



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:40 AM UTC

PDB ID : 3FVT / pdb\_00003fvt  
Title : Crystal Structure of Acetyl Xylan Esterase from *Bacillus pumilus*, monoclinic crystal form II  
Authors : Krastanova, I.; Cassetta, A.; Lamba, D.  
Deposited on : 2009-01-16  
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

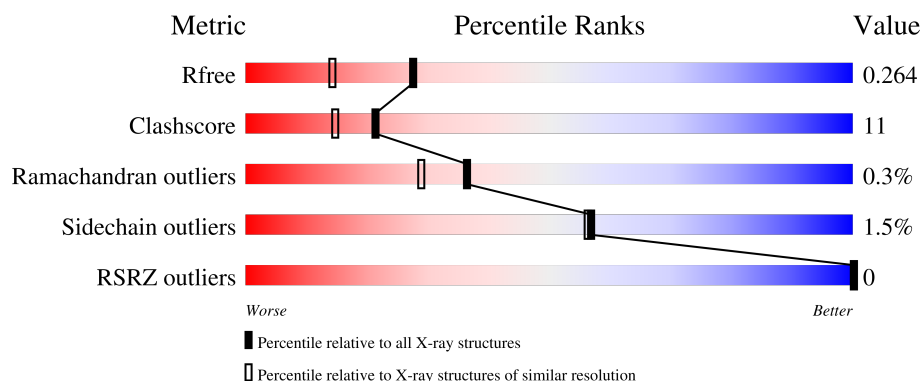
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 7789 (1.90-1.90)                                      |
| Clashscore            | 190562                      | 8410 (1.90-1.90)                                      |
| Ramachandran outliers | 187476                      | 8333 (1.90-1.90)                                      |
| Sidechain outliers    | 187428                      | 8333 (1.90-1.90)                                      |
| RSRZ outliers         | 180081                      | 7790 (1.90-1.90)                                      |

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                                                   |
|-----|-------|--------|----------------------------------------------------------------------------------------------------|
| 1   | A     | 320    | <br>78% 20% .. |
| 1   | B     | 320    | <br>79% 18% .. |
| 1   | C     | 320    | <br>76% 21% .. |
| 1   | D     | 320    | <br>76% 22% .. |
| 1   | E     | 320    | <br>82% 15% .. |

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| Mol | Chain | Length | Quality of chain                                                                              |
|-----|-------|--------|-----------------------------------------------------------------------------------------------|
| 1   | F     | 320    |  74% 23% .  |
| 1   | G     | 320    |  72% 25% .. |
| 1   | H     | 320    |  71% 26% .. |
| 1   | I     | 320    |  77% 20% .. |
| 1   | L     | 320    |  73% 25% .. |
| 1   | M     | 320    |  75% 22% .. |
| 1   | N     | 320    |  79% 19% .. |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 3   | GOL  | G     | 2274 | -         | -        | X       | -                |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 33650 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Acetyl xylan esterase.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 318      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2544  | 1652 | 417 | 471 | 4 |         |         |       |
| 1   | B     | 317      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2536  | 1647 | 416 | 470 | 3 |         |         |       |
| 1   | C     | 316      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2528  | 1641 | 415 | 469 | 3 |         |         |       |
| 1   | D     | 317      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2536  | 1647 | 416 | 470 | 3 |         |         |       |
| 1   | E     | 317      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2536  | 1647 | 416 | 470 | 3 |         |         |       |
| 1   | F     | 319      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2550  | 1654 | 418 | 475 | 3 |         |         |       |
| 1   | G     | 317      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2536  | 1647 | 416 | 470 | 3 |         |         |       |
| 1   | H     | 317      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2536  | 1647 | 416 | 470 | 3 |         |         |       |
| 1   | I     | 317      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2536  | 1647 | 416 | 470 | 3 |         |         |       |
| 1   | L     | 317      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2536  | 1647 | 416 | 470 | 3 |         |         |       |
| 1   | M     | 318      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2544  | 1652 | 417 | 471 | 4 |         |         |       |
| 1   | N     | 318      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2544  | 1652 | 417 | 471 | 4 |         |         |       |

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

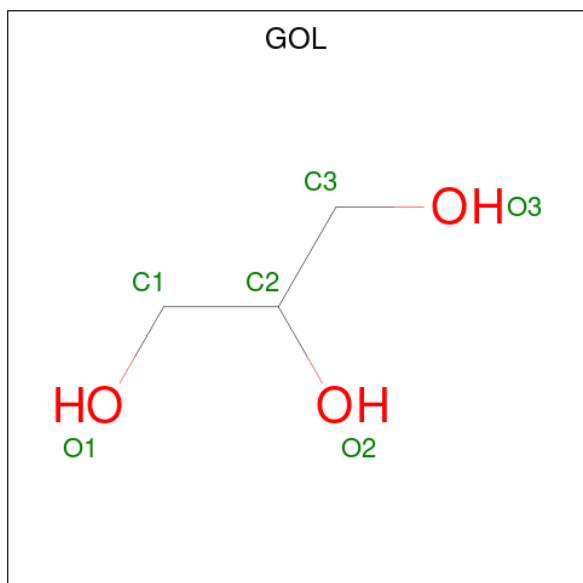
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | A     | 2        | Total | Cl | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | B     | 2        | Total | Cl | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | C     | 2        | Total | Cl | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | D     | 2        | Total | Cl | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | E     | 2        | Total | Cl | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | F     | 2        | Total | Cl | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | G     | 2        | Total | Cl | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | H     | 2        | Total | Cl | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | I     | 2        | Total | Cl | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | L     | 2        | Total | Cl | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | M     | 2        | Total | Cl | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | N     | 2        | Total | Cl | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | G     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms |     |  | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|--|---------|---------|
| 4   | A     | 332      | Total | O   |  | 0       | 0       |
|     |       |          | 332   | 332 |  |         |         |
| 4   | B     | 303      | Total | O   |  | 0       | 0       |
|     |       |          | 303   | 303 |  |         |         |
| 4   | C     | 296      | Total | O   |  | 0       | 0       |
|     |       |          | 296   | 296 |  |         |         |
| 4   | D     | 266      | Total | O   |  | 0       | 0       |
|     |       |          | 266   | 266 |  |         |         |
| 4   | E     | 295      | Total | O   |  | 0       | 0       |
|     |       |          | 295   | 295 |  |         |         |
| 4   | F     | 267      | Total | O   |  | 0       | 0       |
|     |       |          | 267   | 267 |  |         |         |
| 4   | G     | 196      | Total | O   |  | 0       | 0       |
|     |       |          | 196   | 196 |  |         |         |
| 4   | H     | 206      | Total | O   |  | 0       | 0       |
|     |       |          | 206   | 206 |  |         |         |
| 4   | I     | 270      | Total | O   |  | 0       | 0       |
|     |       |          | 270   | 270 |  |         |         |
| 4   | L     | 265      | Total | O   |  | 0       | 0       |
|     |       |          | 265   | 265 |  |         |         |
| 4   | M     | 213      | Total | O   |  | 0       | 0       |
|     |       |          | 213   | 213 |  |         |         |
| 4   | N     | 243      | Total | O   |  | 0       | 0       |
|     |       |          | 243   | 243 |  |         |         |

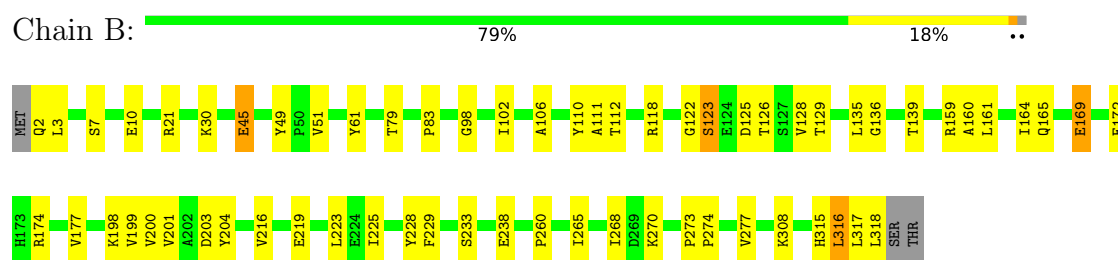
### 3 Residue-property plots

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

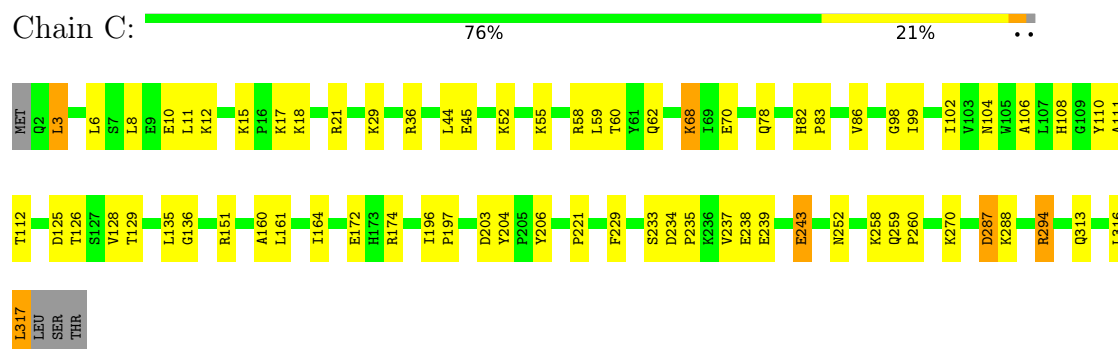
- Molecule 1: Acetyl xylan esterase



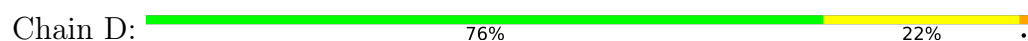
- Molecule 1: Acetyl xylan esterase

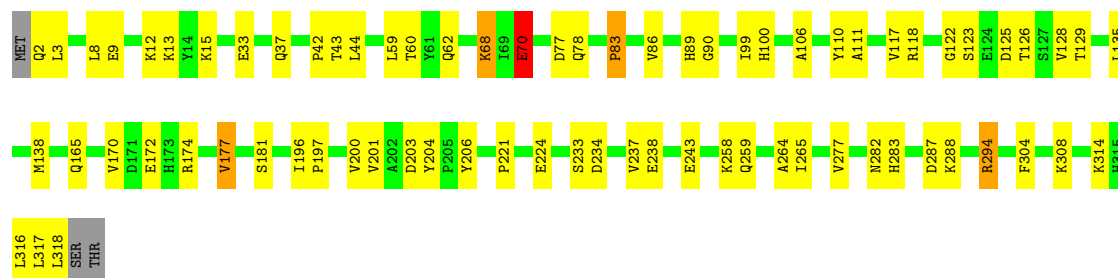


- Molecule 1: Acetyl xylan esterase



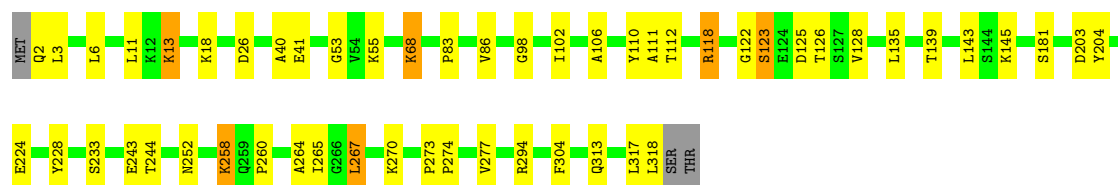
- Molecule 1: Acetyl xylan esterase





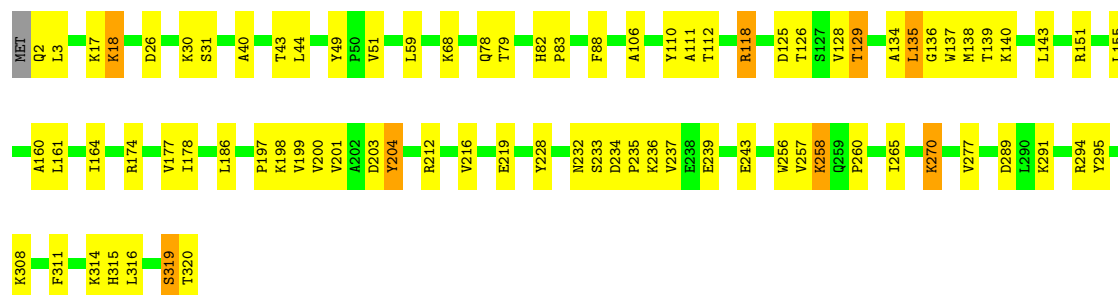
- Molecule 1: Acetyl xylan esterase

Chain E: 82% 15% ..



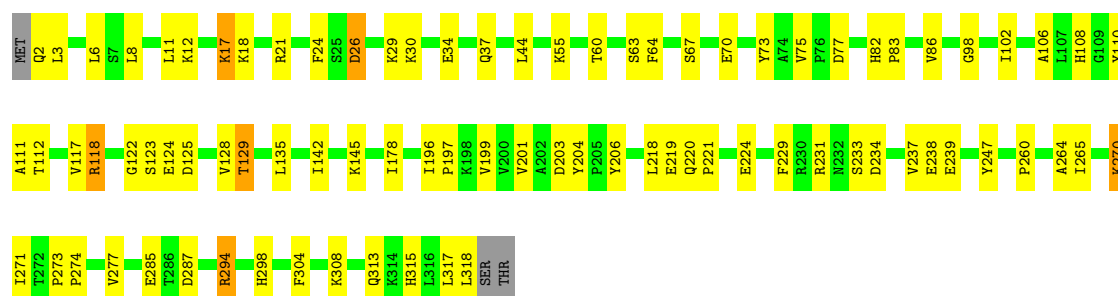
- Molecule 1: Acetyl xylan esterase

Chain F: 74% 23% .



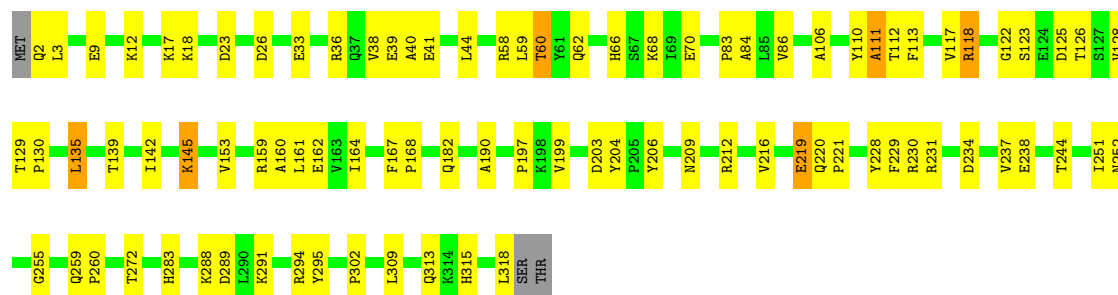
- Molecule 1: Acetyl xylan esterase

Chain G: 72% 25% ..



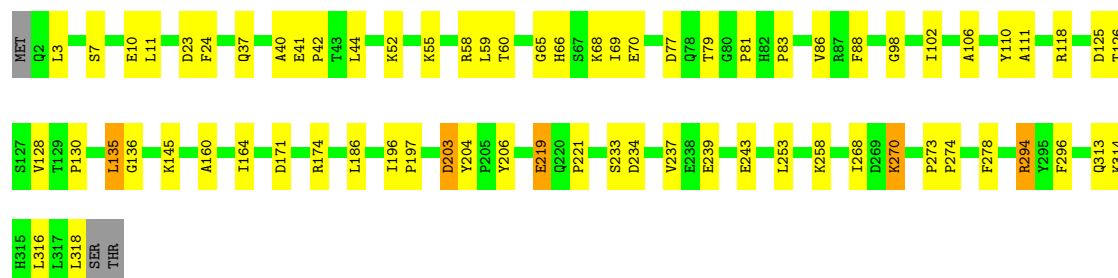
- Molecule 1: Acetyl xylan esterase

Chain H: 71% 26% ..



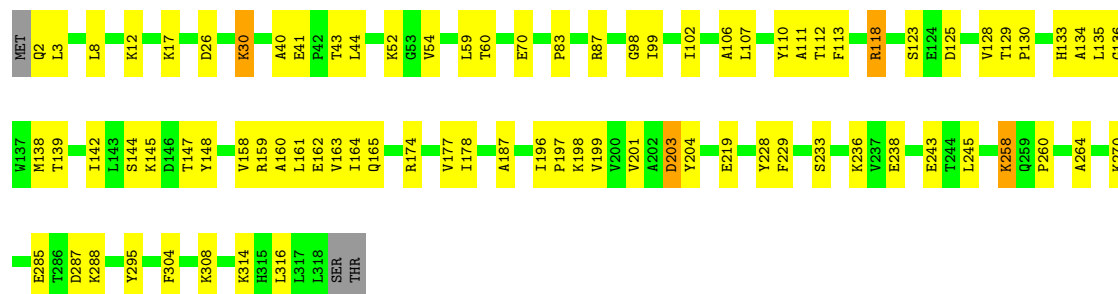
- Molecule 1: Acetyl xylan esterase

Chain I: 77% 20% ..



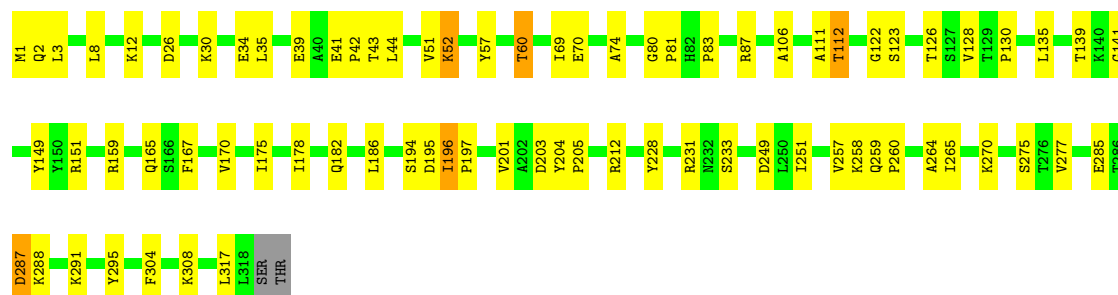
- Molecule 1: Acetyl xylan esterase

Chain L: 73% 25% ..



- Molecule 1: Acetyl xylan esterase

Chain M: 75% 22% ..



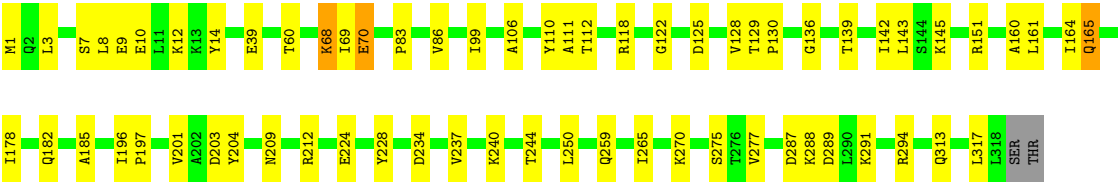
- Molecule 1: Acetyl xylan esterase

Chain N: 

79%

19%

..



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 144.04Å 87.20Å 184.82Å<br>90.00° 112.87° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 29.74 – 1.90<br>29.74 – 1.90                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 89.9 (29.74-1.90)<br>89.7 (29.74-1.90)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.09                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.30 (at 1.89Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.2                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.211 , 0.264<br>0.211 , 0.264                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 29799 reflections (9.97%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 22.1                                                        | Xtriage          |
| Anisotropy                                                              | 0.185                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.35 , 23.8                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$ | Xtriage          |
| Estimated twinning fraction                                             | 0.296 for h,-k,-h-l                                         | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.97                                                        | EDS              |
| Total number of atoms                                                   | 33650                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 22.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.61         | 0/2616  | 1.00        | 13/3551 (0.4%)   |
| 1   | B     | 0.60         | 0/2608  | 0.98        | 5/3541 (0.1%)    |
| 1   | C     | 0.58         | 0/2600  | 1.00        | 13/3530 (0.4%)   |
| 1   | D     | 0.57         | 0/2608  | 0.98        | 10/3541 (0.3%)   |
| 1   | E     | 0.58         | 0/2608  | 0.96        | 8/3541 (0.2%)    |
| 1   | F     | 0.56         | 0/2622  | 1.00        | 16/3559 (0.4%)   |
| 1   | G     | 0.52         | 0/2608  | 0.97        | 13/3541 (0.4%)   |
| 1   | H     | 0.50         | 0/2608  | 0.95        | 10/3541 (0.3%)   |
| 1   | I     | 0.57         | 0/2608  | 0.97        | 7/3541 (0.2%)    |
| 1   | L     | 0.57         | 0/2608  | 0.98        | 9/3541 (0.3%)    |
| 1   | M     | 0.51         | 0/2616  | 0.96        | 11/3551 (0.3%)   |
| 1   | N     | 0.56         | 0/2616  | 0.95        | 10/3551 (0.3%)   |
| All | All   | 0.56         | 0/31326 | 0.98        | 125/42529 (0.3%) |

There are no bond length outliers.

All (125) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | D     | 111 | ALA  | N-CA-C | -7.87 | 97.21       | 109.25   |
| 1   | F     | 83  | PRO  | N-CA-C | -7.64 | 100.52      | 111.22   |
| 1   | N     | 83  | PRO  | N-CA-C | -7.62 | 99.99       | 111.57   |
| 1   | E     | 111 | ALA  | N-CA-C | -7.61 | 98.19       | 109.15   |
| 1   | B     | 83  | PRO  | N-CA-C | -7.58 | 100.04      | 111.41   |
| 1   | A     | 233 | SER  | N-CA-C | 7.46  | 122.02      | 113.15   |
| 1   | A     | 83  | PRO  | N-CA-C | -7.37 | 100.36      | 111.41   |
| 1   | I     | 111 | ALA  | N-CA-C | -7.34 | 98.58       | 109.15   |
| 1   | B     | 233 | SER  | N-CA-C | 7.24  | 121.97      | 113.20   |
| 1   | H     | 83  | PRO  | N-CA-C | -7.21 | 99.64       | 111.68   |
| 1   | E     | 294 | ARG  | N-CA-C | 7.03  | 119.84      | 111.33   |
| 1   | L     | 83  | PRO  | N-CA-C | -6.87 | 101.11      | 111.41   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | C     | 111 | ALA  | N-CA-C | -6.86 | 99.27       | 109.15   |
| 1   | C     | 83  | PRO  | N-CA-C | -6.80 | 101.23      | 111.57   |
| 1   | E     | 83  | PRO  | N-CA-C | -6.72 | 101.33      | 111.41   |
| 1   | E     | 233 | SER  | N-CA-C | 6.72  | 121.33      | 113.20   |
| 1   | F     | 233 | SER  | N-CA-C | 6.71  | 121.18      | 113.19   |
| 1   | M     | 83  | PRO  | N-CA-C | -6.71 | 100.71      | 111.38   |
| 1   | G     | 108 | HIS  | N-CA-C | -6.70 | 105.07      | 113.18   |
| 1   | M     | 111 | ALA  | N-CA-C | -6.67 | 99.78       | 109.59   |
| 1   | D     | 83  | PRO  | N-CA-C | -6.66 | 101.43      | 111.41   |
| 1   | I     | 83  | PRO  | N-CA-C | -6.63 | 101.93      | 111.22   |
| 1   | A     | 99  | ILE  | N-CA-C | 6.62  | 118.16      | 110.62   |
| 1   | G     | 112 | THR  | N-CA-C | 6.59  | 119.67      | 109.07   |
| 1   | A     | 111 | ALA  | N-CA-C | -6.57 | 98.49       | 108.67   |
| 1   | G     | 83  | PRO  | N-CA-C | -6.56 | 101.56      | 111.41   |
| 1   | E     | 86  | VAL  | N-CA-C | -6.48 | 98.41       | 107.80   |
| 1   | M     | 233 | SER  | N-CA-C | 6.45  | 121.01      | 113.20   |
| 1   | C     | 233 | SER  | N-CA-C | 6.44  | 120.98      | 113.18   |
| 1   | N     | 224 | GLU  | N-CA-C | -6.38 | 104.42      | 111.82   |
| 1   | L     | 99  | ILE  | N-CA-C | 6.35  | 117.09      | 110.62   |
| 1   | C     | 99  | ILE  | N-CA-C | 6.33  | 117.84      | 110.62   |
| 1   | D     | 233 | SER  | N-CA-C | 6.32  | 120.59      | 113.01   |
| 1   | L     | 233 | SER  | N-CA-C | 6.30  | 120.82      | 113.20   |
| 1   | F     | 82  | HIS  | CA-C-N | -6.26 | 114.20      | 120.21   |
| 1   | F     | 82  | HIS  | C-N-CA | -6.26 | 114.20      | 120.21   |
| 1   | F     | 151 | ARG  | N-CA-C | -6.23 | 104.42      | 111.14   |
| 1   | H     | 111 | ALA  | N-CA-C | -6.21 | 99.05       | 108.67   |
| 1   | N     | 99  | ILE  | N-CA-C | 6.18  | 116.85      | 110.36   |
| 1   | C     | 15  | LYS  | CA-C-N | 6.18  | 126.13      | 119.76   |
| 1   | C     | 15  | LYS  | C-N-CA | 6.18  | 126.13      | 119.76   |
| 1   | F     | 112 | THR  | N-CA-C | 6.17  | 118.96      | 108.90   |
| 1   | N     | 111 | ALA  | N-CA-C | -6.16 | 100.53      | 109.59   |
| 1   | L     | 111 | ALA  | N-CA-C | -6.15 | 100.29      | 109.15   |
| 1   | I     | 86  | VAL  | N-CA-C | -6.12 | 98.93       | 107.80   |
| 1   | G     | 224 | GLU  | N-CA-C | -6.08 | 104.72      | 111.71   |
| 1   | G     | 233 | SER  | N-CA-C | 6.04  | 120.25      | 113.01   |
| 1   | G     | 142 | ILE  | N-CA-C | 6.03  | 120.57      | 111.89   |
| 1   | A     | 316 | LEU  | N-CA-C | 5.97  | 120.12      | 112.12   |
| 1   | N     | 151 | ARG  | N-CA-C | -5.93 | 104.74      | 111.14   |
| 1   | M     | 112 | THR  | N-CA-C | 5.93  | 118.56      | 108.90   |
| 1   | C     | 294 | ARG  | N-CA-C | 5.90  | 117.71      | 111.28   |
| 1   | C     | 58  | ARG  | N-CA-C | -5.88 | 99.15       | 108.73   |
| 1   | C     | 151 | ARG  | N-CA-C | -5.88 | 104.79      | 111.14   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | D     | 243 | GLU  | N-CA-C  | -5.86 | 104.80      | 111.07   |
| 1   | F     | 294 | ARG  | N-CA-C  | 5.85  | 118.12      | 111.11   |
| 1   | F     | 129 | THR  | N-CA-C  | -5.81 | 100.21      | 109.04   |
| 1   | H     | 295 | TYR  | N-CA-C  | 5.78  | 119.95      | 113.02   |
| 1   | A     | 288 | LYS  | N-CA-C  | 5.76  | 117.83      | 109.07   |
| 1   | N     | 182 | GLN  | N-CA-C  | -5.76 | 104.36      | 111.33   |
| 1   | M     | 151 | ARG  | N-CA-C  | -5.74 | 104.72      | 110.97   |
| 1   | M     | 196 | ILE  | CB-CA-C | -5.73 | 108.28      | 114.35   |
| 1   | F     | 111 | ALA  | N-CA-C  | -5.73 | 100.90      | 109.15   |
| 1   | C     | 112 | THR  | N-CA-C  | 5.71  | 118.21      | 108.90   |
| 1   | B     | 111 | ALA  | N-CA-C  | -5.69 | 100.96      | 109.15   |
| 1   | D     | 170 | VAL  | N-CA-C  | 5.64  | 116.06      | 108.17   |
| 1   | A     | 86  | VAL  | N-CA-C  | -5.63 | 99.63       | 107.80   |
| 1   | A     | 254 | ALA  | N-CA-C  | 5.63  | 118.14      | 111.33   |
| 1   | D     | 70  | GLU  | N-CA-C  | 5.60  | 116.75      | 108.86   |
| 1   | H     | 112 | THR  | N-CA-C  | 5.59  | 118.51      | 109.40   |
| 1   | A     | 118 | ARG  | N-CA-C  | 5.57  | 122.66      | 110.80   |
| 1   | C     | 86  | VAL  | N-CA-C  | -5.57 | 99.72       | 107.80   |
| 1   | H     | 288 | LYS  | N-CA-C  | 5.57  | 118.15      | 109.52   |
| 1   | C     | 243 | GLU  | N-CA-C  | -5.56 | 105.12      | 111.07   |
| 1   | G     | 82  | HIS  | CA-C-N  | -5.51 | 114.58      | 120.03   |
| 1   | G     | 82  | HIS  | C-N-CA  | -5.51 | 114.58      | 120.03   |
| 1   | B     | 112 | THR  | N-CA-C  | 5.50  | 117.86      | 108.90   |
| 1   | A     | 58  | ARG  | N-CA-C  | -5.46 | 99.84       | 108.73   |
| 1   | D     | 288 | LYS  | N-CA-C  | 5.45  | 117.47      | 109.24   |
| 1   | G     | 86  | VAL  | N-CA-C  | -5.45 | 99.90       | 107.80   |
| 1   | E     | 112 | THR  | N-CA-C  | 5.41  | 117.71      | 108.90   |
| 1   | N     | 70  | GLU  | N-CA-C  | 5.40  | 117.19      | 109.14   |
| 1   | G     | 129 | THR  | CA-C-N  | 5.40  | 124.85      | 119.24   |
| 1   | G     | 129 | THR  | C-N-CA  | 5.40  | 124.85      | 119.24   |
| 1   | F     | 138 | MET  | N-CA-C  | 5.35  | 118.60      | 111.75   |
| 1   | L     | 243 | GLU  | N-CA-C  | -5.35 | 105.35      | 111.07   |
| 1   | E     | 224 | GLU  | N-CA-C  | -5.34 | 105.63      | 111.82   |
| 1   | G     | 294 | ARG  | N-CA-C  | 5.34  | 117.79      | 111.33   |
| 1   | F     | 295 | TYR  | N-CA-C  | 5.31  | 119.39      | 113.02   |
| 1   | F     | 40  | ALA  | N-CA-C  | 5.30  | 117.75      | 111.33   |
| 1   | H     | 272 | THR  | CA-C-N  | 5.30  | 125.84      | 120.38   |
| 1   | H     | 272 | THR  | C-N-CA  | 5.30  | 125.84      | 120.38   |
| 1   | L     | 138 | MET  | N-CA-C  | 5.27  | 118.50      | 111.75   |
| 1   | A     | 260 | PRO  | N-CA-C  | -5.25 | 102.95      | 111.03   |
| 1   | G     | 111 | ALA  | N-CA-C  | -5.24 | 100.25      | 108.63   |
| 1   | N     | 112 | THR  | N-CA-C  | 5.23  | 117.43      | 108.90   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | M     | 167 | PHE  | CA-C-N | 5.22  | 124.67      | 119.24   |
| 1   | M     | 167 | PHE  | C-N-CA | 5.22  | 124.67      | 119.24   |
| 1   | D     | 238 | GLU  | N-CA-C | -5.22 | 105.67      | 111.36   |
| 1   | M     | 170 | VAL  | N-CA-C | 5.21  | 115.46      | 108.17   |
| 1   | F     | 204 | TYR  | CA-C-N | 5.21  | 125.21      | 119.90   |
| 1   | F     | 204 | TYR  | C-N-CA | 5.21  | 125.21      | 119.90   |
| 1   | N     | 287 | ASP  | N-CA-C | -5.19 | 102.23      | 109.96   |
| 1   | I     | 58  | ARG  | N-CA-C | -5.18 | 100.80      | 109.24   |
| 1   | C     | 288 | LYS  | N-CA-C | 5.17  | 117.05      | 109.24   |
| 1   | H     | 86  | VAL  | N-CA-C | -5.17 | 100.31      | 107.80   |
| 1   | N     | 288 | LYS  | N-CA-C | 5.16  | 116.92      | 109.07   |
| 1   | A     | 110 | TYR  | N-CA-C | 5.15  | 117.36      | 109.07   |
| 1   | E     | 267 | LEU  | N-CA-C | 5.14  | 118.65      | 112.38   |
| 1   | I     | 233 | SER  | N-CA-C | 5.14  | 119.18      | 113.01   |
| 1   | M     | 288 | LYS  | N-CA-C | 5.14  | 116.80      | 109.14   |
| 1   | A     | 295 | TYR  | N-CA-C | 5.13  | 119.18      | 113.02   |
| 1   | F     | 319 | SER  | N-CA-C | 5.13  | 114.39      | 108.49   |
| 1   | H     | 182 | GLN  | N-CA-C | -5.11 | 105.71      | 111.28   |
| 1   | L     | 295 | TYR  | N-CA-C | 5.11  | 119.15      | 113.02   |
| 1   | I     | 294 | ARG  | N-CA-C | 5.09  | 116.83      | 111.28   |
| 1   | L     | 112 | THR  | N-CA-C | 5.09  | 116.71      | 108.41   |
| 1   | D     | 86  | VAL  | N-CA-C | -5.09 | 99.84       | 107.37   |
| 1   | D     | 294 | ARG  | N-CA-C | 5.08  | 117.47      | 111.33   |
| 1   | B     | 316 | LEU  | N-CA-C | 5.07  | 118.91      | 112.12   |
| 1   | I     | 243 | GLU  | N-CA-C | -5.06 | 105.65      | 111.07   |
| 1   | L     | 288 | LYS  | N-CA-C | 5.06  | 116.50      | 108.96   |
| 1   | M     | 295 | TYR  | N-CA-C | 5.04  | 119.41      | 113.16   |
| 1   | H     | 58  | ARG  | N-CA-C | -5.02 | 100.33      | 108.52   |
| 1   | F     | 260 | PRO  | N-CA-C | -5.01 | 103.31      | 111.03   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2544  | 0        | 2494     | 60      | 0            |
| 1   | B     | 2536  | 0        | 2482     | 50      | 0            |
| 1   | C     | 2528  | 0        | 2471     | 48      | 0            |
| 1   | D     | 2536  | 0        | 2482     | 55      | 0            |
| 1   | E     | 2536  | 0        | 2482     | 43      | 0            |
| 1   | F     | 2550  | 0        | 2494     | 76      | 0            |
| 1   | G     | 2536  | 0        | 2482     | 70      | 0            |
| 1   | H     | 2536  | 0        | 2482     | 71      | 0            |
| 1   | I     | 2536  | 0        | 2482     | 54      | 0            |
| 1   | L     | 2536  | 0        | 2482     | 65      | 0            |
| 1   | M     | 2544  | 0        | 2494     | 61      | 0            |
| 1   | N     | 2544  | 0        | 2494     | 43      | 0            |
| 2   | A     | 2     | 0        | 0        | 0       | 0            |
| 2   | B     | 2     | 0        | 0        | 0       | 0            |
| 2   | C     | 2     | 0        | 0        | 0       | 0            |
| 2   | D     | 2     | 0        | 0        | 0       | 0            |
| 2   | E     | 2     | 0        | 0        | 0       | 0            |
| 2   | F     | 2     | 0        | 0        | 0       | 0            |
| 2   | G     | 2     | 0        | 0        | 0       | 0            |
| 2   | H     | 2     | 0        | 0        | 0       | 0            |
| 2   | I     | 2     | 0        | 0        | 0       | 0            |
| 2   | L     | 2     | 0        | 0        | 0       | 0            |
| 2   | M     | 2     | 0        | 0        | 1       | 0            |
| 2   | N     | 2     | 0        | 0        | 0       | 0            |
| 3   | E     | 6     | 0        | 8        | 1       | 0            |
| 3   | G     | 6     | 0        | 8        | 8       | 0            |
| 4   | A     | 332   | 0        | 0        | 6       | 0            |
| 4   | B     | 303   | 0        | 0        | 13      | 0            |
| 4   | C     | 296   | 0        | 0        | 11      | 0            |
| 4   | D     | 266   | 0        | 0        | 11      | 0            |
| 4   | E     | 295   | 0        | 0        | 11      | 0            |
| 4   | F     | 267   | 0        | 0        | 7       | 0            |
| 4   | G     | 196   | 0        | 0        | 3       | 0            |
| 4   | H     | 206   | 0        | 0        | 6       | 0            |
| 4   | I     | 270   | 0        | 0        | 5       | 0            |
| 4   | L     | 265   | 0        | 0        | 8       | 0            |
| 4   | M     | 213   | 0        | 0        | 13      | 0            |
| 4   | N     | 243   | 0        | 0        | 2       | 0            |
| All | All   | 33650 | 0        | 29837    | 660     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (660) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:1:MET:HE3    | 1:N:270:LYS:HD3  | 1.31                     | 1.12              |
| 1:H:62:GLN:NE2   | 1:H:68:LYS:HD3   | 1.73                     | 1.04              |
| 1:A:1:MET:HG2    | 1:A:2:GLN:H      | 1.23                     | 1.04              |
| 3:G:2274:GOL:H11 | 1:M:135:LEU:HD11 | 1.38                     | 1.03              |
| 1:F:198:LYS:HZ1  | 1:F:320:THR:HB   | 1.22                     | 1.01              |
| 1:C:8:LEU:HG     | 1:C:12:LYS:HE2   | 1.44                     | 0.98              |
| 1:G:221:PRO:HB3  | 3:G:2274:GOL:H12 | 1.49                     | 0.95              |
| 1:I:55:LYS:HE2   | 1:I:77:ASP:HA    | 1.48                     | 0.95              |
| 1:H:313:GLN:HG2  | 1:H:318:LEU:HG   | 1.51                     | 0.93              |
| 1:B:165:GLN:HG3  | 4:B:2904:HOH:O   | 1.69                     | 0.92              |
| 1:G:220:GLN:HB3  | 3:G:2274:GOL:H2  | 1.52                     | 0.91              |
| 1:F:30:LYS:HE2   | 4:F:1088:HOH:O   | 1.70                     | 0.91              |
| 1:G:239:GLU:HB3  | 4:G:2741:HOH:O   | 1.68                     | 0.90              |
| 1:E:128:VAL:HG23 | 1:F:126:THR:HA   | 1.52                     | 0.90              |
| 1:H:23:ASP:OD2   | 1:H:26:ASP:HB3   | 1.72                     | 0.90              |
| 1:G:220:GLN:CB   | 3:G:2274:GOL:H2  | 2.03                     | 0.89              |
| 1:G:17:LYS:HA    | 1:G:17:LYS:HE2   | 1.51                     | 0.89              |
| 1:G:178:ILE:HG22 | 1:G:201:VAL:HB   | 1.55                     | 0.89              |
| 1:A:26:ASP:O     | 1:A:30:LYS:HD3   | 1.72                     | 0.88              |
| 1:C:68:LYS:HZ2   | 1:C:68:LYS:HB2   | 1.39                     | 0.86              |
| 1:B:165:GLN:CG   | 4:B:2904:HOH:O   | 2.23                     | 0.86              |
| 1:H:18:LYS:HE3   | 1:H:252:ASN:HA   | 1.57                     | 0.84              |
| 1:E:126:THR:HA   | 1:F:128:VAL:HG13 | 1.60                     | 0.84              |
| 1:G:17:LYS:HD3   | 1:G:18:LYS:N     | 1.91                     | 0.84              |
| 1:M:285:GLU:HG2  | 4:M:3021:HOH:O   | 1.78                     | 0.84              |
| 1:H:289:ASP:OD2  | 1:H:291:LYS:HE2  | 1.78                     | 0.83              |
| 1:B:201:VAL:HG11 | 1:B:308:LYS:HG3  | 1.61                     | 0.82              |
| 1:G:17:LYS:HD3   | 1:G:18:LYS:H     | 1.45                     | 0.82              |
| 1:G:34:GLU:HA    | 1:G:37:GLN:NE2   | 1.93                     | 0.82              |
| 1:M:74:ALA:HB3   | 4:M:559:HOH:O    | 1.78                     | 0.82              |
| 1:I:60:THR:HG22  | 1:I:70:GLU:HG2   | 1.62                     | 0.82              |
| 1:M:201:VAL:HG11 | 1:M:308:LYS:HG3  | 1.63                     | 0.81              |
| 1:H:60:THR:OG1   | 1:H:68:LYS:HE2   | 1.82                     | 0.80              |
| 1:A:3:LEU:H      | 1:A:3:LEU:HD22   | 1.45                     | 0.79              |
| 1:C:17:LYS:HG2   | 4:C:1597:HOH:O   | 1.82                     | 0.79              |
| 1:A:60:THR:HG22  | 1:A:70:GLU:HG2   | 1.64                     | 0.79              |
| 1:H:23:ASP:HB3   | 4:H:2347:HOH:O   | 1.84                     | 0.78              |
| 1:H:62:GLN:HE22  | 1:H:68:LYS:HD3   | 1.48                     | 0.78              |
| 1:A:1:MET:HG2    | 1:A:2:GLN:N      | 1.97                     | 0.77              |
| 1:D:9:GLU:O      | 1:D:13:LYS:HE2   | 1.85                     | 0.77              |
| 1:F:201:VAL:HG11 | 1:F:308:LYS:HG3  | 1.66                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:23:ASP:HB3   | 4:H:2945:HOH:O   | 1.84                     | 0.77              |
| 1:M:8:LEU:HG     | 1:M:12:LYS:HE3   | 1.66                     | 0.76              |
| 1:C:68:LYS:HB2   | 1:C:68:LYS:NZ    | 1.99                     | 0.76              |
| 1:N:1:MET:HE3    | 1:N:270:LYS:CD   | 2.15                     | 0.76              |
| 1:M:258:LYS:HE2  | 1:M:258:LYS:HA   | 1.67                     | 0.75              |
| 1:F:198:LYS:HZ1  | 1:F:320:THR:CB   | 1.99                     | 0.75              |
| 1:C:270:LYS:HD3  | 4:C:1478:HOH:O   | 1.86                     | 0.74              |
| 1:C:243:GLU:HG2  | 4:C:2005:HOH:O   | 1.88                     | 0.74              |
| 1:H:60:THR:HG22  | 1:H:70:GLU:HG2   | 1.69                     | 0.74              |
| 1:E:2:GLN:N      | 4:E:1244:HOH:O   | 2.20                     | 0.73              |
| 1:B:126:THR:HA   | 1:D:128:VAL:HG13 | 1.70                     | 0.73              |
| 1:G:124:GLU:HB2  | 4:M:2819:HOH:O   | 1.89                     | 0.72              |
| 1:F:78:GLN:HG2   | 1:F:79:THR:N     | 2.03                     | 0.72              |
| 1:A:1:MET:HE2    | 1:A:2:GLN:O      | 1.90                     | 0.72              |
| 1:N:3:LEU:HD21   | 1:N:294:ARG:CZ   | 2.19                     | 0.72              |
| 1:A:3:LEU:HD21   | 1:A:294:ARG:CZ   | 2.19                     | 0.72              |
| 1:D:8:LEU:HG     | 1:D:12:LYS:HE3   | 1.72                     | 0.71              |
| 1:A:126:THR:HA   | 1:C:128:VAL:HG13 | 1.73                     | 0.71              |
| 1:A:219:GLU:HG3  | 1:A:270:LYS:HZ2  | 1.55                     | 0.71              |
| 1:F:2:GLN:OE1    | 1:F:3:LEU:HD22   | 1.91                     | 0.71              |
| 1:M:1:MET:HG3    | 1:M:2:GLN:N      | 2.05                     | 0.70              |
| 1:N:234:ASP:HB3  | 1:N:237:VAL:HG23 | 1.71                     | 0.70              |
| 1:M:112:THR:HB   | 4:M:559:HOH:O    | 1.90                     | 0.70              |
| 1:N:60:THR:HB    | 1:N:68:LYS:HD2   | 1.72                     | 0.70              |
| 1:N:1:MET:CE     | 1:N:270:LYS:HD3  | 2.16                     | 0.70              |
| 1:C:258:LYS:HE2  | 1:C:258:LYS:HA   | 1.73                     | 0.70              |
| 1:G:3:LEU:HD21   | 1:G:294:ARG:CZ   | 2.21                     | 0.70              |
| 1:L:287:ASP:HB3  | 4:L:436:HOH:O    | 1.91                     | 0.70              |
| 1:H:62:GLN:NE2   | 1:H:68:LYS:CD    | 2.55                     | 0.69              |
| 1:B:7:SER:OG     | 1:B:10:GLU:HG3   | 1.92                     | 0.69              |
| 1:B:79:THR:HG23  | 4:B:837:HOH:O    | 1.92                     | 0.69              |
| 1:D:172:GLU:HG2  | 4:D:1813:HOH:O   | 1.93                     | 0.69              |
| 1:C:60:THR:HG22  | 1:C:70:GLU:HG2   | 1.75                     | 0.68              |
| 1:F:3:LEU:HD22   | 1:F:3:LEU:H      | 1.58                     | 0.68              |
| 1:F:174:ARG:HD3  | 1:F:320:THR:HG23 | 1.75                     | 0.68              |
| 1:F:265:ILE:HD13 | 1:F:277:VAL:HG21 | 1.73                     | 0.68              |
| 1:E:135:LEU:HD21 | 1:F:136:GLY:HA2  | 1.75                     | 0.68              |
| 1:B:265:ILE:HD13 | 1:B:277:VAL:HG21 | 1.76                     | 0.67              |
| 1:F:174:ARG:CG   | 1:F:320:THR:HG23 | 2.24                     | 0.67              |
| 1:L:60:THR:HG22  | 1:L:70:GLU:HG2   | 1.74                     | 0.67              |
| 1:D:174:ARG:HD2  | 1:D:316:LEU:O    | 1.95                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:7:SER:OG     | 1:N:9:GLU:HG2    | 1.94                     | 0.67              |
| 1:M:122:GLY:O    | 1:M:123:SER:HB2  | 1.94                     | 0.67              |
| 1:F:161:LEU:HD13 | 1:F:197:PRO:HD3  | 1.75                     | 0.67              |
| 1:A:313:GLN:HE21 | 1:A:317:LEU:HD23 | 1.60                     | 0.67              |
| 1:F:232:ASN:HB3  | 4:F:2376:HOH:O   | 1.93                     | 0.67              |
| 1:B:2:GLN:OE1    | 1:B:3:LEU:HD22   | 1.94                     | 0.67              |
| 1:C:234:ASP:HB3  | 1:C:237:VAL:HG23 | 1.76                     | 0.66              |
| 1:C:21:ARG:HG2   | 1:C:243:GLU:OE2  | 1.96                     | 0.66              |
| 1:G:17:LYS:HA    | 1:G:17:LYS:CE    | 2.22                     | 0.66              |
| 1:H:206:TYR:OH   | 1:H:221:PRO:HG2  | 1.95                     | 0.66              |
| 1:G:206:TYR:OH   | 1:G:221:PRO:HG2  | 1.96                     | 0.66              |
| 1:A:46:SER:HB2   | 4:A:2941:HOH:O   | 1.96                     | 0.65              |
| 1:F:174:ARG:HG2  | 1:F:320:THR:CG2  | 2.27                     | 0.65              |
| 1:G:118:ARG:HB3  | 1:G:125:ASP:HB2  | 1.78                     | 0.65              |
| 1:A:128:VAL:HG13 | 1:C:126:THR:HA   | 1.78                     | 0.65              |
| 1:L:160:ALA:O    | 1:L:164:ILE:HG12 | 1.97                     | 0.65              |
| 1:A:143:LEU:O    | 1:A:240:LYS:HE3  | 1.96                     | 0.64              |
| 1:G:265:ILE:HD13 | 1:G:277:VAL:HG21 | 1.79                     | 0.64              |
| 1:D:2:GLN:N      | 4:D:792:HOH:O    | 2.31                     | 0.64              |
| 1:I:135:LEU:HD22 | 1:L:135:LEU:CD2  | 2.28                     | 0.64              |
| 1:B:219:GLU:OE2  | 1:B:270:LYS:HB2  | 1.98                     | 0.64              |
| 1:I:135:LEU:HD21 | 1:L:136:GLY:HA2  | 1.78                     | 0.64              |
| 1:I:313:GLN:O    | 1:I:318:LEU:HG   | 1.97                     | 0.64              |
| 1:M:249:ASP:OD1  | 1:M:251:ILE:HG12 | 1.97                     | 0.64              |
| 1:F:178:ILE:HG22 | 1:F:201:VAL:HB   | 1.80                     | 0.64              |
| 1:G:201:VAL:HG11 | 1:G:308:LYS:HG3  | 1.80                     | 0.64              |
| 1:I:270:LYS:HB2  | 1:I:270:LYS:NZ   | 2.11                     | 0.64              |
| 1:L:8:LEU:HG     | 1:L:12:LYS:HE3   | 1.78                     | 0.64              |
| 1:I:126:THR:HA   | 1:L:128:VAL:HG13 | 1.79                     | 0.63              |
| 1:I:10:GLU:HG2   | 4:I:2287:HOH:O   | 1.97                     | 0.63              |
| 1:I:160:ALA:O    | 1:I:164:ILE:HG12 | 1.98                     | 0.63              |
| 1:B:98:GLY:O     | 1:B:102:ILE:HG12 | 1.98                     | 0.63              |
| 1:B:128:VAL:HG13 | 1:D:126:THR:HA   | 1.79                     | 0.63              |
| 1:E:135:LEU:HD23 | 1:F:137:TRP:CZ3  | 2.32                     | 0.63              |
| 3:E:2273:GOL:H2  | 4:E:2972:HOH:O   | 1.98                     | 0.63              |
| 1:D:89:HIS:HD2   | 1:D:90:GLY:O     | 1.80                     | 0.63              |
| 1:F:234:ASP:HB3  | 1:F:237:VAL:HG23 | 1.81                     | 0.63              |
| 1:N:160:ALA:O    | 1:N:164:ILE:HG12 | 1.99                     | 0.63              |
| 1:D:89:HIS:HE1   | 1:D:117:VAL:H    | 1.46                     | 0.63              |
| 1:G:317:LEU:O    | 1:G:318:LEU:C    | 2.42                     | 0.62              |
| 1:L:158:VAL:O    | 1:L:162:GLU:HG3  | 1.99                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:258:LYS:HA   | 1:L:258:LYS:HZ3  | 1.64                     | 0.62              |
| 1:E:135:LEU:CD1  | 1:F:135:LEU:HD22 | 2.30                     | 0.62              |
| 1:I:3:LEU:HD21   | 1:I:294:ARG:CZ   | 2.30                     | 0.62              |
| 1:M:178:ILE:HG22 | 1:M:201:VAL:HB   | 1.80                     | 0.62              |
| 1:H:84:ALA:HB1   | 1:H:111:ALA:O    | 1.99                     | 0.62              |
| 1:L:145:LYS:HE2  | 4:L:1633:HOH:O   | 1.99                     | 0.62              |
| 1:A:33:GLU:O     | 1:A:37:GLN:HG3   | 2.00                     | 0.62              |
| 1:F:174:ARG:HD2  | 1:F:316:LEU:O    | 2.00                     | 0.62              |
| 1:D:106:ALA:HA   | 1:D:110:TYR:O    | 1.99                     | 0.62              |
| 1:D:118:ARG:HB3  | 1:D:125:ASP:HB2  | 1.81                     | 0.61              |
| 1:H:106:ALA:HA   | 1:H:110:TYR:O    | 2.00                     | 0.61              |
| 1:H:206:TYR:CZ   | 1:H:221:PRO:HG2  | 2.36                     | 0.61              |
| 1:B:199:VAL:HG12 | 1:B:260:PRO:HG2  | 1.82                     | 0.61              |
| 1:H:135:LEU:CD2  | 1:N:136:GLY:HA2  | 2.30                     | 0.61              |
| 1:E:2:GLN:N      | 4:E:1399:HOH:O   | 2.33                     | 0.61              |
| 1:A:178:ILE:HG22 | 1:A:201:VAL:HB   | 1.82                     | 0.61              |
| 1:D:201:VAL:HG11 | 1:D:308:LYS:HG3  | 1.83                     | 0.61              |
| 1:H:128:VAL:O    | 1:H:130:PRO:HD3  | 1.99                     | 0.61              |
| 1:A:1:MET:HB3    | 1:A:268:ILE:HB   | 1.82                     | 0.60              |
| 1:B:177:VAL:CG2  | 1:B:200:VAL:HG22 | 2.31                     | 0.60              |
| 1:F:17:LYS:N     | 1:F:17:LYS:HE2   | 2.15                     | 0.60              |
| 1:D:89:HIS:CE1   | 1:D:117:VAL:H    | 2.18                     | 0.60              |
| 1:A:3:LEU:HD21   | 1:A:294:ARG:NH2  | 2.15                     | 0.60              |
| 1:C:62:GLN:HE22  | 1:C:68:LYS:HZ2   | 1.50                     | 0.60              |
| 1:C:260:PRO:HA   | 1:C:287:ASP:HB2  | 1.83                     | 0.60              |
| 1:H:3:LEU:HD22   | 1:H:3:LEU:H      | 1.67                     | 0.60              |
| 4:H:1512:HOH:O   | 1:N:122:GLY:HA2  | 2.01                     | 0.60              |
| 1:D:3:LEU:H      | 1:D:3:LEU:HD22   | 1.66                     | 0.60              |
| 1:B:318:LEU:C    | 1:B:318:LEU:HD12 | 2.27                     | 0.59              |
| 1:F:235:PRO:O    | 1:F:239:GLU:HG3  | 2.03                     | 0.59              |
| 1:M:264:ALA:HB2  | 1:M:304:PHE:CE1  | 2.37                     | 0.59              |
| 1:H:3:LEU:HD21   | 1:H:294:ARG:CZ   | 2.33                     | 0.59              |
| 1:C:44:LEU:HD13  | 1:C:59:LEU:HD13  | 1.83                     | 0.59              |
| 1:L:54:VAL:CG2   | 1:L:107:LEU:HD23 | 2.32                     | 0.59              |
| 1:G:3:LEU:HD22   | 1:G:3:LEU:H      | 1.67                     | 0.59              |
| 1:F:160:ALA:O    | 1:F:164:ILE:HG12 | 2.02                     | 0.58              |
| 1:F:174:ARG:CD   | 1:F:320:THR:HG23 | 2.33                     | 0.58              |
| 1:L:43:THR:C     | 1:L:44:LEU:HD22  | 2.28                     | 0.58              |
| 1:A:128:VAL:HG13 | 1:C:125:ASP:O    | 2.03                     | 0.58              |
| 1:E:135:LEU:CD2  | 1:F:136:GLY:HA2  | 2.32                     | 0.58              |
| 1:H:2:GLN:OE1    | 1:H:3:LEU:HD22   | 2.04                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:258:LYS:HE2  | 4:I:346:HOH:O    | 2.03                     | 0.58              |
| 1:F:257:VAL:C    | 1:F:258:LYS:HE3  | 2.29                     | 0.58              |
| 1:M:41:GLU:HG3   | 4:M:1987:HOH:O   | 2.03                     | 0.58              |
| 1:L:161:LEU:HD13 | 1:L:197:PRO:HD3  | 1.86                     | 0.58              |
| 1:D:2:GLN:N      | 4:D:2936:HOH:O   | 2.36                     | 0.58              |
| 1:C:78:GLN:NE2   | 4:C:2992:HOH:O   | 2.36                     | 0.58              |
| 1:G:313:GLN:HG3  | 1:G:317:LEU:HD23 | 1.84                     | 0.58              |
| 1:H:135:LEU:HD21 | 1:N:136:GLY:HA2  | 1.86                     | 0.58              |
| 1:G:231:ARG:HG3  | 1:G:231:ARG:HH11 | 1.67                     | 0.58              |
| 1:H:203:ASP:O    | 1:H:204:TYR:C    | 2.47                     | 0.58              |
| 1:N:118:ARG:HB3  | 1:N:125:ASP:HB2  | 1.86                     | 0.58              |
| 1:G:220:GLN:HB2  | 3:G:2274:GOL:H2  | 1.82                     | 0.57              |
| 1:I:135:LEU:CD2  | 1:L:136:GLY:HA2  | 2.34                     | 0.57              |
| 1:M:1:MET:CE     | 1:M:2:GLN:H      | 2.17                     | 0.57              |
| 1:L:52:LYS:HD3   | 4:L:2354:HOH:O   | 2.03                     | 0.57              |
| 1:F:139:THR:HG21 | 1:F:228:TYR:HB2  | 1.86                     | 0.57              |
| 1:I:206:TYR:OH   | 1:I:221:PRO:HG2  | 2.04                     | 0.57              |
| 1:M:165:GLN:NE2  | 4:M:2520:HOH:O   | 2.36                     | 0.57              |
| 1:H:234:ASP:HB3  | 1:H:237:VAL:HG23 | 1.85                     | 0.57              |
| 1:L:2:GLN:N      | 4:L:730:HOH:O    | 2.36                     | 0.57              |
| 1:L:17:LYS:HE2   | 1:L:17:LYS:HA    | 1.85                     | 0.57              |
| 1:F:177:VAL:CG2  | 1:F:200:VAL:HG22 | 2.34                     | 0.57              |
| 1:M:182:GLN:O    | 1:M:186:LEU:HG   | 2.05                     | 0.57              |
| 1:L:54:VAL:HG23  | 1:L:107:LEU:HD23 | 1.86                     | 0.57              |
| 1:A:118:ARG:HB3  | 1:A:125:ASP:HB2  | 1.87                     | 0.57              |
| 1:D:287:ASP:HA   | 4:D:2626:HOH:O   | 2.05                     | 0.57              |
| 1:G:60:THR:HG22  | 1:G:70:GLU:HG2   | 1.85                     | 0.57              |
| 1:H:125:ASP:O    | 1:N:128:VAL:HG13 | 2.05                     | 0.57              |
| 1:I:106:ALA:HA   | 1:I:110:TYR:O    | 2.04                     | 0.57              |
| 1:I:135:LEU:HD22 | 1:L:135:LEU:HD21 | 1.85                     | 0.57              |
| 1:A:26:ASP:HB3   | 1:A:30:LYS:NZ    | 2.20                     | 0.57              |
| 1:A:44:LEU:CD1   | 1:A:59:LEU:HB2   | 2.35                     | 0.56              |
| 1:D:60:THR:HB    | 1:D:68:LYS:HD2   | 1.87                     | 0.56              |
| 1:F:43:THR:O     | 1:F:44:LEU:HD12  | 2.06                     | 0.56              |
| 1:F:174:ARG:HG2  | 1:F:320:THR:HG23 | 1.84                     | 0.56              |
| 1:E:2:GLN:N      | 4:E:523:HOH:O    | 2.38                     | 0.56              |
| 1:D:3:LEU:HD21   | 1:D:294:ARG:CZ   | 2.34                     | 0.56              |
| 1:H:84:ALA:HB2   | 1:H:111:ALA:HB3  | 1.88                     | 0.56              |
| 1:B:30:LYS:HB2   | 4:B:2802:HOH:O   | 2.05                     | 0.56              |
| 1:G:264:ALA:HB2  | 1:G:304:PHE:CZ   | 2.41                     | 0.56              |
| 1:M:141:GLY:HA2  | 2:M:321:CL:CL    | 2.43                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:205:PRO:HD2  | 1:M:277:VAL:HG13 | 1.87                     | 0.56              |
| 1:A:135:LEU:HD11 | 1:C:136:GLY:HA2  | 1.88                     | 0.56              |
| 1:I:135:LEU:HD21 | 1:L:136:GLY:CA   | 2.36                     | 0.56              |
| 1:G:313:GLN:HE21 | 1:G:317:LEU:CD2  | 2.19                     | 0.56              |
| 1:H:139:THR:HG21 | 1:H:228:TYR:HB2  | 1.88                     | 0.56              |
| 1:A:219:GLU:HG3  | 1:A:270:LYS:NZ   | 2.21                     | 0.56              |
| 1:B:135:LEU:HD23 | 1:B:136:GLY:N    | 2.21                     | 0.56              |
| 1:G:206:TYR:CZ   | 1:G:221:PRO:HG2  | 2.42                     | 0.55              |
| 1:H:126:THR:HA   | 1:N:128:VAL:HG13 | 1.87                     | 0.55              |
| 1:L:270:LYS:HD2  | 4:L:1218:HOH:O   | 2.06                     | 0.55              |
| 1:A:7:SER:OG     | 1:A:10:GLU:HG3   | 2.07                     | 0.55              |
| 1:B:45:GLU:CD    | 4:B:781:HOH:O    | 2.49                     | 0.55              |
| 1:C:18:LYS:HE3   | 1:C:252:ASN:HA   | 1.87                     | 0.55              |
| 1:I:135:LEU:CD2  | 1:L:135:LEU:HD23 | 2.36                     | 0.55              |
| 1:A:60:THR:CG2   | 1:A:70:GLU:HG2   | 2.36                     | 0.55              |
| 1:G:98:GLY:O     | 1:G:102:ILE:HG12 | 2.05                     | 0.55              |
| 1:A:135:LEU:CD1  | 1:C:136:GLY:HA2  | 2.37                     | 0.55              |
| 1:C:174:ARG:C    | 1:C:316:LEU:HD22 | 2.32                     | 0.55              |
| 1:I:37:GLN:NE2   | 4:I:1916:HOH:O   | 2.40                     | 0.55              |
| 1:I:52:LYS:HD3   | 1:I:52:LYS:C     | 2.31                     | 0.55              |
| 1:F:43:THR:C     | 1:F:44:LEU:HD12  | 2.31                     | 0.55              |
| 1:A:1:MET:N      | 1:A:268:ILE:HD12 | 2.22                     | 0.55              |
| 1:B:125:ASP:O    | 1:D:128:VAL:HG13 | 2.06                     | 0.55              |
| 1:G:26:ASP:OD2   | 1:G:30:LYS:HE2   | 2.06                     | 0.55              |
| 1:L:128:VAL:O    | 1:L:130:PRO:HD3  | 2.07                     | 0.55              |
| 1:A:1:MET:CG     | 1:A:2:GLN:H      | 1.97                     | 0.55              |
| 1:A:219:GLU:CG   | 1:A:270:LYS:HZ2  | 2.19                     | 0.55              |
| 1:H:44:LEU:HD21  | 1:H:59:LEU:HD13  | 1.89                     | 0.55              |
| 1:H:251:ILE:HB   | 1:H:283:HIS:CD2  | 2.42                     | 0.55              |
| 1:L:17:LYS:HE2   | 1:L:17:LYS:CA    | 2.37                     | 0.55              |
| 1:F:2:GLN:N      | 4:F:1430:HOH:O   | 2.40                     | 0.55              |
| 1:N:165:GLN:O    | 1:N:165:GLN:HG2  | 2.06                     | 0.55              |
| 1:A:201:VAL:HG11 | 1:A:308:LYS:HG3  | 1.88                     | 0.54              |
| 1:C:160:ALA:O    | 1:C:164:ILE:HG12 | 2.08                     | 0.54              |
| 1:M:203:ASP:O    | 1:M:204:TYR:C    | 2.49                     | 0.54              |
| 1:A:1:MET:HE1    | 1:A:4:PHE:CD1    | 2.43                     | 0.54              |
| 1:H:230:ARG:NH2  | 4:H:1925:HOH:O   | 2.40                     | 0.54              |
| 1:I:234:ASP:HB3  | 1:I:237:VAL:HG23 | 1.89                     | 0.54              |
| 1:I:239:GLU:HG3  | 4:I:1087:HOH:O   | 2.07                     | 0.54              |
| 1:G:317:LEU:O    | 1:G:317:LEU:HG   | 2.08                     | 0.54              |
| 1:D:62:GLN:HE22  | 1:D:68:LYS:HD3   | 1.72                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:169:GLU:CD   | 4:B:1448:HOH:O   | 2.50                     | 0.54              |
| 1:C:197:PRO:O    | 1:C:259:GLN:HG2  | 2.07                     | 0.54              |
| 1:M:265:ILE:HD13 | 1:M:277:VAL:HG21 | 1.88                     | 0.54              |
| 1:D:62:GLN:NE2   | 1:D:68:LYS:HD3   | 2.22                     | 0.54              |
| 1:H:313:GLN:HG2  | 1:H:318:LEU:CG   | 2.32                     | 0.54              |
| 1:C:78:GLN:HG2   | 1:C:82:HIS:HE1   | 1.73                     | 0.54              |
| 1:I:270:LYS:HB2  | 1:I:270:LYS:HZ2  | 1.73                     | 0.54              |
| 1:I:219:GLU:HG3  | 1:I:270:LYS:HZ1  | 1.73                     | 0.53              |
| 1:I:174:ARG:C    | 1:I:316:LEU:HD22 | 2.33                     | 0.53              |
| 1:L:203:ASP:O    | 1:L:204:TYR:C    | 2.51                     | 0.53              |
| 1:E:128:VAL:CG2  | 1:F:126:THR:HA   | 2.31                     | 0.53              |
| 1:F:270:LYS:HB2  | 1:F:270:LYS:NZ   | 2.22                     | 0.53              |
| 1:G:318:LEU:HD12 | 1:G:318:LEU:H    | 1.73                     | 0.53              |
| 1:D:206:TYR:CZ   | 1:D:221:PRO:HG2  | 2.43                     | 0.53              |
| 1:E:18:LYS:HE3   | 1:E:252:ASN:HA   | 1.90                     | 0.53              |
| 1:E:53:GLY:HA3   | 4:E:2136:HOH:O   | 2.09                     | 0.53              |
| 1:F:311:PHE:O    | 1:F:314:LYS:HG2  | 2.08                     | 0.53              |
| 1:N:178:ILE:HG22 | 1:N:201:VAL:HB   | 1.91                     | 0.53              |
| 1:B:2:GLN:N      | 4:B:908:HOH:O    | 2.41                     | 0.53              |
| 1:F:26:ASP:O     | 1:F:30:LYS:HG3   | 2.08                     | 0.52              |
| 1:I:11:LEU:HB3   | 1:I:278:PHE:CD1  | 2.43                     | 0.52              |
| 1:E:135:LEU:HD13 | 1:F:135:LEU:CD2  | 2.39                     | 0.52              |
| 1:L:30:LYS:NZ    | 4:L:893:HOH:O    | 2.43                     | 0.52              |
| 1:L:174:ARG:HD2  | 1:L:316:LEU:O    | 2.08                     | 0.52              |
| 1:N:3:LEU:CD2    | 1:N:294:ARG:CZ   | 2.87                     | 0.52              |
| 1:B:135:LEU:HD23 | 1:B:135:LEU:C    | 2.33                     | 0.52              |
| 1:H:212:ARG:O    | 1:H:216:VAL:HG23 | 2.09                     | 0.52              |
| 1:M:106:ALA:HB2  | 4:M:559:HOH:O    | 2.09                     | 0.52              |
| 1:E:258:LYS:HA   | 1:E:258:LYS:HZ3  | 1.73                     | 0.52              |
| 1:F:319:SER:OG   | 1:F:320:THR:N    | 2.42                     | 0.52              |
| 1:H:231:ARG:HG3  | 1:H:231:ARG:HH11 | 1.74                     | 0.52              |
| 1:A:128:VAL:HG12 | 1:A:129:THR:N    | 2.23                     | 0.52              |
| 1:H:122:GLY:O    | 1:H:123:SER:HB2  | 2.10                     | 0.51              |
| 1:A:3:LEU:H      | 1:A:3:LEU:CD2    | 2.20                     | 0.51              |
| 1:B:21:ARG:HG2   | 4:B:2589:HOH:O   | 2.10                     | 0.51              |
| 1:D:181:SER:HA   | 1:D:204:TYR:O    | 2.10                     | 0.51              |
| 3:G:2274:GOL:H31 | 1:M:135:LEU:CD1  | 2.39                     | 0.51              |
| 1:A:1:MET:SD     | 1:A:270:LYS:HG3  | 2.51                     | 0.51              |
| 1:D:128:VAL:HG12 | 1:D:129:THR:N    | 2.26                     | 0.51              |
| 1:G:264:ALA:HB2  | 1:G:304:PHE:CE1  | 2.46                     | 0.51              |
| 1:L:258:LYS:NZ   | 1:L:258:LYS:HB3  | 2.25                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:234:ASP:HB3  | 1:G:237:VAL:HG23 | 1.90                     | 0.51              |
| 1:E:55:LYS:NZ    | 4:E:867:HOH:O    | 2.43                     | 0.51              |
| 1:L:87:ARG:HG2   | 1:L:87:ARG:HH11  | 1.76                     | 0.51              |
| 1:L:178:ILE:HG22 | 1:L:201:VAL:HB   | 1.92                     | 0.51              |
| 1:N:128:VAL:HG12 | 1:N:129:THR:N    | 2.25                     | 0.51              |
| 1:E:313:GLN:HG2  | 1:E:318:LEU:HG   | 1.92                     | 0.51              |
| 1:L:201:VAL:HG11 | 1:L:308:LYS:HG3  | 1.93                     | 0.51              |
| 1:M:60:THR:HG22  | 1:M:70:GLU:HG2   | 1.92                     | 0.51              |
| 1:B:229:PHE:CE1  | 1:B:238:GLU:HA   | 2.45                     | 0.51              |
| 1:H:160:ALA:O    | 1:H:164:ILE:HG12 | 2.10                     | 0.51              |
| 1:L:26:ASP:O     | 1:L:30:LYS:HE3   | 2.11                     | 0.51              |
| 1:D:177:VAL:CG2  | 1:D:200:VAL:HG22 | 2.41                     | 0.50              |
| 1:L:139:THR:HG21 | 1:L:228:TYR:HB2  | 1.93                     | 0.50              |
| 1:E:98:GLY:O     | 1:E:102:ILE:HG12 | 2.11                     | 0.50              |
| 1:I:206:TYR:CZ   | 1:I:221:PRO:HG2  | 2.46                     | 0.50              |
| 1:F:174:ARG:HG2  | 1:F:320:THR:HG21 | 1.94                     | 0.50              |
| 1:G:271:ILE:HD12 | 1:G:298:HIS:CD2  | 2.46                     | 0.50              |
| 1:A:138:MET:HB2  | 1:A:224:GLU:OE1  | 2.11                     | 0.50              |
| 1:B:223:LEU:HB3  | 4:B:765:HOH:O    | 2.11                     | 0.50              |
| 1:C:206:TYR:CZ   | 1:C:221:PRO:HG2  | 2.47                     | 0.50              |
| 1:D:203:ASP:O    | 1:D:204:TYR:C    | 2.54                     | 0.50              |
| 1:E:118:ARG:HB3  | 1:E:125:ASP:HB2  | 1.93                     | 0.50              |
| 1:E:135:LEU:HD13 | 1:F:135:LEU:HD22 | 1.93                     | 0.50              |
| 1:F:17:LYS:HE3   | 4:F:1748:HOH:O   | 2.12                     | 0.50              |
| 1:I:3:LEU:H      | 1:I:3:LEU:HD22   | 1.76                     | 0.50              |
| 1:I:118:ARG:HB3  | 1:I:125:ASP:HB2  | 1.93                     | 0.50              |
| 1:M:231:ARG:HG3  | 1:M:231:ARG:HH11 | 1.77                     | 0.50              |
| 1:N:8:LEU:HG     | 1:N:12:LYS:HE3   | 1.93                     | 0.50              |
| 1:A:203:ASP:O    | 1:A:204:TYR:C    | 2.54                     | 0.50              |
| 1:I:135:LEU:HD22 | 1:L:135:LEU:HD23 | 1.93                     | 0.50              |
| 1:I:314:LYS:HA   | 1:I:318:LEU:HD12 | 1.93                     | 0.50              |
| 1:A:1:MET:SD     | 1:A:270:LYS:CG   | 3.00                     | 0.50              |
| 1:D:206:TYR:OH   | 1:D:221:PRO:HG2  | 2.12                     | 0.50              |
| 1:C:29:LYS:HE2   | 4:C:2947:HOH:O   | 2.13                     | 0.49              |
| 1:E:55:LYS:NZ    | 4:E:1646:HOH:O   | 2.28                     | 0.49              |
| 1:G:73:TYR:CE2   | 1:G:75:VAL:CG2   | 2.95                     | 0.49              |
| 1:I:125:ASP:O    | 1:L:128:VAL:HG13 | 2.12                     | 0.49              |
| 1:L:142:ILE:HD13 | 1:L:148:TYR:CE1  | 2.47                     | 0.49              |
| 1:I:98:GLY:O     | 1:I:102:ILE:HG12 | 2.12                     | 0.49              |
| 1:L:264:ALA:HB2  | 1:L:304:PHE:CE1  | 2.47                     | 0.49              |
| 1:N:203:ASP:O    | 1:N:204:TYR:C    | 2.55                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:287:ASP:HB3  | 4:D:2042:HOH:O   | 2.13                     | 0.49              |
| 1:G:128:VAL:HG13 | 1:M:126:THR:HA   | 1.94                     | 0.49              |
| 1:G:203:ASP:O    | 1:G:204:TYR:C    | 2.56                     | 0.49              |
| 1:C:10:GLU:HG2   | 4:C:2045:HOH:O   | 2.12                     | 0.49              |
| 1:F:198:LYS:NZ   | 1:F:320:THR:CG2  | 2.75                     | 0.49              |
| 1:M:139:THR:HG21 | 1:M:228:TYR:HB2  | 1.95                     | 0.49              |
| 1:B:198:LYS:HE3  | 4:B:2267:HOH:O   | 2.11                     | 0.49              |
| 1:C:128:VAL:HG12 | 1:C:129:THR:N    | 2.27                     | 0.49              |
| 1:E:265:ILE:HD13 | 1:E:277:VAL:HG21 | 1.93                     | 0.49              |
| 1:N:106:ALA:HA   | 1:N:110:TYR:O    | 2.12                     | 0.49              |
| 1:A:270:LYS:NZ   | 1:A:270:LYS:HB2  | 2.27                     | 0.49              |
| 1:B:160:ALA:O    | 1:B:164:ILE:HG12 | 2.12                     | 0.49              |
| 1:D:60:THR:HG22  | 1:D:70:GLU:HB3   | 1.94                     | 0.49              |
| 1:I:313:GLN:HG2  | 1:I:318:LEU:HD21 | 1.94                     | 0.49              |
| 1:M:80:GLY:HA3   | 1:M:81:PRO:C     | 2.38                     | 0.49              |
| 1:C:62:GLN:HE22  | 1:C:68:LYS:NZ    | 2.11                     | 0.49              |
| 1:E:106:ALA:HA   | 1:E:110:TYR:O    | 2.12                     | 0.49              |
| 1:F:270:LYS:HB2  | 1:F:270:LYS:HZ2  | 1.76                     | 0.49              |
| 1:I:135:LEU:HD23 | 1:I:136:GLY:N    | 2.28                     | 0.49              |
| 1:L:106:ALA:HA   | 1:L:110:TYR:O    | 2.13                     | 0.48              |
| 1:H:219:GLU:CD   | 1:H:220:GLN:H    | 2.20                     | 0.48              |
| 1:F:49:TYR:HD1   | 1:F:51:VAL:HG12  | 1.78                     | 0.48              |
| 1:M:51:VAL:HG22  | 1:M:52:LYS:N     | 2.28                     | 0.48              |
| 1:G:117:VAL:O    | 1:G:118:ARG:C    | 2.57                     | 0.48              |
| 1:H:302:PRO:HB3  | 4:M:1899:HOH:O   | 2.14                     | 0.48              |
| 1:N:313:GLN:HE21 | 1:N:317:LEU:HD23 | 1.78                     | 0.48              |
| 1:A:23:ASP:OD2   | 1:A:145:LYS:NZ   | 2.46                     | 0.48              |
| 1:D:177:VAL:HG23 | 1:D:200:VAL:HG22 | 1.95                     | 0.48              |
| 1:E:13:LYS:HB2   | 1:E:13:LYS:NZ    | 2.28                     | 0.48              |
| 1:F:106:ALA:HA   | 1:F:110:TYR:O    | 2.14                     | 0.48              |
| 1:F:289:ASP:HB2  | 4:F:2248:HOH:O   | 2.14                     | 0.48              |
| 1:G:135:LEU:HD22 | 1:M:135:LEU:HD22 | 1.96                     | 0.48              |
| 1:H:126:THR:HA   | 1:N:128:VAL:HG22 | 1.94                     | 0.48              |
| 1:D:99:ILE:HG23  | 1:D:100:HIS:N    | 2.29                     | 0.48              |
| 1:L:236:LYS:N    | 1:L:236:LYS:HE2  | 2.28                     | 0.48              |
| 1:M:249:ASP:CG   | 1:M:251:ILE:HG12 | 2.38                     | 0.48              |
| 1:C:172:GLU:HG2  | 4:C:435:HOH:O    | 2.12                     | 0.48              |
| 1:D:78:GLN:NE2   | 4:D:2467:HOH:O   | 2.47                     | 0.48              |
| 1:N:3:LEU:HD21   | 1:N:294:ARG:NE   | 2.27                     | 0.48              |
| 1:N:265:ILE:HD13 | 1:N:277:VAL:HG21 | 1.94                     | 0.48              |
| 1:C:45:GLU:HG3   | 4:C:437:HOH:O    | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:203:ASP:O    | 1:C:204:TYR:C    | 2.54                     | 0.48              |
| 1:M:30:LYS:O     | 1:M:34:GLU:HG3   | 2.13                     | 0.48              |
| 1:M:260:PRO:HA   | 1:M:287:ASP:O    | 2.13                     | 0.48              |
| 1:C:3:LEU:CD1    | 1:C:294:ARG:NH1  | 2.77                     | 0.48              |
| 1:E:145:LYS:HA   | 1:E:244:THR:HG23 | 1.96                     | 0.48              |
| 1:F:18:LYS:NZ    | 1:F:18:LYS:CB    | 2.77                     | 0.48              |
| 1:C:161:LEU:HD13 | 1:C:197:PRO:HD3  | 1.95                     | 0.47              |
| 1:F:234:ASP:HB3  | 1:F:237:VAL:CG2  | 2.44                     | 0.47              |
| 1:G:122:GLY:O    | 1:G:123:SER:HB2  | 2.14                     | 0.47              |
| 1:H:9:GLU:HA     | 1:H:12:LYS:HD2   | 1.94                     | 0.47              |
| 1:M:1:MET:HE2    | 1:M:2:GLN:O      | 2.14                     | 0.47              |
| 1:M:257:VAL:O    | 1:M:258:LYS:HE3  | 2.14                     | 0.47              |
| 1:B:49:TYR:HD1   | 1:B:51:VAL:HG12  | 1.78                     | 0.47              |
| 1:N:143:LEU:C    | 1:N:240:LYS:HZ1  | 2.20                     | 0.47              |
| 1:A:1:MET:H3     | 1:A:268:ILE:HD12 | 1.78                     | 0.47              |
| 1:E:128:VAL:HG23 | 1:F:125:ASP:O    | 2.14                     | 0.47              |
| 1:L:314:LYS:HD2  | 4:L:3127:HOH:O   | 2.13                     | 0.47              |
| 1:N:128:VAL:CG1  | 1:N:129:THR:N    | 2.77                     | 0.47              |
| 1:B:216:VAL:HG13 | 4:B:3011:HOH:O   | 2.14                     | 0.47              |
| 1:F:31:SER:HB3   | 1:F:155:LEU:HD11 | 1.96                     | 0.47              |
| 1:F:78:GLN:HG2   | 1:F:79:THR:H     | 1.78                     | 0.47              |
| 1:A:260:PRO:HA   | 1:A:287:ASP:O    | 2.15                     | 0.47              |
| 1:B:165:GLN:C    | 1:B:165:GLN:CD   | 2.83                     | 0.47              |
| 1:E:6:LEU:HB2    | 1:E:11:LEU:CD2   | 2.45                     | 0.47              |
| 1:I:128:VAL:O    | 1:I:130:PRO:HD3  | 2.14                     | 0.47              |
| 1:L:40:ALA:O     | 1:L:41:GLU:C     | 2.56                     | 0.47              |
| 1:M:194:SER:OG   | 1:M:196:ILE:HD13 | 2.15                     | 0.47              |
| 1:A:106:ALA:HA   | 1:A:110:TYR:O    | 2.14                     | 0.47              |
| 1:G:55:LYS:HE3   | 1:G:77:ASP:OD1   | 2.14                     | 0.47              |
| 1:H:59:LEU:HD23  | 1:H:113:PHE:CD1  | 2.49                     | 0.47              |
| 1:I:40:ALA:O     | 1:I:41:GLU:C     | 2.56                     | 0.47              |
| 1:M:1:MET:HE2    | 1:M:2:GLN:H      | 1.78                     | 0.47              |
| 1:B:61:TYR:CE2   | 1:B:159:ARG:HG3  | 2.49                     | 0.47              |
| 1:C:6:LEU:HB2    | 1:C:11:LEU:CD2   | 2.45                     | 0.47              |
| 1:F:203:ASP:O    | 1:F:204:TYR:C    | 2.57                     | 0.47              |
| 1:G:106:ALA:HA   | 1:G:110:TYR:O    | 2.14                     | 0.47              |
| 1:G:229:PHE:CE1  | 1:G:238:GLU:HA   | 2.49                     | 0.47              |
| 1:I:68:LYS:NZ    | 4:I:2902:HOH:O   | 2.45                     | 0.47              |
| 1:A:1:MET:SD     | 1:A:270:LYS:HD3  | 2.55                     | 0.47              |
| 1:M:1:MET:HG3    | 1:M:2:GLN:H      | 1.77                     | 0.47              |
| 1:A:13:LYS:HE3   | 4:A:1904:HOH:O   | 2.14                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:139:THR:HG21 | 1:E:228:TYR:HB2  | 1.96                     | 0.46              |
| 1:I:3:LEU:HD21   | 1:I:294:ARG:NH2  | 2.30                     | 0.46              |
| 1:I:273:PRO:HA   | 1:I:274:PRO:HD3  | 1.87                     | 0.46              |
| 1:A:178:ILE:HD12 | 4:A:3099:HOH:O   | 2.16                     | 0.46              |
| 1:C:98:GLY:O     | 1:C:102:ILE:HG12 | 2.15                     | 0.46              |
| 1:G:318:LEU:H    | 1:G:318:LEU:CD1  | 2.29                     | 0.46              |
| 1:L:219:GLU:CD   | 1:L:270:LYS:HZ3  | 2.24                     | 0.46              |
| 1:A:3:LEU:HD22   | 1:A:3:LEU:N      | 2.22                     | 0.46              |
| 1:E:258:LYS:HA   | 1:E:258:LYS:NZ   | 2.30                     | 0.46              |
| 1:F:198:LYS:NZ   | 1:F:320:THR:HB   | 2.10                     | 0.46              |
| 1:H:145:LYS:HA   | 1:H:244:THR:HG23 | 1.98                     | 0.46              |
| 1:N:197:PRO:O    | 1:N:259:GLN:HG2  | 2.14                     | 0.46              |
| 1:N:289:ASP:OD2  | 1:N:291:LYS:HE2  | 2.16                     | 0.46              |
| 1:E:264:ALA:HB2  | 1:E:304:PHE:CE1  | 2.50                     | 0.46              |
| 1:G:128:VAL:HG12 | 1:G:129:THR:N    | 2.29                     | 0.46              |
| 1:H:60:THR:CG2   | 1:H:70:GLU:HG2   | 2.44                     | 0.46              |
| 1:D:258:LYS:HD2  | 4:D:2817:HOH:O   | 2.15                     | 0.46              |
| 1:D:264:ALA:HB2  | 1:D:304:PHE:CE1  | 2.50                     | 0.46              |
| 1:H:33:GLU:OE2   | 1:H:36:ARG:NH2   | 2.48                     | 0.46              |
| 1:M:149:TYR:HA   | 4:M:2599:HOH:O   | 2.15                     | 0.46              |
| 1:H:229:PHE:CE1  | 1:H:238:GLU:HA   | 2.50                     | 0.46              |
| 1:G:6:LEU:HB2    | 1:G:11:LEU:CD2   | 2.46                     | 0.46              |
| 1:B:139:THR:HG21 | 1:B:228:TYR:HB2  | 1.98                     | 0.46              |
| 1:D:2:GLN:O      | 1:D:3:LEU:C      | 2.59                     | 0.46              |
| 1:L:128:VAL:HG12 | 1:L:129:THR:N    | 2.30                     | 0.46              |
| 1:M:35:LEU:O     | 1:M:159:ARG:NH2  | 2.49                     | 0.46              |
| 1:N:14:TYR:OH    | 1:N:209:ASN:ND2  | 2.43                     | 0.46              |
| 1:A:196:ILE:HB   | 1:A:197:PRO:HD3  | 1.98                     | 0.46              |
| 1:N:86:VAL:HG21  | 1:N:161:LEU:HD23 | 1.98                     | 0.46              |
| 1:G:313:GLN:HG3  | 1:G:317:LEU:CD2  | 2.45                     | 0.46              |
| 1:I:81:PRO:HB2   | 1:I:171:ASP:HB2  | 1.98                     | 0.45              |
| 1:L:159:ARG:O    | 1:L:163:VAL:HG23 | 2.16                     | 0.45              |
| 1:H:161:LEU:HD11 | 1:H:190:ALA:HB1  | 1.96                     | 0.45              |
| 1:F:319:SER:O    | 1:F:320:THR:OXT  | 2.33                     | 0.45              |
| 1:L:196:ILE:N    | 1:L:197:PRO:HD2  | 2.31                     | 0.45              |
| 1:H:161:LEU:HD22 | 1:H:197:PRO:HG3  | 1.98                     | 0.45              |
| 1:L:8:LEU:O      | 1:L:12:LYS:HG3   | 2.16                     | 0.45              |
| 1:F:139:THR:HG21 | 1:F:228:TYR:CB   | 2.46                     | 0.45              |
| 1:H:135:LEU:HD23 | 1:N:136:GLY:HA2  | 1.96                     | 0.45              |
| 1:I:196:ILE:HB   | 1:I:197:PRO:HD3  | 1.97                     | 0.45              |
| 1:B:61:TYR:CD2   | 1:B:159:ARG:HG3  | 2.52                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:2:GLN:N      | 4:G:2046:HOH:O   | 2.48                     | 0.45              |
| 1:M:128:VAL:O    | 1:M:130:PRO:HD3  | 2.16                     | 0.45              |
| 1:B:199:VAL:HG11 | 1:B:315:HIS:CB   | 2.47                     | 0.45              |
| 1:D:122:GLY:O    | 1:D:123:SER:HB2  | 2.16                     | 0.45              |
| 1:F:258:LYS:HE3  | 1:F:258:LYS:N    | 2.31                     | 0.45              |
| 1:L:264:ALA:HB2  | 1:L:304:PHE:CD1  | 2.52                     | 0.45              |
| 1:N:212:ARG:HE   | 1:N:275:SER:CB   | 2.30                     | 0.45              |
| 1:B:45:GLU:HG2   | 4:B:781:HOH:O    | 2.18                     | 0.45              |
| 1:F:256:TRP:O    | 1:F:258:LYS:HE3  | 2.17                     | 0.45              |
| 1:L:133:HIS:HD2  | 1:L:134:ALA:O    | 2.00                     | 0.45              |
| 1:B:136:GLY:HA2  | 1:D:135:LEU:CD1  | 2.47                     | 0.44              |
| 1:E:135:LEU:HD11 | 1:F:135:LEU:HD22 | 1.99                     | 0.44              |
| 1:I:7:SER:OG     | 1:I:10:GLU:HG3   | 2.17                     | 0.44              |
| 1:A:41:GLU:HG2   | 4:A:2438:HOH:O   | 2.16                     | 0.44              |
| 1:D:265:ILE:HD13 | 1:D:277:VAL:HG21 | 1.98                     | 0.44              |
| 1:E:122:GLY:O    | 1:E:123:SER:HB2  | 2.18                     | 0.44              |
| 1:A:2:GLN:OE1    | 1:A:3:LEU:HD22   | 2.17                     | 0.44              |
| 1:D:43:THR:HB    | 4:D:2766:HOH:O   | 2.16                     | 0.44              |
| 1:D:314:LYS:HA   | 1:D:318:LEU:HD12 | 1.97                     | 0.44              |
| 1:E:273:PRO:HA   | 1:E:274:PRO:HD3  | 1.92                     | 0.44              |
| 1:N:60:THR:HA    | 1:N:69:ILE:O     | 2.18                     | 0.44              |
| 1:C:21:ARG:HG2   | 1:C:243:GLU:CD   | 2.42                     | 0.44              |
| 1:E:181:SER:HA   | 1:E:204:TYR:O    | 2.17                     | 0.44              |
| 1:G:229:PHE:CZ   | 1:G:238:GLU:HG3  | 2.53                     | 0.44              |
| 1:M:43:THR:HG23  | 4:M:2387:HOH:O   | 2.17                     | 0.44              |
| 1:B:203:ASP:O    | 1:B:204:TYR:C    | 2.60                     | 0.44              |
| 1:N:60:THR:HG22  | 1:N:70:GLU:HG2   | 2.00                     | 0.44              |
| 1:C:235:PRO:O    | 1:C:239:GLU:HG3  | 2.18                     | 0.44              |
| 1:H:17:LYS:HD3   | 1:H:17:LYS:N     | 2.33                     | 0.44              |
| 1:M:87:ARG:HG2   | 1:M:178:ILE:HG13 | 1.99                     | 0.44              |
| 1:N:139:THR:HG21 | 1:N:228:TYR:HB2  | 1.99                     | 0.44              |
| 1:F:243:GLU:CD   | 4:F:724:HOH:O    | 2.60                     | 0.44              |
| 1:H:23:ASP:CB    | 4:H:2945:HOH:O   | 2.55                     | 0.44              |
| 1:L:98:GLY:O     | 1:L:102:ILE:HG12 | 2.18                     | 0.44              |
| 1:N:130:PRO:HA   | 4:N:3010:HOH:O   | 2.18                     | 0.44              |
| 1:C:55:LYS:HE3   | 4:C:589:HOH:O    | 2.18                     | 0.44              |
| 1:C:135:LEU:C    | 1:C:135:LEU:HD23 | 2.42                     | 0.44              |
| 1:D:42:PRO:HD2   | 4:D:2954:HOH:O   | 2.18                     | 0.44              |
| 1:H:128:VAL:CG1  | 1:H:129:THR:N    | 2.81                     | 0.44              |
| 1:M:26:ASP:HB2   | 4:M:2877:HOH:O   | 2.17                     | 0.44              |
| 1:D:33:GLU:O     | 1:D:37:GLN:HG3   | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:118:ARG:HB3  | 1:F:125:ASP:HB2  | 2.00                     | 0.43              |
| 1:G:145:LYS:HD3  | 1:G:247:TYR:CZ   | 2.53                     | 0.43              |
| 1:M:195:ASP:OD2  | 1:M:195:ASP:N    | 2.45                     | 0.43              |
| 1:B:165:GLN:HG2  | 1:B:172:GLU:HB2  | 1.99                     | 0.43              |
| 1:D:2:GLN:OE1    | 1:D:3:LEU:HD22   | 2.18                     | 0.43              |
| 1:D:83:PRO:HG3   | 1:D:317:LEU:HD12 | 1.99                     | 0.43              |
| 1:H:209:ASN:ND2  | 1:H:212:ARG:HB3  | 2.32                     | 0.43              |
| 1:L:2:GLN:N      | 4:L:2621:HOH:O   | 2.50                     | 0.43              |
| 1:L:258:LYS:NZ   | 1:L:258:LYS:CB   | 2.81                     | 0.43              |
| 1:M:197:PRO:O    | 1:M:259:GLN:HG2  | 2.18                     | 0.43              |
| 1:B:174:ARG:HD2  | 1:B:316:LEU:O    | 2.18                     | 0.43              |
| 1:E:258:LYS:HE2  | 4:E:858:HOH:O    | 2.18                     | 0.43              |
| 1:L:270:LYS:NZ   | 1:L:270:LYS:HB2  | 2.33                     | 0.43              |
| 1:A:128:VAL:CG1  | 1:A:129:THR:N    | 2.81                     | 0.43              |
| 1:B:317:LEU:O    | 1:B:318:LEU:O    | 2.36                     | 0.43              |
| 1:F:129:THR:OG1  | 1:F:140:LYS:HE3  | 2.18                     | 0.43              |
| 1:G:199:VAL:HG11 | 1:G:315:HIS:HB2  | 2.00                     | 0.43              |
| 1:L:258:LYS:HB3  | 1:L:258:LYS:HZ2  | 1.82                     | 0.43              |
| 1:M:257:VAL:O    | 1:M:258:LYS:CE   | 2.65                     | 0.43              |
| 1:F:44:LEU:HD11  | 1:F:59:LEU:HD13  | 2.00                     | 0.43              |
| 1:G:3:LEU:HD22   | 1:G:3:LEU:N      | 2.33                     | 0.43              |
| 1:L:229:PHE:CE1  | 1:L:238:GLU:HA   | 2.54                     | 0.43              |
| 1:B:161:LEU:HD21 | 1:B:177:VAL:CG1  | 2.48                     | 0.43              |
| 1:D:2:GLN:N      | 4:D:2966:HOH:O   | 2.51                     | 0.43              |
| 1:F:289:ASP:OD2  | 1:F:291:LYS:NZ   | 2.50                     | 0.43              |
| 1:G:220:GLN:HB3  | 3:G:2274:GOL:C2  | 2.35                     | 0.43              |
| 1:I:88:PHE:HB3   | 1:I:186:LEU:HD12 | 2.00                     | 0.43              |
| 1:N:9:GLU:CG     | 1:N:10:GLU:N     | 2.82                     | 0.43              |
| 1:A:289:ASP:OD2  | 4:A:2829:HOH:O   | 2.22                     | 0.43              |
| 1:B:2:GLN:HG3    | 1:B:3:LEU:H      | 1.84                     | 0.43              |
| 1:B:128:VAL:HG12 | 1:B:129:THR:N    | 2.33                     | 0.43              |
| 1:D:44:LEU:HD21  | 1:D:59:LEU:HD13  | 2.00                     | 0.43              |
| 1:I:203:ASP:O    | 1:I:204:TYR:C    | 2.61                     | 0.43              |
| 1:L:144:SER:HB3  | 1:L:147:THR:OG1  | 2.18                     | 0.43              |
| 1:E:270:LYS:HD3  | 4:E:2634:HOH:O   | 2.19                     | 0.43              |
| 1:G:3:LEU:HD21   | 1:G:294:ARG:NE   | 2.33                     | 0.43              |
| 1:L:258:LYS:HZ3  | 1:L:258:LYS:CA   | 2.31                     | 0.43              |
| 1:M:44:LEU:HD11  | 1:M:57:TYR:HB2   | 1.99                     | 0.43              |
| 1:M:212:ARG:HE   | 1:M:275:SER:CB   | 2.32                     | 0.43              |
| 1:E:243:GLU:HG2  | 4:E:1172:HOH:O   | 2.18                     | 0.43              |
| 1:F:88:PHE:HB3   | 1:F:186:LEU:HD12 | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:236:LYS:HE2  | 4:F:1539:HOH:O   | 2.19                     | 0.43              |
| 1:G:218:LEU:C    | 1:G:219:GLU:HG2  | 2.44                     | 0.43              |
| 1:G:219:GLU:OE2  | 1:G:270:LYS:NZ   | 2.52                     | 0.43              |
| 1:I:42:PRO:HA    | 1:I:60:THR:O     | 2.19                     | 0.43              |
| 1:L:142:ILE:HD11 | 1:L:245:LEU:HG   | 2.01                     | 0.43              |
| 1:E:317:LEU:HD12 | 1:E:317:LEU:HA   | 1.88                     | 0.43              |
| 1:G:313:GLN:HE21 | 1:G:317:LEU:HD22 | 1.84                     | 0.43              |
| 1:H:3:LEU:HD21   | 1:H:294:ARG:NH2  | 2.34                     | 0.43              |
| 1:H:117:VAL:HG13 | 1:H:153:VAL:CG1  | 2.49                     | 0.43              |
| 1:H:309:LEU:O    | 1:H:313:GLN:HB2  | 2.19                     | 0.43              |
| 1:M:265:ILE:O    | 1:M:265:ILE:HG23 | 2.19                     | 0.43              |
| 1:F:134:ALA:O    | 1:F:135:LEU:C    | 2.63                     | 0.42              |
| 1:H:219:GLU:OE1  | 1:H:220:GLN:HG2  | 2.19                     | 0.42              |
| 1:G:6:LEU:HB2    | 1:G:11:LEU:HD23  | 2.00                     | 0.42              |
| 1:M:175:ILE:HD12 | 1:M:196:ILE:CG2  | 2.49                     | 0.42              |
| 1:C:104:ASN:O    | 1:C:108:HIS:HD2  | 2.02                     | 0.42              |
| 1:D:42:PRO:HA    | 1:D:60:THR:O     | 2.18                     | 0.42              |
| 1:E:68:LYS:HE3   | 4:E:918:HOH:O    | 2.19                     | 0.42              |
| 1:E:267:LEU:HA   | 1:E:267:LEU:HD23 | 1.77                     | 0.42              |
| 1:F:212:ARG:HG3  | 1:F:212:ARG:HH11 | 1.83                     | 0.42              |
| 1:F:212:ARG:CZ   | 1:F:216:VAL:HG21 | 2.49                     | 0.42              |
| 1:G:21:ARG:HG2   | 4:G:2808:HOH:O   | 2.19                     | 0.42              |
| 1:H:39:GLU:HG3   | 4:H:2923:HOH:O   | 2.20                     | 0.42              |
| 1:H:231:ARG:HG3  | 1:H:231:ARG:NH1  | 2.34                     | 0.42              |
| 1:B:106:ALA:HA   | 1:B:110:TYR:O    | 2.20                     | 0.42              |
| 1:B:225:ILE:HG22 | 1:B:229:PHE:CE2  | 2.55                     | 0.42              |
| 1:F:270:LYS:NZ   | 1:F:270:LYS:CB   | 2.82                     | 0.42              |
| 1:G:63:SER:O     | 1:G:64:PHE:C     | 2.63                     | 0.42              |
| 1:H:199:VAL:HG11 | 1:H:315:HIS:CG   | 2.54                     | 0.42              |
| 1:L:59:LEU:HD23  | 1:L:113:PHE:CE1  | 2.55                     | 0.42              |
| 1:M:291:LYS:NZ   | 4:M:1950:HOH:O   | 2.52                     | 0.42              |
| 1:C:52:LYS:HG3   | 4:C:2957:HOH:O   | 2.19                     | 0.42              |
| 1:C:196:ILE:N    | 1:C:197:PRO:HD2  | 2.35                     | 0.42              |
| 1:D:196:ILE:HB   | 1:D:197:PRO:HD3  | 2.01                     | 0.42              |
| 1:G:260:PRO:HA   | 1:G:287:ASP:O    | 2.20                     | 0.42              |
| 1:H:38:VAL:HG22  | 1:H:66:HIS:CE1   | 2.54                     | 0.42              |
| 1:M:60:THR:HA    | 1:M:69:ILE:O     | 2.20                     | 0.42              |
| 1:B:21:ARG:CG    | 4:B:2589:HOH:O   | 2.67                     | 0.42              |
| 1:D:15:LYS:NZ    | 1:D:282:ASN:O    | 2.49                     | 0.42              |
| 1:H:142:ILE:HG12 | 1:H:142:ILE:O    | 2.19                     | 0.42              |
| 1:B:273:PRO:HA   | 1:B:274:PRO:HD3  | 1.92                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:229:PHE:CE1  | 1:C:238:GLU:HA   | 2.54                     | 0.42              |
| 1:E:143:LEU:HD23 | 1:E:143:LEU:HA   | 1.86                     | 0.42              |
| 1:F:199:VAL:HG11 | 1:F:315:HIS:CG   | 2.55                     | 0.42              |
| 1:H:117:VAL:O    | 1:H:118:ARG:C    | 2.63                     | 0.42              |
| 1:H:118:ARG:HB3  | 1:H:125:ASP:HB2  | 2.02                     | 0.42              |
| 1:H:234:ASP:HB3  | 1:H:237:VAL:CG2  | 2.50                     | 0.42              |
| 1:L:198:LYS:HG2  | 1:L:199:VAL:HG13 | 2.01                     | 0.42              |
| 1:M:1:MET:SD     | 1:M:270:LYS:HG2  | 2.60                     | 0.42              |
| 1:F:128:VAL:HG12 | 1:F:129:THR:N    | 2.34                     | 0.42              |
| 1:G:24:PHE:CE1   | 1:G:247:TYR:HA   | 2.55                     | 0.42              |
| 1:H:259:GLN:O    | 1:H:260:PRO:C    | 2.62                     | 0.42              |
| 1:L:17:LYS:HE2   | 1:L:17:LYS:N     | 2.35                     | 0.42              |
| 1:L:118:ARG:HB3  | 1:L:125:ASP:HB2  | 2.01                     | 0.42              |
| 1:M:264:ALA:HB2  | 1:M:304:PHE:CD1  | 2.55                     | 0.42              |
| 1:B:122:GLY:O    | 1:B:123:SER:HB2  | 2.20                     | 0.41              |
| 1:B:268:ILE:O    | 1:B:270:LYS:HD2  | 2.20                     | 0.41              |
| 1:D:165:GLN:NE2  | 4:D:1945:HOH:O   | 2.52                     | 0.41              |
| 1:F:2:GLN:OE1    | 1:F:3:LEU:CD2    | 2.66                     | 0.41              |
| 1:H:159:ARG:NE   | 1:H:162:GLU:OE1  | 2.45                     | 0.41              |
| 1:M:8:LEU:O      | 1:M:12:LYS:HG3   | 2.19                     | 0.41              |
| 1:M:39:GLU:HB3   | 4:M:2348:HOH:O   | 2.20                     | 0.41              |
| 1:G:34:GLU:HG2   | 1:G:37:GLN:HE22  | 1.84                     | 0.41              |
| 1:H:145:LYS:H    | 1:H:145:LYS:HD3  | 1.84                     | 0.41              |
| 1:H:219:GLU:OE1  | 1:H:220:GLN:N    | 2.43                     | 0.41              |
| 1:M:196:ILE:N    | 1:M:197:PRO:CD   | 2.83                     | 0.41              |
| 1:N:142:ILE:O    | 1:N:142:ILE:HG12 | 2.20                     | 0.41              |
| 1:G:26:ASP:O     | 1:G:30:LYS:HG3   | 2.20                     | 0.41              |
| 1:G:273:PRO:HA   | 1:G:274:PRO:HD3  | 1.95                     | 0.41              |
| 1:A:139:THR:HG21 | 1:A:228:TYR:HB2  | 2.02                     | 0.41              |
| 1:B:177:VAL:HG23 | 1:B:200:VAL:HG22 | 2.01                     | 0.41              |
| 1:E:313:GLN:HA   | 1:E:317:LEU:HB2  | 2.03                     | 0.41              |
| 1:A:206:TYR:CZ   | 1:A:221:PRO:HG2  | 2.56                     | 0.41              |
| 1:C:36:ARG:HD3   | 4:C:2468:HOH:O   | 2.20                     | 0.41              |
| 1:C:106:ALA:HA   | 1:C:110:TYR:O    | 2.21                     | 0.41              |
| 1:E:40:ALA:O     | 1:E:41:GLU:C     | 2.62                     | 0.41              |
| 1:G:73:TYR:CZ    | 1:G:75:VAL:HG22  | 2.55                     | 0.41              |
| 1:H:139:THR:HG21 | 1:H:228:TYR:CB   | 2.49                     | 0.41              |
| 1:I:268:ILE:HG12 | 1:I:296:PHE:O    | 2.21                     | 0.41              |
| 1:M:1:MET:CG     | 1:M:2:GLN:N      | 2.81                     | 0.41              |
| 1:A:195:ASP:OD2  | 1:A:195:ASP:C    | 2.64                     | 0.41              |
| 1:C:21:ARG:CG    | 1:C:243:GLU:OE2  | 2.67                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:319:SER:O    | 1:F:320:THR:C    | 2.64                     | 0.41              |
| 1:I:23:ASP:OD2   | 1:I:145:LYS:NZ   | 2.54                     | 0.41              |
| 1:N:39:GLU:CD    | 4:N:2862:HOH:O   | 2.63                     | 0.41              |
| 1:F:256:TRP:O    | 1:F:258:LYS:CE   | 2.69                     | 0.41              |
| 1:H:167:PHE:HA   | 1:H:168:PRO:HD2  | 1.89                     | 0.41              |
| 1:L:60:THR:CG2   | 1:L:70:GLU:HG2   | 2.47                     | 0.41              |
| 1:M:41:GLU:N     | 1:M:42:PRO:CD    | 2.84                     | 0.41              |
| 1:N:185:ALA:HA   | 1:N:250:LEU:HD11 | 2.03                     | 0.41              |
| 1:A:203:ASP:OD1  | 1:A:203:ASP:N    | 2.53                     | 0.41              |
| 1:A:313:GLN:HG3  | 1:A:317:LEU:HD23 | 2.03                     | 0.41              |
| 1:E:203:ASP:O    | 1:E:204:TYR:C    | 2.62                     | 0.41              |
| 3:G:2274:GOL:H31 | 1:M:135:LEU:HD13 | 2.03                     | 0.41              |
| 1:H:128:VAL:HG12 | 1:H:129:THR:N    | 2.35                     | 0.41              |
| 1:I:3:LEU:HD22   | 1:I:3:LEU:N      | 2.36                     | 0.41              |
| 1:I:234:ASP:HB3  | 1:I:237:VAL:CG2  | 2.50                     | 0.41              |
| 1:L:177:VAL:HG23 | 1:L:187:ALA:HB1  | 2.01                     | 0.41              |
| 1:B:2:GLN:HG3    | 1:B:3:LEU:N      | 2.36                     | 0.41              |
| 1:D:197:PRO:O    | 1:D:259:GLN:HG2  | 2.20                     | 0.41              |
| 1:G:8:LEU:HG     | 1:G:12:LYS:HE2   | 2.03                     | 0.41              |
| 1:G:29:LYS:HE2   | 1:G:29:LYS:HB3   | 1.87                     | 0.41              |
| 1:H:40:ALA:O     | 1:H:41:GLU:C     | 2.64                     | 0.41              |
| 1:L:54:VAL:HG21  | 1:L:107:LEU:HD23 | 2.01                     | 0.41              |
| 1:L:260:PRO:HA   | 1:L:287:ASP:O    | 2.21                     | 0.41              |
| 1:M:231:ARG:HG3  | 1:M:231:ARG:NH1  | 2.36                     | 0.41              |
| 1:N:196:ILE:HB   | 1:N:197:PRO:HD3  | 2.03                     | 0.41              |
| 1:A:235:PRO:O    | 1:A:239:GLU:HG3  | 2.21                     | 0.40              |
| 1:C:313:GLN:HA   | 1:C:317:LEU:HB2  | 2.03                     | 0.40              |
| 1:D:77:ASP:O     | 1:D:77:ASP:OD1   | 2.39                     | 0.40              |
| 1:G:231:ARG:HG3  | 1:G:231:ARG:NH1  | 2.34                     | 0.40              |
| 1:I:44:LEU:HD13  | 1:I:59:LEU:HD13  | 2.02                     | 0.40              |
| 1:I:55:LYS:HE2   | 1:I:77:ASP:CA    | 2.36                     | 0.40              |
| 1:A:180:GLY:HA2  | 1:A:203:ASP:HB2  | 2.02                     | 0.40              |
| 1:D:15:LYS:NZ    | 1:D:283:HIS:HA   | 2.35                     | 0.40              |
| 1:D:138:MET:HB2  | 1:D:224:GLU:OE1  | 2.22                     | 0.40              |
| 1:F:143:LEU:HD23 | 1:F:143:LEU:HA   | 1.71                     | 0.40              |
| 1:G:196:ILE:N    | 1:G:197:PRO:CD   | 2.84                     | 0.40              |
| 1:N:145:LYS:HA   | 1:N:244:THR:HG23 | 2.03                     | 0.40              |
| 1:G:199:VAL:HG11 | 1:G:315:HIS:CB   | 2.51                     | 0.40              |
| 1:G:44:LEU:HD12  | 1:G:44:LEU:HA    | 1.97                     | 0.40              |
| 1:I:24:PHE:HZ    | 1:I:253:LEU:HD23 | 1.86                     | 0.40              |
| 1:A:2:GLN:OE1    | 1:A:2:GLN:HA     | 2.20                     | 0.40              |

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| Atom-1          | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|----------------|--------------------------|-------------------|
| 1:A:232:ASN:ND2 | 4:A:2033:HOH:O | 2.50                     | 0.40              |
| 1:D:234:ASP:O   | 1:D:237:VAL:HB | 2.22                     | 0.40              |
| 1:I:60:THR:HA   | 1:I:69:ILE:O   | 2.22                     | 0.40              |
| 1:I:65:GLY:O    | 1:I:66:HIS:HB2 | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 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     | 316/320 (99%)   | 303 (96%)  | 11 (4%)  | 2 (1%)   | 21          | 13  |
| 1   | B     | 315/320 (98%)   | 302 (96%)  | 11 (4%)  | 2 (1%)   | 21          | 13  |
| 1   | C     | 314/320 (98%)   | 298 (95%)  | 16 (5%)  | 0        | 100         | 100 |
| 1   | D     | 315/320 (98%)   | 296 (94%)  | 19 (6%)  | 0        | 100         | 100 |
| 1   | E     | 315/320 (98%)   | 303 (96%)  | 10 (3%)  | 2 (1%)   | 21          | 13  |
| 1   | F     | 317/320 (99%)   | 303 (96%)  | 13 (4%)  | 1 (0%)   | 36          | 29  |
| 1   | G     | 315/320 (98%)   | 298 (95%)  | 16 (5%)  | 1 (0%)   | 36          | 29  |
| 1   | H     | 315/320 (98%)   | 298 (95%)  | 15 (5%)  | 2 (1%)   | 21          | 13  |
| 1   | I     | 315/320 (98%)   | 303 (96%)  | 12 (4%)  | 0        | 100         | 100 |
| 1   | L     | 315/320 (98%)   | 299 (95%)  | 14 (4%)  | 2 (1%)   | 21          | 13  |
| 1   | M     | 316/320 (99%)   | 296 (94%)  | 19 (6%)  | 1 (0%)   | 36          | 29  |
| 1   | N     | 316/320 (99%)   | 297 (94%)  | 19 (6%)  | 0        | 100         | 100 |
| All | All   | 3784/3840 (98%) | 3596 (95%) | 175 (5%) | 13 (0%)  | 36          | 29  |

All (13) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 317 | LEU  |
| 1   | B     | 118 | ARG  |
| 1   | E     | 118 | ARG  |
| 1   | F     | 118 | ARG  |
| 1   | G     | 118 | ARG  |
| 1   | H     | 118 | ARG  |
| 1   | L     | 118 | ARG  |
| 1   | L     | 123 | SER  |
| 1   | A     | 118 | ARG  |
| 1   | H     | 255 | GLY  |
| 1   | A     | 123 | SER  |
| 1   | B     | 123 | SER  |
| 1   | E     | 123 | SER  |

### 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     | 268/270 (99%)   | 266 (99%)  | 2 (1%)   | 76          | 78 |
| 1   | B     | 267/270 (99%)   | 265 (99%)  | 2 (1%)   | 76          | 78 |
| 1   | C     | 266/270 (98%)   | 262 (98%)  | 4 (2%)   | 57          | 56 |
| 1   | D     | 267/270 (99%)   | 264 (99%)  | 3 (1%)   | 65          | 67 |
| 1   | E     | 267/270 (99%)   | 261 (98%)  | 6 (2%)   | 45          | 42 |
| 1   | F     | 269/270 (100%)  | 263 (98%)  | 6 (2%)   | 45          | 42 |
| 1   | G     | 267/270 (99%)   | 262 (98%)  | 5 (2%)   | 50          | 47 |
| 1   | H     | 267/270 (99%)   | 263 (98%)  | 4 (2%)   | 57          | 56 |
| 1   | I     | 267/270 (99%)   | 262 (98%)  | 5 (2%)   | 50          | 47 |
| 1   | L     | 267/270 (99%)   | 261 (98%)  | 6 (2%)   | 45          | 42 |
| 1   | M     | 268/270 (99%)   | 264 (98%)  | 4 (2%)   | 57          | 56 |
| 1   | N     | 268/270 (99%)   | 266 (99%)  | 2 (1%)   | 76          | 78 |
| All | All   | 3208/3240 (99%) | 3159 (98%) | 49 (2%)  | 57          | 56 |

All (49) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 67  | SER  |
| 1   | A     | 270 | LYS  |
| 1   | B     | 45  | GLU  |
| 1   | B     | 169 | GLU  |
| 1   | C     | 3   | LEU  |
| 1   | C     | 68  | LYS  |
| 1   | C     | 287 | ASP  |
| 1   | C     | 317 | LEU  |
| 1   | D     | 68  | LYS  |
| 1   | D     | 70  | GLU  |
| 1   | D     | 177 | VAL  |
| 1   | E     | 3   | LEU  |
| 1   | E     | 13  | LYS  |
| 1   | E     | 26  | ASP  |
| 1   | E     | 68  | LYS  |
| 1   | E     | 258 | LYS  |
| 1   | E     | 260 | PRO  |
| 1   | F     | 18  | LYS  |
| 1   | F     | 68  | LYS  |
| 1   | F     | 135 | LEU  |
| 1   | F     | 219 | GLU  |
| 1   | F     | 258 | LYS  |
| 1   | F     | 270 | LYS  |
| 1   | G     | 17  | LYS  |
| 1   | G     | 26  | ASP  |
| 1   | G     | 67  | SER  |
| 1   | G     | 270 | LYS  |
| 1   | G     | 285 | GLU  |
| 1   | H     | 60  | THR  |
| 1   | H     | 135 | LEU  |
| 1   | H     | 145 | LYS  |
| 1   | H     | 219 | GLU  |
| 1   | I     | 79  | THR  |
| 1   | I     | 135 | LEU  |
| 1   | I     | 203 | ASP  |
| 1   | I     | 219 | GLU  |
| 1   | I     | 270 | LYS  |
| 1   | L     | 3   | LEU  |
| 1   | L     | 30  | LYS  |
| 1   | L     | 165 | GLN  |
| 1   | L     | 203 | ASP  |
| 1   | L     | 258 | LYS  |
| 1   | L     | 285 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 3   | LEU  |
| 1   | M     | 52  | LYS  |
| 1   | M     | 60  | THR  |
| 1   | M     | 287 | ASP  |
| 1   | N     | 68  | LYS  |
| 1   | N     | 165 | GLN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 173 | HIS  |
| 1   | A     | 220 | GLN  |
| 1   | A     | 313 | GLN  |
| 1   | B     | 92  | ASN  |
| 1   | B     | 165 | GLN  |
| 1   | B     | 232 | ASN  |
| 1   | C     | 62  | GLN  |
| 1   | C     | 82  | HIS  |
| 1   | C     | 173 | HIS  |
| 1   | C     | 232 | ASN  |
| 1   | C     | 305 | GLN  |
| 1   | D     | 62  | GLN  |
| 1   | D     | 78  | GLN  |
| 1   | D     | 89  | HIS  |
| 1   | D     | 232 | ASN  |
| 1   | E     | 220 | GLN  |
| 1   | E     | 232 | ASN  |
| 1   | F     | 37  | GLN  |
| 1   | F     | 62  | GLN  |
| 1   | F     | 220 | GLN  |
| 1   | F     | 298 | HIS  |
| 1   | G     | 37  | GLN  |
| 1   | G     | 82  | HIS  |
| 1   | G     | 232 | ASN  |
| 1   | G     | 313 | GLN  |
| 1   | H     | 62  | GLN  |
| 1   | H     | 82  | HIS  |
| 1   | H     | 165 | GLN  |
| 1   | H     | 220 | GLN  |
| 1   | H     | 298 | HIS  |
| 1   | I     | 37  | GLN  |
| 1   | I     | 62  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 220 | GLN  |
| 1   | I     | 305 | GLN  |
| 1   | L     | 133 | HIS  |
| 1   | L     | 165 | GLN  |
| 1   | L     | 173 | HIS  |
| 1   | L     | 220 | GLN  |
| 1   | M     | 220 | GLN  |
| 1   | M     | 232 | ASN  |
| 1   | N     | 37  | GLN  |
| 1   | N     | 165 | GLN  |
| 1   | N     | 173 | HIS  |
| 1   | N     | 209 | ASN  |
| 1   | N     | 313 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 24 are monoatomic - leaving 2 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 3   | GOL  | E     | 2273 | -    | 5,5,5        | 0.34 | 0           | 5,5,5       | 0.20 | 0           |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | GOL  | G     | 2274 | -    | 5,5,5        | 0.32 | 0        | 5,5,5       | 0.14 | 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 |
|-----|------|-------|------|------|---------|----------|-------|
| 3   | GOL  | E     | 2273 | -    | -       | 0/4/4/4  | -     |
| 3   | GOL  | G     | 2274 | -    | -       | 0/4/4/4  | -     |

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.

2 monomers are involved in 9 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | E     | 2273 | GOL  | 1       | 0            |
| 3   | G     | 2274 | GOL  | 8       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2   | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|-----------|-----------------------|-------|
| 1   | A     | 318/320 (99%)   | -1.63  | 0 100 100 | 10, 16, 28, 45        | 0     |
| 1   | B     | 317/320 (99%)   | -1.62  | 0 100 100 | 11, 16, 27, 48        | 0     |
| 1   | C     | 316/320 (98%)   | -1.60  | 0 100 100 | 11, 17, 29, 36        | 0     |
| 1   | D     | 317/320 (99%)   | -1.58  | 0 100 100 | 9, 19, 30, 44         | 0     |
| 1   | E     | 317/320 (99%)   | -1.62  | 0 100 100 | 11, 17, 28, 41        | 0     |
| 1   | F     | 319/320 (99%)   | -1.58  | 0 100 100 | 11, 19, 31, 46        | 0     |
| 1   | G     | 317/320 (99%)   | -1.49  | 0 100 100 | 16, 24, 36, 51        | 0     |
| 1   | H     | 317/320 (99%)   | -1.48  | 0 100 100 | 15, 25, 40, 52        | 0     |
| 1   | I     | 317/320 (99%)   | -1.61  | 0 100 100 | 12, 19, 31, 43        | 0     |
| 1   | L     | 317/320 (99%)   | -1.56  | 0 100 100 | 12, 20, 32, 42        | 0     |
| 1   | M     | 318/320 (99%)   | -1.45  | 0 100 100 | 16, 25, 39, 49        | 0     |
| 1   | N     | 318/320 (99%)   | -1.57  | 0 100 100 | 13, 20, 33, 46        | 0     |
| All | All   | 3808/3840 (99%) | -1.57  | 0 100 100 | 9, 20, 33, 52         | 0     |

There are no RSRZ outliers to report.

### 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 oligosaccharides in this entry.

## 6.4 Ligands ⓘ

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 3   | GOL  | E     | 2273 | 6/6   | 0.98 | 0.06 | 41,42,43,44                | 0     |
| 2   | CL   | N     | 321  | 1/1   | 0.99 | 0.03 | 32,32,32,32                | 0     |
| 2   | CL   | M     | 322  | 1/1   | 0.99 | 0.05 | 33,33,33,33                | 0     |
| 3   | GOL  | G     | 2274 | 6/6   | 0.99 | 0.06 | 18,32,38,40                | 0     |
| 2   | CL   | C     | 321  | 1/1   | 1.00 | 0.02 | 27,27,27,27                | 0     |
| 2   | CL   | C     | 322  | 1/1   | 1.00 | 0.01 | 18,18,18,18                | 0     |
| 2   | CL   | D     | 321  | 1/1   | 1.00 | 0.03 | 20,20,20,20                | 0     |
| 2   | CL   | D     | 322  | 1/1   | 1.00 | 0.02 | 25,25,25,25                | 0     |
| 2   | CL   | E     | 321  | 1/1   | 1.00 | 0.02 | 33,33,33,33                | 0     |
| 2   | CL   | E     | 322  | 1/1   | 1.00 | 0.02 | 20,20,20,20                | 0     |
| 2   | CL   | F     | 321  | 1/1   | 1.00 | 0.01 | 23,23,23,23                | 0     |
| 2   | CL   | F     | 322  | 1/1   | 1.00 | 0.02 | 31,31,31,31                | 0     |
| 2   | CL   | G     | 321  | 1/1   | 1.00 | 0.02 | 29,29,29,29                | 0     |
| 2   | CL   | G     | 322  | 1/1   | 1.00 | 0.03 | 32,32,32,32                | 0     |
| 2   | CL   | H     | 321  | 1/1   | 1.00 | 0.03 | 34,34,34,34                | 0     |
| 2   | CL   | H     | 322  | 1/1   | 1.00 | 0.02 | 22,22,22,22                | 0     |
| 2   | CL   | I     | 321  | 1/1   | 1.00 | 0.01 | 19,19,19,19                | 0     |
| 2   | CL   | I     | 322  | 1/1   | 1.00 | 0.02 | 32,32,32,32                | 0     |
| 2   | CL   | L     | 321  | 1/1   | 1.00 | 0.02 | 25,25,25,25                | 0     |
| 2   | CL   | L     | 322  | 1/1   | 1.00 | 0.01 | 19,19,19,19                | 0     |
| 2   | CL   | M     | 321  | 1/1   | 1.00 | 0.02 | 22,22,22,22                | 0     |
| 2   | CL   | A     | 321  | 1/1   | 1.00 | 0.02 | 34,34,34,34                | 0     |
| 2   | CL   | A     | 322  | 1/1   | 1.00 | 0.02 | 20,20,20,20                | 0     |
| 2   | CL   | N     | 322  | 1/1   | 1.00 | 0.02 | 30,30,30,30                | 0     |
| 2   | CL   | B     | 321  | 1/1   | 1.00 | 0.02 | 18,18,18,18                | 0     |
| 2   | CL   | B     | 322  | 1/1   | 1.00 | 0.01 | 24,24,24,24                | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.