



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 06:56 am BST

PDB ID : 2G3M  
Title : Crystal structure of the Sulfolobus solfataricus alpha-glucosidase MalA  
Authors : Ernst, H.A.; Lo Leggio, L.; Willemoes, M.; Leonard, G.; Blum, P.; Larsen, S.  
Deposited on : 2006-02-20  
Resolution : 2.55 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

|                                |   |  |
|--------------------------------|---|--|
| MolProbity                     | : | 4.02b-467  |
| Xtriage (Phenix)               | : | 1.13   |
| EDS                            | : | 2.11   |
| Percentile statistics          | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac                         | : | 5.8.0158   |
| CCP4                           | : | 7.0.044 (Gargrove)   |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)  |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)  |
| Validation Pipeline (wwPDB-VP) | : | 2.11   |

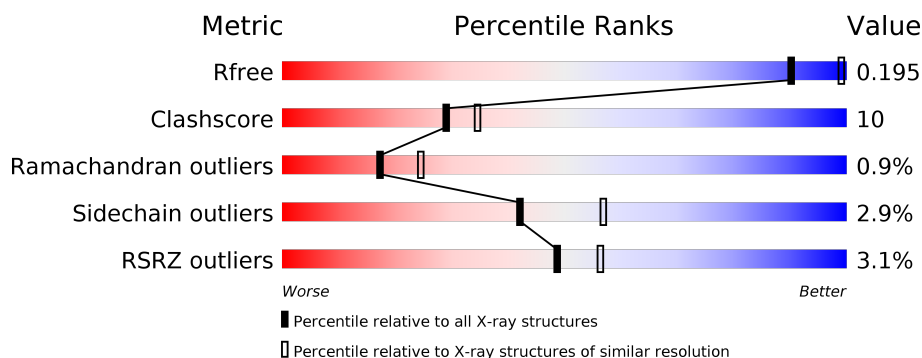
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 1284 (2.56-2.52)                                      |
| Clashscore            | 141614                      | 1332 (2.56-2.52)                                      |
| Ramachandran outliers | 138981                      | 1315 (2.56-2.52)                                      |
| Sidechain outliers    | 138945                      | 1315 (2.56-2.52)                                      |
| RSRZ outliers         | 127900                      | 1272 (2.56-2.52)                                      |

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

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | A     | 693    | <div> <div>3%</div> <div> <div></div> <div>76%</div> <div>23%</div> </div> <div></div> </div> |
| 1   | B     | 693    | <div> <div>2%</div> <div> <div></div> <div>76%</div> <div>23%</div> </div> <div></div> </div> |
| 1   | C     | 693    | <div> <div>4%</div> <div> <div></div> <div>75%</div> <div>24%</div> </div> <div></div> </div> |
| 1   | D     | 693    | <div> <div>3%</div> <div> <div></div> <div>75%</div> <div>24%</div> </div> <div></div> </div> |
| 1   | E     | 693    | <div> <div>2%</div> <div> <div></div> <div>78%</div> <div>20%</div> </div> <div></div> </div> |
| 1   | F     | 693    | <div> <div>3%</div> <div> <div></div> <div>76%</div> <div>22%</div> </div> <div></div> </div> |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 35378 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 Alpha-glucosidase.

| Mol | Chain | Residues | Atoms |      |     |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|---------|-------|
| 1   | A     | 691      | Total | C    | N   | O    | S  | 0       | 1       | 0     |
|     |       |          | 5684  | 3703 | 919 | 1047 | 15 |         |         |       |
| 1   | B     | 691      | Total | C    | N   | O    | S  | 0       | 1       | 0     |
|     |       |          | 5684  | 3703 | 919 | 1047 | 15 |         |         |       |
| 1   | C     | 691      | Total | C    | N   | O    | S  | 0       | 1       | 0     |
|     |       |          | 5684  | 3703 | 919 | 1047 | 15 |         |         |       |
| 1   | D     | 691      | Total | C    | N   | O    | S  | 0       | 1       | 0     |
|     |       |          | 5684  | 3703 | 919 | 1047 | 15 |         |         |       |
| 1   | E     | 691      | Total | C    | N   | O    | S  | 0       | 1       | 0     |
|     |       |          | 5684  | 3703 | 919 | 1047 | 15 |         |         |       |
| 1   | F     | 692      | Total | C    | N   | O    | S  | 0       | 1       | 0     |
|     |       |          | 5695  | 3709 | 923 | 1048 | 15 |         |         |       |

There are 24 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| A     | 1       | MET      | -      | CLONING ARTIFACT | UNP O59645 |
| A     | 2       | ARG      | -      | CLONING ARTIFACT | UNP O59645 |
| A     | 3       | ILE      | -      | CLONING ARTIFACT | UNP O59645 |
| A     | 4       | LEU      | -      | CLONING ARTIFACT | UNP O59645 |
| B     | 1       | MET      | -      | CLONING ARTIFACT | UNP O59645 |
| B     | 2       | ARG      | -      | CLONING ARTIFACT | UNP O59645 |
| B     | 3       | ILE      | -      | CLONING ARTIFACT | UNP O59645 |
| B     | 4       | LEU      | -      | CLONING ARTIFACT | UNP O59645 |
| C     | 1       | MET      | -      | CLONING ARTIFACT | UNP O59645 |
| C     | 2       | ARG      | -      | CLONING ARTIFACT | UNP O59645 |
| C     | 3       | ILE      | -      | CLONING ARTIFACT | UNP O59645 |
| C     | 4       | LEU      | -      | CLONING ARTIFACT | UNP O59645 |
| D     | 1       | MET      | -      | CLONING ARTIFACT | UNP O59645 |
| D     | 2       | ARG      | -      | CLONING ARTIFACT | UNP O59645 |
| D     | 3       | ILE      | -      | CLONING ARTIFACT | UNP O59645 |
| D     | 4       | LEU      | -      | CLONING ARTIFACT | UNP O59645 |
| E     | 1       | MET      | -      | CLONING ARTIFACT | UNP O59645 |

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| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| E     | 2       | ARG      | -      | CLONING ARTIFACT | UNP O59645 |
| E     | 3       | ILE      | -      | CLONING ARTIFACT | UNP O59645 |
| E     | 4       | LEU      | -      | CLONING ARTIFACT | UNP O59645 |
| F     | 1       | MET      | -      | CLONING ARTIFACT | UNP O59645 |
| F     | 2       | ARG      | -      | CLONING ARTIFACT | UNP O59645 |
| F     | 3       | ILE      | -      | CLONING ARTIFACT | UNP O59645 |
| F     | 4       | LEU      | -      | CLONING ARTIFACT | UNP O59645 |

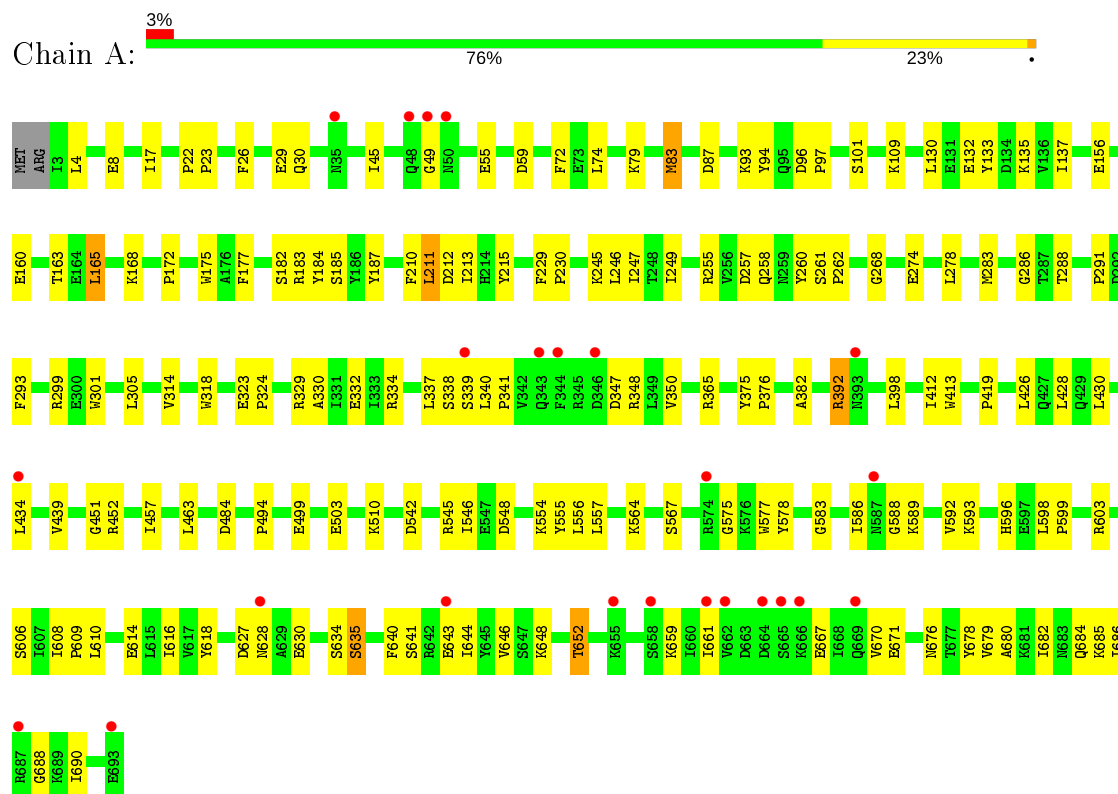
- Molecule 2 is water.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 2   | A     | 213      | Total O<br>213 213 | 0       | 0       |
| 2   | B     | 210      | Total O<br>210 210 | 0       | 0       |
| 2   | C     | 178      | Total O<br>178 178 | 0       | 0       |
| 2   | D     | 221      | Total O<br>221 221 | 0       | 0       |
| 2   | E     | 249      | Total O<br>249 249 | 0       | 0       |
| 2   | F     | 192      | Total O<br>192 192 | 0       | 0       |

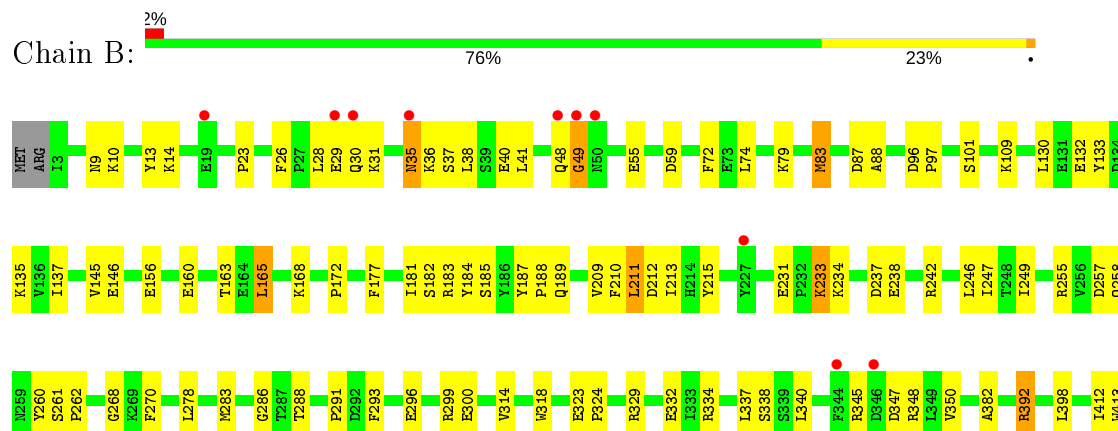
### 3 Residue-property plots

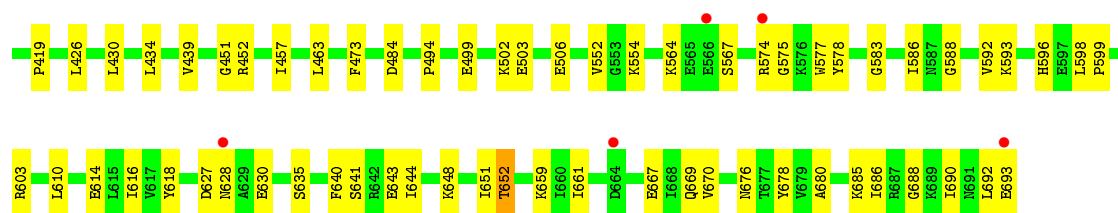
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: Alpha-glucosidase

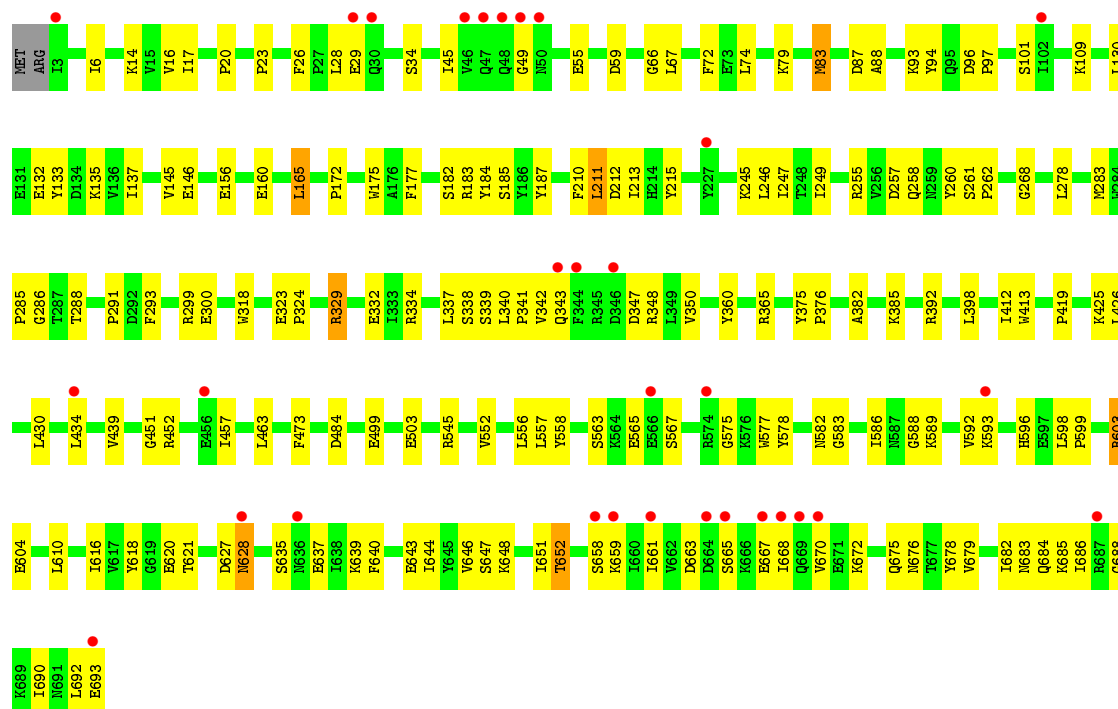
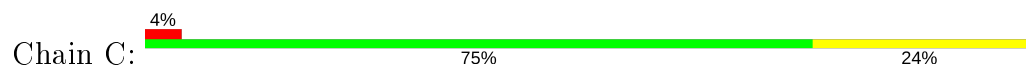


#### • Molecule 1: Alpha-glucosidase

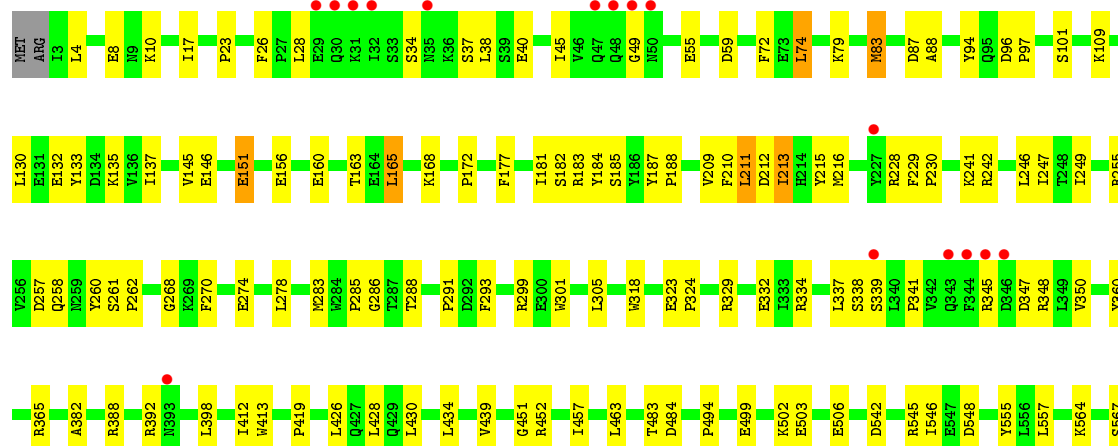
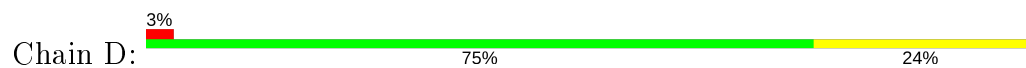


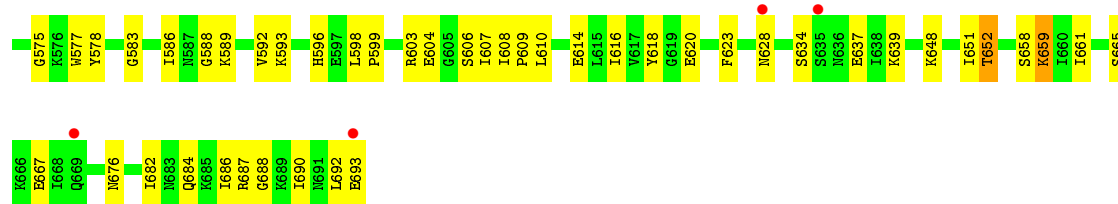


● Molecule 1: Alpha-glucosidase

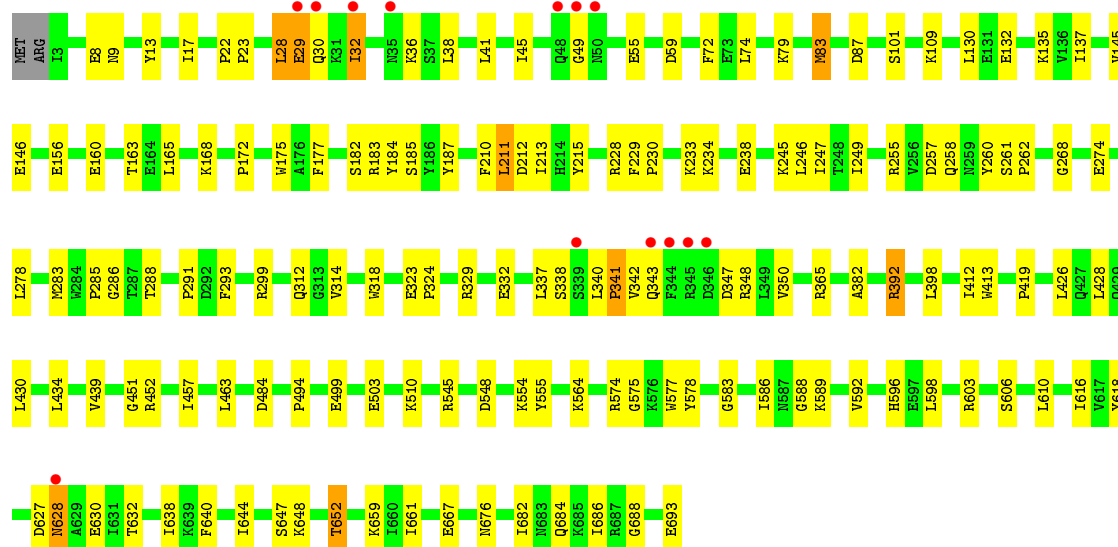
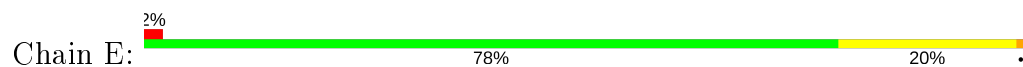


● Molecule 1: Alpha-glucosidase

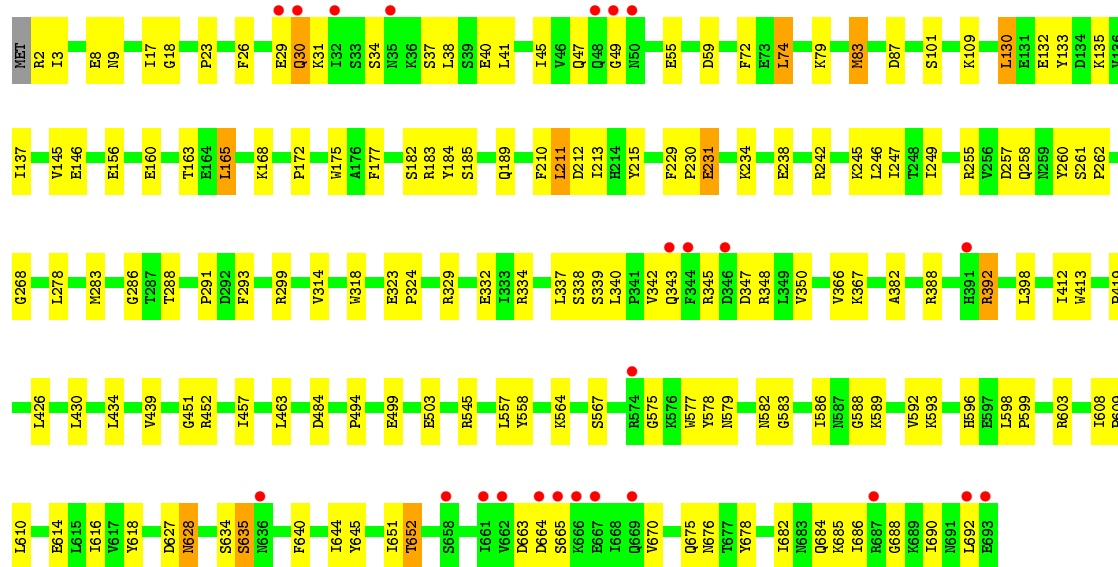
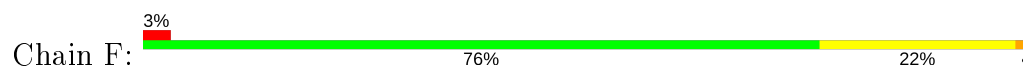




● Molecule 1: Alpha-glucosidase



● Molecule 1: Alpha-glucosidase



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1 21 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 103.17Å 173.56Å 154.08Å<br>90.00° 108.00° 90.00°            | Depositor        |
| Resolution (Å)  | 34.25 – 2.55<br>34.25 – 2.55                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.9 (34.25-2.55)<br>100.0 (34.25-2.55)                     | Depositor<br>EDS |
| $R_{merge}$   | 0.09  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 5.95 (at 2.54Å)   | Xtriage          |
| Refinement program  | CNS 1.1   | Depositor        |
| R, $R_{free}$   | 0.170 , 0.195<br>0.171 , 0.195                              | Depositor<br>DCC |
| $R_{free}$ test set   | 8380 reflections (5.01%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 33.7  | Xtriage          |
| Anisotropy  | 0.344   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.36 , 41.6   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction   | 0.018 for h,-k,-h-l   | Xtriage          |
| $F_o, F_c$ correlation  | 0.95  | EDS              |
| Total number of atoms   | 35378   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 34.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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](#)

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     | 0.36         | 0/5838      | 0.61        | 0/7902      |
| 1   | B     | 0.36         | 0/5838      | 0.61        | 0/7902      |
| 1   | C     | 0.36         | 0/5838      | 0.60        | 0/7902      |
| 1   | D     | 0.37         | 0/5838      | 0.61        | 0/7902      |
| 1   | E     | 0.37         | 0/5838      | 0.62        | 0/7902      |
| 1   | F     | 0.36         | 0/5849      | 0.61        | 0/7916      |
| All | All   | 0.36         | 0/35039     | 0.61        | 0/47426     |

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     | 5684  | 0        | 5651     | 109     | 0            |
| 1   | B     | 5684  | 0        | 5651     | 115     | 0            |
| 1   | C     | 5684  | 0        | 5651     | 125     | 0            |
| 1   | D     | 5684  | 0        | 5651     | 127     | 0            |
| 1   | E     | 5684  | 0        | 5651     | 111     | 0            |
| 1   | F     | 5695  | 0        | 5664     | 123     | 0            |
| 2   | A     | 213   | 0        | 0        | 2       | 0            |
| 2   | B     | 210   | 0        | 0        | 3       | 0            |
| 2   | C     | 178   | 0        | 0        | 2       | 0            |
| 2   | D     | 221   | 0        | 0        | 3       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | E     | 249   | 0        | 0        | 4       | 0            |
| 2   | F     | 192   | 0        | 0        | 4       | 0            |
| All | All   | 35378 | 0        | 33919    | 651     | 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 10.

All (651) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:661:ILE:HG12 | 1:D:667:GLU:HG2  | 1.41                     | 1.02              |
| 1:A:258:GLN:HG3  | 1:E:278:LEU:HD21 | 1.51                     | 0.93              |
| 1:D:564:LYS:H    | 1:D:564:LYS:HD2  | 1.31                     | 0.91              |
| 1:B:564:LYS:H    | 1:B:564:LYS:HD2  | 1.37                     | 0.88              |
| 1:B:35:ASN:H     | 1:B:35:ASN:HD22  | 1.23                     | 0.85              |
| 1:B:258:GLN:HG3  | 1:D:278:LEU:HD21 | 1.58                     | 0.85              |
| 1:E:163:THR:HG22 | 1:E:168:LYS:HD3  | 1.57                     | 0.83              |
| 1:C:686:ILE:HD13 | 1:C:690:ILE:HD11 | 1.57                     | 0.83              |
| 1:C:278:LEU:HD21 | 1:F:258:GLN:HG3  | 1.58                     | 0.83              |
| 1:C:299:ARG:HG3  | 1:C:382:ALA:HB2  | 1.60                     | 0.82              |
| 1:C:596:HIS:HD2  | 1:C:598:LEU:H    | 1.26                     | 0.82              |
| 1:C:332:GLU:HG3  | 1:F:332:GLU:HG3  | 1.60                     | 0.81              |
| 1:A:686:ILE:HD13 | 1:A:690:ILE:HD11 | 1.63                     | 0.81              |
| 1:D:341:PRO:HA   | 1:F:345:ARG:NH1  | 1.97                     | 0.80              |
| 1:B:278:LEU:HD21 | 1:D:258:GLN:HG3  | 1.61                     | 0.79              |
| 1:E:577:TRP:CZ3  | 1:E:603:ARG:HB3  | 2.16                     | 0.79              |
| 1:A:670:VAL:CG1  | 1:A:678:TYR:HB3  | 2.11                     | 0.79              |
| 1:D:651:ILE:HD13 | 1:D:692:LEU:HD21 | 1.65                     | 0.78              |
| 1:C:299:ARG:CG   | 1:C:382:ALA:HB2  | 2.14                     | 0.78              |
| 1:D:299:ARG:HG3  | 1:D:382:ALA:HB2  | 1.66                     | 0.78              |
| 1:A:610:LEU:HD11 | 1:A:616:ILE:HD11 | 1.66                     | 0.77              |
| 1:A:163:THR:HG22 | 1:A:168:LYS:HD3  | 1.67                     | 0.77              |
| 1:B:564:LYS:N    | 1:B:564:LYS:HD2  | 1.98                     | 0.77              |
| 1:E:299:ARG:HG3  | 1:E:382:ALA:HB2  | 1.66                     | 0.77              |
| 1:F:163:THR:HG22 | 1:F:168:LYS:HD3  | 1.68                     | 0.76              |
| 1:C:596:HIS:CD2  | 1:C:598:LEU:H    | 2.02                     | 0.76              |
| 1:D:618:TYR:HB2  | 1:D:652:THR:HG23 | 1.66                     | 0.76              |
| 1:F:8:GLU:HB2    | 1:F:34:SER:HB2   | 1.68                     | 0.75              |
| 1:D:163:THR:HG22 | 1:D:168:LYS:HD3  | 1.69                     | 0.75              |
| 1:D:564:LYS:HD2  | 1:D:564:LYS:N    | 2.02                     | 0.75              |
| 1:E:163:THR:CG2  | 1:E:168:LYS:HD3  | 2.17                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:596:HIS:HD2  | 1:F:598:LEU:H    | 1.35                     | 0.74              |
| 1:B:314:VAL:O    | 1:B:392:ARG:NH2  | 2.20                     | 0.74              |
| 1:B:35:ASN:H     | 1:B:35:ASN:ND2   | 1.86                     | 0.73              |
| 1:B:347:ASP:O    | 1:B:350:VAL:HG12 | 1.89                     | 0.73              |
| 1:B:299:ARG:HG2  | 1:B:382:ALA:HB2  | 1.70                     | 0.73              |
| 1:C:567:SER:OG   | 1:C:593:LYS:HE3  | 1.89                     | 0.73              |
| 1:F:37:SER:OG    | 1:F:40:GLU:HG3   | 1.88                     | 0.73              |
| 1:B:299:ARG:CG   | 1:B:382:ALA:HB2  | 2.19                     | 0.72              |
| 1:B:37:SER:OG    | 1:B:40:GLU:HG3   | 1.89                     | 0.72              |
| 1:E:596:HIS:HD2  | 1:E:598:LEU:H    | 1.37                     | 0.72              |
| 1:E:299:ARG:CG   | 1:E:382:ALA:HB2  | 2.18                     | 0.72              |
| 1:E:38:LEU:HD21  | 1:E:45:ILE:HD12  | 1.71                     | 0.72              |
| 1:B:651:ILE:HD13 | 1:B:692:LEU:HD21 | 1.72                     | 0.72              |
| 1:F:596:HIS:CD2  | 1:F:598:LEU:H    | 2.08                     | 0.72              |
| 1:B:596:HIS:HD2  | 1:B:598:LEU:H    | 1.36                     | 0.71              |
| 1:A:686:ILE:CD1  | 1:A:690:ILE:HD11 | 2.20                     | 0.71              |
| 1:B:36:LYS:HE3   | 2:B:896:HOH:O    | 1.89                     | 0.71              |
| 1:D:686:ILE:HD13 | 1:D:690:ILE:HD11 | 1.72                     | 0.71              |
| 1:C:618:TYR:HB2  | 1:C:652:THR:HG23 | 1.71                     | 0.70              |
| 1:C:258:GLN:HG3  | 1:F:278:LEU:HD21 | 1.71                     | 0.70              |
| 1:A:258:GLN:CG   | 1:E:278:LEU:HD21 | 2.19                     | 0.70              |
| 1:B:686:ILE:HD13 | 1:B:690:ILE:HD11 | 1.72                     | 0.70              |
| 1:A:670:VAL:HG11 | 1:A:678:TYR:HB3  | 1.71                     | 0.70              |
| 1:C:425:LYS:HG3  | 2:C:832:HOH:O    | 1.92                     | 0.70              |
| 1:D:299:ARG:CG   | 1:D:382:ALA:HB2  | 2.22                     | 0.69              |
| 1:A:286:GLY:O    | 1:A:288:THR:HG23 | 1.93                     | 0.69              |
| 1:A:8:GLU:O      | 1:A:30:GLN:HG3   | 1.93                     | 0.69              |
| 1:C:17:ILE:HD11  | 1:C:45:ILE:HD13  | 1.74                     | 0.69              |
| 1:E:13:TYR:CE2   | 1:E:36:LYS:HG3   | 2.27                     | 0.69              |
| 1:B:268:GLY:H    | 1:D:258:GLN:HG2  | 1.59                     | 0.68              |
| 1:C:286:GLY:O    | 1:C:288:THR:HG23 | 1.94                     | 0.68              |
| 1:A:630:GLU:HB2  | 1:A:641:SER:HB3  | 1.76                     | 0.68              |
| 1:F:299:ARG:CG   | 1:F:382:ALA:HB2  | 2.24                     | 0.68              |
| 1:F:610:LEU:HD11 | 1:F:616:ILE:HD11 | 1.74                     | 0.67              |
| 1:A:314:VAL:O    | 1:A:392:ARG:NH2  | 2.28                     | 0.67              |
| 1:B:233:LYS:HE3  | 1:B:237:ASP:OD2  | 1.94                     | 0.67              |
| 1:B:286:GLY:O    | 1:B:288:THR:HG23 | 1.94                     | 0.67              |
| 1:C:278:LEU:HD21 | 1:F:258:GLN:CG   | 2.25                     | 0.67              |
| 1:B:185:SER:OG   | 1:B:212:ASP:HB3  | 1.95                     | 0.67              |
| 1:B:14:LYS:HD2   | 1:B:28:LEU:HD12  | 1.76                     | 0.67              |
| 1:A:278:LEU:HD21 | 1:E:258:GLN:HG3  | 1.76                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:646:VAL:HG21 | 1:C:686:ILE:HD12 | 1.77                     | 0.67              |
| 1:D:286:GLY:O    | 1:D:288:THR:HG23 | 1.95                     | 0.67              |
| 1:A:567:SER:OG   | 1:A:593:LYS:HE3  | 1.95                     | 0.66              |
| 1:C:563:SER:OG   | 1:C:565:GLU:HG2  | 1.95                     | 0.66              |
| 1:E:286:GLY:O    | 1:E:288:THR:HG23 | 1.95                     | 0.66              |
| 1:B:258:GLN:HG2  | 1:D:268:GLY:H    | 1.60                     | 0.66              |
| 1:B:258:GLN:CG   | 1:D:278:LEU:HD21 | 2.23                     | 0.66              |
| 1:F:38:LEU:HD21  | 1:F:45:ILE:HD12  | 1.76                     | 0.66              |
| 1:E:314:VAL:O    | 1:E:392:ARG:NH2  | 2.29                     | 0.66              |
| 1:F:286:GLY:O    | 1:F:288:THR:HG23 | 1.96                     | 0.66              |
| 1:D:577:TRP:CZ3  | 1:D:603:ARG:HB3  | 2.31                     | 0.66              |
| 1:C:337:LEU:HD21 | 1:F:337:LEU:HD21 | 1.76                     | 0.65              |
| 1:F:686:ILE:CD1  | 1:F:690:ILE:HD11 | 2.27                     | 0.65              |
| 1:C:185:SER:OG   | 1:C:212:ASP:HB3  | 1.95                     | 0.65              |
| 1:A:185:SER:OG   | 1:A:212:ASP:HB3  | 1.96                     | 0.65              |
| 1:B:278:LEU:HD21 | 1:D:258:GLN:CG   | 2.27                     | 0.65              |
| 1:A:452:ARG:HD3  | 1:A:484:ASP:O    | 1.97                     | 0.65              |
| 1:E:185:SER:OG   | 1:E:212:ASP:HB3  | 1.97                     | 0.65              |
| 1:F:185:SER:OG   | 1:F:212:ASP:HB3  | 1.97                     | 0.65              |
| 1:E:30:GLN:O     | 1:E:32:ILE:HG22  | 1.97                     | 0.65              |
| 1:F:651:ILE:HD13 | 1:F:692:LEU:HD21 | 1.78                     | 0.65              |
| 1:A:163:THR:CG2  | 1:A:168:LYS:HD3  | 2.26                     | 0.64              |
| 1:D:564:LYS:CD   | 1:D:564:LYS:H    | 2.08                     | 0.64              |
| 1:D:185:SER:OG   | 1:D:212:ASP:HB3  | 1.96                     | 0.64              |
| 1:F:682:ILE:HG22 | 1:F:684:GLN:HG2  | 1.80                     | 0.64              |
| 1:B:334:ARG:O    | 1:B:338:SER:HB2  | 1.98                     | 0.64              |
| 1:B:337:LEU:HD21 | 1:D:337:LEU:HD21 | 1.79                     | 0.64              |
| 1:F:23:PRO:HG3   | 2:F:722:HOH:O    | 1.97                     | 0.63              |
| 1:B:564:LYS:H    | 1:B:564:LYS:CD   | 2.11                     | 0.63              |
| 1:C:258:GLN:HG2  | 1:F:268:GLY:H    | 1.63                     | 0.63              |
| 1:C:23:PRO:HG3   | 2:C:722:HOH:O    | 1.98                     | 0.63              |
| 1:B:452:ARG:HD3  | 1:B:484:ASP:O    | 1.99                     | 0.63              |
| 1:C:332:GLU:CG   | 1:F:332:GLU:HG3  | 2.28                     | 0.63              |
| 1:E:452:ARG:HD3  | 1:E:484:ASP:O    | 1.99                     | 0.63              |
| 1:F:452:ARG:HD3  | 1:F:484:ASP:O    | 1.98                     | 0.63              |
| 1:F:567:SER:OG   | 1:F:593:LYS:HE3  | 1.98                     | 0.63              |
| 1:E:554:LYS:O    | 1:E:603:ARG:HD3  | 1.99                     | 0.63              |
| 1:A:577:TRP:CZ3  | 1:A:603:ARG:HB3  | 2.33                     | 0.63              |
| 1:B:23:PRO:HG3   | 2:B:722:HOH:O    | 1.99                     | 0.63              |
| 1:D:452:ARG:HD3  | 1:D:484:ASP:O    | 1.97                     | 0.63              |
| 1:B:574:ARG:HD3  | 2:B:876:HOH:O    | 1.99                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:577:TRP:CZ3  | 1:B:603:ARG:HB3  | 2.34                     | 0.63              |
| 1:F:610:LEU:HB2  | 1:F:614:GLU:HB3  | 1.79                     | 0.63              |
| 1:A:596:HIS:HD2  | 1:A:598:LEU:H    | 1.46                     | 0.62              |
| 1:F:575:GLY:O    | 1:F:588:GLY:N    | 2.33                     | 0.62              |
| 1:F:618:TYR:HB2  | 1:F:652:THR:HG23 | 1.80                     | 0.62              |
| 1:C:339:SER:HB3  | 1:D:339:SER:CB   | 2.29                     | 0.62              |
| 1:A:261:SER:HB3  | 1:A:262:PRO:HD3  | 1.81                     | 0.62              |
| 1:C:452:ARG:HD3  | 1:C:484:ASP:O    | 1.99                     | 0.62              |
| 1:D:87:ASP:O     | 1:D:348:ARG:HD3  | 2.00                     | 0.62              |
| 1:B:87:ASP:O     | 1:B:348:ARG:HD3  | 2.00                     | 0.62              |
| 1:D:323:GLU:N    | 1:D:324:PRO:HA   | 2.15                     | 0.62              |
| 1:F:686:ILE:HD13 | 1:F:690:ILE:HD11 | 1.82                     | 0.62              |
| 1:B:163:THR:HG22 | 1:B:168:LYS:HD3  | 1.82                     | 0.61              |
| 1:A:299:ARG:CG   | 1:A:382:ALA:HB2  | 2.29                     | 0.61              |
| 1:E:574:ARG:HD3  | 2:E:893:HOH:O    | 2.00                     | 0.61              |
| 1:F:87:ASP:O     | 1:F:348:ARG:HD3  | 2.00                     | 0.61              |
| 1:F:299:ARG:HG2  | 1:F:382:ALA:HB2  | 1.81                     | 0.61              |
| 1:C:683:ASN:H    | 1:C:683:ASN:HD22 | 1.47                     | 0.61              |
| 1:D:23:PRO:HG3   | 2:D:721:HOH:O    | 2.00                     | 0.61              |
| 1:F:17:ILE:HD11  | 1:F:45:ILE:HD13  | 1.83                     | 0.61              |
| 1:B:596:HIS:CD2  | 1:B:598:LEU:H    | 2.17                     | 0.61              |
| 1:F:261:SER:HB3  | 1:F:262:PRO:HD3  | 1.82                     | 0.61              |
| 1:B:55:GLU:HG2   | 1:B:137:ILE:HG12 | 1.82                     | 0.61              |
| 1:C:261:SER:HB3  | 1:C:262:PRO:HD3  | 1.83                     | 0.61              |
| 1:C:627:ASP:O    | 1:C:628:ASN:HB3  | 1.99                     | 0.61              |
| 1:A:661:ILE:HG12 | 1:A:667:GLU:HG2  | 1.83                     | 0.60              |
| 1:B:261:SER:HB3  | 1:B:262:PRO:HD3  | 1.82                     | 0.60              |
| 1:C:26:PHE:HB3   | 1:C:165:LEU:HD22 | 1.83                     | 0.60              |
| 1:B:9:ASN:ND2    | 1:B:10:LYS:HG3   | 2.15                     | 0.60              |
| 1:B:578:TYR:CE1  | 1:B:583:GLY:HA2  | 2.36                     | 0.60              |
| 1:C:668:ILE:HD13 | 1:C:682:ILE:HA   | 1.83                     | 0.60              |
| 1:D:261:SER:HB3  | 1:D:262:PRO:HD3  | 1.83                     | 0.60              |
| 1:E:323:GLU:N    | 1:E:324:PRO:HA   | 2.16                     | 0.60              |
| 1:F:340:LEU:HB3  | 1:F:342:VAL:HG12 | 1.83                     | 0.60              |
| 1:E:23:PRO:HG3   | 2:E:723:HOH:O    | 2.01                     | 0.60              |
| 1:E:575:GLY:O    | 1:E:588:GLY:N    | 2.34                     | 0.60              |
| 1:C:618:TYR:HB2  | 1:C:652:THR:CG2  | 2.31                     | 0.60              |
| 1:D:575:GLY:O    | 1:D:588:GLY:N    | 2.33                     | 0.60              |
| 1:F:347:ASP:O    | 1:F:350:VAL:HG12 | 2.02                     | 0.60              |
| 1:A:330:ALA:O    | 1:A:334:ARG:HG2  | 2.02                     | 0.60              |
| 1:F:323:GLU:N    | 1:F:324:PRO:HA   | 2.17                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:23:PRO:HG3   | 2:A:720:HOH:O    | 2.01                     | 0.60              |
| 1:C:683:ASN:N    | 1:C:683:ASN:HD22 | 1.98                     | 0.60              |
| 1:A:596:HIS:CD2  | 1:A:598:LEU:H    | 2.20                     | 0.60              |
| 1:B:575:GLY:O    | 1:B:588:GLY:N    | 2.35                     | 0.60              |
| 1:B:323:GLU:N    | 1:B:324:PRO:HA   | 2.17                     | 0.59              |
| 1:C:575:GLY:O    | 1:C:588:GLY:N    | 2.33                     | 0.59              |
| 1:A:17:ILE:HD11  | 1:A:45:ILE:HD13  | 1.84                     | 0.59              |
| 1:C:268:GLY:H    | 1:F:258:GLN:HG2  | 1.67                     | 0.59              |
| 1:B:26:PHE:HB3   | 1:B:165:LEU:HD22 | 1.83                     | 0.59              |
| 1:A:323:GLU:N    | 1:A:324:PRO:HA   | 2.17                     | 0.59              |
| 1:D:607:ILE:C    | 1:D:608:ILE:HD12 | 2.23                     | 0.59              |
| 1:E:596:HIS:CD2  | 1:E:598:LEU:H    | 2.20                     | 0.59              |
| 1:C:334:ARG:O    | 1:C:338:SER:HB2  | 2.02                     | 0.59              |
| 1:E:55:GLU:HG2   | 1:E:137:ILE:HG12 | 1.85                     | 0.59              |
| 1:C:323:GLU:N    | 1:C:324:PRO:HA   | 2.17                     | 0.59              |
| 1:F:577:TRP:CZ3  | 1:F:603:ARG:HB3  | 2.38                     | 0.59              |
| 1:A:575:GLY:O    | 1:A:588:GLY:N    | 2.34                     | 0.58              |
| 1:D:132:GLU:HG3  | 2:D:832:HOH:O    | 2.03                     | 0.58              |
| 1:E:618:TYR:HB2  | 1:E:652:THR:HG23 | 1.86                     | 0.58              |
| 1:A:339:SER:HB2  | 1:F:339:SER:HB3  | 1.84                     | 0.58              |
| 1:B:643:GLU:OE2  | 1:B:685:LYS:HD3  | 2.03                     | 0.58              |
| 1:C:557:LEU:C    | 1:C:557:LEU:HD23 | 2.23                     | 0.58              |
| 1:B:268:GLY:N    | 1:D:258:GLN:HG2  | 2.19                     | 0.58              |
| 1:F:557:LEU:HD23 | 1:F:558:TYR:N    | 2.17                     | 0.58              |
| 1:B:340:LEU:HD11 | 1:E:340:LEU:HD13 | 1.85                     | 0.58              |
| 1:C:686:ILE:CD1  | 1:C:690:ILE:HD11 | 2.29                     | 0.58              |
| 1:D:614:GLU:HG2  | 1:D:648:LYS:HB3  | 1.83                     | 0.58              |
| 1:A:87:ASP:O     | 1:A:348:ARG:HD3  | 2.04                     | 0.58              |
| 1:D:55:GLU:HG2   | 1:D:137:ILE:HG12 | 1.86                     | 0.58              |
| 1:E:261:SER:HB3  | 1:E:262:PRO:HD3  | 1.86                     | 0.58              |
| 1:B:618:TYR:HB2  | 1:B:652:THR:HG23 | 1.84                     | 0.58              |
| 1:A:419:PRO:HG2  | 1:A:457:ILE:HG23 | 1.85                     | 0.58              |
| 1:D:499:GLU:O    | 1:D:503:GLU:HG3  | 2.04                     | 0.58              |
| 1:F:55:GLU:HG2   | 1:F:137:ILE:HG12 | 1.86                     | 0.57              |
| 1:F:412:ILE:HD12 | 1:F:439:VAL:HG11 | 1.87                     | 0.57              |
| 1:B:35:ASN:N     | 1:B:35:ASN:HD22  | 1.91                     | 0.57              |
| 1:C:87:ASP:O     | 1:C:348:ARG:HD3  | 2.04                     | 0.57              |
| 1:E:419:PRO:HG2  | 1:E:457:ILE:HG23 | 1.87                     | 0.57              |
| 1:E:8:GLU:O      | 1:E:32:ILE:HG23  | 2.04                     | 0.57              |
| 1:A:337:LEU:HD21 | 1:E:337:LEU:HD21 | 1.87                     | 0.57              |
| 1:B:499:GLU:O    | 1:B:503:GLU:HG3  | 2.05                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:26:PHE:HB3   | 1:D:165:LEU:HD22 | 1.87                     | 0.57              |
| 1:A:55:GLU:HG2   | 1:A:137:ILE:HG12 | 1.86                     | 0.57              |
| 1:D:686:ILE:CD1  | 1:D:690:ILE:HD11 | 2.35                     | 0.57              |
| 1:E:661:ILE:CD1  | 1:E:693:GLU:HG3  | 2.35                     | 0.57              |
| 1:C:258:GLN:HG2  | 1:F:268:GLY:N    | 2.19                     | 0.57              |
| 1:F:618:TYR:HB2  | 1:F:652:THR:CG2  | 2.35                     | 0.57              |
| 1:C:14:LYS:HD2   | 1:C:28:LEU:HD12  | 1.87                     | 0.56              |
| 1:D:360:TYR:CZ   | 1:D:365:ARG:HD2  | 2.40                     | 0.56              |
| 1:D:659:LYS:HB3  | 1:D:659:LYS:NZ   | 2.20                     | 0.56              |
| 1:B:255:ARG:HG2  | 1:B:257:ASP:HB2  | 1.87                     | 0.56              |
| 1:B:258:GLN:HG2  | 1:D:268:GLY:N    | 2.20                     | 0.56              |
| 1:A:255:ARG:HG2  | 1:A:257:ASP:HB2  | 1.87                     | 0.56              |
| 1:C:156:GLU:O    | 1:C:160:GLU:HG3  | 2.05                     | 0.56              |
| 1:F:293:PHE:O    | 1:F:299:ARG:HD3  | 2.05                     | 0.56              |
| 1:C:55:GLU:HG2   | 1:C:137:ILE:HG12 | 1.86                     | 0.56              |
| 1:C:347:ASP:O    | 1:C:350:VAL:HG12 | 2.05                     | 0.56              |
| 1:A:412:ILE:HD12 | 1:A:439:VAL:HG11 | 1.87                     | 0.56              |
| 1:E:59:ASP:OD2   | 1:E:109:LYS:HD2  | 2.06                     | 0.56              |
| 1:F:156:GLU:O    | 1:F:160:GLU:HG3  | 2.06                     | 0.56              |
| 1:C:419:PRO:HG2  | 1:C:457:ILE:HG23 | 1.88                     | 0.55              |
| 1:D:255:ARG:HG2  | 1:D:257:ASP:HB2  | 1.88                     | 0.55              |
| 1:E:342:VAL:CG1  | 1:F:342:VAL:HG23 | 2.36                     | 0.55              |
| 1:E:610:LEU:HD11 | 1:E:616:ILE:HD11 | 1.88                     | 0.55              |
| 1:F:342:VAL:HG22 | 1:F:343:GLN:N    | 2.21                     | 0.55              |
| 1:E:156:GLU:O    | 1:E:160:GLU:HG3  | 2.06                     | 0.55              |
| 1:F:255:ARG:HG2  | 1:F:257:ASP:HB2  | 1.88                     | 0.55              |
| 1:F:499:GLU:O    | 1:F:503:GLU:HG3  | 2.07                     | 0.55              |
| 1:A:643:GLU:OE2  | 1:A:685:LYS:HD2  | 2.06                     | 0.55              |
| 1:B:59:ASP:OD2   | 1:B:109:LYS:HD2  | 2.06                     | 0.55              |
| 1:B:412:ILE:HD12 | 1:B:439:VAL:HG11 | 1.88                     | 0.55              |
| 1:D:618:TYR:HB2  | 1:D:652:THR:CG2  | 2.34                     | 0.55              |
| 1:F:419:PRO:HG2  | 1:F:457:ILE:HG23 | 1.88                     | 0.55              |
| 1:D:163:THR:CG2  | 1:D:168:LYS:HD3  | 2.37                     | 0.55              |
| 1:D:419:PRO:HG2  | 1:D:457:ILE:HG23 | 1.87                     | 0.55              |
| 1:C:255:ARG:HG2  | 1:C:257:ASP:HB2  | 1.87                     | 0.55              |
| 1:A:156:GLU:O    | 1:A:160:GLU:HG3  | 2.06                     | 0.55              |
| 1:D:578:TYR:CE1  | 1:D:583:GLY:HA2  | 2.42                     | 0.55              |
| 1:D:334:ARG:O    | 1:D:338:SER:HB2  | 2.07                     | 0.55              |
| 1:B:614:GLU:HG2  | 1:B:648:LYS:HB3  | 1.87                     | 0.55              |
| 1:C:651:ILE:HD13 | 1:C:692:LEU:HD21 | 1.89                     | 0.55              |
| 1:D:156:GLU:O    | 1:D:160:GLU:HG3  | 2.07                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:234:LYS:O    | 1:E:238:GLU:HG3  | 2.07                     | 0.55              |
| 1:D:637:GLU:OE2  | 1:D:639:LYS:HE3  | 2.08                     | 0.54              |
| 1:B:661:ILE:HG12 | 1:B:667:GLU:HG2  | 1.88                     | 0.54              |
| 1:B:419:PRO:HG2  | 1:B:457:ILE:HG23 | 1.88                     | 0.54              |
| 1:C:59:ASP:OD2   | 1:C:109:LYS:HD2  | 2.07                     | 0.54              |
| 1:C:299:ARG:HG2  | 1:C:382:ALA:HB2  | 1.90                     | 0.54              |
| 1:F:334:ARG:O    | 1:F:338:SER:HB3  | 2.06                     | 0.54              |
| 1:D:59:ASP:OD2   | 1:D:109:LYS:HD2  | 2.07                     | 0.54              |
| 1:E:87:ASP:O     | 1:E:348:ARG:HD3  | 2.08                     | 0.54              |
| 1:F:59:ASP:OD2   | 1:F:109:LYS:HD2  | 2.07                     | 0.54              |
| 1:F:675:GLN:HG2  | 1:F:676:ASN:ND2  | 2.23                     | 0.54              |
| 1:E:412:ILE:HD12 | 1:E:439:VAL:HG11 | 1.89                     | 0.54              |
| 1:F:132:GLU:HG3  | 2:F:826:HOH:O    | 2.07                     | 0.54              |
| 1:A:618:TYR:HB2  | 1:A:652:THR:HG23 | 1.90                     | 0.54              |
| 1:C:577:TRP:CZ3  | 1:C:603:ARG:HB3  | 2.42                     | 0.54              |
| 1:E:342:VAL:HG11 | 1:F:342:VAL:HG23 | 1.89                     | 0.54              |
| 1:E:342:VAL:HG12 | 1:E:343:GLN:N    | 2.22                     | 0.54              |
| 1:E:578:TYR:CE1  | 1:E:583:GLY:HA2  | 2.43                     | 0.54              |
| 1:F:163:THR:CG2  | 1:F:168:LYS:HD3  | 2.35                     | 0.54              |
| 1:A:299:ARG:HG3  | 1:A:382:ALA:HB2  | 1.90                     | 0.54              |
| 1:E:255:ARG:HG2  | 1:E:257:ASP:HB2  | 1.89                     | 0.53              |
| 1:D:652:THR:HA   | 1:D:676:ASN:O    | 2.08                     | 0.53              |
| 1:E:682:ILE:HG22 | 1:E:684:GLN:HG2  | 1.91                     | 0.53              |
| 1:C:682:ILE:HG22 | 1:C:684:GLN:HG2  | 1.91                     | 0.53              |
| 1:E:577:TRP:CH2  | 1:E:603:ARG:HB3  | 2.43                     | 0.53              |
| 1:B:651:ILE:HD13 | 1:B:692:LEU:CD2  | 2.38                     | 0.53              |
| 1:E:659:LYS:HD2  | 1:E:667:GLU:HG3  | 1.90                     | 0.53              |
| 1:A:652:THR:HA   | 1:A:676:ASN:O    | 2.09                     | 0.53              |
| 1:A:59:ASP:OD2   | 1:A:109:LYS:HD2  | 2.08                     | 0.53              |
| 1:C:499:GLU:O    | 1:C:503:GLU:HG3  | 2.08                     | 0.53              |
| 1:D:83:MET:HG3   | 1:D:101:SER:HB3  | 1.91                     | 0.53              |
| 1:D:412:ILE:HD12 | 1:D:439:VAL:HG11 | 1.89                     | 0.53              |
| 1:A:268:GLY:H    | 1:E:258:GLN:HG2  | 1.74                     | 0.53              |
| 1:B:299:ARG:HG3  | 1:B:382:ALA:HB2  | 1.91                     | 0.53              |
| 1:B:652:THR:HA   | 1:B:676:ASN:O    | 2.09                     | 0.53              |
| 1:C:182:SER:HB2  | 1:C:210:PHE:HB2  | 1.91                     | 0.52              |
| 1:B:234:LYS:O    | 1:B:238:GLU:HG3  | 2.09                     | 0.52              |
| 1:A:334:ARG:O    | 1:A:338:SER:HB3  | 2.09                     | 0.52              |
| 1:B:156:GLU:O    | 1:B:160:GLU:HG3  | 2.09                     | 0.52              |
| 1:C:412:ILE:HD12 | 1:C:439:VAL:HG11 | 1.89                     | 0.52              |
| 1:D:596:HIS:CD2  | 1:D:598:LEU:H    | 2.27                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:182:SER:HB2  | 1:F:210:PHE:HB2  | 1.92                     | 0.52              |
| 1:C:578:TYR:CE1  | 1:C:583:GLY:HA2  | 2.44                     | 0.52              |
| 1:C:652:THR:HA   | 1:C:676:ASN:O    | 2.10                     | 0.52              |
| 1:D:388:ARG:HD3  | 2:D:850:HOH:O    | 2.08                     | 0.52              |
| 1:D:10:LYS:O     | 1:D:10:LYS:HG2   | 2.10                     | 0.52              |
| 1:D:651:ILE:HD13 | 1:D:692:LEU:CD2  | 2.38                     | 0.52              |
| 1:C:17:ILE:HD11  | 1:C:45:ILE:CD1   | 2.39                     | 0.52              |
| 1:F:234:LYS:O    | 1:F:238:GLU:HG3  | 2.09                     | 0.52              |
| 1:A:274:GLU:O    | 1:A:365:ARG:NH2  | 2.43                     | 0.52              |
| 1:E:342:VAL:CG1  | 1:E:343:GLN:N    | 2.73                     | 0.52              |
| 1:F:299:ARG:HG3  | 1:F:382:ALA:HB2  | 1.90                     | 0.52              |
| 1:A:586:ILE:HD13 | 1:A:592:VAL:HG11 | 1.92                     | 0.51              |
| 1:C:258:GLN:CG   | 1:F:278:LEU:HD21 | 2.38                     | 0.51              |
| 1:A:268:GLY:N    | 1:E:258:GLN:HG2  | 2.25                     | 0.51              |
| 1:A:557:LEU:HD23 | 1:A:557:LEU:C    | 2.30                     | 0.51              |
| 1:D:293:PHE:O    | 1:D:299:ARG:HD3  | 2.10                     | 0.51              |
| 1:A:554:LYS:O    | 1:A:603:ARG:HD3  | 2.11                     | 0.51              |
| 1:B:163:THR:CG2  | 1:B:168:LYS:HD3  | 2.41                     | 0.51              |
| 1:B:35:ASN:N     | 1:B:35:ASN:ND2   | 2.51                     | 0.51              |
| 1:E:274:GLU:O    | 1:E:365:ARG:NH2  | 2.38                     | 0.51              |
| 1:B:340:LEU:CD1  | 1:E:340:LEU:HD13 | 2.41                     | 0.51              |
| 1:C:6:ILE:HG22   | 1:C:34:SER:HB2   | 1.92                     | 0.51              |
| 1:A:499:GLU:O    | 1:A:503:GLU:HG3  | 2.11                     | 0.51              |
| 1:A:679:VAL:HG12 | 1:A:680:ALA:N    | 2.26                     | 0.51              |
| 1:D:586:ILE:HD13 | 1:D:592:VAL:HG11 | 1.93                     | 0.51              |
| 1:E:652:THR:HA   | 1:E:676:ASN:O    | 2.11                     | 0.51              |
| 1:A:299:ARG:HG2  | 1:A:382:ALA:HB2  | 1.91                     | 0.51              |
| 1:A:132:GLU:HG3  | 2:A:835:HOH:O    | 2.11                     | 0.50              |
| 1:A:578:TYR:CE1  | 1:A:583:GLY:HA2  | 2.46                     | 0.50              |
| 1:B:172:PRO:HG2  | 1:B:177:PHE:CE1  | 2.46                     | 0.50              |
| 1:B:72:PHE:CZ    | 1:B:79:LYS:HE2   | 2.46                     | 0.50              |
| 1:E:182:SER:HB2  | 1:E:210:PHE:HB2  | 1.93                     | 0.50              |
| 1:C:268:GLY:N    | 1:F:258:GLN:HG2  | 2.26                     | 0.50              |
| 1:C:675:GLN:HG2  | 1:C:676:ASN:ND2  | 2.26                     | 0.50              |
| 1:E:640:PHE:CE2  | 1:E:644:ILE:HD11 | 2.46                     | 0.50              |
| 1:D:72:PHE:CZ    | 1:D:79:LYS:HE2   | 2.47                     | 0.50              |
| 1:A:132:GLU:HB3  | 1:A:135:LYS:HB2  | 1.93                     | 0.50              |
| 1:C:291:PRO:HG2  | 1:C:293:PHE:CE2  | 2.46                     | 0.50              |
| 1:F:586:ILE:HD13 | 1:F:592:VAL:HG11 | 1.94                     | 0.50              |
| 1:A:293:PHE:O    | 1:A:299:ARG:HD3  | 2.11                     | 0.50              |
| 1:D:341:PRO:HA   | 1:F:345:ARG:HH12 | 1.75                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:659:LYS:HA   | 1:A:670:VAL:HG23 | 1.93                     | 0.50              |
| 1:B:686:ILE:CD1  | 1:B:690:ILE:HD11 | 2.39                     | 0.50              |
| 1:B:692:LEU:HD12 | 1:B:692:LEU:N    | 2.27                     | 0.50              |
| 1:D:172:PRO:HG2  | 1:D:177:PHE:CE1  | 2.47                     | 0.50              |
| 1:D:229:PHE:N    | 1:D:230:PRO:HD3  | 2.25                     | 0.50              |
| 1:D:682:ILE:HG22 | 1:D:684:GLN:HG2  | 1.94                     | 0.50              |
| 1:E:347:ASP:O    | 1:E:350:VAL:HG12 | 2.11                     | 0.50              |
| 1:F:291:PRO:HG2  | 1:F:293:PHE:CE2  | 2.47                     | 0.50              |
| 1:A:172:PRO:HG2  | 1:A:177:PHE:CE1  | 2.46                     | 0.50              |
| 1:A:211:LEU:HD22 | 1:A:246:LEU:HD11 | 1.93                     | 0.50              |
| 1:B:586:ILE:HD13 | 1:B:592:VAL:HG11 | 1.94                     | 0.50              |
| 1:C:211:LEU:HD22 | 1:C:246:LEU:HD11 | 1.94                     | 0.50              |
| 1:E:229:PHE:N    | 1:E:230:PRO:HD3  | 2.26                     | 0.50              |
| 1:E:564:LYS:HD2  | 1:E:564:LYS:N    | 2.27                     | 0.50              |
| 1:E:72:PHE:CZ    | 1:E:79:LYS:HE2   | 2.47                     | 0.50              |
| 1:A:339:SER:HB2  | 1:F:339:SER:CB   | 2.41                     | 0.50              |
| 1:A:83:MET:HG3   | 1:A:101:SER:HB3  | 1.93                     | 0.49              |
| 1:B:293:PHE:O    | 1:B:299:ARG:HD3  | 2.12                     | 0.49              |
| 1:B:627:ASP:O    | 1:B:628:ASN:CG   | 2.51                     | 0.49              |
| 1:D:181:ILE:CG1  | 1:D:209:VAL:HG12 | 2.41                     | 0.49              |
| 1:C:586:ILE:HD13 | 1:C:592:VAL:HG11 | 1.94                     | 0.49              |
| 1:A:291:PRO:HG2  | 1:A:293:PHE:CE2  | 2.47                     | 0.49              |
| 1:A:682:ILE:HG22 | 1:A:684:GLN:HG2  | 1.94                     | 0.49              |
| 1:A:72:PHE:CZ    | 1:A:79:LYS:HE2   | 2.48                     | 0.49              |
| 1:C:648:LYS:HD2  | 1:C:679:VAL:HG11 | 1.94                     | 0.49              |
| 1:F:257:ASP:HB3  | 1:F:260:TYR:CB   | 2.42                     | 0.49              |
| 1:C:172:PRO:HG2  | 1:C:177:PHE:CE1  | 2.48                     | 0.49              |
| 1:C:451:GLY:O    | 1:C:452:ARG:HG3  | 2.12                     | 0.49              |
| 1:C:72:PHE:CZ    | 1:C:79:LYS:HE2   | 2.48                     | 0.49              |
| 1:B:554:LYS:O    | 1:B:603:ARG:HD3  | 2.13                     | 0.49              |
| 1:E:586:ILE:HD13 | 1:E:592:VAL:HG11 | 1.94                     | 0.49              |
| 1:C:683:ASN:N    | 1:C:683:ASN:ND2  | 2.60                     | 0.49              |
| 1:C:83:MET:HG3   | 1:C:101:SER:HB3  | 1.94                     | 0.49              |
| 1:E:291:PRO:HG2  | 1:E:293:PHE:CE2  | 2.48                     | 0.49              |
| 1:F:132:GLU:HB3  | 1:F:135:LYS:HB2  | 1.95                     | 0.49              |
| 1:F:610:LEU:HD11 | 1:F:616:ILE:CD1  | 2.43                     | 0.49              |
| 1:F:72:PHE:CZ    | 1:F:79:LYS:HE2   | 2.47                     | 0.49              |
| 1:D:257:ASP:HB3  | 1:D:260:TYR:CB   | 2.43                     | 0.49              |
| 1:B:610:LEU:HD11 | 1:B:616:ILE:HD11 | 1.95                     | 0.48              |
| 1:E:132:GLU:HB3  | 1:E:135:LYS:HB2  | 1.95                     | 0.48              |
| 1:B:257:ASP:HB3  | 1:B:260:TYR:CB   | 2.42                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:291:PRO:HG2  | 1:B:293:PHE:CE2  | 2.47                     | 0.48              |
| 1:D:291:PRO:HG2  | 1:D:293:PHE:CE2  | 2.47                     | 0.48              |
| 1:E:659:LYS:HD2  | 1:E:667:GLU:CG   | 2.43                     | 0.48              |
| 1:D:133:TYR:HB3  | 1:E:187:TYR:O    | 2.12                     | 0.48              |
| 1:D:301:TRP:CZ2  | 1:D:305:LEU:HD11 | 2.48                     | 0.48              |
| 1:E:392:ARG:NH1  | 2:E:905:HOH:O    | 2.46                     | 0.48              |
| 1:E:564:LYS:H    | 1:E:564:LYS:HD2  | 1.77                     | 0.48              |
| 1:A:556:LEU:HD23 | 1:A:557:LEU:N    | 2.28                     | 0.48              |
| 1:E:312:GLN:HG2  | 2:E:929:HOH:O    | 2.12                     | 0.48              |
| 1:B:211:LEU:HD22 | 1:B:246:LEU:HD11 | 1.95                     | 0.48              |
| 1:C:300:GLU:HG2  | 1:C:385:LYS:NZ   | 2.29                     | 0.48              |
| 1:A:589:LYS:HA   | 1:A:589:LYS:HD2  | 1.67                     | 0.48              |
| 1:B:567:SER:OG   | 1:B:593:LYS:HE3  | 2.12                     | 0.48              |
| 1:E:172:PRO:HG2  | 1:E:177:PHE:CE1  | 2.49                     | 0.48              |
| 1:D:545:ARG:HB2  | 1:E:494:PRO:HG3  | 1.96                     | 0.48              |
| 1:B:181:ILE:CG1  | 1:B:209:VAL:HG12 | 2.43                     | 0.48              |
| 1:E:499:GLU:O    | 1:E:503:GLU:HG3  | 2.13                     | 0.48              |
| 1:E:83:MET:HG3   | 1:E:101:SER:HB3  | 1.94                     | 0.48              |
| 1:F:17:ILE:HD11  | 1:F:45:ILE:CD1   | 2.43                     | 0.48              |
| 1:B:13:TYR:OH    | 1:B:36:LYS:HD2   | 2.13                     | 0.48              |
| 1:E:211:LEU:HD22 | 1:E:246:LEU:HD11 | 1.95                     | 0.48              |
| 1:E:247:ILE:N    | 1:E:247:ILE:HD12 | 2.29                     | 0.48              |
| 1:F:172:PRO:HG2  | 1:F:177:PHE:CE1  | 2.48                     | 0.48              |
| 1:F:189:GLN:HE22 | 1:F:231:GLU:HB2  | 1.78                     | 0.48              |
| 1:C:659:LYS:HA   | 1:C:670:VAL:HG23 | 1.96                     | 0.48              |
| 1:B:630:GLU:HB2  | 1:B:641:SER:HB3  | 1.95                     | 0.48              |
| 1:E:661:ILE:HD13 | 1:E:693:GLU:HG3  | 1.96                     | 0.48              |
| 1:F:211:LEU:HD22 | 1:F:246:LEU:HD11 | 1.96                     | 0.48              |
| 1:F:31:LYS:HG3   | 1:F:31:LYS:O     | 2.13                     | 0.48              |
| 1:A:257:ASP:HB3  | 1:A:260:TYR:CB   | 2.44                     | 0.47              |
| 1:A:182:SER:HB2  | 1:A:210:PHE:HB2  | 1.96                     | 0.47              |
| 1:A:494:PRO:HG3  | 1:C:545:ARG:HB2  | 1.96                     | 0.47              |
| 1:A:347:ASP:O    | 1:A:350:VAL:HG12 | 2.13                     | 0.47              |
| 1:C:339:SER:HB3  | 1:D:339:SER:HB3  | 1.96                     | 0.47              |
| 1:E:17:ILE:HD11  | 1:E:45:ILE:HD13  | 1.95                     | 0.47              |
| 1:B:132:GLU:HB3  | 1:B:135:LYS:HB2  | 1.95                     | 0.47              |
| 1:F:645:TYR:HA   | 1:F:685:LYS:HA   | 1.97                     | 0.47              |
| 1:A:133:TYR:HB3  | 1:B:187:TYR:O    | 2.13                     | 0.47              |
| 1:A:247:ILE:N    | 1:A:247:ILE:HD12 | 2.29                     | 0.47              |
| 1:B:182:SER:HB2  | 1:B:210:PHE:HB2  | 1.96                     | 0.47              |
| 1:B:189:GLN:HE22 | 1:B:231:GLU:HB2  | 1.78                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:672:LYS:HD2  | 1:C:678:TYR:CE1  | 2.49                     | 0.47              |
| 1:F:83:MET:HG3   | 1:F:101:SER:HB3  | 1.96                     | 0.47              |
| 1:A:278:LEU:HD21 | 1:E:258:GLN:CG   | 2.45                     | 0.47              |
| 1:B:83:MET:HG3   | 1:B:101:SER:HB3  | 1.95                     | 0.47              |
| 1:B:670:VAL:HG22 | 1:B:680:ALA:HB2  | 1.97                     | 0.47              |
| 1:D:451:GLY:O    | 1:D:452:ARG:HG3  | 2.14                     | 0.47              |
| 1:A:17:ILE:HD11  | 1:A:45:ILE:CD1   | 2.45                     | 0.47              |
| 1:B:247:ILE:HD12 | 1:B:247:ILE:N    | 2.30                     | 0.47              |
| 1:C:132:GLU:HB3  | 1:C:135:LYS:HB2  | 1.97                     | 0.47              |
| 1:C:257:ASP:HB3  | 1:C:260:TYR:CB   | 2.44                     | 0.47              |
| 1:C:640:PHE:CE2  | 1:C:644:ILE:HD11 | 2.49                     | 0.47              |
| 1:D:132:GLU:HB3  | 1:D:135:LYS:HB2  | 1.97                     | 0.47              |
| 1:D:610:LEU:HD11 | 1:D:616:ILE:HD11 | 1.97                     | 0.47              |
| 1:B:296:GLU:O    | 1:B:300:GLU:HG3  | 2.15                     | 0.47              |
| 1:D:181:ILE:HG13 | 1:D:209:VAL:HG12 | 1.97                     | 0.47              |
| 1:F:26:PHE:HB3   | 1:F:165:LEU:HD22 | 1.95                     | 0.47              |
| 1:F:388:ARG:HD3  | 2:F:840:HOH:O    | 2.15                     | 0.47              |
| 1:A:332:GLU:HG2  | 1:E:332:GLU:HG3  | 1.97                     | 0.46              |
| 1:A:451:GLY:O    | 1:A:452:ARG:HG3  | 2.14                     | 0.46              |
| 1:E:293:PHE:O    | 1:E:299:ARG:HD3  | 2.15                     | 0.46              |
| 1:C:661:ILE:HD11 | 1:C:693:GLU:CD   | 2.35                     | 0.46              |
| 1:D:345:ARG:O    | 1:D:345:ARG:HG3  | 2.15                     | 0.46              |
| 1:D:37:SER:OG    | 1:D:40:GLU:HG3   | 2.14                     | 0.46              |
| 1:E:299:ARG:HG2  | 1:E:382:ALA:HB2  | 1.95                     | 0.46              |
| 1:C:183:ARG:HG2  | 1:C:184:TYR:N    | 2.31                     | 0.46              |
| 1:C:643:GLU:CD   | 1:C:685:LYS:HD3  | 2.35                     | 0.46              |
| 1:D:247:ILE:HD12 | 1:D:247:ILE:N    | 2.29                     | 0.46              |
| 1:E:257:ASP:HB3  | 1:E:260:TYR:CB   | 2.44                     | 0.46              |
| 1:E:555:TYR:HB3  | 1:E:606:SER:HB3  | 1.96                     | 0.46              |
| 1:B:659:LYS:HE3  | 1:B:693:GLU:HG3  | 1.98                     | 0.46              |
| 1:D:187:TYR:O    | 1:F:133:TYR:HB3  | 2.16                     | 0.46              |
| 1:E:342:VAL:HG11 | 1:F:342:VAL:CG2  | 2.45                     | 0.46              |
| 1:D:211:LEU:HD22 | 1:D:246:LEU:HD11 | 1.97                     | 0.46              |
| 1:E:175:TRP:CE3  | 1:E:245:LYS:HG3  | 2.50                     | 0.46              |
| 1:A:682:ILE:CG2  | 1:A:684:GLN:HG2  | 2.46                     | 0.46              |
| 1:B:640:PHE:CE2  | 1:B:644:ILE:HD11 | 2.51                     | 0.46              |
| 1:C:16:VAL:HG13  | 1:C:20:PRO:HG2   | 1.97                     | 0.46              |
| 1:F:183:ARG:HG2  | 1:F:184:TYR:N    | 2.30                     | 0.46              |
| 1:F:2:ARG:HG2    | 1:F:47:GLN:OE1   | 2.16                     | 0.46              |
| 1:C:247:ILE:N    | 1:C:247:ILE:HD12 | 2.30                     | 0.46              |
| 1:B:670:VAL:CG1  | 1:B:678:TYR:HB3  | 2.46                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:187:TYR:O    | 1:C:133:TYR:HB3  | 2.15                     | 0.46              |
| 1:D:608:ILE:HD12 | 1:D:608:ILE:N    | 2.31                     | 0.46              |
| 1:C:596:HIS:HD2  | 1:C:598:LEU:N    | 2.05                     | 0.46              |
| 1:C:692:LEU:N    | 1:C:692:LEU:HD12 | 2.31                     | 0.46              |
| 1:D:228:ARG:C    | 1:D:230:PRO:HD3  | 2.37                     | 0.46              |
| 1:A:183:ARG:HG2  | 1:A:184:TYR:N    | 2.31                     | 0.45              |
| 1:B:183:ARG:HG2  | 1:B:184:TYR:N    | 2.31                     | 0.45              |
| 1:C:360:TYR:CE2  | 1:C:365:ARG:HD2  | 2.51                     | 0.45              |
| 1:F:3:ILE:HB     | 1:F:18:GLY:HA2   | 1.98                     | 0.45              |
| 1:A:26:PHE:HB3   | 1:A:165:LEU:HD22 | 1.99                     | 0.45              |
| 1:D:88:ALA:C     | 1:D:348:ARG:HD2  | 2.37                     | 0.45              |
| 1:C:183:ARG:O    | 1:C:185:SER:HA   | 2.16                     | 0.45              |
| 1:C:360:TYR:CZ   | 1:C:365:ARG:HD2  | 2.51                     | 0.45              |
| 1:D:182:SER:HB2  | 1:D:210:PHE:HB2  | 1.97                     | 0.45              |
| 1:E:183:ARG:HG2  | 1:E:184:TYR:N    | 2.31                     | 0.45              |
| 1:C:557:LEU:HD23 | 1:C:558:TYR:N    | 2.31                     | 0.45              |
| 1:D:589:LYS:HD2  | 1:D:589:LYS:HA   | 1.66                     | 0.45              |
| 1:F:242:ARG:HH11 | 1:F:242:ARG:HG3  | 1.82                     | 0.45              |
| 1:F:247:ILE:HD12 | 1:F:247:ILE:N    | 2.31                     | 0.45              |
| 1:A:229:PHE:N    | 1:A:230:PRO:HD3  | 2.30                     | 0.45              |
| 1:D:8:GLU:HB2    | 1:D:34:SER:HB2   | 1.98                     | 0.45              |
| 1:D:609:PRO:HG2  | 1:D:623:PHE:HE2  | 1.82                     | 0.45              |
| 1:D:687:ARG:HB3  | 1:D:687:ARG:NH1  | 2.32                     | 0.45              |
| 1:A:258:GLN:CD   | 1:E:278:LEU:HD21 | 2.37                     | 0.45              |
| 1:A:646:VAL:HG21 | 1:A:686:ILE:HD12 | 1.99                     | 0.45              |
| 1:A:258:GLN:HG2  | 1:E:268:GLY:H    | 1.80                     | 0.45              |
| 1:F:451:GLY:O    | 1:F:452:ARG:HG3  | 2.17                     | 0.45              |
| 1:A:340:LEU:HD13 | 1:F:340:LEU:HD13 | 1.99                     | 0.45              |
| 1:B:618:TYR:HB2  | 1:B:652:THR:CG2  | 2.45                     | 0.45              |
| 1:E:183:ARG:O    | 1:E:185:SER:HA   | 2.16                     | 0.45              |
| 1:E:451:GLY:O    | 1:E:452:ARG:HG3  | 2.15                     | 0.45              |
| 1:B:451:GLY:O    | 1:B:452:ARG:HG3  | 2.17                     | 0.45              |
| 1:F:670:VAL:CG1  | 1:F:678:TYR:HB3  | 2.47                     | 0.45              |
| 1:A:564:LYS:HD3  | 1:A:564:LYS:N    | 2.32                     | 0.44              |
| 1:B:249:ILE:HA   | 1:B:318:TRP:HB3  | 2.00                     | 0.44              |
| 1:A:249:ILE:HA   | 1:A:318:TRP:HB3  | 2.00                     | 0.44              |
| 1:C:620:GLU:O    | 1:C:621:THR:HB   | 2.18                     | 0.44              |
| 1:C:658:SER:HB2  | 1:C:693:GLU:O    | 2.17                     | 0.44              |
| 1:D:183:ARG:HG2  | 1:D:184:TYR:N    | 2.32                     | 0.44              |
| 1:D:360:TYR:CE2  | 1:D:365:ARG:HD2  | 2.52                     | 0.44              |
| 1:E:9:ASN:OD1    | 1:E:29:GLU:HB2   | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:38:LEU:HD21  | 1:F:45:ILE:CD1   | 2.46                     | 0.44              |
| 1:F:17:ILE:CD1   | 1:F:45:ILE:HD13  | 2.47                     | 0.44              |
| 1:A:640:PHE:CE2  | 1:A:644:ILE:HD11 | 2.53                     | 0.44              |
| 1:A:670:VAL:HG12 | 1:A:671:GLU:N    | 2.32                     | 0.44              |
| 1:B:242:ARG:HG3  | 1:B:242:ARG:HH11 | 1.82                     | 0.44              |
| 1:C:96:ASP:OD1   | 1:C:97:PRO:HA    | 2.18                     | 0.44              |
| 1:D:151:GLU:HA   | 1:D:151:GLU:OE1  | 2.16                     | 0.44              |
| 1:D:241:LYS:CE   | 1:D:242:ARG:HH12 | 2.30                     | 0.44              |
| 1:B:270:PHE:N    | 1:D:258:GLN:OE1  | 2.38                     | 0.44              |
| 1:F:175:TRP:CE3  | 1:F:245:LYS:HG3  | 2.53                     | 0.44              |
| 1:F:557:LEU:C    | 1:F:557:LEU:HD23 | 2.38                     | 0.44              |
| 1:E:340:LEU:HD12 | 1:E:341:PRO:HD2  | 2.00                     | 0.44              |
| 1:F:651:ILE:HD13 | 1:F:692:LEU:CD2  | 2.45                     | 0.44              |
| 1:E:28:LEU:O     | 1:E:29:GLU:C     | 2.55                     | 0.43              |
| 1:F:640:PHE:CD2  | 1:F:644:ILE:HD11 | 2.53                     | 0.43              |
| 1:A:22:PRO:HA    | 1:A:23:PRO:HD3   | 1.89                     | 0.43              |
| 1:C:285:PRO:HD2  | 1:C:288:THR:HG21 | 2.00                     | 0.43              |
| 1:C:342:VAL:HG22 | 1:C:343:GLN:H    | 1.83                     | 0.43              |
| 1:C:663:ASP:C    | 1:C:665:SER:H    | 2.22                     | 0.43              |
| 1:B:332:GLU:CG   | 1:D:332:GLU:HG3  | 2.47                     | 0.43              |
| 1:A:172:PRO:HG2  | 1:A:177:PHE:HE1  | 1.83                     | 0.43              |
| 1:B:183:ARG:O    | 1:B:185:SER:HA   | 2.19                     | 0.43              |
| 1:C:610:LEU:HD11 | 1:C:616:ILE:HD11 | 1.98                     | 0.43              |
| 1:B:669:GLN:HA   | 1:B:669:GLN:OE1  | 2.19                     | 0.43              |
| 1:C:473:PHE:CG   | 1:C:552:VAL:HG21 | 2.53                     | 0.43              |
| 1:C:637:GLU:OE1  | 1:C:639:LYS:HE3  | 2.18                     | 0.43              |
| 1:B:88:ALA:O     | 1:B:348:ARG:HD2  | 2.19                     | 0.43              |
| 1:E:249:ILE:HA   | 1:E:318:TRP:HB3  | 2.01                     | 0.43              |
| 1:F:229:PHE:N    | 1:F:230:PRO:HD3  | 2.33                     | 0.43              |
| 1:F:627:ASP:O    | 1:F:628:ASN:HB3  | 2.18                     | 0.43              |
| 1:F:634:SER:O    | 1:F:635:SER:C    | 2.56                     | 0.43              |
| 1:F:640:PHE:CE2  | 1:F:644:ILE:HD11 | 2.54                     | 0.43              |
| 1:B:133:TYR:HB3  | 1:C:187:TYR:O    | 2.18                     | 0.43              |
| 1:C:300:GLU:HG2  | 1:C:385:LYS:HZ1  | 1.82                     | 0.43              |
| 1:C:672:LYS:HD2  | 1:C:678:TYR:HE1  | 1.81                     | 0.43              |
| 1:F:314:VAL:O    | 1:F:392:ARG:NH2  | 2.51                     | 0.43              |
| 1:F:652:THR:HA   | 1:F:676:ASN:O    | 2.19                     | 0.43              |
| 1:F:9:ASN:OD1    | 1:F:30:GLN:HB2   | 2.19                     | 0.43              |
| 1:B:145:VAL:HG22 | 1:B:146:GLU:N    | 2.34                     | 0.43              |
| 1:B:257:ASP:HB3  | 1:B:260:TYR:HB3  | 2.00                     | 0.43              |
| 1:C:340:LEU:HA   | 1:C:340:LEU:HD12 | 1.81                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:347:ASP:O    | 1:D:350:VAL:HG12 | 2.19                     | 0.43              |
| 1:F:257:ASP:HB3  | 1:F:260:TYR:HB2  | 2.01                     | 0.43              |
| 1:F:257:ASP:HB3  | 1:F:260:TYR:HB3  | 2.00                     | 0.43              |
| 1:D:183:ARG:O    | 1:D:185:SER:HA   | 2.18                     | 0.43              |
| 1:D:215:TYR:C    | 1:D:215:TYR:CD1  | 2.92                     | 0.43              |
| 1:E:215:TYR:C    | 1:E:215:TYR:CD1  | 2.92                     | 0.43              |
| 1:E:13:TYR:HE2   | 1:E:36:LYS:HG3   | 1.79                     | 0.43              |
| 1:C:329:ARG:HB3  | 1:C:350:VAL:HG22 | 2.00                     | 0.43              |
| 1:C:556:LEU:HD23 | 1:C:557:LEU:N    | 2.34                     | 0.43              |
| 1:D:299:ARG:HG2  | 1:D:382:ALA:HB2  | 2.01                     | 0.43              |
| 1:D:567:SER:OG   | 1:D:593:LYS:HE3  | 2.18                     | 0.43              |
| 1:E:228:ARG:C    | 1:E:230:PRO:HD3  | 2.39                     | 0.43              |
| 1:F:183:ARG:O    | 1:F:185:SER:HA   | 2.19                     | 0.43              |
| 1:B:31:LYS:O     | 1:B:31:LYS:HG3   | 2.19                     | 0.42              |
| 1:C:556:LEU:HD23 | 1:C:556:LEU:C    | 2.40                     | 0.42              |
| 1:F:215:TYR:CD1  | 1:F:215:TYR:C    | 2.93                     | 0.42              |
| 1:A:686:ILE:HD13 | 1:A:690:ILE:CD1  | 2.43                     | 0.42              |
| 1:A:183:ARG:O    | 1:A:185:SER:HA   | 2.19                     | 0.42              |
| 1:B:172:PRO:HG2  | 1:B:177:PHE:HE1  | 1.83                     | 0.42              |
| 1:D:96:ASP:OD1   | 1:D:97:PRO:HA    | 2.19                     | 0.42              |
| 1:B:258:GLN:OE1  | 1:D:270:PHE:N    | 2.38                     | 0.42              |
| 1:C:342:VAL:HG22 | 1:C:343:GLN:N    | 2.34                     | 0.42              |
| 1:E:285:PRO:HD2  | 1:E:288:THR:HG21 | 2.02                     | 0.42              |
| 1:C:257:ASP:HB3  | 1:C:260:TYR:HB2  | 2.02                     | 0.42              |
| 1:D:257:ASP:HB3  | 1:D:260:TYR:HB3  | 2.02                     | 0.42              |
| 1:A:555:TYR:HB3  | 1:A:606:SER:HB3  | 2.01                     | 0.42              |
| 1:A:93:LYS:O     | 1:A:94:TYR:HB2   | 2.19                     | 0.42              |
| 1:B:473:PHE:CG   | 1:B:552:VAL:HG21 | 2.54                     | 0.42              |
| 1:C:604:GLU:HA   | 1:C:618:TYR:CE2  | 2.55                     | 0.42              |
| 1:D:609:PRO:CG   | 1:D:623:PHE:HE2  | 2.32                     | 0.42              |
| 1:E:661:ILE:HD12 | 1:E:661:ILE:N    | 2.34                     | 0.42              |
| 1:C:249:ILE:HA   | 1:C:318:TRP:HB3  | 2.02                     | 0.42              |
| 1:C:589:LYS:HD2  | 1:C:589:LYS:HA   | 1.68                     | 0.42              |
| 1:B:258:GLN:CD   | 1:D:278:LEU:HD21 | 2.40                     | 0.42              |
| 1:F:145:VAL:HG22 | 1:F:146:GLU:N    | 2.35                     | 0.42              |
| 1:D:257:ASP:HB3  | 1:D:260:TYR:HB2  | 2.01                     | 0.42              |
| 1:E:647:SER:OG   | 1:E:648:LYS:N    | 2.52                     | 0.42              |
| 1:F:249:ILE:HA   | 1:F:318:TRP:HB3  | 2.01                     | 0.42              |
| 1:A:215:TYR:C    | 1:A:215:TYR:CD1  | 2.94                     | 0.42              |
| 1:A:375:TYR:N    | 1:A:376:PRO:HD2  | 2.35                     | 0.42              |
| 1:A:428:LEU:HD23 | 1:A:548:ASP:HA   | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:241:LYS:CE   | 1:D:242:ARG:NH1  | 2.83                     | 0.42              |
| 1:D:94:TYR:CZ    | 1:E:452:ARG:HG2  | 2.55                     | 0.42              |
| 1:F:340:LEU:C    | 1:F:342:VAL:H    | 2.23                     | 0.42              |
| 1:B:502:LYS:O    | 1:B:506:GLU:HG3  | 2.20                     | 0.41              |
| 1:C:659:LYS:HD2  | 1:C:667:GLU:OE2  | 2.20                     | 0.41              |
| 1:B:257:ASP:HB3  | 1:B:260:TYR:HB2  | 2.01                     | 0.41              |
| 1:D:241:LYS:HE3  | 1:D:242:ARG:NH1  | 2.36                     | 0.41              |
| 1:E:257:ASP:HB3  | 1:E:260:TYR:HB2  | 2.02                     | 0.41              |
| 1:F:589:LYS:HD2  | 1:F:589:LYS:HA   | 1.68                     | 0.41              |
| 1:A:257:ASP:HB3  | 1:A:260:TYR:HB2  | 2.01                     | 0.41              |
| 1:C:215:TYR:C    | 1:C:215:TYR:CD1  | 2.93                     | 0.41              |
| 1:C:582:ASN:OD1  | 1:C:582:ASN:C    | 2.59                     | 0.41              |
| 1:D:28:LEU:HA    | 1:D:28:LEU:HD23  | 1.90                     | 0.41              |
| 1:F:578:TYR:CE1  | 1:F:583:GLY:HA2  | 2.55                     | 0.41              |
| 1:D:555:TYR:HB3  | 1:D:606:SER:OG   | 2.20                     | 0.41              |
| 1:A:340:LEU:HD12 | 1:A:341:PRO:HD2  | 2.01                     | 0.41              |
| 1:A:627:ASP:O    | 1:A:628:ASN:CG   | 2.59                     | 0.41              |
| 1:A:545:ARG:HB2  | 1:B:494:PRO:HG3  | 2.02                     | 0.41              |
| 1:C:66:GLY:O     | 1:C:67:LEU:HB2   | 2.20                     | 0.41              |
| 1:D:213:ILE:HG22 | 1:D:216:MET:HE3  | 2.03                     | 0.41              |
| 1:D:658:SER:N    | 1:D:693:GLU:O    | 2.49                     | 0.41              |
| 1:E:22:PRO:HA    | 1:E:23:PRO:HD3   | 1.89                     | 0.41              |
| 1:E:340:LEU:O    | 1:E:342:VAL:N    | 2.45                     | 0.41              |
| 1:E:589:LYS:HA   | 1:E:589:LYS:HD2  | 1.68                     | 0.41              |
| 1:B:215:TYR:CD1  | 1:B:215:TYR:C    | 2.94                     | 0.41              |
| 1:F:172:PRO:HG2  | 1:F:177:PHE:HE1  | 1.86                     | 0.41              |
| 1:F:74:LEU:HA    | 1:F:74:LEU:HD12  | 1.86                     | 0.41              |
| 1:A:510:LYS:HE2  | 1:A:610:LEU:HD13 | 2.03                     | 0.41              |
| 1:A:542:ASP:O    | 1:A:546:ILE:HD13 | 2.20                     | 0.41              |
| 1:A:634:SER:O    | 1:A:635:SER:C    | 2.59                     | 0.41              |
| 1:C:575:GLY:O    | 1:C:588:GLY:CA   | 2.68                     | 0.41              |
| 1:D:249:ILE:HA   | 1:D:318:TRP:HB3  | 2.01                     | 0.41              |
| 1:D:428:LEU:HD23 | 1:D:548:ASP:HA   | 2.03                     | 0.41              |
| 1:D:483:THR:HG22 | 1:F:130:LEU:HD22 | 2.03                     | 0.41              |
| 1:F:175:TRP:CD2  | 1:F:245:LYS:HG3  | 2.56                     | 0.41              |
| 1:F:564:LYS:HG3  | 2:F:867:HOH:O    | 2.20                     | 0.41              |
| 1:A:608:ILE:HA   | 1:A:609:PRO:HD3  | 1.89                     | 0.41              |
| 1:B:187:TYR:HB2  | 1:B:188:PRO:HA   | 2.03                     | 0.41              |
| 1:B:96:ASP:OD1   | 1:B:97:PRO:HA    | 2.21                     | 0.41              |
| 1:C:575:GLY:O    | 1:C:588:GLY:HA3  | 2.21                     | 0.41              |
| 1:E:510:LYS:HE2  | 1:E:610:LEU:HD13 | 2.01                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:682:ILE:HG21 | 1:E:686:ILE:HD11 | 2.02                     | 0.41              |
| 1:F:345:ARG:O    | 1:F:345:ARG:HG3  | 2.21                     | 0.41              |
| 1:F:579:ASN:HB3  | 1:F:582:ASN:OD1  | 2.21                     | 0.41              |
| 1:C:257:ASP:HB3  | 1:C:260:TYR:HB3  | 2.03                     | 0.41              |
| 1:E:340:LEU:HD12 | 1:E:340:LEU:HA   | 1.88                     | 0.41              |
| 1:E:632:THR:O    | 1:E:638:ILE:HA   | 2.20                     | 0.41              |
| 1:F:608:ILE:HA   | 1:F:609:PRO:HD3  | 1.80                     | 0.41              |
| 1:B:38:LEU:HA    | 1:B:38:LEU:HD12  | 1.93                     | 0.41              |
| 1:C:375:TYR:N    | 1:C:376:PRO:HD2  | 2.35                     | 0.41              |
| 1:D:274:GLU:O    | 1:D:365:ARG:NH2  | 2.54                     | 0.41              |
| 1:D:557:LEU:C    | 1:D:557:LEU:HD23 | 2.42                     | 0.41              |
| 1:A:175:TRP:CE3  | 1:A:245:LYS:HG3  | 2.54                     | 0.41              |
| 1:A:614:GLU:HG2  | 1:A:648:LYS:HB3  | 2.03                     | 0.41              |
| 1:C:145:VAL:HG22 | 1:C:146:GLU:N    | 2.36                     | 0.41              |
| 1:C:175:TRP:CE3  | 1:C:245:LYS:HG3  | 2.55                     | 0.41              |
| 1:C:88:ALA:C     | 1:C:348:ARG:HD2  | 2.41                     | 0.41              |
| 1:D:502:LYS:O    | 1:D:506:GLU:HG3  | 2.21                     | 0.41              |
| 1:E:257:ASP:HB3  | 1:E:260:TYR:HB3  | 2.03                     | 0.41              |
| 1:E:428:LEU:HD23 | 1:E:548:ASP:HA   | 2.02                     | 0.41              |
| 1:E:627:ASP:O    | 1:E:628:ASN:HB3  | 2.21                     | 0.41              |
| 1:C:183:ARG:C    | 1:C:185:SER:HA   | 2.41                     | 0.40              |
| 1:C:182:SER:CB   | 1:C:210:PHE:HB2  | 2.51                     | 0.40              |
| 1:D:285:PRO:HD2  | 1:D:288:THR:HG21 | 2.03                     | 0.40              |
| 1:D:596:HIS:HD2  | 1:D:598:LEU:H    | 1.69                     | 0.40              |
| 1:D:604:GLU:HA   | 1:D:618:TYR:CE2  | 2.56                     | 0.40              |
| 1:F:575:GLY:O    | 1:F:588:GLY:CA   | 2.69                     | 0.40              |
| 1:B:48:GLN:HB3   | 1:B:49:GLY:H     | 1.65                     | 0.40              |
| 1:C:172:PRO:HG2  | 1:C:177:PHE:HE1  | 1.86                     | 0.40              |
| 1:D:17:ILE:HD11  | 1:D:45:ILE:HD13  | 2.02                     | 0.40              |
| 1:D:74:LEU:HD12  | 1:D:74:LEU:HA    | 1.86                     | 0.40              |
| 1:D:494:PRO:HG3  | 1:F:545:ARG:HB2  | 2.02                     | 0.40              |
| 1:A:301:TRP:CZ2  | 1:A:305:LEU:HD11 | 2.57                     | 0.40              |
| 1:A:96:ASP:OD1   | 1:A:97:PRO:HA    | 2.21                     | 0.40              |
| 1:C:93:LYS:O     | 1:C:94:TYR:HB2   | 2.21                     | 0.40              |
| 1:D:145:VAL:HG22 | 1:D:146:GLU:N    | 2.36                     | 0.40              |
| 1:D:187:TYR:HB2  | 1:D:188:PRO:HA   | 2.03                     | 0.40              |
| 1:D:4:LEU:HD21   | 1:D:38:LEU:HD13  | 2.03                     | 0.40              |
| 1:E:145:VAL:HG22 | 1:E:146:GLU:N    | 2.36                     | 0.40              |
| 1:E:545:ARG:HB2  | 1:F:494:PRO:HG3  | 2.03                     | 0.40              |
| 1:E:575:GLY:O    | 1:E:588:GLY:CA   | 2.69                     | 0.40              |
| 1:F:366:VAL:HG12 | 1:F:367:LYS:O    | 2.22                     | 0.40              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:345:ARG:HE  | 1:C:341:PRO:HA   | 1.86                     | 0.40              |
| 1:E:555:TYR:HB3 | 1:E:606:SER:CB   | 2.52                     | 0.40              |
| 1:D:542:ASP:O   | 1:D:546:ILE:HD13 | 2.21                     | 0.40              |
| 1:D:620:GLU:HG2 | 1:D:634:SER:HA   | 2.04                     | 0.40              |
| 1:F:663:ASP:C   | 1:F:665:SER:H    | 2.25                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|----------|-------------|----|
| 1   | A     | 690/693 (100%)   | 651 (94%)  | 33 (5%)  | 6 (1%)   | 17          | 24 |
| 1   | B     | 690/693 (100%)   | 653 (95%)  | 31 (4%)  | 6 (1%)   | 17          | 24 |
| 1   | C     | 690/693 (100%)   | 648 (94%)  | 35 (5%)  | 7 (1%)   | 15          | 22 |
| 1   | D     | 690/693 (100%)   | 652 (94%)  | 34 (5%)  | 4 (1%)   | 25          | 34 |
| 1   | E     | 690/693 (100%)   | 649 (94%)  | 35 (5%)  | 6 (1%)   | 17          | 24 |
| 1   | F     | 691/693 (100%)   | 649 (94%)  | 34 (5%)  | 8 (1%)   | 13          | 17 |
| All | All   | 4141/4158 (100%) | 3902 (94%) | 202 (5%) | 37 (1%)  | 17          | 24 |

All (37) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 29  | GLU  |
| 1   | C     | 29  | GLU  |
| 1   | E     | 29  | GLU  |
| 1   | F     | 635 | SER  |
| 1   | C     | 635 | SER  |
| 1   | F     | 29  | GLU  |
| 1   | A     | 29  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 635 | SER  |
| 1   | A     | 688 | GLY  |
| 1   | D     | 688 | GLY  |
| 1   | F     | 664 | ASP  |
| 1   | B     | 635 | SER  |
| 1   | C     | 688 | GLY  |
| 1   | D     | 599 | PRO  |
| 1   | E     | 338 | SER  |
| 1   | E     | 341 | PRO  |
| 1   | E     | 688 | GLY  |
| 1   | A     | 599 | PRO  |
| 1   | C     | 599 | PRO  |
| 1   | C     | 647 | SER  |
| 1   | F     | 30  | GLN  |
| 1   | B     | 688 | GLY  |
| 1   | F     | 599 | PRO  |
| 1   | A     | 49  | GLY  |
| 1   | B     | 49  | GLY  |
| 1   | C     | 49  | GLY  |
| 1   | D     | 49  | GLY  |
| 1   | D     | 213 | ILE  |
| 1   | E     | 49  | GLY  |
| 1   | F     | 49  | GLY  |
| 1   | F     | 688 | GLY  |
| 1   | A     | 213 | ILE  |
| 1   | B     | 213 | ILE  |
| 1   | B     | 599 | PRO  |
| 1   | C     | 213 | ILE  |
| 1   | E     | 213 | ILE  |
| 1   | F     | 213 | ILE  |

### 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     | 623/624 (100%) | 607 (97%) | 16 (3%)  | 46 61       |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|-------------|----|
| 1   | B     | 623/624 (100%)   | 604 (97%)  | 19 (3%)  | 41          | 55 |
| 1   | C     | 623/624 (100%)   | 606 (97%)  | 17 (3%)  | 44          | 59 |
| 1   | D     | 623/624 (100%)   | 604 (97%)  | 19 (3%)  | 41          | 55 |
| 1   | E     | 623/624 (100%)   | 602 (97%)  | 21 (3%)  | 37          | 50 |
| 1   | F     | 624/624 (100%)   | 606 (97%)  | 18 (3%)  | 42          | 57 |
| All | All   | 3739/3744 (100%) | 3629 (97%) | 110 (3%) | 42          | 57 |

All (110) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 4   | LEU  |
| 1   | A     | 74  | LEU  |
| 1   | A     | 83  | MET  |
| 1   | A     | 130 | LEU  |
| 1   | A     | 165 | LEU  |
| 1   | A     | 211 | LEU  |
| 1   | A     | 283 | MET  |
| 1   | A     | 329 | ARG  |
| 1   | A     | 392 | ARG  |
| 1   | A     | 398 | LEU  |
| 1   | A     | 413 | TRP  |
| 1   | A     | 426 | LEU  |
| 1   | A     | 430 | LEU  |
| 1   | A     | 434 | LEU  |
| 1   | A     | 463 | LEU  |
| 1   | A     | 652 | THR  |
| 1   | B     | 30  | GLN  |
| 1   | B     | 35  | ASN  |
| 1   | B     | 41  | LEU  |
| 1   | B     | 74  | LEU  |
| 1   | B     | 83  | MET  |
| 1   | B     | 130 | LEU  |
| 1   | B     | 165 | LEU  |
| 1   | B     | 211 | LEU  |
| 1   | B     | 233 | LYS  |
| 1   | B     | 283 | MET  |
| 1   | B     | 329 | ARG  |
| 1   | B     | 392 | ARG  |
| 1   | B     | 398 | LEU  |
| 1   | B     | 413 | TRP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 426 | LEU  |
| 1   | B     | 430 | LEU  |
| 1   | B     | 434 | LEU  |
| 1   | B     | 463 | LEU  |
| 1   | B     | 652 | THR  |
| 1   | C     | 74  | LEU  |
| 1   | C     | 83  | MET  |
| 1   | C     | 130 | LEU  |
| 1   | C     | 165 | LEU  |
| 1   | C     | 211 | LEU  |
| 1   | C     | 283 | MET  |
| 1   | C     | 329 | ARG  |
| 1   | C     | 392 | ARG  |
| 1   | C     | 398 | LEU  |
| 1   | C     | 413 | TRP  |
| 1   | C     | 426 | LEU  |
| 1   | C     | 430 | LEU  |
| 1   | C     | 434 | LEU  |
| 1   | C     | 463 | LEU  |
| 1   | C     | 603 | ARG  |
| 1   | C     | 628 | ASN  |
| 1   | C     | 652 | THR  |
| 1   | D     | 74  | LEU  |
| 1   | D     | 83  | MET  |
| 1   | D     | 130 | LEU  |
| 1   | D     | 151 | GLU  |
| 1   | D     | 165 | LEU  |
| 1   | D     | 211 | LEU  |
| 1   | D     | 283 | MET  |
| 1   | D     | 329 | ARG  |
| 1   | D     | 392 | ARG  |
| 1   | D     | 398 | LEU  |
| 1   | D     | 413 | TRP  |
| 1   | D     | 426 | LEU  |
| 1   | D     | 430 | LEU  |
| 1   | D     | 434 | LEU  |
| 1   | D     | 463 | LEU  |
| 1   | D     | 628 | ASN  |
| 1   | D     | 652 | THR  |
| 1   | D     | 659 | LYS  |
| 1   | D     | 665 | SER  |
| 1   | E     | 28  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 32  | ILE  |
| 1   | E     | 41  | LEU  |
| 1   | E     | 74  | LEU  |
| 1   | E     | 83  | MET  |
| 1   | E     | 130 | LEU  |
| 1   | E     | 165 | LEU  |
| 1   | E     | 211 | LEU  |
| 1   | E     | 233 | LYS  |
| 1   | E     | 283 | MET  |
| 1   | E     | 329 | ARG  |
| 1   | E     | 392 | ARG  |
| 1   | E     | 398 | LEU  |
| 1   | E     | 413 | TRP  |
| 1   | E     | 426 | LEU  |
| 1   | E     | 430 | LEU  |
| 1   | E     | 434 | LEU  |
| 1   | E     | 463 | LEU  |
| 1   | E     | 628 | ASN  |
| 1   | E     | 630 | GLU  |
| 1   | E     | 652 | THR  |
| 1   | F     | 41  | LEU  |
| 1   | F     | 74  | LEU  |
| 1   | F     | 83  | MET  |
| 1   | F     | 130 | LEU  |
| 1   | F     | 165 | LEU  |
| 1   | F     | 211 | LEU  |
| 1   | F     | 231 | GLU  |
| 1   | F     | 283 | MET  |
| 1   | F     | 329 | ARG  |
| 1   | F     | 392 | ARG  |
| 1   | F     | 398 | LEU  |
| 1   | F     | 413 | TRP  |
| 1   | F     | 426 | LEU  |
| 1   | F     | 430 | LEU  |
| 1   | F     | 434 | LEU  |
| 1   | F     | 463 | LEU  |
| 1   | F     | 628 | ASN  |
| 1   | F     | 652 | THR  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 35  | ASN  |
| 1   | A     | 48  | GLN  |
| 1   | A     | 343 | GLN  |
| 1   | A     | 596 | HIS  |
| 1   | B     | 9   | ASN  |
| 1   | B     | 30  | GLN  |
| 1   | B     | 35  | ASN  |
| 1   | B     | 48  | GLN  |
| 1   | B     | 343 | GLN  |
| 1   | B     | 596 | HIS  |
| 1   | C     | 48  | GLN  |
| 1   | C     | 343 | GLN  |
| 1   | C     | 596 | HIS  |
| 1   | C     | 675 | GLN  |
| 1   | C     | 676 | ASN  |
| 1   | C     | 683 | ASN  |
| 1   | D     | 9   | ASN  |
| 1   | D     | 48  | GLN  |
| 1   | D     | 243 | ASN  |
| 1   | D     | 343 | GLN  |
| 1   | D     | 596 | HIS  |
| 1   | E     | 48  | GLN  |
| 1   | E     | 243 | ASN  |
| 1   | E     | 343 | GLN  |
| 1   | E     | 596 | HIS  |
| 1   | E     | 669 | GLN  |
| 1   | F     | 48  | GLN  |
| 1   | F     | 343 | GLN  |
| 1   | F     | 596 | HIS  |
| 1   | F     | 675 | GLN  |
| 1   | F     | 676 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2  |    |    | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------|----|----|-----------------------|-------|
| 1   | A     | 691/693 (99%)   | -0.11  | 24 (3%)  | 44 | 51 | 21, 31, 60, 74        | 0     |
| 1   | B     | 691/693 (99%)   | -0.11  | 15 (2%)  | 62 | 68 | 21, 32, 59, 78        | 0     |
| 1   | C     | 691/693 (99%)   | -0.04  | 31 (4%)  | 33 | 40 | 22, 32, 66, 84        | 0     |
| 1   | D     | 691/693 (99%)   | -0.14  | 20 (2%)  | 51 | 59 | 20, 30, 54, 78        | 0     |
| 1   | E     | 691/693 (99%)   | -0.18  | 13 (1%)  | 66 | 73 | 18, 30, 50, 80        | 0     |
| 1   | F     | 692/693 (99%)   | -0.09  | 24 (3%)  | 44 | 51 | 19, 31, 63, 83        | 0     |
| All | All   | 4147/4158 (99%) | -0.11  | 127 (3%) | 49 | 56 | 18, 31, 60, 84        | 0     |

All (127) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 49  | GLY  | 7.0  |
| 1   | B     | 30  | GLN  | 5.0  |
| 1   | D     | 49  | GLY  | 4.7  |
| 1   | E     | 30  | GLN  | 4.6  |
| 1   | A     | 693 | GLU  | 4.6  |
| 1   | F     | 693 | GLU  | 4.4  |
| 1   | C     | 687 | ARG  | 4.1  |
| 1   | C     | 628 | ASN  | 4.0  |
| 1   | C     | 50  | ASN  | 3.8  |
| 1   | F     | 29  | GLU  | 3.8  |
| 1   | C     | 667 | GLU  | 3.7  |
| 1   | F     | 661 | ILE  | 3.7  |
| 1   | E     | 29  | GLU  | 3.7  |
| 1   | C     | 661 | ILE  | 3.7  |
| 1   | C     | 693 | GLU  | 3.7  |
| 1   | C     | 49  | GLY  | 3.6  |
| 1   | E     | 49  | GLY  | 3.6  |
| 1   | E     | 50  | ASN  | 3.6  |
| 1   | D     | 35  | ASN  | 3.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 30  | GLN  | 3.6  |
| 1   | F     | 48  | GLN  | 3.5  |
| 1   | B     | 344 | PHE  | 3.5  |
| 1   | D     | 50  | ASN  | 3.4  |
| 1   | C     | 668 | ILE  | 3.4  |
| 1   | F     | 664 | ASP  | 3.4  |
| 1   | B     | 29  | GLU  | 3.3  |
| 1   | C     | 29  | GLU  | 3.3  |
| 1   | D     | 30  | GLN  | 3.3  |
| 1   | D     | 346 | ASP  | 3.3  |
| 1   | D     | 48  | GLN  | 3.3  |
| 1   | B     | 49  | GLY  | 3.2  |
| 1   | B     | 346 | ASP  | 3.2  |
| 1   | A     | 664 | ASP  | 3.1  |
| 1   | D     | 343 | GLN  | 3.1  |
| 1   | D     | 669 | GLN  | 3.1  |
| 1   | F     | 346 | ASP  | 3.1  |
| 1   | C     | 574 | ARG  | 3.1  |
| 1   | A     | 662 | VAL  | 3.0  |
| 1   | F     | 574 | ARG  | 3.0  |
| 1   | A     | 346 | ASP  | 3.0  |
| 1   | B     | 50  | ASN  | 3.0  |
| 1   | C     | 669 | GLN  | 2.9  |
| 1   | B     | 664 | ASP  | 2.9  |
| 1   | A     | 339 | SER  | 2.9  |
| 1   | D     | 29  | GLU  | 2.9  |
| 1   | C     | 658 | SER  | 2.8  |
| 1   | D     | 345 | ARG  | 2.8  |
| 1   | A     | 35  | ASN  | 2.8  |
| 1   | A     | 48  | GLN  | 2.8  |
| 1   | B     | 227 | TYR  | 2.8  |
| 1   | C     | 346 | ASP  | 2.7  |
| 1   | E     | 344 | PHE  | 2.7  |
| 1   | F     | 343 | GLN  | 2.7  |
| 1   | C     | 48  | GLN  | 2.7  |
| 1   | A     | 393 | ASN  | 2.7  |
| 1   | F     | 35  | ASN  | 2.7  |
| 1   | F     | 50  | ASN  | 2.6  |
| 1   | E     | 345 | ARG  | 2.6  |
| 1   | B     | 628 | ASN  | 2.6  |
| 1   | E     | 343 | GLN  | 2.6  |
| 1   | C     | 659 | LYS  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 31  | LYS  | 2.6  |
| 1   | D     | 635 | SER  | 2.6  |
| 1   | A     | 665 | SER  | 2.5  |
| 1   | F     | 687 | ARG  | 2.5  |
| 1   | A     | 49  | GLY  | 2.5  |
| 1   | E     | 35  | ASN  | 2.5  |
| 1   | D     | 344 | PHE  | 2.5  |
| 1   | A     | 343 | GLN  | 2.5  |
| 1   | C     | 664 | ASP  | 2.5  |
| 1   | E     | 628 | ASN  | 2.5  |
| 1   | A     | 666 | LYS  | 2.4  |
| 1   | A     | 661 | ILE  | 2.4  |
| 1   | D     | 47  | GLN  | 2.4  |
| 1   | A     | 669 | GLN  | 2.4  |
| 1   | C     | 593 | LYS  | 2.4  |
| 1   | A     | 628 | ASN  | 2.4  |
| 1   | C     | 3   | ILE  | 2.4  |
| 1   | C     | 344 | PHE  | 2.4  |
| 1   | C     | 636 | ASN  | 2.4  |
| 1   | C     | 665 | SER  | 2.4  |
| 1   | F     | 665 | SER  | 2.4  |
| 1   | F     | 692 | LEU  | 2.4  |
| 1   | C     | 670 | VAL  | 2.3  |
| 1   | B     | 574 | ARG  | 2.3  |
| 1   | E     | 346 | ASP  | 2.3  |
| 1   | B     | 48  | GLN  | 2.3  |
| 1   | D     | 693 | GLU  | 2.3  |
| 1   | C     | 47  | GLN  | 2.3  |
| 1   | F     | 662 | VAL  | 2.3  |
| 1   | E     | 339 | SER  | 2.3  |
| 1   | F     | 669 | GLN  | 2.3  |
| 1   | C     | 30  | GLN  | 2.3  |
| 1   | A     | 574 | ARG  | 2.2  |
| 1   | A     | 655 | LYS  | 2.2  |
| 1   | B     | 35  | ASN  | 2.2  |
| 1   | A     | 643 | GLU  | 2.2  |
| 1   | B     | 19  | GLU  | 2.2  |
| 1   | A     | 687 | ARG  | 2.2  |
| 1   | C     | 102 | ILE  | 2.2  |
| 1   | E     | 32  | ILE  | 2.2  |
| 1   | F     | 32  | ILE  | 2.2  |
| 1   | A     | 587 | ASN  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 227 | TYR  | 2.2  |
| 1   | B     | 566 | GLU  | 2.2  |
| 1   | E     | 48  | GLN  | 2.2  |
| 1   | C     | 434 | LEU  | 2.2  |
| 1   | C     | 566 | GLU  | 2.2  |
| 1   | A     | 50  | ASN  | 2.1  |
| 1   | C     | 343 | GLN  | 2.1  |
| 1   | F     | 344 | PHE  | 2.1  |
| 1   | F     | 666 | LYS  | 2.1  |
| 1   | F     | 658 | SER  | 2.1  |
| 1   | C     | 456 | GLU  | 2.1  |
| 1   | A     | 344 | PHE  | 2.1  |
| 1   | D     | 393 | ASN  | 2.1  |
| 1   | C     | 227 | TYR  | 2.1  |
| 1   | D     | 339 | SER  | 2.1  |
| 1   | F     | 391 | HIS  | 2.0  |
| 1   | B     | 693 | GLU  | 2.0  |
| 1   | D     | 32  | ILE  | 2.0  |
| 1   | A     | 658 | SER  | 2.0  |
| 1   | D     | 628 | ASN  | 2.0  |
| 1   | F     | 636 | ASN  | 2.0  |
| 1   | F     | 667 | GLU  | 2.0  |
| 1   | C     | 46  | VAL  | 2.0  |
| 1   | A     | 434 | LEU  | 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.