



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 12:02 AM GMT

PDB ID : 3E6A  
Title : Crystal structure and Functional Analysis of Glyceraldehyde-3-phosphat  
eDehydrogenase from Oryza Sativa  
Authors : Tien, Y.C.; Lin, Y.H.; Chang, S.L.; Chen, C.J.  
Deposited on : 2008-08-15  
Resolution : 3.77 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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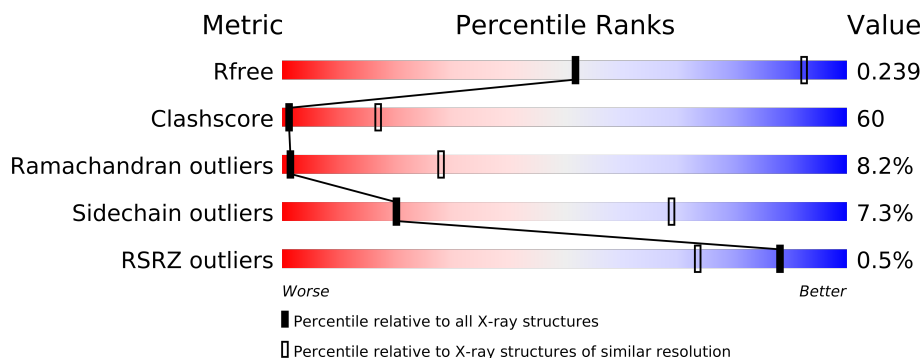
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.77 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 66092                       | 1139 (4.16-3.40)                                      |
| Clashscore            | 79885                       | 1069 (4.06-3.50)                                      |
| Ramachandran outliers | 78287                       | 1019 (4.06-3.50)                                      |
| Sidechain outliers    | 78261                       | 1012 (4.06-3.50)                                      |
| RSRZ outliers         | 66119                       | 1140 (4.16-3.40)                                      |

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 336    |                  |
| 1   | B     | 336    |                  |
| 1   | C     | 336    |                  |
| 1   | O     | 336    |                  |

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 2   | SO4  | C     | 6926 | -        | X                |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10312 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Glyceraldehyde-3-phosphatedehydrogenase, cytosolic.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | O     | 335      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2544  | 1616 | 430 | 489 | 9 |         |         |       |
| 1   | A     | 334      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2539  | 1614 | 429 | 487 | 9 |         |         |       |
| 1   | B     | 335      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2544  | 1616 | 430 | 489 | 9 |         |         |       |
| 1   | C     | 335      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2544  | 1616 | 430 | 489 | 9 |         |         |       |

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | O     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | O     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 3 is water.

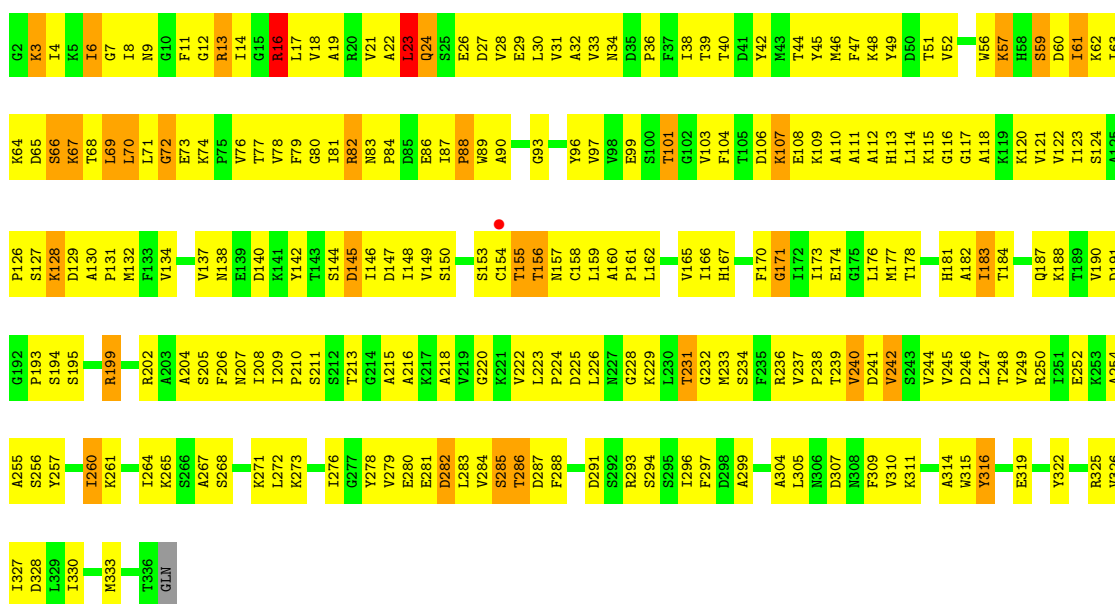
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | O     | 29       | Total | O  | 0       | 0       |
|     |       |          | 29    | 29 |         |         |
| 3   | A     | 23       | Total | O  | 0       | 0       |
|     |       |          | 23    | 23 |         |         |
| 3   | B     | 23       | Total | O  | 0       | 0       |
|     |       |          | 23    | 23 |         |         |
| 3   | C     | 26       | Total | O  | 0       | 0       |
|     |       |          | 26    | 26 |         |         |

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

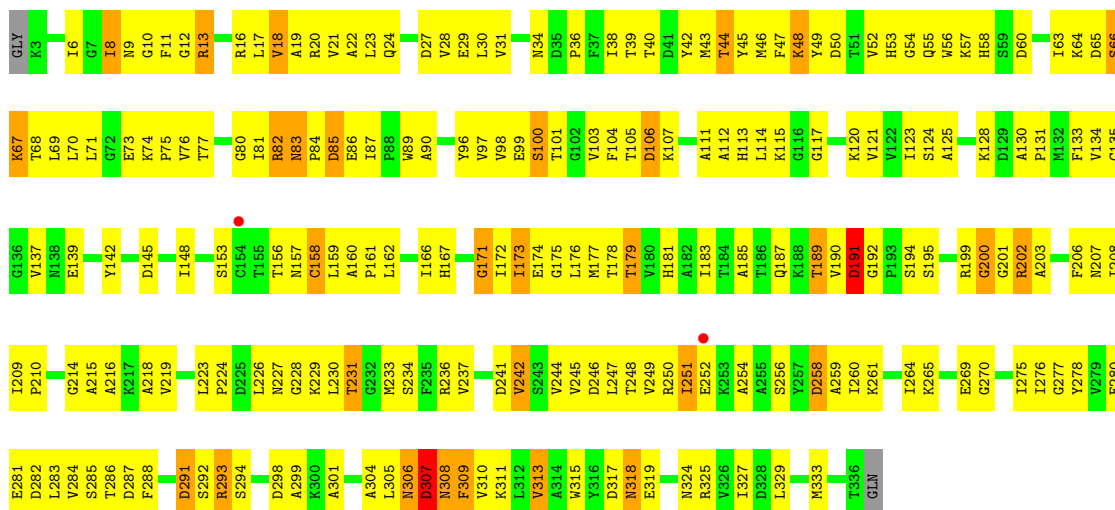
- Molecule 1: Glyceraldehyde-3-phosphatedehydrogenase, cytosolic

Chain O: 



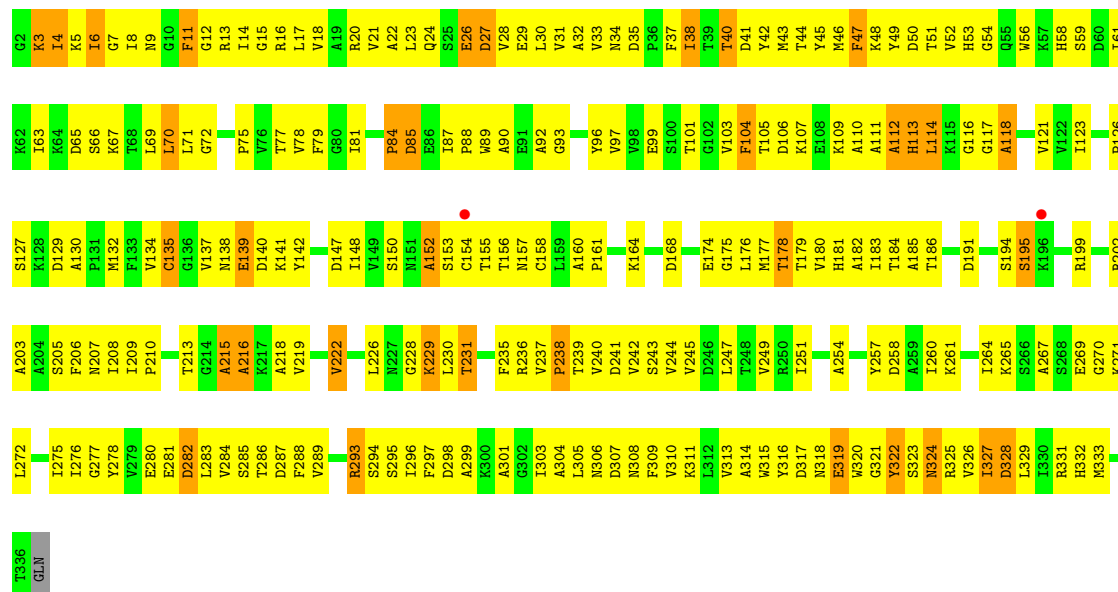
- Molecule 1: Glyceraldehyde-3-phosphatedehydrogenase, cytosolic

Chain A: 



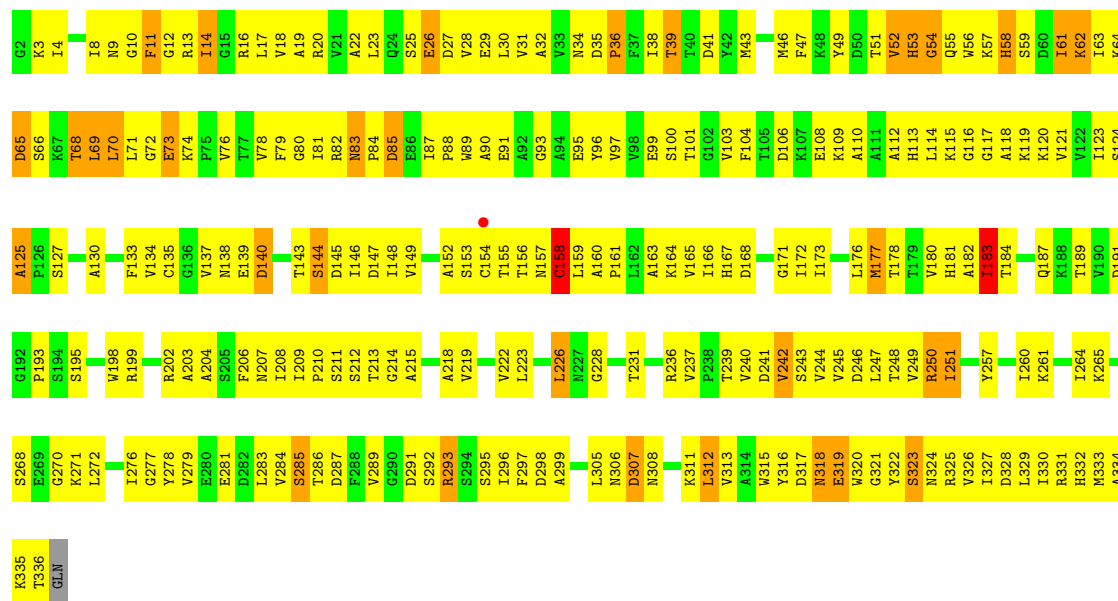
• Molecule 1: Glyceraldehyde-3-phosphatedehydrogenase, cytosolic

Chain B:



• Molecule 1: Glyceraldehyde-3-phosphatedehydrogenase, cytosolic

Chain C:



## 4 Data and refinement statistics

| Property                                                                | Value                                                                                                      | Source           |
|-------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                                                                   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 76.26Å 127.42Å 77.39Å<br>90.00° 118.05° 90.00°                                                             | Depositor        |
| Resolution (Å)                                                          | 30.00 – 3.77<br>26.61 – 3.51                                                                               | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.1 (30.00-3.77)<br>98.9 (26.61-3.51)                                                                     | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                                                                            | Depositor        |
| $R_{sym}$                                                               | 0.33                                                                                                       | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 4.60 (at 3.55Å)                                                                                            | Xtriage          |
| Refinement program                                                      | CNS                                                                                                        | Depositor        |
| R, $R_{free}$                                                           | 0.196 , 0.210<br>0.223 , 0.239                                                                             | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 675 reflections (5.41%)                                                                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 38.3                                                                                                       | Xtriage          |
| Anisotropy                                                              | 1.061                                                                                                      | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.36 , -9.7                                                                                                | EDS              |
| Estimated twinning fraction                                             | 0.010 for -h-l,k,h<br>0.010 for l,k,-h-l<br>0.037 for h,-k,-h-l<br>0.034 for -h-l,-k,l<br>0.033 for l,-k,h | Xtriage          |
| L-test for twinning                                                     | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$                                                | Xtriage          |
| Outliers                                                                | 0 of 16104 reflections                                                                                     | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.86                                                                                                       | EDS              |
| Total number of atoms                                                   | 10312                                                                                                      | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 0.0                                                                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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     | 0.32         | 0/2586  | 0.60        | 0/3504         |
| 1   | B     | 0.34         | 0/2591  | 0.62        | 0/3510         |
| 1   | C     | 0.33         | 0/2591  | 0.64        | 0/3510         |
| 1   | O     | 0.34         | 0/2591  | 0.72        | 6/3510 (0.2%)  |
| All | All   | 0.33         | 0/10359 | 0.65        | 6/14034 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |

There are no bond length outliers.

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | O     | 16  | ARG  | O-C-N  | 8.49  | 136.28      | 122.70   |
| 1   | O     | 16  | ARG  | CA-C-N | -7.60 | 100.47      | 117.20   |
| 1   | O     | 195 | SER  | CA-C-O | -6.68 | 106.07      | 120.10   |
| 1   | O     | 16  | ARG  | N-CA-C | 6.62  | 128.88      | 111.00   |
| 1   | O     | 195 | SER  | CA-C-N | 5.81  | 129.98      | 117.20   |
| 1   | O     | 16  | ARG  | C-N-CA | -5.54 | 107.84      | 121.70   |

There are no chirality outliers.

All (1) planarity outliers are listed below:



| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 13  | ARG  | Sidechain |

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2539  | 0        | 2562     | 328     | 0            |
| 1   | B     | 2544  | 0        | 2568     | 322     | 0            |
| 1   | C     | 2544  | 0        | 2568     | 345     | 0            |
| 1   | O     | 2544  | 0        | 2568     | 364     | 0            |
| 2   | A     | 10    | 0        | 0        | 3       | 0            |
| 2   | B     | 10    | 0        | 0        | 1       | 0            |
| 2   | C     | 10    | 0        | 0        | 11      | 0            |
| 2   | O     | 10    | 0        | 0        | 1       | 0            |
| 3   | A     | 23    | 0        | 0        | 0       | 19           |
| 3   | B     | 23    | 0        | 0        | 7       | 10           |
| 3   | C     | 26    | 0        | 0        | 0       | 18           |
| 3   | O     | 29    | 0        | 0        | 1       | 9            |
| All | All   | 10312 | 0        | 10266    | 1227    | 29           |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 60.

All (1227) close contacts within the same asymmetric unit are listed below.

| Atom-1          | Atom-2           | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 1:O:240:VAL:HB  | 1:B:206:PHE:CE1  | 1.42        | 1.55     |
| 1:A:42:TYR:CZ   | 1:A:46:MET:HE2   | 1.66        | 1.31     |
| 1:O:206:PHE:CE2 | 1:B:240:VAL:HB   | 1.71        | 1.25     |
| 1:A:11:PHE:CE2  | 1:A:16:ARG:CD    | 2.21        | 1.24     |
| 1:A:42:TYR:CE2  | 1:A:46:MET:CE    | 2.20        | 1.23     |
| 1:C:215:ALA:HB2 | 2:C:6926:SO4:O3  | 1.37        | 1.20     |
| 1:O:240:VAL:CB  | 1:B:206:PHE:CE1  | 2.25        | 1.18     |
| 1:O:12:GLY:O    | 1:O:16:ARG:HD3   | 1.43        | 1.18     |
| 1:B:205:SER:O   | 1:B:206:PHE:CD2  | 1.97        | 1.17     |
| 1:A:158:CYS:SG  | 1:A:245:VAL:HG21 | 1.87        | 1.14     |
| 1:A:11:PHE:CE2  | 1:A:16:ARG:HD3   | 1.81        | 1.14     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:O:240:VAL:HB   | 1:B:206:PHE:CD1  | 1.84        | 1.13     |
| 1:A:46:MET:HE3   | 1:C:193:PRO:HA   | 1.21        | 1.12     |
| 1:A:42:TYR:CZ    | 1:A:46:MET:CE    | 2.32        | 1.11     |
| 1:A:11:PHE:CE2   | 1:A:16:ARG:HG2   | 1.86        | 1.10     |
| 1:O:288:PHE:HE1  | 1:O:315:TRP:CG   | 1.71        | 1.08     |
| 1:B:110:ALA:HB2  | 1:B:123:ILE:HD11 | 1.35        | 1.08     |
| 1:O:206:PHE:CE2  | 1:B:240:VAL:CB   | 2.39        | 1.04     |
| 1:A:11:PHE:CE2   | 1:A:16:ARG:CG    | 2.41        | 1.04     |
| 1:B:216:ALA:HB1  | 1:B:231:THR:HA   | 1.39        | 1.03     |
| 1:C:64:LYS:HB2   | 1:C:70:LEU:HD22  | 1.40        | 1.03     |
| 1:A:42:TYR:CE2   | 1:A:46:MET:HE3   | 1.94        | 1.03     |
| 1:O:288:PHE:CE1  | 1:O:315:TRP:CG   | 2.47        | 1.01     |
| 1:A:173:ILE:HD11 | 1:A:252:GLU:N    | 1.74        | 1.00     |
| 1:O:170:PHE:CE2  | 1:O:260:ILE:HD12 | 1.96        | 1.00     |
| 1:B:205:SER:O    | 1:B:206:PHE:HD2  | 1.37        | 0.99     |
| 1:B:35:ASP:OD1   | 1:B:38:ILE:HD13  | 1.61        | 0.99     |
| 1:C:23:LEU:HD11  | 1:C:71:LEU:HD23  | 1.45        | 0.99     |
| 1:A:42:TYR:HD1   | 1:C:198:TRP:CE2  | 1.81        | 0.98     |
| 1:O:288:PHE:HE1  | 1:O:315:TRP:CD1  | 1.81        | 0.98     |
| 1:A:13:ARG:NH1   | 1:A:50:ASP:OD2   | 1.96        | 0.98     |
| 1:B:288:PHE:HE2  | 1:B:315:TRP:CG   | 1.83        | 0.97     |
| 1:B:288:PHE:CE2  | 1:B:315:TRP:CG   | 2.52        | 0.97     |
| 1:O:48:LYS:CE    | 1:O:49:TYR:HE2   | 1.79        | 0.95     |
| 1:A:42:TYR:OH    | 1:A:46:MET:HE2   | 1.65        | 0.95     |
| 1:B:4:ILE:HD11   | 1:B:28:VAL:HG22  | 1.49        | 0.95     |
| 1:O:176:LEU:HD13 | 1:C:311:LYS:HB2  | 1.44        | 0.95     |
| 1:B:239:THR:HG21 | 3:B:6956:HOH:O   | 1.66        | 0.94     |
| 1:A:248:THR:HG23 | 1:B:176:LEU:HD12 | 1.49        | 0.94     |
| 1:O:240:VAL:HB   | 1:B:206:PHE:HE1  | 1.13        | 0.94     |
| 1:O:206:PHE:CD2  | 1:B:240:VAL:HB   | 2.00        | 0.94     |
| 1:A:42:TYR:OH    | 1:A:46:MET:CE    | 2.16        | 0.94     |
| 1:C:215:ALA:CB   | 2:C:6926:SO4:O3  | 2.16        | 0.94     |
| 1:O:48:LYS:HE2   | 1:O:49:TYR:HE2   | 1.29        | 0.94     |
| 1:A:42:TYR:CD1   | 1:C:198:TRP:CE2  | 2.56        | 0.93     |
| 1:B:103:VAL:HG23 | 1:B:104:PHE:H    | 1.34        | 0.93     |
| 1:O:64:LYS:HG3   | 1:O:70:LEU:HB2   | 1.49        | 0.93     |
| 1:A:11:PHE:CD2   | 1:A:16:ARG:HG2   | 2.05        | 0.92     |
| 1:B:160:ALA:HB3  | 1:B:161:PRO:HD3  | 1.52        | 0.91     |
| 1:A:114:LEU:HD11 | 1:A:148:ILE:HD11 | 1.52        | 0.91     |
| 1:O:48:LYS:CD    | 1:O:49:TYR:HE2   | 1.84        | 0.90     |
| 1:C:213:THR:OG1  | 2:C:6926:SO4:S   | 2.29        | 0.90     |
| 1:A:11:PHE:HE2   | 1:A:16:ARG:CD    | 1.76        | 0.90     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:24:GLN:HE21  | 1:A:58:HIS:CD2   | 1.90        | 0.89     |
| 1:C:38:ILE:HG12  | 1:C:46:MET:HE2   | 1.53        | 0.88     |
| 1:O:48:LYS:CD    | 1:O:49:TYR:CE2   | 2.56        | 0.88     |
| 1:O:99:GLU:HB2   | 1:O:123:ILE:HA   | 1.54        | 0.88     |
| 1:A:160:ALA:HB3  | 1:A:161:PRO:HD3  | 1.56        | 0.88     |
| 1:C:181:HIS:HB3  | 1:C:236:ARG:HE   | 1.38        | 0.87     |
| 1:C:11:PHE:CZ    | 1:C:16:ARG:HG2   | 2.10        | 0.87     |
| 1:O:48:LYS:HE2   | 1:O:49:TYR:CE2   | 2.09        | 0.87     |
| 1:A:208:ILE:HG23 | 1:A:237:VAL:HG12 | 1.57        | 0.87     |
| 1:O:44:THR:HG22  | 1:O:69:LEU:HD11  | 1.57        | 0.87     |
| 1:C:158:CYS:HA   | 1:C:295:SER:HB2  | 1.57        | 0.86     |
| 1:C:272:LEU:HB3  | 1:C:276:ILE:HD13 | 1.54        | 0.86     |
| 1:A:158:CYS:SG   | 1:A:245:VAL:CG2  | 2.62        | 0.86     |
| 1:O:57:LYS:NZ    | 1:O:61:ILE:CD1   | 2.38        | 0.86     |
| 1:A:42:TYR:HE2   | 1:A:46:MET:HE3   | 1.35        | 0.86     |
| 1:C:83:ASN:HD22  | 1:C:84:PRO:CD    | 1.89        | 0.86     |
| 1:A:55:GLN:OE1   | 1:A:57:LYS:HG2   | 1.75        | 0.86     |
| 1:O:162:LEU:O    | 1:O:166:ILE:HD13 | 1.75        | 0.86     |
| 1:O:206:PHE:HE2  | 1:B:240:VAL:CB   | 1.88        | 0.85     |
| 1:O:282:ASP:HA   | 1:C:199:ARG:HE   | 1.39        | 0.85     |
| 1:O:63:ILE:H     | 1:O:63:ILE:HD12  | 1.42        | 0.85     |
| 1:B:21:VAL:HB    | 1:B:327:ILE:HD12 | 1.58        | 0.85     |
| 1:O:140:ASP:OD2  | 3:O:6937:HOH:O   | 1.95        | 0.84     |
| 1:A:42:TYR:CE2   | 1:A:46:MET:SD    | 2.69        | 0.84     |
| 1:O:183:ILE:O    | 1:O:183:ILE:HD13 | 1.77        | 0.84     |
| 1:C:261:LYS:HE3  | 1:C:299:ALA:HB1  | 1.60        | 0.84     |
| 1:C:34:ASN:HB2   | 1:C:79:PHE:HB2   | 1.60        | 0.83     |
| 1:C:83:ASN:HD22  | 1:C:84:PRO:HD2   | 1.43        | 0.83     |
| 1:O:57:LYS:HZ1   | 1:O:61:ILE:HD11  | 1.40        | 0.83     |
| 1:B:138:ASN:HB2  | 1:B:141:LYS:HG3  | 1.61        | 0.83     |
| 1:C:249:VAL:HG22 | 1:C:250:ARG:H    | 1.42        | 0.82     |
| 1:B:110:ALA:CB   | 1:B:123:ILE:HD11 | 2.08        | 0.82     |
| 1:B:90:ALA:HB2   | 1:B:117:GLY:HA3  | 1.59        | 0.82     |
| 1:O:90:ALA:HB2   | 1:O:117:GLY:HA3  | 1.61        | 0.82     |
| 1:O:82:ARG:HH11  | 1:O:82:ARG:HB2   | 1.43        | 0.82     |
| 1:O:222:VAL:HG23 | 1:O:223:LEU:H    | 1.44        | 0.81     |
| 1:B:288:PHE:CE2  | 1:B:315:TRP:CB   | 2.62        | 0.81     |
| 1:A:175:GLY:HA3  | 1:A:249:VAL:HG23 | 1.61        | 0.81     |
| 1:A:24:GLN:HE21  | 1:A:58:HIS:CG    | 1.98        | 0.81     |
| 1:O:79:PHE:HB3   | 1:O:81:ILE:HD12  | 1.62        | 0.81     |
| 1:A:252:GLU:HA   | 1:A:252:GLU:OE2  | 1.80        | 0.80     |
| 1:A:233:MET:SD   | 1:B:311:LYS:HD3  | 2.21        | 0.80     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:O:57:LYS:HZ3   | 1:O:61:ILE:HD13  | 1.47        | 0.80     |
| 1:A:29:GLU:HG3   | 1:A:74:LYS:HZ1   | 1.47        | 0.80     |
| 1:O:264:ILE:HD12 | 1:O:297:PHE:CG   | 2.17        | 0.79     |
| 1:A:11:PHE:HE2   | 1:A:16:ARG:HD3   | 1.31        | 0.79     |
| 1:O:240:VAL:CB   | 1:B:206:PHE:HE1  | 1.77        | 0.79     |
| 1:C:88:PRO:HB2   | 1:C:91:GLU:HB3   | 1.64        | 0.79     |
| 1:B:324:ASN:N    | 1:B:324:ASN:HD22 | 1.81        | 0.79     |
| 1:B:134:VAL:HG23 | 1:B:222:VAL:HG11 | 1.64        | 0.79     |
| 1:A:46:MET:CE    | 1:C:193:PRO:HA   | 2.10        | 0.79     |
| 1:O:237:VAL:HG11 | 1:C:237:VAL:HG11 | 1.65        | 0.79     |
| 1:O:23:LEU:H     | 1:O:23:LEU:HD23  | 1.48        | 0.79     |
| 1:O:280:GLU:HG2  | 1:O:299:ALA:HB3  | 1.64        | 0.79     |
| 1:B:286:THR:HG21 | 1:C:51:THR:HG23  | 1.64        | 0.79     |
| 1:A:19:ALA:O     | 1:A:23:LEU:HD13  | 1.82        | 0.79     |
| 1:A:11:PHE:CD2   | 1:A:16:ARG:HD3   | 2.18        | 0.78     |
| 1:A:38:ILE:HD12  | 1:A:43:MET:HG2   | 1.63        | 0.78     |
| 1:O:272:LEU:HB3  | 1:O:276:ILE:HG22 | 1.64        | 0.78     |
| 1:O:97:VAL:HB    | 1:O:121:VAL:HG22 | 1.63        | 0.78     |
| 1:O:48:LYS:HD3   | 1:O:49:TYR:CE2   | 2.17        | 0.78     |
| 1:A:81:ILE:HD12  | 1:A:81:ILE:H     | 1.47        | 0.78     |
| 1:A:29:GLU:HG3   | 1:A:74:LYS:NZ    | 1.99        | 0.78     |
| 1:A:64:LYS:HB2   | 1:A:70:LEU:HD21  | 1.66        | 0.78     |
| 1:C:61:ILE:HD13  | 1:C:71:LEU:HD12  | 1.66        | 0.77     |
| 1:O:61:ILE:HD12  | 1:O:61:ILE:N     | 1.99        | 0.77     |
| 1:C:161:PRO:O    | 1:C:165:VAL:HG23 | 1.84        | 0.77     |
| 1:O:48:LYS:CE    | 1:O:49:TYR:CE2   | 2.64        | 0.77     |
| 1:O:34:ASN:HB2   | 1:O:79:PHE:HB2   | 1.66        | 0.77     |
| 1:O:81:ILE:HD13  | 1:O:88:PRO:HD2   | 1.66        | 0.77     |
| 1:C:14:ILE:HD12  | 1:C:14:ILE:H     | 1.50        | 0.77     |
| 1:A:100:SER:HA   | 1:A:124:SER:OG   | 1.85        | 0.77     |
| 1:O:51:THR:HG23  | 1:A:286:THR:HG21 | 1.67        | 0.77     |
| 1:B:294:SER:OG   | 1:B:325:ARG:HD2  | 1.85        | 0.77     |
| 1:A:11:PHE:CD2   | 1:A:16:ARG:CG    | 2.66        | 0.76     |
| 1:O:68:THR:O     | 1:O:69:LEU:HB2   | 1.85        | 0.76     |
| 1:A:251:ILE:HD13 | 1:A:251:ILE:H    | 1.50        | 0.76     |
| 1:O:48:LYS:HG2   | 1:O:49:TYR:CD2   | 2.21        | 0.76     |
| 1:A:206:PHE:CE2  | 1:C:240:VAL:HB   | 2.21        | 0.76     |
| 1:A:281:GLU:HB2  | 1:A:283:LEU:HD21 | 1.68        | 0.76     |
| 1:A:173:ILE:N    | 1:A:173:ILE:CD1  | 2.49        | 0.76     |
| 1:O:199:ARG:HH11 | 1:O:199:ARG:HG3  | 1.51        | 0.76     |
| 1:B:257:TYR:HA   | 1:B:260:ILE:HD12 | 1.66        | 0.76     |
| 1:C:29:GLU:HG3   | 1:C:31:VAL:HG13  | 1.68        | 0.76     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:O:82:ARG:HH11  | 1:O:82:ARG:CB    | 1.99        | 0.75     |
| 1:C:62:LYS:HG3   | 1:C:70:LEU:HD23  | 1.69        | 0.75     |
| 1:A:284:VAL:HG11 | 1:B:209:ILE:HG12 | 1.68        | 0.75     |
| 1:A:101:THR:OG1  | 1:A:103:VAL:HG22 | 1.86        | 0.75     |
| 1:C:153:SER:CB   | 2:C:6926:SO4:O1  | 2.35        | 0.75     |
| 1:O:112:ALA:HA   | 1:O:115:LYS:NZ   | 2.01        | 0.75     |
| 1:C:73:GLU:HB3   | 1:C:74:LYS:HE3   | 1.68        | 0.75     |
| 1:A:305:LEU:HB2  | 1:B:176:LEU:HD21 | 1.67        | 0.75     |
| 1:A:305:LEU:HD13 | 1:B:231:THR:HG22 | 1.68        | 0.75     |
| 1:A:11:PHE:CZ    | 1:A:16:ARG:HG2   | 2.22        | 0.74     |
| 1:A:18:VAL:HG13  | 1:A:327:ILE:HD11 | 1.68        | 0.74     |
| 1:O:240:VAL:CA   | 1:B:206:PHE:HE1  | 1.98        | 0.74     |
| 1:C:181:HIS:HB3  | 1:C:236:ARG:NE   | 2.01        | 0.74     |
| 1:B:182:ALA:HB1  | 1:B:239:THR:O    | 1.86        | 0.74     |
| 1:C:38:ILE:HG12  | 1:C:46:MET:CE    | 2.18        | 0.74     |
| 1:O:84:PRO:HA    | 1:O:87:ILE:HD12  | 1.67        | 0.74     |
| 1:O:245:VAL:HG23 | 1:O:316:TYR:CE2  | 2.23        | 0.73     |
| 1:C:158:CYS:SG   | 1:C:245:VAL:HG21 | 2.28        | 0.73     |
| 1:O:48:LYS:HG2   | 1:O:49:TYR:CE2   | 2.23        | 0.73     |
| 1:B:177:MET:HG2  | 1:B:178:THR:N    | 2.01        | 0.73     |
| 1:A:177:MET:HG2  | 1:A:178:THR:N    | 2.03        | 0.73     |
| 1:O:193:PRO:CG   | 1:B:38:ILE:HD11  | 2.17        | 0.73     |
| 1:O:206:PHE:HE2  | 1:B:240:VAL:CA   | 2.01        | 0.73     |
| 1:A:13:ARG:NH2   | 1:A:52:VAL:HG12  | 2.04        | 0.73     |
| 1:O:57:LYS:HZ1   | 1:O:61:ILE:CD1   | 1.99        | 0.73     |
| 1:A:233:MET:SD   | 1:B:311:LYS:CD   | 2.77        | 0.73     |
| 1:B:288:PHE:CD2  | 1:B:315:TRP:HB3  | 2.23        | 0.72     |
| 1:C:161:PRO:HB3  | 1:C:276:ILE:HD11 | 1.72        | 0.72     |
| 1:O:96:TYR:HA    | 1:O:120:LYS:O    | 1.89        | 0.72     |
| 1:B:63:ILE:H     | 1:B:63:ILE:HD12  | 1.54        | 0.72     |
| 1:O:31:VAL:HG21  | 1:O:93:GLY:O     | 1.90        | 0.72     |
| 1:A:305:LEU:HD11 | 1:B:228:GLY:O    | 1.90        | 0.72     |
| 1:A:203:ALA:HB3  | 1:A:207:ASN:OD1  | 1.90        | 0.72     |
| 1:C:35:ASP:OD1   | 1:C:38:ILE:HD12  | 1.89        | 0.72     |
| 1:A:24:GLN:NE2   | 1:A:58:HIS:CD2   | 2.58        | 0.72     |
| 1:B:59:SER:HB2   | 1:B:72:GLY:HA3   | 1.71        | 0.72     |
| 1:O:183:ILE:H    | 1:O:183:ILE:HD12 | 1.55        | 0.71     |
| 1:O:19:ALA:O     | 1:O:23:LEU:HD23  | 1.90        | 0.71     |
| 1:A:157:ASN:O    | 1:A:294:SER:HB3  | 1.89        | 0.71     |
| 1:A:100:SER:O    | 1:A:100:SER:OG   | 2.07        | 0.71     |
| 1:A:215:ALA:HB2  | 2:A:6923:SO4:O3  | 1.90        | 0.71     |
| 1:B:42:TYR:O     | 1:B:46:MET:HG3   | 1.91        | 0.71     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:O:57:LYS:NZ    | 1:O:61:ILE:HD13  | 2.01        | 0.71     |
| 1:B:215:ALA:O    | 1:B:219:VAL:HG23 | 1.90        | 0.71     |
| 1:C:4:ILE:HG21   | 1:C:330:ILE:HG22 | 1.72        | 0.71     |
| 1:A:11:PHE:CE2   | 1:A:16:ARG:HD2   | 2.23        | 0.71     |
| 1:A:173:ILE:N    | 1:A:173:ILE:HD12 | 2.05        | 0.71     |
| 1:A:64:LYS:HB2   | 1:A:70:LEU:CD2   | 2.20        | 0.71     |
| 1:A:64:LYS:HD3   | 1:A:68:THR:HG21  | 1.72        | 0.71     |
| 1:C:213:THR:OG1  | 2:C:6926:SO4:O2  | 2.05        | 0.71     |
| 1:C:16:ARG:O     | 1:C:19:ALA:HB3   | 1.91        | 0.71     |
| 1:O:240:VAL:CA   | 1:B:206:PHE:CE1  | 2.73        | 0.71     |
| 1:C:199:ARG:HH11 | 1:C:210:PRO:HB2  | 1.56        | 0.70     |
| 1:C:68:THR:HA    | 1:C:78:VAL:HG23  | 1.71        | 0.70     |
| 1:C:23:LEU:CD1   | 1:C:71:LEU:HD23  | 2.21        | 0.70     |
| 1:A:172:ILE:HD12 | 1:A:226:LEU:HD21 | 1.73        | 0.70     |
| 1:B:288:PHE:HE2  | 1:B:315:TRP:CD1  | 2.09        | 0.70     |
| 1:B:127:SER:HB3  | 1:B:130:ALA:HB3  | 1.71        | 0.70     |
| 1:C:11:PHE:CE1   | 1:C:16:ARG:HG2   | 2.27        | 0.70     |
| 1:B:81:ILE:HD13  | 1:B:87:ILE:HA    | 1.72        | 0.70     |
| 1:O:206:PHE:CE2  | 1:B:240:VAL:CA   | 2.74        | 0.70     |
| 1:O:208:ILE:HD12 | 1:C:315:TRP:HZ3  | 1.55        | 0.70     |
| 1:O:16:ARG:O     | 1:O:19:ALA:HB3   | 1.92        | 0.70     |
| 1:O:104:PHE:HD1  | 1:O:109:LYS:HB3  | 1.56        | 0.70     |
| 1:O:228:GLY:O    | 1:C:305:LEU:HD11 | 1.92        | 0.69     |
| 1:A:83:ASN:HD22  | 1:A:83:ASN:N     | 1.89        | 0.69     |
| 1:O:285:SER:HB3  | 1:C:208:ILE:HB   | 1.74        | 0.69     |
| 1:O:57:LYS:NZ    | 1:O:61:ILE:HD11  | 2.01        | 0.69     |
| 1:A:176:LEU:HD21 | 1:B:305:LEU:HB2  | 1.73        | 0.69     |
| 1:O:199:ARG:NH1  | 1:O:199:ARG:HG3  | 2.07        | 0.69     |
| 1:O:127:SER:CB   | 1:O:130:ALA:HB3  | 2.22        | 0.69     |
| 1:A:183:ILE:HD12 | 1:C:189:THR:HB   | 1.75        | 0.69     |
| 1:C:153:SER:OG   | 2:C:6926:SO4:O1  | 2.09        | 0.69     |
| 1:A:285:SER:HA   | 1:A:315:TRP:CZ3  | 2.28        | 0.69     |
| 1:C:199:ARG:NH1  | 1:C:210:PRO:HB2  | 2.08        | 0.69     |
| 1:B:205:SER:HA   | 1:B:238:PRO:HG3  | 1.75        | 0.68     |
| 1:C:213:THR:OG1  | 2:C:6926:SO4:O3  | 2.10        | 0.68     |
| 1:B:6:ILE:HG22   | 1:B:96:TYR:HB2   | 1.75        | 0.68     |
| 1:O:288:PHE:CE1  | 1:O:315:TRP:CD1  | 2.73        | 0.68     |
| 1:A:202:ARG:HH21 | 1:C:51:THR:N     | 1.92        | 0.68     |
| 1:A:142:TYR:HE2  | 1:A:333:MET:HA   | 1.58        | 0.68     |
| 1:O:81:ILE:HD13  | 1:O:87:ILE:HA    | 1.75        | 0.68     |
| 1:C:264:ILE:HD12 | 1:C:297:PHE:CG   | 2.28        | 0.68     |
| 1:B:38:ILE:N     | 1:B:38:ILE:CD1   | 2.57        | 0.67     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:4:ILE:CD1    | 1:B:28:VAL:HG22  | 2.24        | 0.67     |
| 1:O:222:VAL:HG23 | 1:O:223:LEU:N    | 2.09        | 0.67     |
| 1:A:309:PHE:HE2  | 1:B:175:GLY:H    | 1.41        | 0.67     |
| 1:O:57:LYS:HA    | 1:O:57:LYS:HE3   | 1.76        | 0.67     |
| 1:O:183:ILE:HD12 | 1:O:239:THR:O    | 1.94        | 0.67     |
| 1:O:23:LEU:HD11  | 1:O:47:PHE:CZ    | 2.30        | 0.67     |
| 1:C:69:LEU:O     | 1:C:70:LEU:HB2   | 1.94        | 0.67     |
| 1:B:6:ILE:CG2    | 1:B:96:TYR:HB2   | 2.24        | 0.67     |
| 1:O:59:SER:O     | 1:O:72:GLY:HA3   | 1.94        | 0.67     |
| 1:C:134:VAL:HG22 | 1:C:152:ALA:HB2  | 1.76        | 0.67     |
| 1:C:158:CYS:O    | 1:C:161:PRO:HD2  | 1.94        | 0.67     |
| 1:C:81:ILE:HD13  | 1:C:87:ILE:HA    | 1.76        | 0.67     |
| 1:A:84:PRO:HB2   | 1:A:112:ALA:HB3  | 1.76        | 0.67     |
| 1:O:256:SER:O    | 1:O:260:ILE:HD13 | 1.94        | 0.67     |
| 1:A:84:PRO:HA    | 1:A:87:ILE:HD11  | 1.76        | 0.67     |
| 1:O:59:SER:O     | 1:O:60:ASP:HB3   | 1.95        | 0.67     |
| 1:O:208:ILE:H    | 1:C:285:SER:HB2  | 1.60        | 0.66     |
| 1:C:88:PRO:HB2   | 1:C:91:GLU:CB    | 2.24        | 0.66     |
| 1:C:172:ILE:HG23 | 1:C:249:VAL:CG2  | 2.25        | 0.66     |
| 1:O:254:ALA:HA   | 1:O:307:ASP:O    | 1.95        | 0.66     |
| 1:O:215:ALA:O    | 1:O:218:ALA:HB3  | 1.95        | 0.66     |
| 1:C:215:ALA:HB2  | 2:C:6926:SO4:S   | 2.35        | 0.66     |
| 1:A:142:TYR:CE2  | 1:A:333:MET:HG2  | 2.31        | 0.66     |
| 1:O:288:PHE:CE1  | 1:O:315:TRP:CB   | 2.78        | 0.66     |
| 1:C:159:LEU:HD13 | 1:C:245:VAL:HG11 | 1.75        | 0.66     |
| 1:C:159:LEU:HD11 | 1:C:247:LEU:HD22 | 1.76        | 0.66     |
| 1:O:68:THR:O     | 1:O:69:LEU:CB    | 2.42        | 0.66     |
| 1:B:205:SER:C    | 1:B:206:PHE:CD2  | 2.68        | 0.66     |
| 1:B:111:ALA:HA   | 1:B:148:ILE:HD11 | 1.78        | 0.66     |
| 1:B:216:ALA:HB1  | 1:B:231:THR:CA   | 2.20        | 0.66     |
| 1:O:211:SER:O    | 1:O:234:SER:HB3  | 1.94        | 0.66     |
| 1:A:69:LEU:O     | 1:A:75:PRO:HA    | 1.95        | 0.66     |
| 1:A:258:ASP:HA   | 1:A:261:LYS:HD3  | 1.77        | 0.66     |
| 1:B:243:SER:HB2  | 1:B:316:TYR:CE1  | 2.30        | 0.66     |
| 1:O:176:LEU:HD23 | 1:O:231:THR:HG23 | 1.77        | 0.65     |
| 1:O:264:ILE:HD12 | 1:O:297:PHE:CD2  | 2.31        | 0.65     |
| 1:C:90:ALA:HB2   | 1:C:117:GLY:O    | 1.96        | 0.65     |
| 1:O:48:LYS:CG    | 1:O:49:TYR:CE2   | 2.80        | 0.65     |
| 1:O:18:VAL:HG13  | 1:O:327:ILE:HD11 | 1.79        | 0.65     |
| 1:C:31:VAL:HG21  | 1:C:93:GLY:O     | 1.96        | 0.65     |
| 1:O:9:ASN:ND2    | 1:O:87:ILE:HD13  | 2.12        | 0.65     |
| 1:A:305:LEU:HD23 | 1:A:309:PHE:HD2  | 1.61        | 0.64     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:C:251:ILE:H    | 1:C:251:ILE:HD13 | 1.62        | 0.64     |
| 1:A:237:VAL:HG11 | 1:B:237:VAL:HG11 | 1.77        | 0.64     |
| 1:A:176:LEU:O    | 1:A:247:LEU:HD12 | 1.97        | 0.64     |
| 1:A:44:THR:CG2   | 1:A:69:LEU:HD11  | 2.28        | 0.64     |
| 1:A:260:ILE:O    | 1:A:264:ILE:HG12 | 1.97        | 0.64     |
| 1:A:30:LEU:HD23  | 1:A:31:VAL:N     | 2.12        | 0.64     |
| 1:O:161:PRO:O    | 1:O:165:VAL:HG23 | 1.96        | 0.64     |
| 1:O:12:GLY:O     | 1:O:16:ARG:CD    | 2.35        | 0.64     |
| 1:A:208:ILE:O    | 1:A:210:PRO:HD3  | 1.97        | 0.64     |
| 1:C:83:ASN:ND2   | 1:C:84:PRO:HD2   | 2.13        | 0.64     |
| 1:O:296:ILE:HB   | 1:O:315:TRP:HB2  | 1.80        | 0.64     |
| 1:O:260:ILE:N    | 1:O:260:ILE:HD13 | 2.13        | 0.64     |
| 1:O:166:ILE:H    | 1:O:166:ILE:HD12 | 1.63        | 0.64     |
| 1:O:284:VAL:HG11 | 1:C:209:ILE:HG12 | 1.80        | 0.63     |
| 1:A:246:ASP:OD1  | 1:B:178:THR:HG21 | 1.97        | 0.63     |
| 1:A:131:PRO:HD2  | 1:A:148:ILE:O    | 1.97        | 0.63     |
| 1:C:11:PHE:CE1   | 1:C:16:ARG:HA    | 2.33        | 0.63     |
| 1:B:56:TRP:HD1   | 1:B:61:ILE:HD11  | 1.64        | 0.63     |
| 1:B:158:CYS:HG   | 1:B:316:TYR:HD2  | 1.45        | 0.63     |
| 1:C:251:ILE:HD13 | 1:C:308:ASN:O    | 1.99        | 0.63     |
| 1:B:59:SER:HB2   | 1:B:72:GLY:CA    | 2.28        | 0.63     |
| 1:O:194:SER:H    | 1:B:42:TYR:HE2   | 1.41        | 0.63     |
| 1:C:327:ILE:HA   | 1:C:330:ILE:HD12 | 1.78        | 0.63     |
| 1:C:83:ASN:HD22  | 1:C:84:PRO:N     | 1.97        | 0.63     |
| 1:C:4:ILE:HG21   | 1:C:330:ILE:CG2  | 2.27        | 0.63     |
| 1:C:161:PRO:HB3  | 1:C:276:ILE:CD1  | 2.28        | 0.63     |
| 1:B:327:ILE:O    | 1:B:327:ILE:HG22 | 1.97        | 0.63     |
| 1:O:205:SER:O    | 1:O:206:PHE:HD1  | 1.82        | 0.63     |
| 1:B:103:VAL:HG23 | 1:B:104:PHE:N    | 2.11        | 0.63     |
| 1:A:66:SER:C     | 1:A:68:THR:H     | 2.01        | 0.63     |
| 1:A:67:LYS:O     | 1:A:77:THR:HA    | 1.99        | 0.63     |
| 1:O:247:LEU:HG   | 1:O:249:VAL:HG13 | 1.80        | 0.63     |
| 1:O:257:TYR:CD2  | 1:O:261:LYS:HD2  | 2.34        | 0.62     |
| 1:O:282:ASP:HB3  | 1:C:199:ARG:HG3  | 1.81        | 0.62     |
| 1:A:42:TYR:HE2   | 1:A:46:MET:CE    | 1.88        | 0.62     |
| 1:B:89:TRP:NE1   | 1:B:113:HIS:ND1  | 2.43        | 0.62     |
| 1:A:173:ILE:CD1  | 1:A:252:GLU:N    | 2.57        | 0.62     |
| 1:C:249:VAL:HG22 | 1:C:250:ARG:N    | 2.11        | 0.62     |
| 1:B:325:ARG:HH11 | 1:B:325:ARG:HG2  | 1.63        | 0.62     |
| 1:O:64:LYS:HG3   | 1:O:70:LEU:CB    | 2.28        | 0.62     |
| 1:B:126:PRO:HD3  | 1:B:153:SER:HB3  | 1.81        | 0.62     |
| 1:A:90:ALA:HB2   | 1:A:117:GLY:HA3  | 1.82        | 0.62     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:285:SER:CB   | 3:B:6956:HOH:O   | 2.48        | 0.62     |
| 1:A:43:MET:C     | 1:A:45:TYR:H     | 2.02        | 0.62     |
| 1:C:11:PHE:H     | 1:C:35:ASP:HB2   | 1.63        | 0.62     |
| 1:O:288:PHE:CD1  | 1:O:315:TRP:CB   | 2.83        | 0.61     |
| 1:O:84:PRO:HA    | 1:O:87:ILE:CD1   | 2.29        | 0.61     |
| 1:A:42:TYR:CE1   | 1:C:198:TRP:CD1  | 2.88        | 0.61     |
| 1:B:177:MET:HG2  | 1:B:178:THR:H    | 1.65        | 0.61     |
| 1:B:85:ASP:H     | 1:B:112:ALA:HB1  | 1.66        | 0.61     |
| 1:O:113:HIS:O    | 1:O:118:ALA:HB3  | 2.00        | 0.61     |
| 1:O:248:THR:HG23 | 1:C:176:LEU:HD12 | 1.82        | 0.61     |
| 1:O:122:VAL:HG13 | 1:O:149:VAL:HG23 | 1.82        | 0.61     |
| 1:C:219:VAL:HG12 | 1:C:223:LEU:HB2  | 1.82        | 0.61     |
| 1:B:288:PHE:CD2  | 1:B:315:TRP:CB   | 2.83        | 0.61     |
| 1:B:181:HIS:O    | 1:B:236:ARG:HA   | 2.00        | 0.61     |
| 1:B:142:TYR:CZ   | 1:B:333:MET:HG2  | 2.34        | 0.61     |
| 1:O:288:PHE:CD1  | 1:O:315:TRP:HB3  | 2.35        | 0.61     |
| 1:C:272:LEU:HD13 | 1:C:276:ILE:CD1  | 2.30        | 0.61     |
| 1:O:111:ALA:O    | 1:O:114:LEU:HD23 | 2.00        | 0.61     |
| 1:O:99:GLU:OE2   | 1:O:99:GLU:HA    | 2.01        | 0.61     |
| 1:A:265:LYS:HG2  | 1:A:269:GLU:OE2  | 2.00        | 0.61     |
| 1:A:158:CYS:HG   | 1:A:245:VAL:CG2  | 2.13        | 0.61     |
| 1:A:42:TYR:HD1   | 1:C:198:TRP:CZ2  | 2.19        | 0.61     |
| 1:O:213:THR:HG22 | 1:O:233:MET:HA   | 1.82        | 0.61     |
| 1:C:208:ILE:O    | 1:C:210:PRO:HD3  | 2.01        | 0.60     |
| 1:C:306:ASN:O    | 1:C:308:ASN:N    | 2.33        | 0.60     |
| 1:C:137:VAL:HG21 | 1:C:160:ALA:HB1  | 1.82        | 0.60     |
| 1:O:178:THR:O    | 1:O:246:ASP:HB3  | 2.02        | 0.60     |
| 1:O:310:VAL:HG22 | 1:O:311:LYS:N    | 2.16        | 0.60     |
| 1:O:18:VAL:HG13  | 1:O:327:ILE:CD1  | 2.32        | 0.60     |
| 1:A:43:MET:O     | 1:A:45:TYR:N     | 2.34        | 0.60     |
| 1:C:138:ASN:C    | 1:C:140:ASP:H    | 2.04        | 0.60     |
| 1:B:324:ASN:O    | 1:B:328:ASP:HB2  | 2.00        | 0.60     |
| 1:O:245:VAL:HG12 | 1:O:246:ASP:N    | 2.16        | 0.60     |
| 1:B:215:ALA:HA   | 1:B:218:ALA:HB3  | 1.83        | 0.60     |
| 1:C:8:ILE:HG22   | 1:C:10:GLY:H     | 1.66        | 0.60     |
| 1:B:140:ASP:C    | 1:B:142:TYR:H    | 2.03        | 0.60     |
| 1:O:309:PHE:CZ   | 1:C:176:LEU:HG   | 2.36        | 0.60     |
| 1:B:261:LYS:HE3  | 1:B:299:ALA:HB1  | 1.84        | 0.60     |
| 1:A:18:VAL:HG13  | 1:A:327:ILE:CD1  | 2.31        | 0.60     |
| 1:A:55:GLN:OE1   | 1:A:57:LYS:CG    | 2.50        | 0.60     |
| 1:O:177:MET:C    | 1:O:177:MET:SD   | 2.79        | 0.60     |
| 1:B:121:VAL:HB   | 1:B:148:ILE:HD13 | 1.83        | 0.59     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:16:ARG:HD2   | 1:B:47:PHE:HA    | 1.84        | 0.59     |
| 1:B:244:VAL:CG2  | 1:B:313:VAL:HG13 | 2.32        | 0.59     |
| 1:C:38:ILE:CG1   | 1:C:46:MET:HE2   | 2.29        | 0.59     |
| 1:O:160:ALA:HB3  | 1:O:161:PRO:HD3  | 1.84        | 0.59     |
| 1:O:284:VAL:HB   | 1:C:207:ASN:HD22 | 1.67        | 0.59     |
| 1:A:175:GLY:CA   | 1:A:249:VAL:HG23 | 2.31        | 0.59     |
| 1:A:11:PHE:HZ    | 1:A:47:PHE:HD2   | 1.50        | 0.59     |
| 1:C:64:LYS:O     | 1:C:68:THR:HG23  | 2.03        | 0.59     |
| 1:O:106:ASP:OD1  | 1:O:128:LYS:HE2  | 2.03        | 0.59     |
| 1:C:154:CYS:SG   | 1:C:181:HIS:CE1  | 2.95        | 0.59     |
| 1:A:244:VAL:CG2  | 1:A:313:VAL:HG23 | 2.32        | 0.59     |
| 1:A:251:ILE:HD13 | 1:A:251:ILE:N    | 2.16        | 0.59     |
| 1:B:281:GLU:O    | 1:B:283:LEU:N    | 2.35        | 0.59     |
| 1:C:264:ILE:HD12 | 1:C:297:PHE:CD1  | 2.38        | 0.59     |
| 1:O:288:PHE:CD1  | 1:O:315:TRP:CG   | 2.88        | 0.59     |
| 1:A:254:ALA:HB2  | 1:A:308:ASN:ND2  | 2.16        | 0.59     |
| 1:O:202:ARG:HG3  | 1:C:284:VAL:HG11 | 1.84        | 0.59     |
| 1:B:56:TRP:CD1   | 1:B:61:ILE:HD11  | 2.38        | 0.59     |
| 1:O:191:ASP:HA   | 1:O:202:ARG:HA   | 1.83        | 0.59     |
| 1:C:199:ARG:HB3  | 1:C:209:ILE:HG23 | 1.84        | 0.59     |
| 1:B:324:ASN:H    | 1:B:324:ASN:HD22 | 1.50        | 0.59     |
| 1:O:226:LEU:HA   | 1:O:229:LYS:HD2  | 1.85        | 0.59     |
| 1:O:190:VAL:CG2  | 1:B:185:ALA:HB2  | 2.32        | 0.59     |
| 1:C:127:SER:CB   | 1:C:130:ALA:HB3  | 2.33        | 0.59     |
| 1:A:230:LEU:O    | 1:A:231:THR:HB   | 2.02        | 0.59     |
| 1:O:187:GLN:HB3  | 1:O:204:ALA:HB2  | 1.85        | 0.59     |
| 1:C:65:ASP:OD2   | 1:C:65:ASP:C     | 2.42        | 0.59     |
| 1:O:72:GLY:O     | 1:O:73:GLU:HB2   | 2.01        | 0.59     |
| 1:O:79:PHE:HB3   | 1:O:81:ILE:CD1   | 2.33        | 0.59     |
| 1:C:329:LEU:O    | 1:C:333:MET:N    | 2.34        | 0.59     |
| 1:A:298:ASP:OD1  | 1:A:301:ALA:HB2  | 2.03        | 0.59     |
| 1:O:170:PHE:CZ   | 1:O:260:ILE:HD12 | 2.37        | 0.58     |
| 1:O:261:LYS:HE3  | 1:O:299:ALA:HB1  | 1.84        | 0.58     |
| 1:B:16:ARG:O     | 1:B:20:ARG:HG3   | 2.02        | 0.58     |
| 1:O:202:ARG:NH1  | 1:C:284:VAL:HG22 | 2.17        | 0.58     |
| 1:C:9:ASN:O      | 1:C:101:THR:HG23 | 2.03        | 0.58     |
| 1:O:157:ASN:O    | 1:O:294:SER:HB3  | 2.03        | 0.58     |
| 1:O:166:ILE:H    | 1:O:166:ILE:CD1  | 2.16        | 0.58     |
| 1:A:48:LYS:HE2   | 1:A:49:TYR:CE1   | 2.39        | 0.58     |
| 1:C:215:ALA:CA   | 2:C:6926:SO4:O3  | 2.50        | 0.58     |
| 1:B:230:LEU:O    | 1:B:231:THR:HB   | 2.02        | 0.58     |
| 1:O:183:ILE:HG23 | 1:O:237:VAL:O    | 2.03        | 0.58     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:C:172:ILE:HG12 | 1:C:249:VAL:HG21 | 1.84        | 0.58     |
| 1:B:257:TYR:O    | 1:B:261:LYS:HG3  | 2.03        | 0.58     |
| 1:A:44:THR:HG23  | 1:A:69:LEU:HD11  | 1.84        | 0.58     |
| 1:O:315:TRP:O    | 1:O:316:TYR:HB3  | 2.04        | 0.58     |
| 1:C:14:ILE:O     | 1:C:18:VAL:HG23  | 2.04        | 0.58     |
| 1:B:40:THR:OG1   | 1:B:78:VAL:HG21  | 2.04        | 0.58     |
| 1:O:205:SER:O    | 1:O:206:PHE:CD1  | 2.57        | 0.58     |
| 1:A:172:ILE:C    | 1:A:173:ILE:HD12 | 2.24        | 0.58     |
| 1:B:22:ALA:HB2   | 1:B:327:ILE:HD13 | 1.85        | 0.58     |
| 1:O:178:THR:HG23 | 1:O:233:MET:HG3  | 1.86        | 0.58     |
| 1:B:11:PHE:CD2   | 1:B:16:ARG:HG2   | 2.39        | 0.58     |
| 1:O:305:LEU:HD11 | 1:C:228:GLY:O    | 2.04        | 0.58     |
| 1:B:27:ASP:OD2   | 1:B:331:ARG:HG3  | 2.03        | 0.58     |
| 1:O:278:TYR:OH   | 1:O:280:GLU:OE1  | 2.13        | 0.58     |
| 1:B:152:ALA:HB1  | 1:B:156:THR:HB   | 1.86        | 0.58     |
| 1:C:61:ILE:HD13  | 1:C:71:LEU:CD1   | 2.33        | 0.58     |
| 1:O:155:THR:O    | 1:O:157:ASN:N    | 2.37        | 0.57     |
| 1:C:241:ASP:OD1  | 1:C:319:GLU:HG3  | 2.04        | 0.57     |
| 1:A:42:TYR:CD1   | 1:C:198:TRP:NE1  | 2.71        | 0.57     |
| 1:O:193:PRO:HB3  | 1:B:38:ILE:CD1   | 2.33        | 0.57     |
| 1:B:275:ILE:HG22 | 1:B:275:ILE:O    | 2.03        | 0.57     |
| 1:O:155:THR:HG22 | 1:O:156:THR:N    | 2.20        | 0.57     |
| 1:B:325:ARG:NE   | 1:B:325:ARG:HA   | 2.20        | 0.57     |
| 1:A:162:LEU:O    | 1:A:166:ILE:HD13 | 2.04        | 0.57     |
| 1:C:16:ARG:NH1   | 1:C:16:ARG:HG3   | 2.18        | 0.57     |
| 1:A:208:ILE:HD11 | 3:B:6956:HOH:O   | 2.03        | 0.57     |
| 1:A:111:ALA:HB1  | 1:A:114:LEU:HD12 | 1.86        | 0.57     |
| 1:O:57:LYS:CA    | 1:O:57:LYS:HE3   | 2.34        | 0.57     |
| 1:O:9:ASN:HD22   | 1:O:89:TRP:HZ2   | 1.52        | 0.57     |
| 1:C:110:ALA:CB   | 1:C:123:ILE:HD11 | 2.35        | 0.57     |
| 1:C:158:CYS:C    | 1:C:161:PRO:HD2  | 2.23        | 0.57     |
| 1:O:81:ILE:CD1   | 1:O:88:PRO:HD2   | 2.32        | 0.57     |
| 1:A:179:THR:HG23 | 1:A:234:SER:CB   | 2.35        | 0.57     |
| 1:O:48:LYS:CG    | 1:O:49:TYR:HE2   | 2.17        | 0.57     |
| 1:A:107:LYS:HA   | 1:A:148:ILE:HG21 | 1.87        | 0.57     |
| 1:O:57:LYS:H     | 1:O:57:LYS:HE3   | 1.69        | 0.57     |
| 1:O:81:ILE:HD13  | 1:O:88:PRO:CD    | 2.35        | 0.57     |
| 1:A:16:ARG:O     | 1:A:19:ALA:HB3   | 2.05        | 0.57     |
| 1:A:66:SER:O     | 1:A:68:THR:N     | 2.38        | 0.57     |
| 1:O:106:ASP:CB   | 1:O:128:LYS:HE2  | 2.35        | 0.57     |
| 1:O:260:ILE:CD1  | 1:O:260:ILE:N    | 2.68        | 0.57     |
| 1:B:160:ALA:HB3  | 1:B:161:PRO:CD   | 2.30        | 0.57     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:23:LEU:HD21  | 1:A:71:LEU:HG    | 1.85        | 0.56     |
| 1:O:281:GLU:O    | 1:O:283:LEU:HG   | 2.05        | 0.56     |
| 1:C:176:LEU:HD22 | 1:C:231:THR:HG23 | 1.87        | 0.56     |
| 1:C:16:ARG:HG3   | 1:C:16:ARG:HH11  | 1.70        | 0.56     |
| 1:O:166:ILE:N    | 1:O:166:ILE:HD12 | 2.20        | 0.56     |
| 1:C:34:ASN:CB    | 1:C:79:PHE:HB2   | 2.34        | 0.56     |
| 1:B:181:HIS:O    | 1:B:236:ARG:HD3  | 2.05        | 0.56     |
| 1:A:24:GLN:HG3   | 1:A:56:TRP:CH2   | 2.39        | 0.56     |
| 1:C:213:THR:HG23 | 1:C:213:THR:O    | 2.06        | 0.56     |
| 1:O:206:PHE:HE2  | 1:B:240:VAL:HA   | 1.67        | 0.56     |
| 1:O:82:ARG:NH1   | 1:O:82:ARG:HB2   | 2.17        | 0.56     |
| 1:O:240:VAL:HG22 | 1:O:241:ASP:N    | 2.19        | 0.56     |
| 1:A:31:VAL:C     | 1:A:76:VAL:HG13  | 2.25        | 0.56     |
| 1:C:106:ASP:HB2  | 1:C:109:LYS:HB2  | 1.87        | 0.56     |
| 1:C:211:SER:OG   | 1:C:212:SER:N    | 2.39        | 0.56     |
| 1:A:173:ILE:HD13 | 1:A:251:ILE:HA   | 1.87        | 0.56     |
| 1:A:113:HIS:HB2  | 1:A:121:VAL:CG2  | 2.36        | 0.56     |
| 1:O:286:THR:OG1  | 1:C:207:ASN:ND2  | 2.39        | 0.56     |
| 1:O:239:THR:HG21 | 1:C:208:ILE:HG13 | 1.86        | 0.56     |
| 1:O:240:VAL:HA   | 1:B:206:PHE:HE1  | 1.70        | 0.56     |
| 1:O:199:ARG:HD3  | 1:C:283:LEU:O    | 2.06        | 0.56     |
| 1:A:42:TYR:HE1   | 1:C:198:TRP:CG   | 2.23        | 0.56     |
| 1:O:182:ALA:HB1  | 1:O:239:THR:O    | 2.06        | 0.56     |
| 1:A:282:ASP:HB3  | 1:B:199:ARG:HG2  | 1.87        | 0.56     |
| 1:O:68:THR:HG22  | 1:O:69:LEU:N     | 2.21        | 0.56     |
| 1:A:24:GLN:HG3   | 1:A:56:TRP:HH2   | 1.71        | 0.56     |
| 1:C:272:LEU:CB   | 1:C:276:ILE:HD13 | 2.29        | 0.56     |
| 1:B:6:ILE:HD12   | 1:B:28:VAL:HG12  | 1.86        | 0.56     |
| 1:C:81:ILE:CD1   | 1:C:87:ILE:HA    | 2.36        | 0.56     |
| 1:C:173:ILE:HD12 | 1:C:250:ARG:HD2  | 1.88        | 0.56     |
| 1:C:264:ILE:HD12 | 1:C:297:PHE:CD2  | 2.41        | 0.56     |
| 1:C:181:HIS:HB3  | 1:C:236:ARG:CD   | 2.36        | 0.56     |
| 1:A:216:ALA:HB3  | 1:A:231:THR:HA   | 1.88        | 0.56     |
| 1:O:83:ASN:HB2   | 1:O:86:GLU:HG3   | 1.87        | 0.56     |
| 1:A:22:ALA:HA    | 1:A:28:VAL:HG13  | 1.88        | 0.56     |
| 1:O:206:PHE:CE2  | 1:B:240:VAL:CG2  | 2.88        | 0.56     |
| 1:B:272:LEU:O    | 1:B:276:ILE:HG22 | 2.06        | 0.56     |
| 1:A:245:VAL:O    | 1:A:313:VAL:HA   | 2.06        | 0.55     |
| 1:O:112:ALA:HA   | 1:O:115:LYS:HZ3  | 1.69        | 0.55     |
| 1:C:242:VAL:HA   | 1:C:317:ASP:HA   | 1.88        | 0.55     |
| 1:B:49:TYR:CD1   | 1:C:283:LEU:HD11 | 2.41        | 0.55     |
| 1:A:9:ASN:HD22   | 1:A:113:HIS:HE1  | 1.54        | 0.55     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:O:245:VAL:CG1  | 1:O:246:ASP:N    | 2.68        | 0.55     |
| 1:C:134:VAL:HG23 | 1:C:222:VAL:HG11 | 1.88        | 0.55     |
| 1:C:13:ARG:NH2   | 1:C:319:GLU:OE1  | 2.39        | 0.55     |
| 1:C:178:THR:O    | 1:C:246:ASP:HB3  | 2.06        | 0.55     |
| 1:C:276:ILE:N    | 1:C:276:ILE:HD12 | 2.21        | 0.55     |
| 1:C:25:SER:OG    | 1:C:28:VAL:HB    | 2.06        | 0.55     |
| 1:B:20:ARG:O     | 1:B:24:GLN:HB2   | 2.06        | 0.55     |
| 1:A:207:ASN:HD22 | 1:B:284:VAL:CG2  | 2.19        | 0.55     |
| 1:A:21:VAL:HG11  | 1:A:327:ILE:HG13 | 1.88        | 0.55     |
| 1:C:101:THR:O    | 1:C:103:VAL:HG23 | 2.06        | 0.55     |
| 1:C:137:VAL:HG12 | 1:C:138:ASN:N    | 2.21        | 0.55     |
| 1:O:256:SER:O    | 1:O:260:ILE:CD1  | 2.55        | 0.55     |
| 1:B:280:GLU:HG2  | 1:B:299:ALA:HB3  | 1.89        | 0.55     |
| 1:O:44:THR:HG22  | 1:O:69:LEU:CD1   | 2.34        | 0.55     |
| 1:O:134:VAL:CG2  | 1:O:222:VAL:HG11 | 2.36        | 0.55     |
| 1:O:242:VAL:HG21 | 1:O:285:SER:O    | 2.06        | 0.55     |
| 1:B:158:CYS:HA   | 1:B:295:SER:HB2  | 1.89        | 0.55     |
| 1:B:156:THR:HG23 | 1:B:219:VAL:HG22 | 1.89        | 0.55     |
| 1:A:9:ASN:O      | 1:A:101:THR:HG22 | 2.05        | 0.55     |
| 1:A:42:TYR:CE1   | 1:C:198:TRP:CG   | 2.95        | 0.55     |
| 1:C:134:VAL:HG22 | 1:C:152:ALA:CB   | 2.36        | 0.55     |
| 1:C:11:PHE:N     | 1:C:35:ASP:HB2   | 2.22        | 0.55     |
| 1:O:115:LYS:HD2  | 1:O:115:LYS:H    | 1.70        | 0.55     |
| 1:B:265:LYS:O    | 1:B:269:GLU:HG3  | 2.07        | 0.55     |
| 1:A:318:ASN:ND2  | 1:A:319:GLU:HG3  | 2.20        | 0.55     |
| 1:B:17:LEU:CD1   | 1:B:319:GLU:HB3  | 2.37        | 0.55     |
| 1:A:153:SER:HB2  | 2:A:6923:SO4:O4  | 2.07        | 0.55     |
| 1:A:97:VAL:HG11  | 1:A:113:HIS:CG   | 2.42        | 0.55     |
| 1:A:167:HIS:HB2  | 1:A:172:ILE:CD1  | 2.37        | 0.55     |
| 1:B:49:TYR:CE1   | 1:C:283:LEU:HD11 | 2.41        | 0.55     |
| 1:C:283:LEU:HG   | 1:C:287:ASP:OD2  | 2.06        | 0.55     |
| 1:O:181:HIS:O    | 1:O:237:VAL:HG22 | 2.07        | 0.54     |
| 1:O:48:LYS:CG    | 1:O:49:TYR:CD2   | 2.90        | 0.54     |
| 1:O:267:ALA:O    | 1:O:272:LEU:HB2  | 2.07        | 0.54     |
| 1:A:66:SER:C     | 1:A:68:THR:N     | 2.61        | 0.54     |
| 1:O:8:ILE:O      | 1:O:33:VAL:HA    | 2.07        | 0.54     |
| 1:C:17:LEU:HD23  | 1:C:20:ARG:HD2   | 1.89        | 0.54     |
| 1:C:3:LYS:HE2    | 1:C:26:GLU:O     | 2.06        | 0.54     |
| 1:B:23:LEU:CD1   | 1:B:71:LEU:HG    | 2.38        | 0.54     |
| 1:O:288:PHE:HD1  | 1:O:315:TRP:HB3  | 1.72        | 0.54     |
| 1:C:177:MET:HG3  | 1:C:245:VAL:HG13 | 1.90        | 0.54     |
| 1:O:49:TYR:HD2   | 1:O:49:TYR:N     | 2.06        | 0.54     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:C:73:GLU:CB    | 1:C:74:LYS:HE3   | 2.35        | 0.54     |
| 1:A:265:LYS:HB2  | 1:A:278:TYR:CD1  | 2.41        | 0.54     |
| 1:A:294:SER:OG   | 1:A:325:ARG:HD2  | 2.07        | 0.54     |
| 1:C:61:ILE:CD1   | 1:C:71:LEU:HD12  | 2.35        | 0.54     |
| 1:B:325:ARG:HG2  | 1:B:325:ARG:NH1  | 2.19        | 0.54     |
| 1:O:287:ASP:OD1  | 1:A:49:TYR:HB3   | 2.07        | 0.54     |
| 1:B:103:VAL:O    | 1:B:105:THR:N    | 2.39        | 0.54     |
| 1:B:38:ILE:HD13  | 1:B:38:ILE:N     | 2.23        | 0.54     |
| 1:O:205:SER:C    | 1:O:206:PHE:CD1  | 2.80        | 0.54     |
| 1:O:208:ILE:HD12 | 1:C:315:TRP:CZ3  | 2.41        | 0.54     |
| 1:O:62:LYS:HE2   | 1:O:70:LEU:HD23  | 1.87        | 0.54     |
| 1:B:71:LEU:N     | 1:B:71:LEU:HD22  | 2.22        | 0.54     |
| 1:C:276:ILE:HG22 | 1:C:277:GLY:N    | 2.23        | 0.54     |
| 1:C:84:PRO:HA    | 1:C:87:ILE:CD1   | 2.37        | 0.54     |
| 1:B:17:LEU:HD21  | 1:B:53:HIS:CD2   | 2.42        | 0.54     |
| 1:A:173:ILE:HD11 | 1:A:252:GLU:CA   | 2.37        | 0.54     |
| 1:O:40:THR:O     | 1:O:44:THR:HG23  | 2.07        | 0.54     |
| 1:B:132:MET:HA   | 1:B:150:SER:O    | 2.08        | 0.54     |
| 1:A:38:ILE:HG13  | 1:A:43:MET:HE2   | 1.90        | 0.54     |
| 1:O:284:VAL:CG1  | 1:C:209:ILE:HG12 | 2.37        | 0.54     |
| 1:O:309:PHE:CE2  | 1:C:176:LEU:HG   | 2.43        | 0.54     |
| 1:B:61:ILE:N     | 1:B:61:ILE:HD12  | 2.23        | 0.54     |
| 1:A:42:TYR:CZ    | 1:A:46:MET:HE3   | 2.26        | 0.54     |
| 1:C:159:LEU:HD22 | 1:C:177:MET:SD   | 2.48        | 0.54     |
| 1:O:48:LYS:HG2   | 1:O:49:TYR:HD2   | 1.72        | 0.54     |
| 1:A:208:ILE:CD1  | 3:B:6956:HOH:O   | 2.55        | 0.54     |
| 1:A:87:ILE:HD13  | 1:A:89:TRP:CZ2   | 2.43        | 0.54     |
| 1:O:120:LYS:HD3  | 1:O:147:ASP:OD1  | 2.08        | 0.54     |
| 1:C:158:CYS:SG   | 1:C:245:VAL:CG2  | 2.96        | 0.53     |
| 1:B:152:ALA:HB3  | 1:B:157:ASN:ND2  | 2.22        | 0.53     |
| 1:C:148:ILE:HD12 | 1:C:148:ILE:N    | 2.23        | 0.53     |
| 1:A:60:ASP:OD2   | 1:A:60:ASP:N     | 2.41        | 0.53     |
| 1:C:272:LEU:HD13 | 1:C:276:ILE:HD13 | 1.88        | 0.53     |
| 1:O:84:PRO:HB2   | 1:O:112:ALA:HB3  | 1.88        | 0.53     |
| 1:O:32:ALA:HA    | 1:O:77:THR:O     | 2.08        | 0.53     |
| 1:O:120:LYS:HE2  | 1:O:146:ILE:O    | 2.08        | 0.53     |
| 1:O:131:PRO:HD2  | 1:O:148:ILE:O    | 2.08        | 0.53     |
| 1:O:282:ASP:HA   | 1:C:199:ARG:NE   | 2.18        | 0.53     |
| 1:A:308:ASN:O    | 1:A:309:PHE:HB2  | 2.08        | 0.53     |
| 1:O:99:GLU:CB    | 1:O:123:ILE:HA   | 2.31        | 0.53     |
| 1:A:9:ASN:ND2    | 1:A:34:ASN:HD22  | 2.07        | 0.53     |
| 1:O:241:ASP:O    | 1:O:242:VAL:HB   | 2.08        | 0.53     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:252:GLU:CA   | 1:A:252:GLU:OE2  | 2.55        | 0.53     |
| 1:A:114:LEU:HD11 | 1:A:148:ILE:CD1  | 2.32        | 0.53     |
| 1:C:87:ILE:HG21  | 1:C:89:TRP:CZ2   | 2.44        | 0.53     |
| 1:O:271:LYS:HG3  | 1:O:272:LEU:N    | 2.24        | 0.53     |
| 1:O:165:VAL:HG21 | 1:O:276:ILE:HD13 | 1.91        | 0.53     |
| 1:A:124:SER:O    | 1:A:125:ALA:HB2  | 2.09        | 0.53     |
| 1:O:106:ASP:HB3  | 1:O:128:LYS:HE2  | 1.91        | 0.53     |
| 1:B:322:TYR:O    | 1:B:325:ARG:HB2  | 2.08        | 0.53     |
| 1:O:144:SER:O    | 1:O:146:ILE:N    | 2.42        | 0.53     |
| 1:B:8:ILE:HD12   | 1:B:8:ILE:N      | 2.24        | 0.53     |
| 1:A:49:TYR:HD1   | 1:A:55:GLN:HG3   | 1.74        | 0.53     |
| 1:A:173:ILE:HD11 | 1:A:252:GLU:H    | 1.70        | 0.53     |
| 1:C:36:PRO:HA    | 1:C:80:GLY:HA2   | 1.90        | 0.53     |
| 1:B:288:PHE:CE2  | 1:B:315:TRP:HB2  | 2.40        | 0.53     |
| 1:A:202:ARG:HH21 | 1:C:51:THR:H     | 1.57        | 0.53     |
| 1:A:183:ILE:HG22 | 1:A:187:GLN:NE2  | 2.24        | 0.53     |
| 1:B:329:LEU:O    | 1:B:333:MET:HB2  | 2.08        | 0.53     |
| 1:O:206:PHE:CD2  | 1:B:240:VAL:CB   | 2.81        | 0.53     |
| 1:O:49:TYR:CE1   | 1:A:283:LEU:HD22 | 2.44        | 0.53     |
| 1:O:44:THR:OG1   | 1:O:45:TYR:N     | 2.42        | 0.53     |
| 1:B:52:VAL:HG11  | 1:B:241:ASP:HB2  | 1.90        | 0.53     |
| 1:A:39:THR:HG22  | 1:A:40:THR:N     | 2.24        | 0.53     |
| 1:B:105:THR:HA   | 1:B:123:ILE:HD12 | 1.91        | 0.53     |
| 1:A:85:ASP:HA    | 1:A:112:ALA:O    | 2.08        | 0.53     |
| 1:C:215:ALA:N    | 2:C:6926:SO4:O3  | 2.42        | 0.52     |
| 1:A:285:SER:HA   | 1:A:315:TRP:HZ3  | 1.72        | 0.52     |
| 1:B:265:LYS:HE2  | 1:B:269:GLU:OE1  | 2.09        | 0.52     |
| 1:O:65:ASP:O     | 1:O:65:ASP:OD1   | 2.26        | 0.52     |
| 1:A:17:LEU:HD23  | 1:A:20:ARG:HD2   | 1.91        | 0.52     |
| 1:A:42:TYR:CE2   | 1:A:46:MET:HE2   | 2.01        | 0.52     |
| 1:O:296:ILE:O    | 1:O:314:ALA:HA   | 2.09        | 0.52     |
| 1:C:35:ASP:CG    | 1:C:38:ILE:HD12  | 2.29        | 0.52     |
| 1:B:219:VAL:HA   | 1:B:222:VAL:HG22 | 1.90        | 0.52     |
| 1:B:261:LYS:HB3  | 1:B:278:TYR:OH   | 2.09        | 0.52     |
| 1:B:160:ALA:CB   | 1:B:161:PRO:HD3  | 2.33        | 0.52     |
| 1:A:189:THR:HB   | 1:C:183:ILE:HD12 | 1.91        | 0.52     |
| 1:C:176:LEU:HD22 | 1:C:231:THR:CG2  | 2.39        | 0.52     |
| 1:B:6:ILE:HD12   | 1:B:28:VAL:CG1   | 2.40        | 0.52     |
| 1:B:303:ILE:HG22 | 1:B:311:LYS:HB3  | 1.91        | 0.52     |
| 1:A:207:ASN:HB2  | 1:A:209:ILE:HD11 | 1.92        | 0.52     |
| 1:C:18:VAL:HG12  | 1:C:327:ILE:HD11 | 1.92        | 0.52     |
| 1:B:251:ILE:HG13 | 1:B:308:ASN:HA   | 1.91        | 0.52     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:C:97:VAL:HB    | 1:C:121:VAL:HG22 | 1.92        | 0.52     |
| 1:O:113:HIS:CB   | 1:O:121:VAL:HG21 | 2.39        | 0.52     |
| 1:A:42:TYR:CD1   | 1:C:198:TRP:CD2  | 2.97        | 0.52     |
| 1:B:134:VAL:CG2  | 1:B:222:VAL:HG11 | 2.37        | 0.52     |
| 1:A:42:TYR:OH    | 1:A:46:MET:HE3   | 2.05        | 0.52     |
| 1:A:48:LYS:HG2   | 1:A:49:TYR:CD1   | 2.45        | 0.52     |
| 1:A:265:LYS:HB2  | 1:A:278:TYR:CE1  | 2.45        | 0.52     |
| 1:C:127:SER:HB3  | 1:C:130:ALA:HB3  | 1.91        | 0.52     |
| 1:A:36:PRO:CB    | 1:A:82:ARG:HE    | 2.23        | 0.52     |
| 1:A:167:HIS:HB2  | 1:A:172:ILE:HD12 | 1.91        | 0.52     |
| 1:O:123:ILE:HD11 | 1:O:148:ILE:CG2  | 2.40        | 0.52     |
| 1:O:153:SER:O    | 1:O:154:CYS:C    | 2.48        | 0.52     |
| 1:O:36:PRO:HG3   | 1:O:80:GLY:C     | 2.30        | 0.52     |
| 1:O:9:ASN:HD21   | 1:O:87:ILE:HD13  | 1.75        | 0.52     |
| 1:O:132:MET:HA   | 1:O:150:SER:O    | 2.10        | 0.52     |
| 1:O:23:LEU:O     | 1:O:24:GLN:HB2   | 2.09        | 0.52     |
| 1:O:193:PRO:CB   | 1:B:38:ILE:HD11  | 2.40        | 0.52     |
| 1:O:49:TYR:CD2   | 1:O:49:TYR:N     | 2.76        | 0.52     |
| 1:O:40:THR:CG2   | 1:O:69:LEU:HD13  | 2.39        | 0.52     |
| 1:O:142:TYR:CE1  | 1:O:146:ILE:HB   | 2.45        | 0.52     |
| 1:B:63:ILE:N     | 1:B:63:ILE:HD12  | 2.24        | 0.52     |
| 1:C:63:ILE:N     | 1:C:63:ILE:HD12  | 2.24        | 0.52     |
| 1:A:207:ASN:HB2  | 1:A:209:ILE:CD1  | 2.40        | 0.52     |
| 1:C:10:GLY:HA3   | 1:C:100:SER:C    | 2.30        | 0.52     |
| 1:C:167:HIS:ND1  | 1:C:226:LEU:HD21 | 2.25        | 0.52     |
| 1:O:52:VAL:HG11  | 1:O:241:ASP:OD1  | 2.10        | 0.51     |
| 1:C:138:ASN:C    | 1:C:140:ASP:N    | 2.62        | 0.51     |
| 1:B:285:SER:HB2  | 3:B:6956:HOH:O   | 2.07        | 0.51     |
| 1:B:24:GLN:NE2   | 1:B:58:HIS:HB3   | 2.24        | 0.51     |
| 1:C:264:ILE:O    | 1:C:268:SER:HB3  | 2.10        | 0.51     |
| 1:O:311:LYS:HB2  | 1:C:176:LEU:CD1  | 2.41        | 0.51     |
| 1:A:254:ALA:HA   | 1:A:307:ASP:O    | 2.09        | 0.51     |
| 1:B:161:PRO:O    | 1:B:164:LYS:HB3  | 2.10        | 0.51     |
| 1:O:162:LEU:O    | 1:O:166:ILE:CD1  | 2.53        | 0.51     |
| 1:B:324:ASN:N    | 1:B:324:ASN:ND2  | 2.53        | 0.51     |
| 1:C:173:ILE:HB   | 1:C:250:ARG:O    | 2.11        | 0.51     |
| 1:C:250:ARG:HD3  | 1:C:308:ASN:O    | 2.10        | 0.51     |
| 1:C:327:ILE:O    | 1:C:330:ILE:N    | 2.40        | 0.51     |
| 1:O:184:THR:HG23 | 1:O:236:ARG:NH2  | 2.25        | 0.51     |
| 1:B:107:LYS:O    | 1:B:111:ALA:HB2  | 2.09        | 0.51     |
| 1:A:13:ARG:NH2   | 1:A:52:VAL:CG1   | 2.72        | 0.51     |
| 1:O:66:SER:O     | 1:O:67:LYS:HG3   | 2.11        | 0.51     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:C:81:ILE:HD12  | 1:C:87:ILE:HG23  | 1.91        | 0.51     |
| 1:O:310:VAL:HG22 | 1:O:311:LYS:H    | 1.75        | 0.51     |
| 1:O:261:LYS:HA   | 1:O:297:PHE:HE2  | 1.75        | 0.51     |
| 1:C:172:ILE:HG23 | 1:C:249:VAL:HG23 | 1.91        | 0.51     |
| 1:B:219:VAL:HA   | 1:B:222:VAL:CG2  | 2.41        | 0.51     |
| 1:B:332:HIS:C    | 1:B:332:HIS:ND1  | 2.64        | 0.51     |
| 1:B:228:GLY:O    | 1:B:230:LEU:N    | 2.44        | 0.51     |
| 1:O:176:LEU:HB3  | 1:C:311:LYS:HE2  | 1.93        | 0.51     |
| 1:O:57:LYS:HZ3   | 1:O:61:ILE:CD1   | 2.08        | 0.51     |
| 1:B:126:PRO:CD   | 1:B:153:SER:HB3  | 2.41        | 0.51     |
| 1:O:250:ARG:HH11 | 1:O:250:ARG:HB2  | 1.76        | 0.51     |
| 1:B:121:VAL:HB   | 1:B:148:ILE:CD1  | 2.40        | 0.51     |
| 1:O:202:ARG:NH1  | 1:B:45:TYR:OH    | 2.42        | 0.51     |
| 1:O:104:PHE:O    | 1:O:110:ALA:HB2  | 2.10        | 0.51     |
| 1:C:143:THR:O    | 1:C:145:ASP:N    | 2.44        | 0.51     |
| 1:O:57:LYS:N     | 1:O:57:LYS:HE3   | 2.26        | 0.51     |
| 1:O:113:HIS:HB2  | 1:O:121:VAL:HG21 | 1.92        | 0.51     |
| 1:C:17:LEU:HD22  | 1:C:320:TRP:HE3  | 1.75        | 0.51     |
| 1:B:164:LYS:HG3  | 1:B:168:ASP:OD2  | 2.11        | 0.51     |
| 1:O:63:ILE:H     | 1:O:63:ILE:CD1   | 2.19        | 0.51     |
| 1:A:207:ASN:ND2  | 1:B:286:THR:OG1  | 2.43        | 0.51     |
| 1:C:166:ILE:HG13 | 1:C:312:LEU:CD1  | 2.41        | 0.51     |
| 1:B:272:LEU:HD23 | 1:B:275:ILE:HG22 | 1.92        | 0.51     |
| 1:O:6:ILE:HA     | 1:O:96:TYR:O     | 2.10        | 0.51     |
| 1:B:177:MET:CE   | 1:B:179:THR:HG23 | 2.42        | 0.50     |
| 1:C:328:ASP:HA   | 1:C:331:ARG:HD2  | 1.93        | 0.50     |
| 1:A:63:ILE:HD12  | 1:A:63:ILE:N     | 2.26        | 0.50     |
| 1:B:51:THR:O     | 1:B:51:THR:HG22  | 2.10        | 0.50     |
| 1:C:181:HIS:CB   | 1:C:236:ARG:HE   | 2.16        | 0.50     |
| 1:C:31:VAL:C     | 1:C:76:VAL:HG13  | 2.32        | 0.50     |
| 1:C:264:ILE:HG21 | 1:C:297:PHE:HB2  | 1.92        | 0.50     |
| 1:C:181:HIS:HB3  | 1:C:236:ARG:HD3  | 1.92        | 0.50     |
| 1:O:49:TYR:HE1   | 1:A:283:LEU:HD13 | 1.76        | 0.50     |
| 1:O:294:SER:OG   | 1:O:325:ARG:HD2  | 2.11        | 0.50     |
| 1:B:24:GLN:HE21  | 1:B:58:HIS:HB3   | 1.76        | 0.50     |
| 1:A:276:ILE:HG13 | 1:A:277:GLY:N    | 2.26        | 0.50     |
| 1:O:176:LEU:CD2  | 1:O:231:THR:HG23 | 2.41        | 0.50     |
| 1:B:77:THR:HG22  | 1:B:78:VAL:N     | 2.25        | 0.50     |
| 1:B:112:ALA:O    | 1:B:113:HIS:C    | 2.50        | 0.50     |
| 1:O:60:ASP:C     | 1:O:61:ILE:HD12  | 2.31        | 0.50     |
| 1:C:52:VAL:HG22  | 1:C:240:VAL:HG21 | 1.93        | 0.50     |
| 1:O:159:LEU:HD13 | 1:O:177:MET:HG3  | 1.92        | 0.50     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:17:LEU:HD22  | 1:B:320:TRP:HE3  | 1.76        | 0.50     |
| 1:C:324:ASN:O    | 1:C:325:ARG:C    | 2.50        | 0.50     |
| 1:C:244:VAL:HG12 | 1:C:245:VAL:N    | 2.26        | 0.50     |
| 1:A:137:VAL:HG21 | 1:A:160:ALA:HB1  | 1.92        | 0.50     |
| 1:A:215:ALA:O    | 1:A:219:VAL:HG23 | 2.11        | 0.50     |
| 1:A:305:LEU:HD13 | 1:B:231:THR:CG2  | 2.40        | 0.50     |
| 1:B:288:PHE:CE2  | 1:B:315:TRP:CD1  | 2.92        | 0.50     |
| 1:B:29:GLU:O     | 1:B:31:VAL:HG13  | 2.12        | 0.50     |
| 1:C:244:VAL:HG22 | 1:C:315:TRP:CD2  | 2.47        | 0.50     |
| 1:B:228:GLY:C    | 1:B:230:LEU:H    | 2.14        | 0.50     |
| 1:C:289:VAL:HA   | 1:C:317:ASP:OD2  | 2.12        | 0.50     |
| 1:A:30:LEU:HD22  | 1:A:76:VAL:HG11  | 1.93        | 0.50     |
| 1:C:296:ILE:N    | 1:C:296:ILE:HD12 | 2.25        | 0.50     |
| 1:C:156:THR:O    | 1:C:158:CYS:N    | 2.40        | 0.50     |
| 1:O:222:VAL:CG2  | 1:O:223:LEU:H    | 2.21        | 0.50     |
| 1:A:97:VAL:O     | 1:A:121:VAL:HG13 | 2.12        | 0.50     |
| 1:B:30:LEU:HD23  | 1:B:31:VAL:N     | 2.26        | 0.50     |
| 1:C:96:TYR:OH    | 1:C:334:ALA:HB2  | 2.11        | 0.50     |
| 1:B:81:ILE:CD1   | 1:B:87:ILE:HA    | 2.41        | 0.50     |
| 1:B:18:VAL:CG1   | 1:B:327:ILE:HD11 | 2.42        | 0.50     |
| 1:O:9:ASN:O      | 1:O:101:THR:HG22 | 2.11        | 0.50     |
| 1:C:291:ASP:OD1  | 1:C:293:ARG:HB2  | 2.11        | 0.50     |
| 1:A:159:LEU:HD22 | 1:A:177:MET:SD   | 2.52        | 0.49     |
| 1:C:148:ILE:HD12 | 1:C:148:ILE:H    | 1.76        | 0.49     |
| 1:B:107:LYS:HA   | 1:B:148:ILE:HG21 | 1.94        | 0.49     |
| 1:O:231:THR:OG1  | 1:O:232:GLY:N    | 2.45        | 0.49     |
| 1:O:255:ALA:N    | 1:O:307:ASP:HB3  | 2.27        | 0.49     |
| 1:B:33:VAL:HG12  | 1:B:34:ASN:N     | 2.27        | 0.49     |
| 1:A:304:ALA:HB1  | 1:A:310:VAL:HG12 | 1.93        | 0.49     |
| 1:C:323:SER:O    | 1:C:326:VAL:HB   | 2.13        | 0.49     |
| 1:O:137:VAL:HG11 | 1:O:223:LEU:HD22 | 1.93        | 0.49     |
| 1:A:291:ASP:OD1  | 1:A:293:ARG:NE   | 2.45        | 0.49     |
| 1:C:250:ARG:HG2  | 1:C:250:ARG:HH21 | 1.78        | 0.49     |
| 1:A:203:ALA:HB1  | 1:A:206:PHE:HB2  | 1.93        | 0.49     |
| 1:A:174:GLU:OE1  | 1:B:306:ASN:ND2  | 2.32        | 0.49     |
| 1:C:95:GLU:O     | 1:C:119:LYS:HB2  | 2.12        | 0.49     |
| 1:C:176:LEU:O    | 1:C:247:LEU:HD12 | 2.11        | 0.49     |
| 1:O:193:PRO:HG3  | 1:B:38:ILE:HD11  | 1.94        | 0.49     |
| 1:O:193:PRO:HB3  | 1:B:38:ILE:HD11  | 1.93        | 0.49     |
| 1:O:282:ASP:HB3  | 1:C:199:ARG:CG   | 2.42        | 0.49     |
| 1:C:180:VAL:HG12 | 1:C:237:VAL:HG22 | 1.94        | 0.49     |
| 1:A:158:CYS:O    | 1:A:161:PRO:HD2  | 2.12        | 0.49     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:O:126:PRO:HG3  | 1:O:153:SER:HB3  | 1.94        | 0.49     |
| 1:B:322:TYR:CD2  | 1:B:322:TYR:C    | 2.85        | 0.49     |
| 1:B:296:ILE:O    | 1:B:314:ALA:HA   | 2.12        | 0.49     |
| 1:C:244:VAL:CG1  | 1:C:245:VAL:N    | 2.76        | 0.49     |
| 1:A:158:CYS:HB2  | 1:A:294:SER:O    | 2.13        | 0.49     |
| 1:B:106:ASP:O    | 1:B:107:LYS:C    | 2.50        | 0.49     |
| 1:O:155:THR:O    | 1:O:158:CYS:N    | 2.43        | 0.49     |
| 1:O:22:ALA:O     | 1:O:24:GLN:N     | 2.44        | 0.49     |
| 1:O:106:ASP:OD1  | 1:O:128:LYS:HG2  | 2.13        | 0.49     |
| 1:B:276:ILE:HG13 | 1:B:295:SER:O    | 2.12        | 0.49     |
| 1:B:158:CYS:SG   | 1:B:316:TYR:CD2  | 3.06        | 0.49     |
| 1:B:199:ARG:HH11 | 1:B:210:PRO:CG   | 2.24        | 0.49     |
| 1:C:250:ARG:HA   | 1:C:308:ASN:O    | 2.12        | 0.49     |
| 1:B:303:ILE:HG12 | 1:B:304:ALA:N    | 2.27        | 0.49     |
| 1:A:200:GLY:HA2  | 1:A:209:ILE:HG21 | 1.94        | 0.49     |
| 1:A:84:PRO:HA    | 1:A:87:ILE:CD1   | 2.43        | 0.49     |
| 1:C:153:SER:HB2  | 2:C:6926:SO4:O1  | 2.13        | 0.49     |
| 1:A:135:CYS:HB2  | 1:A:325:ARG:HD3  | 1.94        | 0.49     |
| 1:A:29:GLU:CG    | 1:A:74:LYS:HZ1   | 2.23        | 0.49     |
| 1:A:142:TYR:CZ   | 1:A:333:MET:HG2  | 2.48        | 0.49     |
| 1:O:244:VAL:HG22 | 1:O:245:VAL:O    | 2.12        | 0.48     |
| 1:B:226:LEU:HA   | 1:B:229:LYS:HD2  | 1.94        | 0.48     |
| 1:B:254:ALA:HA   | 1:B:307:ASP:O    | 2.13        | 0.48     |
| 1:O:48:LYS:C     | 1:O:49:TYR:HD2   | 2.17        | 0.48     |
| 1:O:257:TYR:CE2  | 1:O:261:LYS:HD2  | 2.48        | 0.48     |
| 1:B:18:VAL:HG13  | 1:B:327:ILE:HD11 | 1.94        | 0.48     |
| 1:B:117:GLY:O    | 1:B:118:ALA:C    | 2.52        | 0.48     |
| 1:O:103:VAL:HG23 | 1:O:104:PHE:CE2  | 2.47        | 0.48     |
| 1:O:283:LEU:HD13 | 1:O:288:PHE:CE2  | 2.48        | 0.48     |
| 1:C:62:LYS:O     | 1:C:70:LEU:HB3   | 2.14        | 0.48     |
| 1:A:208:ILE:HG13 | 3:B:6956:HOH:O   | 2.13        | 0.48     |
| 1:A:285:SER:CA   | 1:A:315:TRP:CZ3  | 2.97        | 0.48     |
| 1:B:49:TYR:HE2   | 1:C:281:GLU:OE2  | 1.96        | 0.48     |
| 1:A:265:LYS:HD2  | 1:A:278:TYR:CE2  | 2.48        | 0.48     |
| 1:A:256:SER:O    | 1:A:259:ALA:HB3  | 2.13        | 0.48     |
| 1:B:101:THR:OG1  | 1:B:103:VAL:HG22 | 2.13        | 0.48     |
| 1:C:38:ILE:HG21  | 1:C:46:MET:HE2   | 1.96        | 0.48     |
| 1:B:14:ILE:O     | 1:B:18:VAL:HG23  | 2.12        | 0.48     |
| 1:B:272:LEU:HD23 | 1:B:275:ILE:CG2  | 2.43        | 0.48     |
| 1:A:284:VAL:HG12 | 1:B:209:ILE:HA   | 1.95        | 0.48     |
| 1:B:219:VAL:O    | 1:B:219:VAL:HG12 | 2.14        | 0.48     |
| 1:B:77:THR:CG2   | 1:B:78:VAL:N     | 2.76        | 0.48     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:139:GLU:H    | 1:A:139:GLU:CD   | 2.17        | 0.48     |
| 1:B:139:GLU:HG2  | 1:B:139:GLU:O    | 2.12        | 0.48     |
| 1:C:160:ALA:HB3  | 1:C:161:PRO:HD3  | 1.94        | 0.48     |
| 1:A:305:LEU:O    | 1:A:306:ASN:HB3  | 2.14        | 0.48     |
| 1:O:36:PRO:HG2   | 1:O:82:ARG:HG2   | 1.94        | 0.48     |
| 1:O:115:LYS:O    | 1:O:116:GLY:C    | 2.51        | 0.48     |
| 1:C:14:ILE:HD12  | 1:C:14:ILE:N     | 2.26        | 0.48     |
| 1:O:13:ARG:HG2   | 1:O:319:GLU:OE2  | 2.13        | 0.48     |
| 1:A:309:PHE:HE2  | 1:B:175:GLY:N    | 2.07        | 0.48     |
| 1:C:11:PHE:CE2   | 1:C:43:MET:HG3   | 2.48        | 0.48     |
| 1:A:130:ALA:CB   | 1:A:148:ILE:HG22 | 2.44        | 0.48     |
| 1:O:7:GLY:O      | 1:O:97:VAL:HG13  | 2.14        | 0.48     |
| 1:A:233:MET:CE   | 1:B:301:ALA:O    | 2.62        | 0.48     |
| 1:B:40:THR:O     | 1:B:43:MET:HB3   | 2.12        | 0.48     |
| 1:C:180:VAL:O    | 1:C:243:SER:HB3  | 2.13        | 0.48     |
| 1:C:322:TYR:O    | 1:C:324:ASN:N    | 2.47        | 0.48     |
| 1:A:84:PRO:C     | 1:A:86:GLU:H     | 2.17        | 0.48     |
| 1:C:110:ALA:HB3  | 1:C:123:ILE:HD11 | 1.95        | 0.48     |
| 1:A:49:TYR:CD1   | 1:A:55:GLN:HG3   | 2.49        | 0.47     |
| 1:C:292:SER:HA   | 1:C:321:GLY:HA2  | 1.96        | 0.47     |
| 1:O:245:VAL:HG23 | 1:O:316:TYR:HE2  | 1.75        | 0.47     |
| 1:B:107:LYS:O    | 1:B:111:ALA:N    | 2.44        | 0.47     |
| 1:B:283:LEU:HD21 | 1:C:49:TYR:CZ    | 2.49        | 0.47     |
| 1:A:84:PRO:HB2   | 1:A:112:ALA:CB   | 2.43        | 0.47     |
| 1:A:166:ILE:HD11 | 1:A:264:ILE:HD11 | 1.95        | 0.47     |
| 1:C:82:ARG:HG2   | 1:C:82:ARG:O     | 2.14        | 0.47     |
| 1:A:171:GLY:O    | 1:A:251:ILE:HA   | 2.14        | 0.47     |
| 1:C:34:ASN:O     | 1:C:34:ASN:CG    | 2.51        | 0.47     |
| 1:A:175:GLY:HA2  | 1:B:309:PHE:CE2  | 2.49        | 0.47     |
| 1:O:65:ASP:O     | 1:O:66:SER:C     | 2.51        | 0.47     |
| 1:B:65:ASP:O     | 1:B:67:LYS:N     | 2.47        | 0.47     |
| 1:C:322:TYR:O    | 1:C:323:SER:C    | 2.53        | 0.47     |
| 1:O:183:ILE:O    | 1:O:183:ILE:CD1  | 2.55        | 0.47     |
| 1:A:90:ALA:HB2   | 1:A:117:GLY:O    | 2.14        | 0.47     |
| 1:A:11:PHE:HZ    | 1:A:47:PHE:CD2   | 2.31        | 0.47     |
| 1:C:244:VAL:CG2  | 1:C:315:TRP:CE3  | 2.98        | 0.47     |
| 1:C:247:LEU:HD12 | 1:C:248:THR:N    | 2.29        | 0.47     |
| 1:A:287:ASP:CG   | 1:B:202:ARG:HH22 | 2.17        | 0.47     |
| 1:O:112:ALA:HA   | 1:O:115:LYS:HZ2  | 1.76        | 0.47     |
| 1:C:334:ALA:C    | 1:C:336:THR:H    | 2.18        | 0.47     |
| 1:O:21:VAL:HG12  | 1:O:21:VAL:O     | 2.13        | 0.47     |
| 1:A:113:HIS:HB2  | 1:A:121:VAL:HG21 | 1.96        | 0.47     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:O:215:ALA:HB2  | 2:O:6921:SO4:O4  | 2.14        | 0.47     |
| 1:B:22:ALA:C     | 1:B:24:GLN:H     | 2.18        | 0.47     |
| 1:A:23:LEU:CD2   | 1:A:71:LEU:HG    | 2.44        | 0.47     |
| 1:C:199:ARG:O    | 1:C:202:ARG:HG2  | 2.15        | 0.47     |
| 1:O:206:PHE:HE2  | 1:B:240:VAL:CG2  | 2.26        | 0.47     |
| 1:O:250:ARG:CB   | 1:O:250:ARG:NH1  | 2.78        | 0.47     |
| 1:B:229:LYS:O    | 1:B:230:LEU:HD23 | 2.14        | 0.47     |
| 1:O:79:PHE:CB    | 1:O:81:ILE:HD12  | 2.40        | 0.47     |
| 1:B:49:TYR:HB3   | 1:C:287:ASP:OD1  | 2.15        | 0.47     |
| 1:A:84:PRO:O     | 1:A:86:GLU:N     | 2.48        | 0.47     |
| 1:A:162:LEU:O    | 1:A:166:ILE:CD1  | 2.63        | 0.47     |
| 1:O:19:ALA:O     | 1:O:23:LEU:CD2   | 2.63        | 0.47     |
| 1:B:275:ILE:O    | 1:B:275:ILE:CG2  | 2.63        | 0.47     |
| 1:C:257:TYR:CE2  | 1:C:261:LYS:HD2  | 2.49        | 0.47     |
| 1:B:49:TYR:CZ    | 1:C:283:LEU:HD11 | 2.49        | 0.47     |
| 1:B:264:ILE:HG21 | 1:B:297:PHE:CD2  | 2.50        | 0.47     |
| 1:B:44:THR:HG21  | 1:B:63:ILE:HD11  | 1.97        | 0.47     |
| 1:C:135:CYS:HB2  | 1:C:325:ARG:HD3  | 1.97        | 0.47     |
| 1:A:173:ILE:HD13 | 1:A:251:ILE:CA   | 2.45        | 0.47     |
| 1:O:193:PRO:HB3  | 1:B:38:ILE:HD12  | 1.96        | 0.47     |
| 1:C:279:VAL:HG23 | 1:C:298:ASP:HA   | 1.97        | 0.47     |
| 1:C:291:ASP:OD1  | 1:C:293:ARG:HD3  | 2.15        | 0.47     |
| 1:C:114:LEU:C    | 1:C:116:GLY:H    | 2.18        | 0.47     |
| 1:C:28:VAL:HG12  | 1:C:29:GLU:N     | 2.30        | 0.46     |
| 1:O:264:ILE:O    | 1:O:267:ALA:HB3  | 2.16        | 0.46     |
| 1:B:287:ASP:OD1  | 1:C:49:TYR:HB3   | 2.14        | 0.46     |
| 1:A:181:HIS:O    | 1:A:236:ARG:HA   | 2.15        | 0.46     |
| 1:A:178:THR:HB   | 1:A:246:ASP:HB3  | 1.97        | 0.46     |
| 1:O:106:ASP:CG   | 1:O:128:LYS:HE2  | 2.35        | 0.46     |
| 1:A:189:THR:HB   | 1:C:183:ILE:CD1  | 2.45        | 0.46     |
| 1:A:283:LEU:N    | 1:A:283:LEU:HD23 | 2.31        | 0.46     |
| 1:A:81:ILE:H     | 1:A:81:ILE:CD1   | 2.22        | 0.46     |
| 1:O:28:VAL:HG22  | 1:O:29:GLU:N     | 2.29        | 0.46     |
| 1:A:43:MET:C     | 1:A:45:TYR:N     | 2.69        | 0.46     |
| 1:C:12:GLY:HA2   | 1:C:16:ARG:HH12  | 1.81        | 0.46     |
| 1:A:87:ILE:HB    | 1:A:89:TRP:NE1   | 2.30        | 0.46     |
| 1:A:83:ASN:N     | 1:A:83:ASN:ND2   | 2.57        | 0.46     |
| 1:C:99:GLU:OE2   | 1:C:104:PHE:HB2  | 2.16        | 0.46     |
| 1:A:158:CYS:HG   | 1:A:245:VAL:HG23 | 1.78        | 0.46     |
| 1:O:138:ASN:OD1  | 1:O:222:VAL:HG12 | 2.15        | 0.46     |
| 1:A:329:LEU:O    | 1:A:333:MET:HG3  | 2.15        | 0.46     |
| 1:C:206:PHE:O    | 1:C:207:ASN:OD1  | 2.34        | 0.46     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:215:ALA:HB2  | 2:B:6924:SO4:O3  | 2.16        | 0.46     |
| 1:A:134:VAL:HG21 | 1:A:156:THR:HG22 | 1.97        | 0.46     |
| 1:A:16:ARG:NE    | 1:A:46:MET:O     | 2.49        | 0.46     |
| 1:C:39:THR:O     | 1:C:43:MET:HB2   | 2.16        | 0.46     |
| 1:A:70:LEU:HD22  | 1:A:70:LEU:N     | 2.30        | 0.46     |
| 1:C:265:LYS:O    | 1:C:268:SER:N    | 2.49        | 0.46     |
| 1:C:99:GLU:OE1   | 1:C:99:GLU:HA    | 2.15        | 0.46     |
| 1:C:17:LEU:HA    | 1:C:20:ARG:HD2   | 1.98        | 0.46     |
| 1:A:73:GLU:HA    | 1:A:73:GLU:OE2   | 2.15        | 0.46     |
| 1:A:99:GLU:HB3   | 1:A:123:ILE:HA   | 1.98        | 0.46     |
| 1:A:114:LEU:CD1  | 1:A:148:ILE:HD11 | 2.37        | 0.46     |
| 1:O:9:ASN:HD21   | 1:O:87:ILE:CD1   | 2.29        | 0.46     |
| 1:C:49:TYR:CE1   | 1:C:55:GLN:NE2   | 2.84        | 0.46     |
| 1:A:87:ILE:HD13  | 1:A:89:TRP:HZ2   | 1.80        | 0.46     |
| 1:O:206:PHE:CD2  | 1:B:240:VAL:CG2  | 2.99        | 0.46     |
| 1:O:61:ILE:CD1   | 1:O:61:ILE:N     | 2.71        | 0.46     |
| 1:O:158:CYS:O    | 1:O:161:PRO:HD2  | 2.15        | 0.46     |
| 1:A:230:LEU:O    | 1:A:231:THR:CB   | 2.64        | 0.46     |
| 1:A:203:ALA:CB   | 1:A:206:PHE:HB2  | 2.46        | 0.46     |
| 1:A:203:ALA:O    | 1:A:209:ILE:HD11 | 2.16        | 0.46     |
| 1:O:218:ALA:C    | 1:O:220:GLY:N    | 2.69        | 0.46     |
| 1:B:140:ASP:C    | 1:B:142:TYR:N    | 2.69        | 0.46     |
| 1:O:170:PHE:CE2  | 1:O:260:ILE:CD1  | 2.86        | 0.46     |
| 1:B:210:PRO:HB3  | 1:B:235:PHE:CD1  | 2.51        | 0.46     |
| 1:A:191:ASP:OD1  | 1:C:51:THR:HB    | 2.16        | 0.46     |
| 1:B:286:THR:O    | 1:B:289:VAL:HG23 | 2.16        | 0.46     |
| 1:B:49:TYR:CE2   | 1:C:281:GLU:OE2  | 2.69        | 0.46     |
| 1:A:115:LYS:C    | 1:A:117:GLY:H    | 2.20        | 0.46     |
| 1:A:199:ARG:C    | 1:A:201:GLY:H    | 2.20        | 0.46     |
| 1:C:187:GLN:NE2  | 1:C:204:ALA:CB   | 2.79        | 0.46     |
| 1:B:184:THR:C    | 1:B:186:THR:H    | 2.20        | 0.45     |
| 1:B:322:TYR:HD2  | 1:B:322:TYR:C    | 2.20        | 0.45     |
| 1:B:296:ILE:N    | 1:B:296:ILE:HD12 | 2.31        | 0.45     |
| 1:B:46:MET:O     | 1:B:48:LYS:N     | 2.49        | 0.45     |
| 1:C:260:ILE:O    | 1:C:264:ILE:HG13 | 2.16        | 0.45     |
| 1:B:277:GLY:HA3  | 1:B:293:ARG:NH2  | 2.30        | 0.45     |
| 1:A:96:TYR:HA    | 1:A:120:LYS:O    | 2.16        | 0.45     |
| 1:C:139:GLU:HG3  | 1:C:332:HIS:CD2  | 2.51        | 0.45     |
| 1:A:42:TYR:HD1   | 1:C:198:TRP:CD2  | 2.29        | 0.45     |
| 1:B:4:ILE:HG13   | 1:B:28:VAL:HA    | 1.98        | 0.45     |
| 1:C:85:ASP:OD1   | 1:C:112:ALA:HB1  | 2.15        | 0.45     |
| 1:B:49:TYR:CG    | 1:C:283:LEU:HD11 | 2.52        | 0.45     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:C:279:VAL:HG22 | 1:C:297:PHE:O    | 2.16        | 0.45     |
| 1:A:166:ILE:CD1  | 1:A:264:ILE:HD11 | 2.47        | 0.45     |
| 1:O:333:MET:HB3  | 1:O:333:MET:HE2  | 1.81        | 0.45     |
| 1:A:85:ASP:N     | 1:A:85:ASP:OD2   | 2.47        | 0.45     |
| 1:O:142:TYR:HE1  | 1:O:146:ILE:HB   | 1.79        | 0.45     |
| 1:A:12:GLY:O     | 1:A:16:ARG:HG3   | 2.16        | 0.45     |
| 1:O:173:ILE:HG13 | 1:O:252:GLU:HB3  | 1.98        | 0.45     |
| 1:A:248:THR:HG1  | 1:A:311:LYS:HZ3  | 1.63        | 0.45     |
| 1:O:49:TYR:CD1   | 1:A:283:LEU:HD22 | 2.52        | 0.45     |
| 1:A:291:ASP:O    | 1:A:293:ARG:N    | 2.50        | 0.45     |
| 1:O:209:ILE:HA   | 1:O:210:PRO:HD3  | 1.76        | 0.45     |
| 1:B:174:GLU:HA   | 1:B:229:LYS:O    | 2.16        | 0.45     |
| 1:A:130:ALA:HB2  | 1:A:148:ILE:HG22 | 1.99        | 0.45     |
| 1:A:284:VAL:O    | 1:A:287:ASP:HB2  | 2.17        | 0.45     |
| 1:C:278:TYR:CE1  | 1:C:299:ALA:HB2  | 2.51        | 0.45     |
| 1:B:44:THR:HG21  | 1:B:63:ILE:HG13  | 1.99        | 0.45     |
| 1:O:255:ALA:O    | 1:O:307:ASP:HA   | 2.15        | 0.45     |
| 1:B:5:LYS:HB2    | 1:B:93:GLY:O     | 2.16        | 0.45     |
| 1:C:243:SER:HB2  | 1:C:316:TYR:CZ   | 2.51        | 0.45     |
| 1:O:183:ILE:HD11 | 1:O:240:VAL:HA   | 1.99        | 0.45     |
| 1:O:284:VAL:HG22 | 1:C:202:ARG:NH1  | 2.32        | 0.45     |
| 1:C:11:PHE:HE1   | 1:C:16:ARG:HA    | 1.81        | 0.45     |
| 1:O:276:ILE:HG23 | 1:O:276:ILE:O    | 2.16        | 0.45     |
| 1:A:97:VAL:HG21  | 1:A:113:HIS:HB3  | 1.98        | 0.45     |
| 1:O:127:SER:HB3  | 1:O:130:ALA:HB3  | 1.96        | 0.45     |
| 1:B:79:PHE:CZ    | 1:B:88:PRO:HG2   | 2.52        | 0.45     |
| 1:C:138:ASN:O    | 1:C:140:ASP:N    | 2.50        | 0.45     |
| 1:A:283:LEU:HD12 | 1:A:288:PHE:CE1  | 2.52        | 0.45     |
| 1:C:123:ILE:HG22 | 1:C:125:ALA:O    | 2.17        | 0.45     |
| 1:O:184:THR:HG23 | 1:O:236:ARG:HH22 | 1.82        | 0.45     |
| 1:A:106:ASP:OD2  | 1:A:128:LYS:HE2  | 2.17        | 0.45     |
| 1:B:213:THR:O    | 1:B:213:THR:HG23 | 2.17        | 0.45     |
| 1:B:247:LEU:HD11 | 1:B:249:VAL:HB   | 1.99        | 0.45     |
| 1:A:55:GLN:HG2   | 1:A:56:TRP:N     | 2.31        | 0.45     |
| 1:B:228:GLY:C    | 1:B:230:LEU:N    | 2.71        | 0.45     |
| 1:A:207:ASN:HD22 | 1:B:284:VAL:HG23 | 1.80        | 0.45     |
| 1:C:35:ASP:HA    | 1:C:36:PRO:HD2   | 1.77        | 0.45     |
| 1:A:13:ARG:HH21  | 1:A:52:VAL:HG12  | 1.79        | 0.45     |
| 1:C:89:TRP:NE1   | 1:C:113:HIS:ND1  | 2.65        | 0.45     |
| 1:B:265:LYS:C    | 1:B:267:ALA:H    | 2.19        | 0.45     |
| 1:B:320:TRP:O    | 1:B:323:SER:HB2  | 2.17        | 0.45     |
| 1:O:206:PHE:CE2  | 1:B:240:VAL:HG23 | 2.52        | 0.44     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:281:GLU:CB   | 1:A:283:LEU:HD21 | 2.42        | 0.44     |
| 1:B:183:ILE:HG12 | 1:B:239:THR:O    | 2.16        | 0.44     |
| 1:C:9:ASN:HB3    | 1:C:99:GLU:OE1   | 2.16        | 0.44     |
| 1:C:82:ARG:HH11  | 1:C:82:ARG:HG3   | 1.82        | 0.44     |
| 1:B:65:ASP:C     | 1:B:67:LYS:H     | 2.20        | 0.44     |
| 1:A:38:ILE:HG22  | 1:A:42:TYR:CD2   | 2.52        | 0.44     |
| 1:C:198:TRP:O    | 1:C:199:ARG:C    | 2.56        | 0.44     |
| 1:A:306:ASN:C    | 1:A:308:ASN:H    | 2.20        | 0.44     |
| 1:A:173:ILE:CD1  | 1:A:252:GLU:HG2  | 2.47        | 0.44     |
| 1:O:97:VAL:O     | 1:O:121:VAL:HG13 | 2.18        | 0.44     |
| 1:B:286:THR:CG2  | 1:C:51:THR:HG23  | 2.39        | 0.44     |
| 1:O:8:ILE:HB     | 1:O:33:VAL:HG12  | 1.98        | 0.44     |
| 1:C:219:VAL:O    | 1:C:223:LEU:N    | 2.48        | 0.44     |
| 1:C:124:SER:O    | 1:C:125:ALA:HB2  | 2.17        | 0.44     |
| 1:C:95:GLU:HG2   | 1:C:119:LYS:HG3  | 1.99        | 0.44     |
| 1:C:154:CYS:SG   | 1:C:155:THR:N    | 2.91        | 0.44     |
| 1:C:38:ILE:CG2   | 1:C:46:MET:HE2   | 2.47        | 0.44     |
| 1:A:106:ASP:CG   | 1:A:128:LYS:HE2  | 2.37        | 0.44     |
| 1:A:11:PHE:CD2   | 1:A:16:ARG:CD    | 2.79        | 0.44     |
| 1:O:283:LEU:HD13 | 1:O:288:PHE:HE2  | 1.82        | 0.44     |
| 1:B:107:LYS:N    | 1:B:129:ASP:OD1  | 2.41        | 0.44     |
| 1:A:281:GLU:HB2  | 1:A:283:LEU:CD2  | 2.43        | 0.44     |
| 1:O:174:GLU:HB2  | 1:C:305:LEU:HD23 | 1.99        | 0.44     |
| 1:C:264:ILE:HG21 | 1:C:297:PHE:CB   | 2.47        | 0.44     |
| 1:O:107:LYS:O    | 1:O:111:ALA:HB2  | 2.17        | 0.44     |
| 1:A:36:PRO:HB3   | 1:A:80:GLY:O     | 2.17        | 0.44     |
| 1:O:4:ILE:HD13   | 1:O:330:ILE:HG22 | 2.00        | 0.44     |
| 1:C:325:ARG:NE   | 1:C:325:ARG:HA   | 2.32        | 0.44     |
| 1:O:40:THR:HG23  | 1:O:69:LEU:HD13  | 1.98        | 0.44     |
| 1:C:56:TRP:CZ2   | 1:C:58:HIS:HB3   | 2.53        | 0.44     |
| 1:A:244:VAL:HG22 | 1:A:313:VAL:HG23 | 1.99        | 0.44     |
| 1:C:30:LEU:O     | 1:C:76:VAL:HG22  | 2.18        | 0.44     |
| 1:B:152:ALA:HB3  | 1:B:157:ASN:HD21 | 1.82        | 0.44     |
| 1:O:191:ASP:OD1  | 1:O:202:ARG:NE   | 2.50        | 0.44     |
| 1:C:293:ARG:HB2  | 1:C:296:ILE:HD11 | 2.00        | 0.44     |
| 1:B:70:LEU:HD12  | 1:B:75:PRO:N     | 2.33        | 0.44     |
| 1:A:242:VAL:HA   | 1:A:317:ASP:HA   | 1.99        | 0.44     |
| 1:C:17:LEU:HD22  | 1:C:320:TRP:CE3  | 2.52        | 0.44     |
| 1:A:291:ASP:OD1  | 1:A:293:ARG:HB2  | 2.18        | 0.44     |
| 1:B:7:GLY:O      | 1:B:97:VAL:HA    | 2.18        | 0.44     |
| 1:B:147:ASP:N    | 1:B:147:ASP:OD2  | 2.50        | 0.44     |
| 1:O:124:SER:C    | 1:O:322:TYR:OH   | 2.56        | 0.44     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:153:SER:CB   | 2:A:6923:SO4:O4  | 2.66        | 0.44     |
| 1:O:77:THR:HG21  | 1:O:79:PHE:CZ    | 2.53        | 0.44     |
| 1:C:13:ARG:HH21  | 1:C:52:VAL:HG21  | 1.83        | 0.44     |
| 1:O:183:ILE:CD1  | 1:O:183:ILE:H    | 2.26        | 0.44     |
| 1:O:250:ARG:HG3  | 1:O:309:PHE:CD1  | 2.53        | 0.44     |
| 1:B:9:ASN:ND2    | 1:B:99:GLU:OE1   | 2.51        | 0.44     |
| 1:C:63:ILE:HG22  | 1:C:65:ASP:O     | 2.18        | 0.44     |
| 1:O:165:VAL:HB   | 1:O:166:ILE:HD12 | 1.99        | 0.44     |
| 1:B:284:VAL:HG22 | 1:B:287:ASP:OD2  | 2.18        | 0.44     |
| 1:A:241:ASP:CG   | 1:A:242:VAL:H    | 2.21        | 0.44     |
| 1:C:152:ALA:HB1  | 1:C:156:THR:HB   | 2.00        | 0.43     |
| 1:C:159:LEU:CD1  | 1:C:247:LEU:HD22 | 2.47        | 0.43     |
| 1:C:83:ASN:ND2   | 1:C:84:PRO:N     | 2.65        | 0.43     |
| 1:O:162:LEU:CD1  | 1:O:264:ILE:HD11 | 2.48        | 0.43     |
| 1:O:264:ILE:O    | 1:O:268:SER:N    | 2.51        | 0.43     |
| 1:O:81:ILE:HB    | 1:O:87:ILE:HG12  | 1.99        | 0.43     |
| 1:B:257:TYR:CD2  | 1:B:261:LYS:HD2  | 2.52        | 0.43     |
| 1:C:72:GLY:O     | 1:C:73:GLU:HB2   | 2.17        | 0.43     |
| 1:B:298:ASP:OD2  | 1:B:315:TRP:NE1  | 2.52        | 0.43     |
| 1:A:285:SER:HB3  | 1:B:208:ILE:HB   | 2.00        | 0.43     |
| 1:O:30:LEU:HD12  | 1:O:31:VAL:N     | 2.33        | 0.43     |
| 1:C:61:ILE:HG23  | 1:C:61:ILE:O     | 2.18        | 0.43     |
| 1:O:153:SER:O    | 1:O:155:THR:N    | 2.51        | 0.43     |
| 1:O:240:VAL:CG1  | 1:B:206:PHE:CE1  | 2.99        | 0.43     |
| 1:A:137:VAL:HG12 | 1:A:223:LEU:HD21 | 1.99        | 0.43     |
| 1:B:112:ALA:O    | 1:B:114:LEU:N    | 2.52        | 0.43     |
| 1:O:199:ARG:O    | 1:O:202:ARG:HG2  | 2.17        | 0.43     |
| 1:A:90:ALA:HB2   | 1:A:117:GLY:CA   | 2.47        | 0.43     |
| 1:O:145:ASP:OD2  | 1:O:145:ASP:N    | 2.52        | 0.43     |
| 1:O:284:VAL:HG12 | 1:C:209:ILE:HA   | 2.00        | 0.43     |
| 1:O:23:LEU:HD11  | 1:O:47:PHE:HZ    | 1.78        | 0.43     |
| 1:A:153:SER:O    | 1:A:157:ASN:HB2  | 2.17        | 0.43     |
| 1:B:111:ALA:HA   | 1:B:148:ILE:CD1  | 2.47        | 0.43     |
| 1:C:65:ASP:OD2   | 1:C:66:SER:N     | 2.51        | 0.43     |
| 1:B:27:ASP:OD1   | 1:B:28:VAL:HG23  | 2.19        | 0.43     |
| 1:C:84:PRO:HA    | 1:C:87:ILE:HD12  | 2.01        | 0.43     |
| 1:O:268:SER:O    | 1:O:273:LYS:HA   | 2.17        | 0.43     |
| 1:B:326:VAL:C    | 1:B:328:ASP:H    | 2.22        | 0.43     |
| 1:C:52:VAL:O     | 1:C:54:GLY:N     | 2.44        | 0.43     |
| 1:A:48:LYS:HE2   | 1:A:49:TYR:CZ    | 2.53        | 0.43     |
| 1:O:296:ILE:N    | 1:O:296:ILE:HD12 | 2.33        | 0.43     |
| 1:B:84:PRO:O     | 1:B:87:ILE:HG13  | 2.19        | 0.43     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:243:SER:HB2  | 1:B:316:TYR:CZ   | 2.53        | 0.43     |
| 1:C:317:ASP:O    | 1:C:318:ASN:C    | 2.56        | 0.43     |
| 1:A:6:ILE:HD13   | 1:A:28:VAL:HG21  | 2.01        | 0.43     |
| 1:C:97:VAL:O     | 1:C:121:VAL:HG13 | 2.19        | 0.43     |
| 1:B:85:ASP:N     | 1:B:112:ALA:HB1  | 2.32        | 0.43     |
| 1:C:249:VAL:CG2  | 1:C:250:ARG:H    | 2.21        | 0.43     |
| 1:B:87:ILE:O     | 1:B:116:GLY:HA3  | 2.18        | 0.43     |
| 1:A:285:SER:CA   | 1:A:315:TRP:HZ3  | 2.32        | 0.43     |
| 1:B:21:VAL:HG21  | 1:B:324:ASN:ND2  | 2.33        | 0.43     |
| 1:A:233:MET:SD   | 1:B:311:LYS:HD2  | 2.57        | 0.43     |
| 1:A:241:ASP:OD1  | 1:A:318:ASN:OD1  | 2.37        | 0.43     |
| 1:C:96:TYR:CD2   | 1:C:120:LYS:HB2  | 2.53        | 0.43     |
| 1:C:164:LYS:HG2  | 1:C:168:ASP:OD2  | 2.18        | 0.43     |
| 1:B:180:VAL:O    | 1:B:180:VAL:HG12 | 2.18        | 0.43     |
| 1:O:3:LYS:HG2    | 1:O:26:GLU:O     | 2.18        | 0.43     |
| 1:C:133:PHE:HA   | 1:C:138:ASN:HD21 | 1.83        | 0.43     |
| 1:O:206:PHE:C    | 1:O:207:ASN:OD1  | 2.57        | 0.43     |
| 1:A:226:LEU:HA   | 1:A:226:LEU:HD23 | 1.88        | 0.43     |
| 1:B:161:PRO:HB3  | 1:B:272:LEU:HD22 | 2.01        | 0.43     |
| 1:O:166:ILE:N    | 1:O:166:ILE:CD1  | 2.80        | 0.43     |
| 1:C:13:ARG:NH2   | 1:C:52:VAL:HG21  | 2.34        | 0.43     |
| 1:B:260:ILE:HG22 | 1:B:264:ILE:HD12 | 2.00        | 0.43     |
| 1:A:57:LYS:O     | 1:A:58:HIS:C     | 2.57        | 0.43     |
| 1:O:279:VAL:HG11 | 1:O:283:LEU:HD12 | 2.00        | 0.43     |
| 1:A:9:ASN:ND2    | 1:A:87:ILE:HD11  | 2.34        | 0.43     |
| 1:B:44:THR:HG21  | 1:B:63:ILE:CD1   | 2.49        | 0.43     |
| 1:O:38:ILE:HG23  | 1:O:42:TYR:CD2   | 2.54        | 0.43     |
| 1:O:279:VAL:HG11 | 1:O:283:LEU:CD1  | 2.49        | 0.42     |
| 1:O:250:ARG:CB   | 1:O:250:ARG:HH11 | 2.32        | 0.42     |
| 1:A:305:LEU:O    | 1:A:306:ASN:CB   | 2.67        | 0.42     |
| 1:A:284:VAL:CG2  | 1:B:207:ASN:ND2  | 2.82        | 0.42     |
| 1:B:22:ALA:C     | 1:B:24:GLN:N     | 2.71        | 0.42     |
| 1:A:206:PHE:HZ   | 1:C:239:THR:O    | 2.01        | 0.42     |
| 1:B:283:LEU:O    | 1:B:284:VAL:HG13 | 2.19        | 0.42     |
| 1:C:241:ASP:O    | 1:C:242:VAL:HB   | 2.18        | 0.42     |
| 1:O:322:TYR:O    | 1:O:326:VAL:HG23 | 2.19        | 0.42     |
| 1:C:57:LYS:HA    | 1:C:57:LYS:HD3   | 1.77        | 0.42     |
| 1:C:244:VAL:CG1  | 1:C:313:VAL:HG13 | 2.49        | 0.42     |
| 1:C:19:ALA:HB1   | 1:C:30:LEU:HD22  | 2.01        | 0.42     |
| 1:C:84:PRO:HB2   | 1:C:112:ALA:HB3  | 2.00        | 0.42     |
| 1:B:11:PHE:CE2   | 1:B:16:ARG:HG2   | 2.54        | 0.42     |
| 1:A:175:GLY:O    | 1:B:305:LEU:HD22 | 2.19        | 0.42     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:O:8:ILE:HG12   | 1:O:30:LEU:HD13  | 2.01        | 0.42     |
| 1:B:13:ARG:NH1   | 1:B:50:ASP:OD2   | 2.44        | 0.42     |
| 1:O:283:LEU:HD21 | 1:A:49:TYR:CD2   | 2.54        | 0.42     |
| 1:C:153:SER:H    | 1:C:157:ASN:ND2  | 2.16        | 0.42     |
| 1:A:251:ILE:N    | 1:A:251:ILE:CD1  | 2.82        | 0.42     |
| 1:A:50:ASP:HB3   | 1:A:54:GLY:O     | 2.18        | 0.42     |
| 1:O:294:SER:OG   | 1:O:325:ARG:NH1  | 2.52        | 0.42     |
| 1:B:303:ILE:CG1  | 1:B:304:ALA:N    | 2.81        | 0.42     |
| 1:C:53:HIS:HE1   | 1:C:241:ASP:OD2  | 2.02        | 0.42     |
| 1:C:260:ILE:HG21 | 1:C:312:LEU:HD22 | 2.02        | 0.42     |
| 1:A:298:ASP:CG   | 1:A:301:ALA:HB2  | 2.39        | 0.42     |
| 1:A:199:ARG:HG3  | 1:B:282:ASP:HB3  | 2.00        | 0.42     |
| 1:O:3:LYS:NZ     | 1:O:74:LYS:NZ    | 2.67        | 0.42     |
| 1:A:11:PHE:HE2   | 1:A:16:ARG:HD2   | 1.63        | 0.42     |
| 1:C:154:CYS:HA   | 1:C:322:TYR:CD1  | 2.55        | 0.42     |
| 1:C:272:LEU:HD13 | 1:C:276:ILE:HD11 | 2.02        | 0.42     |
| 1:O:304:ALA:HB2  | 1:O:310:VAL:HG23 | 2.02        | 0.42     |
| 1:C:90:ALA:HB3   | 1:C:117:GLY:HA3  | 2.01        | 0.42     |
| 1:B:244:VAL:HG21 | 1:B:313:VAL:HG13 | 2.01        | 0.42     |
| 1:B:107:LYS:O    | 1:B:111:ALA:CB   | 2.67        | 0.42     |
| 1:C:22:ALA:HA    | 1:C:25:SER:OG    | 2.20        | 0.42     |
| 1:A:207:ASN:ND2  | 1:B:284:VAL:CG2  | 2.82        | 0.42     |
| 1:B:135:CYS:HB2  | 1:B:325:ARG:HD3  | 2.01        | 0.42     |
| 1:O:187:GLN:HB3  | 1:O:204:ALA:CB   | 2.49        | 0.42     |
| 1:O:17:LEU:CD1   | 1:O:319:GLU:HB3  | 2.49        | 0.42     |
| 1:O:213:THR:HG22 | 1:O:233:MET:CA   | 2.47        | 0.42     |
| 1:B:110:ALA:HB1  | 1:B:121:VAL:HG11 | 2.00        | 0.42     |
| 1:C:39:THR:O     | 1:C:43:MET:N     | 2.41        | 0.42     |
| 1:O:68:THR:O     | 1:O:76:VAL:O     | 2.36        | 0.42     |
| 1:A:249:VAL:HG22 | 1:A:250:ARG:N    | 2.34        | 0.42     |
| 1:C:52:VAL:CG2   | 1:C:240:VAL:HG21 | 2.49        | 0.42     |
| 1:A:9:ASN:CG     | 1:A:34:ASN:HD22  | 2.22        | 0.42     |
| 1:B:71:LEU:H     | 1:B:71:LEU:HD22  | 1.84        | 0.42     |
| 1:B:51:THR:HG23  | 1:C:286:THR:HG21 | 2.02        | 0.42     |
| 1:C:32:ALA:N     | 1:C:76:VAL:HG13  | 2.34        | 0.42     |
| 1:O:45:TYR:OH    | 1:B:202:ARG:NH1  | 2.53        | 0.42     |
| 1:C:306:ASN:C    | 1:C:308:ASN:H    | 2.21        | 0.42     |
| 1:B:244:VAL:HG22 | 1:B:245:VAL:N    | 2.35        | 0.42     |
| 1:C:293:ARG:HH21 | 1:C:293:ARG:CG   | 2.33        | 0.42     |
| 1:A:42:TYR:HA    | 1:C:198:TRP:CH2  | 2.54        | 0.42     |
| 1:A:158:CYS:SG   | 1:A:159:LEU:N    | 2.93        | 0.42     |
| 1:B:84:PRO:HB2   | 1:B:112:ALA:CB   | 2.50        | 0.42     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:O:137:VAL:CG1  | 1:O:223:LEU:HD22 | 2.49        | 0.42     |
| 1:A:231:THR:HG22 | 1:B:305:LEU:HD13 | 2.01        | 0.42     |
| 1:C:149:VAL:HG21 | 1:C:333:MET:SD   | 2.60        | 0.42     |
| 1:A:298:ASP:HB3  | 1:A:301:ALA:CB   | 2.50        | 0.42     |
| 1:C:293:ARG:HG2  | 1:C:293:ARG:NH2  | 2.35        | 0.42     |
| 1:C:95:GLU:HG2   | 1:C:119:LYS:HB2  | 2.01        | 0.42     |
| 1:B:113:HIS:O    | 1:B:116:GLY:N    | 2.52        | 0.42     |
| 1:B:9:ASN:HD22   | 1:B:99:GLU:CD    | 2.22        | 0.42     |
| 1:O:223:LEU:CB   | 1:O:226:LEU:HD12 | 2.50        | 0.42     |
| 1:B:321:GLY:O    | 1:B:322:TYR:C    | 2.57        | 0.42     |
| 1:C:120:LYS:HA   | 1:C:147:ASP:O    | 2.20        | 0.42     |
| 1:B:32:ALA:HB2   | 1:B:92:ALA:CB    | 2.50        | 0.42     |
| 1:A:229:LYS:O    | 1:A:230:LEU:HD23 | 2.19        | 0.42     |
| 1:O:9:ASN:ND2    | 1:O:113:HIS:HE1  | 2.17        | 0.42     |
| 1:C:104:PHE:O    | 1:C:110:ALA:HB2  | 2.20        | 0.42     |
| 1:A:71:LEU:HD13  | 1:A:71:LEU:HA    | 1.90        | 0.41     |
| 1:C:270:GLY:C    | 1:C:272:LEU:H    | 2.24        | 0.41     |
| 1:C:276:ILE:CG2  | 1:C:277:GLY:N    | 2.83        | 0.41     |
| 1:A:173:ILE:HG13 | 1:A:252:GLU:CD   | 2.40        | 0.41     |
| 1:A:285:SER:OG   | 1:B:207:ASN:HA   | 2.19        | 0.41     |
| 1:O:106:ASP:O    | 1:O:108:GLU:N    | 2.53        | 0.41     |
| 1:C:184:THR:HG23 | 1:C:236:ARG:CZ   | 2.50        | 0.41     |
| 1:A:137:VAL:CG1  | 1:A:223:LEU:HD21 | 2.50        | 0.41     |
| 1:B:111:ALA:O    | 1:B:114:LEU:HD12 | 2.20        | 0.41     |
| 1:B:89:TRP:HB2   | 1:B:118:ALA:H    | 1.84        | 0.41     |
| 1:C:65:ASP:OD2   | 1:C:68:THR:HG22  | 2.20        | 0.41     |
| 1:O:188:LYS:HE3  | 1:O:193:PRO:O    | 2.21        | 0.41     |
| 1:O:128:LYS:HE3  | 1:O:129:ASP:CG   | 2.40        | 0.41     |
| 1:A:291:ASP:OD2  | 1:A:293:ARG:NH2  | 2.54        | 0.41     |
| 1:A:190:VAL:O    | 1:A:192:GLY:N    | 2.53        | 0.41     |
| 1:O:208:ILE:HG13 | 1:C:285:SER:HB2  | 2.03        | 0.41     |
| 1:C:69:LEU:HD22  | 1:C:78:VAL:CG2   | 2.50        | 0.41     |
| 1:C:16:ARG:HH11  | 1:C:16:ARG:CG    | 2.32        | 0.41     |
| 1:C:25:SER:C     | 1:C:27:ASP:H     | 2.23        | 0.41     |
| 1:O:199:ARG:CG   | 1:O:199:ARG:HH11 | 2.21        | 0.41     |
| 1:B:278:TYR:CE1  | 1:B:299:ALA:HB2  | 2.54        | 0.41     |
| 1:A:183:ILE:HG22 | 1:A:187:GLN:HE22 | 1.84        | 0.41     |
| 1:O:247:LEU:CG   | 1:O:249:VAL:HG13 | 2.47        | 0.41     |
| 1:C:219:VAL:O    | 1:C:223:LEU:HB2  | 2.20        | 0.41     |
| 1:B:85:ASP:HB3   | 1:B:112:ALA:HB1  | 2.01        | 0.41     |
| 1:B:37:PHE:C     | 1:B:38:ILE:HD12  | 2.40        | 0.41     |
| 1:B:208:ILE:O    | 1:B:210:PRO:HD3  | 2.21        | 0.41     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:324:ASN:H    | 1:B:324:ASN:ND2  | 2.14        | 0.41     |
| 1:B:317:ASP:O    | 1:B:318:ASN:C    | 2.58        | 0.41     |
| 1:A:39:THR:O     | 1:A:43:MET:HG3   | 2.21        | 0.41     |
| 1:B:81:ILE:HB    | 1:B:87:ILE:HG12  | 2.01        | 0.41     |
| 1:A:284:VAL:HB   | 1:A:285:SER:H    | 1.70        | 0.41     |
| 1:O:120:LYS:NZ   | 1:O:142:TYR:OH   | 2.51        | 0.41     |
| 1:C:10:GLY:HA3   | 1:C:100:SER:O    | 2.20        | 0.41     |
| 1:A:11:PHE:HB3   | 1:A:38:ILE:HD11  | 2.03        | 0.41     |
| 1:O:173:ILE:HB   | 1:O:250:ARG:O    | 2.21        | 0.41     |
| 1:A:208:ILE:CG1  | 3:B:6956:HOH:O   | 2.68        | 0.41     |
| 1:O:264:ILE:HD12 | 1:O:297:PHE:CD1  | 2.55        | 0.41     |
| 1:B:153:SER:O    | 1:B:155:THR:N    | 2.53        | 0.41     |
| 1:B:12:GLY:O     | 1:B:15:GLY:N     | 2.53        | 0.41     |
| 1:B:26:GLU:H     | 1:B:26:GLU:CD    | 2.24        | 0.41     |
| 1:O:167:HIS:ND1  | 1:O:171:GLY:HA2  | 2.35        | 0.41     |
| 1:C:214:GLY:O    | 1:C:218:ALA:N    | 2.54        | 0.41     |
| 1:B:113:HIS:O    | 1:B:114:LEU:C    | 2.59        | 0.41     |
| 1:A:307:ASP:N    | 1:A:307:ASP:OD1  | 2.54        | 0.41     |
| 1:O:156:THR:C    | 1:O:158:CYS:H    | 2.23        | 0.41     |
| 1:C:182:ALA:O    | 1:C:183:ILE:C    | 2.59        | 0.41     |
| 1:C:334:ALA:O    | 1:C:336:THR:N    | 2.53        | 0.41     |
| 1:C:81:ILE:HG22  | 1:C:83:ASN:H     | 1.85        | 0.41     |
| 1:A:227:ASN:C    | 1:A:229:LYS:H    | 2.24        | 0.41     |
| 1:A:9:ASN:ND2    | 1:A:113:HIS:HE1  | 2.17        | 0.41     |
| 1:C:292:SER:HB2  | 1:C:324:ASN:ND2  | 2.35        | 0.41     |
| 1:O:310:VAL:CG2  | 1:O:311:LYS:N    | 2.82        | 0.41     |
| 1:B:114:LEU:HD23 | 1:B:118:ALA:O    | 2.20        | 0.41     |
| 1:C:69:LEU:CD2   | 1:C:78:VAL:HG22  | 2.51        | 0.41     |
| 1:O:265:LYS:O    | 1:O:268:SER:N    | 2.53        | 0.41     |
| 1:B:296:ILE:HG22 | 1:B:297:PHE:N    | 2.35        | 0.41     |
| 1:A:133:PHE:CE2  | 1:A:142:TYR:HB2  | 2.55        | 0.41     |
| 1:A:291:ASP:C    | 1:A:293:ARG:H    | 2.23        | 0.41     |
| 1:B:3:LYS:HE3    | 1:B:26:GLU:C     | 2.42        | 0.41     |
| 1:A:8:ILE:HG23   | 1:A:98:VAL:HB    | 2.03        | 0.41     |
| 1:C:181:HIS:HD2  | 1:C:243:SER:OG   | 2.04        | 0.41     |
| 1:O:285:SER:HA   | 1:O:315:TRP:CZ3  | 2.56        | 0.41     |
| 1:C:23:LEU:HD12  | 1:C:47:PHE:HZ    | 1.85        | 0.41     |
| 1:A:111:ALA:HA   | 1:A:148:ILE:HD11 | 2.02        | 0.41     |
| 1:B:327:ILE:O    | 1:B:327:ILE:CG2  | 2.68        | 0.41     |
| 1:C:53:HIS:NE2   | 1:C:319:GLU:OE1  | 2.40        | 0.41     |
| 1:B:265:LYS:C    | 1:B:267:ALA:N    | 2.75        | 0.41     |
| 1:O:183:ILE:CD1  | 1:O:240:VAL:HA   | 2.51        | 0.40     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:O:239:THR:HG21 | 1:C:208:ILE:CG1  | 2.49        | 0.40     |
| 1:C:159:LEU:HD13 | 1:C:245:VAL:CG1  | 2.49        | 0.40     |
| 1:C:177:MET:HG2  | 1:C:178:THR:N    | 2.35        | 0.40     |
| 1:B:106:ASP:OD1  | 1:B:109:LYS:HD2  | 2.21        | 0.40     |
| 1:C:19:ALA:O     | 1:C:23:LEU:HG    | 2.22        | 0.40     |
| 1:O:68:THR:O     | 1:O:78:VAL:HG23  | 2.20        | 0.40     |
| 1:O:89:TRP:NE1   | 1:O:113:HIS:ND1  | 2.65        | 0.40     |
| 1:B:304:ALA:CB   | 1:B:310:VAL:HG12 | 2.51        | 0.40     |
| 1:B:306:ASN:C    | 1:B:308:ASN:H    | 2.25        | 0.40     |
| 1:A:214:GLY:O    | 1:A:218:ALA:N    | 2.51        | 0.40     |
| 1:A:275:ILE:O    | 1:A:294:SER:N    | 2.47        | 0.40     |
| 1:A:52:VAL:HG13  | 1:A:53:HIS:CD2   | 2.55        | 0.40     |
| 1:O:63:ILE:HD12  | 1:O:63:ILE:N     | 2.23        | 0.40     |
| 1:O:86:GLU:O     | 1:O:87:ILE:C     | 2.60        | 0.40     |
| 1:B:293:ARG:NH2  | 1:B:293:ARG:HG2  | 2.35        | 0.40     |
| 1:A:56:TRP:CD1   | 1:A:56:TRP:O     | 2.74        | 0.40     |
| 1:O:207:ASN:HB3  | 1:C:285:SER:HB3  | 2.02        | 0.40     |
| 1:B:104:PHE:HA   | 1:B:109:LYS:HD3  | 2.03        | 0.40     |
| 1:B:99:GLU:HB3   | 1:B:123:ILE:HD13 | 2.03        | 0.40     |
| 1:A:173:ILE:CD1  | 1:A:251:ILE:C    | 2.90        | 0.40     |
| 1:A:84:PRO:HG3   | 1:A:104:PHE:CE2  | 2.57        | 0.40     |
| 1:C:143:THR:O    | 1:C:144:SER:C    | 2.59        | 0.40     |
| 1:C:114:LEU:HA   | 1:C:118:ALA:HB3  | 2.04        | 0.40     |
| 1:B:194:SER:O    | 1:B:195:SER:C    | 2.59        | 0.40     |
| 1:O:245:VAL:CG1  | 1:O:246:ASP:H    | 2.33        | 0.40     |
| 1:O:174:GLU:HB2  | 1:C:305:LEU:CD2  | 2.50        | 0.40     |
| 1:O:216:ALA:C    | 1:O:218:ALA:N    | 2.71        | 0.40     |
| 1:B:244:VAL:CG2  | 1:B:245:VAL:N    | 2.83        | 0.40     |
| 1:B:293:ARG:HH21 | 1:B:293:ARG:HG2  | 1.85        | 0.40     |
| 1:O:14:ILE:HG12  | 1:O:322:TYR:HD2  | 1.86        | 0.40     |
| 1:B:271:LYS:N    | 1:B:271:LYS:HD2  | 2.37        | 0.40     |
| 1:A:38:ILE:HG21  | 1:A:46:MET:SD    | 2.61        | 0.40     |
| 1:O:311:LYS:HB2  | 1:C:176:LEU:HD12 | 2.03        | 0.40     |
| 1:B:183:ILE:O    | 1:B:184:THR:HG23 | 2.22        | 0.40     |
| 1:B:202:ARG:O    | 1:B:203:ALA:C    | 2.59        | 0.40     |
| 1:O:9:ASN:HD22   | 1:O:113:HIS:HE1  | 1.69        | 0.40     |
| 1:B:153:SER:HA   | 1:B:322:TYR:HE1  | 1.87        | 0.40     |
| 1:A:9:ASN:ND2    | 1:A:87:ILE:CD1   | 2.85        | 0.40     |
| 1:C:95:GLU:HB3   | 1:C:96:TYR:CD1   | 2.57        | 0.40     |
| 1:B:26:GLU:N     | 1:B:26:GLU:OE1   | 2.52        | 0.40     |

All (29) 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                | Distance(Å) | Clash(Å) |
|----------------|-----------------------|-------------|----------|
| 3:A:6940:HOH:O | 3:C:6947:HOH:O[2_644] | 0.07        | 2.13     |
| 3:B:6960:HOH:O | 3:C:6948:HOH:O[1_455] | 0.13        | 2.07     |
| 3:O:6950:HOH:O | 3:A:6928:HOH:O[1_455] | 0.14        | 2.06     |
| 3:O:6940:HOH:O | 3:A:6939:HOH:O[1_455] | 0.20        | 2.00     |
| 3:O:6933:HOH:O | 3:A:6933:HOH:O[1_556] | 0.21        | 1.99     |
| 3:A:6939:HOH:O | 3:C:6937:HOH:O[2_645] | 0.30        | 1.90     |
| 3:A:6932:HOH:O | 3:C:6941:HOH:O[2_645] | 0.33        | 1.87     |
| 3:A:6946:HOH:O | 3:C:6946:HOH:O[2_644] | 0.33        | 1.87     |
| 3:B:6944:HOH:O | 3:C:6951:HOH:O[1_454] | 0.35        | 1.85     |
| 3:O:6951:HOH:O | 3:A:6945:HOH:O[1_656] | 0.36        | 1.84     |
| 3:A:6936:HOH:O | 3:B:6963:HOH:O[2_544] | 0.36        | 1.84     |
| 3:A:6937:HOH:O | 3:C:6952:HOH:O[2_645] | 0.36        | 1.84     |
| 3:A:6938:HOH:O | 3:C:6930:HOH:O[2_645] | 0.36        | 1.84     |
| 3:O:6948:HOH:O | 3:B:6959:HOH:O[2_545] | 0.38        | 1.82     |
| 3:O:6948:HOH:O | 3:B:6962:HOH:O[2_544] | 0.38        | 1.82     |
| 3:B:6959:HOH:O | 3:B:6962:HOH:O[1_556] | 0.40        | 1.80     |
| 3:A:6941:HOH:O | 3:C:6939:HOH:O[2_544] | 0.45        | 1.75     |
| 3:B:6961:HOH:O | 3:C:6949:HOH:O[1_454] | 0.45        | 1.75     |
| 3:A:6934:HOH:O | 3:C:6934:HOH:O[2_645] | 0.46        | 1.74     |
| 3:O:6940:HOH:O | 3:C:6937:HOH:O[2_545] | 0.50        | 1.70     |
| 3:A:6937:HOH:O | 3:B:6957:HOH:O[2_544] | 0.51        | 1.69     |
| 3:A:6945:HOH:O | 3:C:6944:HOH:O[2_544] | 0.53        | 1.67     |
| 3:A:6944:HOH:O | 3:C:6930:HOH:O[2_544] | 0.60        | 1.60     |
| 3:A:6938:HOH:O | 3:A:6944:HOH:O[1_656] | 0.61        | 1.59     |
| 3:A:6943:HOH:O | 3:C:6953:HOH:O[1_554] | 0.61        | 1.59     |
| 3:B:6957:HOH:O | 3:C:6952:HOH:O[1_454] | 0.62        | 1.58     |
| 3:O:6951:HOH:O | 3:C:6944:HOH:O[2_645] | 0.71        | 1.49     |
| 3:B:6953:HOH:O | 3:C:6950:HOH:O[1_454] | 1.17        | 1.03     |
| 3:O:6942:HOH:O | 3:A:6924:HOH:O[1_556] | 1.33        | 0.87     |

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 1   | A     | 332/336 (99%) | 255 (77%) | 51 (15%) | 26 (8%)  | 1           | 30 |
| 1   | B     | 333/336 (99%) | 233 (70%) | 70 (21%) | 30 (9%)  | 1           | 25 |

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| Mol | Chain | Analysed        | Favoured  | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|-----------|-----------|----------|-------------|----|
| 1   | C     | 333/336 (99%)   | 236 (71%) | 67 (20%)  | 30 (9%)  | 1           | 25 |
| 1   | O     | 333/336 (99%)   | 246 (74%) | 64 (19%)  | 23 (7%)  | 2           | 35 |
| All | All   | 1331/1344 (99%) | 970 (73%) | 252 (19%) | 109 (8%) | 1           | 28 |

All (109) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 24  | GLN  |
| 1   | O     | 56  | TRP  |
| 1   | O     | 67  | LYS  |
| 1   | O     | 69  | LEU  |
| 1   | O     | 145 | ASP  |
| 1   | O     | 156 | THR  |
| 1   | O     | 242 | VAL  |
| 1   | O     | 285 | SER  |
| 1   | A     | 44  | THR  |
| 1   | A     | 191 | ASP  |
| 1   | A     | 202 | ARG  |
| 1   | A     | 231 | THR  |
| 1   | A     | 292 | SER  |
| 1   | A     | 309 | PHE  |
| 1   | B     | 152 | ALA  |
| 1   | B     | 242 | VAL  |
| 1   | B     | 282 | ASP  |
| 1   | C     | 53  | HIS  |
| 1   | C     | 69  | LEU  |
| 1   | C     | 70  | LEU  |
| 1   | C     | 144 | SER  |
| 1   | C     | 285 | SER  |
| 1   | C     | 307 | ASP  |
| 1   | O     | 3   | LYS  |
| 1   | O     | 59  | SER  |
| 1   | O     | 70  | LEU  |
| 1   | O     | 72  | GLY  |
| 1   | O     | 107 | LYS  |
| 1   | O     | 155 | THR  |
| 1   | O     | 171 | GLY  |
| 1   | O     | 282 | ASP  |
| 1   | A     | 48  | LYS  |
| 1   | A     | 67  | LYS  |
| 1   | A     | 85  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 171 | GLY  |
| 1   | A     | 194 | SER  |
| 1   | A     | 242 | VAL  |
| 1   | A     | 299 | ALA  |
| 1   | A     | 306 | ASN  |
| 1   | B     | 4   | ILE  |
| 1   | B     | 47  | PHE  |
| 1   | B     | 66  | SER  |
| 1   | B     | 70  | LEU  |
| 1   | B     | 84  | PRO  |
| 1   | B     | 85  | ASP  |
| 1   | B     | 104 | PHE  |
| 1   | B     | 113 | HIS  |
| 1   | B     | 135 | CYS  |
| 1   | B     | 137 | VAL  |
| 1   | B     | 216 | ALA  |
| 1   | B     | 229 | LYS  |
| 1   | B     | 231 | THR  |
| 1   | C     | 54  | GLY  |
| 1   | C     | 59  | SER  |
| 1   | C     | 61  | ILE  |
| 1   | C     | 115 | LYS  |
| 1   | C     | 158 | CYS  |
| 1   | C     | 171 | GLY  |
| 1   | C     | 191 | ASP  |
| 1   | C     | 195 | SER  |
| 1   | C     | 203 | ALA  |
| 1   | C     | 242 | VAL  |
| 1   | C     | 271 | LYS  |
| 1   | C     | 323 | SER  |
| 1   | C     | 335 | LYS  |
| 1   | O     | 66  | SER  |
| 1   | A     | 65  | ASP  |
| 1   | A     | 195 | SER  |
| 1   | A     | 228 | GLY  |
| 1   | A     | 307 | ASP  |
| 1   | B     | 118 | ALA  |
| 1   | B     | 154 | CYS  |
| 1   | B     | 195 | SER  |
| 1   | B     | 270 | GLY  |
| 1   | B     | 319 | GLU  |
| 1   | C     | 58  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 146 | ILE  |
| 1   | C     | 318 | ASN  |
| 1   | O     | 23  | LEU  |
| 1   | O     | 231 | THR  |
| 1   | O     | 316 | TYR  |
| 1   | A     | 291 | ASP  |
| 1   | B     | 54  | GLY  |
| 1   | B     | 69  | LEU  |
| 1   | B     | 112 | ALA  |
| 1   | B     | 114 | LEU  |
| 1   | B     | 238 | PRO  |
| 1   | C     | 226 | LEU  |
| 1   | C     | 319 | GLU  |
| 1   | A     | 185 | ALA  |
| 1   | A     | 318 | ASN  |
| 1   | B     | 3   | LYS  |
| 1   | B     | 40  | THR  |
| 1   | C     | 26  | GLU  |
| 1   | C     | 36  | PRO  |
| 1   | C     | 163 | ALA  |
| 1   | O     | 238 | PRO  |
| 1   | A     | 66  | SER  |
| 1   | A     | 200 | GLY  |
| 1   | A     | 224 | PRO  |
| 1   | B     | 215 | ALA  |
| 1   | B     | 327 | ILE  |
| 1   | C     | 125 | ALA  |
| 1   | C     | 183 | ILE  |
| 1   | A     | 270 | GLY  |
| 1   | C     | 52  | VAL  |
| 1   | O     | 88  | PRO  |
| 1   | O     | 224 | PRO  |
| 1   | A     | 10  | GLY  |

### 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     | 274/276 (99%)    | 252 (92%)  | 22 (8%)  | 17          | 65 |
| 1   | B     | 275/276 (100%)   | 260 (94%)  | 15 (6%)  | 30          | 79 |
| 1   | C     | 275/276 (100%)   | 255 (93%)  | 20 (7%)  | 20          | 69 |
| 1   | O     | 275/276 (100%)   | 252 (92%)  | 23 (8%)  | 16          | 63 |
| All | All   | 1099/1104 (100%) | 1019 (93%) | 80 (7%)  | 20          | 69 |

All (80) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 6   | ILE  |
| 1   | O     | 11  | PHE  |
| 1   | O     | 13  | ARG  |
| 1   | O     | 16  | ARG  |
| 1   | O     | 23  | LEU  |
| 1   | O     | 27  | ASP  |
| 1   | O     | 39  | THR  |
| 1   | O     | 46  | MET  |
| 1   | O     | 57  | LYS  |
| 1   | O     | 61  | ILE  |
| 1   | O     | 71  | LEU  |
| 1   | O     | 82  | ARG  |
| 1   | O     | 101 | THR  |
| 1   | O     | 128 | LYS  |
| 1   | O     | 183 | ILE  |
| 1   | O     | 199 | ARG  |
| 1   | O     | 225 | ASP  |
| 1   | O     | 240 | VAL  |
| 1   | O     | 260 | ILE  |
| 1   | O     | 286 | THR  |
| 1   | O     | 291 | ASP  |
| 1   | O     | 293 | ARG  |
| 1   | O     | 328 | ASP  |
| 1   | A     | 8   | ILE  |
| 1   | A     | 18  | VAL  |
| 1   | A     | 27  | ASP  |
| 1   | A     | 82  | ARG  |
| 1   | A     | 83  | ASN  |
| 1   | A     | 100 | SER  |
| 1   | A     | 105 | THR  |
| 1   | A     | 106 | ASP  |
| 1   | A     | 145 | ASP  |
| 1   | A     | 158 | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 173 | ILE  |
| 1   | A     | 179 | THR  |
| 1   | A     | 189 | THR  |
| 1   | A     | 191 | ASP  |
| 1   | A     | 251 | ILE  |
| 1   | A     | 258 | ASP  |
| 1   | A     | 280 | GLU  |
| 1   | A     | 293 | ARG  |
| 1   | A     | 307 | ASP  |
| 1   | A     | 308 | ASN  |
| 1   | A     | 313 | VAL  |
| 1   | A     | 324 | ASN  |
| 1   | B     | 6   | ILE  |
| 1   | B     | 11  | PHE  |
| 1   | B     | 26  | GLU  |
| 1   | B     | 27  | ASP  |
| 1   | B     | 38  | ILE  |
| 1   | B     | 41  | ASP  |
| 1   | B     | 139 | GLU  |
| 1   | B     | 178 | THR  |
| 1   | B     | 191 | ASP  |
| 1   | B     | 222 | VAL  |
| 1   | B     | 258 | ASP  |
| 1   | B     | 293 | ARG  |
| 1   | B     | 322 | TYR  |
| 1   | B     | 324 | ASN  |
| 1   | B     | 328 | ASP  |
| 1   | C     | 11  | PHE  |
| 1   | C     | 14  | ILE  |
| 1   | C     | 39  | THR  |
| 1   | C     | 41  | ASP  |
| 1   | C     | 62  | LYS  |
| 1   | C     | 65  | ASP  |
| 1   | C     | 68  | THR  |
| 1   | C     | 73  | GLU  |
| 1   | C     | 83  | ASN  |
| 1   | C     | 85  | ASP  |
| 1   | C     | 108 | GLU  |
| 1   | C     | 140 | ASP  |
| 1   | C     | 158 | CYS  |
| 1   | C     | 177 | MET  |
| 1   | C     | 183 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 250 | ARG  |
| 1   | C     | 251 | ILE  |
| 1   | C     | 293 | ARG  |
| 1   | C     | 307 | ASP  |
| 1   | C     | 312 | LEU  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 9   | ASN  |
| 1   | O     | 83  | ASN  |
| 1   | O     | 187 | GLN  |
| 1   | O     | 227 | ASN  |
| 1   | O     | 324 | ASN  |
| 1   | A     | 9   | ASN  |
| 1   | A     | 24  | GLN  |
| 1   | A     | 34  | ASN  |
| 1   | A     | 53  | HIS  |
| 1   | A     | 58  | HIS  |
| 1   | A     | 83  | ASN  |
| 1   | A     | 187 | GLN  |
| 1   | A     | 308 | ASN  |
| 1   | A     | 318 | ASN  |
| 1   | B     | 9   | ASN  |
| 1   | B     | 24  | GLN  |
| 1   | B     | 53  | HIS  |
| 1   | B     | 157 | ASN  |
| 1   | B     | 207 | ASN  |
| 1   | B     | 324 | ASN  |
| 1   | C     | 24  | GLN  |
| 1   | C     | 55  | GLN  |
| 1   | C     | 83  | ASN  |
| 1   | C     | 157 | ASN  |
| 1   | C     | 181 | HIS  |
| 1   | C     | 207 | ASN  |
| 1   | C     | 324 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

8 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   | SO4  | A     | 6922 | -    | 4,4,4        | 0.18 | 0           | 6,6,6       | 0.08 | 0           |
| 2   | SO4  | A     | 6923 | -    | 4,4,4        | 0.28 | 0           | 6,6,6       | 0.09 | 0           |
| 2   | SO4  | B     | 6924 | -    | 4,4,4        | 0.25 | 0           | 6,6,6       | 0.12 | 0           |
| 2   | SO4  | B     | 6925 | -    | 4,4,4        | 0.17 | 0           | 6,6,6       | 0.09 | 0           |
| 2   | SO4  | C     | 6926 | -    | 4,4,4        | 0.36 | 0           | 6,6,6       | 0.15 | 0           |
| 2   | SO4  | C     | 6927 | -    | 4,4,4        | 0.29 | 0           | 6,6,6       | 0.06 | 0           |
| 2   | SO4  | O     | 6920 | -    | 4,4,4        | 0.23 | 0           | 6,6,6       | 0.10 | 0           |
| 2   | SO4  | O     | 6921 | -    | 4,4,4        | 0.26 | 0           | 6,6,6       | 0.07 | 0           |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 2   | SO4  | A     | 6922 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 2   | SO4  | A     | 6923 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 2   | SO4  | B     | 6924 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 2   | SO4  | B     | 6925 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 2   | SO4  | C     | 6926 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 2   | SO4  | C     | 6927 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 2   | SO4  | O     | 6920 | -    | -       | 0/0/0/0  | 0/0/0/0 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 2   | SO4  | O     | 6921 | -    | -       | 0/0/0/0  | 0/0/0/0 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 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     | 334/336 (99%)   | -0.02  | 2 (0%) 86 70 | 0, 0, 0, 0            | 2 (0%) |
| 1   | B     | 335/336 (99%)   | -0.03  | 2 (0%) 86 70 | 0, 0, 0, 0            | 2 (0%) |
| 1   | C     | 335/336 (99%)   | 0.00   | 1 (0%) 91 83 | 0, 0, 0, 0            | 2 (0%) |
| 1   | O     | 335/336 (99%)   | -0.02  | 1 (0%) 91 83 | 0, 0, 0, 0            | 2 (0%) |
| All | All   | 1339/1344 (99%) | -0.02  | 6 (0%) 88 79 | 0, 0, 0, 0            | 8 (0%) |

All (6) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 154 | CYS  | 3.6  |
| 1   | C     | 154 | CYS  | 3.2  |
| 1   | B     | 154 | CYS  | 2.9  |
| 1   | A     | 252 | GLU  | 2.8  |
| 1   | B     | 196 | LYS  | 2.2  |
| 1   | O     | 154 | CYS  | 2.1  |

### 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. LLDF column lists the quality of electron



density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|----------------------------|-------|
| 2   | SO4  | C     | 6926 | 5/5   | 0.51 | 1.76  | 0,0,0,0                    | 0     |
| 2   | SO4  | C     | 6927 | 5/5   | 0.33 | 0.15  | 0,0,0,0                    | 0     |
| 2   | SO4  | B     | 6924 | 5/5   | 0.29 | 0.15  | 0,0,0,0                    | 0     |
| 2   | SO4  | O     | 6921 | 5/5   | 0.20 | 0.07  | 0,0,0,0                    | 0     |
| 2   | SO4  | O     | 6920 | 5/5   | 0.28 | -0.07 | 0,0,0,0                    | 0     |
| 2   | SO4  | A     | 6923 | 5/5   | 0.27 | -0.13 | 0,0,0,0                    | 0     |
| 2   | SO4  | B     | 6925 | 5/5   | 0.19 | -0.61 | 0,0,0,0                    | 0     |
| 2   | SO4  | A     | 6922 | 5/5   | 0.20 | -0.98 | 0,0,0,0                    | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.