



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:00 AM UTC

PDB ID : 7D5Z / pdb\_00007d5z  
Title : Crystal structure of EBV gH/gL bound with neutralizing antibody 1D8  
Authors : Zhu, Q.; Shan, S.; Yu, J.; Wang, X.; Zhang, L.; Zeng, M.  
Deposited on : 2020-09-28  
Resolution : 4.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

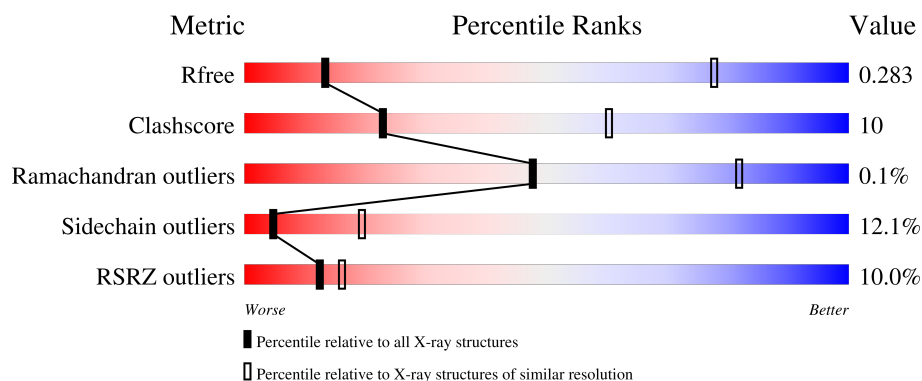
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.20 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1004 (4.52-3.88)                                      |
| Clashscore            | 190562                      | 1019 (4.50-3.90)                                      |
| Ramachandran outliers | 187476                      | 1020 (4.56-3.84)                                      |
| Sidechain outliers    | 187428                      | 1006 (4.56-3.84)                                      |
| RSRZ outliers         | 180081                      | 1001 (4.52-3.88)                                      |

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

| Mol | Chain | Length | Quality of chain                                                                                              |
|-----|-------|--------|---------------------------------------------------------------------------------------------------------------|
| 1   | A     | 665    | <div> <div>9%</div> <div> <div></div> <div>71%</div> <div>24%</div> <div>••</div> </div> </div>               |
| 1   | E     | 665    | <div> <div>17%</div> <div> <div></div> <div>72%</div> <div>24%</div> <div>••</div> </div> </div>              |
| 1   | I     | 665    | <div> <div>8%</div> <div> <div></div> <div>70%</div> <div>26%</div> <div>••</div> </div> </div>               |
| 1   | M     | 665    | <div> <div>7%</div> <div> <div></div> <div>69%</div> <div>26%</div> <div>••</div> </div> </div>               |
| 2   | B     | 112    | <div> <div>7%</div> <div> <div></div> <div>59%</div> <div>23%</div> <div>•</div> <div>16%</div> </div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | F     | 112    |                  |
| 2   | J     | 112    |                  |
| 2   | N     | 112    |                  |
| 3   | C     | 233    |                  |
| 3   | G     | 233    |                  |
| 3   | K     | 233    |                  |
| 3   | O     | 233    |                  |
| 4   | D     | 470    |                  |
| 4   | H     | 470    |                  |
| 4   | L     | 470    |                  |
| 4   | P     | 470    |                  |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36304 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 Envelope glycoprotein H.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | M     | 655      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 5099  | 3270 | 842 | 955 | 32 |         |         |       |
| 1   | A     | 655      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 5099  | 3270 | 842 | 955 | 32 |         |         |       |
| 1   | E     | 655      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 5099  | 3270 | 842 | 955 | 32 |         |         |       |
| 1   | I     | 655      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 5099  | 3270 | 842 | 955 | 32 |         |         |       |

There are 20 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| M     | 680     | HIS      | -      | expression tag | UNP Q3KSQ3 |
| M     | 681     | HIS      | -      | expression tag | UNP Q3KSQ3 |
| M     | 682     | HIS      | -      | expression tag | UNP Q3KSQ3 |
| M     | 683     | HIS      | -      | expression tag | UNP Q3KSQ3 |
| M     | 684     | HIS      | -      | expression tag | UNP Q3KSQ3 |
| A     | 680     | HIS      | -      | expression tag | UNP Q3KSQ3 |
| A     | 681     | HIS      | -      | expression tag | UNP Q3KSQ3 |
| A     | 682     | HIS      | -      | expression tag | UNP Q3KSQ3 |
| A     | 683     | HIS      | -      | expression tag | UNP Q3KSQ3 |
| A     | 684     | HIS      | -      | expression tag | UNP Q3KSQ3 |
| E     | 680     | HIS      | -      | expression tag | UNP Q3KSQ3 |
| E     | 681     | HIS      | -      | expression tag | UNP Q3KSQ3 |
| E     | 682     | HIS      | -      | expression tag | UNP Q3KSQ3 |
| E     | 683     | HIS      | -      | expression tag | UNP Q3KSQ3 |
| E     | 684     | HIS      | -      | expression tag | UNP Q3KSQ3 |
| I     | 680     | HIS      | -      | expression tag | UNP Q3KSQ3 |
| I     | 681     | HIS      | -      | expression tag | UNP Q3KSQ3 |
| I     | 682     | HIS      | -      | expression tag | UNP Q3KSQ3 |
| I     | 683     | HIS      | -      | expression tag | UNP Q3KSQ3 |
| I     | 684     | HIS      | -      | expression tag | UNP Q3KSQ3 |

- Molecule 2 is a protein called Envelope glycoprotein L.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | N     | 94       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 719   | 454 | 120 | 141 | 4 |         |         |       |
| 2   | B     | 94       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 719   | 454 | 120 | 141 | 4 |         |         |       |
| 2   | F     | 94       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 719   | 454 | 120 | 141 | 4 |         |         |       |
| 2   | J     | 94       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 719   | 454 | 120 | 141 | 4 |         |         |       |

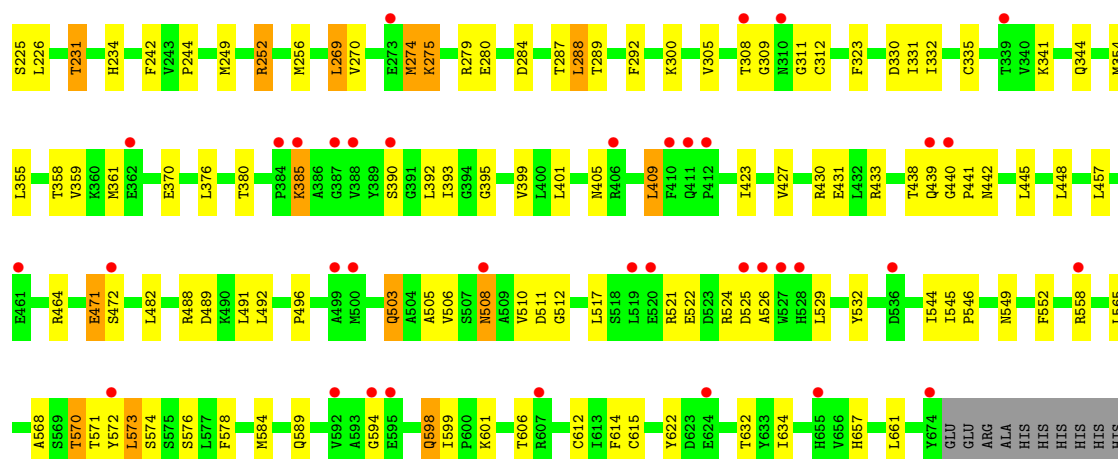
- Molecule 3 is a protein called light chain of 1D8.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | O     | 213      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1647  | 1035 | 278 | 329 | 5 |         |         |       |
| 3   | C     | 213      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1647  | 1035 | 278 | 329 | 5 |         |         |       |
| 3   | G     | 213      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1647  | 1035 | 278 | 329 | 5 |         |         |       |
| 3   | K     | 213      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1647  | 1035 | 278 | 329 | 5 |         |         |       |

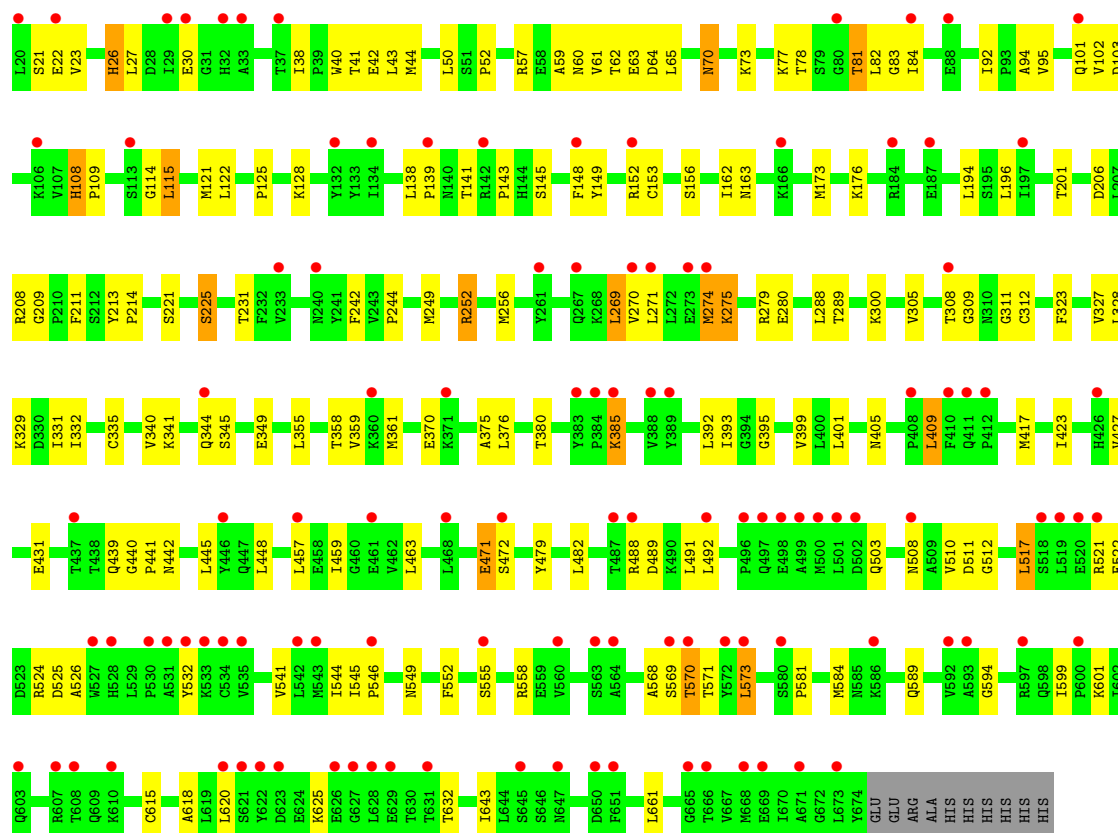
- Molecule 4 is a protein called heavy chain of 1D8.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4   | P     | 214      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1611  | 1021 | 273 | 307 | 10 |         |         |       |
| 4   | D     | 214      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1611  | 1021 | 273 | 307 | 10 |         |         |       |
| 4   | H     | 214      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1611  | 1021 | 273 | 307 | 10 |         |         |       |
| 4   | L     | 214      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1611  | 1021 | 273 | 307 | 10 |         |         |       |

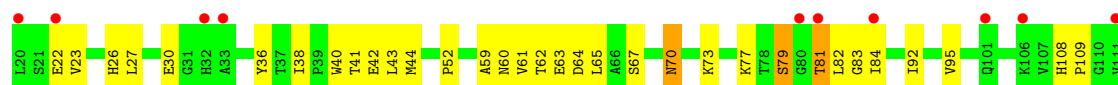


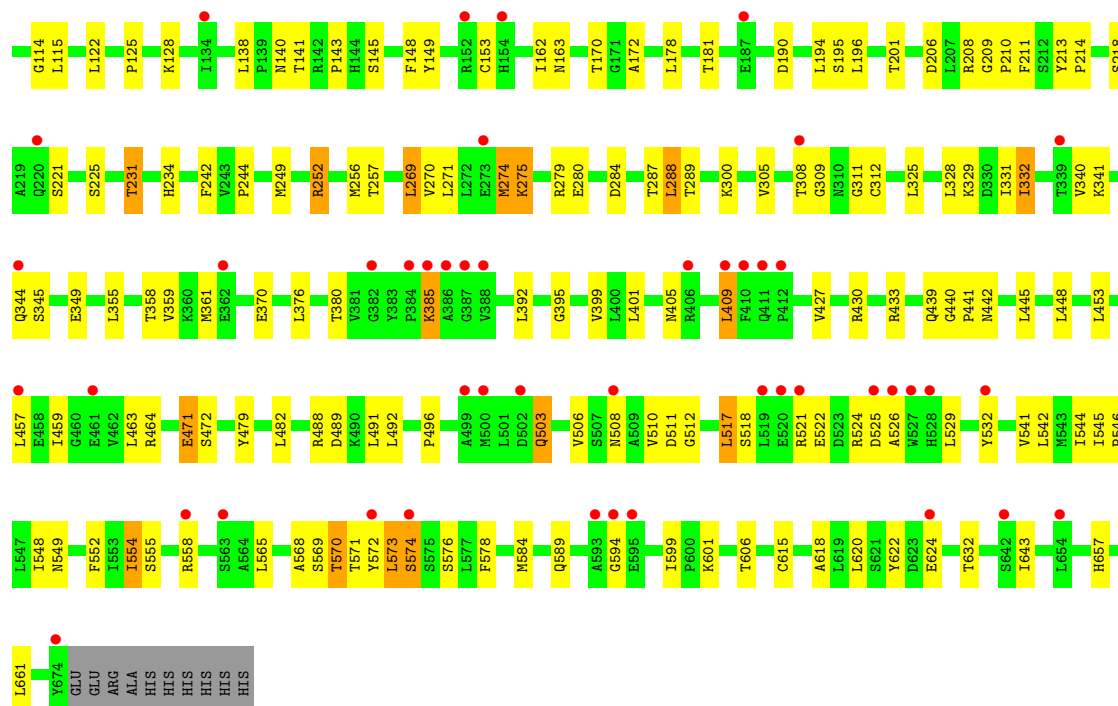


• Molecule 1: Envelope glycoprotein H

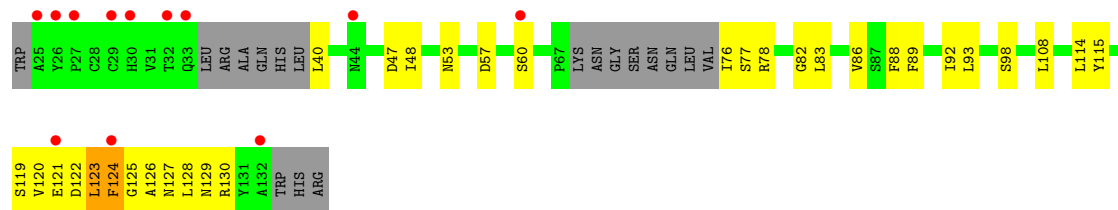


• Molecule 1: Envelope glycoprotein H





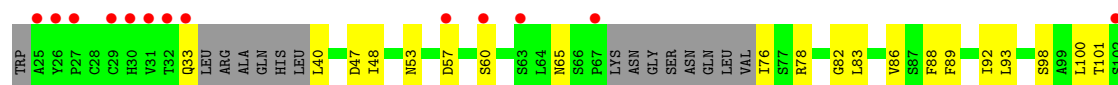
• Molecule 2: Envelope glycoprotein L



• Molecule 2: Envelope glycoprotein L

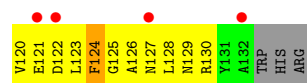
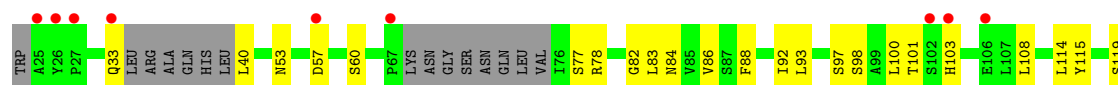


• Molecule 2: Envelope glycoprotein L

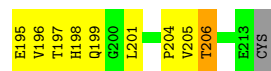




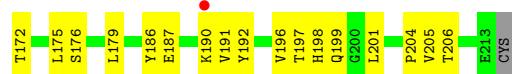
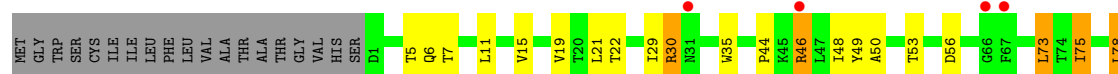
• Molecule 2: Envelope glycoprotein L



• Molecule 3: light chain of 1D8



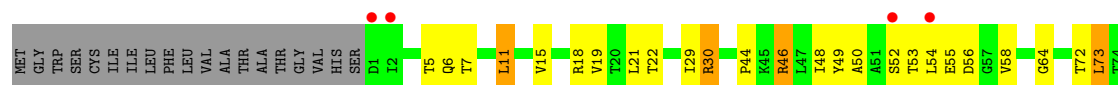
• Molecule 3: light chain of 1D8



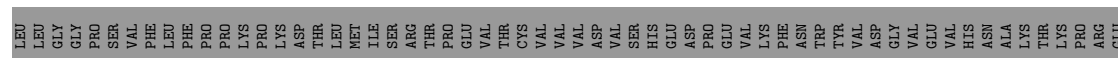
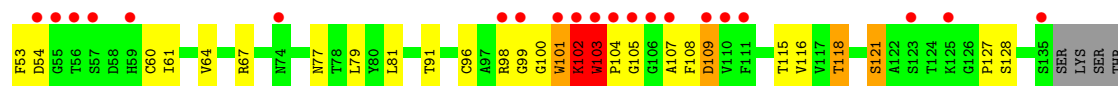
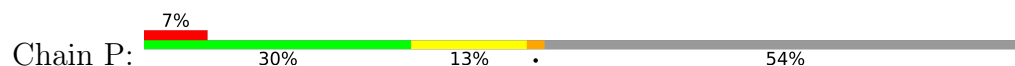
• Molecule 3: light chain of 1D8



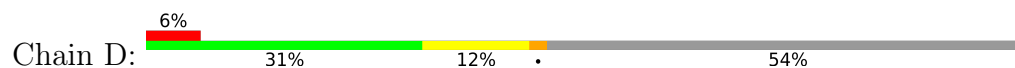
- Molecule 3: light chain of 1D8

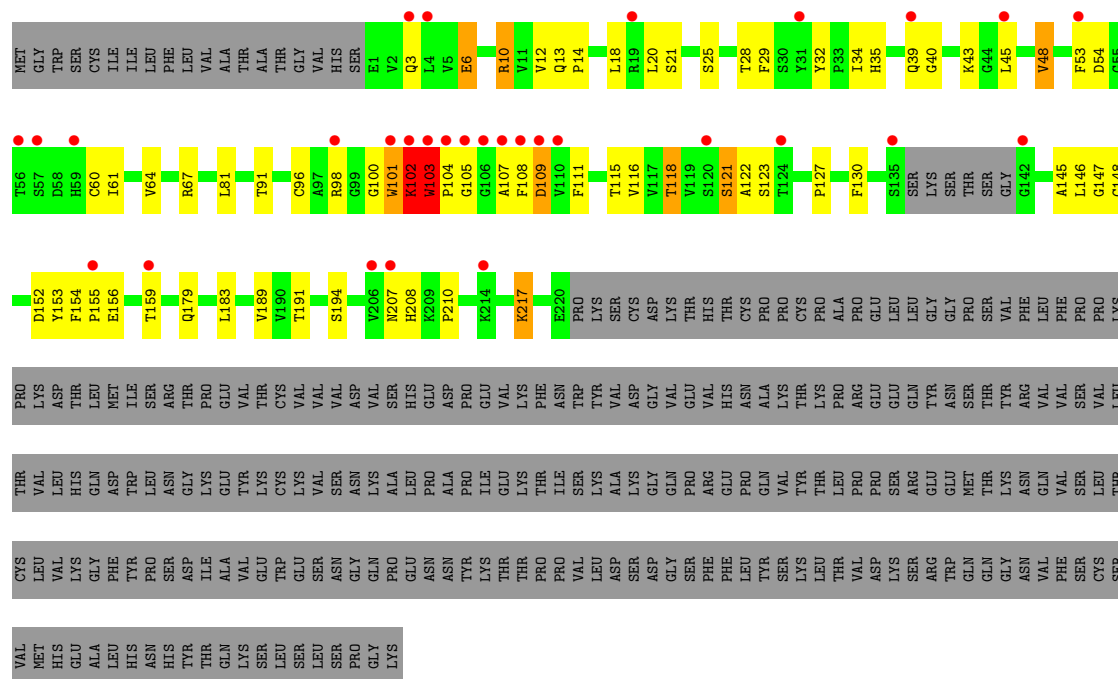


- Molecule 4: heavy chain of 1D8

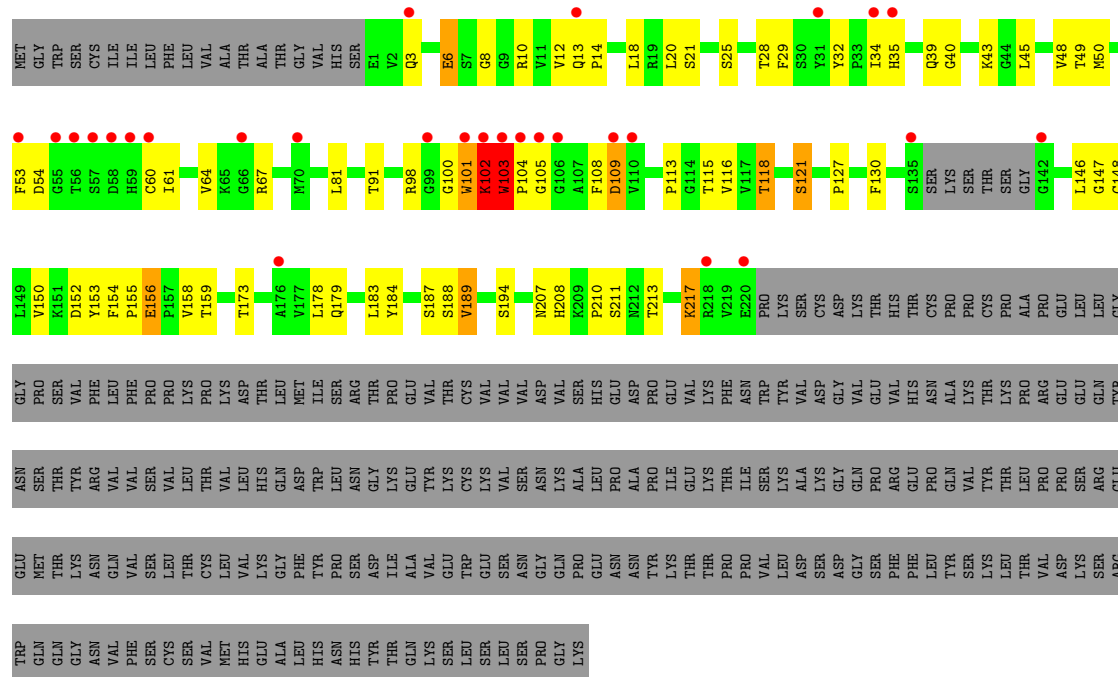
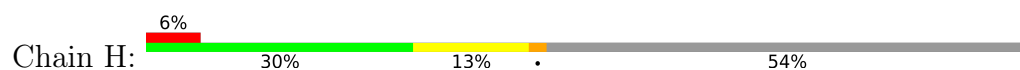


- Molecule 4: heavy chain of 1D8

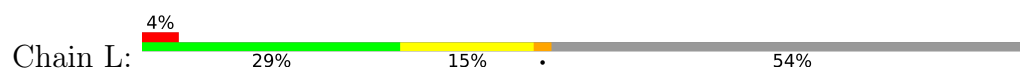




### • Molecule 4: heavy chain of 1D8



### • Molecule 4: heavy chain of 1D8



[illegible]

## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 41 21 2                                                   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 212.87Å 212.87Å 598.13Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 50.03 – 4.20<br>50.03 – 4.20                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.4 (50.03-4.20)<br>99.8 (50.03-4.20)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.13                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.91 (at 4.14Å)                                             | Xtrriage         |
| Refinement program                                                      | PHENIX 1.18.2_3874                                          | Depositor        |
| R, $R_{free}$                                                           | 0.246 , 0.277<br>0.254 , 0.283                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 5096 reflections (5.05%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 127.2                                                       | Xtrriage         |
| Anisotropy                                                              | 0.104                                                       | Xtrriage         |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 214.9                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$ | Xtrriage         |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtrriage         |
| $F_o, F_c$ correlation                                                  | 0.87                                                        | EDS              |
| Total number of atoms                                                   | 36304                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 153.0                                                       | wwPDB-VP         |

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.10 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1713e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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     | 0.17         | 0/5208  | 0.45        | 0/7067          |
| 1   | E     | 0.18         | 0/5208  | 0.44        | 0/7067          |
| 1   | I     | 0.18         | 0/5208  | 0.44        | 0/7067          |
| 1   | M     | 0.17         | 0/5208  | 0.43        | 0/7067          |
| 2   | B     | 0.19         | 0/729   | 0.42        | 0/987           |
| 2   | F     | 0.18         | 0/729   | 0.42        | 0/987           |
| 2   | J     | 0.18         | 0/729   | 0.41        | 0/987           |
| 2   | N     | 0.18         | 0/729   | 0.42        | 0/987           |
| 3   | C     | 0.21         | 0/1686  | 0.48        | 0/2294          |
| 3   | G     | 0.19         | 0/1686  | 0.47        | 0/2294          |
| 3   | K     | 0.19         | 0/1686  | 0.48        | 0/2294          |
| 3   | O     | 0.20         | 0/1686  | 0.47        | 0/2294          |
| 4   | D     | 0.20         | 0/1653  | 0.50        | 3/2249 (0.1%)   |
| 4   | H     | 0.23         | 0/1653  | 0.52        | 3/2249 (0.1%)   |
| 4   | L     | 0.21         | 0/1653  | 0.52        | 3/2249 (0.1%)   |
| 4   | P     | 0.20         | 0/1653  | 0.50        | 3/2249 (0.1%)   |
| All | All   | 0.19         | 0/37104 | 0.46        | 12/50388 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 3   | C     | 0                   | 2                   |
| 3   | G     | 0                   | 1                   |
| 3   | K     | 0                   | 2                   |
| 3   | O     | 0                   | 1                   |
| 4   | D     | 0                   | 2                   |
| 4   | H     | 0                   | 2                   |
| 4   | L     | 0                   | 2                   |
| 4   | P     | 0                   | 2                   |
| All | All   | 0                   | 14                  |

There are no bond length outliers.

All (12) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|-----|------|--------|------|------------------------|---------------------|
| 4   | H     | 103 | TRP  | N-CA-C | 8.07 | 127.65                 | 109.81              |
| 4   | L     | 103 | TRP  | N-CA-C | 7.97 | 127.44                 | 109.81              |
| 4   | D     | 103 | TRP  | N-CA-C | 7.75 | 126.93                 | 109.81              |
| 4   | P     | 103 | TRP  | N-CA-C | 7.71 | 126.85                 | 109.81              |
| 4   | L     | 102 | LYS  | CA-C-N | 6.19 | 136.91                 | 121.80              |
| 4   | L     | 102 | LYS  | C-N-CA | 6.19 | 136.91                 | 121.80              |
| 4   | H     | 102 | LYS  | CA-C-N | 6.12 | 136.74                 | 121.80              |
| 4   | H     | 102 | LYS  | C-N-CA | 6.12 | 136.74                 | 121.80              |
| 4   | P     | 102 | LYS  | CA-C-N | 5.93 | 136.27                 | 121.80              |
| 4   | P     | 102 | LYS  | C-N-CA | 5.93 | 136.27                 | 121.80              |
| 4   | D     | 102 | LYS  | CA-C-N | 5.92 | 136.25                 | 121.80              |
| 4   | D     | 102 | LYS  | C-N-CA | 5.92 | 136.25                 | 121.80              |

There are no chirality outliers.

All (14) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 3   | C     | 106 | ILE  | Peptide |
| 3   | C     | 29  | ILE  | Peptide |
| 4   | D     | 102 | LYS  | Peptide |
| 4   | D     | 121 | SER  | Peptide |
| 3   | G     | 29  | ILE  | Peptide |
| 4   | H     | 102 | LYS  | Peptide |
| 4   | H     | 121 | SER  | Peptide |
| 3   | K     | 106 | ILE  | Peptide |
| 3   | K     | 29  | ILE  | Peptide |
| 4   | L     | 102 | LYS  | Peptide |
| 4   | L     | 121 | SER  | Peptide |
| 3   | O     | 29  | ILE  | Peptide |
| 4   | P     | 102 | LYS  | Peptide |
| 4   | P     | 121 | SER  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 5099  | 0        | 5119     | 98      | 0            |
| 1   | E     | 5099  | 0        | 5119     | 95      | 0            |
| 1   | I     | 5099  | 0        | 5119     | 106     | 0            |
| 1   | M     | 5099  | 0        | 5119     | 109     | 0            |
| 2   | B     | 719   | 0        | 703      | 16      | 0            |
| 2   | F     | 719   | 0        | 703      | 19      | 0            |
| 2   | J     | 719   | 0        | 703      | 20      | 0            |
| 2   | N     | 719   | 0        | 703      | 18      | 0            |
| 3   | C     | 1647  | 0        | 1598     | 39      | 0            |
| 3   | G     | 1647  | 0        | 1598     | 37      | 0            |
| 3   | K     | 1647  | 0        | 1598     | 40      | 0            |
| 3   | O     | 1647  | 0        | 1598     | 32      | 0            |
| 4   | D     | 1611  | 0        | 1568     | 44      | 0            |
| 4   | H     | 1611  | 0        | 1568     | 47      | 0            |
| 4   | L     | 1611  | 0        | 1568     | 50      | 0            |
| 4   | P     | 1611  | 0        | 1568     | 55      | 0            |
| All | All   | 36304 | 0        | 35952    | 750     | 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 (750) 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:M:201:THR:HG22 | 1:M:225:SER:HB2  | 1.53                     | 0.88              |
| 3:K:75:ILE:HG12  | 3:K:78:LEU:HD23  | 1.59                     | 0.84              |
| 1:I:201:THR:HG22 | 1:I:225:SER:HB2  | 1.59                     | 0.84              |
| 1:I:526:ALA:HB1  | 1:I:532:TYR:HE2  | 1.44                     | 0.82              |
| 3:G:75:ILE:HG12  | 3:G:78:LEU:HD23  | 1.62                     | 0.81              |
| 1:A:201:THR:HG22 | 1:A:225:SER:HB2  | 1.62                     | 0.81              |
| 3:C:75:ILE:HG12  | 3:C:78:LEU:HD23  | 1.63                     | 0.80              |
| 1:A:81:THR:HG21  | 2:J:125:GLY:HA2  | 1.62                     | 0.78              |
| 1:M:81:THR:HG21  | 2:F:125:GLY:HA2  | 1.66                     | 0.78              |
| 2:B:125:GLY:HA2  | 1:I:81:THR:HG21  | 1.68                     | 0.76              |
| 1:A:526:ALA:HB1  | 1:A:532:TYR:HE2  | 1.52                     | 0.74              |
| 1:E:114:GLY:HA2  | 1:E:358:THR:HG21 | 1.69                     | 0.74              |
| 1:E:141:THR:HG23 | 1:E:143:PRO:HD2  | 1.70                     | 0.74              |
| 2:N:125:GLY:HA2  | 1:E:81:THR:HG21  | 1.70                     | 0.73              |
| 1:A:570:THR:OG1  | 1:A:571:THR:N    | 2.19                     | 0.73              |
| 1:I:114:GLY:HA2  | 1:I:358:THR:HG21 | 1.71                     | 0.73              |
| 1:M:526:ALA:HB1  | 1:M:532:TYR:HE2  | 1.54                     | 0.72              |
| 1:A:114:GLY:HA2  | 1:A:358:THR:HG21 | 1.71                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:60:ASN:HB3   | 1:E:63:GLU:HB2   | 1.71                     | 0.72              |
| 1:M:448:LEU:HD13 | 1:M:546:PRO:HD2  | 1.72                     | 0.72              |
| 1:E:526:ALA:HB1  | 1:E:532:TYR:HE2  | 1.55                     | 0.71              |
| 4:L:20:LEU:HD12  | 4:L:81:LEU:HD23  | 1.71                     | 0.71              |
| 1:A:448:LEU:HD13 | 1:A:546:PRO:HD2  | 1.72                     | 0.71              |
| 1:A:60:ASN:HB3   | 1:A:63:GLU:HB2   | 1.73                     | 0.71              |
| 1:M:570:THR:OG1  | 1:M:571:THR:N    | 2.22                     | 0.71              |
| 1:E:522:GLU:HG3  | 1:E:524:ARG:HG2  | 1.72                     | 0.70              |
| 2:J:93:LEU:HB2   | 2:J:108:LEU:HD13 | 1.74                     | 0.70              |
| 1:I:570:THR:OG1  | 1:I:571:THR:N    | 2.20                     | 0.70              |
| 3:C:108:ARG:HH22 | 3:C:111:ALA:HB3  | 1.58                     | 0.69              |
| 1:M:114:GLY:HA2  | 1:M:358:THR:HG21 | 1.74                     | 0.69              |
| 1:E:570:THR:OG1  | 1:E:571:THR:N    | 2.23                     | 0.69              |
| 1:M:522:GLU:HG3  | 1:M:524:ARG:HG2  | 1.74                     | 0.69              |
| 4:D:20:LEU:HD12  | 4:D:81:LEU:HD23  | 1.75                     | 0.69              |
| 1:E:201:THR:HG22 | 1:E:225:SER:HB2  | 1.73                     | 0.69              |
| 1:E:361:MET:HE2  | 1:E:392:LEU:HA   | 1.74                     | 0.69              |
| 1:I:361:MET:HE2  | 1:I:392:LEU:HA   | 1.75                     | 0.69              |
| 1:M:82:LEU:HG    | 1:M:83:GLY:H     | 1.58                     | 0.69              |
| 3:O:75:ILE:HG12  | 3:O:78:LEU:HD23  | 1.74                     | 0.69              |
| 1:I:122:LEU:HA   | 1:I:312:CYS:HA   | 1.75                     | 0.69              |
| 1:I:448:LEU:HD13 | 1:I:546:PRO:HD2  | 1.75                     | 0.68              |
| 1:M:60:ASN:HB3   | 1:M:63:GLU:HB2   | 1.75                     | 0.68              |
| 1:E:122:LEU:HA   | 1:E:312:CYS:HA   | 1.76                     | 0.68              |
| 1:A:122:LEU:HA   | 1:A:312:CYS:HA   | 1.76                     | 0.68              |
| 1:I:269:LEU:HD12 | 1:I:331:ILE:HG23 | 1.75                     | 0.68              |
| 2:B:60:SER:HB3   | 2:B:83:LEU:HG    | 1.76                     | 0.67              |
| 3:C:197:THR:HG23 | 3:C:204:PRO:HG3  | 1.76                     | 0.67              |
| 1:I:565:LEU:HD11 | 1:I:578:PHE:HB3  | 1.75                     | 0.67              |
| 2:N:60:SER:HB3   | 2:N:83:LEU:HG    | 1.77                     | 0.67              |
| 4:P:14:PRO:HD2   | 4:P:121:SER:HB3  | 1.75                     | 0.67              |
| 1:M:275:LYS:HE2  | 1:M:512:GLY:HA3  | 1.77                     | 0.66              |
| 2:B:93:LEU:HB2   | 2:B:108:LEU:HD13 | 1.78                     | 0.66              |
| 3:K:197:THR:HG23 | 3:K:204:PRO:HG3  | 1.77                     | 0.66              |
| 1:A:522:GLU:HG3  | 1:A:524:ARG:HG2  | 1.77                     | 0.66              |
| 1:E:482:LEU:HD22 | 1:E:544:ILE:HB   | 1.78                     | 0.66              |
| 1:M:361:MET:HE2  | 1:M:392:LEU:HA   | 1.78                     | 0.65              |
| 1:A:361:MET:HE2  | 1:A:392:LEU:HA   | 1.78                     | 0.65              |
| 1:I:60:ASN:HB3   | 1:I:63:GLU:HB2   | 1.77                     | 0.65              |
| 1:M:122:LEU:HA   | 1:M:312:CYS:HA   | 1.79                     | 0.65              |
| 2:F:93:LEU:HB2   | 2:F:108:LEU:HD13 | 1.79                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:H:20:LEU:HD12  | 4:H:81:LEU:HD23  | 1.79                     | 0.65              |
| 1:E:526:ALA:HB1  | 1:E:532:TYR:CE2  | 2.31                     | 0.65              |
| 1:M:401:LEU:O    | 1:M:405:ASN:ND2  | 2.30                     | 0.64              |
| 3:O:108:ARG:HH22 | 3:O:111:ALA:HB3  | 1.62                     | 0.64              |
| 1:M:269:LEU:HD12 | 1:M:331:ILE:HG23 | 1.80                     | 0.64              |
| 1:I:522:GLU:HG3  | 1:I:524:ARG:HG2  | 1.79                     | 0.64              |
| 2:N:121:GLU:HB3  | 2:F:121:GLU:HB3  | 1.79                     | 0.64              |
| 1:E:541:VAL:HA   | 1:E:555:SER:HB3  | 1.80                     | 0.64              |
| 4:P:40:GLY:HA3   | 4:P:43:LYS:HE3   | 1.80                     | 0.63              |
| 2:N:93:LEU:HB2   | 2:N:108:LEU:HD13 | 1.78                     | 0.63              |
| 2:J:60:SER:HB3   | 2:J:83:LEU:HG    | 1.78                     | 0.63              |
| 1:I:82:LEU:HG    | 1:I:83:GLY:H     | 1.63                     | 0.63              |
| 1:E:279:ARG:HG3  | 1:E:280:GLU:H    | 1.64                     | 0.63              |
| 4:D:39:GLN:HB2   | 4:D:45:LEU:HD23  | 1.80                     | 0.63              |
| 1:I:526:ALA:HB1  | 1:I:532:TYR:CE2  | 2.30                     | 0.63              |
| 4:L:53:PHE:CD1   | 4:L:103:TRP:HB2  | 2.33                     | 0.63              |
| 1:A:275:LYS:HE2  | 1:A:512:GLY:HA3  | 1.81                     | 0.63              |
| 2:F:60:SER:HB3   | 2:F:83:LEU:HG    | 1.79                     | 0.63              |
| 3:K:108:ARG:HH22 | 3:K:111:ALA:HB3  | 1.63                     | 0.63              |
| 1:M:242:PHE:CZ   | 1:M:244:PRO:HG3  | 2.34                     | 0.62              |
| 1:M:526:ALA:HB1  | 1:M:532:TYR:CE2  | 2.33                     | 0.62              |
| 1:A:82:LEU:HG    | 1:A:83:GLY:H     | 1.64                     | 0.62              |
| 4:P:20:LEU:HD12  | 4:P:81:LEU:HD23  | 1.81                     | 0.62              |
| 1:I:361:MET:HE3  | 1:I:395:GLY:HA3  | 1.80                     | 0.62              |
| 1:A:361:MET:HE3  | 1:A:395:GLY:HA3  | 1.81                     | 0.62              |
| 1:A:565:LEU:HD11 | 1:A:578:PHE:HB3  | 1.82                     | 0.62              |
| 4:D:127:PRO:HB3  | 4:D:153:TYR:HB3  | 1.82                     | 0.62              |
| 4:D:14:PRO:HD2   | 4:D:121:SER:HB3  | 1.82                     | 0.61              |
| 4:D:53:PHE:CD1   | 4:D:103:TRP:HB2  | 2.35                     | 0.61              |
| 1:I:242:PHE:CZ   | 1:I:244:PRO:HG3  | 2.35                     | 0.61              |
| 1:E:82:LEU:HG    | 1:E:83:GLY:H     | 1.66                     | 0.61              |
| 3:O:19:VAL:HB    | 3:O:75:ILE:HG23  | 1.83                     | 0.61              |
| 1:A:526:ALA:HB1  | 1:A:532:TYR:CE2  | 2.33                     | 0.61              |
| 1:A:589:GLN:H    | 1:A:589:GLN:CD   | 2.09                     | 0.61              |
| 2:B:125:GLY:HA2  | 1:I:81:THR:CG2   | 2.30                     | 0.61              |
| 1:E:448:LEU:HD13 | 1:E:546:PRO:HD2  | 1.83                     | 0.61              |
| 1:M:81:THR:CG2   | 2:F:125:GLY:HA2  | 2.30                     | 0.60              |
| 3:K:146:VAL:HG22 | 3:K:196:VAL:HG22 | 1.83                     | 0.60              |
| 4:H:53:PHE:CD1   | 4:H:103:TRP:HB2  | 2.36                     | 0.60              |
| 1:A:81:THR:CG2   | 2:J:125:GLY:HA2  | 2.31                     | 0.60              |
| 1:I:279:ARG:HG3  | 1:I:280:GLU:H    | 1.67                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:91:THR:HG23  | 4:D:118:THR:HA   | 1.83                     | 0.60              |
| 1:E:488:ARG:NH1  | 1:E:511:ASP:OD1  | 2.35                     | 0.59              |
| 1:A:269:LEU:HD12 | 1:A:331:ILE:HG23 | 1.83                     | 0.59              |
| 4:L:40:GLY:HA3   | 4:L:43:LYS:HE3   | 1.83                     | 0.59              |
| 4:L:91:THR:HG23  | 4:L:118:THR:HA   | 1.84                     | 0.59              |
| 4:P:53:PHE:CD1   | 4:P:103:TRP:HB2  | 2.36                     | 0.59              |
| 4:H:40:GLY:HA3   | 4:H:43:LYS:HE3   | 1.84                     | 0.59              |
| 1:I:401:LEU:O    | 1:I:405:ASN:ND2  | 2.35                     | 0.59              |
| 1:A:279:ARG:HG3  | 1:A:280:GLU:H    | 1.65                     | 0.59              |
| 1:E:138:LEU:HD13 | 1:E:148:PHE:HB3  | 1.84                     | 0.59              |
| 1:I:482:LEU:HD22 | 1:I:544:ILE:HB   | 1.82                     | 0.59              |
| 4:L:127:PRO:HB3  | 4:L:153:TYR:HB3  | 1.85                     | 0.59              |
| 1:A:401:LEU:O    | 1:A:405:ASN:ND2  | 2.36                     | 0.59              |
| 4:P:127:PRO:HB3  | 4:P:153:TYR:HB3  | 1.84                     | 0.59              |
| 1:E:275:LYS:HE2  | 1:E:512:GLY:HA3  | 1.83                     | 0.59              |
| 1:A:209:GLY:O    | 2:B:115:TYR:OH   | 2.21                     | 0.58              |
| 4:L:20:LEU:HB2   | 4:L:81:LEU:HB3   | 1.85                     | 0.58              |
| 1:M:138:LEU:HD13 | 1:M:148:PHE:HB3  | 1.84                     | 0.58              |
| 1:M:279:ARG:HG3  | 1:M:280:GLU:H    | 1.68                     | 0.58              |
| 1:M:589:GLN:CD   | 1:M:589:GLN:H    | 2.11                     | 0.58              |
| 1:M:86:LEU:N     | 1:M:221:SER:OG   | 2.34                     | 0.58              |
| 3:K:132:VAL:HB   | 3:K:179:LEU:HB3  | 1.86                     | 0.58              |
| 4:P:39:GLN:HB2   | 4:P:45:LEU:HD23  | 1.85                     | 0.58              |
| 1:A:138:LEU:HD13 | 1:A:148:PHE:HB3  | 1.84                     | 0.58              |
| 1:I:311:GLY:HA2  | 4:L:101:TRP:CE3  | 2.38                     | 0.58              |
| 3:O:132:VAL:HB   | 3:O:179:LEU:HB3  | 1.86                     | 0.58              |
| 1:A:242:PHE:CZ   | 1:A:244:PRO:HG3  | 2.39                     | 0.58              |
| 1:E:573:LEU:HD13 | 1:E:625:LYS:HG2  | 1.86                     | 0.58              |
| 3:K:85:THR:HA    | 3:K:103:LYS:HA   | 1.85                     | 0.58              |
| 4:L:208:HIS:CD2  | 4:L:210:PRO:HD2  | 2.39                     | 0.58              |
| 1:M:82:LEU:CG    | 1:M:83:GLY:H     | 2.16                     | 0.57              |
| 1:I:503:GLN:HA   | 1:I:506:VAL:HB   | 1.85                     | 0.57              |
| 4:P:91:THR:HG23  | 4:P:118:THR:HA   | 1.87                     | 0.57              |
| 1:A:311:GLY:HA2  | 4:D:101:TRP:CE3  | 2.38                     | 0.57              |
| 2:N:125:GLY:HA2  | 1:E:81:THR:CG2   | 2.33                     | 0.57              |
| 4:P:208:HIS:CD2  | 4:P:210:PRO:HD2  | 2.39                     | 0.57              |
| 1:A:568:ALA:HA   | 1:A:599:ILE:HD13 | 1.85                     | 0.57              |
| 1:A:482:LEU:HD22 | 1:A:544:ILE:HB   | 1.85                     | 0.57              |
| 4:D:152:ASP:OD1  | 4:D:179:GLN:NE2  | 2.38                     | 0.57              |
| 1:E:70:ASN:HA    | 1:E:73:LYS:HE3   | 1.86                     | 0.57              |
| 1:I:589:GLN:H    | 1:I:589:GLN:CD   | 2.11                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:568:ALA:HA   | 1:I:599:ILE:HD13 | 1.87                     | 0.57              |
| 4:H:208:HIS:CD2  | 4:H:210:PRO:HD2  | 2.40                     | 0.56              |
| 1:I:40:TRP:HB3   | 1:I:44:MET:HE3   | 1.86                     | 0.56              |
| 4:H:14:PRO:HD2   | 4:H:121:SER:HB3  | 1.85                     | 0.56              |
| 1:M:311:GLY:HA2  | 4:P:101:TRP:CE3  | 2.39                     | 0.56              |
| 1:M:361:MET:HE3  | 1:M:395:GLY:HA3  | 1.86                     | 0.56              |
| 1:E:44:MET:HE2   | 1:E:52:PRO:HD2   | 1.88                     | 0.56              |
| 1:E:242:PHE:CZ   | 1:E:244:PRO:HG3  | 2.40                     | 0.56              |
| 1:E:632:THR:HG21 | 1:E:643:ILE:HD11 | 1.87                     | 0.56              |
| 3:G:197:THR:HG23 | 3:G:204:PRO:HG3  | 1.86                     | 0.56              |
| 4:D:159:THR:HB   | 4:D:207:ASN:HB3  | 1.87                     | 0.56              |
| 3:C:19:VAL:HB    | 3:C:75:ILE:HG23  | 1.88                     | 0.56              |
| 1:I:571:THR:HG23 | 1:I:574:SER:H    | 1.70                     | 0.56              |
| 4:D:152:ASP:HB3  | 4:D:183:LEU:HD13 | 1.88                     | 0.56              |
| 1:I:138:LEU:HD13 | 1:I:148:PHE:HB3  | 1.86                     | 0.56              |
| 3:C:108:ARG:CZ   | 3:C:172:THR:HG22 | 2.36                     | 0.56              |
| 4:H:91:THR:HG23  | 4:H:118:THR:HA   | 1.88                     | 0.56              |
| 4:L:147:GLY:HA3  | 4:L:189:VAL:HG12 | 1.88                     | 0.56              |
| 3:K:50:ALA:HB3   | 3:K:53:THR:HG23  | 1.88                     | 0.56              |
| 4:H:61:ILE:HG22  | 4:H:64:VAL:HG22  | 1.87                     | 0.55              |
| 1:M:572:TYR:CE1  | 1:A:170:THR:HG21 | 2.41                     | 0.55              |
| 1:M:482:LEU:HD22 | 1:M:544:ILE:HB   | 1.87                     | 0.55              |
| 4:H:127:PRO:HB3  | 4:H:153:TYR:HB3  | 1.88                     | 0.55              |
| 4:P:32:TYR:HE1   | 4:P:101:TRP:HD1  | 1.53                     | 0.55              |
| 1:I:92:ILE:O     | 4:L:102:LYS:HD3  | 2.07                     | 0.55              |
| 1:I:275:LYS:HE2  | 1:I:512:GLY:HA3  | 1.88                     | 0.55              |
| 4:L:34:ILE:HG22  | 4:L:35:HIS:N     | 2.21                     | 0.55              |
| 2:N:124:PHE:C    | 2:N:126:ALA:H    | 2.15                     | 0.55              |
| 3:K:108:ARG:CZ   | 3:K:172:THR:HG22 | 2.36                     | 0.55              |
| 3:C:132:VAL:HB   | 3:C:179:LEU:HB3  | 1.89                     | 0.54              |
| 4:L:39:GLN:HB2   | 4:L:45:LEU:HD23  | 1.89                     | 0.54              |
| 4:L:152:ASP:OD1  | 4:L:179:GLN:NE2  | 2.38                     | 0.54              |
| 4:D:208:HIS:CD2  | 4:D:210:PRO:HD2  | 2.41                     | 0.54              |
| 1:I:64:ASP:N     | 1:I:64:ASP:OD1   | 2.40                     | 0.54              |
| 1:A:64:ASP:OD1   | 1:A:64:ASP:N     | 2.40                     | 0.54              |
| 1:M:568:ALA:HA   | 1:M:599:ILE:HD13 | 1.90                     | 0.54              |
| 1:A:40:TRP:HB3   | 1:A:44:MET:HE3   | 1.90                     | 0.54              |
| 1:I:70:ASN:HA    | 1:I:73:LYS:HE3   | 1.89                     | 0.54              |
| 1:A:380:THR:HG22 | 1:A:427:VAL:HG22 | 1.90                     | 0.54              |
| 1:E:361:MET:HE3  | 1:E:395:GLY:HA3  | 1.89                     | 0.54              |
| 1:I:44:MET:HE2   | 1:I:52:PRO:HD2   | 1.89                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:O:108:ARG:CZ   | 3:O:172:THR:HG22 | 2.37                     | 0.54              |
| 1:E:279:ARG:HG3  | 1:E:280:GLU:N    | 2.24                     | 0.53              |
| 1:E:401:LEU:O    | 1:E:405:ASN:ND2  | 2.40                     | 0.53              |
| 3:G:50:ALA:HB3   | 3:G:53:THR:HG23  | 1.91                     | 0.53              |
| 4:D:20:LEU:HB2   | 4:D:81:LEU:HB3   | 1.91                     | 0.53              |
| 1:M:464:ARG:HB2  | 1:M:496:PRO:HG3  | 1.90                     | 0.53              |
| 3:G:108:ARG:CZ   | 3:G:172:THR:HG22 | 2.38                     | 0.53              |
| 1:M:448:LEU:HD22 | 1:M:546:PRO:O    | 2.09                     | 0.53              |
| 1:A:385:LYS:HG2  | 1:A:385:LYS:O    | 2.09                     | 0.53              |
| 2:B:57:ASP:HB3   | 2:B:130:ARG:NH2  | 2.24                     | 0.53              |
| 1:E:128:LYS:NZ   | 3:G:56:ASP:OD1   | 2.36                     | 0.53              |
| 1:A:503:GLN:HA   | 1:A:506:VAL:HB   | 1.91                     | 0.53              |
| 4:D:32:TYR:HE1   | 4:D:101:TRP:HD1  | 1.55                     | 0.53              |
| 1:I:270:VAL:HG12 | 1:I:274:MET:HE3  | 1.91                     | 0.53              |
| 4:P:6:GLU:HG2    | 4:P:96:CYS:SG    | 2.48                     | 0.52              |
| 1:E:269:LEU:HD12 | 1:E:331:ILE:HG23 | 1.91                     | 0.52              |
| 1:I:622:TYR:CE1  | 1:I:657:HIS:HB2  | 2.44                     | 0.52              |
| 1:E:82:LEU:CG    | 1:E:83:GLY:H     | 2.22                     | 0.52              |
| 1:E:311:GLY:HA2  | 4:H:101:TRP:CE3  | 2.44                     | 0.52              |
| 1:I:385:LYS:O    | 1:I:385:LYS:HG2  | 2.08                     | 0.52              |
| 1:E:393:ILE:HG12 | 1:E:431:GLU:HG3  | 1.91                     | 0.52              |
| 1:I:140:ASN:HA   | 1:I:145:SER:HB3  | 1.91                     | 0.52              |
| 2:B:124:PHE:C    | 2:B:126:ALA:H    | 2.17                     | 0.52              |
| 1:A:44:MET:HE2   | 1:A:52:PRO:HD2   | 1.92                     | 0.52              |
| 1:A:249:MET:SD   | 1:A:289:THR:HG23 | 2.50                     | 0.52              |
| 3:C:50:ALA:HB3   | 3:C:53:THR:HG23  | 1.91                     | 0.52              |
| 1:I:210:PRO:HB3  | 2:J:83:LEU:HD13  | 1.90                     | 0.52              |
| 4:H:6:GLU:HG3    | 4:H:113:PRO:HD2  | 1.91                     | 0.52              |
| 3:G:19:VAL:HB    | 3:G:75:ILE:HG23  | 1.92                     | 0.52              |
| 1:I:92:ILE:HB    | 4:L:102:LYS:HE2  | 1.91                     | 0.52              |
| 3:C:91:HIS:HB2   | 3:C:96:TRP:CZ2   | 2.45                     | 0.52              |
| 1:M:140:ASN:HA   | 1:M:145:SER:HB3  | 1.91                     | 0.52              |
| 4:P:101:TRP:HZ2  | 4:P:107:ALA:HB3  | 1.74                     | 0.52              |
| 4:P:152:ASP:HA   | 4:P:183:LEU:HB3  | 1.92                     | 0.52              |
| 4:D:64:VAL:HA    | 4:D:67:ARG:HH11  | 1.74                     | 0.51              |
| 1:A:488:ARG:NH1  | 1:A:511:ASP:OD1  | 2.42                     | 0.51              |
| 3:G:94:TYR:HB3   | 3:G:96:TRP:CD1   | 2.46                     | 0.51              |
| 1:I:82:LEU:CG    | 1:I:83:GLY:H     | 2.23                     | 0.51              |
| 4:L:152:ASP:HB3  | 4:L:183:LEU:HD13 | 1.91                     | 0.51              |
| 1:M:503:GLN:HA   | 1:M:506:VAL:HB   | 1.91                     | 0.51              |
| 2:J:57:ASP:HB3   | 2:J:130:ARG:NH2  | 2.26                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:92:ILE:O     | 4:H:102:LYS:HD3  | 2.11                     | 0.51              |
| 1:M:64:ASP:OD1   | 1:M:64:ASP:N     | 2.43                     | 0.51              |
| 4:H:34:ILE:HG22  | 4:H:35:HIS:N     | 2.26                     | 0.51              |
| 1:M:92:ILE:O     | 4:P:102:LYS:HD3  | 2.11                     | 0.51              |
| 1:A:59:ALA:HB1   | 2:B:84:ASN:HB3   | 1.93                     | 0.51              |
| 4:P:20:LEU:HB2   | 4:P:81:LEU:HB3   | 1.93                     | 0.51              |
| 1:E:115:LEU:HD11 | 1:E:375:ALA:HB2  | 1.92                     | 0.51              |
| 4:L:34:ILE:CG2   | 4:L:35:HIS:N     | 2.74                     | 0.51              |
| 1:M:385:LYS:O    | 1:M:385:LYS:HG2  | 2.09                     | 0.51              |
| 4:L:173:THR:HG23 | 4:L:188:SER:HB2  | 1.91                     | 0.50              |
| 3:O:140:TYR:CG   | 3:O:141:PRO:HA   | 2.45                     | 0.50              |
| 1:E:40:TRP:HB3   | 1:E:44:MET:HE3   | 1.92                     | 0.50              |
| 1:I:309:GLY:HA3  | 4:L:32:TYR:OH    | 2.12                     | 0.50              |
| 4:P:64:VAL:HA    | 4:P:67:ARG:HH11  | 1.75                     | 0.50              |
| 1:A:82:LEU:CG    | 1:A:83:GLY:H     | 2.23                     | 0.50              |
| 1:A:491:LEU:HB2  | 1:A:510:VAL:HG13 | 1.92                     | 0.50              |
| 1:M:571:THR:HG23 | 1:M:573:LEU:H    | 1.76                     | 0.50              |
| 2:N:57:ASP:HB3   | 2:N:130:ARG:NH2  | 2.26                     | 0.50              |
| 1:A:73:LYS:HZ1   | 1:I:79:SER:HB3   | 1.77                     | 0.50              |
| 1:E:94:ALA:HB1   | 4:H:104:PRO:HD3  | 1.92                     | 0.50              |
| 3:G:85:THR:HA    | 3:G:103:LYS:HA   | 1.92                     | 0.50              |
| 1:M:82:LEU:CD2   | 2:F:129:ASN:H    | 2.25                     | 0.50              |
| 1:M:181:THR:HG23 | 1:M:195:SER:HB3  | 1.94                     | 0.50              |
| 1:M:558:ARG:NH2  | 1:M:594:GLY:O    | 2.44                     | 0.50              |
| 3:O:94:TYR:HB3   | 3:O:96:TRP:CD1   | 2.47                     | 0.50              |
| 3:O:198:HIS:HB3  | 3:O:201:LEU:HG   | 1.92                     | 0.50              |
| 4:D:61:ILE:HG22  | 4:D:64:VAL:HG22  | 1.92                     | 0.50              |
| 1:E:558:ARG:NH2  | 1:E:594:GLY:O    | 2.44                     | 0.50              |
| 1:I:488:ARG:NH1  | 1:I:511:ASP:OD1  | 2.44                     | 0.50              |
| 1:I:570:THR:HG1  | 1:I:571:THR:H    | 1.58                     | 0.50              |
| 3:K:136:LEU:HB2  | 3:K:175:LEU:HB3  | 1.94                     | 0.50              |
| 4:L:14:PRO:HD2   | 4:L:121:SER:HB3  | 1.93                     | 0.50              |
| 1:A:86:LEU:N     | 1:A:221:SER:OG   | 2.38                     | 0.50              |
| 4:H:152:ASP:HB3  | 4:H:183:LEU:HD13 | 1.94                     | 0.50              |
| 1:A:140:ASN:HA   | 1:A:145:SER:HB3  | 1.94                     | 0.50              |
| 3:C:21:LEU:HD22  | 3:C:102:THR:HG21 | 1.94                     | 0.50              |
| 1:E:589:GLN:CD   | 1:E:589:GLN:H    | 2.19                     | 0.50              |
| 1:I:491:LEU:HB2  | 1:I:510:VAL:HG13 | 1.94                     | 0.50              |
| 1:A:558:ARG:NH2  | 1:A:594:GLY:O    | 2.44                     | 0.49              |
| 1:I:548:ILE:O    | 1:I:549:ASN:HB2  | 2.12                     | 0.49              |
| 4:L:159:THR:HB   | 4:L:207:ASN:HB3  | 1.93                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:571:THR:HG23 | 1:A:573:LEU:H    | 1.77                     | 0.49              |
| 2:F:57:ASP:HB3   | 2:F:130:ARG:NH2  | 2.26                     | 0.49              |
| 2:B:82:GLY:O     | 2:B:86:VAL:HG23  | 2.12                     | 0.49              |
| 4:D:103:TRP:CD1  | 4:D:104:PRO:HD3  | 2.47                     | 0.49              |
| 2:B:121:GLU:HB3  | 2:J:121:GLU:HB3  | 1.94                     | 0.49              |
| 1:E:249:MET:SD   | 1:E:289:THR:HG23 | 2.53                     | 0.49              |
| 3:G:108:ARG:HH22 | 3:G:111:ALA:HB3  | 1.76                     | 0.49              |
| 4:H:32:TYR:HE1   | 4:H:101:TRP:HD1  | 1.59                     | 0.49              |
| 1:I:209:GLY:O    | 2:J:115:TYR:OH   | 2.24                     | 0.49              |
| 1:I:542:LEU:HB2  | 1:I:554:ILE:HG22 | 1.94                     | 0.49              |
| 3:C:146:VAL:HG22 | 3:C:196:VAL:HG22 | 1.95                     | 0.49              |
| 4:D:147:GLY:HA3  | 4:D:189:VAL:HG12 | 1.94                     | 0.49              |
| 4:H:147:GLY:HA3  | 4:H:189:VAL:HG12 | 1.94                     | 0.49              |
| 1:M:270:VAL:HG12 | 1:M:274:MET:HE3  | 1.94                     | 0.49              |
| 3:C:94:TYR:HB3   | 3:C:96:TRP:CD1   | 2.48                     | 0.49              |
| 4:P:152:ASP:OD1  | 4:P:179:GLN:NE2  | 2.45                     | 0.49              |
| 4:D:100:GLY:HA2  | 4:D:105:GLY:O    | 2.12                     | 0.49              |
| 1:E:305:VAL:O    | 1:E:308:THR:HG22 | 2.13                     | 0.49              |
| 4:P:12:VAL:HG11  | 4:P:18:LEU:HB2   | 1.94                     | 0.49              |
| 1:A:270:VAL:HG12 | 1:A:274:MET:HE3  | 1.95                     | 0.49              |
| 1:E:479:TYR:HA   | 1:E:517:LEU:HD23 | 1.95                     | 0.49              |
| 3:G:11:LEU:HD22  | 3:G:104:VAL:HG22 | 1.95                     | 0.49              |
| 1:I:305:VAL:O    | 1:I:308:THR:HG22 | 2.12                     | 0.49              |
| 1:M:232:PHE:HE1  | 1:E:73:LYS:HD3   | 1.76                     | 0.48              |
| 4:H:152:ASP:OD1  | 4:H:179:GLN:NE2  | 2.46                     | 0.48              |
| 1:A:448:LEU:HD22 | 1:A:546:PRO:O    | 2.14                     | 0.48              |
| 3:G:136:LEU:HD13 | 3:G:175:LEU:HD22 | 1.94                     | 0.48              |
| 4:P:100:GLY:HA2  | 4:P:105:GLY:O    | 2.13                     | 0.48              |
| 1:A:305:VAL:O    | 1:A:308:THR:HG22 | 2.14                     | 0.48              |
| 1:A:439:GLN:C    | 1:A:441:PRO:HD2  | 2.38                     | 0.48              |
| 2:B:88:PHE:O     | 2:B:92:ILE:HG12  | 2.13                     | 0.48              |
| 1:E:491:LEU:HB2  | 1:E:510:VAL:HG13 | 1.96                     | 0.48              |
| 1:M:565:LEU:HD11 | 1:M:578:PHE:HB3  | 1.96                     | 0.48              |
| 4:P:13:GLN:HG3   | 4:P:121:SER:HB3  | 1.95                     | 0.48              |
| 1:E:385:LYS:O    | 1:E:385:LYS:HG2  | 2.12                     | 0.48              |
| 3:K:91:HIS:HB2   | 3:K:96:TRP:CZ2   | 2.49                     | 0.48              |
| 1:M:40:TRP:HB3   | 1:M:44:MET:HE3   | 1.96                     | 0.48              |
| 1:I:141:THR:HG23 | 1:I:143:PRO:HD2  | 1.95                     | 0.48              |
| 3:C:136:LEU:HD13 | 3:C:175:LEU:HD22 | 1.95                     | 0.48              |
| 1:I:448:LEU:HD22 | 1:I:546:PRO:O    | 2.14                     | 0.48              |
| 3:K:140:TYR:CG   | 3:K:141:PRO:HA   | 2.49                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:284:ASP:OD1  | 1:M:287:THR:OG1  | 2.28                     | 0.48              |
| 3:O:46:ARG:HG2   | 4:P:109:ASP:HA   | 1.95                     | 0.48              |
| 3:O:48:ILE:HD12  | 3:O:73:LEU:HD12  | 1.96                     | 0.48              |
| 1:A:128:LYS:NZ   | 3:C:56:ASP:OD1   | 2.46                     | 0.48              |
| 4:D:152:ASP:HA   | 4:D:183:LEU:HB3  | 1.95                     | 0.48              |
| 2:N:123:LEU:HD13 | 2:N:123:LEU:HA   | 1.72                     | 0.47              |
| 3:O:91:HIS:HB2   | 3:O:96:TRP:CZ2   | 2.48                     | 0.47              |
| 4:P:103:TRP:CD1  | 4:P:104:PRO:HD3  | 2.49                     | 0.47              |
| 1:E:309:GLY:HA3  | 4:H:32:TYR:OH    | 2.14                     | 0.47              |
| 2:F:82:GLY:O     | 2:F:86:VAL:HG23  | 2.14                     | 0.47              |
| 3:K:11:LEU:HD22  | 3:K:104:VAL:HG22 | 1.96                     | 0.47              |
| 1:M:572:TYR:CG   | 1:M:572:TYR:O    | 2.67                     | 0.47              |
| 3:O:136:LEU:HD13 | 3:O:175:LEU:HD22 | 1.95                     | 0.47              |
| 1:A:231:THR:HB   | 1:A:234:HIS:H    | 1.78                     | 0.47              |
| 3:C:30:ARG:H     | 3:C:30:ARG:HG3   | 1.48                     | 0.47              |
| 1:M:141:THR:HG23 | 1:M:143:PRO:HD2  | 1.96                     | 0.47              |
| 1:M:305:VAL:O    | 1:M:308:THR:HG22 | 2.14                     | 0.47              |
| 2:N:82:GLY:O     | 2:N:86:VAL:HG23  | 2.14                     | 0.47              |
| 4:P:152:ASP:HB3  | 4:P:183:LEU:HD13 | 1.97                     | 0.47              |
| 1:A:430:ARG:HA   | 1:A:433:ARG:HG3  | 1.97                     | 0.47              |
| 1:E:92:ILE:HB    | 4:H:102:LYS:HE2  | 1.97                     | 0.47              |
| 1:M:376:LEU:HD11 | 1:M:399:VAL:HG21 | 1.97                     | 0.47              |
| 1:M:380:THR:HG22 | 1:M:427:VAL:HG22 | 1.97                     | 0.47              |
| 3:C:85:THR:HA    | 3:C:103:LYS:HA   | 1.96                     | 0.47              |
| 1:E:108:HIS:ND1  | 1:E:109:PRO:HD2  | 2.30                     | 0.47              |
| 4:H:178:LEU:HD12 | 4:H:184:TYR:CZ   | 2.49                     | 0.47              |
| 1:I:329:LYS:HZ3  | 1:I:340:VAL:HB   | 1.79                     | 0.47              |
| 3:O:146:VAL:HG22 | 3:O:196:VAL:HG22 | 1.96                     | 0.47              |
| 4:P:61:ILE:HG22  | 4:P:64:VAL:HG22  | 1.95                     | 0.47              |
| 3:K:48:ILE:HD12  | 3:K:73:LEU:HD12  | 1.97                     | 0.47              |
| 1:M:622:TYR:CE1  | 1:M:657:HIS:HB2  | 2.50                     | 0.47              |
| 3:O:11:LEU:HD22  | 3:O:104:VAL:HG22 | 1.97                     | 0.47              |
| 3:O:85:THR:HA    | 3:O:103:LYS:HA   | 1.96                     | 0.47              |
| 4:P:4:LEU:HD11   | 4:P:98:ARG:HG2   | 1.97                     | 0.47              |
| 1:A:214:PRO:O    | 2:J:125:GLY:HA3  | 2.14                     | 0.47              |
| 1:A:464:ARG:HB2  | 1:A:496:PRO:HG3  | 1.97                     | 0.47              |
| 3:C:140:TYR:CG   | 3:C:141:PRO:HA   | 2.49                     | 0.47              |
| 4:D:34:ILE:HG22  | 4:D:35:HIS:N     | 2.29                     | 0.47              |
| 4:D:145:ALA:HB2  | 4:D:191:THR:HG22 | 1.96                     | 0.47              |
| 1:E:448:LEU:HD22 | 1:E:546:PRO:O    | 2.14                     | 0.47              |
| 3:G:18:ARG:HH11  | 3:G:18:ARG:HB2   | 1.80                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:G:201:LEU:HD13 | 3:G:205:VAL:HG23 | 1.95                     | 0.47              |
| 1:I:618:ALA:HB3  | 1:I:661:LEU:HB2  | 1.97                     | 0.47              |
| 3:K:94:TYR:HB3   | 3:K:96:TRP:CD1   | 2.50                     | 0.47              |
| 3:G:132:VAL:HB   | 3:G:179:LEU:HB3  | 1.96                     | 0.47              |
| 3:O:136:LEU:HB2  | 3:O:175:LEU:HB3  | 1.96                     | 0.47              |
| 3:G:46:ARG:HG2   | 4:H:109:ASP:HA   | 1.97                     | 0.47              |
| 3:O:113:PRO:HD3  | 3:O:198:HIS:ND1  | 2.30                     | 0.47              |
| 3:C:167:ASP:HB3  | 3:C:170:ASP:OD1  | 2.15                     | 0.47              |
| 4:H:34:ILE:CG2   | 4:H:35:HIS:N     | 2.77                     | 0.47              |
| 2:J:88:PHE:O     | 2:J:92:ILE:HG12  | 2.15                     | 0.47              |
| 3:K:7:THR:HG23   | 3:K:22:THR:HB    | 1.96                     | 0.47              |
| 1:M:78:THR:HB    | 1:M:81:THR:HB    | 1.97                     | 0.46              |
| 1:M:271:LEU:O    | 1:M:275:LYS:HD2  | 2.15                     | 0.46              |
| 1:E:26:HIS:HE2   | 2:F:47:ASP:HB3   | 1.80                     | 0.46              |
| 1:E:380:THR:HG22 | 1:E:427:VAL:HG22 | 1.97                     | 0.46              |
| 1:I:439:GLN:C    | 1:I:441:PRO:HD2  | 2.40                     | 0.46              |
| 2:N:129:ASN:H    | 1:E:82:LEU:CD2   | 2.29                     | 0.46              |
| 4:P:34:ILE:HG22  | 4:P:35:HIS:N     | 2.31                     | 0.46              |
| 4:P:10:ARG:HB2   | 4:P:18:LEU:HD21  | 1.98                     | 0.46              |
| 1:A:409:LEU:H    | 1:A:409:LEU:HG   | 1.36                     | 0.46              |
| 1:A:571:THR:HG23 | 1:A:574:SER:H    | 1.80                     | 0.46              |
| 1:I:125:PRO:HA   | 1:I:128:LYS:HE2  | 1.96                     | 0.46              |
| 3:K:6:GLN:HG3    | 3:K:99:GLY:HA3   | 1.96                     | 0.46              |
| 1:M:549:ASN:HA   | 1:M:584:MET:SD   | 2.56                     | 0.46              |
| 2:N:88:PHE:O     | 2:N:92:ILE:HG12  | 2.14                     | 0.46              |
| 2:N:125:GLY:HA3  | 1:E:214:PRO:O    | 2.15                     | 0.46              |
| 3:C:48:ILE:HD12  | 3:C:73:LEU:HD12  | 1.98                     | 0.46              |
| 1:I:380:THR:HG22 | 1:I:427:VAL:HG22 | 1.96                     | 0.46              |
| 4:L:61:ILE:HG22  | 4:L:64:VAL:HG22  | 1.96                     | 0.46              |
| 4:L:211:SER:OG   | 4:L:213:THR:OG1  | 2.25                     | 0.46              |
| 1:A:284:ASP:OD1  | 1:A:287:THR:OG1  | 2.29                     | 0.46              |
| 3:C:46:ARG:HG2   | 4:D:109:ASP:HA   | 1.98                     | 0.46              |
| 1:E:62:THR:HB    | 2:F:33:GLN:HA    | 1.97                     | 0.46              |
| 4:L:7:SER:HG     | 4:L:21:SER:HG    | 1.62                     | 0.46              |
| 4:L:12:VAL:HG11  | 4:L:18:LEU:HB2   | 1.97                     | 0.46              |
| 4:P:102:LYS:HB2  | 4:P:102:LYS:HE3  | 1.85                     | 0.46              |
| 4:H:53:PHE:HB3   | 4:H:103:TRP:HB3  | 1.97                     | 0.46              |
| 3:K:64:GLY:HA2   | 3:K:72:THR:O     | 2.16                     | 0.46              |
| 3:K:163:VAL:HG12 | 3:K:164:THR:O    | 2.15                     | 0.46              |
| 4:L:145:ALA:HB2  | 4:L:191:THR:HG22 | 1.97                     | 0.46              |
| 3:O:167:ASP:HB3  | 3:O:170:ASP:OD1  | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:82:LEU:CD2   | 2:J:129:ASN:H    | 2.28                     | 0.46              |
| 1:A:279:ARG:HG3  | 1:A:280:GLU:N    | 2.30                     | 0.46              |
| 1:A:311:GLY:HA3  | 4:D:101:TRP:HB2  | 1.97                     | 0.46              |
| 1:A:505:ALA:HA   | 1:A:508:ASN:HB2  | 1.97                     | 0.46              |
| 4:D:53:PHE:HB3   | 4:D:103:TRP:CB   | 2.45                     | 0.46              |
| 2:J:97:SER:O     | 4:L:1:GLU:N      | 2.48                     | 0.46              |
| 1:M:279:ARG:HG3  | 1:M:280:GLU:N    | 2.31                     | 0.46              |
| 2:N:122:ASP:HA   | 2:N:124:PHE:CE1  | 2.51                     | 0.46              |
| 4:P:29:PHE:HE1   | 4:P:34:ILE:HD11  | 1.81                     | 0.46              |
| 1:E:209:GLY:O    | 2:F:115:TYR:OH   | 2.32                     | 0.46              |
| 1:E:618:ALA:HB3  | 1:E:661:LEU:HB2  | 1.98                     | 0.46              |
| 3:G:50:ALA:C     | 3:G:52:SER:H     | 2.24                     | 0.46              |
| 3:K:124:GLN:O    | 3:K:127:SER:OG   | 2.34                     | 0.46              |
| 3:K:136:LEU:HD13 | 3:K:175:LEU:HD22 | 1.96                     | 0.46              |
| 1:M:94:ALA:HB1   | 4:P:104:PRO:HD3  | 1.97                     | 0.46              |
| 1:M:618:ALA:HB3  | 1:M:661:LEU:HB2  | 1.98                     | 0.46              |
| 1:E:121:MET:HE2  | 1:E:121:MET:HB3  | 1.80                     | 0.46              |
| 1:E:328:LEU:HG   | 1:E:332:ILE:HD12 | 1.98                     | 0.46              |
| 1:I:275:LYS:HE3  | 1:I:275:LYS:N    | 2.30                     | 0.46              |
| 4:L:32:TYR:HE1   | 4:L:101:TRP:HD1  | 1.64                     | 0.46              |
| 1:A:572:TYR:CG   | 1:A:572:TYR:O    | 2.69                     | 0.45              |
| 2:B:129:ASN:H    | 1:I:82:LEU:CD2   | 2.29                     | 0.45              |
| 3:C:113:PRO:HD3  | 3:C:198:HIS:ND1  | 2.31                     | 0.45              |
| 3:G:140:TYR:CG   | 3:G:141:PRO:HA   | 2.50                     | 0.45              |
| 4:H:12:VAL:HG11  | 4:H:18:LEU:HB2   | 1.97                     | 0.45              |
| 1:I:376:LEU:HD11 | 1:I:399:VAL:HG21 | 1.98                     | 0.45              |
| 1:M:249:MET:SD   | 1:M:289:THR:HG23 | 2.56                     | 0.45              |
| 3:O:107:LYS:HG3  | 3:O:108:ARG:N    | 2.31                     | 0.45              |
| 4:P:5:VAL:O      | 4:P:23:VAL:N     | 2.34                     | 0.45              |
| 4:P:29:PHE:CE1   | 4:P:34:ILE:HD11  | 2.50                     | 0.45              |
| 1:I:328:LEU:HG   | 1:I:332:ILE:HD12 | 1.98                     | 0.45              |
| 1:I:376:LEU:O    | 1:I:380:THR:HG23 | 2.17                     | 0.45              |
| 2:J:82:GLY:O     | 2:J:86:VAL:HG23  | 2.17                     | 0.45              |
| 4:P:98:ARG:HG3   | 4:P:109:ASP:OD1  | 2.16                     | 0.45              |
| 3:C:163:VAL:HG12 | 3:C:164:THR:O    | 2.16                     | 0.45              |
| 2:J:119:SER:HB3  | 2:J:122:ASP:HB2  | 1.99                     | 0.45              |
| 3:K:18:ARG:HB2   | 3:K:18:ARG:HH11  | 1.81                     | 0.45              |
| 4:L:98:ARG:HG3   | 4:L:109:ASP:OD1  | 2.17                     | 0.45              |
| 1:M:344:GLN:HG2  | 1:M:349:GLU:OE2  | 2.16                     | 0.45              |
| 1:M:598:GLN:H    | 1:M:598:GLN:HG2  | 1.58                     | 0.45              |
| 1:A:181:THR:HG23 | 1:A:195:SER:HB3  | 1.99                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:48:VAL:HG12  | 4:D:64:VAL:HG21  | 1.98                     | 0.45              |
| 4:D:64:VAL:HA    | 4:D:67:ARG:NH1   | 2.31                     | 0.45              |
| 2:F:122:ASP:HA   | 2:F:124:PHE:CE1  | 2.51                     | 0.45              |
| 2:B:122:ASP:HA   | 2:B:124:PHE:CE1  | 2.51                     | 0.45              |
| 1:E:409:LEU:H    | 1:E:409:LEU:HG   | 1.50                     | 0.45              |
| 1:E:471:GLU:HG2  | 1:E:472:SER:N    | 2.32                     | 0.45              |
| 1:M:70:ASN:HA    | 1:M:73:LYS:HE3   | 1.99                     | 0.45              |
| 1:M:221:SER:HB3  | 1:M:250:PHE:HE2  | 1.81                     | 0.45              |
| 1:E:439:GLN:C    | 1:E:441:PRO:HD2  | 2.42                     | 0.45              |
| 1:E:549:ASN:HA   | 1:E:584:MET:SD   | 2.57                     | 0.45              |
| 4:H:64:VAL:HA    | 4:H:67:ARG:HH11  | 1.81                     | 0.45              |
| 2:J:124:PHE:C    | 2:J:126:ALA:H    | 2.25                     | 0.45              |
| 3:K:167:ASP:HB3  | 3:K:170:ASP:OD1  | 2.16                     | 0.45              |
| 4:L:53:PHE:HB3   | 4:L:103:TRP:CB   | 2.47                     | 0.45              |
| 1:M:92:ILE:HB    | 4:P:102:LYS:HE2  | 1.99                     | 0.45              |
| 1:M:172:ALA:O    | 1:M:178:LEU:HD12 | 2.17                     | 0.45              |
| 1:M:440:GLY:N    | 1:M:441:PRO:HD2  | 2.32                     | 0.45              |
| 2:B:123:LEU:HD13 | 2:B:123:LEU:HA   | 1.73                     | 0.45              |
| 3:C:198:HIS:HB3  | 3:C:201:LEU:HG   | 1.99                     | 0.45              |
| 4:H:98:ARG:HG3   | 4:H:109:ASP:OD1  | 2.17                     | 0.45              |
| 3:O:50:ALA:HB3   | 3:O:53:THR:HG23  | 1.97                     | 0.45              |
| 1:E:417:MET:HE3  | 1:E:417:MET:HB2  | 1.91                     | 0.45              |
| 1:I:59:ALA:O     | 1:I:61:VAL:N     | 2.50                     | 0.45              |
| 1:I:209:GLY:C    | 1:I:211:PHE:H    | 2.25                     | 0.45              |
| 1:I:440:GLY:N    | 1:I:441:PRO:HD2  | 2.31                     | 0.45              |
| 1:I:518:SER:O    | 1:I:522:GLU:HB2  | 2.17                     | 0.45              |
| 1:A:70:ASN:HA    | 1:A:73:LYS:HE3   | 1.98                     | 0.45              |
| 1:A:440:GLY:N    | 1:A:441:PRO:HD2  | 2.32                     | 0.45              |
| 3:G:91:HIS:HB2   | 3:G:96:TRP:CZ2   | 2.51                     | 0.45              |
| 1:A:622:TYR:CE1  | 1:A:657:HIS:HB2  | 2.52                     | 0.44              |
| 3:C:108:ARG:NH2  | 3:C:140:TYR:HB2  | 2.32                     | 0.44              |
| 4:D:101:TRP:HZ2  | 4:D:107:ALA:HB3  | 1.82                     | 0.44              |
| 1:E:64:ASP:OD1   | 1:E:64:ASP:N     | 2.50                     | 0.44              |
| 1:I:242:PHE:CE1  | 1:I:288:LEU:HB3  | 2.52                     | 0.44              |
| 3:O:94:TYR:HA    | 3:O:95:PRO:C     | 2.42                     | 0.44              |
| 4:P:217:LYS:HA   | 4:P:217:LYS:HD3  | 1.56                     | 0.44              |
| 1:E:345:SER:O    | 1:E:349:GLU:HG3  | 2.17                     | 0.44              |
| 2:F:48:ILE:HD12  | 2:F:89:PHE:HZ    | 1.82                     | 0.44              |
| 3:G:113:PRO:HD3  | 3:G:198:HIS:ND1  | 2.32                     | 0.44              |
| 4:L:35:HIS:CE1   | 4:L:50:MET:HG3   | 2.52                     | 0.44              |
| 1:M:25:LEU:N     | 1:M:36:TYR:O     | 2.42                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:549:ASN:HA   | 1:A:584:MET:SD   | 2.58                     | 0.44              |
| 4:D:34:ILE:CG2   | 4:D:35:HIS:N     | 2.80                     | 0.44              |
| 4:H:217:LYS:HA   | 4:H:217:LYS:HD3  | 1.49                     | 0.44              |
| 1:M:252:ARG:O    | 1:M:256:MET:HB2  | 2.18                     | 0.44              |
| 4:H:159:THR:HB   | 4:H:207:ASN:HB3  | 1.99                     | 0.44              |
| 1:I:541:VAL:HA   | 1:I:555:SER:HB3  | 1.99                     | 0.44              |
| 2:N:48:ILE:HD12  | 2:N:89:PHE:HZ    | 1.83                     | 0.44              |
| 1:E:571:THR:HG23 | 1:E:573:LEU:H    | 1.82                     | 0.44              |
| 1:I:345:SER:O    | 1:I:349:GLU:HG3  | 2.17                     | 0.44              |
| 1:M:489:ASP:OD1  | 1:M:489:ASP:N    | 2.38                     | 0.44              |
| 3:O:195:GLU:HB2  | 3:O:206:THR:HG23 | 2.00                     | 0.44              |
| 2:B:124:PHE:C    | 2:B:126:ALA:N    | 2.76                     | 0.44              |
| 4:D:40:GLY:HA3   | 4:D:43:LYS:HE3   | 1.99                     | 0.44              |
| 3:G:35:TRP:CD2   | 3:G:73:LEU:HB2   | 2.53                     | 0.44              |
| 1:I:325:LEU:O    | 1:I:329:LYS:N    | 2.47                     | 0.44              |
| 4:L:5:VAL:O      | 4:L:23:VAL:N     | 2.41                     | 0.44              |
| 1:M:439:GLN:C    | 1:M:441:PRO:HD2  | 2.43                     | 0.44              |
| 3:O:145:LYS:HB3  | 3:O:197:THR:HB   | 2.00                     | 0.44              |
| 1:A:21:SER:O     | 1:A:40:TRP:HB2   | 2.18                     | 0.44              |
| 1:A:25:LEU:N     | 1:A:36:TYR:O     | 2.42                     | 0.44              |
| 1:A:92:ILE:O     | 4:D:102:LYS:HD3  | 2.18                     | 0.44              |
| 1:A:376:LEU:HD11 | 1:A:399:VAL:HG21 | 1.99                     | 0.44              |
| 3:C:35:TRP:CD2   | 3:C:73:LEU:HB2   | 2.53                     | 0.44              |
| 1:E:201:THR:CG2  | 1:E:225:SER:HB2  | 2.45                     | 0.44              |
| 4:L:100:GLY:C    | 4:L:103:TRP:HA   | 2.42                     | 0.44              |
| 1:M:479:TYR:HA   | 1:M:517:LEU:HD23 | 1.99                     | 0.44              |
| 3:O:30:ARG:H     | 3:O:30:ARG:HG3   | 1.50                     | 0.44              |
| 4:D:12:VAL:HG11  | 4:D:18:LEU:HB2   | 2.00                     | 0.44              |
| 1:E:101:GLN:HE22 | 4:H:101:TRP:HZ3  | 1.66                     | 0.44              |
| 2:F:88:PHE:O     | 2:F:92:ILE:HG12  | 2.17                     | 0.44              |
| 3:G:167:ASP:HB3  | 3:G:170:ASP:OD1  | 2.17                     | 0.44              |
| 4:H:29:PHE:HE1   | 4:H:34:ILE:HD11  | 1.82                     | 0.44              |
| 1:M:101:GLN:HE22 | 4:P:101:TRP:HZ3  | 1.65                     | 0.44              |
| 4:D:217:LYS:HA   | 4:D:217:LYS:HD3  | 1.64                     | 0.44              |
| 1:E:376:LEU:HD11 | 1:E:399:VAL:HG21 | 1.99                     | 0.44              |
| 3:G:81:GLU:H     | 3:G:81:GLU:CD    | 2.25                     | 0.44              |
| 1:I:571:THR:HG23 | 1:I:573:LEU:H    | 1.83                     | 0.44              |
| 4:L:53:PHE:HB3   | 4:L:103:TRP:HB3  | 1.99                     | 0.44              |
| 4:L:217:LYS:HA   | 4:L:217:LYS:HD3  | 1.57                     | 0.44              |
| 4:P:100:GLY:C    | 4:P:103:TRP:HA   | 2.42                     | 0.43              |
| 1:A:242:PHE:CE1  | 1:A:288:LEU:HB3  | 2.53                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:G:64:GLY:HA2   | 3:G:72:THR:O     | 2.17                     | 0.43              |
| 1:I:279:ARG:HG3  | 1:I:280:GLU:N    | 2.31                     | 0.43              |
| 3:K:54:LEU:HD11  | 3:K:58:VAL:O     | 2.18                     | 0.43              |
| 1:M:176:LYS:HA   | 1:M:176:LYS:HD3  | 1.83                     | 0.43              |
| 4:D:29:PHE:HE1   | 4:D:34:ILE:HD11  | 1.83                     | 0.43              |
| 4:D:32:TYR:HE1   | 4:D:101:TRP:CD1  | 2.36                     | 0.43              |
| 3:G:146:VAL:HG22 | 3:G:196:VAL:HG22 | 2.00                     | 0.43              |
| 1:M:409:LEU:H    | 1:M:409:LEU:HG   | 1.41                     | 0.43              |
| 4:P:34:ILE:CG2   | 4:P:35:HIS:N     | 2.81                     | 0.43              |
| 1:A:122:LEU:O    | 1:A:125:PRO:HD2  | 2.18                     | 0.43              |
| 4:D:122:ALA:O    | 4:D:123:SER:OG   | 2.33                     | 0.43              |
| 1:E:242:PHE:CE1  | 1:E:288:LEU:HB3  | 2.53                     | 0.43              |
| 1:E:376:LEU:O    | 1:E:380:THR:HG23 | 2.18                     | 0.43              |
| 2:J:128:LEU:HD23 | 2:J:128:LEU:HA   | 1.82                     | 0.43              |
| 3:K:46:ARG:HG2   | 4:L:109:ASP:HA   | 2.00                     | 0.43              |
| 1:A:309:GLY:HA3  | 4:D:32:TYR:OH    | 2.18                     | 0.43              |
| 1:A:323:PHE:CZ   | 1:A:423:ILE:HA   | 2.53                     | 0.43              |
| 3:C:44:PRO:HB2   | 4:D:111:PHE:CE1  | 2.53                     | 0.43              |
| 1:I:271:LEU:O    | 1:I:275:LYS:HD2  | 2.17                     | 0.43              |
| 3:K:108:ARG:NH2  | 3:K:140:TYR:HB2  | 2.33                     | 0.43              |
| 3:K:134:CYS:HB2  | 3:K:148:TRP:CH2  | 2.54                     | 0.43              |
| 4:L:154:PHE:HA   | 4:L:155:PRO:HA   | 1.79                     | 0.43              |
| 4:P:145:ALA:HB2  | 4:P:191:THR:HG22 | 2.00                     | 0.43              |
| 1:E:122:LEU:O    | 1:E:125:PRO:HD2  | 2.18                     | 0.43              |
| 1:E:440:GLY:N    | 1:E:441:PRO:HD2  | 2.33                     | 0.43              |
| 1:I:122:LEU:O    | 1:I:125:PRO:HD2  | 2.18                     | 0.43              |
| 3:K:19:VAL:HB    | 3:K:75:ILE:HG23  | 2.00                     | 0.43              |
| 3:K:50:ALA:C     | 3:K:52:SER:H     | 2.26                     | 0.43              |
| 1:I:284:ASP:OD1  | 1:I:287:THR:OG1  | 2.25                     | 0.43              |
| 1:M:26:HIS:NE2   | 2:N:47:ASP:OD2   | 2.47                     | 0.43              |
| 1:M:82:LEU:O     | 1:M:219:ALA:HA   | 2.19                     | 0.43              |
| 3:O:7:THR:HG23   | 3:O:22:THR:HB    | 1.99                     | 0.43              |
| 4:H:39:GLN:HB2   | 4:H:45:LEU:HD23  | 2.00                     | 0.43              |
| 1:I:252:ARG:O    | 1:I:256:MET:HB2  | 2.18                     | 0.43              |
| 4:L:48:VAL:HG12  | 4:L:64:VAL:HG21  | 2.01                     | 0.43              |
| 4:P:29:PHE:CD2   | 4:P:77:ASN:HA    | 2.54                     | 0.43              |
| 1:A:56:TRP:NE1   | 1:A:61:VAL:HG21  | 2.33                     | 0.43              |
| 1:A:82:LEU:O     | 1:A:219:ALA:HA   | 2.19                     | 0.43              |
| 4:D:10:ARG:HB2   | 4:D:18:LEU:HD21  | 2.00                     | 0.43              |
| 3:G:19:VAL:HG21  | 3:G:78:LEU:HG    | 2.01                     | 0.43              |
| 4:H:156:GLU:HG3  | 4:H:184:TYR:CD2  | 2.53                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:21:LEU:HD22  | 3:K:102:THR:HG21 | 2.01                     | 0.43              |
| 1:M:44:MET:HE2   | 1:M:52:PRO:HD2   | 2.00                     | 0.43              |
| 4:P:147:GLY:HA3  | 4:P:189:VAL:HG12 | 2.01                     | 0.43              |
| 1:A:59:ALA:O     | 1:A:61:VAL:N     | 2.51                     | 0.43              |
| 1:A:109:PRO:HA   | 1:A:354:MET:HE3  | 2.00                     | 0.43              |
| 1:A:471:GLU:HG2  | 1:A:472:SER:N    | 2.32                     | 0.43              |
| 3:C:148:TRP:CG   | 3:C:179:LEU:HD13 | 2.54                     | 0.43              |
| 4:D:98:ARG:HG3   | 4:D:109:ASP:OD1  | 2.19                     | 0.43              |
| 1:E:152:ARG:NH2  | 1:I:624:GLU:OE2  | 2.52                     | 0.43              |
| 1:I:108:HIS:ND1  | 1:I:109:PRO:HD2  | 2.34                     | 0.43              |
| 1:I:552:PHE:CG   | 1:I:661:LEU:HD23 | 2.53                     | 0.43              |
| 3:K:30:ARG:H     | 3:K:30:ARG:HG3   | 1.42                     | 0.43              |
| 1:M:309:GLY:HA3  | 4:P:32:TYR:OH    | 2.18                     | 0.43              |
| 3:O:64:GLY:HA2   | 3:O:72:THR:O     | 2.18                     | 0.43              |
| 4:P:31:TYR:HA    | 4:P:103:TRP:HZ3  | 1.83                     | 0.43              |
| 1:E:103:ASP:OD2  | 3:G:53:THR:HG22  | 2.19                     | 0.43              |
| 1:E:271:LEU:O    | 1:E:275:LYS:HD2  | 2.19                     | 0.43              |
| 4:L:148:CYS:HB2  | 4:L:162:TRP:CZ2  | 2.54                     | 0.43              |
| 1:E:323:PHE:O    | 1:E:327:VAL:HG23 | 2.18                     | 0.42              |
| 1:E:568:ALA:HA   | 1:E:599:ILE:HD13 | 1.99                     | 0.42              |
| 3:G:163:VAL:HG12 | 3:G:164:THR:O    | 2.19                     | 0.42              |
| 4:H:100:GLY:C    | 4:H:103:TRP:HA   | 2.44                     | 0.42              |
| 1:I:149:TYR:CE2  | 1:I:208:ARG:HA   | 2.54                     | 0.42              |
| 1:I:181:THR:HA   | 1:I:195:SER:HA   | 2.01                     | 0.42              |
| 1:I:190:ASP:OD1  | 1:I:190:ASP:N    | 2.52                     | 0.42              |
| 3:K:81:GLU:H     | 3:K:81:GLU:CD    | 2.24                     | 0.42              |
| 1:M:149:TYR:CE2  | 1:M:208:ARG:HA   | 2.55                     | 0.42              |
| 1:M:482:LEU:HD13 | 1:M:546:PRO:HD3  | 2.01                     | 0.42              |
| 1:A:103:ASP:OD2  | 3:C:53:THR:HG22  | 2.19                     | 0.42              |
| 1:A:552:PHE:CG   | 1:A:661:LEU:HD23 | 2.54                     | 0.42              |
| 3:C:81:GLU:H     | 3:C:81:GLU:CD    | 2.26                     | 0.42              |
| 1:E:139:PRO:HB2  | 1:E:141:THR:HG22 | 2.01                     | 0.42              |
| 3:G:121:SER:OG   | 4:H:130:PHE:HB3  | 2.19                     | 0.42              |
| 1:I:471:GLU:HG2  | 1:I:472:SER:N    | 2.34                     | 0.42              |
| 1:I:558:ARG:NH2  | 1:I:594:GLY:O    | 2.52                     | 0.42              |
| 3:K:115:VAL:HA   | 3:K:135:LEU:O    | 2.19                     | 0.42              |
| 4:L:122:ALA:O    | 4:L:123:SER:OG   | 2.29                     | 0.42              |
| 4:P:48:VAL:HG12  | 4:P:64:VAL:HG21  | 2.01                     | 0.42              |
| 1:A:149:TYR:CE2  | 1:A:208:ARG:HA   | 2.54                     | 0.42              |
| 4:D:6:GLU:HG2    | 4:D:96:CYS:SG    | 2.59                     | 0.42              |
| 4:H:8:GLY:HA3    | 4:H:20:LEU:HA    | 2.00                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:H:173:THR:HG23 | 4:H:188:SER:HB2  | 2.01                     | 0.42              |
| 1:I:172:ALA:O    | 1:I:178:LEU:HD12 | 2.19                     | 0.42              |
| 1:M:103:ASP:OD2  | 3:O:53:THR:HG22  | 2.19                     | 0.42              |
| 1:A:108:HIS:ND1  | 1:A:109:PRO:HD2  | 2.33                     | 0.42              |
| 3:C:145:LYS:HB3  | 3:C:197:THR:HB   | 2.01                     | 0.42              |
| 4:D:100:GLY:C    | 4:D:103:TRP:HA   | 2.44                     | 0.42              |
| 1:E:209:GLY:C    | 1:E:211:PHE:H    | 2.27                     | 0.42              |
| 1:I:430:ARG:HA   | 1:I:433:ARG:HG3  | 2.00                     | 0.42              |
| 1:I:479:TYR:HA   | 1:I:517:LEU:HD23 | 2.00                     | 0.42              |
| 4:L:152:ASP:HA   | 4:L:183:LEU:HB3  | 2.01                     | 0.42              |
| 1:M:125:PRO:HA   | 1:M:128:LYS:HE2  | 2.01                     | 0.42              |
| 3:G:108:ARG:NH2  | 3:G:140:TYR:HB2  | 2.34                     | 0.42              |
| 3:O:81:GLU:H     | 3:O:81:GLU:CD    | 2.27                     | 0.42              |
| 3:C:19:VAL:HG21  | 3:C:78:LEU:HG    | 2.02                     | 0.42              |
| 4:H:35:HIS:CE1   | 4:H:50:MET:HG3   | 2.55                     | 0.42              |
| 1:I:62:THR:HB    | 2:J:33:GLN:HA    | 2.01                     | 0.42              |
| 2:J:122:ASP:HA   | 2:J:124:PHE:CE1  | 2.54                     | 0.42              |
| 3:K:107:LYS:HG3  | 3:K:108:ARG:N    | 2.34                     | 0.42              |
| 4:L:100:GLY:HA2  | 4:L:105:GLY:O    | 2.19                     | 0.42              |
| 4:L:103:TRP:CD1  | 4:L:104:PRO:HD3  | 2.55                     | 0.42              |
| 1:M:108:HIS:ND1  | 1:M:109:PRO:HD2  | 2.34                     | 0.42              |
| 1:M:148:PHE:CZ   | 1:M:197:ILE:CD1  | 3.03                     | 0.42              |
| 1:M:329:LYS:NZ   | 1:M:340:VAL:HB   | 2.35                     | 0.42              |
| 1:A:69:LEU:HD23  | 1:I:79:SER:HA    | 2.02                     | 0.42              |
| 2:F:123:LEU:HD13 | 2:F:123:LEU:HA   | 1.71                     | 0.42              |
| 4:H:32:TYR:HE1   | 4:H:101:TRP:CD1  | 2.38                     | 0.42              |
| 1:I:128:LYS:NZ   | 3:K:56:ASP:OD1   | 2.46                     | 0.42              |
| 1:I:572:TYR:CG   | 1:I:572:TYR:O    | 2.72                     | 0.42              |
| 3:K:150:VAL:HB   | 3:K:155:GLN:HE21 | 1.84                     | 0.42              |
| 1:M:214:PRO:O    | 2:F:125:GLY:HA3  | 2.20                     | 0.42              |
| 4:P:53:PHE:HB3   | 4:P:103:TRP:CB   | 2.48                     | 0.42              |
| 3:C:115:VAL:HA   | 3:C:135:LEU:O    | 2.19                     | 0.42              |
| 1:E:59:ALA:O     | 1:E:61:VAL:N     | 2.53                     | 0.42              |
| 1:I:361:MET:O    | 1:I:395:GLY:HA2  | 2.20                     | 0.42              |
| 1:M:209:GLY:C    | 1:M:211:PHE:H    | 2.28                     | 0.42              |
| 1:M:331:ILE:HA   | 1:M:334:ILE:HG12 | 2.01                     | 0.42              |
| 4:P:159:THR:HB   | 4:P:207:ASN:HB3  | 2.01                     | 0.42              |
| 3:G:115:VAL:HA   | 3:G:135:LEU:O    | 2.19                     | 0.42              |
| 3:G:136:LEU:HB2  | 3:G:175:LEU:HB3  | 2.02                     | 0.42              |
| 4:H:100:GLY:HA2  | 4:H:105:GLY:O    | 2.20                     | 0.42              |
| 4:H:152:ASP:HA   | 4:H:183:LEU:HB3  | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:464:ARG:HB2  | 1:I:496:PRO:HG3  | 2.01                     | 0.42              |
| 1:M:60:ASN:CB    | 1:M:63:GLU:HB2   | 2.47                     | 0.42              |
| 3:C:142:ARG:HD2  | 3:C:163:VAL:HG11 | 2.02                     | 0.42              |
| 3:K:78:LEU:HD23  | 3:K:78:LEU:HA    | 1.93                     | 0.42              |
| 1:M:59:ALA:O     | 1:M:61:VAL:N     | 2.53                     | 0.41              |
| 1:M:181:THR:HA   | 1:M:195:SER:HA   | 2.01                     | 0.41              |
| 1:M:614:PHE:O    | 1:M:634:ILE:HB   | 2.20                     | 0.41              |
| 4:P:53:PHE:HB3   | 4:P:103:TRP:HB3  | 2.01                     | 0.41              |
| 4:P:64:VAL:HA    | 4:P:67:ARG:NH1   | 2.33                     | 0.41              |
| 1:A:181:THR:HA   | 1:A:195:SER:HA   | 2.00                     | 0.41              |
| 1:A:393:ILE:HG12 | 1:A:431:GLU:HG3  | 2.01                     | 0.41              |
| 1:A:614:PHE:O    | 1:A:634:ILE:HB   | 2.20                     | 0.41              |
| 3:G:6:GLN:HG3    | 3:G:99:GLY:HA3   | 2.02                     | 0.41              |
| 4:H:53:PHE:HB3   | 4:H:103:TRP:CB   | 2.50                     | 0.41              |
| 1:I:453:LEU:HD23 | 1:I:453:LEU:HA   | 1.87                     | 0.41              |
| 1:I:459:ILE:O    | 1:I:463:LEU:HG   | 2.20                     | 0.41              |
| 1:E:270:VAL:HG12 | 1:E:274:MET:HE3  | 2.01                     | 0.41              |
| 1:E:323:PHE:CZ   | 1:E:423:ILE:HA   | 2.55                     | 0.41              |
| 1:E:552:PHE:CE2  | 1:E:581:PRO:HB3  | 2.55                     | 0.41              |
| 2:F:47:ASP:HB2   | 2:F:65:ASN:OD1   | 2.20                     | 0.41              |
| 3:G:108:ARG:HD3  | 3:G:171:SER:HB2  | 2.02                     | 0.41              |
| 3:G:186:TYR:HA   | 3:G:192:TYR:OH   | 2.20                     | 0.41              |
| 1:I:329:LYS:NZ   | 1:I:340:VAL:HB   | 2.35                     | 0.41              |
| 4:L:31:TYR:HA    | 4:L:103:TRP:HZ3  | 1.83                     | 0.41              |
| 1:M:539:ASP:OD1  | 1:M:539:ASP:N    | 2.53                     | 0.41              |
| 1:M:583:ILE:HD13 | 1:M:583:ILE:HA   | 1.90                     | 0.41              |
| 4:P:154:PHE:HA   | 4:P:155:PRO:HA   | 1.81                     | 0.41              |
| 1:A:198:PHE:HB2  | 1:A:226:LEU:HD13 | 2.01                     | 0.41              |
| 1:E:176:LYS:HA   | 1:E:176:LYS:HD3  | 1.83                     | 0.41              |
| 1:M:179:MET:HA   | 1:M:196:LEU:O    | 2.20                     | 0.41              |
| 1:A:491:LEU:HD12 | 1:A:510:VAL:HG13 | 2.01                     | 0.41              |
| 3:K:46:ARG:CZ    | 3:K:55:GLU:HB3   | 2.51                     | 0.41              |
| 1:M:169:TYR:OH   | 1:M:292:PHE:HA   | 2.21                     | 0.41              |
| 1:M:275:LYS:HE3  | 1:M:275:LYS:N    | 2.35                     | 0.41              |
| 3:C:6:GLN:HG3    | 3:C:99:GLY:HA3   | 2.02                     | 0.41              |
| 3:C:136:LEU:HB2  | 3:C:175:LEU:HB3  | 2.02                     | 0.41              |
| 1:I:549:ASN:HA   | 1:I:584:MET:SD   | 2.59                     | 0.41              |
| 1:M:50:LEU:HG    | 1:M:52:PRO:HD3   | 2.01                     | 0.41              |
| 1:M:464:ARG:NH2  | 1:M:496:PRO:HB3  | 2.35                     | 0.41              |
| 1:M:541:VAL:HA   | 1:M:555:SER:CB   | 2.50                     | 0.41              |
| 2:N:119:SER:HB3  | 2:N:122:ASP:HB2  | 2.01                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:P:31:TYR:HA    | 4:P:103:TRP:CZ3  | 2.54                     | 0.41              |
| 4:P:32:TYR:HE1   | 4:P:101:TRP:CD1  | 2.34                     | 0.41              |
| 1:A:24:LYS:HA    | 1:A:37:THR:HA    | 2.02                     | 0.41              |
| 3:G:48:ILE:HD12  | 3:G:73:LEU:HD12  | 2.02                     | 0.41              |
| 1:M:209:GLY:O    | 2:N:115:TYR:OH   | 2.34                     | 0.41              |
| 1:M:361:MET:O    | 1:M:395:GLY:HA2  | 2.20                     | 0.41              |
| 1:M:393:ILE:HG12 | 1:M:431:GLU:HG3  | 2.02                     | 0.41              |
| 1:M:552:PHE:CG   | 1:M:661:LEU:HD23 | 2.55                     | 0.41              |
| 4:P:34:ILE:HG21  | 4:P:79:LEU:CD2   | 2.50                     | 0.41              |
| 4:H:154:PHE:HA   | 4:H:155:PRO:HA   | 1.82                     | 0.41              |
| 4:H:211:SER:OG   | 4:H:213:THR:OG1  | 2.29                     | 0.41              |
| 1:I:409:LEU:H    | 1:I:409:LEU:HG   | 1.43                     | 0.41              |
| 4:L:29:PHE:CD2   | 4:L:77:ASN:HA    | 2.56                     | 0.41              |
| 4:L:30:SER:HA    | 4:L:72:ARG:NH2   | 2.35                     | 0.41              |
| 1:M:451:THR:HA   | 1:M:481:SER:HB2  | 2.03                     | 0.41              |
| 1:A:390:SER:OG   | 1:A:438:THR:HB   | 2.20                     | 0.41              |
| 1:E:156:SER:O    | 1:E:173:MET:HG2  | 2.21                     | 0.41              |
| 1:E:329:LYS:NZ   | 1:E:340:VAL:HB   | 2.36                     | 0.41              |
| 1:E:459:ILE:O    | 1:E:463:LEU:HG   | 2.21                     | 0.41              |
| 3:K:44:PRO:HB2   | 4:L:111:PHE:CE1  | 2.55                     | 0.41              |
| 1:M:491:LEU:HD12 | 1:M:510:VAL:HG13 | 2.03                     | 0.41              |
| 3:O:50:ALA:C     | 3:O:52:SER:H     | 2.29                     | 0.41              |
| 3:C:121:SER:OG   | 4:D:130:PHE:HB3  | 2.20                     | 0.41              |
| 3:C:186:TYR:HA   | 3:C:192:TYR:OH   | 2.20                     | 0.41              |
| 4:D:29:PHE:CE1   | 4:D:34:ILE:HD11  | 2.56                     | 0.41              |
| 1:E:50:LEU:HD21  | 2:F:92:ILE:HG23  | 2.03                     | 0.41              |
| 1:E:78:THR:HB    | 1:E:81:THR:HB    | 2.03                     | 0.41              |
| 1:E:92:ILE:C     | 4:H:102:LYS:HD3  | 2.46                     | 0.41              |
| 3:G:35:TRP:CE2   | 3:G:73:LEU:HB2   | 2.56                     | 0.41              |
| 1:I:36:TYR:HD2   | 2:J:103:HIS:CE1  | 2.39                     | 0.41              |
| 1:I:67:SER:HA    | 1:I:70:ASN:HB2   | 2.01                     | 0.41              |
| 1:I:149:TYR:CD2  | 1:I:208:ARG:HA   | 2.56                     | 0.41              |
| 1:I:482:LEU:HD13 | 1:I:546:PRO:HD3  | 2.03                     | 0.41              |
| 1:A:612:CYS:O    | 1:A:614:PHE:N    | 2.54                     | 0.41              |
| 1:E:21:SER:O     | 1:E:40:TRP:HB2   | 2.20                     | 0.41              |
| 1:E:149:TYR:CE2  | 1:E:208:ARG:HA   | 2.56                     | 0.41              |
| 1:I:59:ALA:HB1   | 2:J:84:ASN:HB3   | 2.03                     | 0.41              |
| 3:K:121:SER:OG   | 4:L:130:PHE:HB3  | 2.20                     | 0.41              |
| 1:M:139:PRO:HB2  | 1:M:141:THR:H    | 1.87                     | 0.40              |
| 1:M:156:SER:HB2  | 1:M:342:GLY:O    | 2.21                     | 0.40              |
| 2:N:128:LEU:HD23 | 2:N:128:LEU:HA   | 1.80                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:O:197:THR:HG23 | 3:O:204:PRO:HG3  | 2.02                     | 0.40              |
| 4:P:27:PHE:CE2   | 4:P:98:ARG:HD2   | 2.55                     | 0.40              |
| 4:P:35:HIS:CD2   | 4:P:99:GLY:HA3   | 2.55                     | 0.40              |
| 1:A:179:MET:HA   | 1:A:196:LEU:O    | 2.21                     | 0.40              |
| 1:A:275:LYS:HE3  | 1:A:275:LYS:N    | 2.35                     | 0.40              |
| 4:H:29:PHE:CE1   | 4:H:34:ILE:HD11  | 2.56                     | 0.40              |
| 1:I:231:THR:HB   | 1:I:234:HIS:H    | 1.86                     | 0.40              |
| 1:I:249:MET:SD   | 1:I:289:THR:HG23 | 2.61                     | 0.40              |
| 1:M:311:GLY:HA3  | 4:P:101:TRP:HB2  | 2.02                     | 0.40              |
| 1:M:390:SER:OG   | 1:M:438:THR:HB   | 2.21                     | 0.40              |
| 3:O:108:ARG:NH2  | 3:O:140:TYR:HB2  | 2.35                     | 0.40              |
| 3:C:150:VAL:HG22 | 3:C:192:TYR:CD1  | 2.56                     | 0.40              |
| 1:E:482:LEU:HD13 | 1:E:546:PRO:HD3  | 2.02                     | 0.40              |
| 2:F:128:LEU:HD23 | 2:F:128:LEU:HA   | 1.82                     | 0.40              |
| 1:I:632:THR:HG21 | 1:I:643:ILE:HD11 | 2.03                     | 0.40              |
| 1:A:252:ARG:O    | 1:A:256:MET:HB2  | 2.21                     | 0.40              |
| 4:D:154:PHE:HA   | 4:D:155:PRO:HA   | 1.79                     | 0.40              |
| 4:L:148:CYS:N    | 4:L:188:SER:O    | 2.53                     | 0.40              |
| 1:M:196:LEU:HD12 | 1:M:196:LEU:HA   | 1.84                     | 0.40              |
| 1:M:323:PHE:CZ   | 1:M:423:ILE:HA   | 2.57                     | 0.40              |
| 1:A:149:TYR:CD2  | 1:A:208:ARG:HA   | 2.57                     | 0.40              |
| 1:A:169:TYR:OH   | 1:A:292:PHE:HA   | 2.22                     | 0.40              |
| 3:C:7:THR:HG23   | 3:C:22:THR:HB    | 2.03                     | 0.40              |
| 1:E:252:ARG:O    | 1:E:256:MET:HB2  | 2.21                     | 0.40              |
| 4:H:150:VAL:HG11 | 4:H:158:VAL:HG11 | 2.04                     | 0.40              |
| 4:L:31:TYR:HA    | 4:L:103:TRP:CZ3  | 2.56                     | 0.40              |
| 3:O:148:TRP:CG   | 3:O:179:LEU:HD13 | 2.57                     | 0.40              |
| 1:A:376:LEU:O    | 1:A:380:THR:HG23 | 2.21                     | 0.40              |
| 1:A:598:GLN:H    | 1:A:598:GLN:HG2  | 1.64                     | 0.40              |
| 2:B:125:GLY:HA3  | 1:I:214:PRO:O    | 2.21                     | 0.40              |
| 3:C:107:LYS:HG3  | 3:C:108:ARG:N    | 2.36                     | 0.40              |
| 3:G:96:TRP:CZ3   | 4:H:35:HIS:CE1   | 3.10                     | 0.40              |
| 1:I:79:SER:O     | 1:I:81:THR:HG22  | 2.22                     | 0.40              |
| 3:K:140:TYR:CD1  | 3:K:141:PRO:HA   | 2.57                     | 0.40              |
| 4:L:101:TRP:HZ2  | 4:L:107:ALA:HB3  | 1.87                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 653/665 (98%)   | 609 (93%)  | 44 (7%)  | 0        | 100         | 100 |
| 1   | E     | 653/665 (98%)   | 613 (94%)  | 40 (6%)  | 0        | 100         | 100 |
| 1   | I     | 653/665 (98%)   | 606 (93%)  | 47 (7%)  | 0        | 100         | 100 |
| 1   | M     | 653/665 (98%)   | 606 (93%)  | 47 (7%)  | 0        | 100         | 100 |
| 2   | B     | 88/112 (79%)    | 79 (90%)   | 8 (9%)   | 1 (1%)   | 11          | 45  |
| 2   | F     | 88/112 (79%)    | 80 (91%)   | 6 (7%)   | 2 (2%)   | 5           | 29  |
| 2   | J     | 88/112 (79%)    | 80 (91%)   | 7 (8%)   | 1 (1%)   | 11          | 45  |
| 2   | N     | 88/112 (79%)    | 80 (91%)   | 7 (8%)   | 1 (1%)   | 11          | 45  |
| 3   | C     | 211/233 (91%)   | 200 (95%)  | 11 (5%)  | 0        | 100         | 100 |
| 3   | G     | 211/233 (91%)   | 198 (94%)  | 13 (6%)  | 0        | 100         | 100 |
| 3   | K     | 211/233 (91%)   | 201 (95%)  | 10 (5%)  | 0        | 100         | 100 |
| 3   | O     | 211/233 (91%)   | 199 (94%)  | 12 (6%)  | 0        | 100         | 100 |
| 4   | D     | 210/470 (45%)   | 197 (94%)  | 13 (6%)  | 0        | 100         | 100 |
| 4   | H     | 210/470 (45%)   | 197 (94%)  | 13 (6%)  | 0        | 100         | 100 |
| 4   | L     | 210/470 (45%)   | 196 (93%)  | 14 (7%)  | 0        | 100         | 100 |
| 4   | P     | 210/470 (45%)   | 198 (94%)  | 12 (6%)  | 0        | 100         | 100 |
| All | All   | 4648/5920 (78%) | 4339 (93%) | 304 (6%) | 5 (0%)   | 48          | 82  |

All (5) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | N     | 124 | PHE  |
| 2   | B     | 124 | PHE  |
| 2   | F     | 124 | PHE  |
| 2   | J     | 124 | PHE  |
| 2   | F     | 125 | GLY  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | A     | 561/570 (98%)   | 502 (90%)  | 59 (10%)  | 6           | 23 |
| 1   | E     | 561/570 (98%)   | 500 (89%)  | 61 (11%)  | 6           | 22 |
| 1   | I     | 561/570 (98%)   | 495 (88%)  | 66 (12%)  | 5           | 20 |
| 1   | M     | 561/570 (98%)   | 502 (90%)  | 59 (10%)  | 6           | 23 |
| 2   | B     | 83/99 (84%)     | 73 (88%)   | 10 (12%)  | 5           | 19 |
| 2   | F     | 83/99 (84%)     | 73 (88%)   | 10 (12%)  | 5           | 19 |
| 2   | J     | 83/99 (84%)     | 72 (87%)   | 11 (13%)  | 4           | 17 |
| 2   | N     | 83/99 (84%)     | 73 (88%)   | 10 (12%)  | 5           | 19 |
| 3   | C     | 186/202 (92%)   | 158 (85%)  | 28 (15%)  | 3           | 14 |
| 3   | G     | 186/202 (92%)   | 161 (87%)  | 25 (13%)  | 4           | 17 |
| 3   | K     | 186/202 (92%)   | 162 (87%)  | 24 (13%)  | 4           | 18 |
| 3   | O     | 186/202 (92%)   | 159 (86%)  | 27 (14%)  | 3           | 15 |
| 4   | D     | 180/416 (43%)   | 157 (87%)  | 23 (13%)  | 4           | 18 |
| 4   | H     | 180/416 (43%)   | 154 (86%)  | 26 (14%)  | 3           | 15 |
| 4   | L     | 180/416 (43%)   | 157 (87%)  | 23 (13%)  | 4           | 18 |
| 4   | P     | 180/416 (43%)   | 155 (86%)  | 25 (14%)  | 3           | 16 |
| All | All   | 4040/5148 (78%) | 3553 (88%) | 487 (12%) | 5           | 19 |

All (487) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 22  | GLU  |
| 1   | M     | 23  | VAL  |
| 1   | M     | 26  | HIS  |
| 1   | M     | 27  | LEU  |
| 1   | M     | 30  | GLU  |
| 1   | M     | 38  | ILE  |
| 1   | M     | 42  | GLU  |
| 1   | M     | 43  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 55  | LEU  |
| 1   | M     | 65  | LEU  |
| 1   | M     | 70  | ASN  |
| 1   | M     | 77  | LYS  |
| 1   | M     | 81  | THR  |
| 1   | M     | 84  | ILE  |
| 1   | M     | 95  | VAL  |
| 1   | M     | 102 | VAL  |
| 1   | M     | 115 | LEU  |
| 1   | M     | 153 | CYS  |
| 1   | M     | 163 | ASN  |
| 1   | M     | 194 | LEU  |
| 1   | M     | 196 | LEU  |
| 1   | M     | 213 | TYR  |
| 1   | M     | 231 | THR  |
| 1   | M     | 252 | ARG  |
| 1   | M     | 257 | THR  |
| 1   | M     | 269 | LEU  |
| 1   | M     | 274 | MET  |
| 1   | M     | 275 | LYS  |
| 1   | M     | 300 | LYS  |
| 1   | M     | 335 | CYS  |
| 1   | M     | 341 | LYS  |
| 1   | M     | 344 | GLN  |
| 1   | M     | 355 | LEU  |
| 1   | M     | 359 | VAL  |
| 1   | M     | 370 | GLU  |
| 1   | M     | 385 | LYS  |
| 1   | M     | 409 | LEU  |
| 1   | M     | 442 | ASN  |
| 1   | M     | 445 | LEU  |
| 1   | M     | 457 | LEU  |
| 1   | M     | 471 | GLU  |
| 1   | M     | 489 | ASP  |
| 1   | M     | 492 | LEU  |
| 1   | M     | 503 | GLN  |
| 1   | M     | 508 | ASN  |
| 1   | M     | 517 | LEU  |
| 1   | M     | 521 | ARG  |
| 1   | M     | 525 | ASP  |
| 1   | M     | 529 | LEU  |
| 1   | M     | 545 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 570 | THR  |
| 1   | M     | 573 | LEU  |
| 1   | M     | 576 | SER  |
| 1   | M     | 598 | GLN  |
| 1   | M     | 601 | LYS  |
| 1   | M     | 606 | THR  |
| 1   | M     | 615 | CYS  |
| 1   | M     | 620 | LEU  |
| 1   | M     | 632 | THR  |
| 2   | N     | 40  | LEU  |
| 2   | N     | 53  | ASN  |
| 2   | N     | 76  | ILE  |
| 2   | N     | 77  | SER  |
| 2   | N     | 78  | ARG  |
| 2   | N     | 98  | SER  |
| 2   | N     | 114 | LEU  |
| 2   | N     | 120 | VAL  |
| 2   | N     | 123 | LEU  |
| 2   | N     | 127 | ASN  |
| 3   | O     | 5   | THR  |
| 3   | O     | 11  | LEU  |
| 3   | O     | 15  | VAL  |
| 3   | O     | 27  | GLN  |
| 3   | O     | 30  | ARG  |
| 3   | O     | 46  | ARG  |
| 3   | O     | 49  | TYR  |
| 3   | O     | 75  | ILE  |
| 3   | O     | 78  | LEU  |
| 3   | O     | 83  | PHE  |
| 3   | O     | 85  | THR  |
| 3   | O     | 100 | GLN  |
| 3   | O     | 103 | LYS  |
| 3   | O     | 107 | LYS  |
| 3   | O     | 121 | SER  |
| 3   | O     | 129 | THR  |
| 3   | O     | 133 | VAL  |
| 3   | O     | 143 | GLU  |
| 3   | O     | 147 | GLN  |
| 3   | O     | 154 | LEU  |
| 3   | O     | 176 | SER  |
| 3   | O     | 187 | GLU  |
| 3   | O     | 190 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | O     | 191 | VAL  |
| 3   | O     | 199 | GLN  |
| 3   | O     | 205 | VAL  |
| 3   | O     | 206 | THR  |
| 4   | P     | 3   | GLN  |
| 4   | P     | 6   | GLU  |
| 4   | P     | 13  | GLN  |
| 4   | P     | 25  | SER  |
| 4   | P     | 28  | THR  |
| 4   | P     | 48  | VAL  |
| 4   | P     | 54  | ASP  |
| 4   | P     | 60  | CYS  |
| 4   | P     | 101 | TRP  |
| 4   | P     | 102 | LYS  |
| 4   | P     | 103 | TRP  |
| 4   | P     | 108 | PHE  |
| 4   | P     | 109 | ASP  |
| 4   | P     | 115 | THR  |
| 4   | P     | 116 | VAL  |
| 4   | P     | 118 | THR  |
| 4   | P     | 128 | SER  |
| 4   | P     | 146 | LEU  |
| 4   | P     | 148 | CYS  |
| 4   | P     | 156 | GLU  |
| 4   | P     | 186 | LEU  |
| 4   | P     | 187 | SER  |
| 4   | P     | 189 | VAL  |
| 4   | P     | 194 | SER  |
| 4   | P     | 217 | LYS  |
| 1   | A     | 23  | VAL  |
| 1   | A     | 26  | HIS  |
| 1   | A     | 27  | LEU  |
| 1   | A     | 30  | GLU  |
| 1   | A     | 38  | ILE  |
| 1   | A     | 42  | GLU  |
| 1   | A     | 43  | LEU  |
| 1   | A     | 65  | LEU  |
| 1   | A     | 70  | ASN  |
| 1   | A     | 77  | LYS  |
| 1   | A     | 81  | THR  |
| 1   | A     | 84  | ILE  |
| 1   | A     | 95  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 108 | HIS  |
| 1   | A     | 115 | LEU  |
| 1   | A     | 163 | ASN  |
| 1   | A     | 170 | THR  |
| 1   | A     | 194 | LEU  |
| 1   | A     | 196 | LEU  |
| 1   | A     | 206 | ASP  |
| 1   | A     | 213 | TYR  |
| 1   | A     | 231 | THR  |
| 1   | A     | 252 | ARG  |
| 1   | A     | 269 | LEU  |
| 1   | A     | 274 | MET  |
| 1   | A     | 275 | LYS  |
| 1   | A     | 288 | LEU  |
| 1   | A     | 300 | LYS  |
| 1   | A     | 330 | ASP  |
| 1   | A     | 332 | ILE  |
| 1   | A     | 335 | CYS  |
| 1   | A     | 341 | LYS  |
| 1   | A     | 344 | GLN  |
| 1   | A     | 355 | LEU  |
| 1   | A     | 359 | VAL  |
| 1   | A     | 370 | GLU  |
| 1   | A     | 385 | LYS  |
| 1   | A     | 409 | LEU  |
| 1   | A     | 442 | ASN  |
| 1   | A     | 445 | LEU  |
| 1   | A     | 457 | LEU  |
| 1   | A     | 471 | GLU  |
| 1   | A     | 489 | ASP  |
| 1   | A     | 492 | LEU  |
| 1   | A     | 503 | GLN  |
| 1   | A     | 508 | ASN  |
| 1   | A     | 517 | LEU  |
| 1   | A     | 521 | ARG  |
| 1   | A     | 525 | ASP  |
| 1   | A     | 529 | LEU  |
| 1   | A     | 545 | ILE  |
| 1   | A     | 570 | THR  |
| 1   | A     | 573 | LEU  |
| 1   | A     | 576 | SER  |
| 1   | A     | 598 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 601 | LYS  |
| 1   | A     | 606 | THR  |
| 1   | A     | 615 | CYS  |
| 1   | A     | 632 | THR  |
| 2   | B     | 40  | LEU  |
| 2   | B     | 53  | ASN  |
| 2   | B     | 76  | ILE  |
| 2   | B     | 77  | SER  |
| 2   | B     | 78  | ARG  |
| 2   | B     | 98  | SER  |
| 2   | B     | 100 | LEU  |
| 2   | B     | 114 | LEU  |
| 2   | B     | 123 | LEU  |
| 2   | B     | 127 | ASN  |
| 3   | C     | 5   | THR  |
| 3   | C     | 11  | LEU  |
| 3   | C     | 15  | VAL  |
| 3   | C     | 30  | ARG  |
| 3   | C     | 46  | ARG  |
| 3   | C     | 49  | TYR  |
| 3   | C     | 73  | LEU  |
| 3   | C     | 75  | ILE  |
| 3   | C     | 78  | LEU  |
| 3   | C     | 83  | PHE  |
| 3   | C     | 85  | THR  |
| 3   | C     | 100 | GLN  |
| 3   | C     | 103 | LYS  |
| 3   | C     | 106 | ILE  |
| 3   | C     | 107 | LYS  |
| 3   | C     | 121 | SER  |
| 3   | C     | 129 | THR  |
| 3   | C     | 133 | VAL  |
| 3   | C     | 143 | GLU  |
| 3   | C     | 147 | GLN  |
| 3   | C     | 154 | LEU  |
| 3   | C     | 176 | SER  |
| 3   | C     | 187 | GLU  |
| 3   | C     | 190 | LYS  |
| 3   | C     | 191 | VAL  |
| 3   | C     | 199 | GLN  |
| 3   | C     | 205 | VAL  |
| 3   | C     | 206 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 3   | GLN  |
| 4   | D     | 6   | GLU  |
| 4   | D     | 10  | ARG  |
| 4   | D     | 13  | GLN  |
| 4   | D     | 21  | SER  |
| 4   | D     | 25  | SER  |
| 4   | D     | 28  | THR  |
| 4   | D     | 48  | VAL  |
| 4   | D     | 54  | ASP  |
| 4   | D     | 60  | CYS  |
| 4   | D     | 101 | TRP  |
| 4   | D     | 102 | LYS  |
| 4   | D     | 103 | TRP  |
| 4   | D     | 108 | PHE  |
| 4   | D     | 109 | ASP  |
| 4   | D     | 115 | THR  |
| 4   | D     | 116 | VAL  |
| 4   | D     | 118 | THR  |
| 4   | D     | 146 | LEU  |
| 4   | D     | 148 | CYS  |
| 4   | D     | 156 | GLU  |
| 4   | D     | 194 | SER  |
| 4   | D     | 217 | LYS  |
| 1   | E     | 22  | GLU  |
| 1   | E     | 23  | VAL  |
| 1   | E     | 26  | HIS  |
| 1   | E     | 27  | LEU  |
| 1   | E     | 30  | GLU  |
| 1   | E     | 38  | ILE  |
| 1   | E     | 41  | THR  |
| 1   | E     | 42  | GLU  |
| 1   | E     | 43  | LEU  |
| 1   | E     | 57  | ARG  |
| 1   | E     | 65  | LEU  |
| 1   | E     | 70  | ASN  |
| 1   | E     | 77  | LYS  |
| 1   | E     | 81  | THR  |
| 1   | E     | 84  | ILE  |
| 1   | E     | 95  | VAL  |
| 1   | E     | 102 | VAL  |
| 1   | E     | 108 | HIS  |
| 1   | E     | 115 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 145 | SER  |
| 1   | E     | 153 | CYS  |
| 1   | E     | 162 | ILE  |
| 1   | E     | 163 | ASN  |
| 1   | E     | 194 | LEU  |
| 1   | E     | 196 | LEU  |
| 1   | E     | 206 | ASP  |
| 1   | E     | 213 | TYR  |
| 1   | E     | 221 | SER  |
| 1   | E     | 225 | SER  |
| 1   | E     | 231 | THR  |
| 1   | E     | 252 | ARG  |
| 1   | E     | 269 | LEU  |
| 1   | E     | 274 | MET  |
| 1   | E     | 275 | LYS  |
| 1   | E     | 300 | LYS  |
| 1   | E     | 335 | CYS  |
| 1   | E     | 341 | LYS  |
| 1   | E     | 344 | GLN  |
| 1   | E     | 355 | LEU  |
| 1   | E     | 359 | VAL  |
| 1   | E     | 370 | GLU  |
| 1   | E     | 385 | LYS  |
| 1   | E     | 409 | LEU  |
| 1   | E     | 442 | ASN  |
| 1   | E     | 445 | LEU  |
| 1   | E     | 457 | LEU  |
| 1   | E     | 471 | GLU  |
| 1   | E     | 489 | ASP  |
| 1   | E     | 492 | LEU  |
| 1   | E     | 503 | GLN  |
| 1   | E     | 508 | ASN  |
| 1   | E     | 517 | LEU  |
| 1   | E     | 521 | ARG  |
| 1   | E     | 525 | ASP  |
| 1   | E     | 545 | ILE  |
| 1   | E     | 569 | SER  |
| 1   | E     | 570 | THR  |
| 1   | E     | 573 | LEU  |
| 1   | E     | 601 | LYS  |
| 1   | E     | 615 | CYS  |
| 1   | E     | 620 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | F     | 40  | LEU  |
| 2   | F     | 53  | ASN  |
| 2   | F     | 76  | ILE  |
| 2   | F     | 78  | ARG  |
| 2   | F     | 98  | SER  |
| 2   | F     | 100 | LEU  |
| 2   | F     | 101 | THR  |
| 2   | F     | 114 | LEU  |
| 2   | F     | 123 | LEU  |
| 2   | F     | 127 | ASN  |
| 3   | G     | 5   | THR  |
| 3   | G     | 11  | LEU  |
| 3   | G     | 15  | VAL  |
| 3   | G     | 30  | ARG  |
| 3   | G     | 46  | ARG  |
| 3   | G     | 49  | TYR  |
| 3   | G     | 73  | LEU  |
| 3   | G     | 75  | ILE  |
| 3   | G     | 78  | LEU  |
| 3   | G     | 83  | PHE  |
| 3   | G     | 85  | THR  |
| 3   | G     | 100 | GLN  |
| 3   | G     | 103 | LYS  |
| 3   | G     | 107 | LYS  |
| 3   | G     | 121 | SER  |
| 3   | G     | 129 | THR  |
| 3   | G     | 133 | VAL  |
| 3   | G     | 143 | GLU  |
| 3   | G     | 147 | GLN  |
| 3   | G     | 154 | LEU  |
| 3   | G     | 166 | GLN  |
| 3   | G     | 176 | SER  |
| 3   | G     | 187 | GLU  |
| 3   | G     | 191 | VAL  |
| 3   | G     | 205 | VAL  |
| 4   | H     | 3   | GLN  |
| 4   | H     | 6   | GLU  |
| 4   | H     | 10  | ARG  |
| 4   | H     | 13  | GLN  |
| 4   | H     | 21  | SER  |
| 4   | H     | 25  | SER  |
| 4   | H     | 28  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | H     | 48  | VAL  |
| 4   | H     | 49  | THR  |
| 4   | H     | 54  | ASP  |
| 4   | H     | 60  | CYS  |
| 4   | H     | 101 | TRP  |
| 4   | H     | 102 | LYS  |
| 4   | H     | 103 | TRP  |
| 4   | H     | 108 | PHE  |
| 4   | H     | 109 | ASP  |
| 4   | H     | 115 | THR  |
| 4   | H     | 116 | VAL  |
| 4   | H     | 118 | THR  |
| 4   | H     | 146 | LEU  |
| 4   | H     | 148 | CYS  |
| 4   | H     | 156 | GLU  |
| 4   | H     | 187 | SER  |
| 4   | H     | 189 | VAL  |
| 4   | H     | 194 | SER  |
| 4   | H     | 217 | LYS  |
| 1   | I     | 22  | GLU  |
| 1   | I     | 23  | VAL  |
| 1   | I     | 26  | HIS  |
| 1   | I     | 27  | LEU  |
| 1   | I     | 30  | GLU  |
| 1   | I     | 38  | ILE  |
| 1   | I     | 41  | THR  |
| 1   | I     | 42  | GLU  |
| 1   | I     | 43  | LEU  |
| 1   | I     | 65  | LEU  |
| 1   | I     | 70  | ASN  |
| 1   | I     | 77  | LYS  |
| 1   | I     | 79  | SER  |
| 1   | I     | 81  | THR  |
| 1   | I     | 84  | ILE  |
| 1   | I     | 95  | VAL  |
| 1   | I     | 115 | LEU  |
| 1   | I     | 153 | CYS  |
| 1   | I     | 162 | ILE  |
| 1   | I     | 163 | ASN  |
| 1   | I     | 170 | THR  |
| 1   | I     | 194 | LEU  |
| 1   | I     | 196 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 206 | ASP  |
| 1   | I     | 213 | TYR  |
| 1   | I     | 218 | SER  |
| 1   | I     | 221 | SER  |
| 1   | I     | 231 | THR  |
| 1   | I     | 252 | ARG  |
| 1   | I     | 257 | THR  |
| 1   | I     | 269 | LEU  |
| 1   | I     | 274 | MET  |
| 1   | I     | 275 | LYS  |
| 1   | I     | 288 | LEU  |
| 1   | I     | 300 | LYS  |
| 1   | I     | 332 | ILE  |
| 1   | I     | 341 | LYS  |
| 1   | I     | 344 | GLN  |
| 1   | I     | 355 | LEU  |
| 1   | I     | 359 | VAL  |
| 1   | I     | 370 | GLU  |
| 1   | I     | 385 | LYS  |
| 1   | I     | 409 | LEU  |
| 1   | I     | 442 | ASN  |
| 1   | I     | 445 | LEU  |
| 1   | I     | 457 | LEU  |
| 1   | I     | 471 | GLU  |
| 1   | I     | 489 | ASP  |
| 1   | I     | 492 | LEU  |
| 1   | I     | 503 | GLN  |
| 1   | I     | 508 | ASN  |
| 1   | I     | 517 | LEU  |
| 1   | I     | 521 | ARG  |
| 1   | I     | 525 | ASP  |
| 1   | I     | 529 | LEU  |
| 1   | I     | 545 | ILE  |
| 1   | I     | 554 | ILE  |
| 1   | I     | 569 | SER  |
| 1   | I     | 570 | THR  |
| 1   | I     | 573 | LEU  |
| 1   | I     | 574 | SER  |
| 1   | I     | 576 | SER  |
| 1   | I     | 601 | LYS  |
| 1   | I     | 606 | THR  |
| 1   | I     | 615 | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 620 | LEU  |
| 2   | J     | 40  | LEU  |
| 2   | J     | 53  | ASN  |
| 2   | J     | 77  | SER  |
| 2   | J     | 78  | ARG  |
| 2   | J     | 98  | SER  |
| 2   | J     | 100 | LEU  |
| 2   | J     | 101 | THR  |
| 2   | J     | 114 | LEU  |
| 2   | J     | 120 | VAL  |
| 2   | J     | 123 | LEU  |
| 2   | J     | 127 | ASN  |
| 3   | K     | 5   | THR  |
| 3   | K     | 11  | LEU  |
| 3   | K     | 15  | VAL  |
| 3   | K     | 30  | ARG  |
| 3   | K     | 46  | ARG  |
| 3   | K     | 49  | TYR  |
| 3   | K     | 73  | LEU  |
| 3   | K     | 75  | ILE  |
| 3   | K     | 78  | LEU  |
| 3   | K     | 83  | PHE  |
| 3   | K     | 85  | THR  |
| 3   | K     | 100 | GLN  |
| 3   | K     | 107 | LYS  |
| 3   | K     | 121 | SER  |
| 3   | K     | 129 | THR  |
| 3   | K     | 133 | VAL  |
| 3   | K     | 143 | GLU  |
| 3   | K     | 147 | GLN  |
| 3   | K     | 176 | SER  |
| 3   | K     | 187 | GLU  |
| 3   | K     | 191 | VAL  |
| 3   | K     | 199 | GLN  |
| 3   | K     | 205 | VAL  |
| 3   | K     | 206 | THR  |
| 4   | L     | 3   | GLN  |
| 4   | L     | 6   | GLU  |
| 4   | L     | 10  | ARG  |
| 4   | L     | 13  | GLN  |
| 4   | L     | 21  | SER  |
| 4   | L     | 25  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | L     | 28  | THR  |
| 4   | L     | 48  | VAL  |
| 4   | L     | 54  | ASP  |
| 4   | L     | 60  | CYS  |
| 4   | L     | 101 | TRP  |
| 4   | L     | 102 | LYS  |
| 4   | L     | 103 | TRP  |
| 4   | L     | 108 | PHE  |
| 4   | L     | 109 | ASP  |
| 4   | L     | 115 | THR  |
| 4   | L     | 116 | VAL  |
| 4   | L     | 118 | THR  |
| 4   | L     | 146 | LEU  |
| 4   | L     | 148 | CYS  |
| 4   | L     | 156 | GLU  |
| 4   | L     | 194 | SER  |
| 4   | L     | 217 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 35  | HIS  |
| 1   | M     | 140 | ASN  |
| 1   | M     | 220 | GLN  |
| 1   | M     | 237 | ASN  |
| 1   | M     | 528 | HIS  |
| 3   | O     | 155 | GLN  |
| 4   | P     | 35  | HIS  |
| 4   | P     | 74  | ASN  |
| 1   | A     | 220 | GLN  |
| 1   | A     | 237 | ASN  |
| 1   | A     | 503 | GLN  |
| 2   | B     | 30  | HIS  |
| 3   | C     | 31  | ASN  |
| 4   | D     | 84  | ASN  |
| 1   | E     | 60  | ASN  |
| 1   | E     | 140 | ASN  |
| 1   | E     | 220 | GLN  |
| 2   | F     | 30  | HIS  |
| 3   | G     | 31  | ASN  |
| 3   | G     | 91  | HIS  |
| 4   | H     | 84  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 60  | ASN  |
| 1   | I     | 140 | ASN  |
| 1   | I     | 168 | GLN  |
| 1   | I     | 426 | HIS  |
| 2   | J     | 33  | GLN  |
| 3   | K     | 31  | ASN  |
| 3   | K     | 155 | GLN  |
| 4   | L     | 84  | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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     | 655/665 (98%)   | 0.75   | 59 (9%) 15 18  | 59, 142, 223, 269     | 0     |
| 1   | E     | 655/665 (98%)   | 1.07   | 114 (17%) 4 8  | 64, 184, 281, 343     | 0     |
| 1   | I     | 655/665 (98%)   | 0.70   | 56 (8%) 16 20  | 58, 140, 220, 266     | 0     |
| 1   | M     | 655/665 (98%)   | 0.67   | 49 (7%) 20 22  | 67, 155, 224, 267     | 0     |
| 2   | B     | 94/112 (83%)    | 1.03   | 8 (8%) 16 20   | 96, 169, 218, 269     | 0     |
| 2   | F     | 94/112 (83%)    | 1.03   | 21 (22%) 2 5   | 105, 177, 229, 279    | 0     |
| 2   | J     | 94/112 (83%)    | 0.97   | 13 (13%) 6 10  | 94, 170, 215, 266     | 0     |
| 2   | N     | 94/112 (83%)    | 0.95   | 12 (12%) 7 11  | 104, 186, 232, 277    | 0     |
| 3   | C     | 213/233 (91%)   | 0.31   | 6 (2%) 55 42   | 72, 118, 162, 211     | 0     |
| 3   | G     | 213/233 (91%)   | 0.43   | 5 (2%) 61 47   | 86, 122, 167, 219     | 0     |
| 3   | K     | 213/233 (91%)   | 0.27   | 6 (2%) 55 42   | 72, 115, 156, 202     | 0     |
| 3   | O     | 213/233 (91%)   | 0.40   | 8 (3%) 44 36   | 81, 126, 165, 227     | 0     |
| 4   | D     | 214/470 (45%)   | 0.98   | 30 (14%) 6 10  | 82, 148, 198, 280     | 0     |
| 4   | H     | 214/470 (45%)   | 0.95   | 28 (13%) 7 11  | 81, 146, 196, 265     | 0     |
| 4   | L     | 214/470 (45%)   | 0.78   | 20 (9%) 14 17  | 74, 135, 181, 258     | 0     |
| 4   | P     | 214/470 (45%)   | 1.04   | 34 (15%) 5 8   | 79, 159, 203, 291     | 0     |
| All | All   | 4704/5920 (79%) | 0.76   | 469 (9%) 12 16 | 58, 145, 234, 343     | 0     |

All (469) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4   | L     | 104 | PRO  | 7.9  |
| 4   | H     | 104 | PRO  | 7.7  |
| 1   | E     | 532 | TYR  | 7.5  |
| 4   | L     | 103 | TRP  | 7.1  |
| 4   | P     | 56  | THR  | 6.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 519 | LEU  | 6.9  |
| 1   | E     | 569 | SER  | 6.8  |
| 4   | H     | 103 | TRP  | 6.8  |
| 4   | P     | 104 | PRO  | 6.3  |
| 4   | D     | 104 | PRO  | 6.3  |
| 1   | A     | 500 | MET  | 6.0  |
| 4   | D     | 103 | TRP  | 5.8  |
| 1   | E     | 623 | ASP  | 5.8  |
| 4   | P     | 103 | TRP  | 5.8  |
| 1   | I     | 410 | PHE  | 5.7  |
| 1   | I     | 152 | ARG  | 5.6  |
| 1   | A     | 385 | LYS  | 5.4  |
| 1   | M     | 500 | MET  | 5.3  |
| 4   | D     | 110 | VAL  | 5.3  |
| 1   | E     | 530 | PRO  | 5.2  |
| 4   | L     | 110 | VAL  | 5.2  |
| 1   | E     | 572 | TYR  | 5.2  |
| 2   | J     | 25  | ALA  | 5.1  |
| 4   | P     | 110 | VAL  | 5.1  |
| 1   | I     | 500 | MET  | 5.1  |
| 4   | H     | 56  | THR  | 5.0  |
| 1   | I     | 385 | LYS  | 5.0  |
| 4   | D     | 56  | THR  | 5.0  |
| 1   | E     | 385 | LYS  | 4.9  |
| 1   | A     | 387 | GLY  | 4.9  |
| 1   | M     | 410 | PHE  | 4.6  |
| 1   | E     | 533 | LYS  | 4.6  |
| 4   | H     | 110 | VAL  | 4.5  |
| 1   | E     | 500 | MET  | 4.4  |
| 1   | E     | 564 | ALA  | 4.4  |
| 1   | E     | 607 | ARG  | 4.4  |
| 4   | H     | 105 | GLY  | 4.4  |
| 1   | A     | 410 | PHE  | 4.3  |
| 1   | A     | 624 | GLU  | 4.3  |
| 2   | N     | 27  | PRO  | 4.3  |
| 4   | L     | 56  | THR  | 4.3  |
| 1   | A     | 142 | ARG  | 4.3  |
| 4   | L     | 105 | GLY  | 4.3  |
| 1   | E     | 508 | ASN  | 4.2  |
| 1   | I     | 595 | GLU  | 4.2  |
| 2   | J     | 33  | GLN  | 4.2  |
| 2   | B     | 27  | PRO  | 4.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | F     | 124 | PHE  | 4.2  |
| 1   | I     | 22  | GLU  | 4.2  |
| 1   | I     | 461 | GLU  | 4.2  |
| 4   | D     | 105 | GLY  | 4.1  |
| 1   | A     | 527 | TRP  | 4.1  |
| 1   | E     | 527 | TRP  | 4.1  |
| 2   | F     | 27  | PRO  | 4.1  |
| 1   | M     | 572 | TYR  | 4.0  |
| 4   | H     | 102 | LYS  | 4.0  |
| 1   | A     | 572 | TYR  | 4.0  |
| 1   | I     | 411 | GLN  | 4.0  |
| 1   | A     | 101 | GLN  | 4.0  |
| 1   | E     | 384 | PRO  | 4.0  |
| 1   | E     | 33  | ALA  | 3.9  |
| 1   | I     | 572 | TYR  | 3.9  |
| 2   | N     | 25  | ALA  | 3.9  |
| 1   | E     | 627 | GLY  | 3.9  |
| 1   | M     | 101 | GLN  | 3.9  |
| 1   | E     | 152 | ARG  | 3.9  |
| 4   | P     | 105 | GLY  | 3.9  |
| 4   | P     | 101 | TRP  | 3.8  |
| 1   | A     | 384 | PRO  | 3.8  |
| 1   | E     | 101 | GLN  | 3.8  |
| 1   | E     | 134 | ILE  | 3.8  |
| 1   | I     | 101 | GLN  | 3.8  |
| 1   | E     | 592 | VAL  | 3.8  |
| 4   | H     | 135 | SER  | 3.7  |
| 1   | A     | 499 | ALA  | 3.7  |
| 2   | J     | 127 | ASN  | 3.7  |
| 4   | H     | 58  | ASP  | 3.7  |
| 1   | I     | 384 | PRO  | 3.7  |
| 2   | B     | 33  | GLN  | 3.7  |
| 4   | L     | 102 | LYS  | 3.7  |
| 1   | I     | 528 | HIS  | 3.7  |
| 1   | M     | 80  | GLY  | 3.7  |
| 1   | A     | 41  | THR  | 3.7  |
| 1   | E     | 580 | SER  | 3.6  |
| 4   | D     | 102 | LYS  | 3.6  |
| 1   | I     | 624 | GLU  | 3.6  |
| 2   | B     | 25  | ALA  | 3.6  |
| 3   | O     | 190 | LYS  | 3.6  |
| 1   | E     | 563 | SER  | 3.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | F     | 33  | GLN  | 3.6  |
| 1   | M     | 412 | PRO  | 3.6  |
| 1   | E     | 461 | GLU  | 3.6  |
| 1   | M     | 624 | GLU  | 3.6  |
| 4   | P     | 107 | ALA  | 3.5  |
| 2   | J     | 102 | SER  | 3.5  |
| 1   | I     | 594 | GLY  | 3.5  |
| 1   | E     | 410 | PHE  | 3.5  |
| 1   | I     | 519 | LEU  | 3.5  |
| 4   | P     | 135 | SER  | 3.5  |
| 3   | O     | 83  | PHE  | 3.5  |
| 1   | M     | 133 | TYR  | 3.5  |
| 1   | E     | 520 | GLU  | 3.5  |
| 1   | E     | 492 | LEU  | 3.5  |
| 1   | E     | 499 | ALA  | 3.4  |
| 1   | E     | 531 | ALA  | 3.4  |
| 1   | A     | 528 | HIS  | 3.4  |
| 3   | G     | 83  | PHE  | 3.4  |
| 1   | M     | 608 | THR  | 3.4  |
| 1   | M     | 528 | HIS  | 3.3  |
| 1   | M     | 310 | ASN  | 3.3  |
| 1   | I     | 106 | LYS  | 3.3  |
| 1   | I     | 520 | GLU  | 3.3  |
| 4   | H     | 99  | GLY  | 3.3  |
| 1   | E     | 597 | ARG  | 3.3  |
| 1   | A     | 674 | TYR  | 3.3  |
| 1   | M     | 519 | LEU  | 3.3  |
| 4   | H     | 31  | TYR  | 3.3  |
| 1   | E     | 273 | GLU  | 3.3  |
| 1   | E     | 629 | GLU  | 3.3  |
| 4   | L     | 106 | GLY  | 3.3  |
| 4   | P     | 102 | LYS  | 3.3  |
| 1   | A     | 461 | GLU  | 3.3  |
| 2   | B     | 26  | TYR  | 3.3  |
| 1   | I     | 525 | ASP  | 3.2  |
| 2   | N     | 32  | THR  | 3.2  |
| 1   | E     | 22  | GLU  | 3.2  |
| 1   | I     | 154 | HIS  | 3.2  |
| 1   | A     | 508 | ASN  | 3.2  |
| 1   | E     | 628 | LEU  | 3.2  |
| 2   | N     | 132 | ALA  | 3.2  |
| 4   | D     | 107 | ALA  | 3.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4   | H     | 3   | GLN  | 3.2  |
| 1   | E     | 388 | VAL  | 3.2  |
| 4   | D     | 106 | GLY  | 3.2  |
| 1   | E     | 608 | THR  | 3.1  |
| 2   | F     | 121 | GLU  | 3.1  |
| 4   | D     | 207 | ASN  | 3.1  |
| 4   | L     | 101 | TRP  | 3.1  |
| 4   | D     | 109 | ASP  | 3.1  |
| 1   | E     | 542 | LEU  | 3.1  |
| 1   | A     | 220 | GLN  | 3.1  |
| 4   | L     | 124 | THR  | 3.1  |
| 4   | H     | 55  | GLY  | 3.1  |
| 1   | E     | 20  | LEU  | 3.1  |
| 1   | M     | 411 | GLN  | 3.1  |
| 1   | A     | 525 | ASP  | 3.1  |
| 1   | I     | 521 | ARG  | 3.1  |
| 2   | B     | 124 | PHE  | 3.1  |
| 1   | E     | 139 | PRO  | 3.1  |
| 1   | E     | 535 | VAL  | 3.1  |
| 1   | A     | 558 | ARG  | 3.1  |
| 1   | I     | 387 | GLY  | 3.1  |
| 1   | M     | 607 | ARG  | 3.1  |
| 2   | N     | 33  | GLN  | 3.0  |
| 4   | H     | 101 | TRP  | 3.0  |
| 4   | D     | 59  | HIS  | 3.0  |
| 1   | A     | 595 | GLU  | 3.0  |
| 1   | E     | 528 | HIS  | 3.0  |
| 1   | A     | 362 | GLU  | 3.0  |
| 1   | I     | 20  | LEU  | 3.0  |
| 1   | I     | 674 | TYR  | 3.0  |
| 2   | N     | 121 | GLU  | 3.0  |
| 4   | P     | 39  | GLN  | 3.0  |
| 1   | I     | 558 | ARG  | 3.0  |
| 1   | A     | 655 | HIS  | 3.0  |
| 1   | E     | 468 | LEU  | 3.0  |
| 1   | M     | 508 | ASN  | 3.0  |
| 1   | I     | 362 | GLU  | 3.0  |
| 2   | F     | 57  | ASP  | 3.0  |
| 4   | L     | 31  | TYR  | 3.0  |
| 1   | I     | 563 | SER  | 2.9  |
| 4   | P     | 210 | PRO  | 2.9  |
| 2   | F     | 30  | HIS  | 2.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 502 | ASP  | 2.9  |
| 1   | M     | 499 | ALA  | 2.9  |
| 1   | A     | 520 | GLU  | 2.9  |
| 4   | P     | 45  | LEU  | 2.9  |
| 2   | F     | 103 | HIS  | 2.9  |
| 1   | I     | 508 | ASN  | 2.9  |
| 1   | E     | 586 | LYS  | 2.9  |
| 1   | M     | 132 | TYR  | 2.9  |
| 1   | E     | 389 | TYR  | 2.9  |
| 1   | M     | 295 | SER  | 2.9  |
| 2   | J     | 57  | ASP  | 2.9  |
| 1   | M     | 243 | VAL  | 2.9  |
| 1   | M     | 222 | GLY  | 2.9  |
| 1   | E     | 487 | THR  | 2.9  |
| 4   | D     | 3   | GLN  | 2.9  |
| 4   | D     | 108 | PHE  | 2.9  |
| 1   | A     | 80  | GLY  | 2.9  |
| 1   | E     | 80  | GLY  | 2.9  |
| 1   | E     | 622 | TYR  | 2.8  |
| 1   | E     | 240 | ASN  | 2.8  |
| 3   | K     | 2   | ILE  | 2.8  |
| 4   | H     | 57  | SER  | 2.8  |
| 1   | I     | 527 | TRP  | 2.8  |
| 1   | E     | 457 | LEU  | 2.8  |
| 1   | I     | 654 | LEU  | 2.8  |
| 4   | L     | 218 | ARG  | 2.8  |
| 1   | A     | 472 | SER  | 2.8  |
| 4   | D     | 135 | SER  | 2.8  |
| 4   | H     | 13  | GLN  | 2.8  |
| 3   | O     | 32  | ASN  | 2.8  |
| 1   | I     | 388 | VAL  | 2.8  |
| 2   | B     | 29  | CYS  | 2.8  |
| 1   | M     | 184 | ARG  | 2.8  |
| 4   | H     | 106 | GLY  | 2.8  |
| 1   | A     | 519 | LEU  | 2.8  |
| 3   | K     | 83  | PHE  | 2.8  |
| 2   | J     | 26  | TYR  | 2.7  |
| 3   | O     | 1   | ASP  | 2.7  |
| 4   | P     | 106 | GLY  | 2.7  |
| 1   | E     | 383 | TYR  | 2.7  |
| 1   | A     | 152 | ARG  | 2.7  |
| 4   | P     | 19  | ARG  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4   | L     | 109 | ASP  | 2.7  |
| 1   | E     | 671 | ALA  | 2.7  |
| 2   | F     | 122 | ASP  | 2.7  |
| 4   | P     | 109 | ASP  | 2.7  |
| 1   | I     | 382 | GLY  | 2.7  |
| 1   | M     | 526 | ALA  | 2.7  |
| 1   | M     | 344 | GLN  | 2.7  |
| 1   | A     | 388 | VAL  | 2.7  |
| 1   | E     | 142 | ARG  | 2.7  |
| 1   | E     | 521 | ARG  | 2.7  |
| 1   | M     | 41  | THR  | 2.7  |
| 1   | E     | 446 | TYR  | 2.7  |
| 3   | G     | 2   | ILE  | 2.7  |
| 4   | H     | 109 | ASP  | 2.7  |
| 1   | A     | 273 | GLU  | 2.7  |
| 1   | E     | 30  | GLU  | 2.7  |
| 1   | E     | 106 | LYS  | 2.6  |
| 1   | A     | 412 | PRO  | 2.6  |
| 4   | L     | 59  | HIS  | 2.6  |
| 1   | E     | 647 | ASN  | 2.6  |
| 1   | I     | 344 | GLN  | 2.6  |
| 1   | M     | 472 | SER  | 2.6  |
| 4   | L     | 58  | ASP  | 2.6  |
| 1   | M     | 256 | MET  | 2.6  |
| 4   | D     | 19  | ARG  | 2.6  |
| 1   | M     | 527 | TRP  | 2.6  |
| 4   | H     | 59  | HIS  | 2.6  |
| 1   | E     | 437 | THR  | 2.6  |
| 1   | A     | 21  | SER  | 2.6  |
| 2   | B     | 102 | SER  | 2.6  |
| 4   | L     | 135 | SER  | 2.6  |
| 4   | D     | 101 | TRP  | 2.6  |
| 4   | L     | 66  | GLY  | 2.6  |
| 3   | C     | 129 | THR  | 2.6  |
| 1   | E     | 668 | MET  | 2.6  |
| 4   | P     | 123 | SER  | 2.6  |
| 4   | D     | 45  | LEU  | 2.6  |
| 4   | D     | 98  | ARG  | 2.6  |
| 1   | A     | 22  | GLU  | 2.6  |
| 1   | E     | 570 | THR  | 2.6  |
| 2   | F     | 67  | PRO  | 2.6  |
| 1   | A     | 30  | GLU  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4   | P     | 98  | ARG  | 2.6  |
| 2   | F     | 63  | SER  | 2.6  |
| 1   | A     | 154 | HIS  | 2.6  |
| 1   | E     | 267 | GLN  | 2.6  |
| 4   | P     | 40  | GLY  | 2.6  |
| 1   | I     | 532 | TYR  | 2.6  |
| 1   | A     | 84  | ILE  | 2.5  |
| 4   | P     | 99  | GLY  | 2.5  |
| 4   | D     | 53  | PHE  | 2.5  |
| 1   | E     | 344 | GLN  | 2.5  |
| 1   | E     | 411 | GLN  | 2.5  |
| 2   | N     | 26  | TYR  | 2.5  |
| 1   | E     | 412 | PRO  | 2.5  |
| 1   | A     | 20  | LEU  | 2.5  |
| 1   | E     | 501 | LEU  | 2.5  |
| 1   | I     | 499 | ALA  | 2.5  |
| 1   | M     | 638 | GLU  | 2.5  |
| 3   | K     | 54  | LEU  | 2.5  |
| 1   | E     | 37  | THR  | 2.5  |
| 1   | E     | 666 | THR  | 2.5  |
| 1   | A     | 592 | VAL  | 2.5  |
| 1   | M     | 461 | GLU  | 2.5  |
| 1   | M     | 674 | TYR  | 2.5  |
| 4   | H     | 176 | ALA  | 2.5  |
| 1   | E     | 555 | SER  | 2.5  |
| 4   | P     | 54  | ASP  | 2.5  |
| 3   | K     | 108 | ARG  | 2.5  |
| 3   | G     | 190 | LYS  | 2.5  |
| 1   | E     | 534 | CYS  | 2.4  |
| 1   | E     | 626 | GLU  | 2.4  |
| 4   | D     | 31  | TYR  | 2.4  |
| 1   | A     | 440 | GLY  | 2.4  |
| 1   | M     | 244 | PRO  | 2.4  |
| 1   | E     | 560 | VAL  | 2.4  |
| 4   | P     | 209 | LYS  | 2.4  |
| 2   | N     | 44  | ASN  | 2.4  |
| 1   | I     | 220 | GLN  | 2.4  |
| 2   | F     | 32  | THR  | 2.4  |
| 1   | E     | 573 | LEU  | 2.4  |
| 2   | N     | 124 | PHE  | 2.4  |
| 4   | D     | 39  | GLN  | 2.4  |
| 1   | E     | 610 | LYS  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 645 | SER  | 2.4  |
| 1   | M     | 20  | LEU  | 2.4  |
| 1   | A     | 526 | ALA  | 2.4  |
| 1   | E     | 650 | ASP  | 2.4  |
| 1   | E     | 631 | THR  | 2.4  |
| 1   | I     | 412 | PRO  | 2.4  |
| 4   | P     | 200 | GLN  | 2.4  |
| 4   | P     | 55  | GLY  | 2.4  |
| 4   | L     | 53  | PHE  | 2.4  |
| 1   | E     | 669 | GLU  | 2.4  |
| 2   | J     | 121 | GLU  | 2.4  |
| 4   | D     | 57  | SER  | 2.4  |
| 1   | A     | 151 | LEU  | 2.3  |
| 1   | E     | 29  | ILE  | 2.3  |
| 1   | E     | 84  | ILE  | 2.3  |
| 1   | E     | 187 | GLU  | 2.3  |
| 1   | E     | 497 | GLN  | 2.3  |
| 1   | A     | 339 | THR  | 2.3  |
| 2   | F     | 102 | SER  | 2.3  |
| 1   | E     | 488 | ARG  | 2.3  |
| 4   | P     | 31  | TYR  | 2.3  |
| 1   | M     | 386 | ALA  | 2.3  |
| 4   | D     | 124 | THR  | 2.3  |
| 1   | I     | 574 | SER  | 2.3  |
| 1   | A     | 536 | ASP  | 2.3  |
| 1   | E     | 148 | PHE  | 2.3  |
| 1   | E     | 600 | PRO  | 2.3  |
| 2   | F     | 25  | ALA  | 2.3  |
| 1   | I     | 339 | THR  | 2.3  |
| 4   | H     | 34  | ILE  | 2.3  |
| 2   | F     | 29  | CYS  | 2.3  |
| 4   | P     | 74  | ASN  | 2.3  |
| 1   | M     | 346 | TYR  | 2.3  |
| 2   | N     | 30  | HIS  | 2.3  |
| 4   | P     | 125 | LYS  | 2.3  |
| 1   | E     | 673 | LEU  | 2.3  |
| 1   | M     | 373 | GLU  | 2.3  |
| 4   | P     | 159 | THR  | 2.3  |
| 4   | D     | 155 | PRO  | 2.3  |
| 1   | E     | 270 | VAL  | 2.3  |
| 1   | M     | 137 | MET  | 2.3  |
| 1   | A     | 406 | ARG  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | C     | 67  | PHE  | 2.2  |
| 1   | M     | 432 | LEU  | 2.2  |
| 2   | F     | 125 | GLY  | 2.2  |
| 4   | H     | 142 | GLY  | 2.2  |
| 1   | I     | 33  | ALA  | 2.2  |
| 1   | M     | 558 | ARG  | 2.2  |
| 1   | A     | 411 | GLN  | 2.2  |
| 1   | I     | 273 | GLU  | 2.2  |
| 1   | I     | 134 | ILE  | 2.2  |
| 1   | I     | 308 | THR  | 2.2  |
| 2   | N     | 29  | CYS  | 2.2  |
| 4   | D     | 214 | LYS  | 2.2  |
| 1   | E     | 665 | GLY  | 2.2  |
| 1   | M     | 467 | ALA  | 2.2  |
| 2   | J     | 27  | PRO  | 2.2  |
| 1   | E     | 88  | GLU  | 2.2  |
| 4   | H     | 220 | GLU  | 2.2  |
| 1   | E     | 132 | TYR  | 2.2  |
| 4   | D     | 4   | LEU  | 2.2  |
| 1   | M     | 22  | GLU  | 2.2  |
| 1   | I     | 457 | LEU  | 2.2  |
| 1   | E     | 593 | ALA  | 2.2  |
| 3   | C     | 46  | ARG  | 2.2  |
| 4   | D     | 142 | GLY  | 2.2  |
| 4   | H     | 66  | GLY  | 2.2  |
| 4   | L     | 207 | ASN  | 2.2  |
| 3   | O     | 129 | THR  | 2.2  |
| 1   | M     | 212 | SER  | 2.2  |
| 1   | E     | 518 | SER  | 2.2  |
| 4   | P     | 7   | SER  | 2.2  |
| 4   | L     | 57  | SER  | 2.2  |
| 1   | E     | 603 | GLN  | 2.2  |
| 3   | C     | 190 | LYS  | 2.2  |
| 4   | H     | 218 | ARG  | 2.2  |
| 1   | I     | 593 | ALA  | 2.2  |
| 1   | A     | 197 | ILE  | 2.2  |
| 3   | K     | 52  | SER  | 2.2  |
| 1   | E     | 261 | TYR  | 2.2  |
| 3   | K     | 1   | ASP  | 2.2  |
| 4   | P     | 218 | ARG  | 2.2  |
| 1   | A     | 37  | THR  | 2.2  |
| 4   | H     | 53  | PHE  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | M     | 654 | LEU  | 2.2  |
| 1   | A     | 106 | LYS  | 2.2  |
| 1   | A     | 108 | HIS  | 2.2  |
| 4   | P     | 59  | HIS  | 2.2  |
| 4   | L     | 62  | SER  | 2.2  |
| 3   | G     | 94  | TYR  | 2.2  |
| 4   | H     | 60  | CYS  | 2.2  |
| 1   | I     | 406 | ARG  | 2.2  |
| 1   | M     | 573 | LEU  | 2.1  |
| 1   | E     | 371 | LYS  | 2.1  |
| 1   | E     | 32  | HIS  | 2.1  |
| 1   | A     | 439 | GLN  | 2.1  |
| 1   | A     | 594 | GLY  | 2.1  |
| 3   | C     | 66  | GLY  | 2.1  |
| 1   | M     | 166 | LYS  | 2.1  |
| 1   | E     | 166 | LYS  | 2.1  |
| 1   | I     | 84  | ILE  | 2.1  |
| 2   | B     | 44  | ASN  | 2.1  |
| 3   | O     | 31  | ASN  | 2.1  |
| 4   | D     | 159 | THR  | 2.1  |
| 1   | E     | 233 | VAL  | 2.1  |
| 1   | M     | 197 | ILE  | 2.1  |
| 1   | E     | 274 | MET  | 2.1  |
| 2   | J     | 103 | HIS  | 2.1  |
| 1   | E     | 621 | SER  | 2.1  |
| 2   | N     | 60  | SER  | 2.1  |
| 4   | P     | 57  | SER  | 2.1  |
| 1   | I     | 386 | ALA  | 2.1  |
| 1   | I     | 409 | LEU  | 2.1  |
| 4   | P     | 155 | PRO  | 2.1  |
| 1   | M     | 525 | ASP  | 2.1  |
| 4   | D     | 206 | VAL  | 2.1  |
| 1   | E     | 426 | HIS  | 2.1  |
| 3   | C     | 31  | ASN  | 2.1  |
| 1   | A     | 222 | GLY  | 2.1  |
| 1   | I     | 526 | ALA  | 2.1  |
| 3   | O     | 27  | GLN  | 2.1  |
| 1   | E     | 197 | ILE  | 2.1  |
| 2   | F     | 106 | GLU  | 2.1  |
| 2   | J     | 106 | GLU  | 2.1  |
| 1   | A     | 607 | ARG  | 2.1  |
| 1   | I     | 502 | ASP  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 543 | MET  | 2.1  |
| 1   | E     | 620 | LEU  | 2.1  |
| 1   | I     | 80  | GLY  | 2.1  |
| 2   | J     | 132 | ALA  | 2.1  |
| 3   | G     | 67  | PHE  | 2.1  |
| 1   | M     | 215 | SER  | 2.1  |
| 1   | E     | 271 | LEU  | 2.1  |
| 1   | M     | 391 | GLY  | 2.1  |
| 1   | I     | 32  | HIS  | 2.1  |
| 2   | F     | 109 | THR  | 2.1  |
| 3   | O     | 76  | ASN  | 2.1  |
| 4   | D     | 120 | SER  | 2.1  |
| 1   | E     | 184 | ARG  | 2.0  |
| 1   | A     | 64  | ASP  | 2.0  |
| 2   | F     | 26  | TYR  | 2.0  |
| 2   | J     | 122 | ASP  | 2.0  |
| 1   | A     | 33  | ALA  | 2.0  |
| 1   | E     | 651 | PHE  | 2.0  |
| 1   | A     | 310 | ASN  | 2.0  |
| 1   | E     | 496 | PRO  | 2.0  |
| 1   | I     | 81  | THR  | 2.0  |
| 2   | J     | 67  | PRO  | 2.0  |
| 1   | M     | 595 | GLU  | 2.0  |
| 1   | I     | 187 | GLU  | 2.0  |
| 1   | E     | 113 | SER  | 2.0  |
| 1   | E     | 472 | SER  | 2.0  |
| 1   | I     | 111 | VAL  | 2.0  |
| 2   | F     | 31  | VAL  | 2.0  |
| 1   | A     | 49  | GLY  | 2.0  |
| 4   | H     | 35  | HIS  | 2.0  |
| 1   | E     | 408 | PRO  | 2.0  |
| 1   | E     | 546 | PRO  | 2.0  |
| 1   | A     | 308 | THR  | 2.0  |
| 1   | E     | 498 | GLU  | 2.0  |
| 1   | A     | 24  | LYS  | 2.0  |
| 2   | F     | 60  | SER  | 2.0  |
| 4   | P     | 111 | PHE  | 2.0  |
| 2   | F     | 120 | VAL  | 2.0  |
| 4   | P     | 215 | VAL  | 2.0  |
| 1   | E     | 308 | THR  | 2.0  |
| 4   | H     | 70  | MET  | 2.0  |
| 1   | E     | 360 | LYS  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 390 | SER  | 2.0  |
| 1   | I     | 642 | SER  | 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 oligosaccharides 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.