB2  | 2.22                     | 0.40              |
| 1:A:200:ILE:C    | 1:A:202:ARG:N    | 2.74                     | 0.40              |
| 1:A:533:TRP:HB3  | 1:A:534:PRO:HD2  | 2.03                     | 0.40              |
| 1:A:748:ASP:HB3  | 1:A:756:HIS:CE1  | 2.56                     | 0.40              |
| 1:A:98:VAL:O     | 1:A:99:SER:C     | 2.59                     | 0.40              |
| 3:C:451:PHE:HD1  | 3:C:470:GLN:CB   | 2.34                     | 0.40              |
| 1:A:409:ILE:HG13 | 1:A:443:ILE:HD11 | 1.99                     | 0.40              |
| 3:C:108:VAL:HG11 | 3:C:143:ILE:HD11 | 2.03                     | 0.40              |
| 3:C:184:ASP:CB   | 3:C:185:PRO:HD2  | 2.43                     | 0.40              |
| 1:A:384:GLU:HA   | 1:A:387:VAL:HG23 | 2.04                     | 0.40              |
| 1:A:390:MET:CE   | 1:A:391:LYS:HA   | 2.51                     | 0.40              |
| 1:A:457:LEU:CD2  | 1:A:461:LEU:HG   | 2.52                     | 0.40              |
| 1:A:625:ARG:HD3  | 1:A:625:ARG:HA   | 1.91                     | 0.40              |
| 3:C:184:ASP:N    | 3:C:187:GLY:O    | 2.55                     | 0.40              |
| 3:C:402:ILE:HG22 | 3:C:403:ASP:N    | 2.37                     | 0.40              |
| 3:C:643:SER:O    | 3:C:644:LEU:C    | 2.59                     | 0.40              |
| 3:C:705:ASP:OD1  | 3:C:705:ASP:C    | 2.60                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:329:VAL:O    | 1:A:330:ARG:O    | 2.39                     | 0.40              |
| 3:C:561:TRP:O    | 3:C:587:ILE:HG21 | 2.19                     | 0.40              |
| 4:D:218:THR:CG2  | 4:D:226:VAL:HG13 | 2.52                     | 0.40              |
| 1:A:141:ASP:O    | 1:A:143:CYS:N    | 2.55                     | 0.40              |
| 1:A:274:VAL:HG21 | 1:A:283:GLN:HB2  | 2.04                     | 0.40              |
| 1:A:675:LYS:HD3  | 1:A:675:LYS:HA   | 1.93                     | 0.40              |
| 3:C:412:PRO:O    | 3:C:412:PRO:HG2  | 2.21                     | 0.40              |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------------|--------------------------|-------------------|
| 3:C:103:ARG:NH1 | 3:C:769:LYS:NZ[1_565] | 2.04                     | 0.16              |

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1   | A     | 717/742 (97%)   | 512 (71%)  | 132 (18%) | 73 (10%) | 1           | 12 |
| 2   | B     | 19/117 (16%)    | 14 (74%)   | 4 (21%)   | 1 (5%)   | 2           | 25 |
| 3   | C     | 1095/1159 (94%) | 963 (88%)  | 97 (9%)   | 35 (3%)  | 5           | 36 |
| 4   | D     | 353/382 (92%)   | 326 (92%)  | 22 (6%)   | 5 (1%)   | 13          | 53 |
| All | All   | 2184/2400 (91%) | 1815 (83%) | 255 (12%) | 114 (5%) | 2           | 26 |

All (114) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 56  | ASP  |
| 1   | A     | 58  | TYR  |
| 1   | A     | 76  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 83  | LEU  |
| 1   | A     | 84  | GLU  |
| 1   | A     | 127 | ASP  |
| 1   | A     | 185 | ASP  |
| 1   | A     | 191 | LYS  |
| 1   | A     | 207 | GLU  |
| 1   | A     | 208 | ALA  |
| 1   | A     | 209 | VAL  |
| 1   | A     | 276 | THR  |
| 1   | A     | 330 | ARG  |
| 1   | A     | 483 | CYS  |
| 1   | A     | 517 | ASP  |
| 1   | A     | 587 | LYS  |
| 1   | A     | 606 | ASP  |
| 1   | A     | 616 | ALA  |
| 1   | A     | 633 | CYS  |
| 1   | A     | 644 | LYS  |
| 1   | A     | 660 | PHE  |
| 1   | A     | 661 | LYS  |
| 1   | A     | 710 | LEU  |
| 1   | A     | 752 | PRO  |
| 3   | C     | 367 | LEU  |
| 3   | C     | 430 | VAL  |
| 3   | C     | 583 | GLY  |
| 3   | C     | 598 | SER  |
| 3   | C     | 672 | ASN  |
| 3   | C     | 674 | LYS  |
| 3   | C     | 704 | ILE  |
| 3   | C     | 705 | ASP  |
| 3   | C     | 710 | LEU  |
| 4   | D     | 126 | LEU  |
| 1   | A     | 96  | HIS  |
| 1   | A     | 97  | LYS  |
| 1   | A     | 204 | ARG  |
| 1   | A     | 229 | ASP  |
| 1   | A     | 240 | ASN  |
| 1   | A     | 280 | HIS  |
| 1   | A     | 441 | ARG  |
| 1   | A     | 598 | VAL  |
| 1   | A     | 607 | GLY  |
| 1   | A     | 652 | ASP  |
| 1   | A     | 670 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 691  | ASP  |
| 1   | A     | 711  | GLY  |
| 3   | C     | 549  | SER  |
| 3   | C     | 563  | ASP  |
| 3   | C     | 584  | GLY  |
| 3   | C     | 855  | ASP  |
| 3   | C     | 1110 | ALA  |
| 4   | D     | 120  | ALA  |
| 1   | A     | 55   | PRO  |
| 1   | A     | 71   | ARG  |
| 1   | A     | 75   | SER  |
| 1   | A     | 82   | ASN  |
| 1   | A     | 119  | LEU  |
| 1   | A     | 223  | ASP  |
| 1   | A     | 350  | ALA  |
| 1   | A     | 402  | PRO  |
| 1   | A     | 451  | ALA  |
| 1   | A     | 586  | LYS  |
| 1   | A     | 708  | LYS  |
| 1   | A     | 727  | VAL  |
| 1   | A     | 757  | TYR  |
| 1   | A     | 758  | VAL  |
| 3   | C     | 185  | PRO  |
| 3   | C     | 418  | ASN  |
| 3   | C     | 449  | MET  |
| 3   | C     | 481  | GLN  |
| 3   | C     | 547  | GLY  |
| 3   | C     | 562  | THR  |
| 3   | C     | 624  | SER  |
| 3   | C     | 644  | LEU  |
| 3   | C     | 706  | GLU  |
| 3   | C     | 1109 | VAL  |
| 1   | A     | 54   | LEU  |
| 1   | A     | 91   | GLU  |
| 1   | A     | 189  | GLN  |
| 1   | A     | 228  | LYS  |
| 1   | A     | 293  | GLN  |
| 1   | A     | 325  | LEU  |
| 1   | A     | 377  | GLU  |
| 1   | A     | 514  | ASN  |
| 1   | A     | 610  | PHE  |
| 1   | A     | 617  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 726 | PRO  |
| 2   | B     | 37  | ILE  |
| 3   | C     | 36  | ASN  |
| 3   | C     | 372 | GLN  |
| 3   | C     | 488 | SER  |
| 3   | C     | 503 | CYS  |
| 4   | D     | 119 | HIS  |
| 4   | D     | 190 | GLY  |
| 1   | A     | 51  | ARG  |
| 1   | A     | 201 | GLU  |
| 1   | A     | 233 | LEU  |
| 1   | A     | 378 | VAL  |
| 1   | A     | 440 | PHE  |
| 1   | A     | 597 | LEU  |
| 3   | C     | 242 | GLY  |
| 3   | C     | 592 | LEU  |
| 3   | C     | 460 | CYS  |
| 4   | D     | 291 | ASP  |
| 3   | C     | 493 | PRO  |
| 3   | C     | 551 | GLY  |
| 1   | A     | 306 | GLY  |
| 1   | A     | 618 | GLY  |
| 1   | A     | 619 | ILE  |
| 3   | C     | 406 | GLY  |
| 3   | C     | 712 | ILE  |
| 1   | A     | 519 | GLY  |
| 1   | A     | 405 | PRO  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1   | A     | 631/674 (94%)  | 562 (89%) | 69 (11%) | 7           | 30 |
| 2   | B     | 18/99 (18%)    | 11 (61%)  | 7 (39%)  | 0           | 0  |
| 3   | C     | 957/1015 (94%) | 865 (90%) | 92 (10%) | 10          | 35 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 4   | D     | 304/335 (91%)   | 278 (91%)  | 26 (9%)   | 12          | 42 |
| All | All   | 1910/2123 (90%) | 1716 (90%) | 194 (10%) | 8           | 33 |

All (194) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 64  | ARG  |
| 1   | A     | 79  | ILE  |
| 1   | A     | 90  | VAL  |
| 1   | A     | 93  | LEU  |
| 1   | A     | 95  | SER  |
| 1   | A     | 102 | LEU  |
| 1   | A     | 112 | ASP  |
| 1   | A     | 124 | ASP  |
| 1   | A     | 125 | SER  |
| 1   | A     | 135 | ILE  |
| 1   | A     | 164 | ASN  |
| 1   | A     | 171 | TRP  |
| 1   | A     | 173 | MET  |
| 1   | A     | 175 | LEU  |
| 1   | A     | 182 | ILE  |
| 1   | A     | 183 | ILE  |
| 1   | A     | 199 | LEU  |
| 1   | A     | 205 | SER  |
| 1   | A     | 207 | GLU  |
| 1   | A     | 217 | LEU  |
| 1   | A     | 249 | ARG  |
| 1   | A     | 281 | SER  |
| 1   | A     | 283 | GLN  |
| 1   | A     | 292 | LYS  |
| 1   | A     | 307 | LEU  |
| 1   | A     | 330 | ARG  |
| 1   | A     | 353 | ILE  |
| 1   | A     | 389 | LEU  |
| 1   | A     | 390 | MET  |
| 1   | A     | 394 | PHE  |
| 1   | A     | 402 | PRO  |
| 1   | A     | 422 | LYS  |
| 1   | A     | 428 | GLU  |
| 1   | A     | 429 | LEU  |
| 1   | A     | 439 | LEU  |
| 1   | A     | 444 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 450 | GLU  |
| 1   | A     | 457 | LEU  |
| 1   | A     | 478 | LYS  |
| 1   | A     | 483 | CYS  |
| 1   | A     | 494 | MET  |
| 1   | A     | 498 | MET  |
| 1   | A     | 526 | ASN  |
| 1   | A     | 540 | GLU  |
| 1   | A     | 546 | GLU  |
| 1   | A     | 562 | HIS  |
| 1   | A     | 569 | TRP  |
| 1   | A     | 591 | VAL  |
| 1   | A     | 611 | GLU  |
| 1   | A     | 624 | LEU  |
| 1   | A     | 626 | ARG  |
| 1   | A     | 639 | LEU  |
| 1   | A     | 650 | ASP  |
| 1   | A     | 652 | ASP  |
| 1   | A     | 660 | PHE  |
| 1   | A     | 663 | LYS  |
| 1   | A     | 665 | PHE  |
| 1   | A     | 677 | THR  |
| 1   | A     | 681 | GLN  |
| 1   | A     | 683 | SER  |
| 1   | A     | 687 | ARG  |
| 1   | A     | 691 | ASP  |
| 1   | A     | 692 | ARG  |
| 1   | A     | 706 | MET  |
| 1   | A     | 720 | TYR  |
| 1   | A     | 726 | PRO  |
| 1   | A     | 735 | ARG  |
| 1   | A     | 748 | ASP  |
| 1   | A     | 751 | ASN  |
| 2   | B     | 19  | LYS  |
| 2   | B     | 22  | PHE  |
| 2   | B     | 25  | LYS  |
| 2   | B     | 28  | ASN  |
| 2   | B     | 32  | LEU  |
| 2   | B     | 37  | ILE  |
| 2   | B     | 39  | VAL  |
| 3   | C     | 7   | VAL  |
| 3   | C     | 81  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 99  | ASP  |
| 3   | C     | 133 | LEU  |
| 3   | C     | 159 | LEU  |
| 3   | C     | 167 | VAL  |
| 3   | C     | 189 | HIS  |
| 3   | C     | 191 | LYS  |
| 3   | C     | 241 | ASN  |
| 3   | C     | 304 | LEU  |
| 3   | C     | 314 | LEU  |
| 3   | C     | 334 | VAL  |
| 3   | C     | 339 | ASP  |
| 3   | C     | 360 | VAL  |
| 3   | C     | 370 | GLN  |
| 3   | C     | 396 | ILE  |
| 3   | C     | 403 | ASP  |
| 3   | C     | 410 | LEU  |
| 3   | C     | 412 | PRO  |
| 3   | C     | 414 | ARG  |
| 3   | C     | 419 | ARG  |
| 3   | C     | 420 | GLU  |
| 3   | C     | 452 | VAL  |
| 3   | C     | 454 | ASP  |
| 3   | C     | 469 | ILE  |
| 3   | C     | 473 | SER  |
| 3   | C     | 476 | VAL  |
| 3   | C     | 481 | GLN  |
| 3   | C     | 482 | GLU  |
| 3   | C     | 487 | VAL  |
| 3   | C     | 493 | PRO  |
| 3   | C     | 510 | VAL  |
| 3   | C     | 518 | TYR  |
| 3   | C     | 523 | PRO  |
| 3   | C     | 525 | GLU  |
| 3   | C     | 531 | HIS  |
| 3   | C     | 540 | CYS  |
| 3   | C     | 555 | LEU  |
| 3   | C     | 560 | LEU  |
| 3   | C     | 561 | TRP  |
| 3   | C     | 563 | ASP  |
| 3   | C     | 567 | ARG  |
| 3   | C     | 576 | LEU  |
| 3   | C     | 582 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 587 | ILE  |
| 3   | C     | 594 | THR  |
| 3   | C     | 596 | PHE  |
| 3   | C     | 597 | GLU  |
| 3   | C     | 602 | LEU  |
| 3   | C     | 603 | LEU  |
| 3   | C     | 608 | ASP  |
| 3   | C     | 614 | PHE  |
| 3   | C     | 616 | LEU  |
| 3   | C     | 617 | ASN  |
| 3   | C     | 618 | ILE  |
| 3   | C     | 623 | LEU  |
| 3   | C     | 625 | ASP  |
| 3   | C     | 627 | LYS  |
| 3   | C     | 646 | THR  |
| 3   | C     | 663 | ASN  |
| 3   | C     | 673 | LEU  |
| 3   | C     | 688 | PRO  |
| 3   | C     | 689 | ASP  |
| 3   | C     | 700 | THR  |
| 3   | C     | 701 | ILE  |
| 3   | C     | 703 | THR  |
| 3   | C     | 704 | ILE  |
| 3   | C     | 706 | GLU  |
| 3   | C     | 708 | GLN  |
| 3   | C     | 713 | ARG  |
| 3   | C     | 728 | GLU  |
| 3   | C     | 809 | GLN  |
| 3   | C     | 820 | LYS  |
| 3   | C     | 844 | LYS  |
| 3   | C     | 864 | LYS  |
| 3   | C     | 867 | LYS  |
| 3   | C     | 881 | LEU  |
| 3   | C     | 898 | GLU  |
| 3   | C     | 899 | LEU  |
| 3   | C     | 901 | THR  |
| 3   | C     | 914 | LEU  |
| 3   | C     | 931 | LEU  |
| 3   | C     | 957 | VAL  |
| 3   | C     | 966 | LEU  |
| 3   | C     | 970 | ASN  |
| 3   | C     | 984 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | C     | 1000 | LEU  |
| 3   | C     | 1052 | LEU  |
| 3   | C     | 1086 | THR  |
| 3   | C     | 1093 | LEU  |
| 3   | C     | 1106 | GLN  |
| 3   | C     | 1129 | LEU  |
| 4   | D     | 111  | LYS  |
| 4   | D     | 116  | GLN  |
| 4   | D     | 117  | SER  |
| 4   | D     | 119  | HIS  |
| 4   | D     | 126  | LEU  |
| 4   | D     | 134  | LEU  |
| 4   | D     | 148  | ARG  |
| 4   | D     | 174  | LEU  |
| 4   | D     | 179  | VAL  |
| 4   | D     | 219  | LEU  |
| 4   | D     | 243  | VAL  |
| 4   | D     | 254  | THR  |
| 4   | D     | 262  | LEU  |
| 4   | D     | 274  | GLU  |
| 4   | D     | 293  | LEU  |
| 4   | D     | 299  | VAL  |
| 4   | D     | 308  | LEU  |
| 4   | D     | 312  | LYS  |
| 4   | D     | 321  | MET  |
| 4   | D     | 374  | LEU  |
| 4   | D     | 389  | VAL  |
| 4   | D     | 393  | TYR  |
| 4   | D     | 400  | LEU  |
| 4   | D     | 435  | SER  |
| 4   | D     | 437  | THR  |
| 4   | D     | 453  | ASN  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 74  | GLN  |
| 1   | A     | 92  | ASN  |
| 1   | A     | 145 | GLN  |
| 1   | A     | 189 | GLN  |
| 1   | A     | 283 | GLN  |
| 1   | A     | 309 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 321 | GLN  |
| 1   | A     | 333 | GLN  |
| 1   | A     | 339 | HIS  |
| 1   | A     | 399 | ASN  |
| 1   | A     | 412 | HIS  |
| 1   | A     | 526 | ASN  |
| 1   | A     | 551 | GLN  |
| 1   | A     | 570 | GLN  |
| 1   | A     | 595 | GLN  |
| 1   | A     | 657 | ASN  |
| 1   | A     | 673 | GLN  |
| 1   | A     | 681 | GLN  |
| 1   | A     | 712 | HIS  |
| 1   | A     | 722 | GLN  |
| 1   | A     | 751 | ASN  |
| 1   | A     | 754 | GLN  |
| 1   | A     | 756 | HIS  |
| 2   | B     | 28  | ASN  |
| 3   | C     | 4   | ASN  |
| 3   | C     | 30  | ASN  |
| 3   | C     | 85  | ASN  |
| 3   | C     | 156 | ASN  |
| 3   | C     | 186 | GLN  |
| 3   | C     | 241 | ASN  |
| 3   | C     | 261 | HIS  |
| 3   | C     | 374 | GLN  |
| 3   | C     | 432 | GLN  |
| 3   | C     | 455 | GLN  |
| 3   | C     | 462 | ASN  |
| 3   | C     | 467 | GLN  |
| 3   | C     | 481 | GLN  |
| 3   | C     | 494 | GLN  |
| 3   | C     | 507 | GLN  |
| 3   | C     | 524 | GLN  |
| 3   | C     | 536 | HIS  |
| 3   | C     | 578 | HIS  |
| 3   | C     | 634 | GLN  |
| 3   | C     | 648 | ASN  |
| 3   | C     | 663 | ASN  |
| 3   | C     | 708 | GLN  |
| 3   | C     | 727 | GLN  |
| 3   | C     | 796 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | C     | 885  | ASN  |
| 3   | C     | 904  | ASN  |
| 3   | C     | 907  | ASN  |
| 3   | C     | 908  | ASN  |
| 3   | C     | 1034 | ASN  |
| 3   | C     | 1055 | GLN  |
| 4   | D     | 269  | HIS  |
| 4   | D     | 370  | GLN  |
| 4   | D     | 453  | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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 | $\# Z  > 2$ |
| 5   | 3DR  | E     | 7   | 5    | 8,11,12      | 0.51 | 0           | 8,14,17     | 0.97 | 0           |

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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 5   | 3DR  | E     | 7   | 5    | -       | 0/3/15/16 | 0/1/1/1 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.



There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 719/742 (96%)   | 0.36   | 33 (4%) 33 34 | 288, 322, 371, 414    | 0     |
| 2   | B     | 21/117 (17%)    | 1.04   | 3 (14%) 3 9   | 312, 322, 356, 365    | 0     |
| 3   | C     | 1105/1159 (95%) | 0.33   | 39 (3%) 44 42 | 185, 326, 367, 403    | 0     |
| 4   | D     | 355/382 (92%)   | 0.27   | 8 (2%) 61 58  | 275, 310, 352, 367    | 0     |
| 5   | E     | 11/12 (91%)     | 1.74   | 3 (27%) 1 6   | 342, 359, 437, 441    | 0     |
| 6   | F     | 12/12 (100%)    | 0.59   | 1 (8%) 12 17  | 363, 379, 420, 442    | 0     |
| All | All   | 2223/2424 (91%) | 0.34   | 87 (3%) 40 39 | 185, 322, 367, 442    | 0     |

All (87) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 5   | E     | 1    | DG   | 6.0  |
| 4   | D     | 377  | ILE  | 5.0  |
| 1   | A     | 709  | THR  | 4.6  |
| 5   | E     | 12   | DA   | 4.4  |
| 3   | C     | 1015 | GLN  | 4.4  |
| 1   | A     | 183  | ILE  | 4.3  |
| 1   | A     | 745  | MET  | 4.2  |
| 6   | F     | 12   | DC   | 3.6  |
| 3   | C     | 497  | ASN  | 3.5  |
| 1   | A     | 736  | ILE  | 3.5  |
| 2   | B     | 27   | TRP  | 3.4  |
| 3   | C     | 2    | SER  | 3.4  |
| 1   | A     | 740  | ILE  | 3.3  |
| 1   | A     | 182  | ILE  | 3.3  |
| 1   | A     | 97   | LYS  | 3.3  |
| 2   | B     | 19   | LYS  | 3.3  |
| 3   | C     | 879  | LYS  | 3.3  |
| 1   | A     | 128  | SER  | 3.2  |
| 3   | C     | 1043 | LEU  | 3.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | C     | 856 | GLY  | 3.2  |
| 1   | A     | 420 | GLY  | 3.1  |
| 3   | C     | 943 | GLU  | 3.1  |
| 3   | C     | 246 | LEU  | 3.1  |
| 1   | A     | 727 | VAL  | 3.0  |
| 1   | A     | 567 | LEU  | 3.0  |
| 3   | C     | 766 | SER  | 3.0  |
| 3   | C     | 547 | GLY  | 2.9  |
| 3   | C     | 771 | PHE  | 2.9  |
| 1   | A     | 700 | ILE  | 2.8  |
| 3   | C     | 975 | PHE  | 2.8  |
| 4   | D     | 379 | ALA  | 2.8  |
| 3   | C     | 337 | ASN  | 2.8  |
| 1   | A     | 710 | LEU  | 2.7  |
| 1   | A     | 294 | LEU  | 2.7  |
| 3   | C     | 853 | TYR  | 2.7  |
| 1   | A     | 723 | LEU  | 2.6  |
| 1   | A     | 254 | ARG  | 2.5  |
| 1   | A     | 751 | ASN  | 2.5  |
| 1   | A     | 578 | LEU  | 2.5  |
| 1   | A     | 55  | PRO  | 2.5  |
| 1   | A     | 707 | ARG  | 2.5  |
| 1   | A     | 704 | MET  | 2.5  |
| 3   | C     | 966 | LEU  | 2.4  |
| 3   | C     | 441 | GLU  | 2.4  |
| 3   | C     | 44  | VAL  | 2.4  |
| 4   | D     | 378 | LYS  | 2.4  |
| 1   | A     | 523 | LEU  | 2.4  |
| 3   | C     | 16  | ASN  | 2.4  |
| 1   | A     | 756 | HIS  | 2.4  |
| 1   | A     | 224 | LEU  | 2.4  |
| 4   | D     | 421 | ARG  | 2.3  |
| 5   | E     | 2   | DC   | 2.3  |
| 3   | C     | 965 | PHE  | 2.3  |
| 4   | D     | 101 | GLY  | 2.3  |
| 3   | C     | 855 | ASP  | 2.3  |
| 1   | A     | 754 | GLN  | 2.3  |
| 3   | C     | 942 | PHE  | 2.3  |
| 3   | C     | 979 | LYS  | 2.3  |
| 1   | A     | 654 | PHE  | 2.3  |
| 1   | A     | 661 | LYS  | 2.2  |
| 3   | C     | 685 | ASP  | 2.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | C     | 300 | LEU  | 2.2  |
| 3   | C     | 994 | GLU  | 2.2  |
| 3   | C     | 964 | ASN  | 2.2  |
| 3   | C     | 113 | GLY  | 2.2  |
| 1   | A     | 54  | LEU  | 2.2  |
| 3   | C     | 963 | ASP  | 2.2  |
| 1   | A     | 278 | LEU  | 2.2  |
| 3   | C     | 70  | LYS  | 2.2  |
| 4   | D     | 364 | ILE  | 2.1  |
| 4   | D     | 349 | ILE  | 2.1  |
| 3   | C     | 17  | GLY  | 2.1  |
| 3   | C     | 930 | VAL  | 2.1  |
| 3   | C     | 43  | VAL  | 2.1  |
| 3   | C     | 976 | VAL  | 2.1  |
| 1   | A     | 703 | ILE  | 2.1  |
| 4   | D     | 363 | ILE  | 2.1  |
| 3   | C     | 967 | GLY  | 2.1  |
| 3   | C     | 116 | SER  | 2.1  |
| 3   | C     | 880 | LEU  | 2.1  |
| 2   | B     | 24  | VAL  | 2.0  |
| 3   | C     | 977 | CYS  | 2.0  |
| 3   | C     | 546 | LEU  | 2.0  |
| 1   | A     | 581 | GLU  | 2.0  |
| 1   | A     | 302 | ILE  | 2.0  |
| 1   | A     | 565 | ARG  | 2.0  |
| 3   | C     | 420 | GLU  | 2.0  |

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|----------------------------|-------|
| 5   | 3DR  | E     | 7   | 11/12 | 0.82 | 0.24 | -    | 357,362,366,367            | 0     |

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.