



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:23 am GMT

PDB ID : 1WYV  
Title : Crystal structure of glycine decarboxylase (P-protein) of the glycine cleavage system, in inhibitor-bound form  
Authors : Nakai, T.; Nakagawa, N.; Maoka, N.; Masui, R.; Kuramitsu, S.; Kamiya, N.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2005-02-17  
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

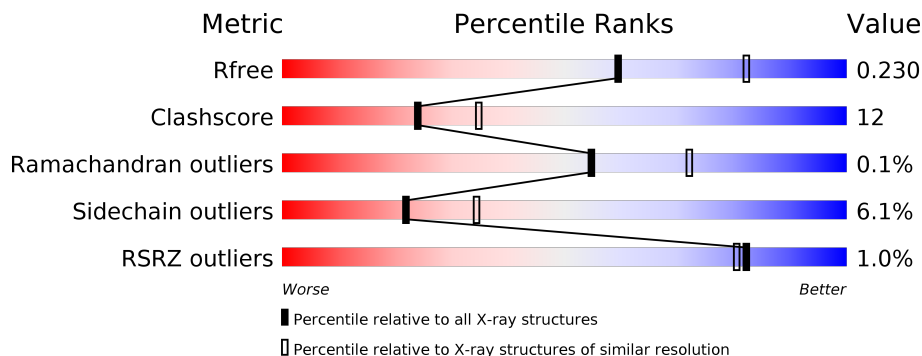
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 100719                      | 3166 (2.40-2.40)                                      |
| Clashscore            | 112137                      | 3674 (2.40-2.40)                                      |
| Ramachandran outliers | 110173                      | 3616 (2.40-2.40)                                      |
| Sidechain outliers    | 110143                      | 3617 (2.40-2.40)                                      |
| RSRZ outliers         | 101464                      | 3195 (2.40-2.40)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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     | 438    | <div> <div>77%</div> <div>19%</div> <div>.</div> </div>               |
| 1   | C     | 438    | <div> <div>77%</div> <div>20%</div> <div>.</div> </div>               |
| 1   | E     | 438    | <div> <div>77%</div> <div>20%</div> <div>.</div> </div>               |
| 1   | G     | 438    | <div> <div>79%</div> <div>18%</div> <div>.</div> </div>               |
| 2   | B     | 474    | <div> <div>%</div> <div>72%</div> <div>25%</div> <div>.</div> </div>  |
| 2   | D     | 474    | <div> <div>3%</div> <div>75%</div> <div>23%</div> <div>.</div> </div> |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 2   | F     | 474    | <div> <div>%</div> <div> <div></div> <div>74%</div> <div>23%</div> <div></div> </div> </div>  |
| 2   | H     | 474    | <div> <div>2%</div> <div> <div></div> <div>70%</div> <div>27%</div> <div></div> </div> </div> |

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   | AOA  | B     | 1476 | -         | -        | -       | X                |
| 3   | PLP  | D     | 2475 | -         | -        | -       | X                |
| 3   | AOA  | D     | 2476 | -         | -        | X       | X                |
| 3   | AOA  | F     | 3476 | -         | -        | X       | X                |
| 3   | AOA  | H     | 4476 | -         | -        | -       | X                |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29408 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.

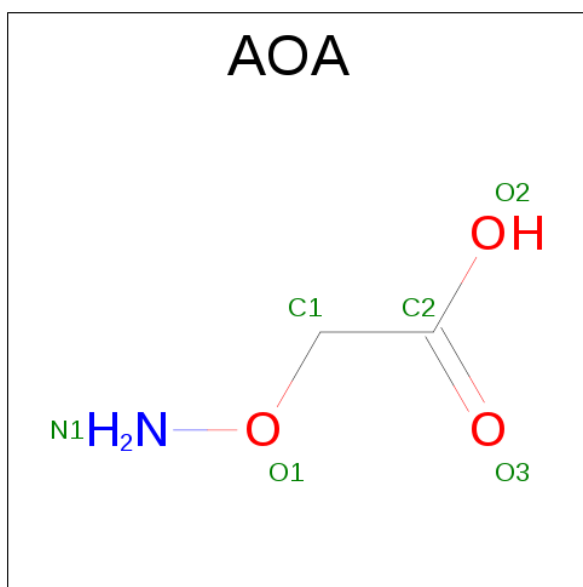
- Molecule 1 is a protein called glycine dehydrogenase (decarboxylating) subunit 1.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 437      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3320  | 2129 | 575 | 607 | 9 |         |         |       |
| 1   | C     | 437      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3320  | 2129 | 575 | 607 | 9 |         |         |       |
| 1   | E     | 437      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3320  | 2129 | 575 | 607 | 9 |         |         |       |
| 1   | G     | 437      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3320  | 2129 | 575 | 607 | 9 |         |         |       |

- Molecule 2 is a protein called glycine dehydrogenase subunit 2 (P-protein).

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 473      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3713  | 2380 | 655 | 666 | 12 |         |         |       |
| 2   | D     | 473      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3713  | 2380 | 655 | 666 | 12 |         |         |       |
| 2   | F     | 473      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3713  | 2380 | 655 | 666 | 12 |         |         |       |
| 2   | H     | 473      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3713  | 2380 | 655 | 666 | 12 |         |         |       |

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: AOA, PLP) (formula:  $C_2H_5NO_3$ ,  $C_8H_{10}NO_6P$ ).



| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 3   | B     | 2        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 21    | 10 | 2 | 8 | 1 |         |         |
| 3   | D     | 2        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 21    | 10 | 2 | 8 | 1 |         |         |
| 3   | F     | 2        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 21    | 10 | 2 | 8 | 1 |         |         |
| 3   | H     | 2        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 21    | 10 | 2 | 8 | 1 |         |         |

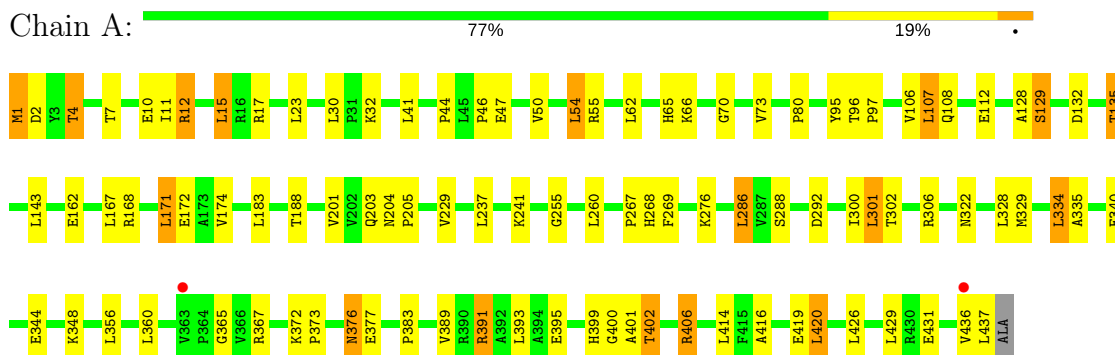
- Molecule 4 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 4   | A     | 162      | Total | O   | 0       | 0       |
|     |       |          | 162   | 162 |         |         |
| 4   | B     | 182      | Total | O   | 0       | 0       |
|     |       |          | 182   | 182 |         |         |
| 4   | C     | 145      | Total | O   | 0       | 0       |
|     |       |          | 145   | 145 |         |         |
| 4   | D     | 117      | Total | O   | 0       | 0       |
|     |       |          | 117   | 117 |         |         |
| 4   | E     | 152      | Total | O   | 0       | 0       |
|     |       |          | 152   | 152 |         |         |
| 4   | F     | 159      | Total | O   | 0       | 0       |
|     |       |          | 159   | 159 |         |         |
| 4   | G     | 150      | Total | O   | 0       | 0       |
|     |       |          | 150   | 150 |         |         |
| 4   | H     | 125      | Total | O   | 0       | 0       |
|     |       |          | 125   | 125 |         |         |

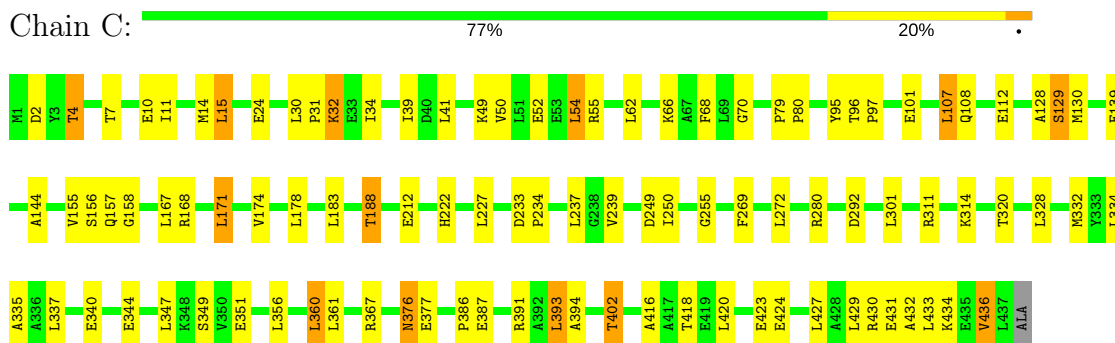
### 3 Residue-property plots

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

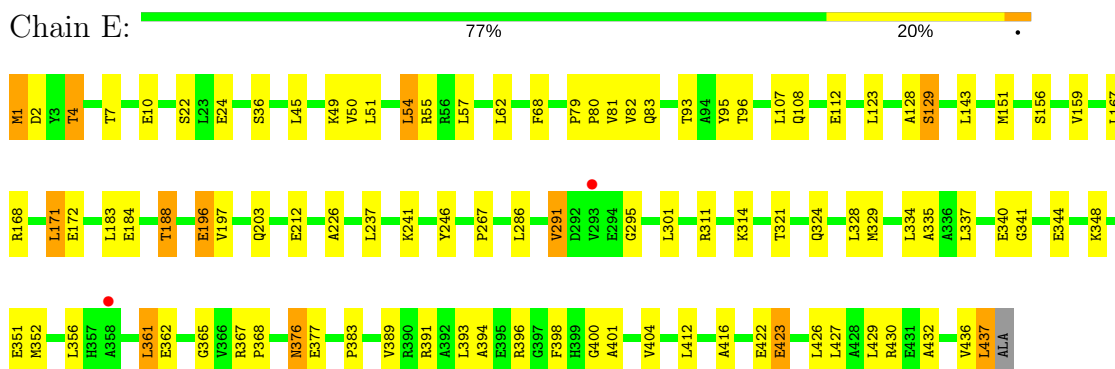
- Molecule 1: glycine dehydrogenase (decarboxylating) subunit 1



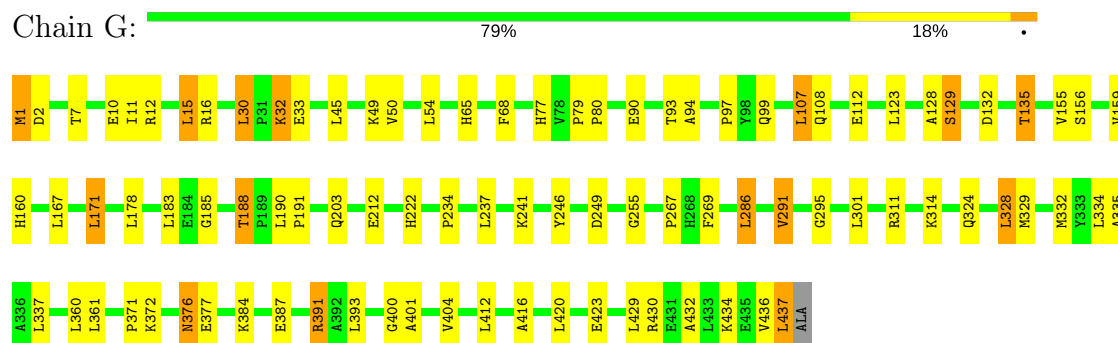
- Molecule 1: glycine dehydrogenase (decarboxylating) subunit 1



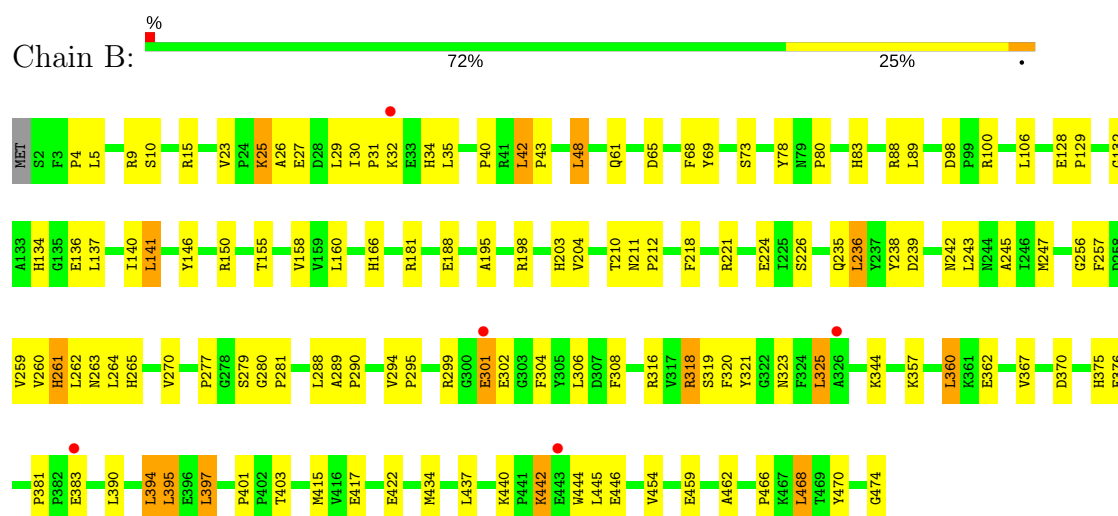
- Molecule 1: glycine dehydrogenase (decarboxylating) subunit 1



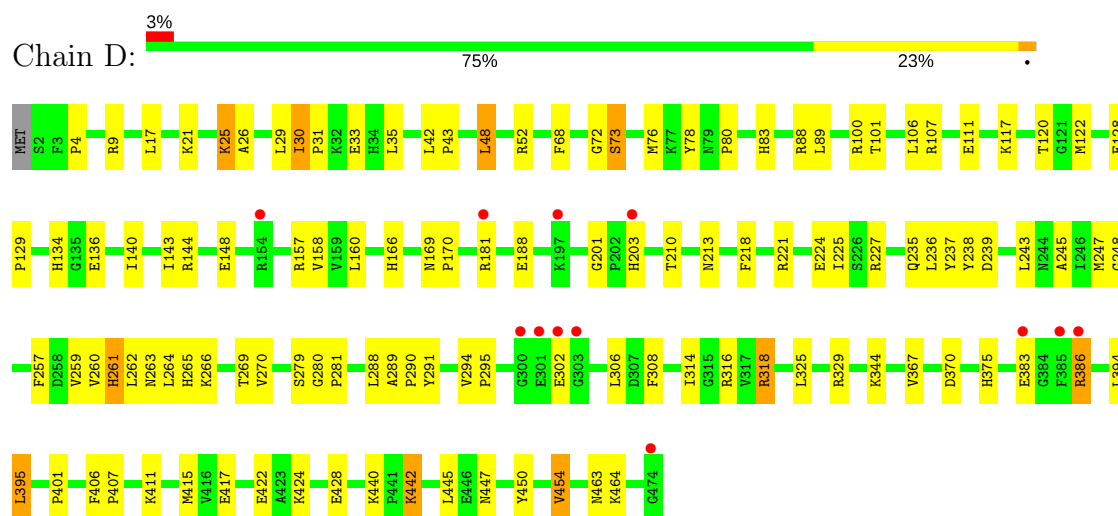
- Molecule 1: glycine dehydrogenase (decarboxylating) subunit 1



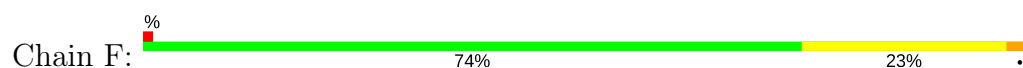
- Molecule 2: glycine dehydrogenase subunit 2 (P-protein)

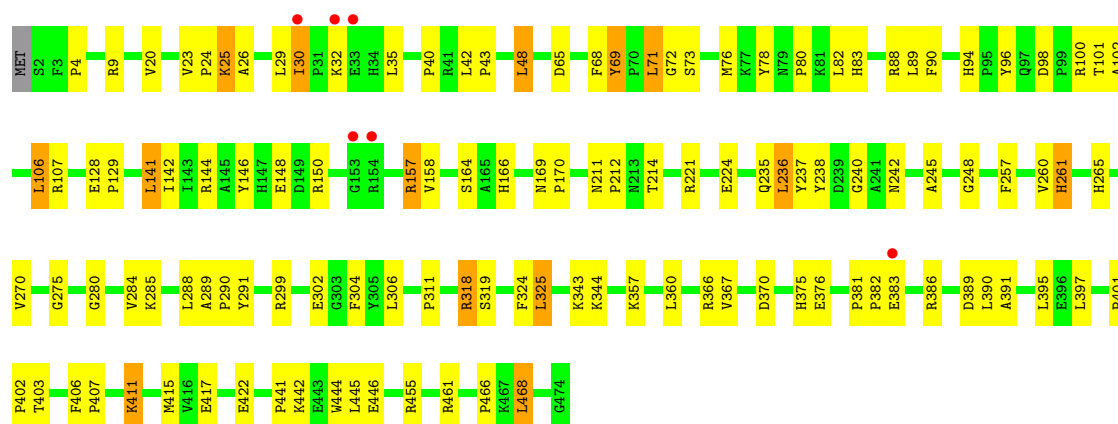


- Molecule 2: glycine dehydrogenase subunit 2 (P-protein)

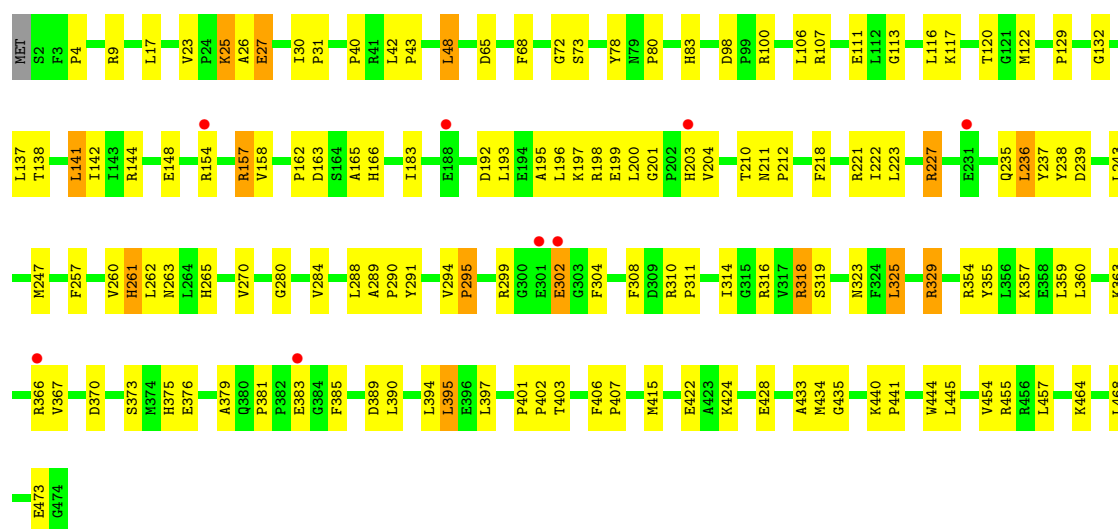


- Molecule 2: glycine dehydrogenase subunit 2 (P-protein)





• Molecule 2: glycine dehydrogenase subunit 2 (P-protein)





## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 134.17Å 166.32Å 190.30Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 47.90 – 2.40<br>47.90 – 2.40                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.7 (47.90-2.40)<br>99.5 (47.90-2.40)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.12  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.72 (at 2.39Å)   | Xtriage          |
| Refinement program  | CNS 1.1   | Depositor        |
| R, $R_{free}$   | 0.188 , 0.230<br>0.188 , 0.230                              | Depositor<br>DCC |
| $R_{free}$ test set   | 8336 reflections (5.03%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 34.6  | Xtriage          |
| Anisotropy  | 0.349   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.35 , 44.1   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.95  | EDS              |
| Total number of atoms   | 29408   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 35.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.91% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

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

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     | 0.35         | 0/3395  | 0.59        | 0/4617  |
| 1   | C     | 0.34         | 0/3395  | 0.59        | 0/4617  |
| 1   | E     | 0.34         | 0/3395  | 0.58        | 0/4617  |
| 1   | G     | 0.33         | 0/3395  | 0.59        | 0/4617  |
| 2   | B     | 0.36         | 0/3808  | 0.61        | 0/5162  |
| 2   | D     | 0.33         | 0/3808  | 0.60        | 0/5162  |
| 2   | F     | 0.35         | 0/3808  | 0.60        | 0/5162  |
| 2   | H     | 0.33         | 0/3808  | 0.60        | 0/5162  |
| All | All   | 0.34         | 0/28812 | 0.60        | 0/39116 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3320  | 0        | 3363     | 78      | 0            |
| 1   | C     | 3320  | 0        | 3363     | 88      | 0            |
| 1   | E     | 3320  | 0        | 3363     | 67      | 0            |
| 1   | G     | 3320  | 0        | 3363     | 74      | 0            |
| 2   | B     | 3713  | 0        | 3745     | 115     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | D     | 3713  | 0        | 3745     | 111     | 0            |
| 2   | F     | 3713  | 0        | 3745     | 110     | 0            |
| 2   | H     | 3713  | 0        | 3745     | 120     | 0            |
| 3   | B     | 21    | 0        | 10       | 3       | 0            |
| 3   | D     | 21    | 0        | 9        | 6       | 0            |
| 3   | F     | 21    | 0        | 9        | 4       | 0            |
| 3   | H     | 21    | 0        | 9        | 2       | 0            |
| 4   | A     | 162   | 0        | 0        | 0       | 0            |
| 4   | B     | 182   | 0        | 0        | 5       | 0            |
| 4   | C     | 145   | 0        | 0        | 6       | 0            |
| 4   | D     | 117   | 0        | 0        | 1       | 0            |
| 4   | E     | 152   | 0        | 0        | 4       | 0            |
| 4   | F     | 159   | 0        | 0        | 3       | 0            |
| 4   | G     | 150   | 0        | 0        | 4       | 0            |
| 4   | H     | 125   | 0        | 0        | 2       | 0            |
| All | All   | 29408 | 0        | 28469    | 707     | 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 12.

All (707) 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) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:30:ILE:HD11  | 2:F:35:LEU:HD21  | 1.49                     | 0.94              |
| 1:C:32:LYS:HD2   | 1:C:32:LYS:H     | 1.33                     | 0.93              |
| 1:C:70:GLY:H     | 1:C:402:THR:HG21 | 1.38                     | 0.89              |
| 2:D:386:ARG:HE   | 2:D:386:ARG:H    | 1.23                     | 0.86              |
| 2:D:386:ARG:NE   | 2:D:386:ARG:H    | 1.75                     | 0.85              |
| 2:F:265:HIS:HA   | 2:F:270:VAL:HB   | 1.57                     | 0.84              |
| 2:H:227:ARG:HH11 | 2:H:227:ARG:HB3  | 1.38                     | 0.84              |
| 2:H:265:HIS:HA   | 2:H:270:VAL:HB   | 1.58                     | 0.84              |
| 1:A:66:LYS:HG2   | 1:A:420:LEU:HD13 | 1.63                     | 0.81              |
| 1:E:335:ALA:HA   | 2:F:43:PRO:HG2   | 1.62                     | 0.81              |
| 2:D:210:THR:HG22 | 2:D:239:ASP:HB3  | 1.63                     | 0.81              |
| 1:G:32:LYS:H     | 1:G:32:LYS:HD3   | 1.45                     | 0.81              |
| 2:H:25:LYS:HE3   | 2:H:26:ALA:H     | 1.45                     | 0.81              |
| 2:F:366:ARG:NH1  | 2:F:382:PRO:HA   | 1.97                     | 0.79              |
| 2:F:72:GLY:HA3   | 2:F:415:MET:HG2  | 1.63                     | 0.79              |
| 2:B:25:LYS:HE3   | 2:B:26:ALA:H     | 1.46                     | 0.78              |
| 2:H:157:ARG:HA   | 2:H:157:ARG:HE   | 1.47                     | 0.78              |
| 1:G:12:ARG:NE    | 1:G:16:ARG:HH21  | 1.81                     | 0.78              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:D:265:HIS:HA   | 2:D:270:VAL:HB    | 1.66                     | 0.77              |
| 1:A:70:GLY:H     | 1:A:402:THR:HG21  | 1.50                     | 0.76              |
| 2:D:25:LYS:HE3   | 2:D:26:ALA:H      | 1.51                     | 0.76              |
| 2:B:357:LYS:NZ   | 2:B:370:ASP:HB2   | 2.01                     | 0.75              |
| 2:D:166:HIS:NE2  | 3:D:2476:AOA:H1C1 | 2.02                     | 0.75              |
| 2:F:4:PRO:HG2    | 2:F:9:ARG:NH2     | 2.02                     | 0.74              |
| 1:G:132:ASP:OD1  | 1:G:135:THR:HB    | 1.88                     | 0.74              |
| 1:C:32:LYS:HD2   | 1:C:32:LYS:N      | 2.03                     | 0.74              |
| 2:B:80:PRO:HG2   | 2:B:83:HIS:CE1    | 2.23                     | 0.74              |
| 2:B:444:TRP:HE3  | 2:B:445:LEU:HD12  | 1.52                     | 0.73              |
| 2:B:367:VAL:CG1  | 2:B:370:ASP:HB3   | 2.18                     | 0.73              |
| 2:F:26:ALA:HB1   | 2:F:35:LEU:HD21   | 1.71                     | 0.73              |
| 1:G:311:ARG:HG3  | 1:G:314:LYS:HB2   | 1.69                     | 0.73              |
| 1:G:97:PRO:HG2   | 1:G:301:LEU:HD21  | 1.69                     | 0.73              |
| 2:B:403:THR:HB   | 2:B:415:MET:HB3   | 1.70                     | 0.72              |
| 1:A:436:VAL:HG23 | 1:A:437:LEU:HD13  | 1.69                     | 0.72              |
| 1:E:83:GLN:HE22  | 1:E:329:MET:CE    | 2.03                     | 0.72              |
| 1:C:234:PRO:HA   | 1:C:237:LEU:HD23  | 1.71                     | 0.72              |
| 2:B:395:LEU:HD13 | 2:B:401:PRO:HD3   | 1.71                     | 0.72              |
| 1:G:377:GLU:HG2  | 1:G:416:ALA:HB2   | 1.72                     | 0.72              |
| 2:F:466:PRO:HB2  | 2:F:468:LEU:HD11  | 1.70                     | 0.71              |
| 1:G:188:THR:HG23 | 1:G:212:GLU:CD    | 2.11                     | 0.71              |
| 1:C:158:GLY:N    | 1:C:183:LEU:HD11  | 2.06                     | 0.71              |
| 1:E:432:ALA:O    | 1:E:436:VAL:HG13  | 1.91                     | 0.71              |
| 2:F:25:LYS:HE3   | 4:F:3599:HOH:O    | 1.89                     | 0.71              |
| 2:D:442:LYS:H    | 2:D:442:LYS:HD2   | 1.55                     | 0.71              |
| 2:B:294:VAL:CG2  | 2:B:308:PHE:HA    | 2.22                     | 0.70              |
| 2:F:284:VAL:HG13 | 2:F:288:LEU:HB2   | 1.72                     | 0.70              |
| 1:C:335:ALA:HA   | 2:D:43:PRO:HG2    | 1.74                     | 0.70              |
| 1:C:95:TYR:HB2   | 2:D:76:MET:CE     | 2.22                     | 0.69              |
| 1:G:107:LEU:HD11 | 1:G:301:LEU:HD22  | 1.72                     | 0.69              |
| 2:D:25:LYS:HE3   | 2:D:26:ALA:N      | 2.06                     | 0.69              |
| 1:E:2:ASP:OD2    | 1:E:4:THR:HB      | 1.92                     | 0.69              |
| 2:H:403:THR:HB   | 2:H:415:MET:HB3   | 1.74                     | 0.69              |
| 2:F:366:ARG:HH12 | 2:F:383:GLU:N     | 1.90                     | 0.68              |
| 1:G:32:LYS:H     | 1:G:32:LYS:CD     | 2.05                     | 0.68              |
| 2:H:454:VAL:HG11 | 2:H:457:LEU:HD21  | 1.76                     | 0.68              |
| 1:E:391:ARG:HG3  | 1:E:391:ARG:HH11  | 1.59                     | 0.68              |
| 2:B:265:HIS:HA   | 2:B:270:VAL:HB    | 1.75                     | 0.67              |
| 2:D:395:LEU:HD13 | 2:D:401:PRO:HD3   | 1.77                     | 0.67              |
| 2:F:144:ARG:O    | 2:F:148:GLU:HG3   | 1.95                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:284:VAL:CG2  | 2:H:288:LEU:HB2  | 2.24                     | 0.67              |
| 1:G:99:GLN:HG3   | 2:H:395:LEU:HD21 | 1.76                     | 0.67              |
| 2:F:367:VAL:CG1  | 2:F:370:ASP:HB3  | 2.24                     | 0.67              |
| 2:D:31:PRO:HB2   | 2:D:33:GLU:OE2   | 1.95                     | 0.66              |
| 1:E:376:ASN:H    | 1:E:376:ASN:HD22 | 1.42                     | 0.66              |
| 1:G:335:ALA:HA   | 2:H:43:PRO:HG2   | 1.76                     | 0.66              |
| 1:C:188:THR:HG23 | 1:C:212:GLU:CD   | 2.15                     | 0.66              |
| 2:D:294:VAL:CG2  | 2:D:308:PHE:HA   | 2.25                     | 0.66              |
| 2:H:294:VAL:CG2  | 2:H:308:PHE:HA   | 2.25                     | 0.66              |
| 2:D:221:ARG:NH2  | 2:D:224:GLU:HG3  | 2.12                     | 0.65              |
| 2:D:166:HIS:NE2  | 3:D:2476:AOA:N1  | 2.45                     | 0.65              |
| 2:D:367:VAL:CG1  | 2:D:370:ASP:HB3  | 2.26                     | 0.65              |
| 1:E:156:SER:OG   | 1:E:188:THR:HG21 | 1.96                     | 0.65              |
| 1:E:4:THR:HG21   | 2:F:344:LYS:HE2  | 1.78                     | 0.65              |
| 1:G:436:VAL:HG23 | 1:G:437:LEU:HD13 | 1.78                     | 0.65              |
| 2:H:25:LYS:HE3   | 2:H:26:ALA:N     | 2.11                     | 0.65              |
| 1:A:4:THR:HG21   | 2:B:344:LYS:HE2  | 1.78                     | 0.65              |
| 2:F:466:PRO:HB2  | 2:F:468:LEU:CD1  | 2.27                     | 0.65              |
| 1:C:156:SER:OG   | 1:C:188:THR:HG21 | 1.97                     | 0.65              |
| 1:E:83:GLN:HE22  | 1:E:329:MET:HE1  | 1.60                     | 0.65              |
| 2:B:158:VAL:HG13 | 2:B:204:VAL:HA   | 1.78                     | 0.64              |
| 2:H:238:TYR:HD2  | 2:H:260:VAL:HG13 | 1.61                     | 0.64              |
| 2:D:238:TYR:HD2  | 2:D:260:VAL:HG13 | 1.60                     | 0.64              |
| 2:D:72:GLY:HA2   | 2:D:417:GLU:HB2  | 1.78                     | 0.64              |
| 1:G:12:ARG:HE    | 1:G:16:ARG:HH21  | 1.43                     | 0.64              |
| 2:B:375:HIS:CE1  | 2:B:376:GLU:HG2  | 2.33                     | 0.64              |
| 2:B:442:LYS:HD2  | 2:B:442:LYS:H    | 1.61                     | 0.64              |
| 2:D:302:GLU:CD   | 2:D:302:GLU:H    | 2.01                     | 0.64              |
| 2:B:78:TYR:HB2   | 2:D:48:LEU:HG    | 1.79                     | 0.64              |
| 1:A:128:ALA:O    | 1:A:129:SER:HB3  | 1.96                     | 0.64              |
| 2:D:4:PRO:HG2    | 2:D:9:ARG:CZ     | 2.28                     | 0.64              |
| 1:A:12:ARG:HG2   | 1:A:12:ARG:HH11  | 1.63                     | 0.64              |
| 2:D:106:LEU:HD11 | 2:D:306:LEU:HD21 | 1.80                     | 0.63              |
| 1:E:340:GLU:O    | 1:E:344:GLU:HG3  | 1.98                     | 0.63              |
| 1:C:66:LYS:HG2   | 1:C:420:LEU:HD13 | 1.81                     | 0.63              |
| 2:F:318:ARG:HD3  | 2:F:319:SER:O    | 1.97                     | 0.63              |
| 1:C:391:ARG:HG3  | 1:C:391:ARG:HH11 | 1.62                     | 0.63              |
| 2:D:144:ARG:O    | 2:D:148:GLU:HG3  | 1.98                     | 0.63              |
| 1:C:432:ALA:O    | 1:C:436:VAL:HG12 | 1.99                     | 0.63              |
| 2:F:236:LEU:HD22 | 2:F:257:PHE:CE1  | 2.34                     | 0.63              |
| 1:A:2:ASP:OD2    | 1:A:4:THR:HB     | 1.99                     | 0.62              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:68:PHE:CE1   | 2:B:422:GLU:HG3   | 2.33                     | 0.62              |
| 1:C:95:TYR:HB2   | 2:D:76:MET:HE1    | 1.81                     | 0.62              |
| 2:B:137:LEU:O    | 2:B:141:LEU:HD22  | 1.99                     | 0.62              |
| 1:C:387:GLU:HG3  | 4:C:577:HOH:O     | 1.98                     | 0.62              |
| 2:H:238:TYR:HB3  | 2:H:260:VAL:HG22  | 1.80                     | 0.62              |
| 2:D:188:GLU:HB2  | 4:D:2565:HOH:O    | 2.00                     | 0.62              |
| 2:H:367:VAL:CG1  | 2:H:370:ASP:HB3   | 2.28                     | 0.62              |
| 1:C:233:ASP:O    | 1:C:237:LEU:HD22  | 2.00                     | 0.62              |
| 2:D:120:THR:HG23 | 2:D:122:MET:HG2   | 1.80                     | 0.62              |
| 2:D:129:PRO:HG2  | 2:D:280:GLY:O     | 2.00                     | 0.62              |
| 1:E:68:PHE:CD2   | 1:E:429:LEU:HD22  | 2.36                     | 0.61              |
| 2:H:193:LEU:O    | 2:H:197:LYS:HG3   | 2.00                     | 0.61              |
| 2:B:30:ILE:HB    | 2:B:35:LEU:HD21   | 1.82                     | 0.61              |
| 1:A:1:MET:HG3    | 1:A:46:PRO:HA     | 1.82                     | 0.61              |
| 2:B:88:ARG:HD3   | 4:B:1580:HOH:O    | 1.99                     | 0.61              |
| 2:B:316:ARG:HG2  | 2:B:316:ARG:HH11  | 1.65                     | 0.61              |
| 1:C:144:ALA:HA   | 1:C:227:LEU:HD12  | 1.83                     | 0.61              |
| 1:A:32:LYS:HD3   | 1:A:32:LYS:H      | 1.66                     | 0.61              |
| 1:A:32:LYS:H     | 1:A:32:LYS:CD     | 2.13                     | 0.60              |
| 1:C:49:LYS:HE3   | 1:C:52:GLU:OE1    | 1.99                     | 0.60              |
| 1:E:128:ALA:O    | 1:E:129:SER:HB3   | 2.00                     | 0.60              |
| 2:F:80:PRO:HG2   | 2:F:83:HIS:CE1    | 2.36                     | 0.60              |
| 1:E:188:THR:HG23 | 1:E:212:GLU:CD    | 2.21                     | 0.60              |
| 1:C:4:THR:HG21   | 2:D:344:LYS:HE2   | 1.84                     | 0.60              |
| 2:F:383:GLU:CD   | 2:F:383:GLU:H     | 2.04                     | 0.60              |
| 2:H:284:VAL:HG22 | 2:H:288:LEU:HB2   | 1.83                     | 0.60              |
| 2:H:80:PRO:HG2   | 2:H:83:HIS:CE1    | 2.37                     | 0.60              |
| 2:B:25:LYS:HG3   | 2:B:27:GLU:HG2    | 1.84                     | 0.60              |
| 2:B:166:HIS:CD2  | 3:B:1476:AOA:H1N1 | 2.20                     | 0.59              |
| 1:E:324:GLN:HE21 | 1:E:328:LEU:HD13  | 1.67                     | 0.59              |
| 1:G:77:HIS:HB2   | 1:G:420:LEU:HD21  | 1.83                     | 0.59              |
| 1:G:97:PRO:HB2   | 1:G:107:LEU:HD22  | 1.84                     | 0.59              |
| 1:C:130:MET:HE3  | 1:C:139:GLU:HB2   | 1.84                     | 0.59              |
| 2:D:411:LYS:NZ   | 2:D:411:LYS:HB3   | 2.17                     | 0.59              |
| 2:D:80:PRO:HG2   | 2:D:83:HIS:CE1    | 2.36                     | 0.59              |
| 2:F:411:LYS:HB2  | 2:F:411:LYS:NZ    | 2.17                     | 0.59              |
| 2:H:83:HIS:HB3   | 2:H:329:ARG:HD2   | 1.83                     | 0.59              |
| 1:C:320:THR:CG2  | 3:D:2476:AOA:H1C2 | 2.33                     | 0.59              |
| 1:G:50:VAL:O     | 1:G:54:LEU:HD23   | 2.03                     | 0.59              |
| 2:B:210:THR:HG22 | 2:B:239:ASP:HB3   | 1.84                     | 0.59              |
| 2:F:68:PHE:CE1   | 2:F:422:GLU:HG3   | 2.37                     | 0.59              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:F:78:TYR:HB2   | 2:H:48:LEU:HG     | 1.85                     | 0.59              |
| 2:B:442:LYS:HD2  | 2:B:442:LYS:N     | 2.17                     | 0.59              |
| 2:B:31:PRO:HG2   | 2:B:34:HIS:HD2    | 1.67                     | 0.59              |
| 2:H:107:ARG:O    | 2:H:111:GLU:HG3   | 2.02                     | 0.59              |
| 2:H:72:GLY:O     | 2:H:73:SER:HB2    | 2.03                     | 0.59              |
| 2:F:4:PRO:HG2    | 2:F:9:ARG:CZ      | 2.32                     | 0.59              |
| 2:B:129:PRO:HG2  | 2:B:280:GLY:O     | 2.02                     | 0.59              |
| 2:H:154:ARG:HG3  | 2:H:154:ARG:HH11  | 1.68                     | 0.59              |
| 2:F:26:ALA:O     | 2:F:30:ILE:HD13   | 2.03                     | 0.58              |
| 2:B:40:PRO:HG2   | 2:B:42:LEU:HD22   | 1.85                     | 0.58              |
| 1:E:376:ASN:H    | 1:E:376:ASN:ND2   | 2.00                     | 0.58              |
| 2:B:370:ASP:HA   | 4:B:1554:HOH:O    | 2.02                     | 0.58              |
| 2:B:442:LYS:O    | 2:B:446:GLU:HG3   | 2.03                     | 0.58              |
| 2:D:30:ILE:HD11  | 2:D:35:LEU:HD21   | 1.86                     | 0.58              |
| 1:A:32:LYS:N     | 1:A:32:LYS:HD3    | 2.19                     | 0.58              |
| 2:D:442:LYS:N    | 2:D:442:LYS:HD2   | 2.18                     | 0.58              |
| 2:B:158:VAL:HG12 | 2:B:203:HIS:O     | 2.04                     | 0.58              |
| 2:H:211:ASN:HA   | 2:H:212:PRO:C     | 2.24                     | 0.58              |
| 2:H:236:LEU:HD22 | 2:H:257:PHE:CE1   | 2.38                     | 0.58              |
| 2:D:83:HIS:HB3   | 2:D:329:ARG:HD2   | 1.85                     | 0.58              |
| 1:A:132:ASP:OD1  | 1:A:135:THR:HB    | 2.04                     | 0.57              |
| 1:A:286:LEU:HB2  | 1:A:306:ARG:NH2   | 2.20                     | 0.57              |
| 1:A:70:GLY:H     | 1:A:402:THR:CG2   | 2.16                     | 0.57              |
| 2:D:291:TYR:O    | 2:D:314:ILE:HG23  | 2.05                     | 0.57              |
| 2:H:210:THR:HG22 | 2:H:239:ASP:HB3   | 1.86                     | 0.57              |
| 2:B:442:LYS:H    | 2:B:442:LYS:CD    | 2.16                     | 0.57              |
| 1:G:33:GLU:H     | 1:G:33:GLU:CD     | 2.06                     | 0.57              |
| 2:H:318:ARG:HD3  | 2:H:319:SER:O     | 2.04                     | 0.57              |
| 2:F:455:ARG:HB3  | 4:F:3565:HOH:O    | 2.03                     | 0.57              |
| 2:B:221:ARG:NH2  | 2:B:224:GLU:HG3   | 2.20                     | 0.57              |
| 2:B:4:PRO:HG2    | 2:B:9:ARG:NH2     | 2.19                     | 0.57              |
| 1:E:351:GLU:OE1  | 2:F:24:PRO:HB3    | 2.05                     | 0.57              |
| 1:G:45:LEU:HD22  | 1:G:49:LYS:HG2    | 1.87                     | 0.57              |
| 2:H:243:LEU:CD1  | 2:H:247:MET:HG2   | 2.34                     | 0.57              |
| 1:E:168:ARG:O    | 1:E:172:GLU:HG3   | 2.05                     | 0.57              |
| 1:C:68:PHE:CD2   | 1:C:429:LEU:HD22  | 2.40                     | 0.56              |
| 2:B:166:HIS:NE2  | 3:B:1476:AOA:H1C2 | 2.20                     | 0.56              |
| 1:C:402:THR:HG22 | 4:C:565:HOH:O     | 2.04                     | 0.56              |
| 2:B:32:LYS:HA    | 2:B:32:LYS:HE3    | 1.86                     | 0.56              |
| 2:D:442:LYS:CD   | 2:D:442:LYS:H     | 2.14                     | 0.56              |
| 1:G:128:ALA:O    | 1:G:129:SER:HB3   | 2.05                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:108:GLN:O    | 1:A:112:GLU:HG3  | 2.05                     | 0.56              |
| 2:H:129:PRO:HG2  | 2:H:280:GLY:O    | 2.05                     | 0.56              |
| 2:B:68:PHE:HE1   | 2:B:422:GLU:HG3  | 1.69                     | 0.56              |
| 1:C:377:GLU:HG2  | 1:C:416:ALA:HB2  | 1.87                     | 0.56              |
| 2:D:424:LYS:O    | 2:D:428:GLU:HG3  | 2.04                     | 0.56              |
| 1:C:391:ARG:NH1  | 2:D:100:ARG:HD2  | 2.20                     | 0.56              |
| 1:A:372:LYS:N    | 1:A:372:LYS:HD2  | 2.21                     | 0.56              |
| 2:B:243:LEU:HD13 | 2:B:247:MET:HB3  | 1.86                     | 0.56              |
| 2:H:262:LEU:O    | 2:H:280:GLY:HA2  | 2.05                     | 0.56              |
| 2:D:4:PRO:HG2    | 2:D:9:ARG:NH2    | 2.20                     | 0.56              |
| 2:F:166:HIS:NE2  | 3:F:3476:AOA:C1  | 2.69                     | 0.56              |
| 2:B:25:LYS:HE3   | 2:B:26:ALA:N     | 2.16                     | 0.56              |
| 2:D:117:LYS:HA   | 2:D:120:THR:HG22 | 1.88                     | 0.56              |
| 2:B:367:VAL:HG11 | 2:B:370:ASP:HB3  | 1.88                     | 0.56              |
| 1:E:128:ALA:O    | 1:E:129:SER:CB   | 2.53                     | 0.55              |
| 1:E:365:GLY:H    | 1:E:367:ARG:NH1  | 2.04                     | 0.55              |
| 1:A:335:ALA:HA   | 2:B:43:PRO:HG2   | 1.89                     | 0.55              |
| 1:C:301:LEU:HD22 | 1:C:301:LEU:N    | 2.21                     | 0.55              |
| 2:H:375:HIS:CE1  | 2:H:376:GLU:HG2  | 2.41                     | 0.55              |
| 2:B:238:TYR:HB3  | 2:B:260:VAL:HG22 | 1.86                     | 0.55              |
| 1:A:128:ALA:O    | 1:A:129:SER:CB   | 2.54                     | 0.55              |
| 2:H:237:TYR:OH   | 2:H:261:HIS:HB3  | 2.06                     | 0.55              |
| 1:C:130:MET:CE   | 1:C:139:GLU:HB2  | 2.36                     | 0.55              |
| 1:A:62:LEU:HD22  | 1:A:399:HIS:NE2  | 2.22                     | 0.55              |
| 2:F:284:VAL:CG1  | 2:F:288:LEU:HB2  | 2.37                     | 0.54              |
| 2:H:116:LEU:O    | 2:H:120:THR:HG22 | 2.07                     | 0.54              |
| 1:E:7:THR:OG1    | 1:E:10:GLU:HG3   | 2.08                     | 0.54              |
| 2:B:383:GLU:H    | 2:B:383:GLU:CD   | 2.10                     | 0.54              |
| 1:A:7:THR:OG1    | 1:A:10:GLU:HG3   | 2.08                     | 0.54              |
| 1:A:167:LEU:HG   | 1:A:171:LEU:HD22 | 1.89                     | 0.54              |
| 2:F:248:GLY:HA3  | 2:F:343:LYS:HG2  | 1.89                     | 0.54              |
| 1:C:222:HIS:HE1  | 1:C:249:ASP:OD2  | 1.89                     | 0.54              |
| 2:H:289:ALA:N    | 2:H:290:PRO:HD2  | 2.23                     | 0.54              |
| 1:C:128:ALA:O    | 1:C:129:SER:CB   | 2.54                     | 0.54              |
| 1:G:156:SER:OG   | 1:G:188:THR:HG21 | 2.08                     | 0.54              |
| 2:B:146:TYR:O    | 2:B:150:ARG:HG3  | 2.06                     | 0.54              |
| 2:D:107:ARG:NH1  | 2:D:111:GLU:OE2  | 2.41                     | 0.54              |
| 1:E:376:ASN:N    | 1:E:376:ASN:HD22 | 2.01                     | 0.54              |
| 2:D:210:THR:OG1  | 2:D:213:ASN:HA   | 2.08                     | 0.54              |
| 2:F:30:ILE:HD13  | 2:F:30:ILE:H     | 1.71                     | 0.54              |
| 2:H:395:LEU:HD13 | 2:H:401:PRO:HD3  | 1.90                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:F:26:ALA:HB1   | 2:F:30:ILE:HD11   | 1.90                     | 0.53              |
| 2:H:265:HIS:CA   | 2:H:270:VAL:HB    | 2.35                     | 0.53              |
| 2:H:40:PRO:HB2   | 2:H:42:LEU:HD13   | 1.89                     | 0.53              |
| 2:B:134:HIS:HE1  | 2:B:318:ARG:HB3   | 1.72                     | 0.53              |
| 2:H:120:THR:HG23 | 2:H:122:MET:H     | 1.72                     | 0.53              |
| 2:H:235:GLN:HE21 | 2:H:288:LEU:HD11  | 1.74                     | 0.53              |
| 2:B:318:ARG:HD3  | 2:B:319:SER:O     | 2.07                     | 0.53              |
| 1:C:50:VAL:O     | 1:C:54:LEU:HD22   | 2.08                     | 0.53              |
| 2:H:302:GLU:OE1  | 2:H:302:GLU:N     | 2.36                     | 0.53              |
| 2:F:25:LYS:HE2   | 2:F:26:ALA:H      | 1.73                     | 0.53              |
| 1:A:276:LYS:HD3  | 2:B:474:GLY:O     | 2.08                     | 0.53              |
| 2:B:444:TRP:CE3  | 2:B:445:LEU:HD12  | 2.40                     | 0.53              |
| 1:G:328:LEU:O    | 1:G:332:MET:HG3   | 2.09                     | 0.53              |
| 2:B:357:LYS:CE   | 2:B:370:ASP:HB2   | 2.39                     | 0.53              |
| 2:B:357:LYS:HZ3  | 2:B:370:ASP:HB2   | 1.73                     | 0.53              |
| 2:F:32:LYS:HD3   | 2:F:32:LYS:O      | 2.08                     | 0.53              |
| 1:C:167:LEU:HG   | 1:C:171:LEU:HD22  | 1.91                     | 0.52              |
| 4:E:586:HOH:O    | 2:F:461:ARG:HD3   | 2.09                     | 0.52              |
| 1:E:356:LEU:HD13 | 1:E:426:LEU:HD22  | 1.91                     | 0.52              |
| 2:H:198:ARG:NH1  | 2:H:198:ARG:HB2   | 2.25                     | 0.52              |
| 2:F:129:PRO:HG2  | 2:F:280:GLY:O     | 2.09                     | 0.52              |
| 2:H:454:VAL:CG1  | 2:H:457:LEU:HD21  | 2.39                     | 0.52              |
| 1:E:51:LEU:HG    | 2:F:82:LEU:HD11   | 1.91                     | 0.52              |
| 2:B:294:VAL:CG2  | 2:B:295:PRO:HA    | 2.39                     | 0.52              |
| 2:B:394:LEU:HD13 | 2:B:437:LEU:HD11  | 1.90                     | 0.52              |
| 2:D:68:PHE:CE1   | 2:D:422:GLU:HG3   | 2.45                     | 0.52              |
| 1:A:143:LEU:HD23 | 1:A:143:LEU:C     | 2.30                     | 0.52              |
| 1:A:300:ILE:CD1  | 2:B:459:GLU:HG2   | 2.40                     | 0.52              |
| 2:B:4:PRO:HG2    | 2:B:9:ARG:CZ      | 2.40                     | 0.52              |
| 2:B:294:VAL:HG22 | 2:B:295:PRO:HA    | 1.90                     | 0.52              |
| 2:D:294:VAL:CG2  | 2:D:295:PRO:HA    | 2.40                     | 0.52              |
| 2:H:98:ASP:OD2   | 2:H:100:ARG:HB2   | 2.10                     | 0.52              |
| 2:F:102:ALA:O    | 2:F:106:LEU:HD22  | 2.10                     | 0.52              |
| 2:H:238:TYR:HB2  | 2:H:257:PHE:CD1   | 2.45                     | 0.52              |
| 1:E:93:THR:HG21  | 2:F:65:ASP:OD1    | 2.10                     | 0.51              |
| 2:B:160:LEU:HD23 | 2:B:181:ARG:HB3   | 1.91                     | 0.51              |
| 1:C:320:THR:HG23 | 3:D:2476:AOA:H1C2 | 1.93                     | 0.51              |
| 2:F:367:VAL:HG11 | 2:F:370:ASP:HB3   | 1.93                     | 0.51              |
| 1:G:32:LYS:N     | 1:G:32:LYS:HD3    | 2.20                     | 0.51              |
| 2:H:243:LEU:HD13 | 2:H:243:LEU:O     | 2.11                     | 0.51              |
| 2:H:290:PRO:HA   | 2:H:310:ARG:HH21  | 1.75                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:441:PRO:HG2  | 2:H:444:TRP:HB2  | 1.92                     | 0.51              |
| 2:B:155:THR:O    | 2:B:203:HIS:HA   | 2.09                     | 0.51              |
| 2:B:238:TYR:HD2  | 2:B:260:VAL:HG13 | 1.74                     | 0.51              |
| 1:G:128:ALA:O    | 1:G:129:SER:CB   | 2.58                     | 0.51              |
| 1:C:30:LEU:HD22  | 2:D:218:PHE:CG   | 2.44                     | 0.51              |
| 2:D:367:VAL:HG12 | 2:D:370:ASP:HB3  | 1.91                     | 0.51              |
| 2:H:424:LYS:O    | 2:H:428:GLU:HG3  | 2.11                     | 0.51              |
| 1:E:57:LEU:CD2   | 2:F:107:ARG:HD2  | 2.41                     | 0.51              |
| 2:F:375:HIS:CE1  | 2:F:376:GLU:HG2  | 2.46                     | 0.51              |
| 1:A:383:PRO:HG2  | 1:A:437:LEU:HG   | 1.92                     | 0.51              |
| 2:B:397:LEU:HD22 | 2:B:437:LEU:HD21 | 1.91                     | 0.51              |
| 2:D:72:GLY:HA3   | 2:D:415:MET:HG2  | 1.93                     | 0.51              |
| 2:F:395:LEU:CD1  | 2:F:401:PRO:HD3  | 2.41                     | 0.51              |
| 1:G:222:HIS:HE1  | 1:G:249:ASP:OD2  | 1.93                     | 0.51              |
| 2:H:383:GLU:CD   | 2:H:383:GLU:H    | 2.14                     | 0.51              |
| 1:C:108:GLN:O    | 1:C:112:GLU:HG3  | 2.10                     | 0.51              |
| 1:G:7:THR:OG1    | 1:G:10:GLU:HG3   | 2.11                     | 0.51              |
| 2:H:381:PRO:HB3  | 2:H:390:LEU:CD1  | 2.40                     | 0.51              |
| 2:D:235:GLN:HE21 | 2:D:288:LEU:HD11 | 1.74                     | 0.51              |
| 2:H:4:PRO:HG2    | 2:H:9:ARG:CZ     | 2.41                     | 0.51              |
| 2:F:142:ILE:HG23 | 2:F:291:TYR:HB2  | 1.91                     | 0.51              |
| 2:H:357:LYS:CE   | 2:H:370:ASP:HB2  | 2.41                     | 0.51              |
| 1:A:406:ARG:HH11 | 1:A:406:ARG:HG2  | 1.75                     | 0.50              |
| 2:B:236:LEU:HD22 | 2:B:257:PHE:CE1  | 2.46                     | 0.50              |
| 1:C:430:ARG:O    | 1:C:434:LYS:HG3  | 2.11                     | 0.50              |
| 2:F:441:PRO:HG2  | 2:F:444:TRP:HB2  | 1.94                     | 0.50              |
| 2:B:294:VAL:HG21 | 2:B:308:PHE:HA   | 1.93                     | 0.50              |
| 1:C:95:TYR:CG    | 1:C:96:THR:N     | 2.79                     | 0.50              |
| 2:D:464:LYS:HA   | 2:D:464:LYS:HE2  | 1.93                     | 0.50              |
| 2:H:113:GLY:O    | 2:H:117:LYS:HG3  | 2.10                     | 0.50              |
| 2:B:245:ALA:HB2  | 2:B:375:HIS:HB3  | 1.92                     | 0.50              |
| 1:C:280:ARG:O    | 1:C:280:ARG:HG2  | 2.10                     | 0.50              |
| 1:C:97:PRO:HG2   | 1:C:301:LEU:HD21 | 1.93                     | 0.50              |
| 2:D:289:ALA:N    | 2:D:290:PRO:HD2  | 2.26                     | 0.50              |
| 2:H:166:HIS:NE2  | 3:H:4476:AOA:N1  | 2.59                     | 0.50              |
| 1:E:212:GLU:HG3  | 4:E:562:HOH:O    | 2.11                     | 0.50              |
| 2:H:142:ILE:HG23 | 2:H:291:TYR:HB2  | 1.93                     | 0.50              |
| 1:E:377:GLU:HG2  | 1:E:416:ALA:HB2  | 1.94                     | 0.50              |
| 1:E:383:PRO:HG2  | 1:E:437:LEU:HG   | 1.92                     | 0.50              |
| 2:H:201:GLY:HA3  | 2:H:203:HIS:CE1  | 2.47                     | 0.50              |
| 2:F:442:LYS:O    | 2:F:446:GLU:HG3  | 2.11                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:430:ARG:O    | 1:G:434:LYS:HG3   | 2.11                     | 0.50              |
| 1:A:340:GLU:O    | 1:A:344:GLU:HG3   | 2.12                     | 0.50              |
| 2:B:188:GLU:HB2  | 4:B:1597:HOH:O    | 2.12                     | 0.50              |
| 2:B:316:ARG:HG2  | 2:B:316:ARG:NH1   | 2.27                     | 0.50              |
| 1:C:128:ALA:O    | 1:C:129:SER:HB3   | 2.12                     | 0.50              |
| 2:F:238:TYR:HB2  | 2:F:257:PHE:CD1   | 2.46                     | 0.50              |
| 1:E:167:LEU:HG   | 1:E:171:LEU:HD22  | 1.93                     | 0.50              |
| 1:G:1:MET:HG2    | 1:G:45:LEU:C      | 2.32                     | 0.49              |
| 2:D:210:THR:CG2  | 2:D:239:ASP:HB3   | 2.39                     | 0.49              |
| 2:H:260:VAL:HG12 | 2:H:261:HIS:N     | 2.26                     | 0.49              |
| 2:H:406:PHE:HA   | 2:H:407:PRO:C     | 2.32                     | 0.49              |
| 2:H:68:PHE:CE1   | 2:H:422:GLU:HG3   | 2.47                     | 0.49              |
| 2:F:166:HIS:HA   | 2:F:406:PHE:CZ    | 2.47                     | 0.49              |
| 2:F:30:ILE:HD11  | 2:F:35:LEU:CD2    | 2.33                     | 0.49              |
| 2:F:69:TYR:HD1   | 2:F:71:LEU:HD22   | 1.77                     | 0.49              |
| 1:G:291:VAL:HG13 | 1:G:295:GLY:HA2   | 1.94                     | 0.49              |
| 2:D:245:ALA:HB2  | 2:D:375:HIS:HB3   | 1.95                     | 0.49              |
| 1:A:377:GLU:HG2  | 1:A:416:ALA:HB2   | 1.94                     | 0.49              |
| 1:G:12:ARG:O     | 1:G:16:ARG:HG3    | 2.13                     | 0.49              |
| 1:A:356:LEU:HB2  | 1:A:426:LEU:HD22  | 1.94                     | 0.49              |
| 2:B:394:LEU:HD23 | 2:B:401:PRO:HA    | 1.94                     | 0.49              |
| 2:F:166:HIS:NE2  | 3:F:3476:AOA:H1C1 | 2.27                     | 0.49              |
| 2:B:318:ARG:NH2  | 2:B:323:ASN:OD1   | 2.46                     | 0.49              |
| 2:F:284:VAL:HG12 | 2:F:285:LYS:O     | 2.13                     | 0.49              |
| 2:F:245:ALA:HB2  | 2:F:375:HIS:HB3   | 1.94                     | 0.49              |
| 1:G:372:LYS:HB2  | 1:G:372:LYS:NZ    | 2.28                     | 0.49              |
| 1:A:73:VAL:HG23  | 2:B:320:PHE:CZ    | 2.48                     | 0.49              |
| 1:C:431:GLU:OE2  | 1:C:434:LYS:HE2   | 2.13                     | 0.49              |
| 2:D:463:ASN:C    | 2:D:464:LYS:HE2   | 2.33                     | 0.49              |
| 1:E:151:MET:HG2  | 4:E:578:HOH:O     | 2.13                     | 0.49              |
| 2:H:294:VAL:CG2  | 2:H:295:PRO:HA    | 2.43                     | 0.49              |
| 1:G:107:LEU:HD11 | 1:G:301:LEU:CD2   | 2.42                     | 0.49              |
| 1:G:286:LEU:HD22 | 2:H:468:LEU:HD12  | 1.94                     | 0.49              |
| 1:A:95:TYR:CG    | 1:A:96:THR:N      | 2.80                     | 0.49              |
| 2:D:261:HIS:C    | 2:D:261:HIS:CD2   | 2.86                     | 0.49              |
| 2:F:78:TYR:CZ    | 2:F:80:PRO:HA     | 2.48                     | 0.49              |
| 2:B:367:VAL:HG12 | 2:B:370:ASP:HB3   | 1.95                     | 0.48              |
| 2:D:294:VAL:HG21 | 2:D:308:PHE:HA    | 1.95                     | 0.48              |
| 1:E:108:GLN:O    | 1:E:112:GLU:HG3   | 2.13                     | 0.48              |
| 2:F:403:THR:HB   | 2:F:415:MET:HB3   | 1.94                     | 0.48              |
| 2:H:318:ARG:NH2  | 2:H:323:ASN:OD1   | 2.46                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:H:4:PRO:HG2    | 2:H:9:ARG:NH2     | 2.28                     | 0.48              |
| 1:C:32:LYS:CD    | 1:C:32:LYS:H      | 2.03                     | 0.48              |
| 2:D:237:TYR:CD1  | 2:D:259:VAL:HG13  | 2.48                     | 0.48              |
| 2:F:128:GLU:N    | 2:F:129:PRO:HD2   | 2.28                     | 0.48              |
| 2:H:144:ARG:HG2  | 2:H:148:GLU:OE1   | 2.13                     | 0.48              |
| 2:F:235:GLN:HE21 | 2:F:288:LEU:HD11  | 1.76                     | 0.48              |
| 2:F:40:PRO:HB2   | 2:F:42:LEU:HD13   | 1.94                     | 0.48              |
| 2:D:383:GLU:CD   | 2:D:383:GLU:H     | 2.15                     | 0.48              |
| 2:H:243:LEU:HD13 | 2:H:247:MET:HG2   | 1.96                     | 0.48              |
| 2:H:455:ARG:HB3  | 4:H:4553:HOH:O    | 2.13                     | 0.48              |
| 1:A:11:ILE:HG22  | 1:A:15:LEU:HD22   | 1.96                     | 0.48              |
| 1:A:376:ASN:H    | 1:A:376:ASN:HD22  | 1.62                     | 0.48              |
| 1:E:362:GLU:OE1  | 1:E:430:ARG:NH1   | 2.47                     | 0.48              |
| 2:F:238:TYR:HB3  | 2:F:260:VAL:HG22  | 1.95                     | 0.48              |
| 1:G:167:LEU:HG   | 1:G:171:LEU:HD22  | 1.96                     | 0.48              |
| 1:C:320:THR:HG21 | 3:D:2476:AOA:H1C2 | 1.96                     | 0.48              |
| 1:E:361:LEU:HD21 | 1:E:368:PRO:HB3   | 1.96                     | 0.48              |
| 2:F:265:HIS:CA   | 2:F:270:VAL:HB    | 2.36                     | 0.48              |
| 1:A:391:ARG:O    | 1:A:395:GLU:HG3   | 2.14                     | 0.48              |
| 1:C:255:GLY:HA3  | 1:C:269:PHE:CE1   | 2.48                     | 0.48              |
| 1:A:300:ILE:HD13 | 2:B:459:GLU:HG2   | 1.96                     | 0.47              |
| 1:C:2:ASP:OD2    | 1:C:4:THR:HB      | 2.14                     | 0.47              |
| 2:D:227:ARG:HG2  | 2:D:227:ARG:HH11  | 1.79                     | 0.47              |
| 2:F:25:LYS:HA    | 2:F:25:LYS:HE2    | 1.96                     | 0.47              |
| 2:H:198:ARG:CB   | 2:H:198:ARG:HH11  | 2.27                     | 0.47              |
| 2:D:166:HIS:NE2  | 3:D:2476:AOA:C1   | 2.73                     | 0.47              |
| 1:E:291:VAL:HG22 | 1:E:295:GLY:C     | 2.35                     | 0.47              |
| 1:G:311:ARG:HG3  | 1:G:314:LYS:CB    | 2.41                     | 0.47              |
| 2:H:402:PRO:HB2  | 2:H:415:MET:O     | 2.14                     | 0.47              |
| 1:A:322:ASN:O    | 2:B:277:PRO:HA    | 2.14                     | 0.47              |
| 1:G:80:PRO:HG2   | 4:G:469:HOH:O     | 2.14                     | 0.47              |
| 2:H:316:ARG:HG2  | 2:H:316:ARG:HH11  | 1.80                     | 0.47              |
| 1:A:260:LEU:HG   | 1:A:329:MET:CE    | 2.44                     | 0.47              |
| 2:D:221:ARG:O    | 2:D:225:ILE:HG13  | 2.14                     | 0.47              |
| 1:G:376:ASN:HD22 | 1:G:376:ASN:H     | 1.60                     | 0.47              |
| 2:H:284:VAL:HG21 | 2:H:288:LEU:HB2   | 1.94                     | 0.47              |
| 1:A:260:LEU:HG   | 1:A:329:MET:HE2   | 1.95                     | 0.47              |
| 2:B:238:TYR:HB2  | 2:B:257:PHE:CD1   | 2.50                     | 0.47              |
| 2:F:166:HIS:HA   | 2:F:406:PHE:HZ    | 1.79                     | 0.47              |
| 2:F:169:ASN:HB2  | 2:F:170:PRO:CD    | 2.45                     | 0.47              |
| 2:F:311:PRO:HG2  | 4:F:3609:HOH:O    | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:69:TYR:HB3   | 2:F:76:MET:HG3   | 1.96                     | 0.47              |
| 2:F:80:PRO:HG2   | 2:F:83:HIS:ND1   | 2.29                     | 0.47              |
| 2:H:25:LYS:HG3   | 2:H:27:GLU:CG    | 2.45                     | 0.47              |
| 1:A:168:ARG:O    | 1:A:172:GLU:HG3  | 2.14                     | 0.47              |
| 1:A:32:LYS:H     | 1:A:32:LYS:CE    | 2.28                     | 0.47              |
| 2:B:381:PRO:HB3  | 2:B:390:LEU:CD1  | 2.45                     | 0.47              |
| 1:E:50:VAL:O     | 1:E:54:LEU:HD22  | 2.15                     | 0.47              |
| 1:C:157:GLN:HB3  | 1:C:183:LEU:HD13 | 1.95                     | 0.47              |
| 2:D:406:PHE:CD1  | 2:D:407:PRO:HA   | 2.50                     | 0.47              |
| 1:E:81:VAL:HG13  | 1:E:82:VAL:N     | 2.29                     | 0.47              |
| 1:A:376:ASN:ND2  | 1:A:376:ASN:H    | 2.12                     | 0.47              |
| 1:E:348:LYS:HE3  | 2:F:20:VAL:HG13  | 1.97                     | 0.47              |
| 2:B:301:GLU:H    | 2:B:301:GLU:HG3  | 1.47                     | 0.47              |
| 2:H:72:GLY:HA3   | 2:H:415:MET:HG2  | 1.97                     | 0.47              |
| 1:A:32:LYS:N     | 1:A:32:LYS:CD    | 2.77                     | 0.47              |
| 1:E:143:LEU:HD23 | 1:E:143:LEU:C    | 2.36                     | 0.47              |
| 2:B:136:GLU:O    | 2:B:140:ILE:HG12 | 2.15                     | 0.46              |
| 2:B:235:GLN:HE21 | 2:B:288:LEU:HD11 | 1.80                     | 0.46              |
| 1:A:162:GLU:HG2  | 2:B:316:ARG:NE   | 2.30                     | 0.46              |
| 1:E:391:ARG:NH1  | 1:E:391:ARG:HG3  | 2.29                     | 0.46              |
| 1:G:1:MET:HG2    | 1:G:45:LEU:O     | 2.15                     | 0.46              |
| 1:A:402:THR:HG23 | 1:A:414:LEU:HB2  | 1.95                     | 0.46              |
| 2:B:466:PRO:HB2  | 2:B:468:LEU:CD1  | 2.46                     | 0.46              |
| 2:F:468:LEU:N    | 2:F:468:LEU:CD1  | 2.78                     | 0.46              |
| 1:E:55:ARG:NH2   | 1:G:65:HIS:NE2   | 2.63                     | 0.46              |
| 2:D:78:TYR:CZ    | 2:D:80:PRO:HA    | 2.50                     | 0.46              |
| 2:H:138:THR:O    | 2:H:142:ILE:HG13 | 2.15                     | 0.46              |
| 2:H:157:ARG:CA   | 2:H:157:ARG:HE   | 2.21                     | 0.46              |
| 2:H:325:LEU:HD12 | 2:H:325:LEU:HA   | 1.80                     | 0.46              |
| 2:F:72:GLY:HA2   | 2:F:417:GLU:HB3  | 1.97                     | 0.46              |
| 2:H:227:ARG:HH11 | 2:H:227:ARG:CB   | 2.19                     | 0.46              |
| 1:C:55:ARG:NH2   | 4:C:494:HOH:O    | 2.48                     | 0.46              |
| 2:D:106:LEU:HD11 | 2:D:306:LEU:CD2  | 2.45                     | 0.46              |
| 2:D:263:ASN:HB2  | 2:D:266:LYS:HB2  | 1.97                     | 0.46              |
| 1:A:376:ASN:N    | 1:A:376:ASN:HD22 | 2.13                     | 0.46              |
| 1:G:112:GLU:HB2  | 4:G:482:HOH:O    | 2.15                     | 0.46              |
| 2:B:48:LEU:HG    | 2:D:78:TYR:HB2   | 1.98                     | 0.46              |
| 1:E:389:VAL:O    | 1:E:393:LEU:HB2  | 2.15                     | 0.46              |
| 2:F:164:SER:HB2  | 2:F:214:THR:OG1  | 2.15                     | 0.46              |
| 1:G:384:LYS:HD2  | 1:G:437:LEU:HD12 | 1.96                     | 0.46              |
| 2:H:30:ILE:HG23  | 2:H:31:PRO:HD2   | 1.96                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:354:ARG:O    | 2:H:357:LYS:HB3  | 2.15                     | 0.46              |
| 2:H:363:LYS:HD2  | 2:H:435:GLY:HA3  | 1.98                     | 0.46              |
| 1:E:241:LYS:HD3  | 1:E:246:TYR:CZ   | 2.50                     | 0.46              |
| 2:B:195:ALA:O    | 2:B:198:ARG:HG2  | 2.15                     | 0.46              |
| 1:C:424:GLU:HG2  | 4:C:538:HOH:O    | 2.15                     | 0.46              |
| 1:E:95:TYR:CG    | 1:E:96:THR:N     | 2.84                     | 0.46              |
| 2:H:381:PRO:HB3  | 2:H:390:LEU:HD12 | 1.98                     | 0.46              |
| 2:H:166:HIS:NE2  | 3:H:4476:AOA:C1  | 2.79                     | 0.46              |
| 1:A:344:GLU:OE1  | 2:B:15:ARG:NH2   | 2.47                     | 0.46              |
| 1:C:239:VAL:HG21 | 1:C:347:LEU:HD21 | 1.97                     | 0.46              |
| 1:C:433:LEU:HA   | 1:C:436:VAL:CG1  | 2.46                     | 0.46              |
| 2:D:245:ALA:HB2  | 2:D:375:HIS:CG   | 2.50                     | 0.46              |
| 2:F:237:TYR:OH   | 2:F:261:HIS:HB3  | 2.16                     | 0.46              |
| 1:A:292:ASP:HB3  | 2:B:454:VAL:HG22 | 1.98                     | 0.45              |
| 1:E:391:ARG:HA   | 2:F:98:ASP:OD2   | 2.16                     | 0.45              |
| 2:F:221:ARG:NH2  | 2:F:224:GLU:HG3  | 2.32                     | 0.45              |
| 2:F:238:TYR:CE2  | 2:F:240:GLY:HA2  | 2.51                     | 0.45              |
| 2:H:195:ALA:HA   | 2:H:198:ARG:NH2  | 2.31                     | 0.45              |
| 2:H:4:PRO:HB3    | 4:H:4548:HOH:O   | 2.16                     | 0.45              |
| 2:B:98:ASP:OD2   | 2:B:100:ARG:HB2  | 2.17                     | 0.45              |
| 1:G:436:VAL:CG2  | 1:G:437:LEU:HD13 | 2.46                     | 0.45              |
| 2:H:196:LEU:HG   | 2:H:200:LEU:HD13 | 1.98                     | 0.45              |
| 1:A:46:PRO:HD3   | 2:D:21:LYS:HG2   | 1.96                     | 0.45              |
| 1:E:45:LEU:HD13  | 1:E:49:LYS:HG3   | 1.98                     | 0.45              |
| 1:G:311:ARG:HG2  | 1:G:311:ARG:HH11 | 1.80                     | 0.45              |
| 1:G:97:PRO:HB2   | 1:G:107:LEU:CD2  | 2.46                     | 0.45              |
| 2:H:162:PRO:HG2  | 2:H:165:ALA:HB2  | 1.97                     | 0.45              |
| 2:B:262:LEU:O    | 2:B:280:GLY:HA2  | 2.16                     | 0.45              |
| 1:E:83:GLN:HE22  | 1:E:329:MET:HE3  | 1.80                     | 0.45              |
| 2:F:211:ASN:HA   | 2:F:212:PRO:C    | 2.37                     | 0.45              |
| 2:F:25:LYS:HE2   | 2:F:26:ALA:N     | 2.31                     | 0.45              |
| 2:F:381:PRO:HB3  | 2:F:390:LEU:CD1  | 2.46                     | 0.45              |
| 1:G:387:GLU:HG3  | 4:G:550:HOH:O    | 2.15                     | 0.45              |
| 1:G:30:LEU:HD13  | 2:H:218:PHE:CE1  | 2.52                     | 0.45              |
| 2:B:31:PRO:HG2   | 2:B:34:HIS:CD2   | 2.50                     | 0.45              |
| 1:G:68:PHE:CD2   | 1:G:429:LEU:HD22 | 2.51                     | 0.45              |
| 1:C:107:LEU:HD11 | 1:C:301:LEU:HD22 | 1.99                     | 0.45              |
| 1:C:328:LEU:O    | 1:C:332:MET:HG3  | 2.16                     | 0.45              |
| 2:D:143:ILE:HD11 | 2:D:259:VAL:HG11 | 1.98                     | 0.45              |
| 2:B:289:ALA:N    | 2:B:290:PRO:HD2  | 2.32                     | 0.45              |
| 2:D:169:ASN:HB2  | 2:D:170:PRO:CD   | 2.47                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:316:ARG:HG2  | 2:D:316:ARG:HH11 | 1.82                     | 0.45              |
| 2:H:440:LYS:HB2  | 2:H:445:LEU:HD21 | 1.98                     | 0.45              |
| 1:A:11:ILE:O     | 1:A:15:LEU:HB2   | 2.17                     | 0.45              |
| 2:B:211:ASN:HA   | 2:B:212:PRO:C    | 2.36                     | 0.45              |
| 2:B:325:LEU:HD12 | 2:B:325:LEU:HA   | 1.84                     | 0.45              |
| 1:C:337:LEU:HD13 | 2:D:17:LEU:HB2   | 1.99                     | 0.45              |
| 2:D:237:TYR:HD1  | 2:D:259:VAL:CG1  | 2.29                     | 0.45              |
| 1:E:196:GLU:CD   | 1:E:196:GLU:H    | 2.21                     | 0.45              |
| 2:F:411:LYS:HZ3  | 2:F:411:LYS:HB2  | 1.80                     | 0.45              |
| 2:F:48:LEU:HG    | 2:H:78:TYR:HB2   | 1.97                     | 0.45              |
| 2:F:391:ALA:O    | 2:F:395:LEU:HD13 | 2.16                     | 0.45              |
| 2:F:261:HIS:CD2  | 2:F:261:HIS:C    | 2.91                     | 0.45              |
| 1:C:311:ARG:NH1  | 1:C:314:LYS:HD3  | 2.32                     | 0.44              |
| 1:C:356:LEU:HG   | 1:C:360:LEU:HD22 | 1.99                     | 0.44              |
| 2:D:33:GLU:CD    | 2:D:33:GLU:H     | 2.20                     | 0.44              |
| 2:F:80:PRO:CG    | 2:F:83:HIS:CE1   | 3.00                     | 0.44              |
| 1:A:406:ARG:HG2  | 1:A:406:ARG:NH1  | 2.32                     | 0.44              |
| 1:A:356:LEU:HD11 | 1:A:429:LEU:HD23 | 1.99                     | 0.44              |
| 1:C:31:PRO:HG2   | 1:C:34:ILE:CD1   | 2.48                     | 0.44              |
| 2:D:395:LEU:CD1  | 2:D:401:PRO:HD3  | 2.45                     | 0.44              |
| 2:H:210:THR:CG2  | 2:H:239:ASP:HB3  | 2.46                     | 0.44              |
| 1:C:7:THR:OG1    | 1:C:10:GLU:HG3   | 2.16                     | 0.44              |
| 1:E:352:MET:HE2  | 1:E:422:GLU:HA   | 1.99                     | 0.44              |
| 2:F:141:LEU:HD12 | 2:F:141:LEU:HA   | 1.80                     | 0.44              |
| 2:H:316:ARG:HG2  | 2:H:316:ARG:NH1  | 2.32                     | 0.44              |
| 1:A:50:VAL:O     | 1:A:54:LEU:HD22  | 2.17                     | 0.44              |
| 1:A:373:PRO:HG3  | 2:B:31:PRO:HG3   | 1.98                     | 0.44              |
| 2:D:464:LYS:HE2  | 2:D:464:LYS:CA   | 2.47                     | 0.44              |
| 1:E:197:VAL:O    | 1:E:226:ALA:HB2  | 2.18                     | 0.44              |
| 1:E:36:SER:HA    | 4:E:560:HOH:O    | 2.17                     | 0.44              |
| 2:F:299:ARG:HB3  | 2:F:304:PHE:CE1  | 2.53                     | 0.44              |
| 2:H:137:LEU:O    | 2:H:141:LEU:HB2  | 2.18                     | 0.44              |
| 1:C:250:ILE:HG23 | 1:C:272:LEU:HD11 | 1.99                     | 0.44              |
| 1:C:30:LEU:HD22  | 2:D:218:PHE:CD1  | 2.52                     | 0.44              |
| 2:D:157:ARG:HA   | 2:D:157:ARG:HE   | 1.83                     | 0.44              |
| 2:D:238:TYR:HB2  | 2:D:257:PHE:CD1  | 2.53                     | 0.44              |
| 1:G:50:VAL:O     | 1:G:54:LEU:CD2   | 2.66                     | 0.44              |
| 2:H:192:ASP:HB3  | 2:H:195:ALA:HB3  | 1.99                     | 0.44              |
| 2:B:245:ALA:HB2  | 2:B:375:HIS:CG   | 2.53                     | 0.44              |
| 2:B:243:LEU:CD1  | 2:B:247:MET:HB3  | 2.46                     | 0.44              |
| 2:B:261:HIS:HA   | 2:B:281:PRO:O    | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:357:LYS:NZ   | 2:F:370:ASP:HB2  | 2.33                     | 0.44              |
| 1:G:255:GLY:HA3  | 1:G:269:PHE:CE1  | 2.52                     | 0.44              |
| 2:H:163:ASP:OD1  | 2:H:163:ASP:N    | 2.49                     | 0.44              |
| 2:H:355:TYR:CE2  | 2:H:359:LEU:HD11 | 2.53                     | 0.44              |
| 2:H:397:LEU:HD23 | 2:H:433:ALA:HB1  | 2.00                     | 0.44              |
| 1:C:433:LEU:O    | 1:C:436:VAL:HG13 | 2.18                     | 0.44              |
| 1:A:201:VAL:HG22 | 1:A:229:VAL:HB   | 2.00                     | 0.44              |
| 2:D:72:GLY:O     | 2:D:73:SER:HB2   | 2.18                     | 0.44              |
| 1:E:57:LEU:HD21  | 2:F:107:ARG:HD2  | 2.00                     | 0.44              |
| 2:F:157:ARG:HG2  | 2:F:157:ARG:HH11 | 1.83                     | 0.44              |
| 1:G:376:ASN:ND2  | 1:G:376:ASN:H    | 2.16                     | 0.44              |
| 2:H:117:LYS:HA   | 2:H:120:THR:HG22 | 1.99                     | 0.44              |
| 2:H:183:ILE:HG22 | 2:H:199:GLU:HG3  | 1.99                     | 0.44              |
| 2:B:394:LEU:HD13 | 2:B:437:LEU:CD1  | 2.47                     | 0.43              |
| 2:H:158:VAL:HG13 | 2:H:204:VAL:HA   | 2.00                     | 0.43              |
| 2:H:25:LYS:HG3   | 2:H:27:GLU:HG3   | 2.00                     | 0.43              |
| 2:B:132:GLY:HA3  | 2:B:263:ASN:ND2  | 2.33                     | 0.43              |
| 2:D:264:LEU:HD22 | 2:D:279:SER:HB3  | 2.00                     | 0.43              |
| 1:E:321:THR:HG23 | 2:F:275:GLY:O    | 2.18                     | 0.43              |
| 2:B:264:LEU:HB2  | 2:B:279:SER:HB3  | 1.99                     | 0.43              |
| 2:D:107:ARG:O    | 2:D:111:GLU:HG3  | 2.17                     | 0.43              |
| 2:D:406:PHE:HA   | 2:D:407:PRO:C    | 2.37                     | 0.43              |
| 1:G:159:VAL:HG22 | 1:G:203:GLN:HB2  | 2.01                     | 0.43              |
| 2:D:80:PRO:HG2   | 2:D:83:HIS:ND1   | 2.34                     | 0.43              |
| 1:G:97:PRO:HG3   | 1:G:107:LEU:HD13 | 2.00                     | 0.43              |
| 1:G:311:ARG:HE   | 1:G:314:LYS:HE3  | 1.82                     | 0.43              |
| 1:A:30:LEU:HD22  | 2:B:218:PHE:CD2  | 2.53                     | 0.43              |
| 1:E:396:ARG:HG3  | 1:E:396:ARG:HH11 | 1.83                     | 0.43              |
| 2:F:24:PRO:HB2   | 2:F:29:LEU:HD21  | 2.00                     | 0.43              |
| 1:G:11:ILE:HG22  | 1:G:15:LEU:HD22  | 2.00                     | 0.43              |
| 2:B:357:LYS:HE3  | 2:B:367:VAL:HG11 | 1.99                     | 0.43              |
| 1:C:391:ARG:HG3  | 1:C:391:ARG:NH1  | 2.32                     | 0.43              |
| 2:D:201:GLY:HA3  | 2:D:203:HIS:CE1  | 2.53                     | 0.43              |
| 2:D:394:LEU:HD23 | 2:D:401:PRO:HA   | 2.01                     | 0.43              |
| 2:B:376:GLU:HB3  | 2:B:417:GLU:HB2  | 2.01                     | 0.43              |
| 1:C:157:GLN:HB3  | 1:C:183:LEU:CD1  | 2.49                     | 0.43              |
| 2:F:146:TYR:O    | 2:F:150:ARG:HG3  | 2.19                     | 0.43              |
| 1:G:93:THR:HG21  | 2:H:65:ASP:OD1   | 2.18                     | 0.43              |
| 1:C:391:ARG:CG   | 1:C:391:ARG:HH11 | 2.31                     | 0.43              |
| 2:D:136:GLU:O    | 2:D:140:ILE:HG12 | 2.19                     | 0.43              |
| 2:D:265:HIS:CA   | 2:D:270:VAL:HB   | 2.42                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:311:ARG:HG3  | 1:E:314:LYS:HB2  | 2.00                     | 0.43              |
| 1:G:329:MET:HE1  | 4:G:575:HOH:O    | 2.19                     | 0.43              |
| 1:G:79:PRO:HA    | 1:G:80:PRO:HD2   | 1.89                     | 0.43              |
| 1:G:337:LEU:HD13 | 2:H:17:LEU:HB2   | 2.01                     | 0.43              |
| 1:A:203:GLN:HG2  | 1:A:205:PRO:O    | 2.19                     | 0.43              |
| 2:B:210:THR:CG2  | 2:B:239:ASP:HB3  | 2.46                     | 0.43              |
| 1:C:340:GLU:O    | 1:C:344:GLU:HG3  | 2.18                     | 0.43              |
| 1:A:47:GLU:OE2   | 2:D:17:LEU:HD22  | 2.19                     | 0.43              |
| 1:G:90:GLU:O     | 1:G:94:ALA:HB2   | 2.18                     | 0.43              |
| 2:B:25:LYS:HE2   | 4:B:1657:HOH:O   | 2.18                     | 0.43              |
| 1:C:301:LEU:HD22 | 1:C:301:LEU:H    | 1.83                     | 0.43              |
| 1:G:391:ARG:HG3  | 1:G:391:ARG:NH1  | 2.34                     | 0.43              |
| 2:F:94:HIS:CE1   | 2:F:96:TYR:HB2   | 2.54                     | 0.42              |
| 1:A:348:LYS:HG3  | 1:A:419:GLU:HA   | 2.02                     | 0.42              |
| 2:B:466:PRO:HB2  | 2:B:468:LEU:HD11 | 2.00                     | 0.42              |
| 1:E:1:MET:HG2    | 1:E:45:LEU:C     | 2.39                     | 0.42              |
| 2:H:294:VAL:HG22 | 2:H:308:PHE:CD1  | 2.54                     | 0.42              |
| 2:H:294:VAL:HG21 | 2:H:308:PHE:HA   | 1.97                     | 0.42              |
| 2:H:366:ARG:O    | 2:H:379:ALA:HA   | 2.20                     | 0.42              |
| 2:B:242:ASN:HB3  | 2:B:375:HIS:CE1  | 2.54                     | 0.42              |
| 1:A:106:VAL:HG23 | 2:B:61:GLN:CD    | 2.40                     | 0.42              |
| 1:C:155:VAL:CG1  | 1:C:178:LEU:HD11 | 2.49                     | 0.42              |
| 1:C:107:LEU:HD11 | 1:C:301:LEU:CD2  | 2.49                     | 0.42              |
| 2:F:106:LEU:HD11 | 2:F:306:LEU:HD21 | 2.01                     | 0.42              |
| 2:F:242:ASN:HB3  | 2:F:375:HIS:CE1  | 2.55                     | 0.42              |
| 2:F:30:ILE:HD13  | 2:F:30:ILE:N     | 2.34                     | 0.42              |
| 2:H:299:ARG:HA   | 2:H:304:PHE:HA   | 2.01                     | 0.42              |
| 1:A:30:LEU:HD22  | 2:B:218:PHE:CG   | 2.54                     | 0.42              |
| 1:C:311:ARG:HG3  | 1:C:314:LYS:HB2  | 2.00                     | 0.42              |
| 2:F:25:LYS:CE    | 2:F:25:LYS:HA    | 2.50                     | 0.42              |
| 1:A:204:ASN:HA   | 1:A:205:PRO:C    | 2.40                     | 0.42              |
| 1:A:389:VAL:O    | 1:A:393:LEU:HB2  | 2.19                     | 0.42              |
| 2:B:40:PRO:CG    | 2:B:42:LEU:HD22  | 2.48                     | 0.42              |
| 2:F:402:PRO:HB2  | 2:F:415:MET:O    | 2.19                     | 0.42              |
| 1:G:185:GLY:O    | 1:G:371:PRO:HG3  | 2.20                     | 0.42              |
| 1:A:97:PRO:HG3   | 1:A:107:LEU:HD13 | 2.01                     | 0.42              |
| 1:C:15:LEU:HA    | 1:C:15:LEU:HD12  | 1.92                     | 0.42              |
| 1:C:31:PRO:O     | 1:C:34:ILE:HG12  | 2.20                     | 0.42              |
| 1:G:311:ARG:HG2  | 1:G:311:ARG:NH1  | 2.35                     | 0.42              |
| 1:G:400:GLY:O    | 1:G:401:ALA:HB3  | 2.19                     | 0.42              |
| 2:B:360:LEU:HD21 | 2:B:434:MET:CE   | 2.50                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:5:LEU:HD13   | 2:B:470:TYR:HD1   | 1.83                     | 0.42              |
| 1:C:49:LYS:HA    | 1:C:49:LYS:HD2    | 1.77                     | 0.42              |
| 1:C:174:VAL:HG22 | 1:C:174:VAL:O     | 2.20                     | 0.42              |
| 2:F:166:HIS:NE2  | 3:F:3476:AOA:N1   | 2.55                     | 0.42              |
| 1:G:291:VAL:CG1  | 1:G:295:GLY:HA2   | 2.50                     | 0.42              |
| 1:G:171:LEU:HA   | 1:G:171:LEU:HD12  | 1.89                     | 0.42              |
| 2:H:381:PRO:HB2  | 2:H:385:PHE:HB2   | 2.02                     | 0.42              |
| 2:H:394:LEU:HA   | 2:H:394:LEU:HD12  | 1.93                     | 0.42              |
| 2:B:226:SER:OG   | 2:B:256:GLY:HA3   | 2.19                     | 0.42              |
| 1:C:349:SER:CB   | 1:C:418:THR:HA    | 2.50                     | 0.42              |
| 1:C:79:PRO:HA    | 1:C:80:PRO:HD2    | 1.88                     | 0.42              |
| 2:D:160:LEU:HD23 | 2:D:181:ARG:HB2   | 2.02                     | 0.42              |
| 1:G:108:GLN:O    | 1:G:112:GLU:HG3   | 2.19                     | 0.42              |
| 1:A:255:GLY:HA3  | 1:A:269:PHE:CZ    | 2.55                     | 0.41              |
| 2:D:128:GLU:N    | 2:D:129:PRO:HD2   | 2.35                     | 0.41              |
| 2:D:237:TYR:HD1  | 2:D:259:VAL:HG13  | 1.85                     | 0.41              |
| 2:D:329:ARG:HH11 | 2:D:329:ARG:HG2   | 1.85                     | 0.41              |
| 1:E:267:PRO:HD2  | 2:F:325:LEU:HB2   | 2.02                     | 0.41              |
| 1:E:337:LEU:O    | 1:E:341:GLY:HA3   | 2.20                     | 0.41              |
| 1:G:241:LYS:HD3  | 1:G:246:TYR:CZ    | 2.55                     | 0.41              |
| 2:H:132:GLY:HA3  | 2:H:263:ASN:HD21  | 1.85                     | 0.41              |
| 1:A:65:HIS:O     | 1:A:66:LYS:HB2    | 2.20                     | 0.41              |
| 1:C:24:GLU:CD    | 1:C:24:GLU:H      | 2.23                     | 0.41              |
| 2:D:262:LEU:O    | 2:D:280:GLY:HA2   | 2.21                     | 0.41              |
| 2:H:78:TYR:CE2   | 2:H:80:PRO:HA     | 2.55                     | 0.41              |
| 1:C:11:ILE:O     | 1:C:15:LEU:HB2    | 2.20                     | 0.41              |
| 1:C:351:GLU:HB2  | 2:D:29:LEU:HD21   | 2.02                     | 0.41              |
| 1:E:394:ALA:HA   | 1:E:398:PHE:O     | 2.20                     | 0.41              |
| 2:F:166:HIS:CD2  | 3:F:3476:AOA:H1N1 | 2.35                     | 0.41              |
| 1:G:155:VAL:CG1  | 1:G:178:LEU:HD11  | 2.50                     | 0.41              |
| 2:H:222:ILE:HG23 | 2:H:223:LEU:N     | 2.34                     | 0.41              |
| 2:H:284:VAL:HG21 | 2:H:288:LEU:CB    | 2.50                     | 0.41              |
| 1:A:365:GLY:H    | 1:A:367:ARG:NH1   | 2.17                     | 0.41              |
| 1:A:400:GLY:O    | 1:A:401:ALA:HB3   | 2.20                     | 0.41              |
| 1:C:157:GLN:O    | 1:C:157:GLN:HG2   | 2.20                     | 0.41              |
| 2:D:447:ASN:HB2  | 2:D:450:TYR:OH    | 2.19                     | 0.41              |
| 2:F:406:PHE:HA   | 2:F:407:PRO:C     | 2.40                     | 0.41              |
| 1:G:404:VAL:HB   | 1:G:412:LEU:HB2   | 2.02                     | 0.41              |
| 2:H:310:ARG:HA   | 2:H:311:PRO:HD2   | 1.85                     | 0.41              |
| 2:F:284:VAL:CG1  | 2:F:285:LYS:O     | 2.68                     | 0.41              |
| 2:F:367:VAL:HG12 | 2:F:370:ASP:HB3   | 2.01                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:166:HIS:NE2  | 3:B:1476:AOA:C1  | 2.83                     | 0.41              |
| 2:B:395:LEU:CD1  | 2:B:401:PRO:HD3  | 2.43                     | 0.41              |
| 1:C:39:ILE:HD12  | 2:D:248:GLY:HA2  | 2.02                     | 0.41              |
| 2:D:157:ARG:HA   | 2:D:157:ARG:NE   | 2.35                     | 0.41              |
| 2:D:80:PRO:HD2   | 2:D:269:THR:HB   | 2.01                     | 0.41              |
| 1:E:143:LEU:HD23 | 1:E:143:LEU:O    | 2.20                     | 0.41              |
| 1:E:400:GLY:O    | 1:E:401:ALA:HB3  | 2.21                     | 0.41              |
| 2:F:90:PHE:HB3   | 2:F:324:PHE:HE2  | 1.85                     | 0.41              |
| 2:H:260:VAL:CG1  | 2:H:261:HIS:N    | 2.83                     | 0.41              |
| 1:A:288:SER:HB2  | 1:A:302:THR:HG21 | 2.03                     | 0.41              |
| 1:A:80:PRO:HG2   | 4:C:489:HOH:O    | 2.20                     | 0.41              |
| 2:B:260:VAL:HG12 | 2:B:261:HIS:N    | 2.35                     | 0.41              |
| 2:B:294:VAL:HG22 | 2:B:295:PRO:CA   | 2.51                     | 0.41              |
| 2:B:65:ASP:O     | 2:D:52:ARG:HG2   | 2.20                     | 0.41              |
| 2:D:30:ILE:N     | 2:D:30:ILE:HD13  | 2.36                     | 0.41              |
| 2:F:366:ARG:HH12 | 2:F:382:PRO:HA   | 1.79                     | 0.41              |
| 2:H:291:TYR:O    | 2:H:314:ILE:HG23 | 2.21                     | 0.41              |
| 1:A:17:ARG:HH21  | 2:B:362:GLU:CD   | 2.24                     | 0.41              |
| 1:A:241:LYS:HB2  | 1:A:241:LYS:HE3  | 1.95                     | 0.41              |
| 2:B:5:LEU:HD13   | 2:B:470:TYR:CD1  | 2.56                     | 0.41              |
| 2:D:261:HIS:HA   | 2:D:281:PRO:O    | 2.21                     | 0.41              |
| 1:A:174:VAL:HG13 | 4:B:1613:HOH:O   | 2.20                     | 0.41              |
| 1:A:62:LEU:HD22  | 1:A:399:HIS:HE2  | 1.85                     | 0.41              |
| 1:C:171:LEU:HD12 | 1:C:171:LEU:HA   | 1.81                     | 0.41              |
| 1:C:158:GLY:CA   | 1:C:183:LEU:HD11 | 2.50                     | 0.41              |
| 1:C:101:GLU:HA   | 2:D:454:VAL:HG12 | 2.03                     | 0.41              |
| 1:E:423:GLU:HA   | 1:E:423:GLU:OE1  | 2.21                     | 0.41              |
| 1:G:159:VAL:O    | 1:G:160:HIS:C    | 2.59                     | 0.41              |
| 1:G:432:ALA:O    | 1:G:436:VAL:HG13 | 2.21                     | 0.41              |
| 1:C:393:LEU:HD13 | 1:C:436:VAL:HG11 | 2.02                     | 0.41              |
| 2:D:136:GLU:HA   | 2:D:237:TYR:OH   | 2.21                     | 0.41              |
| 2:D:80:PRO:CG    | 2:D:83:HIS:CE1   | 3.04                     | 0.41              |
| 2:F:357:LYS:HZ1  | 2:F:370:ASP:HB2  | 1.85                     | 0.41              |
| 2:F:386:ARG:HD3  | 2:F:389:ASP:OD2  | 2.20                     | 0.41              |
| 1:G:267:PRO:HD2  | 2:H:325:LEU:HB2  | 2.03                     | 0.41              |
| 2:H:289:ALA:N    | 2:H:290:PRO:CD   | 2.84                     | 0.41              |
| 1:A:431:GLU:HA   | 1:A:431:GLU:OE1  | 2.20                     | 0.41              |
| 1:C:386:PRO:HG2  | 4:C:577:HOH:O    | 2.20                     | 0.41              |
| 2:D:227:ARG:HG2  | 2:D:227:ARG:NH1  | 2.36                     | 0.41              |
| 1:E:22:SER:OG    | 1:E:24:GLU:HG2   | 2.21                     | 0.41              |
| 2:H:357:LYS:HD2  | 2:H:373:SER:OG   | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:462:ALA:O    | 2:B:466:PRO:HB3  | 2.22                     | 0.40              |
| 1:C:314:LYS:HB3  | 1:C:314:LYS:NZ   | 2.36                     | 0.40              |
| 1:C:394:ALA:HB1  | 2:D:101:THR:HG21 | 2.03                     | 0.40              |
| 2:H:30:ILE:CG2   | 2:H:31:PRO:HD2   | 2.51                     | 0.40              |
| 2:H:367:VAL:HG12 | 2:H:370:ASP:HB3  | 2.02                     | 0.40              |
| 2:H:394:LEU:HD23 | 2:H:401:PRO:HA   | 2.02                     | 0.40              |
| 1:A:1:MET:HE2    | 1:A:44:PRO:HB2   | 2.02                     | 0.40              |
| 1:C:376:ASN:ND2  | 1:C:376:ASN:H    | 2.19                     | 0.40              |
| 1:C:95:TYR:HB2   | 2:D:76:MET:HE2   | 2.02                     | 0.40              |
| 1:E:404:VAL:HB   | 1:E:412:LEU:HB2  | 2.03                     | 0.40              |
| 1:E:79:PRO:HA    | 1:E:80:PRO:HD2   | 1.89                     | 0.40              |
| 1:A:260:LEU:HD23 | 1:A:268:HIS:HA   | 2.03                     | 0.40              |
| 1:A:334:LEU:HA   | 1:A:334:LEU:HD12 | 1.92                     | 0.40              |
| 2:D:134:HIS:HE1  | 2:D:318:ARG:HB3  | 1.86                     | 0.40              |
| 2:D:294:VAL:HG22 | 2:D:295:PRO:HA   | 2.01                     | 0.40              |
| 2:D:302:GLU:CD   | 2:D:302:GLU:N    | 2.71                     | 0.40              |
| 2:F:289:ALA:N    | 2:F:290:PRO:HD2  | 2.37                     | 0.40              |
| 2:B:128:GLU:N    | 2:B:129:PRO:HD2  | 2.36                     | 0.40              |
| 2:D:243:LEU:CD1  | 2:D:247:MET:HG2  | 2.51                     | 0.40              |
| 2:F:366:ARG:HH12 | 2:F:382:PRO:C    | 2.25                     | 0.40              |
| 2:F:366:ARG:HH11 | 2:F:382:PRO:HA   | 1.81                     | 0.40              |
| 1:G:234:PRO:HG3  | 1:G:255:GLY:HA2  | 2.03                     | 0.40              |
| 1:G:324:GLN:HE21 | 1:G:328:LEU:HD13 | 1.86                     | 0.40              |
| 2:H:389:ASP:HB3  | 2:H:445:LEU:HB3  | 2.03                     | 0.40              |
| 1:A:301:LEU:HA   | 1:A:301:LEU:HD12 | 1.91                     | 0.40              |
| 2:B:299:ARG:HB3  | 2:B:304:PHE:CD1  | 2.57                     | 0.40              |
| 1:C:10:GLU:O     | 1:C:14:MET:HG3   | 2.21                     | 0.40              |
| 1:C:168:ARG:HH11 | 1:C:168:ARG:HG3  | 1.87                     | 0.40              |
| 2:D:394:LEU:HD12 | 2:D:394:LEU:HA   | 1.88                     | 0.40              |
| 1:E:159:VAL:HG22 | 1:E:203:GLN:HB2  | 2.04                     | 0.40              |
| 1:E:391:ARG:HD3  | 2:F:100:ARG:NH1  | 2.36                     | 0.40              |
| 1:E:62:LEU:HB3   | 2:F:101:THR:HB   | 2.04                     | 0.40              |
| 1:G:190:LEU:HD12 | 1:G:191:PRO:HD2  | 2.04                     | 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     | 435/438 (99%)   | 416 (96%)  | 18 (4%)  | 1 (0%)   | 51          | 67  |
| 1   | C     | 435/438 (99%)   | 415 (95%)  | 19 (4%)  | 1 (0%)   | 51          | 67  |
| 1   | E     | 435/438 (99%)   | 417 (96%)  | 17 (4%)  | 1 (0%)   | 51          | 67  |
| 1   | G     | 435/438 (99%)   | 416 (96%)  | 18 (4%)  | 1 (0%)   | 51          | 67  |
| 2   | B     | 471/474 (99%)   | 456 (97%)  | 15 (3%)  | 0        | 100         | 100 |
| 2   | D     | 471/474 (99%)   | 456 (97%)  | 15 (3%)  | 0        | 100         | 100 |
| 2   | F     | 471/474 (99%)   | 452 (96%)  | 19 (4%)  | 0        | 100         | 100 |
| 2   | H     | 471/474 (99%)   | 452 (96%)  | 19 (4%)  | 0        | 100         | 100 |
| All | All   | 3624/3648 (99%) | 3480 (96%) | 140 (4%) | 4 (0%)   | 55          | 72  |

All (4) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 129 | SER  |
| 1   | C     | 129 | SER  |
| 1   | E     | 129 | SER  |
| 1   | G     | 129 | 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     | 336/336 (100%) | 311 (93%) | 25 (7%)  | 16          | 25 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|-------------|----|
| 1   | C     | 336/336 (100%)   | 316 (94%)  | 20 (6%)  | 22          | 35 |
| 1   | E     | 336/336 (100%)   | 316 (94%)  | 20 (6%)  | 22          | 35 |
| 1   | G     | 336/336 (100%)   | 313 (93%)  | 23 (7%)  | 18          | 29 |
| 2   | B     | 384/385 (100%)   | 357 (93%)  | 27 (7%)  | 18          | 28 |
| 2   | D     | 384/385 (100%)   | 366 (95%)  | 18 (5%)  | 30          | 48 |
| 2   | F     | 384/385 (100%)   | 361 (94%)  | 23 (6%)  | 22          | 35 |
| 2   | H     | 384/385 (100%)   | 363 (94%)  | 21 (6%)  | 25          | 40 |
| All | All   | 2880/2884 (100%) | 2703 (94%) | 177 (6%) | 22          | 34 |

All (177) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 1   | MET  |
| 1   | A     | 4   | THR  |
| 1   | A     | 12  | ARG  |
| 1   | A     | 15  | LEU  |
| 1   | A     | 23  | LEU  |
| 1   | A     | 41  | LEU  |
| 1   | A     | 54  | LEU  |
| 1   | A     | 55  | ARG  |
| 1   | A     | 107 | LEU  |
| 1   | A     | 135 | THR  |
| 1   | A     | 171 | LEU  |
| 1   | A     | 183 | LEU  |
| 1   | A     | 188 | THR  |
| 1   | A     | 237 | LEU  |
| 1   | A     | 267 | PRO  |
| 1   | A     | 286 | LEU  |
| 1   | A     | 301 | LEU  |
| 1   | A     | 328 | LEU  |
| 1   | A     | 334 | LEU  |
| 1   | A     | 360 | LEU  |
| 1   | A     | 376 | ASN  |
| 1   | A     | 391 | ARG  |
| 1   | A     | 402 | THR  |
| 1   | A     | 406 | ARG  |
| 1   | A     | 420 | LEU  |
| 2   | B     | 10  | SER  |
| 2   | B     | 23  | VAL  |
| 2   | B     | 25  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 29  | LEU  |
| 2   | B     | 42  | LEU  |
| 2   | B     | 48  | LEU  |
| 2   | B     | 69  | TYR  |
| 2   | B     | 73  | SER  |
| 2   | B     | 89  | LEU  |
| 2   | B     | 106 | LEU  |
| 2   | B     | 141 | LEU  |
| 2   | B     | 236 | LEU  |
| 2   | B     | 259 | VAL  |
| 2   | B     | 261 | HIS  |
| 2   | B     | 301 | GLU  |
| 2   | B     | 302 | GLU  |
| 2   | B     | 306 | LEU  |
| 2   | B     | 318 | ARG  |
| 2   | B     | 321 | TYR  |
| 2   | B     | 325 | LEU  |
| 2   | B     | 360 | LEU  |
| 2   | B     | 394 | LEU  |
| 2   | B     | 395 | LEU  |
| 2   | B     | 397 | LEU  |
| 2   | B     | 440 | LYS  |
| 2   | B     | 442 | LYS  |
| 2   | B     | 468 | LEU  |
| 1   | C     | 4   | THR  |
| 1   | C     | 15  | LEU  |
| 1   | C     | 32  | LYS  |
| 1   | C     | 41  | LEU  |
| 1   | C     | 54  | LEU  |
| 1   | C     | 62  | LEU  |
| 1   | C     | 107 | LEU  |
| 1   | C     | 171 | LEU  |
| 1   | C     | 188 | THR  |
| 1   | C     | 292 | ASP  |
| 1   | C     | 334 | LEU  |
| 1   | C     | 360 | LEU  |
| 1   | C     | 361 | LEU  |
| 1   | C     | 367 | ARG  |
| 1   | C     | 376 | ASN  |
| 1   | C     | 393 | LEU  |
| 1   | C     | 402 | THR  |
| 1   | C     | 423 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 427 | LEU  |
| 1   | C     | 436 | VAL  |
| 2   | D     | 25  | LYS  |
| 2   | D     | 30  | ILE  |
| 2   | D     | 42  | LEU  |
| 2   | D     | 48  | LEU  |
| 2   | D     | 73  | SER  |
| 2   | D     | 88  | ARG  |
| 2   | D     | 89  | LEU  |
| 2   | D     | 158 | VAL  |
| 2   | D     | 236 | LEU  |
| 2   | D     | 261 | HIS  |
| 2   | D     | 318 | ARG  |
| 2   | D     | 325 | LEU  |
| 2   | D     | 386 | ARG  |
| 2   | D     | 395 | LEU  |
| 2   | D     | 440 | LYS  |
| 2   | D     | 442 | LYS  |
| 2   | D     | 445 | LEU  |
| 2   | D     | 454 | VAL  |
| 1   | E     | 1   | MET  |
| 1   | E     | 4   | THR  |
| 1   | E     | 54  | LEU  |
| 1   | E     | 107 | LEU  |
| 1   | E     | 123 | LEU  |
| 1   | E     | 171 | LEU  |
| 1   | E     | 183 | LEU  |
| 1   | E     | 184 | GLU  |
| 1   | E     | 188 | THR  |
| 1   | E     | 196 | GLU  |
| 1   | E     | 237 | LEU  |
| 1   | E     | 286 | LEU  |
| 1   | E     | 291 | VAL  |
| 1   | E     | 301 | LEU  |
| 1   | E     | 334 | LEU  |
| 1   | E     | 361 | LEU  |
| 1   | E     | 376 | ASN  |
| 1   | E     | 423 | GLU  |
| 1   | E     | 427 | LEU  |
| 1   | E     | 437 | LEU  |
| 2   | F     | 23  | VAL  |
| 2   | F     | 25  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | F     | 30  | ILE  |
| 2   | F     | 48  | LEU  |
| 2   | F     | 69  | TYR  |
| 2   | F     | 71  | LEU  |
| 2   | F     | 73  | SER  |
| 2   | F     | 88  | ARG  |
| 2   | F     | 89  | LEU  |
| 2   | F     | 106 | LEU  |
| 2   | F     | 141 | LEU  |
| 2   | F     | 157 | ARG  |
| 2   | F     | 158 | VAL  |
| 2   | F     | 236 | LEU  |
| 2   | F     | 261 | HIS  |
| 2   | F     | 302 | GLU  |
| 2   | F     | 318 | ARG  |
| 2   | F     | 325 | LEU  |
| 2   | F     | 360 | LEU  |
| 2   | F     | 397 | LEU  |
| 2   | F     | 411 | LYS  |
| 2   | F     | 445 | LEU  |
| 2   | F     | 468 | LEU  |
| 1   | G     | 1   | MET  |
| 1   | G     | 2   | ASP  |
| 1   | G     | 15  | LEU  |
| 1   | G     | 30  | LEU  |
| 1   | G     | 32  | LYS  |
| 1   | G     | 107 | LEU  |
| 1   | G     | 123 | LEU  |
| 1   | G     | 135 | THR  |
| 1   | G     | 171 | LEU  |
| 1   | G     | 183 | LEU  |
| 1   | G     | 188 | THR  |
| 1   | G     | 237 | LEU  |
| 1   | G     | 286 | LEU  |
| 1   | G     | 291 | VAL  |
| 1   | G     | 328 | LEU  |
| 1   | G     | 334 | LEU  |
| 1   | G     | 360 | LEU  |
| 1   | G     | 361 | LEU  |
| 1   | G     | 376 | ASN  |
| 1   | G     | 391 | ARG  |
| 1   | G     | 393 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 423 | GLU  |
| 1   | G     | 437 | LEU  |
| 2   | H     | 23  | VAL  |
| 2   | H     | 25  | LYS  |
| 2   | H     | 27  | GLU  |
| 2   | H     | 48  | LEU  |
| 2   | H     | 106 | LEU  |
| 2   | H     | 141 | LEU  |
| 2   | H     | 157 | ARG  |
| 2   | H     | 221 | ARG  |
| 2   | H     | 227 | ARG  |
| 2   | H     | 236 | LEU  |
| 2   | H     | 261 | HIS  |
| 2   | H     | 295 | PRO  |
| 2   | H     | 302 | GLU  |
| 2   | H     | 318 | ARG  |
| 2   | H     | 325 | LEU  |
| 2   | H     | 329 | ARG  |
| 2   | H     | 360 | LEU  |
| 2   | H     | 395 | LEU  |
| 2   | H     | 434 | MET  |
| 2   | H     | 464 | LYS  |
| 2   | H     | 473 | GLU  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 83  | GLN  |
| 1   | A     | 376 | ASN  |
| 2   | B     | 34  | HIS  |
| 2   | B     | 235 | GLN  |
| 2   | B     | 263 | ASN  |
| 2   | B     | 380 | GLN  |
| 1   | C     | 83  | GLN  |
| 1   | C     | 222 | HIS  |
| 1   | C     | 376 | ASN  |
| 2   | D     | 179 | GLN  |
| 2   | D     | 235 | GLN  |
| 2   | D     | 263 | ASN  |
| 1   | E     | 60  | GLN  |
| 1   | E     | 83  | GLN  |
| 1   | E     | 376 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | F     | 179 | GLN  |
| 2   | F     | 235 | GLN  |
| 2   | F     | 375 | HIS  |
| 1   | G     | 60  | GLN  |
| 1   | G     | 83  | GLN  |
| 1   | G     | 222 | HIS  |
| 1   | G     | 354 | HIS  |
| 1   | G     | 376 | ASN  |
| 2   | H     | 179 | GLN  |
| 2   | H     | 235 | 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 3   | PLP  | B     | 1475 | 3    | 15,15,16     | 1.68 | 3 (20%)     | 20,22,23    | 1.82 | 3 (15%)     |
| 3   | AOA  | B     | 1476 | 3    | 1,5,5        | 0.34 | 0           | 0,5,5       | 0.00 | -           |
| 3   | PLP  | D     | 2475 | 3    | 15,15,16     | 1.74 | 4 (26%)     | 20,22,23    | 1.93 | 3 (15%)     |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | AOA  | D     | 2476 | 3    | 1,5,5        | 0.59 | 0        | 0,5,5       | 0.00 | -        |
| 3   | PLP  | F     | 3475 | 3    | 15,15,16     | 1.61 | 2 (13%)  | 20,22,23    | 1.82 | 3 (15%)  |
| 3   | AOA  | F     | 3476 | 3    | 1,5,5        | 0.25 | 0        | 0,5,5       | 0.00 | -        |
| 3   | PLP  | H     | 4475 | 3    | 15,15,16     | 1.80 | 3 (20%)  | 20,22,23    | 1.77 | 3 (15%)  |
| 3   | AOA  | H     | 4476 | 3    | 1,5,5        | 0.33 | 0        | 0,5,5       | 0.00 | -        |

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   | PLP  | B     | 1475 | 3    | -       | 0/6/6/8  | 0/1/1/1 |
| 3   | AOA  | B     | 1476 | 3    | -       | 0/0/3/3  | 0/0/0/0 |
| 3   | PLP  | D     | 2475 | 3    | -       | 0/6/6/8  | 0/1/1/1 |
| 3   | AOA  | D     | 2476 | 3    | -       | 0/0/3/3  | 0/0/0/0 |
| 3   | PLP  | F     | 3475 | 3    | -       | 0/6/6/8  | 0/1/1/1 |
| 3   | AOA  | F     | 3476 | 3    | -       | 0/0/3/3  | 0/0/0/0 |
| 3   | PLP  | H     | 4475 | 3    | -       | 0/6/6/8  | 0/1/1/1 |
| 3   | AOA  | H     | 4476 | 3    | -       | 0/0/3/3  | 0/0/0/0 |

All (12) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 3   | D     | 2475 | PLP  | C3-C2  | -2.50 | 1.39        | 1.40     |
| 3   | H     | 4475 | PLP  | C3-C2  | -2.37 | 1.39        | 1.40     |
| 3   | D     | 2475 | PLP  | C2A-C2 | 2.11  | 1.54        | 1.50     |
| 3   | B     | 1475 | PLP  | C2A-C2 | 2.15  | 1.54        | 1.50     |
| 3   | F     | 3475 | PLP  | C2-N1  | 2.56  | 1.39        | 1.33     |
| 3   | H     | 4475 | PLP  | C2-N1  | 2.67  | 1.39        | 1.33     |
| 3   | D     | 2475 | PLP  | C2-N1  | 2.69  | 1.39        | 1.33     |
| 3   | B     | 1475 | PLP  | C2-N1  | 2.79  | 1.39        | 1.33     |
| 3   | F     | 3475 | PLP  | C5-C4  | 3.41  | 1.44        | 1.40     |
| 3   | B     | 1475 | PLP  | C5-C4  | 3.93  | 1.45        | 1.40     |
| 3   | D     | 2475 | PLP  | C5-C4  | 3.96  | 1.45        | 1.40     |
| 3   | H     | 4475 | PLP  | C5-C4  | 4.35  | 1.45        | 1.40     |

All (12) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 3   | D     | 2475 | PLP  | C5A-C5-C6 | -2.43 | 115.14      | 119.33   |
| 3   | B     | 1475 | PLP  | C5A-C5-C6 | -2.38 | 115.24      | 119.33   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3   | H     | 4475 | PLP  | C5A-C5-C6  | -2.33 | 115.33      | 119.33   |
| 3   | D     | 2475 | PLP  | C5-C6-N1   | -2.24 | 120.07      | 123.87   |
| 3   | H     | 4475 | PLP  | C5-C6-N1   | -2.24 | 120.08      | 123.87   |
| 3   | F     | 3475 | PLP  | C5A-C5-C6  | -2.23 | 115.49      | 119.33   |
| 3   | F     | 3475 | PLP  | C5-C6-N1   | -2.08 | 120.35      | 123.87   |
| 3   | B     | 1475 | PLP  | C5-C6-N1   | -2.05 | 120.39      | 123.87   |
| 3   | H     | 4475 | PLP  | O4P-C5A-C5 | 5.92  | 121.23      | 109.32   |
| 3   | F     | 3475 | PLP  | O4P-C5A-C5 | 6.17  | 121.72      | 109.32   |
| 3   | B     | 1475 | PLP  | O4P-C5A-C5 | 6.29  | 121.97      | 109.32   |
| 3   | D     | 2475 | PLP  | O4P-C5A-C5 | 6.70  | 122.80      | 109.32   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 15 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | B     | 1476 | AOA  | 3       | 0            |
| 3   | D     | 2476 | AOA  | 6       | 0            |
| 3   | F     | 3476 | AOA  | 4       | 0            |
| 3   | H     | 4476 | AOA  | 2       | 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     | 437/438 (99%)   | -0.19  | 2 (0%) 90 89  | 20, 33, 48, 55        | 0     |
| 1   | C     | 437/438 (99%)   | -0.26  | 0 100 100     | 20, 34, 49, 59        | 0     |
| 1   | E     | 437/438 (99%)   | -0.21  | 2 (0%) 90 89  | 22, 33, 47, 57        | 0     |
| 1   | G     | 437/438 (99%)   | -0.30  | 0 100 100     | 23, 33, 48, 57        | 0     |
| 2   | B     | 473/474 (99%)   | -0.24  | 5 (1%) 80 79  | 20, 30, 49, 61        | 0     |
| 2   | D     | 473/474 (99%)   | -0.20  | 12 (2%) 58 55 | 24, 36, 56, 72        | 0     |
| 2   | F     | 473/474 (99%)   | -0.21  | 6 (1%) 77 75  | 19, 32, 49, 62        | 0     |
| 2   | H     | 473/474 (99%)   | -0.15  | 8 (1%) 70 68  | 25, 38, 58, 69        | 0     |
| All | All   | 3640/3648 (99%) | -0.22  | 35 (0%) 82 80 | 19, 33, 51, 72        | 0     |

All (35) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | H     | 301 | GLU  | 4.6  |
| 2   | H     | 154 | ARG  | 4.2  |
| 2   | D     | 302 | GLU  | 3.7  |
| 2   | H     | 383 | GLU  | 3.4  |
| 2   | D     | 301 | GLU  | 3.2  |
| 2   | F     | 30  | ILE  | 3.0  |
| 2   | D     | 300 | GLY  | 3.0  |
| 1   | A     | 363 | VAL  | 2.8  |
| 2   | B     | 443 | GLU  | 2.8  |
| 2   | D     | 181 | ARG  | 2.7  |
| 2   | H     | 302 | GLU  | 2.7  |
| 2   | F     | 33  | GLU  | 2.6  |
| 2   | F     | 32  | LYS  | 2.6  |
| 2   | H     | 188 | GLU  | 2.6  |
| 1   | E     | 358 | ALA  | 2.5  |
| 2   | D     | 386 | ARG  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | D     | 197 | LYS  | 2.5  |
| 2   | D     | 383 | GLU  | 2.5  |
| 2   | B     | 32  | LYS  | 2.4  |
| 2   | F     | 154 | ARG  | 2.4  |
| 2   | B     | 301 | GLU  | 2.3  |
| 2   | B     | 383 | GLU  | 2.3  |
| 2   | H     | 366 | ARG  | 2.2  |
| 2   | B     | 326 | ALA  | 2.2  |
| 2   | D     | 474 | GLY  | 2.2  |
| 2   | D     | 154 | ARG  | 2.2  |
| 2   | H     | 203 | HIS  | 2.1  |
| 2   | H     | 231 | GLU  | 2.1  |
| 2   | D     | 203 | HIS  | 2.1  |
| 1   | E     | 293 | VAL  | 2.0  |
| 2   | D     | 385 | PHE  | 2.0  |
| 1   | A     | 436 | VAL  | 2.0  |
| 2   | D     | 303 | GLY  | 2.0  |
| 2   | F     | 153 | GLY  | 2.0  |
| 2   | F     | 383 | GLU  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 3   | AOA  | H     | 4476 | 6/6   | 0.58 | 0.47 | 13.46 | 61,62,63,64                | 0     |
| 3   | AOA  | D     | 2476 | 6/6   | 0.58 | 0.46 | 12.07 | 63,64,67,68                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 3   | AOA  | B     | 1476 | 6/6   | 0.65 | 0.43 | 8.16 | 54,55,62,63                 | 0     |
| 3   | AOA  | F     | 3476 | 6/6   | 0.65 | 0.46 | 6.24 | 57,57,62,63                 | 0     |
| 3   | PLP  | D     | 2475 | 15/16 | 0.94 | 0.24 | 2.11 | 40,60,64,66                 | 0     |
| 3   | PLP  | H     | 4475 | 15/16 | 0.93 | 0.24 | 1.87 | 37,54,59,62                 | 0     |
| 3   | PLP  | B     | 1475 | 15/16 | 0.95 | 0.22 | 1.14 | 32,53,57,60                 | 0     |
| 3   | PLP  | F     | 3475 | 15/16 | 0.96 | 0.21 | 0.65 | 28,51,55,58                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.