



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 10:05 am BST

PDB ID : 3QP5  
Title : Crystal structure of CviR bound to antagonist chlorolactone (CL)  
Authors : Chen, G.; Swem, L.; Swem, D.; Stauff, D.; O'Loughlin, C.; Jeffrey, P.; Bassler, B.; Hughson, F.  
Deposited on : 2011-02-11  
Resolution : 3.25 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

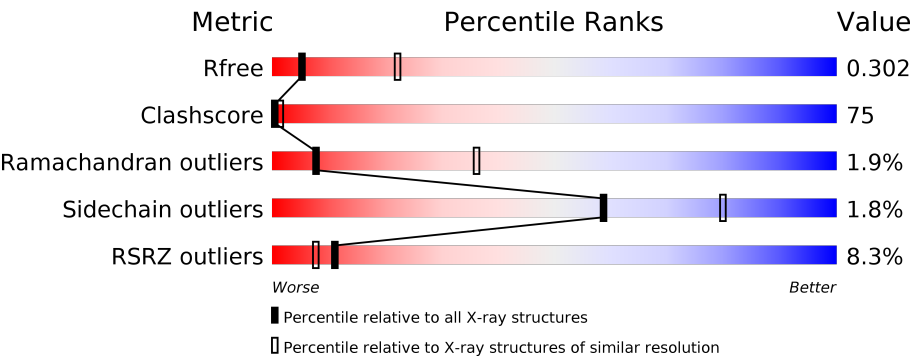
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 1619 (3.28-3.20)                                      |
| Clashscore            | 141614                      | 1755 (3.28-3.20)                                      |
| Ramachandran outliers | 138981                      | 1728 (3.28-3.20)                                      |
| Sidechain outliers    | 138945                      | 1727 (3.28-3.20)                                      |
| RSRZ outliers         | 127900                      | 1567 (3.28-3.20)                                      |

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 265    |                  |
| 1   | B     | 265    |                  |
| 1   | C     | 265    |                  |
| 1   | D     | 265    |                  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | HLC  | A     | 266 | -         | -        | -       | X                |
| 2   | HLC  | C     | 266 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

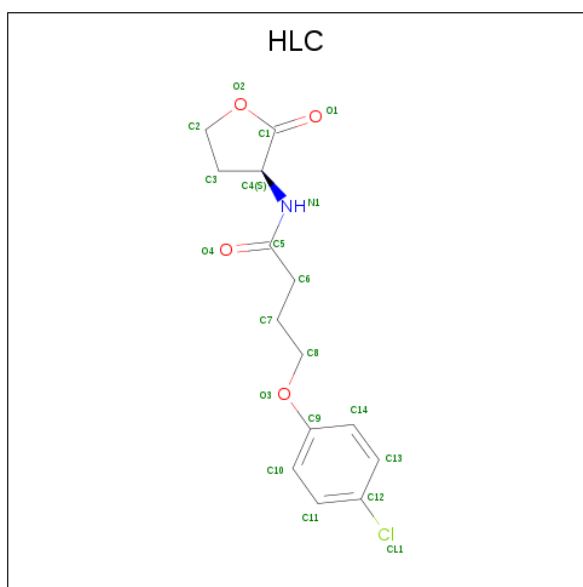
There are 2 unique types of molecules in this entry. The entry contains 7738 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CviR transcriptional regulator.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 251      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1977  | 1240 | 370 | 357 | 10 |         |         |       |
| 1   | B     | 238      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1890  | 1186 | 353 | 342 | 9  |         |         |       |
| 1   | C     | 239      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1902  | 1196 | 354 | 343 | 9  |         |         |       |
| 1   | D     | 238      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1889  | 1186 | 353 | 342 | 8  |         |         |       |

- Molecule 2 is 4-(4-chlorophenoxy)-N-[(3S)-2-oxotetrahydrofuran-3-yl]butanamide (three-letter code: HLC) (formula: C<sub>14</sub>H<sub>16</sub>ClNO<sub>4</sub>).



| Mol | Chain | Residues | Atoms |    |    |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|-----|---------|---------|
| 2   | A     | 1        | Total | C  | Cl | N O | 0       | 0       |
|     |       |          | 20    | 14 | 1  | 1 4 |         |         |
| 2   | B     | 1        | Total | C  | Cl | N O | 0       | 0       |
|     |       |          | 20    | 14 | 1  | 1 4 |         |         |

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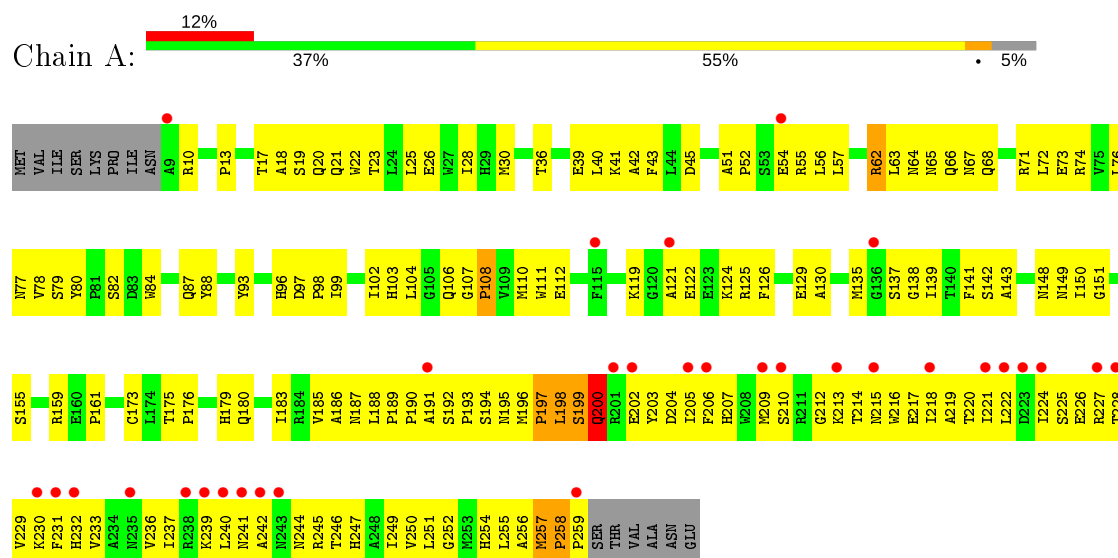
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| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 2   | C     | 1        | Total | C  | Cl | N | O | 0       | 0       |
|     |       |          | 20    | 14 | 1  | 1 | 4 |         |         |
| 2   | D     | 1        | Total | C  | Cl | N | O | 0       | 0       |
|     |       |          | 20    | 14 | 1  | 1 | 4 |         |         |

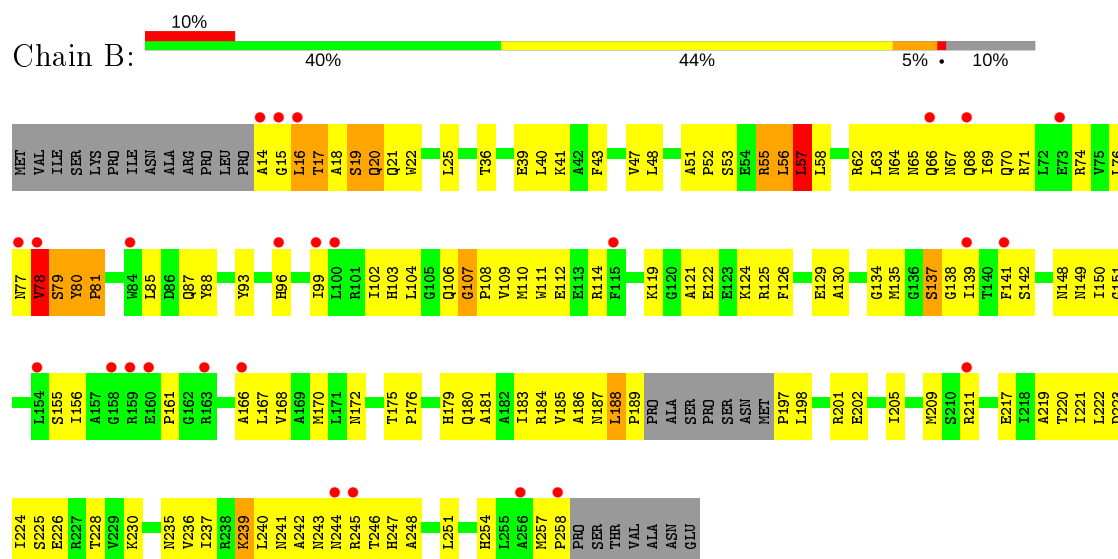
### 3 Residue-property plots [i](#)

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.

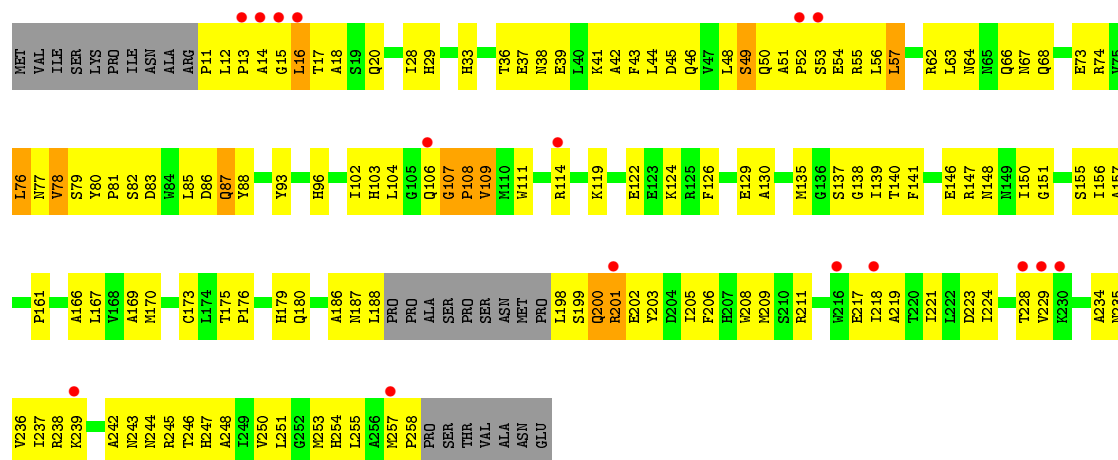
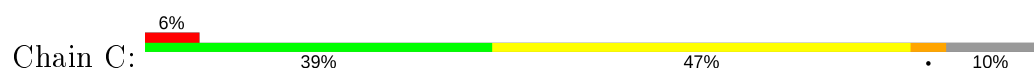
#### • Molecule 1: CviR transcriptional regulator



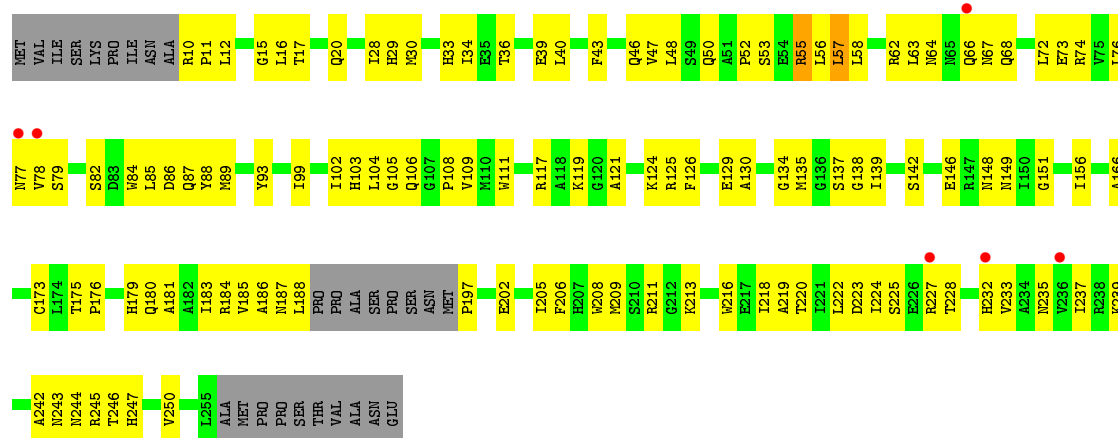
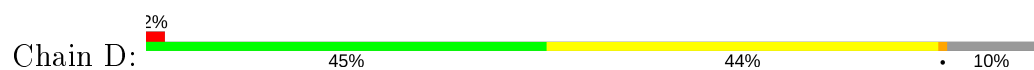
#### • Molecule 1: CviR transcriptional regulator



#### • Molecule 1: CviR transcriptional regulator



• Molecule 1: CviR transcriptional regulator



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | H 3   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 169.32Å 169.32Å 99.84Å<br>90.00° 90.00° 120.00°   | Depositor        |
| Resolution (Å)  | 48.88 – 3.25<br>48.88 – 3.25  | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 94.9 (48.88-3.25)<br>99.2 (48.88-3.25)  | Depositor<br>EDS |
| $R_{merge}$   | 0.06  | Depositor        |
| $R_{sym}$   | 0.06  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.58 (at 3.25Å)   | Xtriage          |
| Refinement program  | PHENIX (phenix.refine: 1.5_2)   | Depositor        |
| R, $R_{free}$   | 0.263 , 0.304<br>0.267 , 0.302  | Depositor<br>DCC |
| $R_{free}$ test set   | 845 reflections (5.06%)   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 90.8  | Xtriage          |
| Anisotropy  | 0.713   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 101.2  | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$   | Xtriage          |
| Estimated twinning fraction   | 0.034 for -2/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+4/3*l,-1/3*h+1/3*k+1/3*l<br>0.034 for -h,1/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+1/3*l<br>0.035 for -1/3*h+1/3*k+4/3*l,-k,2/3*h+1/3*k+1/3*l<br>0.039 for -h,2/3*h+1/3*k+4/3*l,1/3*h+2/3*k-1/3*l<br>0.045 for -1/3*h-2/3*k+4/3*l,-2/3*h-1/3*k-4/3*l,1/3*h-1/3*k-1/3*l<br>0.038 for 1/3*h+2/3*k-4/3*l,-k,-2/3*h-1/3*k-1/3*l<br>0.046 for h,-h-k,-l | Xtriage          |
| $F_o, F_c$ correlation  | 0.91  | EDS              |
| Total number of atoms   | 7738  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 140.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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 ⓘ

### 5.1 Standard geometry ⓘ

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

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     | 0.68         | 1/2021 (0.0%) | 0.83        | 3/2743 (0.1%)   |
| 1   | B     | 0.45         | 0/1927        | 0.65        | 2/2608 (0.1%)   |
| 1   | C     | 0.51         | 0/1941        | 0.69        | 4/2628 (0.2%)   |
| 1   | D     | 0.44         | 0/1927        | 0.68        | 2/2610 (0.1%)   |
| All | All   | 0.53         | 1/7816 (0.0%) | 0.72        | 11/10589 (0.1%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | A     | 258 | PRO  | C-N   | 5.79 | 1.45        | 1.34     |

All (11) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 189 | PRO  | N-CA-CB | 6.86  | 111.53      | 103.30   |
| 1   | B     | 197 | PRO  | N-CA-CB | 6.67  | 111.30      | 103.30   |
| 1   | D     | 197 | PRO  | N-CA-CB | 5.92  | 110.40      | 103.30   |
| 1   | A     | 28  | ILE  | CB-CA-C | -5.88 | 99.85       | 111.60   |
| 1   | C     | 57  | LEU  | N-CA-CB | -5.57 | 99.27       | 110.40   |
| 1   | C     | 49  | SER  | N-CA-C  | -5.34 | 96.58       | 111.00   |
| 1   | D     | 57  | LEU  | N-CA-CB | -5.28 | 99.85       | 110.40   |
| 1   | C     | 78  | VAL  | CB-CA-C | -5.23 | 101.47      | 111.40   |
| 1   | A     | 62  | ARG  | CB-CA-C | 5.05  | 120.51      | 110.40   |
| 1   | B     | 239 | LYS  | N-CA-CB | 5.05  | 119.69      | 110.60   |
| 1   | C     | 87  | GLN  | N-CA-CB | 5.01  | 119.62      | 110.60   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1977  | 0        | 1951     | 381     | 1            |
| 1   | B     | 1890  | 0        | 1873     | 312     | 1            |
| 1   | C     | 1902  | 0        | 1895     | 335     | 1            |
| 1   | D     | 1889  | 0        | 1867     | 231     | 0            |
| 2   | A     | 20    | 0        | 16       | 4       | 0            |
| 2   | B     | 20    | 0        | 16       | 5       | 0            |
| 2   | C     | 20    | 0        | 16       | 13      | 0            |
| 2   | D     | 20    | 0        | 16       | 5       | 0            |
| All | All   | 7738  | 0        | 7650     | 1157    | 2            |

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 75.

All (1157) 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:C:111:TRP:CD2  | 1:C:138:GLY:HA3 | 1.24                     | 1.61              |
| 1:A:57:LEU:HB2   | 1:A:80:TYR:CE2  | 1.18                     | 1.60              |
| 1:A:40:LEU:HD23  | 1:A:76:LEU:CD1  | 1.15                     | 1.56              |
| 1:B:48:LEU:CD2   | 1:B:56:LEU:HD21 | 1.20                     | 1.55              |
| 1:C:111:TRP:CE3  | 1:C:138:GLY:HA3 | 1.40                     | 1.54              |
| 1:A:40:LEU:CD2   | 1:A:76:LEU:CD1  | 1.86                     | 1.51              |
| 1:B:222:LEU:CD2  | 1:D:106:GLN:NE2 | 1.70                     | 1.48              |
| 1:D:57:LEU:HA    | 1:D:77:ASN:ND2  | 1.27                     | 1.48              |
| 1:C:109:VAL:CG1  | 1:C:114:ARG:HD2 | 1.43                     | 1.45              |
| 1:C:247:HIS:NE2  | 1:D:78:VAL:HG22 | 1.33                     | 1.44              |
| 1:B:222:LEU:HD21 | 1:D:106:GLN:NE2 | 1.15                     | 1.43              |
| 1:B:48:LEU:HD22  | 1:B:56:LEU:CD2  | 0.95                     | 1.41              |
| 1:C:109:VAL:CG1  | 1:C:114:ARG:CD  | 1.96                     | 1.41              |
| 1:B:48:LEU:CD2   | 1:B:56:LEU:CD2  | 1.74                     | 1.40              |
| 1:A:254:HIS:O    | 1:A:258:PRO:CD  | 1.67                     | 1.40              |
| 1:D:48:LEU:HD22  | 1:D:56:LEU:CD2  | 1.50                     | 1.38              |
| 1:D:17:THR:OG1   | 1:D:20:GLN:HG3  | 1.23                     | 1.35              |
| 1:A:40:LEU:CD2   | 1:A:76:LEU:HD13 | 1.44                     | 1.35              |
| 1:C:147:ARG:NH2  | 1:C:148:ASN:ND2 | 1.76                     | 1.33              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:17:THR:OG1   | 1:D:20:GLN:CG    | 1.77                     | 1.33              |
| 1:B:187:ASN:CG   | 1:B:188:LEU:HA   | 1.47                     | 1.33              |
| 1:C:111:TRP:CE3  | 1:C:138:GLY:CA   | 2.10                     | 1.33              |
| 1:A:57:LEU:CB    | 1:A:80:TYR:CE2   | 2.11                     | 1.32              |
| 1:C:56:LEU:H     | 1:C:79:SER:CB    | 1.43                     | 1.32              |
| 1:B:67:ASN:HB2   | 1:B:103:HIS:CB   | 1.60                     | 1.32              |
| 1:A:65:ASN:ND2   | 1:D:243:ASN:CG   | 1.84                     | 1.31              |
| 1:B:187:ASN:CB   | 1:B:188:LEU:HA   | 1.41                     | 1.30              |
| 1:C:44:LEU:HD13  | 1:C:77:ASN:ND2   | 1.47                     | 1.29              |
| 1:C:16:LEU:CD2   | 1:C:170:MET:HG2  | 1.59                     | 1.29              |
| 1:D:57:LEU:CA    | 1:D:77:ASN:HD22  | 1.34                     | 1.29              |
| 1:A:205:ILE:O    | 1:A:209:MET:HG2  | 1.29                     | 1.28              |
| 1:C:111:TRP:CD2  | 1:C:138:GLY:CA   | 2.13                     | 1.27              |
| 1:C:109:VAL:HG11 | 1:C:114:ARG:NH1  | 1.48                     | 1.27              |
| 1:A:57:LEU:CB    | 1:A:80:TYR:HE2   | 1.44                     | 1.27              |
| 1:A:203:TYR:O    | 1:A:207:HIS:CB   | 1.82                     | 1.26              |
| 1:A:203:TYR:O    | 1:A:207:HIS:HB2  | 1.08                     | 1.26              |
| 1:D:57:LEU:CA    | 1:D:77:ASN:ND2   | 1.89                     | 1.25              |
| 1:A:65:ASN:ND2   | 1:D:243:ASN:ND2  | 1.85                     | 1.24              |
| 1:B:67:ASN:CB    | 1:B:103:HIS:HB2  | 1.67                     | 1.24              |
| 1:A:65:ASN:HD21  | 1:D:243:ASN:ND2  | 1.29                     | 1.24              |
| 1:A:41:LYS:HD2   | 1:A:41:LYS:O     | 1.35                     | 1.23              |
| 1:C:15:GLY:C     | 1:C:16:LEU:HD12  | 1.57                     | 1.23              |
| 1:C:67:ASN:O     | 1:C:104:LEU:HD13 | 1.35                     | 1.23              |
| 1:C:247:HIS:NE2  | 1:D:78:VAL:CG2   | 2.00                     | 1.22              |
| 1:B:224:ILE:HG21 | 1:B:228:THR:CG2  | 1.70                     | 1.22              |
| 1:D:202:GLU:O    | 1:D:205:ILE:HB   | 1.40                     | 1.22              |
| 1:C:56:LEU:N     | 1:C:79:SER:HB3   | 1.51                     | 1.22              |
| 1:B:57:LEU:CB    | 1:B:77:ASN:HD22  | 1.53                     | 1.21              |
| 1:C:257:MET:HB2  | 1:C:258:PRO:HD3  | 1.23                     | 1.20              |
| 1:B:224:ILE:CG2  | 1:B:228:THR:CG2  | 2.18                     | 1.20              |
| 1:C:147:ARG:HH21 | 1:C:148:ASN:ND2  | 1.36                     | 1.20              |
| 1:B:67:ASN:CB    | 1:B:103:HIS:CB   | 2.18                     | 1.19              |
| 1:B:67:ASN:HB2   | 1:B:103:HIS:CA   | 1.72                     | 1.19              |
| 1:A:227:ARG:HG2  | 1:A:231:PHE:CE2  | 1.78                     | 1.16              |
| 1:B:187:ASN:HB3  | 1:B:188:LEU:HA   | 1.18                     | 1.16              |
| 1:C:17:THR:OG1   | 1:C:20:GLN:HG3   | 1.45                     | 1.16              |
| 1:A:190:PRO:HA   | 1:A:191:ALA:CB   | 1.63                     | 1.16              |
| 1:A:193:PRO:N    | 1:A:194:SER:HA   | 1.50                     | 1.16              |
| 1:C:55:ARG:HA    | 1:C:79:SER:OG    | 1.44                     | 1.15              |
| 1:A:190:PRO:CA   | 1:A:191:ALA:HB3  | 1.77                     | 1.15              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:16:LEU:HD21  | 1:C:170:MET:CG   | 1.76                     | 1.15              |
| 1:C:254:HIS:O    | 1:C:258:PRO:HD2  | 1.47                     | 1.15              |
| 1:D:48:LEU:HD22  | 1:D:56:LEU:HD23  | 1.29                     | 1.14              |
| 1:B:63:LEU:O     | 1:B:149:ASN:HB3  | 1.44                     | 1.14              |
| 1:A:254:HIS:O    | 1:A:258:PRO:HD2  | 1.44                     | 1.14              |
| 1:A:255:LEU:O    | 1:A:259:PRO:CD   | 1.94                     | 1.14              |
| 1:A:65:ASN:HD22  | 1:D:243:ASN:CG   | 1.43                     | 1.13              |
| 1:A:10:ARG:NH1   | 1:A:176:PRO:HB3  | 1.64                     | 1.13              |
| 1:D:40:LEU:HD23  | 1:D:76:LEU:HD23  | 1.13                     | 1.12              |
| 1:C:109:VAL:CG1  | 1:C:114:ARG:HH11 | 1.60                     | 1.12              |
| 1:B:67:ASN:HB3   | 1:B:103:HIS:CG   | 1.85                     | 1.12              |
| 1:B:224:ILE:HG22 | 1:B:228:THR:HB   | 1.13                     | 1.11              |
| 1:A:209:MET:HE3  | 1:A:245:ARG:HE   | 1.07                     | 1.11              |
| 1:B:226:GLU:HG2  | 1:B:230:LYS:HE2  | 1.25                     | 1.11              |
| 1:C:254:HIS:CG   | 1:D:74:ARG:HG3   | 1.86                     | 1.11              |
| 1:A:110:MET:HA   | 1:A:139:ILE:HD13 | 1.33                     | 1.11              |
| 1:D:55:ARG:HA    | 1:D:79:SER:HB3   | 1.18                     | 1.11              |
| 1:B:224:ILE:CG2  | 1:B:228:THR:HG21 | 1.77                     | 1.11              |
| 1:B:57:LEU:CG    | 1:B:77:ASN:HD22  | 1.64                     | 1.11              |
| 1:B:57:LEU:CG    | 1:B:77:ASN:ND2   | 2.14                     | 1.10              |
| 1:B:48:LEU:CD2   | 1:B:56:LEU:HD23  | 1.69                     | 1.10              |
| 1:B:57:LEU:HG    | 1:B:77:ASN:ND2   | 1.64                     | 1.10              |
| 1:B:20:GLN:HE22  | 1:B:166:ALA:CB   | 1.65                     | 1.10              |
| 1:C:111:TRP:HB2  | 1:C:138:GLY:H    | 1.03                     | 1.09              |
| 1:A:255:LEU:O    | 1:A:259:PRO:HD2  | 1.51                     | 1.09              |
| 1:A:110:MET:HA   | 1:A:139:ILE:CD1  | 1.80                     | 1.09              |
| 1:B:67:ASN:HB2   | 1:B:103:HIS:HA   | 1.33                     | 1.09              |
| 1:C:16:LEU:CD2   | 1:C:170:MET:CG   | 2.30                     | 1.09              |
| 1:B:48:LEU:HD22  | 1:B:56:LEU:CG    | 1.83                     | 1.09              |
| 1:C:11:PRO:HG2   | 1:D:33:HIS:CE1   | 1.86                     | 1.09              |
| 1:C:78:VAL:O     | 1:C:78:VAL:HG13  | 1.53                     | 1.09              |
| 1:B:187:ASN:CB   | 1:B:188:LEU:CA   | 2.30                     | 1.08              |
| 1:A:112:GLU:HG2  | 1:A:137:SER:HB3  | 1.35                     | 1.07              |
| 1:A:111:TRP:HB2  | 1:A:138:GLY:H    | 1.19                     | 1.07              |
| 1:A:40:LEU:HD23  | 1:A:76:LEU:HD12  | 1.31                     | 1.07              |
| 1:C:44:LEU:CD1   | 1:C:77:ASN:ND2   | 2.17                     | 1.07              |
| 1:A:55:ARG:HA    | 1:A:79:SER:OG    | 1.55                     | 1.07              |
| 1:A:254:HIS:O    | 1:A:258:PRO:HD3  | 1.50                     | 1.07              |
| 1:C:254:HIS:HB3  | 1:D:74:ARG:HA    | 1.31                     | 1.07              |
| 1:C:219:ALA:HB1  | 1:C:224:ILE:O    | 1.55                     | 1.07              |
| 1:D:74:ARG:HH12  | 1:D:186:ALA:HB2  | 1.16                     | 1.06              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:109:VAL:HG12 | 1:C:114:ARG:HD3  | 1.37                     | 1.06              |
| 1:A:227:ARG:CG   | 1:A:231:PHE:HE2  | 1.68                     | 1.05              |
| 1:A:227:ARG:HG2  | 1:A:231:PHE:HE2  | 0.88                     | 1.04              |
| 1:A:40:LEU:HD23  | 1:A:76:LEU:HD11  | 1.07                     | 1.04              |
| 1:A:77:ASN:OD1   | 1:A:78:VAL:N     | 1.90                     | 1.04              |
| 1:C:86:ASP:OD1   | 1:C:87:GLN:N     | 1.90                     | 1.04              |
| 1:A:254:HIS:ND1  | 1:B:74:ARG:HG3   | 1.72                     | 1.04              |
| 1:A:217:GLU:O    | 1:A:221:ILE:CD1  | 2.05                     | 1.04              |
| 1:A:57:LEU:HB2   | 1:A:80:TYR:CZ    | 1.93                     | 1.03              |
| 1:B:48:LEU:CG    | 1:B:56:LEU:CD2   | 2.36                     | 1.03              |
| 1:B:40:LEU:CD2   | 1:B:76:LEU:HD13  | 1.87                     | 1.03              |
| 1:B:187:ASN:HB3  | 1:B:188:LEU:CA   | 1.86                     | 1.03              |
| 1:D:224:ILE:CG2  | 1:D:228:THR:HB   | 1.88                     | 1.03              |
| 1:B:224:ILE:CG2  | 1:B:228:THR:HB   | 1.87                     | 1.02              |
| 1:C:16:LEU:HD23  | 1:C:170:MET:SD   | 1.99                     | 1.02              |
| 1:B:224:ILE:CG2  | 1:B:228:THR:CB   | 2.37                     | 1.02              |
| 1:C:109:VAL:CG1  | 1:C:114:ARG:HD3  | 1.80                     | 1.02              |
| 1:A:40:LEU:HD21  | 1:A:76:LEU:HD13  | 1.07                     | 1.02              |
| 1:C:53:SER:HB3   | 1:C:156:ILE:CG2  | 1.91                     | 1.01              |
| 1:B:58:LEU:H     | 1:B:77:ASN:HB3   | 1.22                     | 1.01              |
| 1:A:30:MET:HE2   | 1:A:43:PHE:CE1   | 1.96                     | 1.01              |
| 1:A:30:MET:CE    | 1:A:43:PHE:CE1   | 2.44                     | 1.01              |
| 1:B:57:LEU:HB2   | 1:B:77:ASN:HD22  | 1.20                     | 1.01              |
| 1:D:111:TRP:CE3  | 1:D:137:SER:O    | 2.13                     | 1.01              |
| 1:B:67:ASN:CB    | 1:B:103:HIS:CG   | 2.41                     | 1.00              |
| 1:D:111:TRP:HE3  | 1:D:137:SER:O    | 1.45                     | 1.00              |
| 1:B:96:HIS:CD2   | 1:B:122:GLU:CB   | 2.44                     | 1.00              |
| 1:C:109:VAL:HG11 | 1:C:114:ARG:HH11 | 0.90                     | 1.00              |
| 1:D:48:LEU:CD2   | 1:D:56:LEU:HD23  | 1.90                     | 1.00              |
| 1:C:44:LEU:HD12  | 1:C:77:ASN:CG    | 1.82                     | 1.00              |
| 1:A:192:SER:H    | 1:C:49:SER:HB2   | 1.19                     | 1.00              |
| 1:D:56:LEU:H     | 1:D:79:SER:HB2   | 1.26                     | 0.99              |
| 1:A:18:ALA:O     | 1:A:22:TRP:N     | 1.93                     | 0.99              |
| 1:A:102:ILE:CG2  | 1:A:106:GLN:HE21 | 1.76                     | 0.99              |
| 1:A:217:GLU:O    | 1:A:221:ILE:HD12 | 1.62                     | 0.99              |
| 1:D:48:LEU:HD22  | 1:D:56:LEU:HD21  | 1.44                     | 0.99              |
| 1:D:48:LEU:CD2   | 1:D:56:LEU:CD2   | 2.40                     | 0.99              |
| 1:B:57:LEU:HA    | 1:B:77:ASN:HB2   | 1.39                     | 0.98              |
| 1:B:109:VAL:HG21 | 1:B:114:ARG:HH21 | 1.27                     | 0.98              |
| 1:B:187:ASN:CG   | 1:B:188:LEU:CA   | 2.30                     | 0.98              |
| 1:B:78:VAL:HG23  | 1:B:78:VAL:O     | 1.57                     | 0.98              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:109:VAL:HG11 | 1:C:114:ARG:CD   | 1.84                     | 0.98              |
| 1:B:224:ILE:HG22 | 1:B:228:THR:CB   | 1.93                     | 0.98              |
| 1:C:237:ILE:HG23 | 1:C:242:ALA:HB3  | 1.43                     | 0.98              |
| 1:B:222:LEU:HD22 | 1:D:106:GLN:NE2  | 1.77                     | 0.98              |
| 1:D:12:LEU:O     | 1:D:173:CYS:SG   | 2.21                     | 0.98              |
| 1:C:111:TRP:CZ2  | 2:C:266:HLC:H6   | 1.99                     | 0.98              |
| 1:C:55:ARG:HD2   | 1:C:81:PRO:HD3   | 1.43                     | 0.98              |
| 1:A:198:LEU:N    | 1:A:199:SER:HA   | 1.75                     | 0.97              |
| 1:C:217:GLU:O    | 1:C:221:ILE:HG13 | 1.63                     | 0.97              |
| 1:D:17:THR:HG1   | 1:D:20:GLN:CG    | 1.77                     | 0.97              |
| 1:B:224:ILE:HG23 | 1:B:228:THR:HG21 | 1.46                     | 0.97              |
| 1:B:63:LEU:CD2   | 1:B:104:LEU:HD12 | 1.94                     | 0.97              |
| 1:A:242:ALA:HB1  | 1:A:247:HIS:HD1  | 1.28                     | 0.97              |
| 1:C:102:ILE:CG2  | 1:C:114:ARG:HH12 | 1.78                     | 0.96              |
| 1:C:147:ARG:NH2  | 1:C:148:ASN:HD22 | 1.46                     | 0.96              |
| 1:A:10:ARG:HH12  | 1:A:176:PRO:HB3  | 1.31                     | 0.96              |
| 1:B:40:LEU:HD23  | 1:B:76:LEU:HD13  | 1.42                     | 0.96              |
| 1:A:219:ALA:HB2  | 1:A:229:VAL:HG23 | 1.45                     | 0.96              |
| 1:C:44:LEU:CD1   | 1:C:77:ASN:CG    | 2.34                     | 0.96              |
| 1:B:48:LEU:CD1   | 1:B:56:LEU:HD23  | 1.94                     | 0.95              |
| 1:D:56:LEU:H     | 1:D:79:SER:CB    | 1.80                     | 0.95              |
| 1:C:43:PHE:HA    | 1:C:46:GLN:OE1   | 1.64                     | 0.95              |
| 1:B:57:LEU:HD23  | 1:B:57:LEU:C     | 1.87                     | 0.95              |
| 1:A:229:VAL:O    | 1:A:233:VAL:HG23 | 1.66                     | 0.95              |
| 1:A:250:VAL:HG22 | 2:B:266:HLC:CL1  | 2.03                     | 0.95              |
| 1:C:16:LEU:N     | 1:C:16:LEU:CD1   | 2.30                     | 0.95              |
| 1:B:20:GLN:NE2   | 1:B:166:ALA:HB1  | 1.82                     | 0.94              |
| 1:B:48:LEU:CG    | 1:B:56:LEU:HD21  | 1.94                     | 0.94              |
| 1:A:247:HIS:NE2  | 1:B:78:VAL:HA    | 1.81                     | 0.94              |
| 1:D:40:LEU:HD23  | 1:D:76:LEU:CD2   | 1.97                     | 0.94              |
| 1:B:109:VAL:HG21 | 1:B:114:ARG:NH2  | 1.82                     | 0.94              |
| 1:C:13:PRO:HG3   | 1:D:29:HIS:CD2   | 2.03                     | 0.94              |
| 1:C:67:ASN:O     | 1:C:104:LEU:CD1  | 2.15                     | 0.94              |
| 1:D:74:ARG:NH1   | 1:D:186:ALA:HB2  | 1.81                     | 0.94              |
| 1:A:193:PRO:CD   | 1:A:194:SER:HA   | 1.96                     | 0.94              |
| 1:B:56:LEU:H     | 1:B:79:SER:CB    | 1.80                     | 0.94              |
| 1:A:219:ALA:N    | 1:A:229:VAL:HG21 | 1.82                     | 0.94              |
| 1:A:64:ASN:OD1   | 1:A:66:GLN:N     | 1.99                     | 0.94              |
| 1:C:109:VAL:HG13 | 1:C:114:ARG:HD2  | 0.94                     | 0.94              |
| 1:A:41:LYS:C     | 1:A:41:LYS:HD2   | 1.82                     | 0.94              |
| 1:B:224:ILE:HG21 | 1:B:228:THR:HG22 | 1.46                     | 0.94              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:192:SER:CB   | 1:A:194:SER:CB   | 2.45                     | 0.93              |
| 1:A:197:PRO:HB2  | 1:A:199:SER:HB2  | 1.49                     | 0.93              |
| 1:C:111:TRP:HB2  | 1:C:138:GLY:N    | 1.82                     | 0.93              |
| 1:C:13:PRO:HA    | 1:C:173:CYS:SG   | 2.08                     | 0.93              |
| 1:A:30:MET:CE    | 1:A:43:PHE:CD1   | 2.52                     | 0.93              |
| 1:A:254:HIS:CE1  | 1:B:74:ARG:HG3   | 2.03                     | 0.93              |
| 1:C:254:HIS:CG   | 1:D:74:ARG:CG    | 2.52                     | 0.93              |
| 1:B:96:HIS:CD2   | 1:B:122:GLU:HB3  | 2.03                     | 0.93              |
| 1:C:44:LEU:HD12  | 1:C:77:ASN:CB    | 1.99                     | 0.92              |
| 1:A:193:PRO:N    | 1:A:194:SER:CA   | 2.29                     | 0.92              |
| 1:A:251:LEU:HD21 | 1:B:77:ASN:O     | 1.70                     | 0.92              |
| 1:B:77:ASN:O     | 1:B:78:VAL:HG12  | 1.68                     | 0.92              |
| 1:A:198:LEU:N    | 1:A:198:LEU:HD23 | 1.85                     | 0.92              |
| 1:A:246:THR:HA   | 1:A:249:ILE:HD12 | 1.47                     | 0.91              |
| 1:B:40:LEU:HD23  | 1:B:76:LEU:CD1   | 2.00                     | 0.91              |
| 1:A:102:ILE:CG2  | 1:A:106:GLN:NE2  | 2.34                     | 0.91              |
| 1:C:29:HIS:NE2   | 1:D:11:PRO:HA    | 1.85                     | 0.91              |
| 1:A:56:LEU:O     | 1:A:80:TYR:CE2   | 2.24                     | 0.91              |
| 1:B:57:LEU:HA    | 1:B:77:ASN:CB    | 2.00                     | 0.91              |
| 1:C:109:VAL:HG11 | 1:C:114:ARG:CZ   | 2.00                     | 0.91              |
| 1:C:102:ILE:HG23 | 1:C:114:ARG:HH22 | 1.34                     | 0.91              |
| 1:C:15:GLY:C     | 1:C:16:LEU:CD1   | 2.39                     | 0.91              |
| 1:C:119:LYS:HA   | 1:C:124:LYS:HE3  | 1.53                     | 0.90              |
| 1:C:219:ALA:CB   | 1:C:224:ILE:O    | 2.19                     | 0.90              |
| 1:B:96:HIS:CD2   | 1:B:122:GLU:HB2  | 2.06                     | 0.90              |
| 1:D:119:LYS:HA   | 1:D:124:LYS:HE3  | 1.53                     | 0.90              |
| 1:A:202:GLU:O    | 1:A:206:PHE:N    | 2.04                     | 0.90              |
| 1:B:254:HIS:O    | 1:B:258:PRO:HD2  | 1.71                     | 0.90              |
| 1:C:257:MET:CB   | 1:C:258:PRO:HD3  | 1.97                     | 0.90              |
| 1:C:102:ILE:CG2  | 1:C:114:ARG:NH1  | 2.35                     | 0.90              |
| 1:A:111:TRP:HB2  | 1:A:138:GLY:N    | 1.85                     | 0.90              |
| 1:C:254:HIS:CD2  | 1:D:74:ARG:HG3   | 2.06                     | 0.89              |
| 1:A:106:GLN:HG3  | 1:A:106:GLN:O    | 1.71                     | 0.89              |
| 1:A:209:MET:CE   | 1:A:245:ARG:HE   | 1.85                     | 0.89              |
| 1:B:119:LYS:HA   | 1:B:124:LYS:HE3  | 1.52                     | 0.89              |
| 1:B:226:GLU:CG   | 1:B:230:LYS:HE2  | 2.01                     | 0.89              |
| 1:C:109:VAL:HG13 | 1:C:114:ARG:CD   | 1.81                     | 0.89              |
| 1:D:17:THR:HG1   | 1:D:20:GLN:CD    | 1.76                     | 0.89              |
| 1:C:187:ASN:OD1  | 1:C:188:LEU:N    | 2.06                     | 0.89              |
| 1:A:198:LEU:HD23 | 1:A:198:LEU:H    | 1.35                     | 0.89              |
| 1:A:77:ASN:H     | 1:B:251:LEU:CD2  | 1.84                     | 0.89              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:193:PRO:HB2  | 1:A:194:SER:C    | 1.93                     | 0.88              |
| 1:A:193:PRO:HD2  | 1:A:194:SER:O    | 1.72                     | 0.88              |
| 1:C:29:HIS:CD2   | 1:D:11:PRO:HB3   | 2.09                     | 0.88              |
| 1:C:17:THR:HG23  | 1:C:20:GLN:OE1   | 1.73                     | 0.88              |
| 1:B:20:GLN:NE2   | 1:B:166:ALA:CB   | 2.37                     | 0.87              |
| 1:A:102:ILE:HG22 | 1:A:106:GLN:NE2  | 1.89                     | 0.87              |
| 1:A:119:LYS:HA   | 1:A:124:LYS:HE3  | 1.54                     | 0.87              |
| 1:C:17:THR:HG1   | 1:C:20:GLN:HG3   | 1.32                     | 0.87              |
| 1:B:99:ILE:O     | 1:B:102:ILE:HG13 | 1.75                     | 0.87              |
| 1:C:147:ARG:HH22 | 1:C:148:ASN:HD22 | 1.13                     | 0.87              |
| 1:A:192:SER:N    | 1:C:49:SER:HB2   | 1.86                     | 0.87              |
| 1:A:71:ARG:NH2   | 1:C:42:ALA:HB2   | 1.89                     | 0.86              |
| 1:B:48:LEU:CD1   | 1:B:56:LEU:CD2   | 2.53                     | 0.86              |
| 1:C:147:ARG:NH2  | 1:C:148:ASN:CG   | 2.29                     | 0.86              |
| 1:D:57:LEU:HA    | 1:D:77:ASN:HD22  | 0.70                     | 0.86              |
| 1:A:112:GLU:CG   | 1:A:137:SER:HB3  | 2.03                     | 0.86              |
| 1:B:63:LEU:HD21  | 1:B:104:LEU:CD1  | 2.05                     | 0.86              |
| 1:C:48:LEU:HD12  | 1:C:49:SER:N     | 1.90                     | 0.86              |
| 1:A:36:THR:CG2   | 1:A:39:GLU:HG3   | 2.06                     | 0.85              |
| 1:C:52:PRO:HG2   | 1:C:161:PRO:HA   | 1.58                     | 0.85              |
| 1:B:111:TRP:HB2  | 1:B:138:GLY:H    | 1.40                     | 0.85              |
| 1:A:257:MET:HB2  | 1:A:258:PRO:HD3  | 1.57                     | 0.85              |
| 1:D:188:LEU:O    | 1:D:188:LEU:HD13 | 1.76                     | 0.85              |
| 1:A:237:ILE:CD1  | 1:A:245:ARG:HB2  | 2.05                     | 0.85              |
| 1:D:78:VAL:O     | 1:D:78:VAL:HG12  | 1.73                     | 0.85              |
| 1:A:224:ILE:HB   | 1:A:228:THR:HB   | 1.59                     | 0.85              |
| 1:B:63:LEU:HD21  | 1:B:104:LEU:HD12 | 1.56                     | 0.85              |
| 1:C:111:TRP:CE3  | 1:C:138:GLY:N    | 2.44                     | 0.85              |
| 1:A:215:ASN:OD1  | 1:A:230:LYS:HG2  | 1.77                     | 0.85              |
| 1:B:16:LEU:HD23  | 1:B:16:LEU:N     | 1.92                     | 0.85              |
| 1:D:55:ARG:CA    | 1:D:79:SER:HB3   | 2.04                     | 0.85              |
| 1:A:30:MET:HE2   | 1:A:43:PHE:CD1   | 2.11                     | 0.84              |
| 1:A:65:ASN:HD21  | 1:D:243:ASN:HD21 | 1.25                     | 0.84              |
| 1:D:222:LEU:O    | 1:D:223:ASP:HB2  | 1.77                     | 0.84              |
| 1:C:111:TRP:CE2  | 1:C:138:GLY:HA3  | 2.09                     | 0.84              |
| 1:A:210:SER:HA   | 1:A:249:ILE:HG12 | 1.59                     | 0.84              |
| 1:B:226:GLU:HG2  | 1:B:230:LYS:CE   | 2.06                     | 0.84              |
| 1:D:17:THR:OG1   | 1:D:20:GLN:CD    | 2.14                     | 0.84              |
| 1:D:58:LEU:H     | 1:D:77:ASN:HB2   | 1.42                     | 0.84              |
| 1:A:255:LEU:O    | 1:A:259:PRO:HD3  | 1.75                     | 0.84              |
| 1:A:30:MET:CE    | 1:A:43:PHE:HE1   | 1.88                     | 0.84              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:63:LEU:HD11  | 1:C:104:LEU:HD22 | 1.58                     | 0.84              |
| 1:A:216:TRP:CH2  | 1:A:220:THR:OG1  | 2.30                     | 0.84              |
| 1:B:76:LEU:O     | 1:B:76:LEU:HD23  | 1.78                     | 0.84              |
| 1:D:202:GLU:O    | 1:D:205:ILE:CB   | 2.24                     | 0.84              |
| 1:A:219:ALA:CA   | 1:A:229:VAL:CG2  | 2.56                     | 0.84              |
| 1:A:54:GLU:O     | 1:A:79:SER:CB    | 2.25                     | 0.83              |
| 1:A:82:SER:CB    | 1:B:244:ASN:HD21 | 1.90                     | 0.83              |
| 1:D:48:LEU:HD13  | 1:D:56:LEU:HD23  | 1.58                     | 0.83              |
| 1:A:209:MET:HE1  | 1:A:233:VAL:HG21 | 1.61                     | 0.83              |
| 1:C:109:VAL:HG12 | 1:C:114:ARG:CD   | 1.97                     | 0.83              |
| 1:D:99:ILE:O     | 1:D:102:ILE:HG13 | 1.78                     | 0.83              |
| 1:A:30:MET:HE1   | 1:A:43:PHE:CE1   | 2.12                     | 0.83              |
| 1:A:192:SER:C    | 1:A:194:SER:HA   | 1.99                     | 0.83              |
| 1:A:219:ALA:CB   | 1:A:229:VAL:HG23 | 2.08                     | 0.83              |
| 1:B:235:ASN:O    | 1:B:239:LYS:HG3  | 1.77                     | 0.83              |
| 1:C:56:LEU:H     | 1:C:79:SER:HB3   | 0.68                     | 0.83              |
| 1:D:40:LEU:CD2   | 1:D:76:LEU:HD23  | 2.03                     | 0.83              |
| 1:A:224:ILE:HB   | 1:A:228:THR:CB   | 2.09                     | 0.83              |
| 1:B:63:LEU:HD12  | 1:B:150:ILE:O    | 1.78                     | 0.83              |
| 1:D:48:LEU:HD22  | 1:D:56:LEU:CG    | 2.08                     | 0.83              |
| 1:A:215:ASN:HB3  | 1:A:226:GLU:HG3  | 1.59                     | 0.82              |
| 1:B:63:LEU:CD1   | 1:B:150:ILE:C    | 2.47                     | 0.82              |
| 1:A:212:GLY:O    | 1:A:213:LYS:HD2  | 1.80                     | 0.82              |
| 1:B:183:ILE:O    | 1:B:187:ASN:N    | 2.11                     | 0.82              |
| 1:C:11:PRO:CG    | 1:D:33:HIS:CE1   | 2.62                     | 0.82              |
| 1:A:198:LEU:HA   | 1:A:255:LEU:HD11 | 1.62                     | 0.82              |
| 1:C:102:ILE:HG22 | 1:C:114:ARG:CZ   | 2.10                     | 0.82              |
| 1:C:49:SER:OG    | 1:C:50:GLN:OE1   | 1.96                     | 0.82              |
| 2:C:266:HLC:CL1  | 1:D:250:VAL:HG22 | 2.16                     | 0.82              |
| 1:B:221:ILE:HG23 | 1:D:103:HIS:CG   | 2.15                     | 0.81              |
| 1:B:48:LEU:HD13  | 1:B:56:LEU:CD2   | 2.10                     | 0.81              |
| 1:C:16:LEU:N     | 1:C:16:LEU:HD12  | 1.88                     | 0.81              |
| 1:C:82:SER:CB    | 1:D:244:ASN:HD21 | 1.92                     | 0.81              |
| 1:C:108:PRO:O    | 1:C:109:VAL:HG23 | 1.80                     | 0.81              |
| 1:A:36:THR:HG22  | 1:A:39:GLU:HG3   | 1.61                     | 0.81              |
| 1:D:48:LEU:CD1   | 1:D:56:LEU:HD23  | 2.10                     | 0.81              |
| 1:C:257:MET:HB2  | 1:C:258:PRO:CD   | 2.08                     | 0.81              |
| 1:D:57:LEU:HA    | 1:D:77:ASN:CG    | 2.00                     | 0.81              |
| 1:A:237:ILE:HD11 | 1:A:245:ARG:HB2  | 1.61                     | 0.81              |
| 1:A:55:ARG:CA    | 1:A:79:SER:OG    | 2.29                     | 0.81              |
| 1:C:234:ALA:O    | 1:C:238:ARG:HG3  | 1.79                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:20:GLN:HE22  | 1:B:166:ALA:HB1  | 1.37                     | 0.80              |
| 1:C:247:HIS:CD2  | 1:D:78:VAL:HG13  | 2.17                     | 0.80              |
| 1:B:109:VAL:CG2  | 1:B:114:ARG:HH21 | 1.93                     | 0.80              |
| 1:A:17:THR:O     | 1:A:21:GLN:HG3   | 1.80                     | 0.80              |
| 1:B:186:ALA:O    | 1:B:188:LEU:CD1  | 2.30                     | 0.80              |
| 1:B:56:LEU:H     | 1:B:79:SER:HB3   | 1.47                     | 0.80              |
| 1:B:67:ASN:HB2   | 1:B:103:HIS:HB2  | 1.39                     | 0.80              |
| 1:A:57:LEU:CB    | 1:A:80:TYR:CZ    | 2.60                     | 0.80              |
| 1:C:257:MET:SD   | 1:D:72:LEU:O     | 2.40                     | 0.80              |
| 1:C:53:SER:HB3   | 1:C:156:ILE:HG23 | 1.61                     | 0.80              |
| 1:A:192:SER:CB   | 1:A:194:SER:OG   | 2.30                     | 0.80              |
| 1:B:76:LEU:O     | 1:B:76:LEU:CD2   | 2.30                     | 0.80              |
| 1:B:85:LEU:HD22  | 2:B:266:HLC:H14  | 1.62                     | 0.80              |
| 1:D:235:ASN:O    | 1:D:239:LYS:HG3  | 1.82                     | 0.80              |
| 1:D:56:LEU:N     | 1:D:79:SER:HB2   | 1.97                     | 0.79              |
| 1:A:209:MET:HE3  | 1:A:245:ARG:NE   | 1.93                     | 0.79              |
| 1:C:111:TRP:CG   | 1:C:138:GLY:CA   | 2.64                     | 0.79              |
| 1:A:193:PRO:CD   | 1:A:194:SER:O    | 2.30                     | 0.79              |
| 1:C:56:LEU:N     | 1:C:79:SER:CB    | 2.27                     | 0.79              |
| 1:A:254:HIS:O    | 1:A:258:PRO:CG   | 2.29                     | 0.79              |
| 1:B:63:LEU:HD11  | 1:B:151:GLY:CA   | 2.11                     | 0.79              |
| 1:A:193:PRO:CG   | 1:A:194:SER:O    | 2.30                     | 0.79              |
| 1:A:254:HIS:ND1  | 1:B:74:ARG:CG    | 2.46                     | 0.79              |
| 1:A:57:LEU:HB3   | 1:A:80:TYR:OH    | 1.80                     | 0.79              |
| 1:B:181:ALA:O    | 1:B:185:VAL:HG23 | 1.81                     | 0.79              |
| 1:C:16:LEU:HD21  | 1:C:170:MET:HG2  | 0.85                     | 0.79              |
| 1:A:242:ALA:HB1  | 1:A:247:HIS:ND1  | 1.97                     | 0.79              |
| 1:B:77:ASN:O     | 1:B:78:VAL:CG1   | 2.30                     | 0.79              |
| 1:C:247:HIS:NE2  | 1:D:78:VAL:HG13  | 1.97                     | 0.79              |
| 1:C:102:ILE:CG2  | 1:C:114:ARG:HH22 | 1.94                     | 0.79              |
| 1:C:254:HIS:O    | 1:C:258:PRO:CD   | 2.30                     | 0.79              |
| 1:C:254:HIS:ND1  | 1:D:74:ARG:HG2   | 1.98                     | 0.79              |
| 1:D:205:ILE:HD13 | 1:D:222:LEU:HD11 | 1.65                     | 0.79              |
| 1:B:63:LEU:HD22  | 1:B:104:LEU:HD12 | 1.63                     | 0.78              |
| 1:B:63:LEU:CD1   | 1:B:150:ILE:O    | 2.31                     | 0.78              |
| 1:B:57:LEU:CB    | 1:B:77:ASN:ND2   | 2.39                     | 0.78              |
| 1:B:78:VAL:O     | 1:B:78:VAL:CG2   | 2.30                     | 0.78              |
| 1:A:99:ILE:O     | 1:A:102:ILE:HG13 | 1.83                     | 0.78              |
| 1:C:247:HIS:NE2  | 1:D:78:VAL:CG1   | 2.47                     | 0.78              |
| 1:C:111:TRP:CG   | 1:C:138:GLY:HA3  | 2.14                     | 0.78              |
| 1:C:205:ILE:O    | 1:C:209:MET:HG3  | 1.83                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:62:ARG:NE    | 1:A:73:GLU:OE2   | 2.17                     | 0.78              |
| 1:B:58:LEU:N     | 1:B:77:ASN:HB3   | 1.97                     | 0.78              |
| 1:A:36:THR:HG22  | 1:A:39:GLU:CG    | 2.14                     | 0.78              |
| 1:C:147:ARG:CZ   | 1:C:148:ASN:HB3  | 2.14                     | 0.77              |
| 1:A:192:SER:CB   | 1:A:194:SER:HB2  | 2.14                     | 0.77              |
| 1:A:65:ASN:HD22  | 1:D:243:ASN:CB   | 1.98                     | 0.77              |
| 1:A:198:LEU:HA   | 1:A:255:LEU:CD1  | 2.15                     | 0.77              |
| 1:B:244:ASN:OD1  | 1:B:247:HIS:HB3  | 1.85                     | 0.77              |
| 1:C:102:ILE:HG22 | 1:C:114:ARG:NH1  | 1.99                     | 0.77              |
| 1:A:215:ASN:OD1  | 1:A:230:LYS:CG   | 2.32                     | 0.77              |
| 1:C:102:ILE:CG2  | 1:C:114:ARG:NH2  | 2.47                     | 0.77              |
| 1:A:57:LEU:CA    | 1:A:80:TYR:HE2   | 1.96                     | 0.77              |
| 1:B:109:VAL:HG11 | 1:B:114:ARG:NH2  | 2.00                     | 0.77              |
| 1:A:226:GLU:HG2  | 1:A:230:LYS:HE3  | 1.67                     | 0.76              |
| 1:D:78:VAL:CG1   | 1:D:78:VAL:O     | 2.32                     | 0.76              |
| 1:A:112:GLU:CG   | 1:A:137:SER:CB   | 2.63                     | 0.76              |
| 1:A:80:TYR:OH    | 1:A:155:SER:HB2  | 1.84                     | 0.76              |
| 1:B:109:VAL:HG11 | 1:B:114:ARG:NE   | 2.01                     | 0.76              |
| 1:B:57:LEU:HB2   | 1:B:77:ASN:ND2   | 1.98                     | 0.76              |
| 1:C:78:VAL:O     | 1:C:78:VAL:CG1   | 2.30                     | 0.76              |
| 1:C:63:LEU:HD21  | 1:C:104:LEU:CD2  | 2.16                     | 0.75              |
| 1:C:82:SER:OG    | 1:D:246:THR:HG23 | 1.86                     | 0.75              |
| 1:D:188:LEU:HD13 | 1:D:188:LEU:C    | 2.07                     | 0.75              |
| 1:B:56:LEU:N     | 1:B:79:SER:HB3   | 2.02                     | 0.75              |
| 1:D:74:ARG:HH12  | 1:D:186:ALA:CB   | 1.98                     | 0.75              |
| 1:A:112:GLU:HG3  | 1:A:137:SER:HB2  | 1.69                     | 0.75              |
| 1:B:67:ASN:HB3   | 1:B:103:HIS:HB2  | 1.59                     | 0.75              |
| 1:A:217:GLU:O    | 1:A:221:ILE:CG1  | 2.34                     | 0.75              |
| 1:C:63:LEU:HD21  | 1:C:104:LEU:HD22 | 1.67                     | 0.74              |
| 1:B:186:ALA:O    | 1:B:188:LEU:HD12 | 1.88                     | 0.74              |
| 1:C:36:THR:HG22  | 1:C:38:ASN:H     | 1.52                     | 0.74              |
| 1:D:224:ILE:HG22 | 1:D:228:THR:HB   | 1.68                     | 0.74              |
| 1:A:190:PRO:HA   | 1:A:191:ALA:HB3  | 0.80                     | 0.74              |
| 1:A:237:ILE:HG22 | 1:A:242:ALA:O    | 1.87                     | 0.74              |
| 1:C:16:LEU:HD23  | 1:C:170:MET:CG   | 2.10                     | 0.74              |
| 1:A:62:ARG:CG    | 1:A:73:GLU:OE2   | 2.35                     | 0.74              |
| 1:C:56:LEU:O     | 1:C:79:SER:N     | 2.17                     | 0.74              |
| 1:B:48:LEU:HD13  | 1:B:56:LEU:HD23  | 1.68                     | 0.74              |
| 1:C:48:LEU:O     | 1:C:49:SER:C     | 2.22                     | 0.74              |
| 1:B:67:ASN:HD22  | 1:B:103:HIS:HB2  | 1.53                     | 0.73              |
| 1:C:108:PRO:O    | 1:C:109:VAL:CG2  | 2.36                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:36:THR:HG23  | 1:A:39:GLU:H     | 1.52                     | 0.73              |
| 1:C:11:PRO:HG2   | 1:D:33:HIS:HE1   | 1.50                     | 0.73              |
| 1:C:111:TRP:CB   | 1:C:138:GLY:H    | 1.92                     | 0.73              |
| 1:B:224:ILE:HG21 | 1:B:228:THR:HG21 | 1.49                     | 0.73              |
| 1:D:111:TRP:CE3  | 1:D:138:GLY:HA3  | 2.22                     | 0.73              |
| 1:D:48:LEU:CG    | 1:D:56:LEU:HD23  | 2.17                     | 0.73              |
| 1:A:209:MET:CE   | 1:A:233:VAL:HG11 | 2.19                     | 0.73              |
| 1:A:103:HIS:O    | 1:A:106:GLN:HG2  | 1.88                     | 0.73              |
| 1:C:44:LEU:CD1   | 1:C:77:ASN:CB    | 2.66                     | 0.73              |
| 1:B:85:LEU:CD2   | 2:B:266:HLC:H14  | 2.19                     | 0.73              |
| 1:C:254:HIS:ND1  | 1:D:74:ARG:CG    | 2.52                     | 0.73              |
| 1:A:82:SER:HB2   | 1:B:246:THR:HG23 | 1.71                     | 0.73              |
| 1:C:244:ASN:OD1  | 1:C:247:HIS:HB3  | 1.88                     | 0.72              |
| 1:C:111:TRP:CE2  | 2:C:266:HLC:H4   | 2.24                     | 0.72              |
| 1:B:19:SER:O     | 1:B:21:GLN:N     | 2.22                     | 0.72              |
| 1:D:74:ARG:NH1   | 1:D:186:ALA:CB   | 2.53                     | 0.72              |
| 1:A:188:LEU:O    | 1:A:188:LEU:HD12 | 1.90                     | 0.72              |
| 1:B:109:VAL:HG11 | 1:B:114:ARG:CZ   | 2.20                     | 0.72              |
| 1:A:245:ARG:HG2  | 1:A:245:ARG:HH11 | 1.52                     | 0.72              |
| 1:A:17:THR:HG22  | 1:A:18:ALA:N     | 2.04                     | 0.72              |
| 1:B:67:ASN:ND2   | 1:B:103:HIS:HB2  | 2.04                     | 0.72              |
| 1:B:111:TRP:HB2  | 1:B:138:GLY:N    | 2.03                     | 0.72              |
| 1:A:193:PRO:HG2  | 1:A:194:SER:O    | 1.89                     | 0.71              |
| 1:B:57:LEU:CD1   | 1:B:77:ASN:ND2   | 2.52                     | 0.71              |
| 1:A:219:ALA:N    | 1:A:229:VAL:CG2  | 2.52                     | 0.71              |
| 1:C:102:ILE:HG21 | 1:C:114:ARG:HH12 | 1.54                     | 0.71              |
| 1:A:106:GLN:CG   | 1:A:106:GLN:O    | 2.38                     | 0.71              |
| 1:D:244:ASN:OD1  | 1:D:247:HIS:HB3  | 1.91                     | 0.71              |
| 1:A:25:LEU:HD13  | 1:B:25:LEU:HD13  | 1.71                     | 0.71              |
| 1:C:29:HIS:HD2   | 1:D:11:PRO:HB3   | 1.51                     | 0.71              |
| 1:C:15:GLY:O     | 1:C:16:LEU:HD12  | 1.89                     | 0.71              |
| 1:D:29:HIS:O     | 1:D:33:HIS:CD2   | 2.43                     | 0.71              |
| 1:A:217:GLU:O    | 1:A:221:ILE:HG13 | 1.91                     | 0.71              |
| 1:B:99:ILE:HD13  | 1:B:114:ARG:HD2  | 1.72                     | 0.70              |
| 1:C:108:PRO:HG3  | 1:C:141:PHE:CD1  | 2.26                     | 0.70              |
| 1:A:193:PRO:CB   | 1:A:194:SER:C    | 2.59                     | 0.70              |
| 1:C:102:ILE:HG22 | 1:C:114:ARG:NH2  | 2.06                     | 0.70              |
| 1:A:36:THR:O     | 1:A:36:THR:HG23  | 1.90                     | 0.70              |
| 1:D:111:TRP:CZ2  | 2:D:266:HLC:H6   | 2.26                     | 0.70              |
| 1:A:110:MET:HA   | 1:A:139:ILE:HD12 | 1.72                     | 0.70              |
| 1:A:57:LEU:HD23  | 2:A:266:HLC:H9   | 1.72                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:245:ARG:HG2  | 1:A:245:ARG:NH1  | 2.07                     | 0.70              |
| 1:A:64:ASN:OD1   | 1:A:64:ASN:C     | 2.30                     | 0.70              |
| 1:B:48:LEU:CG    | 1:B:56:LEU:HD23  | 2.13                     | 0.70              |
| 1:C:43:PHE:HA    | 1:C:46:GLN:CD    | 2.10                     | 0.70              |
| 1:A:65:ASN:ND2   | 1:D:243:ASN:OD1  | 2.25                     | 0.70              |
| 1:D:17:THR:OG1   | 1:D:20:GLN:CB    | 2.40                     | 0.70              |
| 1:C:17:THR:OG1   | 1:C:20:GLN:CG    | 2.35                     | 0.70              |
| 1:A:210:SER:HB2  | 1:A:249:ILE:HG23 | 1.74                     | 0.69              |
| 1:B:202:GLU:O    | 1:B:205:ILE:HB   | 1.91                     | 0.69              |
| 1:B:48:LEU:HD21  | 1:B:56:LEU:HD23  | 1.72                     | 0.69              |
| 1:A:250:VAL:CG2  | 2:B:266:HLC:CL1  | 2.77                     | 0.69              |
| 1:C:52:PRO:HD3   | 1:C:167:LEU:CD2  | 2.21                     | 0.69              |
| 1:C:64:ASN:ND2   | 1:C:68:GLN:HG2   | 2.07                     | 0.69              |
| 1:C:44:LEU:HD13  | 1:C:77:ASN:HD22  | 1.55                     | 0.69              |
| 1:A:219:ALA:HB2  | 1:A:229:VAL:CG2  | 2.20                     | 0.69              |
| 1:A:219:ALA:HA   | 1:A:229:VAL:CG2  | 2.22                     | 0.69              |
| 1:C:111:TRP:CZ2  | 2:C:266:HLC:C4   | 2.76                     | 0.69              |
| 1:C:64:ASN:HD21  | 1:C:68:GLN:HG2   | 1.56                     | 0.69              |
| 1:A:216:TRP:HZ3  | 1:A:225:SER:HA   | 1.58                     | 0.69              |
| 1:A:202:GLU:OE2  | 1:A:239:LYS:CD   | 2.40                     | 0.69              |
| 1:B:63:LEU:HD11  | 1:B:151:GLY:HA3  | 1.72                     | 0.69              |
| 1:D:187:ASN:O    | 1:D:188:LEU:HB2  | 1.92                     | 0.69              |
| 1:A:10:ARG:HH22  | 1:A:143:ALA:HA   | 1.55                     | 0.69              |
| 1:B:109:VAL:HG11 | 1:B:114:ARG:HE   | 1.58                     | 0.69              |
| 1:C:53:SER:OG    | 1:C:157:ALA:O    | 2.08                     | 0.69              |
| 1:A:10:ARG:NH1   | 1:A:176:PRO:CB   | 2.51                     | 0.69              |
| 1:A:193:PRO:HD2  | 1:A:194:SER:HA   | 1.74                     | 0.68              |
| 1:B:108:PRO:HG3  | 1:B:172:ASN:OD1  | 1.93                     | 0.68              |
| 1:C:36:THR:HG22  | 1:C:37:GLU:N     | 2.07                     | 0.68              |
| 1:D:10:ARG:N     | 1:D:11:PRO:CD    | 2.56                     | 0.68              |
| 1:C:102:ILE:CG2  | 1:C:114:ARG:CZ   | 2.71                     | 0.68              |
| 1:A:54:GLU:O     | 1:A:79:SER:OG    | 2.11                     | 0.68              |
| 1:B:67:ASN:HA    | 1:B:103:HIS:CD2  | 2.29                     | 0.68              |
| 1:C:111:TRP:CH2  | 2:C:266:HLC:H6   | 2.28                     | 0.68              |
| 1:A:102:ILE:HG23 | 1:A:106:GLN:HE21 | 1.55                     | 0.68              |
| 1:A:30:MET:CE    | 1:A:43:PHE:HD1   | 2.04                     | 0.68              |
| 1:C:104:LEU:N    | 1:C:104:LEU:HD12 | 2.09                     | 0.68              |
| 1:A:54:GLU:O     | 1:A:79:SER:HB2   | 1.94                     | 0.68              |
| 1:C:48:LEU:HA    | 1:C:51:ALA:HB3   | 1.76                     | 0.68              |
| 1:A:213:LYS:NZ   | 1:A:217:GLU:HB3  | 2.09                     | 0.68              |
| 1:A:63:LEU:HD21  | 1:A:104:LEU:HD22 | 1.76                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:55:ARG:HA    | 1:D:79:SER:CB    | 2.10                     | 0.68              |
| 1:B:20:GLN:HE22  | 1:B:166:ALA:HB3  | 1.58                     | 0.67              |
| 1:C:108:PRO:HG3  | 1:C:141:PHE:HD1  | 1.59                     | 0.67              |
| 1:D:209:MET:SD   | 1:D:233:VAL:HG13 | 2.34                     | 0.67              |
| 1:B:201:ARG:HD3  | 1:B:201:ARG:O    | 1.95                     | 0.67              |
| 1:C:254:HIS:HB3  | 1:D:74:ARG:CA    | 2.16                     | 0.67              |
| 1:C:80:TYR:OH    | 2:C:266:HLC:O4   | 2.07                     | 0.67              |
| 1:B:188:LEU:N    | 1:B:188:LEU:HD12 | 2.10                     | 0.67              |
| 1:A:112:GLU:HG3  | 1:A:137:SER:CB   | 2.23                     | 0.67              |
| 1:A:257:MET:H    | 1:A:258:PRO:CD   | 2.06                     | 0.67              |
| 1:B:57:LEU:HD12  | 1:B:77:ASN:ND2   | 2.10                     | 0.67              |
| 1:C:55:ARG:CA    | 1:C:79:SER:OG    | 2.35                     | 0.67              |
| 1:B:55:ARG:HA    | 1:B:79:SER:HB3   | 1.76                     | 0.67              |
| 1:A:224:ILE:CB   | 1:A:228:THR:HB   | 2.23                     | 0.67              |
| 1:C:96:HIS:ND1   | 1:C:122:GLU:HB3  | 2.10                     | 0.67              |
| 1:C:36:THR:HB    | 1:C:39:GLU:HG3   | 1.76                     | 0.67              |
| 1:A:30:MET:HE2   | 1:A:43:PHE:HE1   | 1.47                     | 0.67              |
| 1:C:109:VAL:HG11 | 1:C:114:ARG:NE   | 2.10                     | 0.67              |
| 1:B:77:ASN:C     | 1:B:78:VAL:CG1   | 2.63                     | 0.67              |
| 1:A:242:ALA:HB2  | 1:A:251:LEU:HD12 | 1.78                     | 0.66              |
| 1:A:36:THR:O     | 1:A:36:THR:CG2   | 2.41                     | 0.66              |
| 1:B:56:LEU:N     | 1:B:79:SER:CB    | 2.57                     | 0.66              |
| 2:C:266:HLC:CL1  | 1:D:250:VAL:CG2  | 2.80                     | 0.66              |
| 1:C:147:ARG:NH2  | 1:C:148:ASN:CB   | 2.58                     | 0.66              |
| 1:A:209:MET:HE1  | 1:A:233:VAL:HG11 | 1.76                     | 0.66              |
| 1:A:224:ILE:HD12 | 1:A:228:THR:HG22 | 1.76                     | 0.66              |
| 1:D:64:ASN:ND2   | 1:D:68:GLN:HB2   | 2.11                     | 0.66              |
| 1:A:210:SER:CB   | 1:A:249:ILE:HG23 | 2.25                     | 0.66              |
| 1:B:109:VAL:HG11 | 1:B:114:ARG:HH21 | 1.59                     | 0.66              |
| 1:A:112:GLU:HG2  | 1:A:137:SER:CB   | 2.19                     | 0.66              |
| 1:C:16:LEU:HD13  | 1:C:16:LEU:N     | 2.11                     | 0.66              |
| 1:A:202:GLU:OE2  | 1:A:239:LYS:HD2  | 1.96                     | 0.66              |
| 1:B:56:LEU:O     | 1:B:57:LEU:CB    | 2.44                     | 0.65              |
| 1:B:57:LEU:HD23  | 1:B:58:LEU:N     | 2.11                     | 0.65              |
| 1:A:193:PRO:HB2  | 1:A:195:ASN:N    | 2.10                     | 0.65              |
| 1:A:193:PRO:CD   | 1:A:194:SER:CA   | 2.72                     | 0.65              |
| 1:C:77:ASN:O     | 1:C:77:ASN:ND2   | 2.30                     | 0.65              |
| 1:D:63:LEU:HD21  | 1:D:104:LEU:HD22 | 1.79                     | 0.65              |
| 1:A:240:LEU:HD13 | 1:A:252:GLY:HA3  | 1.78                     | 0.65              |
| 1:A:64:ASN:OD1   | 1:A:65:ASN:N     | 2.30                     | 0.65              |
| 1:A:237:ILE:HD13 | 1:A:245:ARG:HB2  | 1.77                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:237:ILE:HG23 | 1:D:242:ALA:HB3  | 1.77                     | 0.65              |
| 1:A:224:ILE:CG1  | 1:A:228:THR:HB   | 2.27                     | 0.65              |
| 1:A:71:ARG:HH21  | 1:C:42:ALA:HB2   | 1.60                     | 0.65              |
| 1:B:88:TYR:HA    | 1:B:93:TYR:HD2   | 1.62                     | 0.65              |
| 1:B:67:ASN:CG    | 1:B:103:HIS:HB2  | 2.16                     | 0.65              |
| 1:B:112:GLU:HG3  | 1:B:137:SER:HB3  | 1.79                     | 0.65              |
| 1:C:17:THR:N     | 1:C:20:GLN:HB2   | 2.11                     | 0.65              |
| 1:B:237:ILE:HG23 | 1:B:242:ALA:HB3  | 1.78                     | 0.65              |
| 1:B:57:LEU:CD2   | 1:B:57:LEU:C     | 2.62                     | 0.65              |
| 1:A:19:SER:OG    | 1:A:20:GLN:N     | 2.30                     | 0.64              |
| 1:A:56:LEU:C     | 1:A:80:TYR:CE2   | 2.69                     | 0.64              |
| 1:D:187:ASN:OD1  | 1:D:188:LEU:N    | 2.30                     | 0.64              |
| 1:C:247:HIS:CE1  | 1:D:78:VAL:CG2   | 2.80                     | 0.64              |
| 1:A:77:ASN:H     | 1:B:251:LEU:HD21 | 1.63                     | 0.64              |
| 1:A:110:MET:CA   | 1:A:139:ILE:CD1  | 2.67                     | 0.64              |
| 1:A:216:TRP:CZ2  | 1:A:220:THR:OG1  | 2.50                     | 0.64              |
| 1:A:71:ARG:NH2   | 1:C:42:ALA:CB    | 2.61                     | 0.64              |
| 1:B:179:HIS:NE2  | 1:B:183:ILE:HD11 | 2.12                     | 0.64              |
| 1:C:200:GLN:OE1  | 1:C:200:GLN:HA   | 1.97                     | 0.64              |
| 1:A:111:TRP:CE3  | 1:A:138:GLY:HA3  | 2.33                     | 0.64              |
| 1:A:56:LEU:O     | 1:A:80:TYR:CD2   | 2.50                     | 0.64              |
| 1:C:139:ILE:HG13 | 1:C:161:PRO:HB2  | 1.80                     | 0.64              |
| 1:A:206:PHE:HD1  | 1:A:209:MET:HB2  | 1.63                     | 0.64              |
| 1:B:96:HIS:HD2   | 1:B:122:GLU:HB2  | 1.56                     | 0.64              |
| 1:C:147:ARG:NH2  | 1:C:148:ASN:HB3  | 2.12                     | 0.64              |
| 1:D:205:ILE:HD13 | 1:D:222:LEU:CD1  | 2.27                     | 0.64              |
| 1:A:197:PRO:HB2  | 1:A:199:SER:CB   | 2.27                     | 0.63              |
| 1:A:206:PHE:CD1  | 1:A:206:PHE:O    | 2.51                     | 0.63              |
| 1:B:57:LEU:HD12  | 1:B:77:ASN:HD21  | 1.63                     | 0.63              |
| 1:C:235:ASN:O    | 1:C:239:LYS:HG3  | 1.98                     | 0.63              |
| 1:A:219:ALA:CA   | 1:A:229:VAL:HG23 | 2.27                     | 0.63              |
| 1:A:209:MET:CE   | 1:A:233:VAL:CG1  | 2.77                     | 0.63              |
| 1:A:96:HIS:ND1   | 1:A:122:GLU:HB3  | 2.14                     | 0.63              |
| 1:B:222:LEU:HD21 | 1:D:106:GLN:CD   | 2.12                     | 0.63              |
| 1:A:71:ARG:HD3   | 1:C:38:ASN:HB3   | 1.79                     | 0.63              |
| 1:C:247:HIS:NE2  | 1:D:78:VAL:CB    | 2.61                     | 0.63              |
| 1:D:36:THR:OG1   | 1:D:39:GLU:HG3   | 1.97                     | 0.63              |
| 1:C:12:LEU:O     | 1:C:173:CYS:SG   | 2.57                     | 0.63              |
| 1:A:257:MET:H    | 1:A:258:PRO:HD2  | 1.63                     | 0.63              |
| 1:B:67:ASN:CB    | 1:B:103:HIS:CD2  | 2.81                     | 0.63              |
| 1:A:190:PRO:O    | 1:C:49:SER:OG    | 2.15                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:237:ILE:CG2  | 1:A:242:ALA:O    | 2.46                     | 0.63              |
| 1:B:64:ASN:ND2   | 1:B:68:GLN:O     | 2.30                     | 0.63              |
| 1:C:17:THR:H     | 1:C:20:GLN:HB2   | 1.64                     | 0.63              |
| 1:A:102:ILE:HG23 | 1:A:106:GLN:NE2  | 2.11                     | 0.63              |
| 1:D:111:TRP:HE3  | 1:D:137:SER:C    | 2.02                     | 0.63              |
| 1:A:226:GLU:CG   | 1:A:230:LYS:HE3  | 2.29                     | 0.62              |
| 1:A:209:MET:HE1  | 1:A:233:VAL:CG2  | 2.28                     | 0.62              |
| 1:C:55:ARG:HD2   | 1:C:81:PRO:CD    | 2.24                     | 0.62              |
| 1:A:209:MET:HE2  | 1:A:233:VAL:CG1  | 2.29                     | 0.62              |
| 1:A:111:TRP:N    | 1:A:138:GLY:O    | 2.27                     | 0.62              |
| 1:D:186:ALA:O    | 1:D:187:ASN:CG   | 2.38                     | 0.62              |
| 1:A:10:ARG:NH2   | 1:A:143:ALA:HA   | 2.14                     | 0.62              |
| 1:B:181:ALA:HA   | 1:B:184:ARG:HH21 | 1.62                     | 0.62              |
| 1:A:233:VAL:HG11 | 1:A:245:ARG:HD2  | 1.81                     | 0.62              |
| 1:A:77:ASN:N     | 1:B:251:LEU:CD2  | 2.62                     | 0.62              |
| 1:A:215:ASN:O    | 1:A:226:GLU:HA   | 2.00                     | 0.62              |
| 1:D:16:LEU:CD2   | 1:D:20:GLN:OE1   | 2.48                     | 0.62              |
| 1:A:241:ASN:HB3  | 1:B:41:LYS:HD2   | 1.81                     | 0.62              |
| 1:B:67:ASN:HB3   | 1:B:103:HIS:CB   | 2.02                     | 0.62              |
| 1:C:81:PRO:O     | 1:C:85:LEU:HG    | 2.00                     | 0.62              |
| 1:C:29:HIS:NE2   | 1:D:11:PRO:CA    | 2.62                     | 0.62              |
| 1:B:63:LEU:HD12  | 1:B:150:ILE:C    | 2.15                     | 0.62              |
| 1:D:17:THR:HG1   | 1:D:20:GLN:CB    | 2.13                     | 0.62              |
| 1:A:96:HIS:CE1   | 1:A:122:GLU:HB3  | 2.35                     | 0.61              |
| 1:B:181:ALA:CA   | 1:B:184:ARG:HH21 | 2.13                     | 0.61              |
| 1:B:20:GLN:CD    | 1:B:166:ALA:HB1  | 2.19                     | 0.61              |
| 1:C:56:LEU:HB3   | 1:C:156:ILE:HG12 | 1.82                     | 0.61              |
| 1:A:242:ALA:CB   | 1:A:247:HIS:HD1  | 2.08                     | 0.61              |
| 1:A:57:LEU:CD2   | 2:A:266:HLC:H9   | 2.30                     | 0.61              |
| 1:C:43:PHE:CD1   | 1:C:46:GLN:OE1   | 2.53                     | 0.61              |
| 1:C:43:PHE:HD1   | 1:C:46:GLN:OE1   | 1.83                     | 0.61              |
| 1:D:58:LEU:N     | 1:D:77:ASN:HB2   | 2.15                     | 0.61              |
| 1:A:57:LEU:CB    | 1:A:80:TYR:OH    | 2.46                     | 0.61              |
| 1:B:109:VAL:CB   | 1:B:114:ARG:HH21 | 2.13                     | 0.61              |
| 1:B:14:ALA:O     | 1:B:16:LEU:CD2   | 2.49                     | 0.61              |
| 1:C:111:TRP:CB   | 1:C:138:GLY:N    | 2.59                     | 0.61              |
| 1:A:179:HIS:NE2  | 1:A:183:ILE:HD11 | 2.15                     | 0.61              |
| 1:B:40:LEU:HD23  | 1:B:76:LEU:CD2   | 2.31                     | 0.61              |
| 1:A:30:MET:HE1   | 1:A:43:PHE:CD1   | 2.30                     | 0.60              |
| 1:B:80:TYR:OH    | 2:B:266:HLC:O4   | 2.18                     | 0.60              |
| 1:C:219:ALA:CA   | 1:C:224:ILE:O    | 2.49                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:88:TYR:HA    | 1:C:93:TYR:HD2   | 1.66                     | 0.60              |
| 1:C:56:LEU:O     | 1:C:79:SER:CB    | 2.49                     | 0.60              |
| 1:D:57:LEU:HA    | 1:D:77:ASN:CB    | 2.32                     | 0.60              |
| 1:A:195:ASN:OD1  | 1:B:188:LEU:CD2  | 2.49                     | 0.60              |
| 1:B:112:GLU:CG   | 1:B:137:SER:HB3  | 2.32                     | 0.60              |
| 1:C:247:HIS:CE1  | 1:D:78:VAL:HG22  | 2.29                     | 0.60              |
| 1:A:192:SER:CB   | 1:A:194:SER:HA   | 2.32                     | 0.60              |
| 1:B:77:ASN:C     | 1:B:78:VAL:HG13  | 2.22                     | 0.60              |
| 1:C:13:PRO:CA    | 1:C:173:CYS:SG   | 2.86                     | 0.60              |
| 1:A:198:LEU:N    | 1:A:199:SER:CA   | 2.59                     | 0.59              |
| 1:B:108:PRO:HG3  | 1:B:141:PHE:HD1  | 1.67                     | 0.59              |
| 1:C:82:SER:OG    | 1:D:244:ASN:ND2  | 2.29                     | 0.59              |
| 1:C:11:PRO:HB2   | 1:D:33:HIS:CE1   | 2.37                     | 0.59              |
| 1:D:56:LEU:N     | 1:D:79:SER:CB    | 2.57                     | 0.59              |
| 1:A:224:ILE:HD12 | 1:A:228:THR:CG2  | 2.31                     | 0.59              |
| 1:C:109:VAL:HG11 | 1:C:114:ARG:HD2  | 1.54                     | 0.59              |
| 1:B:187:ASN:HB3  | 1:B:188:LEU:HG   | 1.85                     | 0.59              |
| 1:B:19:SER:O     | 1:B:22:TRP:N     | 2.36                     | 0.59              |
| 1:B:48:LEU:CB    | 1:B:56:LEU:HD21  | 2.32                     | 0.59              |
| 1:D:48:LEU:HD22  | 1:D:56:LEU:HG    | 1.84                     | 0.59              |
| 1:C:211:ARG:HG2  | 1:C:211:ARG:O    | 2.03                     | 0.59              |
| 1:C:56:LEU:O     | 1:C:79:SER:HB3   | 2.01                     | 0.59              |
| 1:A:255:LEU:C    | 1:A:258:PRO:HD2  | 2.23                     | 0.59              |
| 1:A:40:LEU:CD2   | 1:A:76:LEU:HD11  | 1.89                     | 0.59              |
| 1:B:40:LEU:HD23  | 1:B:76:LEU:HD22  | 1.84                     | 0.59              |
| 1:C:257:MET:CB   | 1:C:258:PRO:CD   | 2.74                     | 0.59              |
| 1:C:82:SER:OG    | 1:D:246:THR:CG2  | 2.50                     | 0.59              |
| 1:D:56:LEU:HD12  | 1:D:77:ASN:OD1   | 2.02                     | 0.59              |
| 1:A:203:TYR:O    | 1:A:207:HIS:HB3  | 1.97                     | 0.59              |
| 1:A:244:ASN:O    | 1:A:247:HIS:HB3  | 2.03                     | 0.59              |
| 1:A:233:VAL:O    | 1:A:236:VAL:HB   | 2.03                     | 0.58              |
| 1:C:96:HIS:CE1   | 1:C:122:GLU:HB3  | 2.38                     | 0.58              |
| 1:D:218:ILE:O    | 1:D:222:LEU:HG   | 2.03                     | 0.58              |
| 1:B:109:VAL:CG1  | 1:B:114:ARG:HH21 | 2.16                     | 0.58              |
| 1:B:166:ALA:O    | 1:B:170:MET:HG3  | 2.01                     | 0.58              |
| 1:D:111:TRP:CE3  | 1:D:137:SER:C    | 2.75                     | 0.58              |
| 1:D:224:ILE:CG2  | 1:D:228:THR:CB   | 2.75                     | 0.58              |
| 1:D:56:LEU:HD12  | 1:D:77:ASN:ND2   | 2.18                     | 0.58              |
| 1:C:63:LEU:CD1   | 1:C:104:LEU:HD22 | 2.30                     | 0.58              |
| 1:C:13:PRO:CG    | 1:D:29:HIS:CD2   | 2.83                     | 0.58              |
| 1:A:227:ARG:O    | 1:A:231:PHE:CD2  | 2.56                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:64:ASN:C     | 1:D:64:ASN:OD1   | 2.41                     | 0.58              |
| 1:A:206:PHE:HE2  | 1:A:252:GLY:O    | 1.85                     | 0.58              |
| 1:C:206:PHE:HA   | 1:C:209:MET:HG3  | 1.85                     | 0.58              |
| 1:A:227:ARG:CG   | 1:A:231:PHE:CE2  | 2.59                     | 0.58              |
| 1:A:192:SER:CB   | 1:A:194:SER:CA   | 2.82                     | 0.58              |
| 1:B:187:ASN:ND2  | 1:B:188:LEU:HA   | 2.17                     | 0.58              |
| 1:B:63:LEU:O     | 1:B:149:ASN:CB   | 2.37                     | 0.58              |
| 1:A:56:LEU:N     | 1:A:79:SER:OG    | 2.37                     | 0.58              |
| 1:C:111:TRP:CZ2  | 2:C:266:HLC:H4   | 2.39                     | 0.58              |
| 1:B:187:ASN:CG   | 1:B:188:LEU:C    | 2.62                     | 0.57              |
| 1:C:175:THR:N    | 1:C:176:PRO:HD2  | 2.19                     | 0.57              |
| 1:D:17:THR:OG1   | 1:D:20:GLN:OE1   | 2.15                     | 0.57              |
| 1:B:56:LEU:O     | 1:B:80:TYR:CD2   | 2.57                     | 0.57              |
| 1:C:108:PRO:C    | 1:C:109:VAL:HG23 | 2.23                     | 0.57              |
| 1:A:199:SER:N    | 1:A:202:GLU:HB2  | 2.20                     | 0.57              |
| 1:B:104:LEU:CD2  | 1:B:142:SER:HB2  | 2.33                     | 0.57              |
| 1:C:52:PRO:HD3   | 1:C:167:LEU:HD21 | 1.85                     | 0.57              |
| 1:A:203:TYR:O    | 1:A:207:HIS:N    | 2.36                     | 0.57              |
| 1:A:88:TYR:HA    | 1:A:93:TYR:HD2   | 1.69                     | 0.57              |
| 1:A:198:LEU:N    | 1:A:198:LEU:CD2  | 2.59                     | 0.57              |
| 1:A:71:ARG:NH2   | 1:C:42:ALA:CA    | 2.68                     | 0.57              |
| 1:B:111:TRP:CE3  | 1:B:138:GLY:HA3  | 2.39                     | 0.57              |
| 1:A:111:TRP:CZ2  | 2:A:266:HLC:H6   | 2.40                     | 0.57              |
| 1:A:148:ASN:OD1  | 1:A:150:ILE:HG22 | 2.05                     | 0.57              |
| 1:A:190:PRO:HB2  | 1:A:192:SER:N    | 2.20                     | 0.57              |
| 1:B:148:ASN:OD1  | 1:B:150:ILE:HG22 | 2.05                     | 0.57              |
| 1:B:43:PHE:O     | 1:B:47:VAL:HG23  | 2.05                     | 0.57              |
| 1:B:63:LEU:HD11  | 1:B:150:ILE:C    | 2.25                     | 0.57              |
| 1:D:179:HIS:NE2  | 1:D:183:ILE:HD11 | 2.19                     | 0.57              |
| 1:B:63:LEU:HB2   | 1:B:149:ASN:C    | 2.25                     | 0.57              |
| 1:B:187:ASN:HB3  | 1:B:188:LEU:CB   | 2.35                     | 0.57              |
| 1:C:53:SER:HB3   | 1:C:156:ILE:HG22 | 1.83                     | 0.57              |
| 1:A:206:PHE:CE2  | 1:A:252:GLY:O    | 2.58                     | 0.56              |
| 1:B:167:LEU:O    | 1:B:168:VAL:C    | 2.43                     | 0.56              |
| 1:C:243:ASN:H    | 1:C:247:HIS:HD1  | 1.52                     | 0.56              |
| 1:C:237:ILE:HG12 | 1:C:248:ALA:HB2  | 1.86                     | 0.56              |
| 1:A:193:PRO:CD   | 1:A:194:SER:C    | 2.73                     | 0.56              |
| 1:A:199:SER:H    | 1:A:202:GLU:HB2  | 1.70                     | 0.56              |
| 1:C:44:LEU:CD1   | 1:C:77:ASN:HB3   | 2.35                     | 0.56              |
| 1:A:209:MET:SD   | 1:A:218:ILE:HD13 | 2.45                     | 0.56              |
| 1:C:102:ILE:HG23 | 1:C:114:ARG:NH2  | 2.08                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:11:PRO:CB    | 1:D:33:HIS:CE1   | 2.88                     | 0.56              |
| 1:A:213:LYS:HE3  | 1:A:217:GLU:CB   | 2.35                     | 0.56              |
| 1:A:25:LEU:CD1   | 1:B:25:LEU:HD13  | 2.35                     | 0.56              |
| 1:B:226:GLU:OE2  | 1:B:230:LYS:HE2  | 2.05                     | 0.56              |
| 1:B:79:SER:O     | 1:B:80:TYR:O     | 2.23                     | 0.56              |
| 1:C:53:SER:CB    | 1:C:157:ALA:O    | 2.52                     | 0.56              |
| 1:C:36:THR:HG22  | 1:C:37:GLU:H     | 1.70                     | 0.56              |
| 1:A:13:PRO:HD3   | 1:A:173:CYS:SG   | 2.45                     | 0.56              |
| 1:A:40:LEU:CD2   | 1:A:76:LEU:HD12  | 2.04                     | 0.56              |
| 1:B:167:LEU:HD12 | 1:B:168:VAL:N    | 2.21                     | 0.56              |
| 1:B:40:LEU:HD22  | 1:B:76:LEU:HD13  | 1.82                     | 0.56              |
| 1:B:237:ILE:HG12 | 1:B:248:ALA:CB   | 2.35                     | 0.56              |
| 1:D:64:ASN:OD1   | 1:D:67:ASN:N     | 2.38                     | 0.56              |
| 1:B:48:LEU:HD13  | 1:B:56:LEU:HD22  | 1.86                     | 0.56              |
| 1:B:57:LEU:HG    | 1:B:77:ASN:CG    | 2.24                     | 0.56              |
| 1:A:41:LYS:CD    | 1:A:41:LYS:O     | 2.30                     | 0.56              |
| 1:B:187:ASN:HB3  | 1:B:188:LEU:CG   | 2.35                     | 0.56              |
| 1:A:77:ASN:N     | 1:B:251:LEU:HD21 | 2.20                     | 0.56              |
| 1:C:11:PRO:HG2   | 1:D:33:HIS:ND1   | 2.18                     | 0.56              |
| 1:C:20:GLN:HE22  | 1:C:166:ALA:CB   | 2.19                     | 0.56              |
| 1:C:62:ARG:HG2   | 1:C:73:GLU:OE2   | 2.06                     | 0.56              |
| 1:D:85:LEU:HD22  | 2:D:266:HLC:H14  | 1.88                     | 0.56              |
| 1:B:36:THR:OG1   | 1:B:39:GLU:HG3   | 2.06                     | 0.56              |
| 1:C:36:THR:CG2   | 1:C:37:GLU:N     | 2.67                     | 0.56              |
| 1:A:198:LEU:HB2  | 1:A:203:TYR:HB2  | 1.88                     | 0.55              |
| 1:B:175:THR:N    | 1:B:176:PRO:HD2  | 2.20                     | 0.55              |
| 1:C:57:LEU:HD11  | 2:C:266:HLC:H13  | 1.87                     | 0.55              |
| 1:A:206:PHE:HA   | 1:A:209:MET:HG2  | 1.89                     | 0.55              |
| 1:A:216:TRP:CZ3  | 1:A:220:THR:OG1  | 2.56                     | 0.55              |
| 1:A:257:MET:N    | 1:A:258:PRO:CD   | 2.69                     | 0.55              |
| 1:C:251:LEU:O    | 1:C:254:HIS:CE1  | 2.60                     | 0.55              |
| 1:D:88:TYR:HA    | 1:D:93:TYR:HD2   | 1.70                     | 0.55              |
| 1:A:17:THR:O     | 1:A:21:GLN:N     | 2.33                     | 0.55              |
| 1:C:36:THR:CG2   | 1:C:37:GLU:H     | 2.19                     | 0.55              |
| 1:A:62:ARG:HG3   | 1:A:73:GLU:OE2   | 2.05                     | 0.55              |
| 1:B:109:VAL:CG1  | 1:B:114:ARG:HE   | 2.17                     | 0.55              |
| 1:A:82:SER:HB3   | 1:B:244:ASN:HD21 | 1.70                     | 0.55              |
| 1:C:63:LEU:CD2   | 1:C:104:LEU:HD22 | 2.36                     | 0.55              |
| 1:C:74:ARG:HD3   | 1:C:76:LEU:HD21  | 1.88                     | 0.55              |
| 1:C:33:HIS:HD2   | 1:D:10:ARG:CB    | 2.20                     | 0.55              |
| 1:A:198:LEU:CB   | 1:A:203:TYR:HB2  | 2.36                     | 0.55              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:108:PRO:HB3 | 1:A:141:PHE:CD1  | 2.42                     | 0.55              |
| 1:B:211:ARG:O   | 1:B:211:ARG:HG2  | 2.06                     | 0.55              |
| 1:B:222:LEU:CD2 | 1:D:106:GLN:CD   | 2.65                     | 0.55              |
| 1:C:48:LEU:HD12 | 1:C:48:LEU:C     | 2.26                     | 0.55              |
| 1:C:111:TRP:CZ3 | 1:C:138:GLY:HA3  | 2.27                     | 0.54              |
| 1:A:255:LEU:C   | 1:A:257:MET:H    | 2.11                     | 0.54              |
| 1:B:63:LEU:HD11 | 1:B:150:ILE:O    | 2.07                     | 0.54              |
| 1:C:56:LEU:HD11 | 1:C:77:ASN:HD21  | 1.72                     | 0.54              |
| 1:C:83:ASP:O    | 1:C:86:ASP:OD1   | 2.26                     | 0.54              |
| 1:D:188:LEU:CD1 | 1:D:188:LEU:C    | 2.75                     | 0.54              |
| 1:A:215:ASN:HB3 | 1:A:226:GLU:CG   | 2.34                     | 0.54              |
| 1:A:56:LEU:HD23 | 1:A:57:LEU:N     | 2.22                     | 0.54              |
| 1:B:56:LEU:O    | 1:B:80:TYR:CE2   | 2.61                     | 0.54              |
| 1:C:111:TRP:HE3 | 1:C:138:GLY:N    | 2.01                     | 0.54              |
| 1:A:254:HIS:CE1 | 1:B:74:ARG:CG    | 2.84                     | 0.54              |
| 1:A:212:GLY:O   | 1:A:213:LYS:CD   | 2.53                     | 0.54              |
| 1:A:36:THR:CG2  | 1:A:39:GLU:H     | 2.19                     | 0.54              |
| 1:B:198:LEU:CD2 | 1:B:236:VAL:HG13 | 2.38                     | 0.54              |
| 1:B:79:SER:O    | 1:B:80:TYR:C     | 2.45                     | 0.54              |
| 1:D:62:ARG:HG2  | 1:D:73:GLU:OE2   | 2.08                     | 0.54              |
| 1:A:193:PRO:HD2 | 1:A:194:SER:C    | 2.28                     | 0.54              |
| 1:A:254:HIS:CE1 | 1:B:74:ARG:CZ    | 2.90                     | 0.54              |
| 1:A:56:LEU:HD22 | 1:A:78:VAL:HG21  | 1.90                     | 0.54              |
| 1:B:180:GLN:OE1 | 1:B:180:GLN:HA   | 2.07                     | 0.54              |
| 1:B:56:LEU:O    | 1:B:57:LEU:HB2   | 2.08                     | 0.54              |
| 1:B:211:ARG:NH1 | 1:D:146:GLU:OE2  | 2.40                     | 0.54              |
| 1:C:104:LEU:N   | 1:C:104:LEU:CD1  | 2.71                     | 0.54              |
| 1:C:45:ASP:O    | 1:C:48:LEU:HG    | 2.08                     | 0.54              |
| 1:A:180:GLN:OE1 | 1:A:180:GLN:HA   | 2.08                     | 0.53              |
| 1:A:242:ALA:CB  | 1:A:247:HIS:ND1  | 2.69                     | 0.53              |
| 1:B:62:ARG:HD2  | 1:B:71:ARG:HH21  | 1.71                     | 0.53              |
| 1:A:17:THR:HG22 | 1:A:18:ALA:H     | 1.69                     | 0.53              |
| 1:B:15:GLY:C    | 1:B:16:LEU:HD23  | 2.29                     | 0.53              |
| 1:C:253:MET:HE2 | 1:C:257:MET:CE   | 2.39                     | 0.53              |
| 1:C:44:LEU:CD1  | 1:C:77:ASN:HD22  | 2.17                     | 0.53              |
| 1:D:56:LEU:HD12 | 1:D:77:ASN:CG    | 2.28                     | 0.53              |
| 1:C:93:TYR:OH   | 1:C:129:GLU:HG2  | 2.08                     | 0.53              |
| 1:A:23:THR:O    | 1:A:26:GLU:HB2   | 2.09                     | 0.53              |
| 1:C:50:GLN:OE1  | 1:C:50:GLN:N     | 2.42                     | 0.53              |
| 1:D:202:GLU:HG2 | 1:D:232:HIS:HB3  | 1.90                     | 0.53              |
| 1:A:96:HIS:CE1  | 1:A:122:GLU:CB   | 2.91                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:175:THR:N    | 1:A:176:PRO:HD2  | 2.24                     | 0.53              |
| 1:C:253:MET:CE   | 1:C:257:MET:HE3  | 2.39                     | 0.53              |
| 1:A:198:LEU:HG   | 1:A:200:GLN:N    | 2.24                     | 0.52              |
| 1:A:245:ARG:HH11 | 1:A:245:ARG:CG   | 2.21                     | 0.52              |
| 1:B:245:ARG:NH1  | 1:B:245:ARG:HG2  | 2.23                     | 0.52              |
| 1:D:58:LEU:H     | 1:D:77:ASN:CB    | 2.16                     | 0.52              |
| 1:A:179:HIS:HE2  | 1:A:183:ILE:HD11 | 1.73                     | 0.52              |
| 1:A:206:PHE:CG   | 1:A:206:PHE:O    | 2.62                     | 0.52              |
| 1:A:206:PHE:HA   | 1:A:209:MET:CG   | 2.38                     | 0.52              |
| 1:A:209:MET:HE1  | 1:A:233:VAL:CG1  | 2.39                     | 0.52              |
| 1:B:14:ALA:O     | 1:B:16:LEU:HD22  | 2.09                     | 0.52              |
| 1:C:111:TRP:CH2  | 2:C:266:HLC:C4   | 2.92                     | 0.52              |
| 1:C:12:LEU:HD12  | 1:C:13:PRO:HD2   | 1.91                     | 0.52              |
| 1:B:179:HIS:HE2  | 1:B:183:ILE:HD11 | 1.72                     | 0.52              |
| 1:C:237:ILE:HG12 | 1:C:248:ALA:CB   | 2.38                     | 0.52              |
| 1:A:198:LEU:H    | 1:A:199:SER:HA   | 1.70                     | 0.52              |
| 1:A:205:ILE:HD13 | 1:A:232:HIS:HB3  | 1.90                     | 0.52              |
| 1:C:33:HIS:CD2   | 1:D:10:ARG:CB    | 2.93                     | 0.52              |
| 1:C:36:THR:HG22  | 1:C:38:ASN:N     | 2.22                     | 0.52              |
| 1:B:167:LEU:HA   | 1:B:170:MET:HB2  | 1.92                     | 0.52              |
| 1:A:205:ILE:CD1  | 1:A:232:HIS:HB3  | 2.40                     | 0.52              |
| 1:B:198:LEU:CD1  | 1:B:236:VAL:HG13 | 2.38                     | 0.52              |
| 1:B:56:LEU:HG    | 1:B:79:SER:OG    | 2.10                     | 0.52              |
| 1:C:224:ILE:CG2  | 1:C:228:THR:HB   | 2.40                     | 0.52              |
| 1:C:111:TRP:HE3  | 1:C:137:SER:C    | 2.13                     | 0.52              |
| 1:C:20:GLN:HE22  | 1:C:166:ALA:HB1  | 1.74                     | 0.52              |
| 1:A:104:LEU:HD12 | 1:A:104:LEU:N    | 2.24                     | 0.52              |
| 1:A:215:ASN:OD1  | 1:A:230:LYS:HG3  | 2.10                     | 0.52              |
| 1:A:36:THR:HG22  | 1:A:39:GLU:CD    | 2.30                     | 0.52              |
| 1:B:151:GLY:HA2  | 1:B:179:HIS:HE1  | 1.75                     | 0.52              |
| 1:D:224:ILE:HG21 | 1:D:228:THR:HB   | 1.87                     | 0.52              |
| 1:A:93:TYR:OH    | 1:A:129:GLU:HG2  | 2.10                     | 0.51              |
| 1:C:245:ARG:HG2  | 1:C:245:ARG:HH11 | 1.75                     | 0.51              |
| 1:C:66:GLN:O     | 1:C:103:HIS:HD2  | 1.93                     | 0.51              |
| 1:A:18:ALA:O     | 1:A:19:SER:C     | 2.45                     | 0.51              |
| 1:B:226:GLU:HG2  | 1:B:230:LYS:HG3  | 1.91                     | 0.51              |
| 1:C:245:ARG:NH1  | 1:C:245:ARG:HG2  | 2.25                     | 0.51              |
| 1:A:213:LYS:CE   | 1:A:217:GLU:HB3  | 2.39                     | 0.51              |
| 1:A:213:LYS:HE3  | 1:A:217:GLU:HB2  | 1.93                     | 0.51              |
| 1:C:64:ASN:OD1   | 1:C:68:GLN:HG2   | 2.10                     | 0.51              |
| 1:D:10:ARG:N     | 1:D:11:PRO:HD2   | 2.24                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:193:PRO:HD2  | 1:A:194:SER:CA   | 2.37                     | 0.51              |
| 1:B:185:VAL:O    | 1:B:185:VAL:HG12 | 2.10                     | 0.51              |
| 1:B:245:ARG:HG2  | 1:B:245:ARG:HH11 | 1.74                     | 0.51              |
| 1:C:106:GLN:O    | 1:C:106:GLN:HG3  | 2.09                     | 0.51              |
| 1:C:48:LEU:HA    | 1:C:51:ALA:CB    | 2.39                     | 0.51              |
| 1:B:187:ASN:C    | 1:B:188:LEU:HD12 | 2.31                     | 0.51              |
| 1:B:57:LEU:O     | 1:B:57:LEU:HD23  | 2.08                     | 0.51              |
| 1:B:57:LEU:CA    | 1:B:77:ASN:CB    | 2.83                     | 0.51              |
| 1:C:42:ALA:O     | 1:C:46:GLN:HG3   | 2.10                     | 0.51              |
| 1:C:82:SER:CB    | 1:D:244:ASN:ND2  | 2.70                     | 0.51              |
| 1:D:20:GLN:HE22  | 1:D:166:ALA:CB   | 2.23                     | 0.51              |
| 1:B:188:LEU:O    | 1:B:189:PRO:C    | 2.49                     | 0.51              |
| 1:D:219:ALA:HB1  | 1:D:224:ILE:O    | 2.11                     | 0.51              |
| 1:C:219:ALA:HA   | 1:C:224:ILE:O    | 2.11                     | 0.51              |
| 1:A:205:ILE:HD13 | 1:A:232:HIS:CB   | 2.40                     | 0.51              |
| 1:A:227:ARG:O    | 1:A:231:PHE:HD2  | 1.92                     | 0.51              |
| 1:C:14:ALA:N     | 1:C:173:CYS:SG   | 2.84                     | 0.51              |
| 1:A:209:MET:HE2  | 1:A:233:VAL:HG13 | 1.92                     | 0.50              |
| 1:B:198:LEU:HD22 | 1:B:236:VAL:HG13 | 1.92                     | 0.50              |
| 1:B:48:LEU:HD22  | 1:B:56:LEU:HD21  | 0.51                     | 0.50              |
| 1:D:185:VAL:O    | 1:D:186:ALA:HB3  | 2.11                     | 0.50              |
| 1:D:17:THR:HG1   | 1:D:20:GLN:HB2   | 1.76                     | 0.50              |
| 1:C:104:LEU:H    | 1:C:104:LEU:CD1  | 2.24                     | 0.50              |
| 1:C:13:PRO:HG3   | 1:D:29:HIS:CG    | 2.46                     | 0.50              |
| 1:D:224:ILE:HG23 | 1:D:228:THR:HB   | 1.86                     | 0.50              |
| 1:A:137:SER:OG   | 1:A:159:ARG:HG2  | 2.11                     | 0.50              |
| 1:B:198:LEU:HD13 | 1:B:236:VAL:HG13 | 1.93                     | 0.50              |
| 1:C:56:LEU:CA    | 1:C:79:SER:HB3   | 2.39                     | 0.50              |
| 1:D:242:ALA:HA   | 1:D:247:HIS:CE1  | 2.46                     | 0.50              |
| 1:A:204:ASP:HB3  | 1:A:222:LEU:HD11 | 1.93                     | 0.50              |
| 1:A:87:GLN:HG2   | 1:A:93:TYR:HE2   | 1.76                     | 0.50              |
| 1:C:64:ASN:CG    | 1:C:68:GLN:HG2   | 2.32                     | 0.50              |
| 1:B:64:ASN:OD1   | 1:B:66:GLN:O     | 2.30                     | 0.50              |
| 1:C:201:ARG:O    | 1:C:205:ILE:HG12 | 2.11                     | 0.50              |
| 1:D:93:TYR:OH    | 1:D:129:GLU:HG2  | 2.12                     | 0.50              |
| 1:A:209:MET:CE   | 1:A:245:ARG:NE   | 2.65                     | 0.50              |
| 1:B:106:GLN:O    | 1:B:107:GLY:O    | 2.30                     | 0.50              |
| 1:B:223:ASP:OD1  | 1:B:223:ASP:O    | 2.30                     | 0.50              |
| 1:A:62:ARG:CD    | 1:A:73:GLU:OE2   | 2.60                     | 0.50              |
| 1:D:186:ALA:O    | 1:D:187:ASN:OD1  | 2.30                     | 0.50              |
| 1:A:194:SER:O    | 1:A:195:ASN:OD1  | 2.30                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:64:ASN:OD1   | 1:B:68:GLN:O     | 2.30                     | 0.50              |
| 1:D:208:TRP:CZ3  | 1:D:211:ARG:HD2  | 2.47                     | 0.50              |
| 1:A:195:ASN:OD1  | 1:B:188:LEU:HD21 | 2.10                     | 0.49              |
| 1:C:130:ALA:HB1  | 1:C:135:MET:HB2  | 1.94                     | 0.49              |
| 1:A:17:THR:CG2   | 1:A:18:ALA:N     | 2.74                     | 0.49              |
| 1:A:192:SER:CA   | 1:A:194:SER:HA   | 2.42                     | 0.49              |
| 1:B:104:LEU:HD22 | 1:B:142:SER:HB2  | 1.93                     | 0.49              |
| 1:C:254:HIS:CB   | 1:D:74:ARG:HA    | 2.22                     | 0.49              |
| 1:B:67:ASN:CA    | 1:B:103:HIS:CD2  | 2.94                     | 0.49              |
| 1:C:93:TYR:CD1   | 1:C:126:PHE:HD1  | 2.30                     | 0.49              |
| 1:B:188:LEU:CD1  | 1:B:188:LEU:N    | 2.75                     | 0.49              |
| 1:D:48:LEU:CD2   | 1:D:56:LEU:HD21  | 2.27                     | 0.49              |
| 1:B:130:ALA:HB1  | 1:B:135:MET:HB2  | 1.95                     | 0.49              |
| 1:B:16:LEU:O     | 1:B:17:THR:O     | 2.31                     | 0.49              |
| 1:B:219:ALA:CB   | 1:B:224:ILE:O    | 2.60                     | 0.49              |
| 1:B:57:LEU:HA    | 1:B:77:ASN:HB3   | 1.91                     | 0.49              |
| 1:D:104:LEU:HG   | 1:D:142:SER:HB2  | 1.94                     | 0.49              |
| 1:C:87:GLN:HG2   | 1:C:93:TYR:HE2   | 1.77                     | 0.49              |
| 1:D:187:ASN:O    | 1:D:188:LEU:CB   | 2.60                     | 0.49              |
| 1:B:93:TYR:OH    | 1:B:129:GLU:HG2  | 2.11                     | 0.49              |
| 1:D:245:ARG:NH1  | 1:D:245:ARG:HG2  | 2.28                     | 0.49              |
| 1:B:225:SER:O    | 1:B:228:THR:HB   | 2.12                     | 0.49              |
| 1:C:106:GLN:O    | 1:C:107:GLY:O    | 2.30                     | 0.49              |
| 1:C:187:ASN:CG   | 1:C:188:LEU:H    | 2.14                     | 0.49              |
| 1:A:130:ALA:HB1  | 1:A:135:MET:HB2  | 1.94                     | 0.49              |
| 1:A:193:PRO:CG   | 1:A:194:SER:C    | 2.81                     | 0.49              |
| 1:B:55:ARG:HH12  | 1:B:134:GLY:HA3  | 1.78                     | 0.49              |
| 1:B:87:GLN:HG2   | 1:B:93:TYR:HE2   | 1.78                     | 0.49              |
| 1:C:111:TRP:CE3  | 1:C:137:SER:C    | 2.86                     | 0.49              |
| 1:C:254:HIS:CB   | 1:D:73:GLU:O     | 2.61                     | 0.49              |
| 1:C:186:ALA:O    | 1:C:187:ASN:OD1  | 2.30                     | 0.48              |
| 1:D:175:THR:N    | 1:D:176:PRO:HD2  | 2.29                     | 0.48              |
| 1:B:67:ASN:HB2   | 1:B:103:HIS:CG   | 2.19                     | 0.48              |
| 1:C:16:LEU:HB3   | 1:C:20:GLN:HB3   | 1.95                     | 0.48              |
| 1:C:16:LEU:HB3   | 1:C:20:GLN:CB    | 2.43                     | 0.48              |
| 1:A:111:TRP:HB2  | 1:A:137:SER:HA   | 1.94                     | 0.48              |
| 1:C:180:GLN:HG3  | 1:D:184:ARG:NH2  | 2.28                     | 0.48              |
| 1:C:87:GLN:NE2   | 1:C:129:GLU:CG   | 2.77                     | 0.48              |
| 1:A:213:LYS:HE3  | 1:A:217:GLU:HB3  | 1.95                     | 0.48              |
| 1:C:111:TRP:CG   | 1:C:138:GLY:N    | 2.81                     | 0.48              |
| 1:B:242:ALA:HA   | 1:B:247:HIS:CE1  | 2.49                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:54:GLU:O     | 1:C:79:SER:OG    | 2.30                     | 0.48              |
| 1:D:15:GLY:O     | 1:D:16:LEU:HG    | 2.14                     | 0.48              |
| 1:B:63:LEU:HB2   | 1:B:149:ASN:CA   | 2.44                     | 0.48              |
| 1:C:14:ALA:CB    | 1:C:169:ALA:HB1  | 2.43                     | 0.48              |
| 1:D:130:ALA:HB1  | 1:D:135:MET:HB2  | 1.96                     | 0.48              |
| 1:D:17:THR:OG1   | 1:D:20:GLN:HB2   | 2.13                     | 0.48              |
| 1:A:199:SER:O    | 1:A:200:GLN:C    | 2.52                     | 0.48              |
| 1:C:104:LEU:H    | 1:C:104:LEU:HD12 | 1.78                     | 0.48              |
| 1:C:111:TRP:CD2  | 1:C:138:GLY:N    | 2.71                     | 0.48              |
| 1:A:219:ALA:CB   | 1:A:229:VAL:CG2  | 2.78                     | 0.48              |
| 1:D:180:GLN:O    | 1:D:184:ARG:HG3  | 2.14                     | 0.48              |
| 1:B:148:ASN:O    | 1:B:149:ASN:C    | 2.51                     | 0.47              |
| 1:C:87:GLN:NE2   | 1:C:129:GLU:HG2  | 2.29                     | 0.47              |
| 1:C:148:ASN:OD1  | 1:C:150:ILE:HG22 | 2.14                     | 0.47              |
| 1:B:226:GLU:CD   | 1:B:230:LYS:HE2  | 2.33                     | 0.47              |
| 1:C:74:ARG:HE    | 1:C:76:LEU:HD23  | 1.78                     | 0.47              |
| 1:B:93:TYR:CD1   | 1:B:126:PHE:HD1  | 2.32                     | 0.47              |
| 1:B:222:LEU:HD23 | 1:D:106:GLN:NE2  | 2.06                     | 0.47              |
| 1:B:17:THR:CG2   | 1:B:18:ALA:N     | 2.77                     | 0.47              |
| 1:B:63:LEU:HG    | 1:B:150:ILE:C    | 2.35                     | 0.47              |
| 1:A:76:LEU:HD23  | 1:A:76:LEU:C     | 2.35                     | 0.47              |
| 1:C:253:MET:CE   | 1:C:257:MET:CE   | 2.93                     | 0.47              |
| 1:A:203:TYR:O    | 1:A:207:HIS:CA   | 2.60                     | 0.47              |
| 1:B:14:ALA:O     | 1:B:16:LEU:HD23  | 2.13                     | 0.47              |
| 1:C:202:GLU:HG2  | 1:C:236:VAL:CG2  | 2.45                     | 0.47              |
| 1:D:108:PRO:HB3  | 1:D:139:ILE:HD11 | 1.96                     | 0.47              |
| 1:D:225:SER:C    | 1:D:227:ARG:N    | 2.68                     | 0.47              |
| 1:D:57:LEU:HD13  | 2:D:266:HLC:H9   | 1.96                     | 0.47              |
| 1:A:104:LEU:HG   | 1:A:142:SER:HB2  | 1.97                     | 0.47              |
| 1:A:205:ILE:O    | 1:A:209:MET:CG   | 2.26                     | 0.47              |
| 1:A:111:TRP:CH2  | 2:A:266:HLC:H6   | 2.49                     | 0.47              |
| 1:B:48:LEU:HD21  | 1:B:56:LEU:CD2   | 2.16                     | 0.47              |
| 1:B:63:LEU:HD11  | 1:B:151:GLY:N    | 2.29                     | 0.47              |
| 1:A:210:SER:HA   | 1:A:249:ILE:CG1  | 2.39                     | 0.47              |
| 1:D:34:ILE:O     | 1:D:184:ARG:HD2  | 2.14                     | 0.47              |
| 1:D:20:GLN:HE22  | 1:D:166:ALA:HB1  | 1.80                     | 0.47              |
| 1:B:108:PRO:HG3  | 1:B:141:PHE:CD1  | 2.47                     | 0.47              |
| 1:B:242:ALA:HB3  | 1:B:248:ALA:HB2  | 1.97                     | 0.47              |
| 1:C:52:PRO:HB2   | 1:C:161:PRO:HG3  | 1.96                     | 0.47              |
| 1:C:198:LEU:HD21 | 1:C:255:LEU:HD13 | 1.96                     | 0.47              |
| 1:D:93:TYR:CD1   | 1:D:126:PHE:HD1  | 2.33                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:57:LEU:HB2   | 1:A:80:TYR:HE2   | 0.70                     | 0.47              |
| 1:A:96:HIS:ND1   | 1:A:122:GLU:CB   | 2.78                     | 0.47              |
| 1:C:247:HIS:CE1  | 1:D:78:VAL:HG21  | 2.50                     | 0.47              |
| 1:D:52:PRO:O     | 1:D:53:SER:HB2   | 2.15                     | 0.47              |
| 1:A:205:ILE:CG2  | 1:A:233:VAL:HG22 | 2.45                     | 0.47              |
| 1:B:87:GLN:NE2   | 1:B:129:GLU:CG   | 2.78                     | 0.47              |
| 1:C:103:HIS:O    | 1:C:106:GLN:HG2  | 2.15                     | 0.47              |
| 1:C:64:ASN:ND2   | 1:C:68:GLN:CG    | 2.75                     | 0.47              |
| 1:C:244:ASN:HD21 | 1:D:82:SER:CB    | 2.28                     | 0.47              |
| 1:A:65:ASN:HD22  | 1:D:243:ASN:HB3  | 1.77                     | 0.46              |
| 1:B:104:LEU:HD23 | 1:B:142:SER:HB2  | 1.96                     | 0.46              |
| 1:B:67:ASN:OD1   | 1:B:68:GLN:N     | 2.48                     | 0.46              |
| 1:B:96:HIS:NE2   | 1:B:122:GLU:HG3  | 2.31                     | 0.46              |
| 1:C:146:GLU:O    | 1:C:147:ARG:C    | 2.53                     | 0.46              |
| 1:A:224:ILE:HG13 | 1:A:228:THR:HB   | 1.98                     | 0.46              |
| 1:A:244:ASN:HB2  | 1:A:247:HIS:HB3  | 1.96                     | 0.46              |
| 1:C:201:ARG:HD3  | 1:C:201:ARG:HA   | 1.43                     | 0.46              |
| 1:C:243:ASN:H    | 1:C:247:HIS:CE1  | 2.33                     | 0.46              |
| 1:B:186:ALA:O    | 1:B:188:LEU:HD11 | 2.12                     | 0.46              |
| 1:B:226:GLU:OE2  | 1:B:230:LYS:CE   | 2.63                     | 0.46              |
| 1:B:51:ALA:HA    | 1:B:52:PRO:HD3   | 1.80                     | 0.46              |
| 1:C:140:THR:CG2  | 1:C:141:PHE:N    | 2.78                     | 0.46              |
| 1:C:29:HIS:CD2   | 1:D:11:PRO:CB    | 2.91                     | 0.46              |
| 1:B:198:LEU:HD22 | 1:B:236:VAL:HA   | 1.97                     | 0.46              |
| 1:D:180:GLN:OE1  | 1:D:180:GLN:HA   | 2.16                     | 0.46              |
| 1:C:109:VAL:CB   | 1:C:114:ARG:HH11 | 2.24                     | 0.46              |
| 1:C:218:ILE:HG22 | 1:C:229:VAL:HG21 | 1.97                     | 0.46              |
| 1:D:16:LEU:HD23  | 1:D:20:GLN:OE1   | 2.15                     | 0.46              |
| 1:C:246:THR:OG1  | 1:D:86:ASP:OD1   | 2.10                     | 0.46              |
| 1:A:36:THR:HG21  | 1:A:39:GLU:HG3   | 1.93                     | 0.46              |
| 1:A:66:GLN:O     | 1:A:103:HIS:HD2  | 1.98                     | 0.46              |
| 1:B:108:PRO:CG   | 1:B:172:ASN:OD1  | 2.63                     | 0.46              |
| 1:D:87:GLN:HG2   | 1:D:93:TYR:HE2   | 1.81                     | 0.46              |
| 1:C:242:ALA:HA   | 1:C:247:HIS:CE1  | 2.51                     | 0.46              |
| 1:C:253:MET:HE2  | 1:C:257:MET:HE3  | 1.98                     | 0.46              |
| 1:D:179:HIS:HE2  | 1:D:183:ILE:HD11 | 1.80                     | 0.46              |
| 1:D:205:ILE:CD1  | 1:D:222:LEU:CD1  | 2.94                     | 0.46              |
| 1:D:48:LEU:HB2   | 1:D:56:LEU:CD2   | 2.46                     | 0.46              |
| 1:B:167:LEU:O    | 1:B:170:MET:N    | 2.49                     | 0.46              |
| 1:C:17:THR:O     | 1:C:20:GLN:N     | 2.49                     | 0.46              |
| 1:B:16:LEU:CD2   | 1:B:16:LEU:N     | 2.64                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:14:ALA:HB1   | 1:C:169:ALA:HB1  | 1.97                     | 0.45              |
| 1:B:110:MET:SD   | 1:B:139:ILE:HD12 | 2.56                     | 0.45              |
| 1:C:16:LEU:CB    | 1:C:20:GLN:CB    | 2.94                     | 0.45              |
| 1:C:180:GLN:OE1  | 1:C:180:GLN:HA   | 2.17                     | 0.45              |
| 1:C:208:TRP:HZ3  | 1:C:211:ARG:HD3  | 1.80                     | 0.45              |
| 1:A:42:ALA:O     | 1:A:45:ASP:HB3   | 2.16                     | 0.45              |
| 1:C:254:HIS:CE1  | 1:D:74:ARG:CG    | 2.99                     | 0.45              |
| 1:A:196:MET:O    | 1:A:197:PRO:O    | 2.35                     | 0.45              |
| 1:B:16:LEU:O     | 1:B:17:THR:C     | 2.54                     | 0.45              |
| 1:B:198:LEU:HD11 | 1:B:240:LEU:HD21 | 1.98                     | 0.45              |
| 1:A:209:MET:CE   | 1:A:233:VAL:CG2  | 2.94                     | 0.45              |
| 1:D:208:TRP:HB3  | 1:D:218:ILE:HG12 | 1.97                     | 0.45              |
| 1:D:56:LEU:CD1   | 1:D:77:ASN:OD1   | 2.65                     | 0.45              |
| 1:C:111:TRP:CZ2  | 2:C:266:HLC:C3   | 2.99                     | 0.45              |
| 1:D:181:ALA:O    | 1:D:184:ARG:HB2  | 2.17                     | 0.45              |
| 1:B:64:ASN:CG    | 1:B:68:GLN:O     | 2.55                     | 0.45              |
| 1:D:216:TRP:CH2  | 1:D:220:THR:HG22 | 2.52                     | 0.45              |
| 1:D:66:GLN:O     | 1:D:103:HIS:HD2  | 1.99                     | 0.45              |
| 1:B:15:GLY:HA3   | 1:B:16:LEU:HA    | 1.51                     | 0.45              |
| 1:C:80:TYR:HA    | 1:C:81:PRO:HD3   | 1.86                     | 0.45              |
| 1:D:206:PHE:HA   | 1:D:209:MET:HG3  | 1.99                     | 0.45              |
| 1:D:216:TRP:HA   | 1:D:216:TRP:CE3  | 2.52                     | 0.45              |
| 1:A:237:ILE:HG12 | 1:A:245:ARG:HA   | 1.99                     | 0.44              |
| 1:B:240:LEU:O    | 1:B:241:ASN:HB2  | 2.16                     | 0.44              |
| 1:C:49:SER:OG    | 1:C:50:GLN:N     | 2.49                     | 0.44              |
| 1:D:48:LEU:HB2   | 1:D:56:LEU:HD21  | 1.98                     | 0.44              |
| 1:A:188:LEU:C    | 1:A:188:LEU:HD12 | 2.36                     | 0.44              |
| 1:A:198:LEU:HD12 | 1:A:203:TYR:CB   | 2.47                     | 0.44              |
| 1:A:210:SER:HB2  | 1:A:249:ILE:CG2  | 2.46                     | 0.44              |
| 1:B:52:PRO:O     | 1:B:161:PRO:HD3  | 2.16                     | 0.44              |
| 1:C:16:LEU:CB    | 1:C:20:GLN:HB3   | 2.47                     | 0.44              |
| 1:C:20:GLN:NE2   | 1:C:166:ALA:HB1  | 2.32                     | 0.44              |
| 1:A:190:PRO:HG2  | 1:C:50:GLN:HE22  | 1.82                     | 0.44              |
| 1:C:52:PRO:HD3   | 1:C:167:LEU:HD23 | 1.98                     | 0.44              |
| 1:A:148:ASN:O    | 1:A:149:ASN:C    | 2.55                     | 0.44              |
| 1:A:52:PRO:O     | 1:A:161:PRO:HD3  | 2.17                     | 0.44              |
| 1:A:214:THR:N    | 1:A:217:GLU:OE1  | 2.41                     | 0.44              |
| 1:A:242:ALA:HA   | 1:A:247:HIS:CE1  | 2.53                     | 0.44              |
| 1:B:223:ASP:CG   | 1:B:223:ASP:O    | 2.55                     | 0.44              |
| 1:A:185:VAL:HG13 | 1:A:186:ALA:N    | 2.32                     | 0.44              |
| 1:B:87:GLN:NE2   | 1:B:129:GLU:HG2  | 2.33                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:19:SER:O     | 1:B:20:GLN:C     | 2.55                     | 0.44              |
| 1:D:245:ARG:HG2  | 1:D:245:ARG:HH11 | 1.81                     | 0.44              |
| 1:B:48:LEU:CB    | 1:B:56:LEU:CD2   | 2.92                     | 0.44              |
| 1:D:111:TRP:CZ3  | 1:D:137:SER:O    | 2.69                     | 0.44              |
| 1:B:243:ASN:H    | 1:B:247:HIS:CE1  | 2.35                     | 0.44              |
| 1:D:148:ASN:O    | 1:D:149:ASN:C    | 2.56                     | 0.44              |
| 1:D:213:LYS:HB2  | 1:D:218:ILE:HG12 | 1.99                     | 0.44              |
| 1:D:87:GLN:NE2   | 1:D:129:GLU:CG   | 2.81                     | 0.44              |
| 1:A:233:VAL:CG1  | 1:A:245:ARG:HD2  | 2.45                     | 0.44              |
| 1:B:217:GLU:O    | 1:B:220:THR:HB   | 2.16                     | 0.44              |
| 1:C:199:SER:O    | 1:C:203:TYR:HB2  | 2.18                     | 0.44              |
| 1:C:251:LEU:O    | 1:C:254:HIS:ND1  | 2.51                     | 0.44              |
| 1:B:63:LEU:CD2   | 1:B:104:LEU:CD1  | 2.71                     | 0.44              |
| 1:D:87:GLN:NE2   | 1:D:129:GLU:HG2  | 2.33                     | 0.44              |
| 1:A:84:TRP:O     | 1:A:88:TYR:HB2   | 2.18                     | 0.43              |
| 1:B:96:HIS:NE2   | 1:B:122:GLU:CB   | 2.79                     | 0.43              |
| 1:C:17:THR:O     | 1:C:18:ALA:C     | 2.57                     | 0.43              |
| 1:D:63:LEU:HD11  | 1:D:151:GLY:HA3  | 2.00                     | 0.43              |
| 1:D:89:MET:HG3   | 2:D:266:HLC:CL1  | 2.55                     | 0.43              |
| 1:A:51:ALA:HA    | 1:A:52:PRO:HD3   | 1.80                     | 0.43              |
| 1:B:121:ALA:O    | 1:B:125:ARG:HB3  | 2.18                     | 0.43              |
| 1:D:225:SER:C    | 1:D:227:ARG:H    | 2.20                     | 0.43              |
| 1:C:82:SER:HG    | 1:D:246:THR:HG23 | 1.81                     | 0.43              |
| 1:C:28:ILE:HG22  | 1:D:28:ILE:HG22  | 2.01                     | 0.43              |
| 1:D:30:MET:HA    | 1:D:33:HIS:HD2   | 1.83                     | 0.43              |
| 1:A:257:MET:CB   | 1:A:258:PRO:HD3  | 2.31                     | 0.43              |
| 1:B:201:ARG:C    | 1:B:201:ARG:HD3  | 2.37                     | 0.43              |
| 1:B:63:LEU:HG    | 1:B:151:GLY:N    | 2.33                     | 0.43              |
| 1:C:64:ASN:HD21  | 1:C:68:GLN:CG    | 2.26                     | 0.43              |
| 1:C:87:GLN:HE22  | 1:C:129:GLU:CG   | 2.32                     | 0.43              |
| 1:A:213:LYS:HZ1  | 1:A:217:GLU:HB3  | 1.82                     | 0.43              |
| 1:B:236:VAL:O    | 1:B:240:LEU:HG   | 2.18                     | 0.43              |
| 1:B:56:LEU:HA    | 1:B:155:SER:O    | 2.18                     | 0.43              |
| 1:D:216:TRP:HA   | 1:D:216:TRP:HE3  | 1.82                     | 0.43              |
| 1:D:76:LEU:O     | 1:D:76:LEU:HG    | 2.19                     | 0.43              |
| 1:A:25:LEU:HD13  | 1:B:25:LEU:CD1   | 2.42                     | 0.43              |
| 1:B:80:TYR:O     | 1:B:81:PRO:O     | 2.37                     | 0.43              |
| 1:D:219:ALA:O    | 1:D:223:ASP:N    | 2.50                     | 0.43              |
| 1:A:111:TRP:CE3  | 1:A:138:GLY:CA   | 3.00                     | 0.43              |
| 1:A:17:THR:HG22  | 1:A:19:SER:H     | 1.83                     | 0.43              |
| 1:A:198:LEU:HD12 | 1:A:203:TYR:HB2  | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:97:ASP:HA    | 1:A:98:PRO:HD3   | 1.77                     | 0.43              |
| 1:A:25:LEU:HD12  | 1:A:25:LEU:HA    | 1.69                     | 0.43              |
| 1:A:71:ARG:HH21  | 1:C:42:ALA:CB    | 2.27                     | 0.43              |
| 1:B:63:LEU:CG    | 1:B:150:ILE:C    | 2.87                     | 0.43              |
| 1:B:63:LEU:HB2   | 1:B:149:ASN:HA   | 2.00                     | 0.43              |
| 1:A:111:TRP:CB   | 1:A:138:GLY:H    | 2.08                     | 0.43              |
| 1:C:237:ILE:HG23 | 1:C:242:ALA:CB   | 2.30                     | 0.43              |
| 1:A:40:LEU:CG    | 1:A:76:LEU:HD11  | 2.44                     | 0.42              |
| 1:B:48:LEU:HB2   | 1:B:56:LEU:CD2   | 2.50                     | 0.42              |
| 1:C:63:LEU:HD21  | 1:C:104:LEU:HD21 | 1.98                     | 0.42              |
| 1:A:107:GLY:HA2  | 1:A:108:PRO:HA   | 1.76                     | 0.42              |
| 1:A:218:ILE:HB   | 1:A:229:VAL:HG11 | 2.01                     | 0.42              |
| 1:B:187:ASN:OD1  | 1:B:188:LEU:C    | 2.58                     | 0.42              |
| 1:D:85:LEU:CD2   | 2:D:266:HLC:H14  | 2.48                     | 0.42              |
| 1:A:104:LEU:CD1  | 1:A:104:LEU:N    | 2.82                     | 0.42              |
| 1:A:209:MET:CE   | 1:A:233:VAL:HG21 | 2.40                     | 0.42              |
| 1:B:237:ILE:HG12 | 1:B:248:ALA:HB2  | 2.00                     | 0.42              |
| 1:C:48:LEU:HD12  | 1:C:49:SER:CA    | 2.47                     | 0.42              |
| 1:C:56:LEU:CD1   | 1:C:77:ASN:HD21  | 2.32                     | 0.42              |
| 1:C:209:MET:HB3  | 1:C:209:MET:HE3  | 1.77                     | 0.42              |
| 1:D:105:GLY:HA2  | 1:D:142:SER:O    | 2.19                     | 0.42              |
| 1:D:55:ARG:HH12  | 1:D:134:GLY:HA3  | 1.84                     | 0.42              |
| 1:D:17:THR:HG23  | 1:D:20:GLN:OE1   | 2.19                     | 0.42              |
| 1:B:107:GLY:HA2  | 1:B:108:PRO:HD3  | 1.82                     | 0.42              |
| 1:A:66:GLN:O     | 1:A:67:ASN:HB2   | 2.20                     | 0.42              |
| 1:A:96:HIS:CE1   | 1:A:122:GLU:HG3  | 2.54                     | 0.42              |
| 1:B:20:GLN:OE1   | 1:B:166:ALA:HB1  | 2.19                     | 0.42              |
| 1:C:108:PRO:C    | 1:C:109:VAL:CG2  | 2.87                     | 0.42              |
| 1:A:62:ARG:C     | 1:A:63:LEU:HD12  | 2.40                     | 0.42              |
| 1:B:219:ALA:HA   | 1:B:224:ILE:O    | 2.20                     | 0.42              |
| 1:C:57:LEU:CD1   | 2:C:266:HLC:H13  | 2.49                     | 0.42              |
| 1:A:138:GLY:O    | 1:A:139:ILE:HD13 | 2.19                     | 0.42              |
| 1:C:96:HIS:CE1   | 1:C:122:GLU:CB   | 3.02                     | 0.42              |
| 1:D:208:TRP:CE3  | 1:D:211:ARG:HD2  | 2.55                     | 0.42              |
| 1:D:48:LEU:HD13  | 1:D:56:LEU:CD2   | 2.41                     | 0.42              |
| 1:C:244:ASN:OD1  | 1:C:247:HIS:CB   | 2.64                     | 0.42              |
| 1:C:82:SER:HA    | 1:C:85:LEU:HD12  | 2.02                     | 0.42              |
| 1:A:190:PRO:CA   | 1:A:191:ALA:CB   | 2.50                     | 0.42              |
| 1:B:48:LEU:HB2   | 1:B:56:LEU:HD21  | 2.00                     | 0.42              |
| 1:C:140:THR:HG22 | 1:C:141:PHE:N    | 2.34                     | 0.42              |
| 1:C:96:HIS:ND1   | 1:C:122:GLU:CB   | 2.82                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:213:LYS:HB2  | 1:D:218:ILE:CG1  | 2.49                     | 0.42              |
| 1:C:247:HIS:CD2  | 1:D:78:VAL:HG22  | 2.34                     | 0.42              |
| 1:A:151:GLY:HA2  | 1:A:179:HIS:HE1  | 1.85                     | 0.41              |
| 1:A:222:LEU:HD23 | 1:A:222:LEU:HA   | 1.85                     | 0.41              |
| 1:B:257:MET:HB2  | 1:B:258:PRO:HD3  | 2.01                     | 0.41              |
| 1:C:56:LEU:HA    | 1:C:155:SER:O    | 2.20                     | 0.41              |
| 1:C:187:ASN:OD1  | 1:C:187:ASN:C    | 2.58                     | 0.41              |
| 1:B:56:LEU:HB3   | 1:B:156:ILE:HG13 | 2.02                     | 0.41              |
| 1:C:151:GLY:HA2  | 1:C:179:HIS:HE1  | 1.85                     | 0.41              |
| 1:C:247:HIS:NE2  | 1:D:78:VAL:HG21  | 2.17                     | 0.41              |
| 1:C:111:TRP:CD2  | 2:C:266:HLC:H4   | 2.55                     | 0.41              |
| 1:D:105:GLY:H    | 1:D:142:SER:CB   | 2.32                     | 0.41              |
| 1:A:41:LYS:C     | 1:A:41:LYS:CD    | 2.56                     | 0.41              |
| 1:C:66:GLN:O     | 1:C:103:HIS:CD2  | 2.72                     | 0.41              |
| 1:C:80:TYR:HB2   | 1:C:85:LEU:HD21  | 2.01                     | 0.41              |
| 1:D:29:HIS:O     | 1:D:33:HIS:HD2   | 1.95                     | 0.41              |
| 1:A:72:LEU:HA    | 1:A:72:LEU:HD23  | 1.81                     | 0.41              |
| 1:A:74:ARG:HG3   | 1:B:254:HIS:CG   | 2.55                     | 0.41              |
| 1:B:219:ALA:HB1  | 1:B:224:ILE:O    | 2.20                     | 0.41              |
| 1:B:76:LEU:C     | 1:B:76:LEU:HD23  | 2.39                     | 0.41              |
| 1:C:111:TRP:CG   | 1:C:138:GLY:C    | 2.93                     | 0.41              |
| 1:C:180:GLN:HG3  | 1:D:184:ARG:HH22 | 1.84                     | 0.41              |
| 1:D:16:LEU:HD22  | 1:D:20:GLN:OE1   | 2.20                     | 0.41              |
| 1:A:255:LEU:O    | 1:A:258:PRO:HD2  | 2.20                     | 0.41              |
| 1:C:186:ALA:O    | 1:C:187:ASN:CG   | 2.59                     | 0.41              |
| 1:A:64:ASN:ND2   | 1:A:68:GLN:HB2   | 2.35                     | 0.41              |
| 1:A:71:ARG:HH12  | 1:C:41:LYS:HB3   | 1.86                     | 0.41              |
| 1:B:226:GLU:O    | 1:B:230:LYS:N    | 2.30                     | 0.41              |
| 1:A:110:MET:CA   | 1:A:139:ILE:HD12 | 2.43                     | 0.41              |
| 1:C:16:LEU:CB    | 1:C:20:GLN:HB2   | 2.51                     | 0.41              |
| 1:A:187:ASN:OD1  | 1:A:187:ASN:O    | 2.38                     | 0.41              |
| 1:B:110:MET:CE   | 1:B:139:ILE:HD12 | 2.50                     | 0.41              |
| 1:B:56:LEU:HB2   | 1:B:57:LEU:H     | 1.60                     | 0.41              |
| 1:B:76:LEU:HD22  | 1:B:76:LEU:O     | 2.15                     | 0.41              |
| 1:C:253:MET:HE1  | 1:C:257:MET:HE3  | 2.03                     | 0.41              |
| 1:A:71:ARG:HH22  | 1:C:42:ALA:N     | 2.18                     | 0.41              |
| 1:A:192:SER:C    | 1:A:194:SER:CA   | 2.80                     | 0.41              |
| 1:A:255:LEU:CA   | 1:A:258:PRO:HD2  | 2.50                     | 0.41              |
| 1:C:243:ASN:ND2  | 1:D:78:VAL:HG11  | 2.36                     | 0.41              |
| 1:A:219:ALA:H    | 1:A:229:VAL:HG21 | 1.74                     | 0.41              |
| 1:A:62:ARG:HG2   | 1:A:73:GLU:OE2   | 2.18                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:223:ASP:OD2  | 1:D:117:ARG:NH1  | 2.54                     | 0.41              |
| 1:D:111:TRP:CE3  | 1:D:138:GLY:CA   | 2.98                     | 0.41              |
| 1:D:84:TRP:O     | 1:D:88:TYR:HB2   | 2.21                     | 0.41              |
| 1:A:214:THR:C    | 1:A:216:TRP:N    | 2.74                     | 0.40              |
| 1:A:218:ILE:HG21 | 1:A:229:VAL:HG13 | 2.02                     | 0.40              |
| 1:A:254:HIS:O    | 1:A:258:PRO:HG2  | 2.16                     | 0.40              |
| 1:B:181:ALA:HA   | 1:B:184:ARG:NH2  | 2.35                     | 0.40              |
| 1:B:52:PRO:O     | 1:B:53:SER:HB2   | 2.21                     | 0.40              |
| 1:B:69:ILE:HG22  | 1:B:70:GLN:N     | 2.36                     | 0.40              |
| 1:D:105:GLY:N    | 1:D:142:SER:OG   | 2.48                     | 0.40              |
| 1:D:56:LEU:HB3   | 1:D:156:ILE:HG12 | 2.03                     | 0.40              |
| 1:D:46:GLN:O     | 1:D:50:GLN:OE1   | 2.39                     | 0.40              |
| 1:A:205:ILE:CD1  | 1:A:232:HIS:CB   | 2.98                     | 0.40              |
| 1:A:258:PRO:N    | 1:A:259:PRO:CD   | 2.83                     | 0.40              |
| 1:A:93:TYR:CD1   | 1:A:126:PHE:HD1  | 2.38                     | 0.40              |
| 1:B:104:LEU:HD13 | 1:B:151:GLY:HA3  | 2.04                     | 0.40              |
| 1:B:63:LEU:CD1   | 1:B:151:GLY:N    | 2.83                     | 0.40              |
| 1:C:224:ILE:HG23 | 1:C:228:THR:HB   | 2.03                     | 0.40              |
| 1:C:250:VAL:O    | 1:C:253:MET:HG2  | 2.21                     | 0.40              |
| 1:C:77:ASN:O     | 1:C:77:ASN:CG    | 2.57                     | 0.40              |
| 1:D:243:ASN:H    | 1:D:247:HIS:CE1  | 2.39                     | 0.40              |
| 1:D:121:ALA:O    | 1:D:125:ARG:HB3  | 2.21                     | 0.40              |
| 1:D:43:PHE:O     | 1:D:47:VAL:HG23  | 2.21                     | 0.40              |
| 1:A:121:ALA:O    | 1:A:125:ARG:HB3  | 2.21                     | 0.40              |
| 1:A:219:ALA:HA   | 1:A:229:VAL:HG22 | 2.02                     | 0.40              |
| 1:A:232:HIS:O    | 1:A:236:VAL:HG23 | 2.21                     | 0.40              |
| 1:B:209:MET:HB3  | 1:B:209:MET:HE3  | 1.90                     | 0.40              |
| 1:B:221:ILE:HA   | 1:D:103:HIS:CE1  | 2.57                     | 0.40              |
| 1:C:211:ARG:CG   | 1:C:211:ARG:O    | 2.68                     | 0.40              |
| 1:D:108:PRO:C    | 1:D:109:VAL:HG23 | 2.42                     | 0.40              |
| 1:C:254:HIS:CE1  | 1:D:74:ARG:HG3   | 2.57                     | 0.40              |

All (2) 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) |
|----------------|------------------------|--------------------------|-------------------|
| 1:C:114:ARG:CG | 1:C:223:ASP:OD2[5_555] | 1.99                     | 0.21              |
| 1:A:45:ASP:OD1 | 1:B:65:ASN:ND2[8_544]  | 2.02                     | 0.18              |

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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     | 249/265 (94%)  | 220 (88%) | 24 (10%)  | 5 (2%)   | 7           | 34  |
| 1   | B     | 234/265 (88%)  | 195 (83%) | 30 (13%)  | 9 (4%)   | 3           | 19  |
| 1   | C     | 235/265 (89%)  | 212 (90%) | 19 (8%)   | 4 (2%)   | 9           | 39  |
| 1   | D     | 234/265 (88%)  | 204 (87%) | 30 (13%)  | 0        | 100         | 100 |
| All | All   | 952/1060 (90%) | 831 (87%) | 103 (11%) | 18 (2%)  | 8           | 36  |

All (18) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 108 | PRO  |
| 1   | B     | 17  | THR  |
| 1   | B     | 19  | SER  |
| 1   | B     | 20  | GLN  |
| 1   | B     | 57  | LEU  |
| 1   | B     | 78  | VAL  |
| 1   | A     | 257 | MET  |
| 1   | B     | 81  | PRO  |
| 1   | B     | 107 | GLY  |
| 1   | C     | 107 | GLY  |
| 1   | A     | 197 | PRO  |
| 1   | A     | 256 | ALA  |
| 1   | C     | 200 | GLN  |
| 1   | A     | 200 | GLN  |
| 1   | B     | 80  | TYR  |
| 1   | C     | 109 | VAL  |
| 1   | C     | 108 | PRO  |
| 1   | B     | 188 | LEU  |

### 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     | 206/223 (92%) | 203 (98%)  | 3 (2%)   | 65          | 83 |
| 1   | B     | 197/223 (88%) | 190 (96%)  | 7 (4%)   | 35          | 66 |
| 1   | C     | 200/223 (90%) | 197 (98%)  | 3 (2%)   | 65          | 83 |
| 1   | D     | 197/223 (88%) | 196 (100%) | 1 (0%)   | 88          | 94 |
| All | All   | 800/892 (90%) | 786 (98%)  | 14 (2%)  | 59          | 80 |

All (14) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 198 | LEU  |
| 1   | A     | 199 | SER  |
| 1   | A     | 200 | GLN  |
| 1   | B     | 16  | LEU  |
| 1   | B     | 55  | ARG  |
| 1   | B     | 56  | LEU  |
| 1   | B     | 57  | LEU  |
| 1   | B     | 78  | VAL  |
| 1   | B     | 79  | SER  |
| 1   | B     | 137 | SER  |
| 1   | C     | 16  | LEU  |
| 1   | C     | 76  | LEU  |
| 1   | C     | 201 | ARG  |
| 1   | D     | 55  | ARG  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 65  | ASN  |
| 1   | A     | 87  | GLN  |
| 1   | A     | 103 | HIS  |
| 1   | A     | 106 | GLN  |
| 1   | A     | 254 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 20  | GLN  |
| 1   | B     | 21  | GLN  |
| 1   | B     | 77  | ASN  |
| 1   | B     | 87  | GLN  |
| 1   | B     | 92  | ASN  |
| 1   | B     | 96  | HIS  |
| 1   | B     | 103 | HIS  |
| 1   | B     | 106 | GLN  |
| 1   | B     | 177 | HIS  |
| 1   | B     | 244 | ASN  |
| 1   | C     | 33  | HIS  |
| 1   | C     | 77  | ASN  |
| 1   | C     | 87  | GLN  |
| 1   | C     | 92  | ASN  |
| 1   | C     | 103 | HIS  |
| 1   | C     | 148 | ASN  |
| 1   | D     | 33  | HIS  |
| 1   | D     | 66  | GLN  |
| 1   | D     | 87  | GLN  |
| 1   | D     | 92  | ASN  |
| 1   | D     | 103 | HIS  |
| 1   | D     | 244 | ASN  |
| 1   | D     | 254 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

4 ligands are 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$ |
| 2   | HLC  | A     | 266 | -    | 21,21,21     | 1.48 | 4 (19%)     | 23,27,27    | 2.53 | 3 (13%)     |
| 2   | HLC  | B     | 266 | -    | 21,21,21     | 1.46 | 4 (19%)     | 23,27,27    | 2.53 | 3 (13%)     |
| 2   | HLC  | C     | 266 | -    | 21,21,21     | 1.47 | 4 (19%)     | 23,27,27    | 2.54 | 3 (13%)     |
| 2   | HLC  | D     | 266 | -    | 21,21,21     | 1.47 | 4 (19%)     | 23,27,27    | 2.54 | 3 (13%)     |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 2   | HLC  | A     | 266 | -    | -       | 3/11/21/21 | 0/2/2/2 |
| 2   | HLC  | B     | 266 | -    | -       | 3/11/21/21 | 0/2/2/2 |
| 2   | HLC  | C     | 266 | -    | -       | 3/11/21/21 | 0/2/2/2 |
| 2   | HLC  | D     | 266 | -    | -       | 3/11/21/21 | 0/2/2/2 |

All (16) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | A     | 266 | HLC  | O2-C1   | 3.93  | 1.43        | 1.35     |
| 2   | C     | 266 | HLC  | O2-C1   | 3.93  | 1.43        | 1.35     |
| 2   | D     | 266 | HLC  | O2-C1   | 3.90  | 1.43        | 1.35     |
| 2   | B     | 266 | HLC  | O2-C1   | 3.87  | 1.43        | 1.35     |
| 2   | B     | 266 | HLC  | C4-C1   | 2.85  | 1.57        | 1.52     |
| 2   | D     | 266 | HLC  | C4-C1   | 2.85  | 1.57        | 1.52     |
| 2   | A     | 266 | HLC  | C4-C1   | 2.84  | 1.57        | 1.52     |
| 2   | C     | 266 | HLC  | C4-C1   | 2.81  | 1.57        | 1.52     |
| 2   | A     | 266 | HLC  | O2-C2   | -2.47 | 1.40        | 1.46     |
| 2   | C     | 266 | HLC  | O2-C2   | -2.42 | 1.40        | 1.46     |
| 2   | B     | 266 | HLC  | O2-C2   | -2.42 | 1.40        | 1.46     |
| 2   | D     | 266 | HLC  | O2-C2   | -2.40 | 1.40        | 1.46     |
| 2   | C     | 266 | HLC  | C12-CL1 | 2.36  | 1.79        | 1.74     |
| 2   | D     | 266 | HLC  | C12-CL1 | 2.36  | 1.79        | 1.74     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2   | B     | 266 | HLC  | C12-CL1 | 2.34 | 1.79        | 1.74     |
| 2   | A     | 266 | HLC  | C12-CL1 | 2.33 | 1.79        | 1.74     |

All (12) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 2   | C     | 266 | HLC  | O2-C1-O1 | -10.00 | 111.05      | 121.42   |
| 2   | D     | 266 | HLC  | O2-C1-O1 | -9.99  | 111.06      | 121.42   |
| 2   | B     | 266 | HLC  | O2-C1-O1 | -9.96  | 111.09      | 121.42   |
| 2   | A     | 266 | HLC  | O2-C1-O1 | -9.95  | 111.10      | 121.42   |
| 2   | D     | 266 | HLC  | C8-O3-C9 | 4.16   | 128.79      | 117.93   |
| 2   | A     | 266 | HLC  | C8-O3-C9 | 4.15   | 128.78      | 117.93   |
| 2   | C     | 266 | HLC  | C8-O3-C9 | 4.15   | 128.77      | 117.93   |
| 2   | B     | 266 | HLC  | C8-O3-C9 | 4.14   | 128.74      | 117.93   |
| 2   | D     | 266 | HLC  | C2-O2-C1 | -3.39  | 107.26      | 110.39   |
| 2   | C     | 266 | HLC  | C2-O2-C1 | -3.38  | 107.27      | 110.39   |
| 2   | A     | 266 | HLC  | C2-O2-C1 | -3.35  | 107.29      | 110.39   |
| 2   | B     | 266 | HLC  | C2-O2-C1 | -3.34  | 107.31      | 110.39   |

There are no chirality outliers.

All (12) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 2   | A     | 266 | HLC  | C10-C9-O3-C8 |
| 2   | D     | 266 | HLC  | C10-C9-O3-C8 |
| 2   | B     | 266 | HLC  | C10-C9-O3-C8 |
| 2   | C     | 266 | HLC  | C10-C9-O3-C8 |
| 2   | A     | 266 | HLC  | C14-C9-O3-C8 |
| 2   | B     | 266 | HLC  | C14-C9-O3-C8 |
| 2   | C     | 266 | HLC  | C14-C9-O3-C8 |
| 2   | D     | 266 | HLC  | C14-C9-O3-C8 |
| 2   | A     | 266 | HLC  | C6-C7-C8-O3  |
| 2   | B     | 266 | HLC  | C6-C7-C8-O3  |
| 2   | C     | 266 | HLC  | C6-C7-C8-O3  |
| 2   | D     | 266 | HLC  | C6-C7-C8-O3  |

There are no ring outliers.

4 monomers are involved in 27 short contacts:

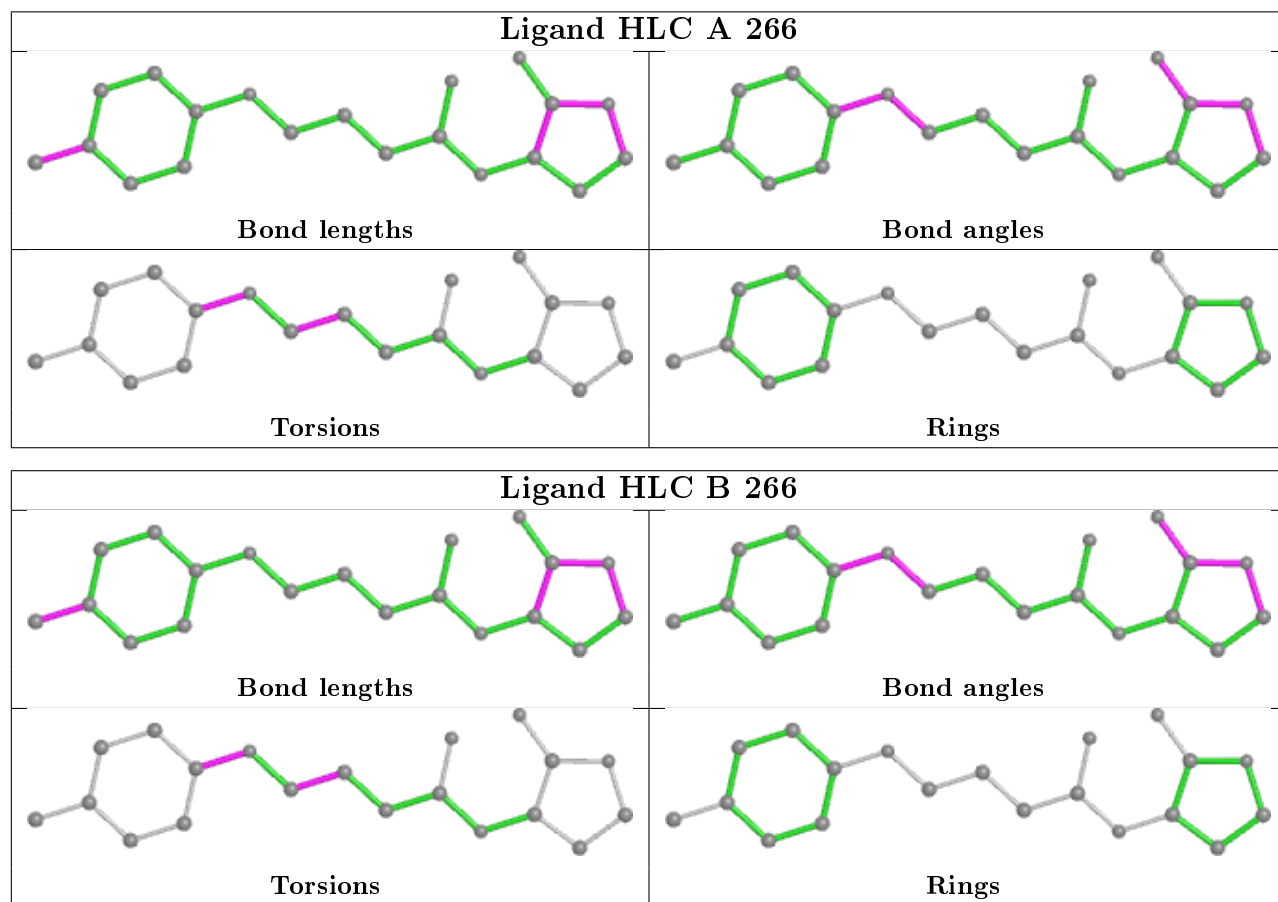
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | A     | 266 | HLC  | 4       | 0            |

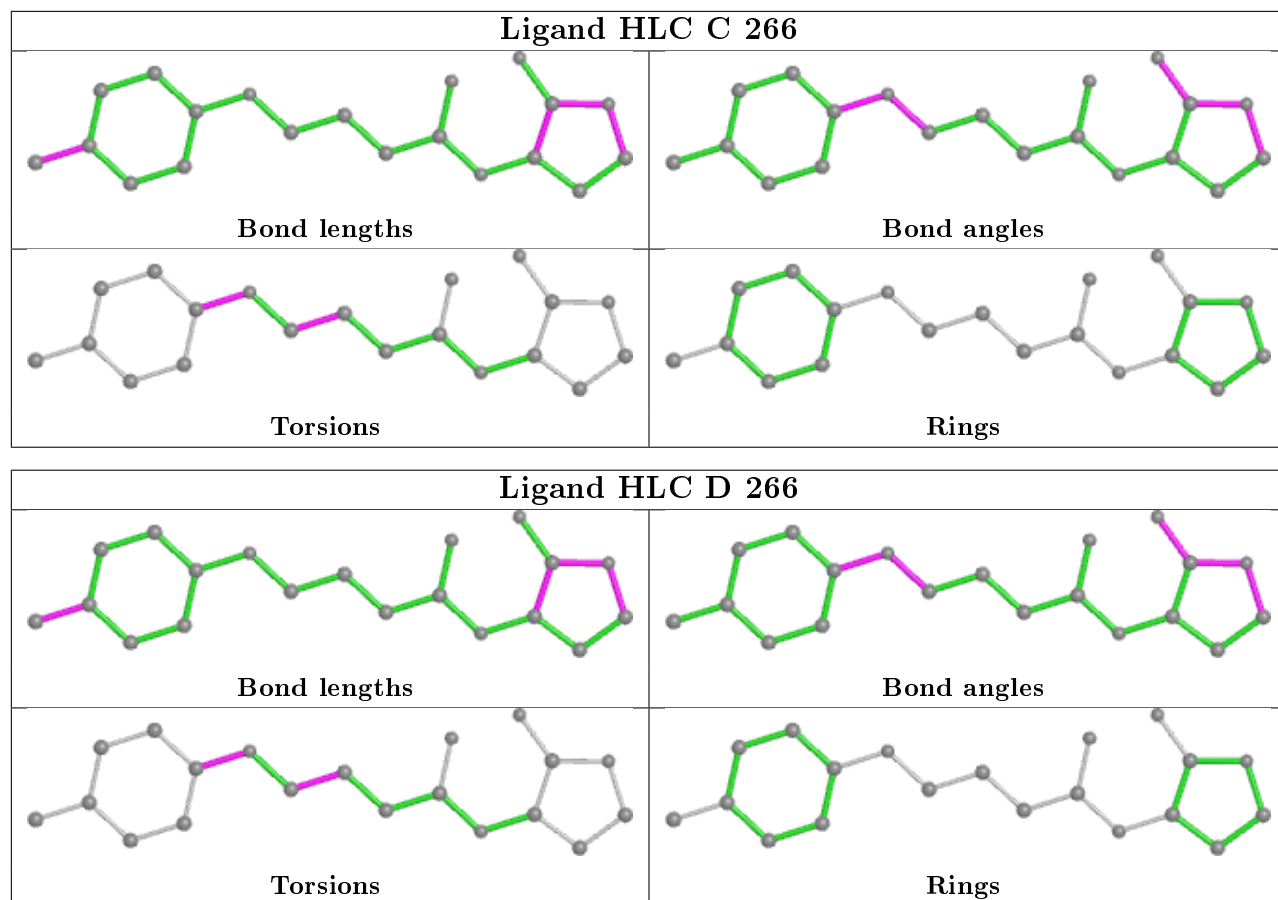
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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | B     | 266 | HLC  | 5       | 0            |
| 2   | C     | 266 | HLC  | 13      | 0            |
| 2   | D     | 266 | HLC  | 5       | 0            |

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 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     | 251/265 (94%)  | 0.72   | 32 (12%) 3 3  | 53, 130, 325, 665     | 0     |
| 1   | B     | 238/265 (89%)  | 0.58   | 26 (10%) 5 4  | 63, 139, 238, 506     | 0     |
| 1   | C     | 239/265 (90%)  | 0.24   | 16 (6%) 17 12 | 55, 112, 209, 315     | 0     |
| 1   | D     | 238/265 (89%)  | 0.08   | 6 (2%) 57 46  | 50, 113, 192, 300     | 0     |
| All | All   | 966/1060 (91%) | 0.41   | 80 (8%) 11 8  | 50, 125, 246, 665     | 0     |

All (80) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 222 | LEU  | 14.5 |
| 1   | A     | 205 | ILE  | 10.3 |
| 1   | A     | 231 | PHE  | 10.0 |
| 1   | A     | 232 | HIS  | 9.2  |
| 1   | A     | 241 | ASN  | 7.7  |
| 1   | A     | 209 | MET  | 7.1  |
| 1   | A     | 221 | ILE  | 6.7  |
| 1   | A     | 259 | PRO  | 6.1  |
| 1   | A     | 202 | GLU  | 5.9  |
| 1   | A     | 227 | ARG  | 5.7  |
| 1   | B     | 78  | VAL  | 5.6  |
| 1   | A     | 218 | ILE  | 5.4  |
| 1   | A     | 230 | LYS  | 5.1  |
| 1   | B     | 14  | ALA  | 4.4  |
| 1   | A     | 215 | ASN  | 4.3  |
| 1   | A     | 223 | ASP  | 4.2  |
| 1   | B     | 244 | ASN  | 4.0  |
| 1   | A     | 238 | ARG  | 4.0  |
| 1   | A     | 224 | ILE  | 3.8  |
| 1   | A     | 235 | ASN  | 3.7  |
| 1   | B     | 15  | GLY  | 3.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 68  | GLN  | 3.7  |
| 1   | B     | 99  | ILE  | 3.6  |
| 1   | C     | 52  | PRO  | 3.6  |
| 1   | B     | 163 | ARG  | 3.5  |
| 1   | A     | 210 | SER  | 3.5  |
| 1   | B     | 77  | ASN  | 3.4  |
| 1   | C     | 257 | MET  | 3.4  |
| 1   | A     | 206 | PHE  | 3.2  |
| 1   | A     | 54  | GLU  | 3.2  |
| 1   | C     | 15  | GLY  | 3.1  |
| 1   | D     | 227 | ARG  | 3.0  |
| 1   | D     | 78  | VAL  | 2.9  |
| 1   | C     | 216 | TRP  | 2.9  |
| 1   | C     | 114 | ARG  | 2.9  |
| 1   | B     | 16  | LEU  | 2.9  |
| 1   | A     | 228 | THR  | 2.9  |
| 1   | C     | 53  | SER  | 2.9  |
| 1   | B     | 258 | PRO  | 2.9  |
| 1   | C     | 201 | ARG  | 2.9  |
| 1   | C     | 13  | PRO  | 2.9  |
| 1   | B     | 154 | LEU  | 2.8  |
| 1   | C     | 228 | THR  | 2.8  |
| 1   | B     | 96  | HIS  | 2.8  |
| 1   | C     | 229 | VAL  | 2.8  |
| 1   | B     | 211 | ARG  | 2.8  |
| 1   | B     | 256 | ALA  | 2.7  |
| 1   | C     | 218 | ILE  | 2.7  |
| 1   | B     | 159 | ARG  | 2.7  |
| 1   | C     | 106 | GLN  | 2.7  |
| 1   | C     | 239 | LYS  | 2.6  |
| 1   | C     | 230 | LYS  | 2.6  |
| 1   | A     | 121 | ALA  | 2.5  |
| 1   | A     | 213 | LYS  | 2.5  |
| 1   | C     | 14  | ALA  | 2.5  |
| 1   | D     | 236 | VAL  | 2.4  |
| 1   | B     | 66  | GLN  | 2.4  |
| 1   | B     | 100 | LEU  | 2.4  |
| 1   | B     | 166 | ALA  | 2.4  |
| 1   | B     | 73  | GLU  | 2.4  |
| 1   | D     | 77  | ASN  | 2.4  |
| 1   | A     | 240 | LEU  | 2.4  |
| 1   | B     | 160 | GLU  | 2.3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 242 | ALA  | 2.3  |
| 1   | C     | 16  | LEU  | 2.3  |
| 1   | A     | 243 | ASN  | 2.2  |
| 1   | A     | 136 | GLY  | 2.2  |
| 1   | B     | 84  | TRP  | 2.2  |
| 1   | A     | 239 | LYS  | 2.2  |
| 1   | A     | 201 | ARG  | 2.2  |
| 1   | B     | 158 | GLY  | 2.2  |
| 1   | A     | 115 | PHE  | 2.2  |
| 1   | D     | 232 | HIS  | 2.2  |
| 1   | B     | 139 | ILE  | 2.1  |
| 1   | B     | 115 | PHE  | 2.1  |
| 1   | D     | 66  | GLN  | 2.1  |
| 1   | B     | 245 | ARG  | 2.1  |
| 1   | A     | 191 | ALA  | 2.1  |
| 1   | A     | 9   | ALA  | 2.1  |
| 1   | B     | 141 | PHE  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

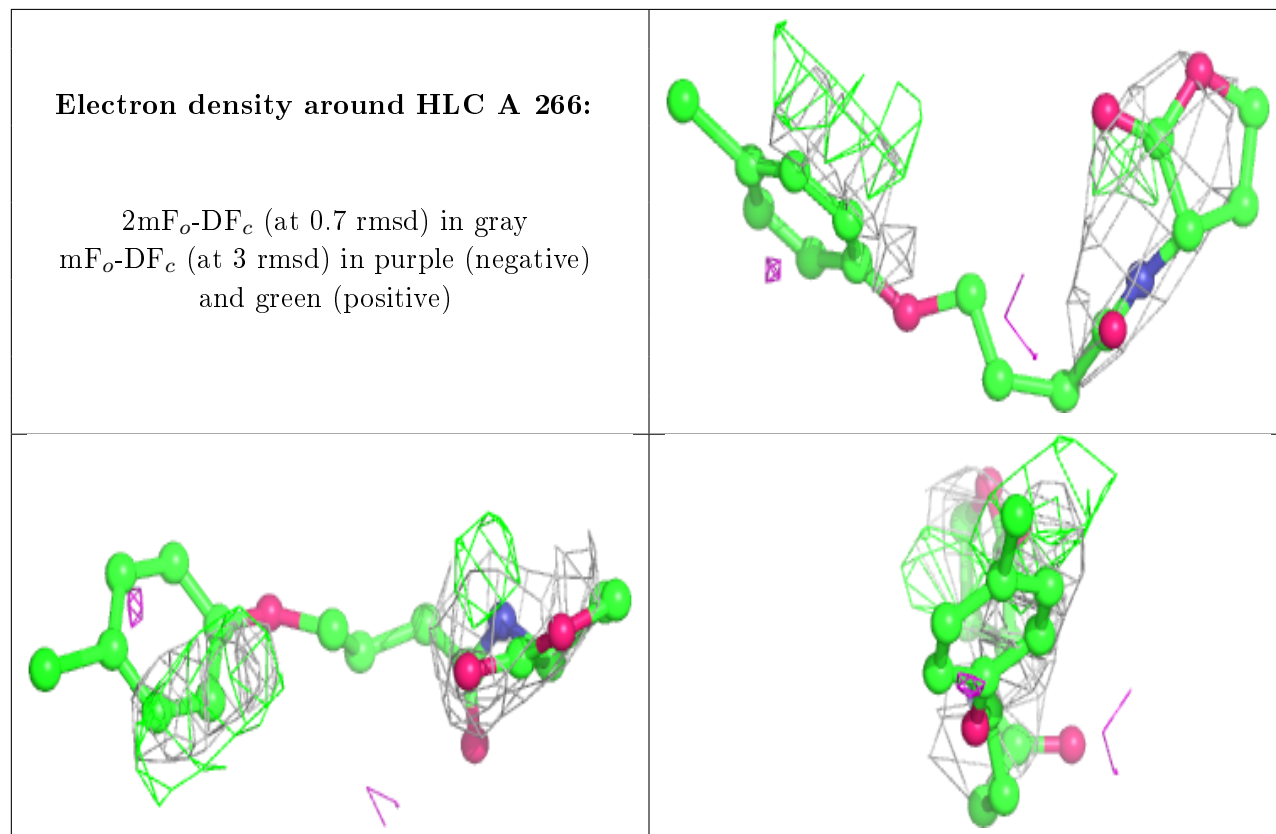
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 2   | HLC  | A     | 266 | 20/20 | 0.70 | 0.71 | 165,196,223,355            | 0     |
| 2   | HLC  | B     | 266 | 20/20 | 0.81 | 0.42 | 150,157,170,363            | 0     |
| 2   | HLC  | C     | 266 | 20/20 | 0.81 | 0.42 | 88,124,168,236             | 0     |
| 2   | HLC  | D     | 266 | 20/20 | 0.87 | 0.35 | 146,171,191,298            | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all

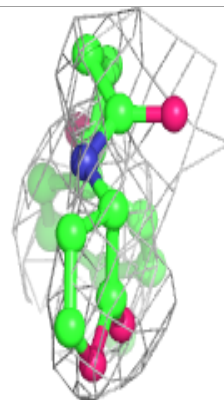
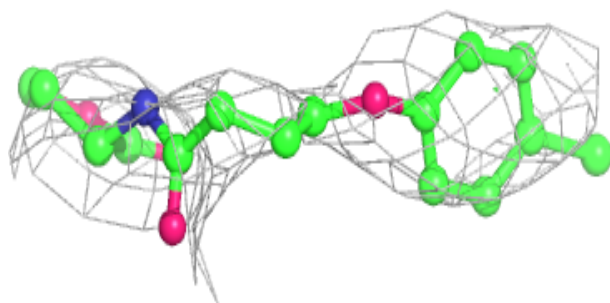
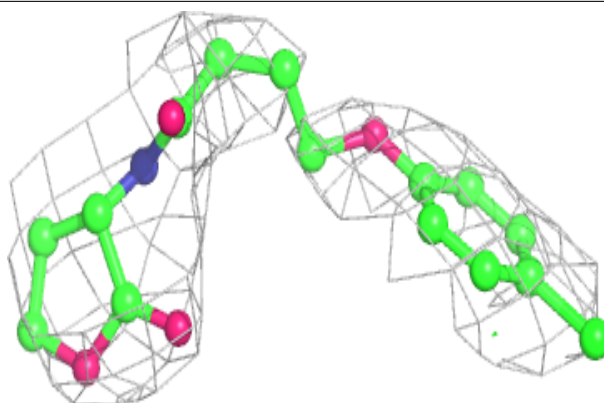


instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

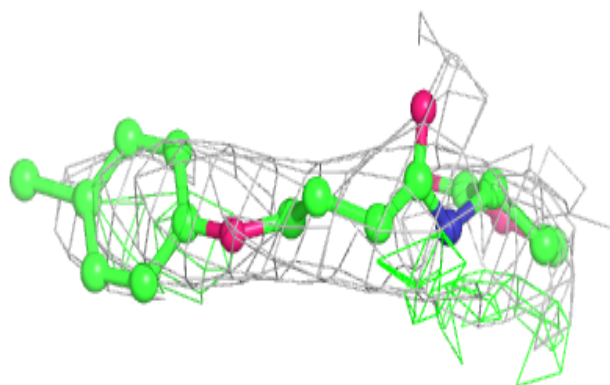
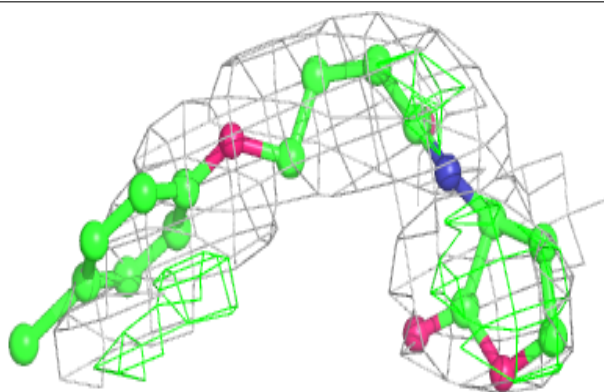


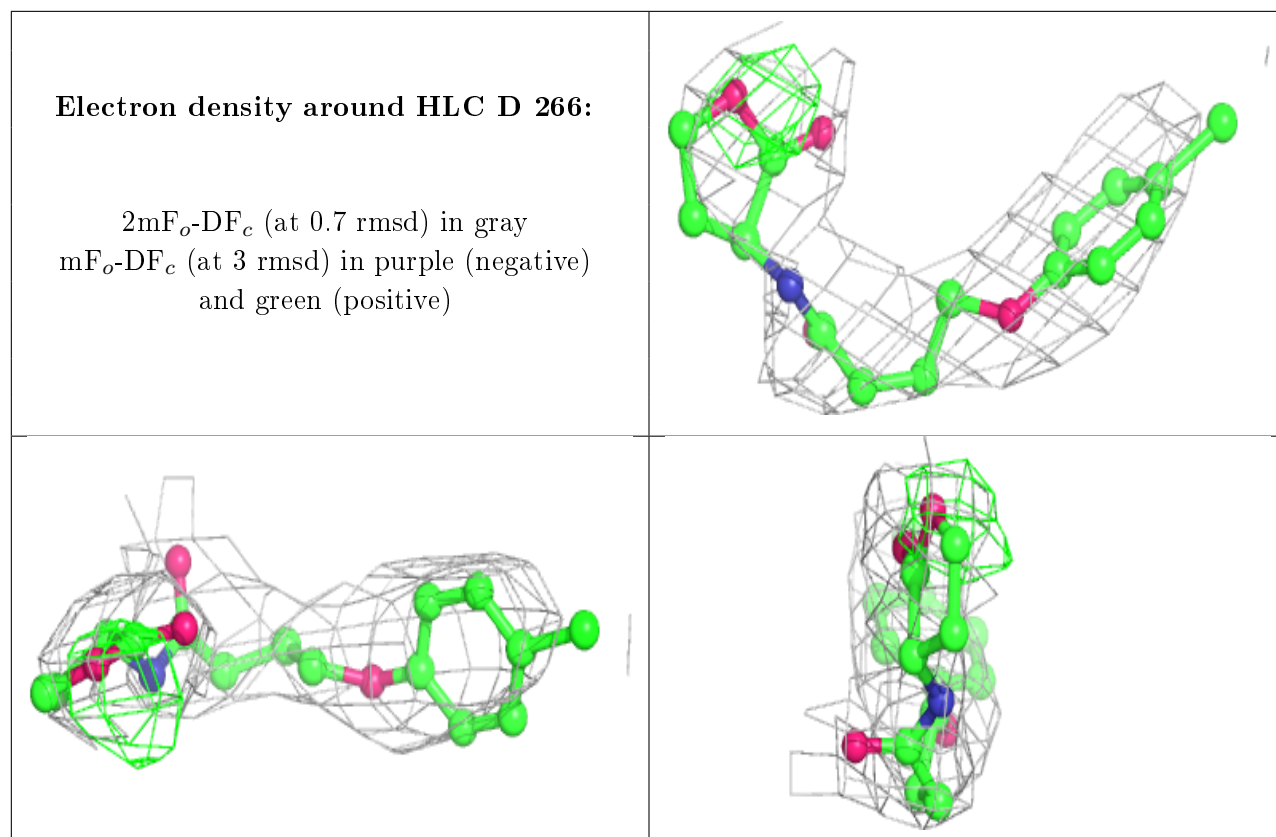
**Electron density around HLC B 266:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around HLC C 266:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.