



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:37 PM UTC

PDB ID : 4R7N / pdb\_00004r7n  
Title : Fab C2E3  
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Kosco-Vilbois, M.; Fischer, N.; Thore, S.; Rousseau, F.  
Deposited on : 2014-08-28  
Resolution : 3.45 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                                                             |

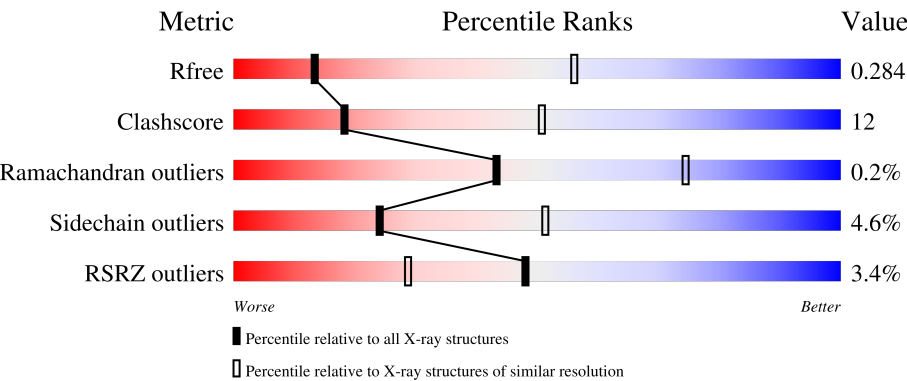
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.45 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 <sub>free</sub>     | 180053                      | 1070 (3.50-3.42)                                      |
| Clashscore            | 190562                      | 1128 (3.50-3.42)                                      |
| Ramachandran outliers | 187476                      | 1101 (3.50-3.42)                                      |
| Sidechain outliers    | 187428                      | 1102 (3.50-3.42)                                      |
| RSRZ outliers         | 180081                      | 1070 (3.50-3.42)                                      |

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     | 225    | <div><div>11%</div><div><div></div><div>68%</div><div>26%</div><div>...</div></div></div> |
| 1   | C     | 225    | <div><div></div><div><div></div><div>73%</div><div>22%</div><div>..</div></div></div>     |
| 1   | E     | 225    | <div><div>11%</div><div><div></div><div>68%</div><div>27%</div><div>..</div></div></div>  |
| 1   | G     | 225    | <div><div>4%</div><div><div></div><div>74%</div><div>20%</div><div>..</div></div></div>   |
| 1   | I     | 225    | <div><div>2%</div><div><div></div><div>74%</div><div>20%</div><div>..</div></div></div>   |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | K     | 225    |                  |
| 1   | M     | 225    |                  |
| 1   | O     | 225    |                  |
| 1   | Q     | 225    |                  |
| 1   | S     | 225    |                  |
| 2   | B     | 214    |                  |
| 2   | D     | 214    |                  |
| 2   | F     | 214    |                  |
| 2   | H     | 214    |                  |
| 2   | J     | 214    |                  |
| 2   | L     | 214    |                  |
| 2   | N     | 214    |                  |
| 2   | P     | 214    |                  |
| 2   | R     | 214    |                  |
| 2   | T     | 214    |                  |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 32933 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 Fab C2E3 Heavy chain.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 218      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1657  | 1056 | 276 | 320 | 5 |         |         |       |
| 1   | C     | 218      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1657  | 1056 | 276 | 320 | 5 |         |         |       |
| 1   | E     | 218      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1657  | 1056 | 276 | 320 | 5 |         |         |       |
| 1   | G     | 218      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1657  | 1056 | 276 | 320 | 5 |         |         |       |
| 1   | I     | 218      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1657  | 1056 | 276 | 320 | 5 |         |         |       |
| 1   | K     | 218      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1657  | 1056 | 276 | 320 | 5 |         |         |       |
| 1   | M     | 218      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1657  | 1056 | 276 | 320 | 5 |         |         |       |
| 1   | O     | 218      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1657  | 1056 | 276 | 320 | 5 |         |         |       |
| 1   | Q     | 218      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1657  | 1056 | 276 | 320 | 5 |         |         |       |
| 1   | S     | 218      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1657  | 1056 | 276 | 320 | 5 |         |         |       |

- Molecule 2 is a protein called Fab C2E3 Light chain.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | B     | 211      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1635  | 1027 | 273 | 331 | 4 |         |         |       |
| 2   | D     | 211      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1635  | 1027 | 273 | 331 | 4 |         |         |       |
| 2   | F     | 211      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1635  | 1027 | 273 | 331 | 4 |         |         |       |
| 2   | H     | 211      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1635  | 1027 | 273 | 331 | 4 |         |         |       |

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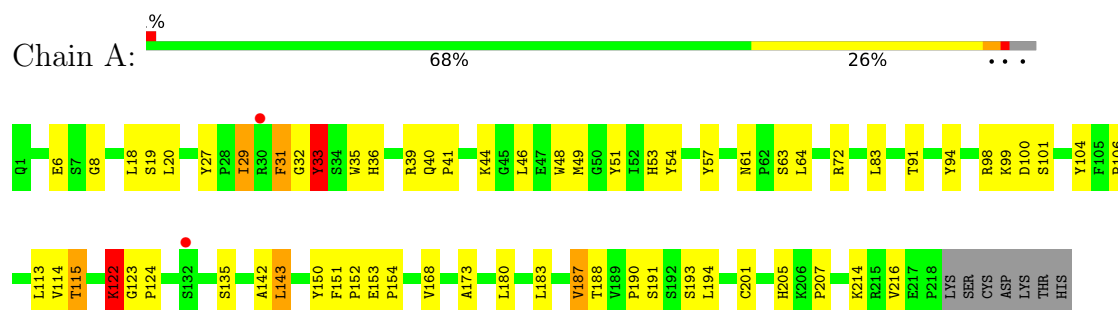
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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | J     | 211      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1635  | 1027 | 273 | 331 | 4 |         |         |       |
| 2   | L     | 211      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1635  | 1027 | 273 | 331 | 4 |         |         |       |
| 2   | N     | 211      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1635  | 1027 | 273 | 331 | 4 |         |         |       |
| 2   | P     | 211      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1635  | 1027 | 273 | 331 | 4 |         |         |       |
| 2   | R     | 213      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1648  | 1034 | 275 | 335 | 4 |         |         |       |
| 2   | T     | 211      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1635  | 1027 | 273 | 331 | 4 |         |         |       |

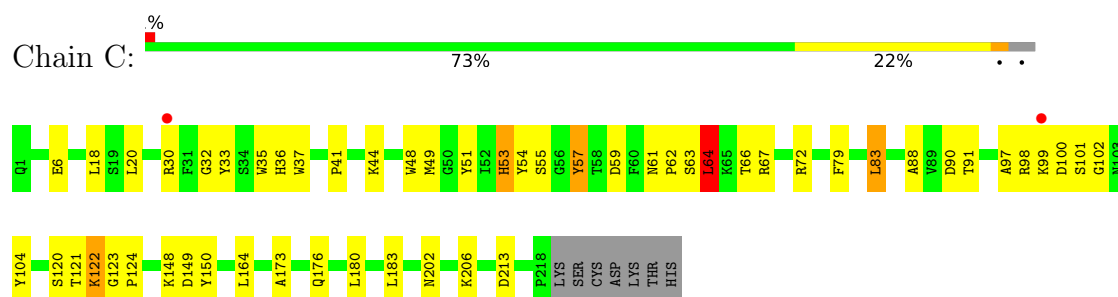
### 3 Residue-property plots

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

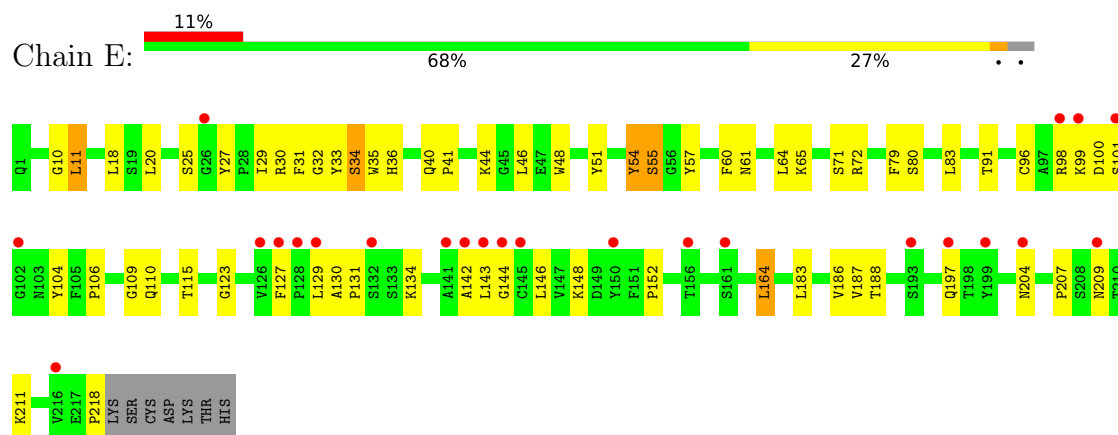
#### • Molecule 1: Fab C2E3 Heavy chain



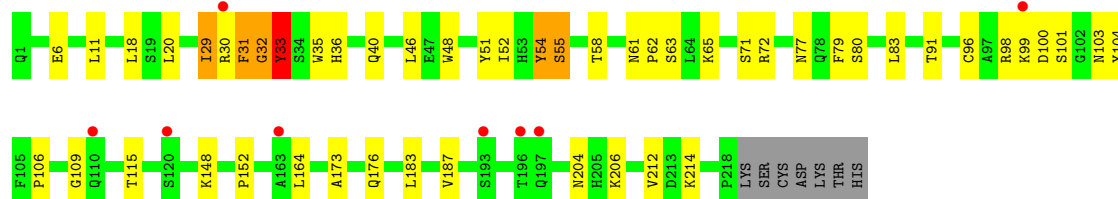
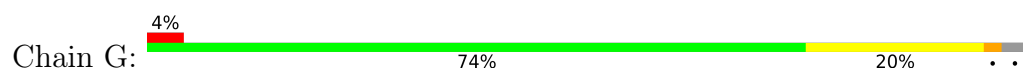
#### • Molecule 1: Fab C2E3 Heavy chain



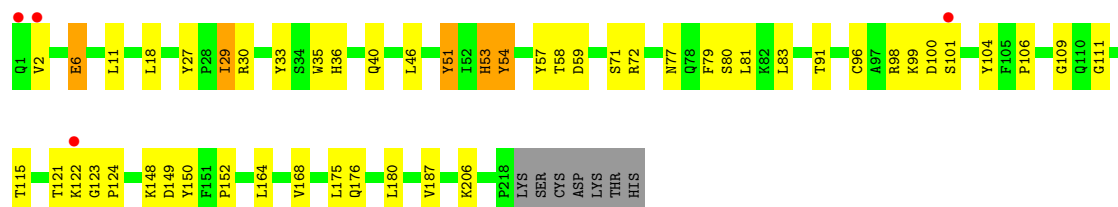
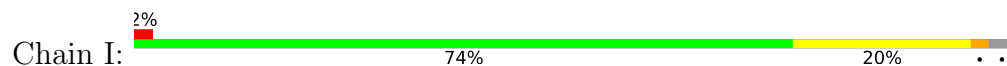
#### • Molecule 1: Fab C2E3 Heavy chain



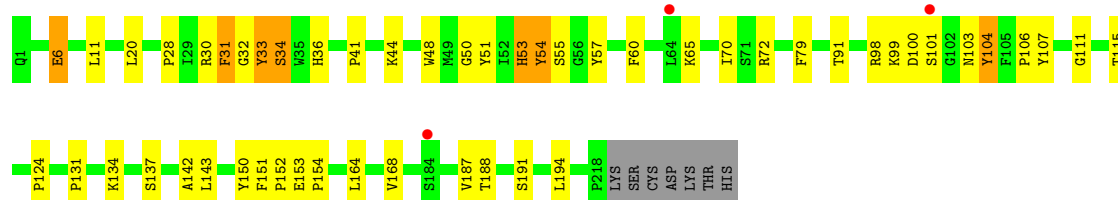
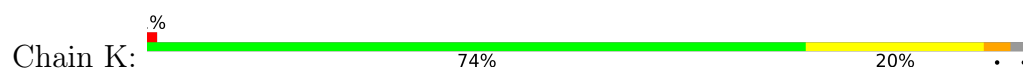
#### • Molecule 1: Fab C2E3 Heavy chain



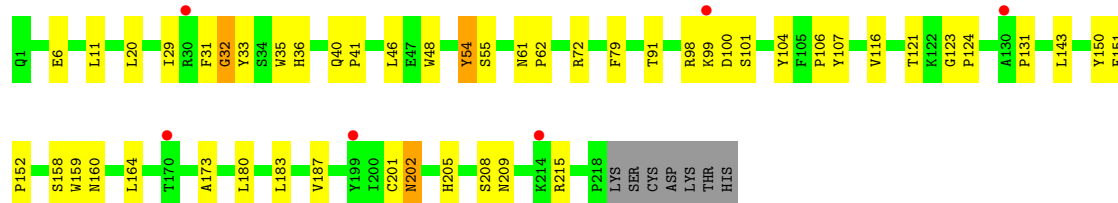
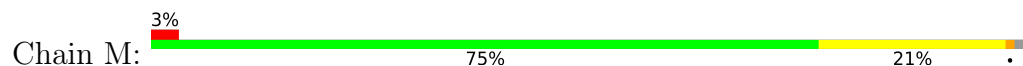
- Molecule 1: Fab C2E3 Heavy chain



- Molecule 1: Fab C2E3 Heavy chain

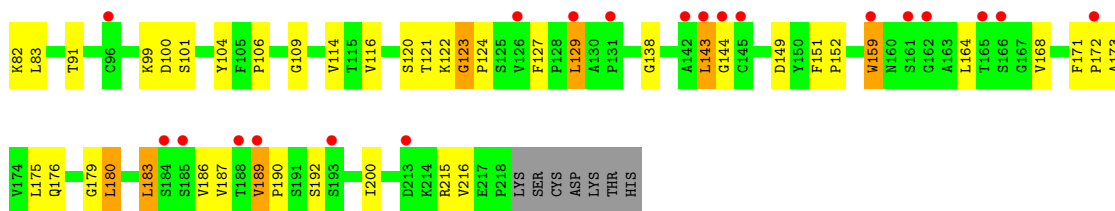


- Molecule 1: Fab C2E3 Heavy chain

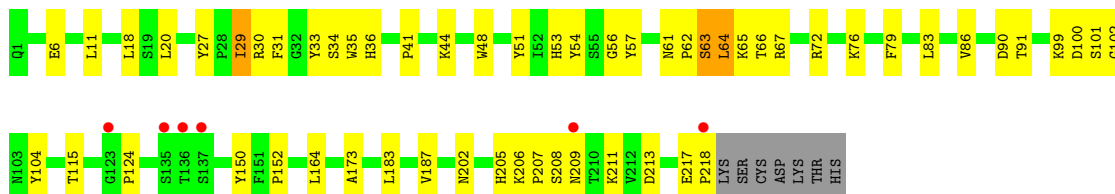
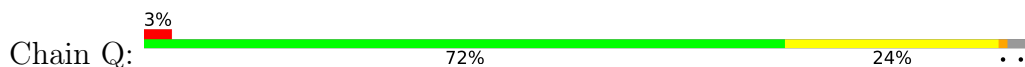


- Molecule 1: Fab C2E3 Heavy chain

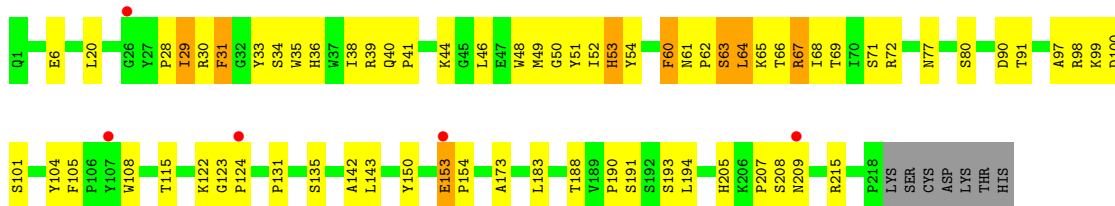




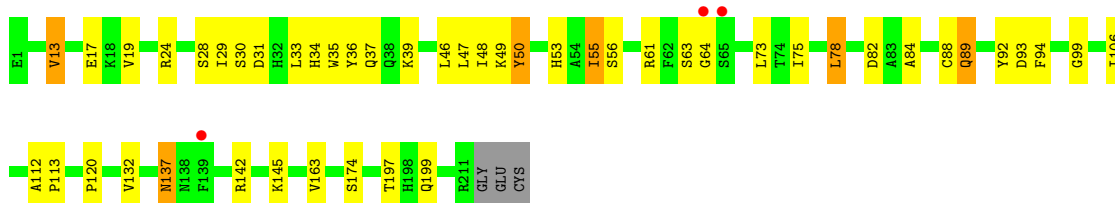
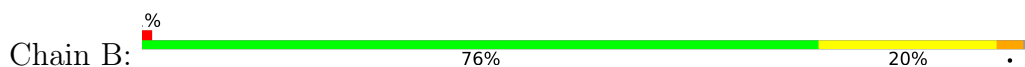
• Molecule 1: Fab C2E3 Heavy chain



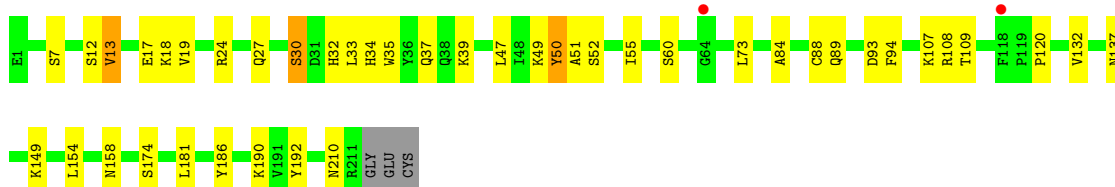
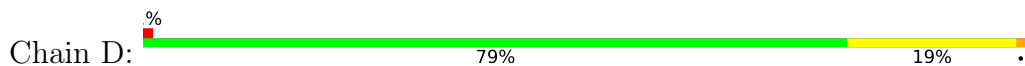
• Molecule 1: Fab C2E3 Heavy chain



• Molecule 2: Fab C2E3 Light chain

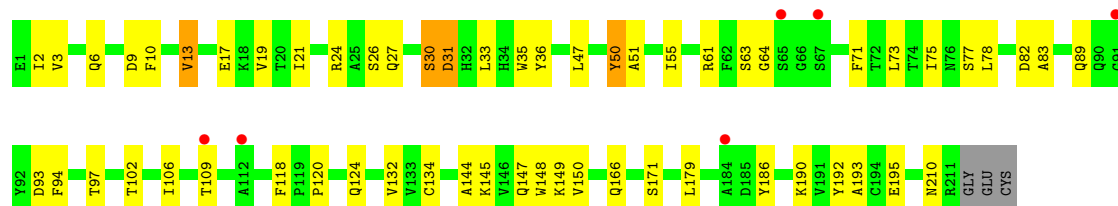


• Molecule 2: Fab C2E3 Light chain



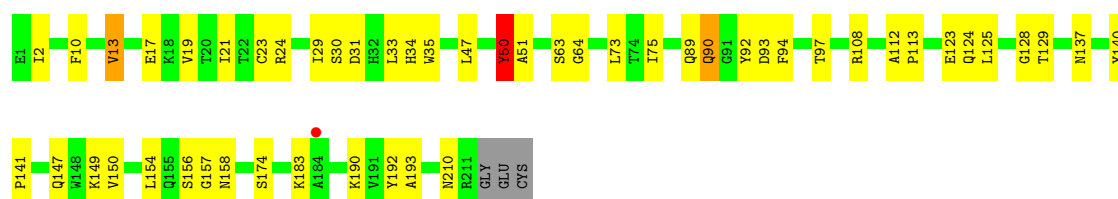
- Molecule 2: Fab C2E3 Light chain

Chain F: 



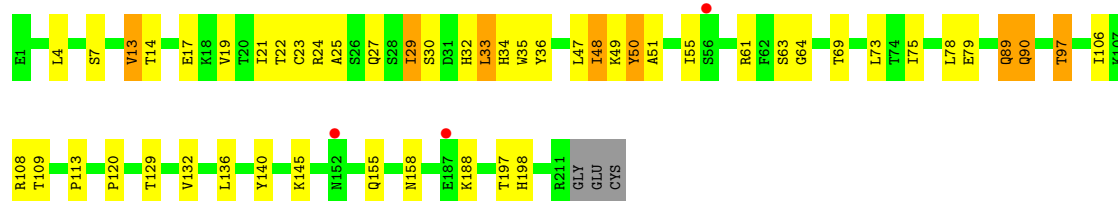
- Molecule 2: Fab C2E3 Light chain

Chain H: 



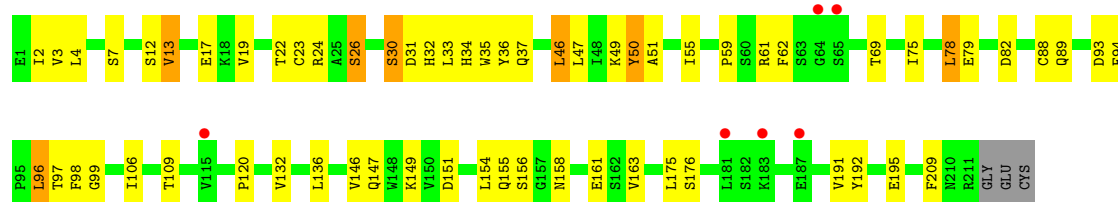
- Molecule 2: Fab C2E3 Light chain

Chain J: 



- Molecule 2: Fab C2E3 Light chain

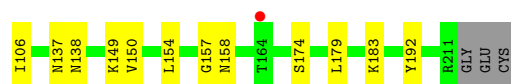
Chain L: 



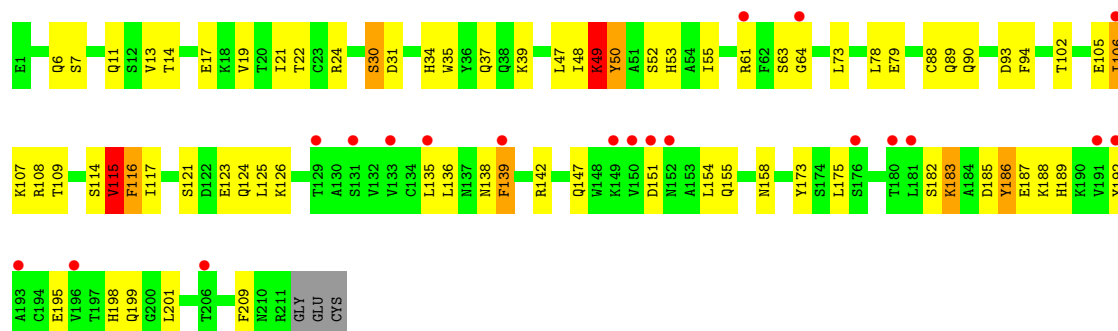
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Chain N: 

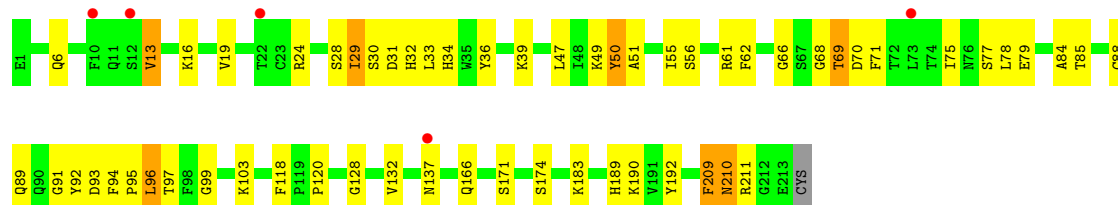
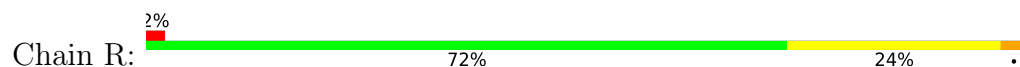




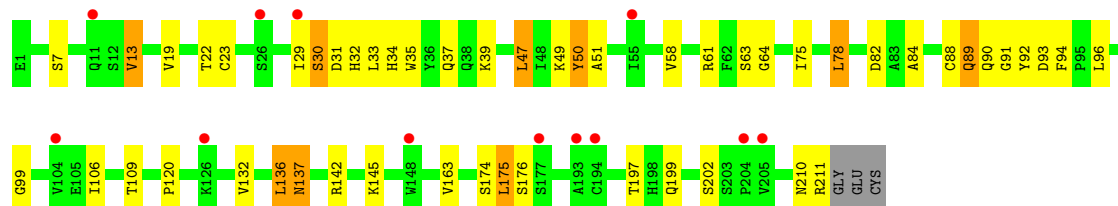
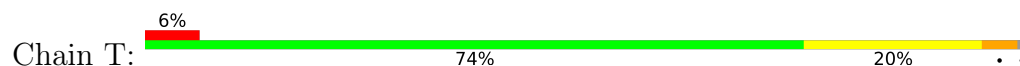
• Molecule 2: Fab C2E3 Light chain



• Molecule 2: Fab C2E3 Light chain



• Molecule 2: Fab C2E3 Light chain



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 2 21                                                   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 178.10Å 208.41Å 214.38Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 48.77 – 3.45<br>48.77 – 3.45                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.9 (48.77-3.45)<br>99.9 (48.77-3.45)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.39 (at 3.48Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (phenix.refine: 1.8.1_1168)                          | Depositor        |
| R, $R_{free}$                                                           | 0.236 , 0.280<br>0.241 , 0.284                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 5006 reflections (4.75%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 101.8                                                       | Xtriage          |
| Anisotropy                                                              | 0.392                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.29 , 119.3                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Estimated twinning fraction                                             | 0.000 for -h,l,k                                            | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                        | EDS              |
| Total number of atoms                                                   | 32933                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 153.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.59 % 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 1.5095e-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

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |         | Bond angles |                 |
|-----|-------|--------------|---------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5         |
| 1   | A     | 0.32         | 0/1705  | 0.78        | 2/2330 (0.1%)   |
| 1   | C     | 0.31         | 0/1705  | 0.79        | 3/2330 (0.1%)   |
| 1   | E     | 0.33         | 0/1705  | 0.81        | 2/2330 (0.1%)   |
| 1   | G     | 0.30         | 0/1705  | 0.76        | 1/2330 (0.0%)   |
| 1   | I     | 0.32         | 0/1705  | 0.80        | 3/2330 (0.1%)   |
| 1   | K     | 0.31         | 0/1705  | 0.76        | 1/2330 (0.0%)   |
| 1   | M     | 0.31         | 0/1705  | 0.81        | 4/2330 (0.2%)   |
| 1   | O     | 0.38         | 0/1705  | 0.85        | 3/2330 (0.1%)   |
| 1   | Q     | 0.31         | 0/1705  | 0.76        | 0/2330          |
| 1   | S     | 0.33         | 0/1705  | 0.79        | 1/2330 (0.0%)   |
| 2   | B     | 0.30         | 0/1672  | 0.74        | 0/2271          |
| 2   | D     | 0.29         | 0/1672  | 0.76        | 2/2271 (0.1%)   |
| 2   | F     | 0.28         | 0/1672  | 0.75        | 2/2271 (0.1%)   |
| 2   | H     | 0.28         | 0/1672  | 0.75        | 1/2271 (0.0%)   |
| 2   | J     | 0.29         | 0/1672  | 0.72        | 1/2271 (0.0%)   |
| 2   | L     | 0.30         | 0/1672  | 0.75        | 2/2271 (0.1%)   |
| 2   | N     | 0.27         | 0/1672  | 0.74        | 1/2271 (0.0%)   |
| 2   | P     | 0.36         | 0/1672  | 0.83        | 5/2271 (0.2%)   |
| 2   | R     | 0.31         | 0/1685  | 0.76        | 3/2288 (0.1%)   |
| 2   | T     | 0.28         | 0/1672  | 0.75        | 3/2271 (0.1%)   |
| All | All   | 0.31         | 0/33783 | 0.77        | 40/46027 (0.1%) |

There are no bond length outliers.

All (40) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | F     | 50  | TYR  | N-CA-C  | 9.39  | 124.68      | 113.23   |
| 2   | H     | 50  | TYR  | N-CA-C  | 8.72  | 123.22      | 112.58   |
| 2   | D     | 50  | TYR  | N-CA-C  | 8.64  | 123.77      | 113.23   |
| 2   | N     | 50  | TYR  | N-CA-C  | 8.07  | 122.57      | 112.24   |
| 1   | M     | 32  | GLY  | N-CA-C  | 7.87  | 125.20      | 111.50   |
| 1   | I     | 29  | ILE  | CB-CA-C | -7.83 | 101.94      | 111.97   |
| 2   | P     | 116 | PHE  | N-CA-C  | 7.42  | 121.03      | 109.52   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | M     | 123 | GLY  | CA-C-N  | 7.39  | 127.31      | 119.85   |
| 1   | M     | 123 | GLY  | C-N-CA  | 7.39  | 127.31      | 119.85   |
| 2   | J     | 50  | TYR  | N-CA-C  | 7.34  | 124.19      | 113.40   |
| 2   | R     | 118 | PHE  | CA-C-N  | 7.18  | 124.91      | 119.66   |
| 2   | R     | 118 | PHE  | C-N-CA  | 7.18  | 124.91      | 119.66   |
| 1   | G     | 32  | GLY  | N-CA-C  | 7.09  | 125.19      | 112.22   |
| 1   | O     | 29  | ILE  | CB-CA-C | -6.77 | 103.35      | 111.81   |
| 2   | L     | 50  | TYR  | N-CA-C  | 6.75  | 125.17      | 110.80   |
| 1   | K     | 32  | GLY  | N-CA-C  | 6.65  | 123.60      | 110.77   |
| 1   | I     | 123 | GLY  | CA-C-N  | 6.46  | 127.91      | 119.84   |
| 1   | I     | 123 | GLY  | C-N-CA  | 6.46  | 127.91      | 119.84   |
| 1   | C     | 97  | ALA  | N-CA-C  | 6.34  | 116.94      | 108.38   |
| 1   | E     | 123 | GLY  | CA-C-N  | 6.31  | 126.22      | 119.85   |
| 1   | E     | 123 | GLY  | C-N-CA  | 6.31  | 126.22      | 119.85   |
| 1   | O     | 123 | GLY  | CA-C-N  | 6.08  | 126.00      | 119.85   |
| 1   | O     | 123 | GLY  | C-N-CA  | 6.08  | 126.00      | 119.85   |
| 2   | R     | 50  | TYR  | N-CA-C  | 5.96  | 125.46      | 113.31   |
| 2   | T     | 50  | TYR  | N-CA-C  | 5.95  | 125.45      | 113.31   |
| 2   | P     | 49  | LYS  | N-CA-C  | -5.88 | 99.59       | 108.46   |
| 2   | T     | 30  | SER  | CB-CA-C | -5.84 | 109.82      | 116.54   |
| 2   | P     | 52  | SER  | N-CA-C  | 5.72  | 118.46      | 111.82   |
| 2   | T     | 137 | ASN  | N-CA-C  | 5.70  | 118.36      | 111.40   |
| 1   | S     | 97  | ALA  | N-CA-C  | 5.39  | 116.47      | 108.60   |
| 1   | A     | 122 | LYS  | N-CA-C  | -5.38 | 101.23      | 109.41   |
| 1   | A     | 29  | ILE  | CB-CA-C | -5.37 | 103.83      | 112.16   |
| 2   | P     | 115 | VAL  | N-CA-C  | 5.31  | 115.54      | 108.27   |
| 1   | C     | 32  | GLY  | N-CA-C  | 5.25  | 125.63      | 113.18   |
| 2   | D     | 30  | SER  | CB-CA-C | -5.19 | 110.57      | 116.54   |
| 2   | L     | 30  | SER  | CB-CA-C | -5.16 | 110.61      | 116.54   |
| 2   | F     | 30  | SER  | CB-CA-C | -5.13 | 110.67      | 116.63   |
| 1   | M     | 41  | PRO  | O-C-N   | 5.13  | 123.67      | 121.31   |
| 1   | C     | 64  | LEU  | N-CA-C  | -5.12 | 105.92      | 113.61   |
| 2   | P     | 30  | SER  | CB-CA-C | -5.04 | 110.74      | 116.54   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1657  | 0        | 1625     | 45      | 0            |
| 1   | C     | 1657  | 0        | 1625     | 33      | 0            |
| 1   | E     | 1657  | 0        | 1625     | 50      | 0            |
| 1   | G     | 1657  | 0        | 1625     | 37      | 0            |
| 1   | I     | 1657  | 0        | 1625     | 30      | 0            |
| 1   | K     | 1657  | 0        | 1625     | 42      | 0            |
| 1   | M     | 1657  | 0        | 1625     | 41      | 0            |
| 1   | O     | 1657  | 0        | 1629     | 61      | 0            |
| 1   | Q     | 1657  | 0        | 1625     | 44      | 0            |
| 1   | S     | 1657  | 0        | 1625     | 49      | 0            |
| 2   | B     | 1635  | 0        | 1587     | 31      | 0            |
| 2   | D     | 1635  | 0        | 1587     | 33      | 0            |
| 2   | F     | 1635  | 0        | 1587     | 43      | 0            |
| 2   | H     | 1635  | 0        | 1587     | 36      | 0            |
| 2   | J     | 1635  | 0        | 1587     | 39      | 0            |
| 2   | L     | 1635  | 0        | 1587     | 47      | 0            |
| 2   | N     | 1635  | 0        | 1587     | 34      | 0            |
| 2   | P     | 1635  | 0        | 1587     | 66      | 0            |
| 2   | R     | 1648  | 0        | 1596     | 46      | 0            |
| 2   | T     | 1635  | 0        | 1587     | 33      | 0            |
| All | All   | 32933 | 0        | 32133    | 785     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (785) 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:K:124:PRO:HB3  | 1:K:150:TYR:HB3 | 1.51                     | 0.93              |
| 1:E:36:HIS:HD2   | 1:E:48:TRP:HE1  | 1.17                     | 0.89              |
| 2:B:29:ILE:HA    | 2:B:92:TYR:HD2  | 1.37                     | 0.89              |
| 2:J:49:LYS:HE3   | 2:J:50:TYR:CE2  | 2.09                     | 0.88              |
| 2:H:29:ILE:HA    | 2:H:92:TYR:HD2  | 1.39                     | 0.86              |
| 1:E:36:HIS:CE1   | 1:E:99:LYS:HB2  | 2.13                     | 0.84              |
| 1:E:129:LEU:HD22 | 1:E:144:GLY:H   | 1.40                     | 0.84              |
| 2:T:90:GLN:HE22  | 2:T:96:LEU:HA   | 1.44                     | 0.83              |
| 1:E:27:TYR:HE2   | 1:E:32:GLY:HA3  | 1.45                     | 0.82              |
| 1:C:124:PRO:HB3  | 1:C:150:TYR:HB3 | 1.60                     | 0.82              |
| 1:K:36:HIS:CE1   | 1:K:99:LYS:HB2  | 2.15                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:36:HIS:NE2   | 1:I:99:LYS:HB2   | 1.96                     | 0.81              |
| 1:O:91:THR:HG22  | 1:O:116:VAL:H    | 1.45                     | 0.80              |
| 2:N:90:GLN:NE2   | 2:N:93:ASP:O     | 2.14                     | 0.80              |
| 2:F:120:PRO:HD3  | 2:F:132:VAL:HG22 | 1.63                     | 0.79              |
| 1:S:54:TYR:O     | 1:S:72:ARG:NH1   | 2.16                     | 0.78              |
| 2:J:49:LYS:HE3   | 2:J:50:TYR:CZ    | 2.19                     | 0.77              |
| 2:R:189:HIS:O    | 2:R:211:ARG:NH2  | 2.18                     | 0.77              |
| 1:C:61:ASN:ND2   | 1:C:62:PRO:O     | 2.18                     | 0.76              |
| 2:P:61:ARG:NH1   | 2:P:79:GLU:OE1   | 2.18                     | 0.76              |
| 2:R:30:SER:N     | 2:R:68:GLY:O     | 2.19                     | 0.76              |
| 2:P:14:THR:HA    | 2:P:107:LYS:HG3  | 1.66                     | 0.75              |
| 1:I:164:LEU:HD21 | 1:I:187:VAL:HG21 | 1.69                     | 0.75              |
| 2:L:136:LEU:HD12 | 2:L:175:LEU:HB3  | 1.69                     | 0.75              |
| 2:B:30:SER:OG    | 2:B:31:ASP:N     | 2.18                     | 0.74              |
| 2:L:163:VAL:HG22 | 2:L:175:LEU:HG   | 1.69                     | 0.74              |
| 1:C:51:TYR:HE1   | 1:C:59:ASP:HB3   | 1.53                     | 0.74              |
| 1:I:124:PRO:HB3  | 1:I:150:TYR:HB3  | 1.68                     | 0.74              |
| 1:M:36:HIS:NE2   | 1:M:99:LYS:HB2   | 2.03                     | 0.74              |
| 2:F:6:GLN:HE21   | 2:F:102:THR:HG23 | 1.53                     | 0.74              |
| 1:M:91:THR:HG22  | 1:M:116:VAL:H    | 1.52                     | 0.73              |
| 1:O:36:HIS:NE2   | 1:O:99:LYS:HB2   | 2.03                     | 0.73              |
| 1:Q:36:HIS:NE2   | 1:Q:99:LYS:HB2   | 2.03                     | 0.73              |
| 2:T:37:GLN:HB2   | 2:T:47:LEU:HD21  | 1.70                     | 0.73              |
| 1:G:33:TYR:O     | 1:G:35:TRP:NE1   | 2.22                     | 0.73              |
| 2:P:6:GLN:HE21   | 2:P:102:THR:HG23 | 1.52                     | 0.73              |
| 1:Q:67:ARG:NH2   | 1:Q:90:ASP:OD2   | 2.21                     | 0.72              |
| 2:P:30:SER:OG    | 2:P:31:ASP:N     | 2.21                     | 0.72              |
| 1:A:36:HIS:NE2   | 1:A:99:LYS:HB2   | 2.04                     | 0.72              |
| 1:K:164:LEU:HD21 | 1:K:187:VAL:HG21 | 1.71                     | 0.71              |
| 1:G:36:HIS:NE2   | 1:G:99:LYS:HB2   | 2.06                     | 0.71              |
| 1:M:208:SER:O    | 1:S:215:ARG:NH1  | 2.24                     | 0.71              |
| 1:S:41:PRO:HG2   | 1:S:44:LYS:HB2   | 1.73                     | 0.71              |
| 2:L:161:GLU:HB3  | 2:L:175:LEU:HD21 | 1.73                     | 0.71              |
| 1:C:67:ARG:NH1   | 1:C:90:ASP:OD2   | 2.22                     | 0.71              |
| 1:G:29:ILE:HG22  | 1:G:35:TRP:CE2   | 2.25                     | 0.70              |
| 1:A:41:PRO:HG2   | 1:A:44:LYS:HB2   | 1.73                     | 0.70              |
| 2:H:30:SER:OG    | 2:H:31:ASP:N     | 2.25                     | 0.70              |
| 2:L:30:SER:OG    | 2:L:31:ASP:N     | 2.24                     | 0.70              |
| 1:K:36:HIS:HD2   | 1:K:48:TRP:HE1   | 1.39                     | 0.70              |
| 1:O:33:TYR:HD1   | 1:O:33:TYR:H     | 1.39                     | 0.70              |
| 2:P:151:ASP:OD2  | 2:P:189:HIS:ND1  | 2.25                     | 0.70              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:L:36:TYR:HE2  | 2:L:89:GLN:HG2   | 1.56                     | 0.70              |
| 1:E:36:HIS:CD2  | 1:E:48:TRP:HE1   | 2.05                     | 0.70              |
| 2:H:29:ILE:HA   | 2:H:92:TYR:CD2   | 2.24                     | 0.69              |
| 2:F:30:SER:OG   | 2:F:31:ASP:N     | 2.24                     | 0.69              |
| 1:S:36:HIS:HE2  | 1:S:99:LYS:HB2   | 1.58                     | 0.68              |
| 2:R:120:PRO:HD3 | 2:R:132:VAL:HG22 | 1.75                     | 0.68              |
| 1:A:40:GLN:HB2  | 1:A:46:LEU:HD23  | 1.76                     | 0.68              |
| 1:A:33:TYR:O    | 1:A:35:TRP:NE1   | 2.27                     | 0.68              |
| 1:C:36:HIS:NE2  | 1:C:99:LYS:HB2   | 2.09                     | 0.68              |
| 1:S:36:HIS:NE2  | 1:S:99:LYS:HB2   | 2.09                     | 0.68              |
| 1:S:40:GLN:HB2  | 1:S:46:LEU:HD23  | 1.75                     | 0.68              |
| 2:R:32:HIS:HB2  | 2:R:91:GLY:O     | 1.94                     | 0.68              |
| 1:E:34:SER:HB2  | 1:E:36:HIS:HE1   | 1.58                     | 0.67              |
| 2:F:21:ILE:HD12 | 2:F:73:LEU:HD23  | 1.75                     | 0.67              |
| 2:N:36:TYR:HE1  | 2:N:89:GLN:HG2   | 1.59                     | 0.67              |
| 1:K:36:HIS:CD2  | 1:K:48:TRP:HE1   | 2.12                     | 0.67              |
| 2:P:21:ILE:HD12 | 2:P:73:LEU:HD23  | 1.76                     | 0.67              |
| 1:O:22:CYS:HB3  | 1:O:79:PHE:HB2   | 1.77                     | 0.66              |
| 1:Q:61:ASN:O    | 1:Q:65:LYS:HG3   | 1.95                     | 0.66              |
| 2:P:155:GLN:OE1 | 2:P:158:ASN:ND2  | 2.29                     | 0.66              |
| 1:E:40:GLN:HB2  | 1:E:46:LEU:HD13  | 1.78                     | 0.66              |
| 1:K:48:TRP:HZ2  | 1:K:51:TYR:HD2   | 1.43                     | 0.66              |
| 1:O:53:HIS:HE1  | 1:O:54:TYR:CE2   | 2.13                     | 0.66              |
| 2:R:137:ASN:O   | 2:R:174:SER:OG   | 2.14                     | 0.66              |
| 1:G:103:ASN:O   | 2:H:89:GLN:NE2   | 2.29                     | 0.66              |
| 2:R:28:SER:HA   | 2:R:69:THR:OG1   | 1.96                     | 0.66              |
| 2:B:46:LEU:HG   | 2:B:55:ILE:HG13  | 1.77                     | 0.65              |
| 1:E:32:GLY:H    | 1:E:54:TYR:HD2   | 1.44                     | 0.65              |
| 1:O:120:SER:OG  | 1:O:121:THR:N    | 2.29                     | 0.65              |
| 1:G:91:THR:HG23 | 1:G:115:THR:HA   | 1.78                     | 0.65              |
| 1:S:39:ARG:HD3  | 1:S:49:MET:HE3   | 1.77                     | 0.65              |
| 1:G:98:ARG:NH1  | 1:G:100:ASP:OD2  | 2.30                     | 0.65              |
| 1:M:54:TYR:HD1  | 1:M:55:SER:N     | 1.95                     | 0.65              |
| 2:N:24:ARG:NH2  | 2:P:17:GLU:OE2   | 2.29                     | 0.64              |
| 1:O:8:GLY:HA3   | 1:O:20:LEU:HD23  | 1.78                     | 0.64              |
| 1:O:149:ASP:HA  | 1:O:180:LEU:HB3  | 1.79                     | 0.64              |
| 2:L:93:ASP:OD1  | 2:L:94:PHE:N     | 2.30                     | 0.64              |
| 1:M:29:ILE:HG22 | 1:M:35:TRP:CE2   | 2.32                     | 0.64              |
| 2:R:192:TYR:HB2 | 2:R:209:PHE:CE1  | 2.33                     | 0.64              |
| 1:S:64:LEU:HD22 | 1:S:67:ARG:HH21  | 1.63                     | 0.64              |
| 1:G:48:TRP:HZ2  | 1:G:51:TYR:HD2   | 1.44                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:192:TYR:HB2  | 2:R:209:PHE:HE1  | 1.61                     | 0.64              |
| 1:G:40:GLN:HB2   | 1:G:46:LEU:HD23  | 1.80                     | 0.64              |
| 1:S:124:PRO:HB3  | 1:S:150:TYR:HB3  | 1.78                     | 0.64              |
| 1:E:144:GLY:HA3  | 1:E:186:VAL:HA   | 1.79                     | 0.64              |
| 2:B:17:GLU:OE2   | 2:J:24:ARG:NH2   | 2.30                     | 0.64              |
| 1:I:91:THR:HG23  | 1:I:115:THR:HA   | 1.79                     | 0.64              |
| 2:H:24:ARG:NH2   | 2:L:17:GLU:OE2   | 2.31                     | 0.64              |
| 1:G:204:ASN:HD21 | 1:G:206:LYS:HE2  | 1.63                     | 0.63              |
| 1:C:104:TYR:CE2  | 2:D:49:LYS:HD3   | 2.33                     | 0.63              |
| 1:M:160:ASN:HD22 | 1:M:164:LEU:HD13 | 1.63                     | 0.63              |
| 1:M:159:TRP:HZ3  | 1:M:187:VAL:HB   | 1.64                     | 0.63              |
| 1:O:36:HIS:HE2   | 1:O:99:LYS:HB2   | 1.62                     | 0.63              |
| 2:J:21:ILE:HD12  | 2:J:73:LEU:HD23  | 1.81                     | 0.63              |
| 1:Q:30:ARG:HA    | 1:Q:54:TYR:HB2   | 1.80                     | 0.63              |
| 1:G:61:ASN:OD1   | 1:G:63:SER:OG    | 2.14                     | 0.62              |
| 1:M:33:TYR:O     | 1:M:35:TRP:NE1   | 2.31                     | 0.62              |
| 2:F:61:ARG:NH2   | 2:F:82:ASP:OD1   | 2.27                     | 0.62              |
| 1:O:33:TYR:N     | 1:O:33:TYR:CD1   | 2.67                     | 0.62              |
| 1:I:51:TYR:HE1   | 1:I:59:ASP:HB3   | 1.64                     | 0.62              |
| 1:K:36:HIS:HE1   | 1:K:99:LYS:HB2   | 1.61                     | 0.62              |
| 1:A:98:ARG:HH21  | 1:A:106:PRO:HG3  | 1.65                     | 0.62              |
| 1:S:29:ILE:HG13  | 1:S:77:ASN:OD1   | 2.00                     | 0.62              |
| 2:H:17:GLU:OE2   | 2:L:24:ARG:NH2   | 2.31                     | 0.62              |
| 2:J:120:PRO:HD3  | 2:J:132:VAL:HG22 | 1.81                     | 0.62              |
| 2:P:115:VAL:HG12 | 2:P:136:LEU:HA   | 1.82                     | 0.62              |
| 1:A:91:THR:HG23  | 1:A:115:THR:HA   | 1.82                     | 0.62              |
| 1:M:40:GLN:HB3   | 1:M:46:LEU:HD23  | 1.81                     | 0.62              |
| 1:O:27:TYR:OH    | 1:O:32:GLY:HA3   | 1.99                     | 0.62              |
| 2:F:50:TYR:N     | 2:F:51:ALA:HA    | 2.15                     | 0.62              |
| 1:S:29:ILE:O     | 1:S:54:TYR:HB3   | 2.01                     | 0.61              |
| 1:S:67:ARG:NH1   | 1:S:90:ASP:OD2   | 2.29                     | 0.61              |
| 2:B:36:TYR:HE1   | 2:B:89:GLN:HG2   | 1.65                     | 0.61              |
| 1:E:29:ILE:HG22  | 1:E:35:TRP:CE2   | 2.35                     | 0.61              |
| 2:D:17:GLU:OE2   | 2:F:24:ARG:NH2   | 2.32                     | 0.61              |
| 2:L:61:ARG:NH1   | 2:L:82:ASP:OD2   | 2.33                     | 0.61              |
| 2:R:50:TYR:N     | 2:R:51:ALA:HA    | 2.15                     | 0.61              |
| 1:S:33:TYR:O     | 1:S:35:TRP:NE1   | 2.33                     | 0.61              |
| 2:F:148:TRP:CD2  | 2:F:179:LEU:HD23 | 2.36                     | 0.61              |
| 1:O:41:PRO:HB2   | 1:O:44:LYS:HE2   | 1.83                     | 0.61              |
| 2:H:50:TYR:N     | 2:H:51:ALA:HA    | 2.16                     | 0.61              |
| 1:A:124:PRO:HB3  | 1:A:150:TYR:HB3  | 1.82                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:159:TRP:HZ3  | 1:O:164:LEU:HD13 | 1.66                     | 0.61              |
| 2:B:29:ILE:HA    | 2:B:92:TYR:CD2   | 2.26                     | 0.60              |
| 1:O:48:TRP:HZ2   | 1:O:51:TYR:HD2   | 1.48                     | 0.60              |
| 2:L:50:TYR:N     | 2:L:51:ALA:HA    | 2.15                     | 0.60              |
| 2:L:147:GLN:HB3  | 2:L:195:GLU:HB3  | 1.83                     | 0.60              |
| 1:S:29:ILE:HD12  | 1:S:30:ARG:H     | 1.65                     | 0.60              |
| 2:F:3:VAL:N      | 2:F:26:SER:OG    | 2.27                     | 0.60              |
| 1:G:54:TYR:HD1   | 1:G:55:SER:N     | 1.98                     | 0.60              |
| 2:D:120:PRO:HD3  | 2:D:132:VAL:HG22 | 1.84                     | 0.60              |
| 2:L:120:PRO:HD3  | 2:L:132:VAL:HG22 | 1.84                     | 0.60              |
| 2:P:106:ILE:HD12 | 2:P:106:ILE:H    | 1.66                     | 0.60              |
| 2:P:107:LYS:HD3  | 2:P:109:THR:HB   | 1.84                     | 0.60              |
| 2:P:125:LEU:HG   | 2:P:183:LYS:HD3  | 1.84                     | 0.59              |
| 1:E:61:ASN:HD22  | 1:E:64:LEU:HD23  | 1.66                     | 0.59              |
| 1:M:124:PRO:HB3  | 1:M:150:TYR:HB3  | 1.85                     | 0.59              |
| 1:M:159:TRP:CZ3  | 1:M:187:VAL:HB   | 2.37                     | 0.59              |
| 2:P:105:GLU:HG3  | 2:P:106:ILE:H    | 1.66                     | 0.59              |
| 2:R:30:SER:OG    | 2:R:31:ASP:N     | 2.35                     | 0.59              |
| 2:B:24:ARG:NH2   | 2:J:17:GLU:OE2   | 2.35                     | 0.59              |
| 1:M:215:ARG:NH2  | 1:S:209:ASN:H    | 1.98                     | 0.59              |
| 2:P:34:HIS:HE1   | 2:P:50:TYR:HD2   | 1.49                     | 0.59              |
| 2:H:137:ASN:O    | 2:H:174:SER:OG   | 2.11                     | 0.59              |
| 1:C:104:TYR:CZ   | 2:D:49:LYS:HD3   | 2.37                     | 0.59              |
| 2:L:3:VAL:N      | 2:L:26:SER:OG    | 2.31                     | 0.59              |
| 2:F:190:LYS:HE3  | 2:F:210:ASN:HB3  | 1.85                     | 0.59              |
| 2:T:50:TYR:N     | 2:T:51:ALA:HA    | 2.18                     | 0.59              |
| 1:O:60:PHE:HB2   | 1:O:65:LYS:HG3   | 1.83                     | 0.59              |
| 1:I:36:HIS:HE2   | 1:I:99:LYS:HB2   | 1.67                     | 0.58              |
| 2:T:120:PRO:HD3  | 2:T:132:VAL:HG22 | 1.86                     | 0.58              |
| 1:I:149:ASP:HA   | 1:I:180:LEU:HB3  | 1.85                     | 0.58              |
| 2:P:105:GLU:HG3  | 2:P:106:ILE:HD12 | 1.84                     | 0.58              |
| 1:S:91:THR:HG23  | 1:S:115:THR:HA   | 1.85                     | 0.58              |
| 1:O:54:TYR:O     | 1:O:72:ARG:NH2   | 2.34                     | 0.58              |
| 1:C:62:PRO:O     | 1:C:63:SER:OG    | 2.21                     | 0.58              |
| 2:D:137:ASN:O    | 2:D:174:SER:OG   | 2.17                     | 0.58              |
| 1:O:173:ALA:HA   | 1:O:183:LEU:HD13 | 1.85                     | 0.58              |
| 2:P:11:GLN:O     | 2:P:105:GLU:N    | 2.31                     | 0.58              |
| 1:E:11:LEU:HB3   | 1:E:152:PRO:HG3  | 1.86                     | 0.58              |
| 2:J:19:VAL:HB    | 2:J:75:ILE:HB    | 1.84                     | 0.58              |
| 1:K:11:LEU:HB2   | 1:K:152:PRO:HG3  | 1.86                     | 0.58              |
| 2:R:36:TYR:OH    | 2:R:89:GLN:NE2   | 2.36                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:91:THR:HG23  | 1:K:115:THR:HA   | 1.85                     | 0.57              |
| 1:O:40:GLN:HB2   | 1:O:46:LEU:HD23  | 1.86                     | 0.57              |
| 1:Q:61:ASN:OD1   | 1:Q:63:SER:OG    | 2.21                     | 0.57              |
| 2:D:50:TYR:N     | 2:D:51:ALA:HA    | 2.20                     | 0.57              |
| 2:N:30:SER:OG    | 2:N:31:ASP:N     | 2.35                     | 0.57              |
| 1:S:67:ARG:NH2   | 1:S:90:ASP:OD1   | 2.34                     | 0.57              |
| 1:S:100:ASP:OD1  | 1:S:101:SER:N    | 2.35                     | 0.57              |
| 2:N:137:ASN:OD1  | 2:N:138:ASN:ND2  | 2.29                     | 0.57              |
| 1:Q:29:ILE:HD12  | 1:Q:30:ARG:H     | 1.69                     | 0.57              |
| 1:C:202:ASN:ND2  | 1:C:213:ASP:OD2  | 2.37                     | 0.57              |
| 1:G:164:LEU:HD21 | 1:G:187:VAL:HG21 | 1.87                     | 0.57              |
| 1:S:123:GLY:H    | 1:S:124:PRO:HD3  | 1.70                     | 0.57              |
| 1:S:205:HIS:ND1  | 1:S:208:SER:OG   | 2.36                     | 0.57              |
| 2:J:78:LEU:HD11  | 2:J:106:ILE:HG12 | 1.87                     | 0.57              |
| 2:N:50:TYR:N     | 2:N:51:ALA:HA    | 2.20                     | 0.57              |
| 2:P:198:HIS:H    | 2:P:201:LEU:HD11 | 1.70                     | 0.57              |
| 1:Q:91:THR:HG23  | 1:Q:115:THR:HA   | 1.87                     | 0.57              |
| 2:T:34:HIS:HD2   | 2:T:89:GLN:HE21  | 1.52                     | 0.57              |
| 2:J:50:TYR:N     | 2:J:51:ALA:HA    | 2.20                     | 0.57              |
| 2:L:49:LYS:HG2   | 2:L:50:TYR:HD2   | 1.69                     | 0.57              |
| 1:O:81:LEU:HD12  | 1:O:82:LYS:N     | 2.20                     | 0.57              |
| 1:S:30:ARG:HA    | 1:S:54:TYR:HB2   | 1.87                     | 0.56              |
| 1:E:48:TRP:HZ2   | 1:E:51:TYR:HD2   | 1.54                     | 0.56              |
| 1:I:40:GLN:HB2   | 1:I:46:LEU:HD23  | 1.87                     | 0.56              |
| 1:O:53:HIS:CE1   | 1:O:54:TYR:CE2   | 2.94                     | 0.56              |
| 1:Q:100:ASP:OD1  | 1:Q:101:SER:N    | 2.34                     | 0.56              |
| 2:F:13:VAL:HB    | 2:F:78:LEU:HD22  | 1.86                     | 0.56              |
| 1:M:33:TYR:CD1   | 1:M:98:ARG:HD2   | 2.41                     | 0.56              |
| 1:Q:164:LEU:HD21 | 1:Q:187:VAL:HG21 | 1.86                     | 0.56              |
| 2:R:190:LYS:HE2  | 2:R:210:ASN:HB3  | 1.87                     | 0.56              |
| 2:F:19:VAL:HB    | 2:F:75:ILE:HB    | 1.88                     | 0.56              |
| 2:T:136:LEU:HD11 | 2:T:175:LEU:HB3  | 1.86                     | 0.56              |
| 1:A:36:HIS:HE2   | 1:A:99:LYS:HB2   | 1.69                     | 0.56              |
| 2:J:33:LEU:HB3   | 2:J:51:ALA:HB2   | 1.86                     | 0.56              |
| 1:Q:54:TYR:O     | 1:Q:72:ARG:NH1   | 2.38                     | 0.56              |
| 1:C:100:ASP:OD1  | 1:C:101:SER:N    | 2.38                     | 0.56              |
| 1:C:120:SER:OG   | 1:C:121:THR:N    | 2.34                     | 0.56              |
| 2:B:88:CYS:O     | 2:B:99:GLY:N     | 2.38                     | 0.56              |
| 2:B:93:ASP:OD1   | 2:B:94:PHE:N     | 2.38                     | 0.56              |
| 1:Q:36:HIS:HE2   | 1:Q:99:LYS:HB2   | 1.69                     | 0.56              |
| 2:B:36:TYR:CE1   | 2:B:89:GLN:HG2   | 2.41                     | 0.55              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:61:ASN:ND2  | 1:A:63:SER:OG    | 2.39                     | 0.55              |
| 1:A:100:ASP:OD1 | 1:A:101:SER:N    | 2.37                     | 0.55              |
| 1:C:148:LYS:NZ  | 1:C:176:GLN:OE1  | 2.34                     | 0.55              |
| 1:E:98:ARG:HG2  | 1:E:100:ASP:H    | 1.71                     | 0.55              |
| 2:T:137:ASN:O   | 2:T:174:SER:OG   | 2.22                     | 0.55              |
| 2:T:30:SER:OG   | 2:T:31:ASP:N     | 2.39                     | 0.55              |
| 2:B:61:ARG:NH2  | 2:B:82:ASP:OD1   | 2.40                     | 0.55              |
| 2:J:4:LEU:HD21  | 2:J:90:GLN:HG3   | 1.87                     | 0.55              |
| 2:N:19:VAL:HB   | 2:N:75:ILE:HB    | 1.89                     | 0.55              |
| 2:P:6:GLN:NE2   | 2:P:102:THR:HG23 | 2.21                     | 0.55              |
| 2:R:16:LYS:HA   | 2:R:77:SER:HB2   | 1.89                     | 0.55              |
| 1:E:36:HIS:HE1  | 1:E:99:LYS:HB2   | 1.70                     | 0.55              |
| 1:K:53:HIS:HD2  | 1:K:57:TYR:CE2   | 2.24                     | 0.55              |
| 1:K:98:ARG:HH21 | 1:K:107:TYR:HE2  | 1.54                     | 0.55              |
| 2:R:93:ASP:OD1  | 2:R:94:PHE:N     | 2.40                     | 0.55              |
| 1:S:29:ILE:HD12 | 1:S:30:ARG:N     | 2.21                     | 0.55              |
| 2:T:47:LEU:HA   | 2:T:58:VAL:HG11  | 1.88                     | 0.55              |
| 2:B:19:VAL:HB   | 2:B:75:ILE:HB    | 1.88                     | 0.55              |
| 1:E:131:PRO:HG2 | 1:E:218:PRO:HG3  | 1.89                     | 0.55              |
| 1:A:54:TYR:O    | 1:A:72:ARG:NH1   | 2.33                     | 0.55              |
| 2:P:7:SER:HG    | 2:P:22:THR:HG1   | 1.48                     | 0.55              |
| 1:A:123:GLY:H   | 1:A:124:PRO:HD3  | 1.72                     | 0.54              |
| 2:D:190:LYS:HE3 | 2:D:210:ASN:HB3  | 1.87                     | 0.54              |
| 2:P:114:SER:H   | 2:P:138:ASN:HB2  | 1.70                     | 0.54              |
| 1:Q:202:ASN:ND2 | 1:Q:213:ASP:OD2  | 2.40                     | 0.54              |
| 1:G:214:LYS:NZ  | 2:H:123:GLU:OE1  | 2.39                     | 0.54              |
| 1:S:50:GLY:HA3  | 1:S:60:PHE:HA    | 1.88                     | 0.54              |
| 1:E:18:LEU:HB3  | 1:E:83:LEU:HB3   | 1.89                     | 0.54              |
| 1:E:33:TYR:O    | 1:E:35:TRP:NE1   | 2.41                     | 0.54              |
| 1:S:153:GLU:HG2 | 1:S:154:PRO:HA   | 1.89                     | 0.54              |
| 1:K:34:SER:HB2  | 1:K:36:HIS:HE1   | 1.73                     | 0.54              |
| 1:O:28:PRO:HG2  | 1:O:31:PHE:HD2   | 1.71                     | 0.54              |
| 1:S:48:TRP:CE3  | 1:S:61:ASN:HB2   | 2.42                     | 0.54              |
| 1:M:152:PRO:O   | 1:M:205:HIS:NE2  | 2.41                     | 0.54              |
| 2:B:120:PRO:HD3 | 2:B:132:VAL:HG22 | 1.89                     | 0.54              |
| 2:L:89:GLN:HB3  | 2:L:98:PHE:CD1   | 2.43                     | 0.54              |
| 1:O:32:GLY:O    | 1:O:54:TYR:CD2   | 2.61                     | 0.54              |
| 1:C:37:TRP:HB3  | 1:C:49:MET:HE3   | 1.89                     | 0.53              |
| 2:N:46:LEU:HG   | 2:N:55:ILE:HG13  | 1.90                     | 0.53              |
| 2:B:55:ILE:O    | 2:B:56:SER:HB3   | 2.08                     | 0.53              |
| 2:D:37:GLN:HB2  | 2:D:47:LEU:HD11  | 1.88                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:4:LEU:HD21   | 2:N:90:GLN:HB3   | 1.90                     | 0.53              |
| 1:Q:33:TYR:O     | 1:Q:35:TRP:NE1   | 2.41                     | 0.53              |
| 2:H:19:VAL:HB    | 2:H:75:ILE:HB    | 1.90                     | 0.53              |
| 2:T:136:LEU:HD11 | 2:T:175:LEU:HD22 | 1.90                     | 0.53              |
| 1:A:180:LEU:HD21 | 1:G:30:ARG:HD2   | 1.89                     | 0.53              |
| 1:E:72:ARG:HA    | 1:E:79:PHE:HA    | 1.90                     | 0.53              |
| 2:P:192:TYR:HB2  | 2:P:209:PHE:HE1  | 1.72                     | 0.53              |
| 2:P:139:PHE:HB3  | 2:P:173:TYR:HB2  | 1.88                     | 0.53              |
| 2:D:33:LEU:HB3   | 2:D:51:ALA:HB2   | 1.90                     | 0.53              |
| 1:O:4:LEU:HD22   | 1:O:109:GLY:HA3  | 1.89                     | 0.53              |
| 1:A:142:ALA:HB2  | 1:A:188:THR:HG22 | 1.91                     | 0.53              |
| 1:I:33:TYR:HB2   | 1:I:98:ARG:HD2   | 1.90                     | 0.53              |
| 2:P:14:THR:HG22  | 2:P:107:LYS:HE3  | 1.90                     | 0.53              |
| 2:T:136:LEU:CD1  | 2:T:175:LEU:HB3  | 2.39                     | 0.53              |
| 2:F:6:GLN:NE2    | 2:F:102:THR:HG23 | 2.21                     | 0.53              |
| 1:M:54:TYR:O     | 1:M:72:ARG:NH1   | 2.41                     | 0.53              |
| 1:M:61:ASN:ND2   | 1:M:62:PRO:O     | 2.41                     | 0.53              |
| 1:C:41:PRO:HB2   | 1:C:44:LYS:HB2   | 1.90                     | 0.52              |
| 2:H:93:ASP:OD1   | 2:H:94:PHE:N     | 2.41                     | 0.52              |
| 2:P:50:TYR:N     | 2:P:50:TYR:CD1   | 2.77                     | 0.52              |
| 1:M:215:ARG:HH22 | 1:S:209:ASN:H    | 1.58                     | 0.52              |
| 2:B:137:ASN:O    | 2:B:174:SER:OG   | 2.22                     | 0.52              |
| 1:I:96:CYS:O     | 1:I:109:GLY:N    | 2.43                     | 0.52              |
| 1:A:98:ARG:HH21  | 1:A:106:PRO:CG   | 2.22                     | 0.52              |
| 2:P:115:VAL:CG1  | 2:P:136:LEU:HG   | 2.39                     | 0.52              |
| 2:P:115:VAL:HG12 | 2:P:136:LEU:HG   | 1.92                     | 0.52              |
| 1:K:191:SER:HA   | 1:K:194:LEU:HD13 | 1.90                     | 0.52              |
| 2:P:108:ARG:HE   | 2:P:108:ARG:HA   | 1.75                     | 0.52              |
| 2:D:108:ARG:NH1  | 2:D:109:THR:O    | 2.43                     | 0.52              |
| 2:L:32:HIS:ND1   | 2:L:50:TYR:HE1   | 2.08                     | 0.52              |
| 1:E:18:LEU:N     | 1:E:83:LEU:O     | 2.35                     | 0.51              |
| 1:G:72:ARG:HA    | 1:G:79:PHE:HA    | 1.91                     | 0.51              |
| 1:M:159:TRP:NE1  | 1:M:201:CYS:HB2  | 2.25                     | 0.51              |
| 1:M:215:ARG:HH12 | 1:S:208:SER:HA   | 1.75                     | 0.51              |
| 2:F:149:LYS:HB2  | 2:F:193:ALA:HB3  | 1.91                     | 0.51              |
| 2:L:7:SER:OG     | 2:L:22:THR:OG1   | 2.26                     | 0.51              |
| 2:L:175:LEU:HD23 | 2:L:176:SER:N    | 2.25                     | 0.51              |
| 2:N:78:LEU:HD11  | 2:N:106:ILE:HG12 | 1.92                     | 0.51              |
| 2:F:83:ALA:HB2   | 2:F:106:ILE:HD13 | 1.91                     | 0.51              |
| 1:G:11:LEU:HB2   | 1:G:152:PRO:HG3  | 1.93                     | 0.51              |
| 1:O:176:GLN:CD   | 1:O:176:GLN:H    | 2.18                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:54:TYR:O     | 1:E:72:ARG:NH1   | 2.42                     | 0.51              |
| 1:M:11:LEU:HB3   | 1:M:152:PRO:HG3  | 1.93                     | 0.51              |
| 1:Q:205:HIS:CD2  | 1:Q:207:PRO:HD2  | 2.46                     | 0.51              |
| 2:T:19:VAL:HB    | 2:T:75:ILE:HB    | 1.92                     | 0.51              |
| 2:T:61:ARG:NH2   | 2:T:82:ASP:OD1   | 2.44                     | 0.51              |
| 1:O:143:LEU:HB2  | 1:O:216:VAL:HG11 | 1.92                     | 0.51              |
| 2:R:47:LEU:HD21  | 2:R:62:PHE:HD2   | 1.76                     | 0.51              |
| 1:O:37:TRP:CE2   | 1:O:81:LEU:HB3   | 2.46                     | 0.51              |
| 1:M:202:ASN:OD1  | 1:M:202:ASN:N    | 2.44                     | 0.51              |
| 1:S:38:ILE:HD12  | 1:S:108:TRP:CH2  | 2.46                     | 0.51              |
| 2:B:63:SER:OG    | 2:B:64:GLY:N     | 2.43                     | 0.51              |
| 1:E:96:CYS:O     | 1:E:109:GLY:N    | 2.44                     | 0.51              |
| 1:Q:62:PRO:HD3   | 2:R:95:PRO:HG2   | 1.92                     | 0.51              |
| 1:C:18:LEU:N     | 1:C:83:LEU:O     | 2.38                     | 0.50              |
| 2:P:116:PHE:O    | 2:P:135:LEU:N    | 2.36                     | 0.50              |
| 2:B:78:LEU:HD11  | 2:B:106:ILE:HG12 | 1.93                     | 0.50              |
| 2:L:155:GLN:OE1  | 2:L:158:ASN:ND2  | 2.35                     | 0.50              |
| 1:S:65:LYS:O     | 1:S:68:ILE:HG22  | 2.11                     | 0.50              |
| 1:A:143:LEU:HD12 | 1:A:143:LEU:H    | 1.76                     | 0.50              |
| 2:D:93:ASP:OD1   | 2:D:94:PHE:N     | 2.44                     | 0.50              |
| 2:F:93:ASP:OD1   | 2:F:94:PHE:N     | 2.44                     | 0.50              |
| 1:M:173:ALA:HB2  | 1:M:183:LEU:HD23 | 1.92                     | 0.50              |
| 1:A:32:GLY:O     | 1:A:54:TYR:HD2   | 1.94                     | 0.50              |
| 1:E:100:ASP:OD1  | 1:E:101:SER:N    | 2.43                     | 0.50              |
| 1:G:52:ILE:HG13  | 1:G:58:THR:HG22  | 1.92                     | 0.50              |
| 1:K:104:TYR:HD1  | 2:L:46:LEU:HD11  | 1.76                     | 0.50              |
| 1:Q:48:TRP:HZ2   | 1:Q:51:TYR:HD2   | 1.58                     | 0.50              |
| 1:M:173:ALA:HA   | 1:M:183:LEU:HB3  | 1.94                     | 0.50              |
| 2:T:33:LEU:HB3   | 2:T:51:ALA:HB2   | 1.93                     | 0.50              |
| 2:T:90:GLN:NE2   | 2:T:96:LEU:HA    | 2.21                     | 0.50              |
| 1:A:190:PRO:O    | 1:A:193:SER:OG   | 2.27                     | 0.50              |
| 2:J:63:SER:OG    | 2:J:64:GLY:N     | 2.45                     | 0.50              |
| 1:K:33:TYR:CD1   | 1:K:33:TYR:N     | 2.80                     | 0.50              |
| 2:P:93:ASP:OD1   | 2:P:94:PHE:N     | 2.44                     | 0.50              |
| 2:P:34:HIS:HE1   | 2:P:50:TYR:CD2   | 2.28                     | 0.50              |
| 2:R:61:ARG:CZ    | 2:R:79:GLU:HG3   | 2.42                     | 0.50              |
| 1:G:148:LYS:NZ   | 1:G:176:GLN:OE1  | 2.38                     | 0.50              |
| 2:H:63:SER:OG    | 2:H:64:GLY:N     | 2.45                     | 0.50              |
| 2:H:156:SER:HB2  | 2:L:156:SER:HB2  | 1.92                     | 0.50              |
| 1:Q:11:LEU:HB3   | 1:Q:152:PRO:HG3  | 1.94                     | 0.50              |
| 1:S:173:ALA:HB2  | 1:S:183:LEU:HD23 | 1.94                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:104:TYR:HB3  | 2:N:34:HIS:CE1   | 2.47                     | 0.49              |
| 1:O:2:VAL:HG22   | 1:O:27:TYR:HB2   | 1.94                     | 0.49              |
| 1:O:33:TYR:HD2   | 1:O:100:ASP:HA   | 1.77                     | 0.49              |
| 2:R:66:GLY:HA3   | 2:R:71:PHE:HD1   | 1.75                     | 0.49              |
| 1:C:33:TYR:O     | 1:C:35:TRP:NE1   | 2.45                     | 0.49              |
| 1:C:72:ARG:HA    | 1:C:79:PHE:HA    | 1.94                     | 0.49              |
| 1:C:173:ALA:HB2  | 1:C:183:LEU:HD23 | 1.93                     | 0.49              |
| 1:M:40:GLN:NE2   | 2:N:38:GLN:OE1   | 2.39                     | 0.49              |
| 2:P:21:ILE:HB    | 2:P:73:LEU:HB3   | 1.93                     | 0.49              |
| 1:A:122:LYS:HG2  | 1:A:123:GLY:HA3  | 1.93                     | 0.49              |
| 1:E:91:THR:HG23  | 1:E:115:THR:HA   | 1.95                     | 0.49              |
| 1:S:28:PRO:HA    | 1:S:77:ASN:HD21  | 1.75                     | 0.49              |
| 1:A:39:ARG:HD3   | 1:A:49:MET:HE3   | 1.93                     | 0.49              |
| 1:C:124:PRO:CB   | 1:C:150:TYR:HB3  | 2.36                     | 0.49              |
| 2:F:78:LEU:HD21  | 2:F:106:ILE:HG13 | 1.94                     | 0.49              |
| 2:N:137:ASN:O    | 2:N:174:SER:OG   | 2.29                     | 0.49              |
| 1:O:164:LEU:HD11 | 1:O:189:VAL:HG21 | 1.95                     | 0.49              |
| 1:O:127:PHE:CZ   | 2:P:124:GLN:HB3  | 2.48                     | 0.49              |
| 1:Q:29:ILE:HG22  | 1:Q:35:TRP:CE2   | 2.47                     | 0.49              |
| 2:R:19:VAL:HB    | 2:R:75:ILE:HB    | 1.94                     | 0.49              |
| 2:T:145:LYS:HB3  | 2:T:197:THR:HB   | 1.95                     | 0.49              |
| 1:A:104:TYR:HB3  | 2:B:34:HIS:CE1   | 2.47                     | 0.49              |
| 1:K:48:TRP:HZ2   | 1:K:51:TYR:CD2   | 2.29                     | 0.49              |
| 2:P:7:SER:OG     | 2:P:22:THR:OG1   | 2.21                     | 0.49              |
| 2:R:49:LYS:C     | 2:R:51:ALA:HA    | 2.37                     | 0.49              |
| 1:S:29:ILE:HG22  | 1:S:35:TRP:CE2   | 2.46                     | 0.49              |
| 1:C:30:ARG:HD2   | 1:M:180:LEU:HD21 | 1.93                     | 0.49              |
| 1:K:168:VAL:HG12 | 1:K:187:VAL:HB   | 1.94                     | 0.49              |
| 2:L:136:LEU:HD11 | 2:L:146:VAL:CG2  | 2.43                     | 0.49              |
| 2:L:151:ASP:HA   | 2:L:191:VAL:HG23 | 1.94                     | 0.49              |
| 1:Q:102:GLY:HA3  | 2:R:50:TYR:OH    | 2.13                     | 0.49              |
| 2:T:93:ASP:OD1   | 2:T:94:PHE:N     | 2.45                     | 0.49              |
| 2:F:132:VAL:HB   | 2:F:179:LEU:HG   | 1.94                     | 0.49              |
| 1:G:100:ASP:OD1  | 1:G:101:SER:N    | 2.40                     | 0.49              |
| 1:E:129:LEU:CD2  | 1:E:144:GLY:H    | 2.18                     | 0.48              |
| 1:I:11:LEU:HB3   | 1:I:152:PRO:HG3  | 1.95                     | 0.48              |
| 2:R:128:GLY:HA2  | 2:R:183:LYS:HE2  | 1.94                     | 0.48              |
| 2:T:49:LYS:C     | 2:T:51:ALA:HA    | 2.38                     | 0.48              |
| 1:Q:41:PRO:HB2   | 1:Q:44:LYS:HB2   | 1.94                     | 0.48              |
| 2:R:47:LEU:HD21  | 2:R:62:PHE:CD2   | 2.47                     | 0.48              |
| 2:B:35:TRP:CZ3   | 2:B:88:CYS:HB3   | 2.48                     | 0.48              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:D:24:ARG:NH2   | 2:F:17:GLU:OE2  | 2.41                     | 0.48              |
| 2:F:61:ARG:HD2   | 2:F:77:SER:O    | 2.12                     | 0.48              |
| 1:K:31:PHE:N     | 1:K:31:PHE:CD1  | 2.81                     | 0.48              |
| 1:Q:34:SER:HB2   | 1:Q:53:HIS:HA   | 1.94                     | 0.48              |
| 2:H:10:PHE:HB3   | 2:L:12:SER:HB3  | 1.95                     | 0.48              |
| 1:I:29:ILE:HD11  | 1:I:77:ASN:C    | 2.39                     | 0.48              |
| 2:N:47:LEU:O     | 2:N:55:ILE:HG12 | 2.13                     | 0.48              |
| 1:A:153:GLU:HG2  | 1:A:154:PRO:HA  | 1.94                     | 0.48              |
| 1:G:33:TYR:CG    | 1:G:98:ARG:HD3  | 2.48                     | 0.48              |
| 2:R:66:GLY:HA3   | 2:R:71:PHE:CD1  | 2.48                     | 0.48              |
| 1:O:129:LEU:HD22 | 1:O:144:GLY:H   | 1.79                     | 0.48              |
| 2:P:49:LYS:HD3   | 2:P:50:TYR:CE1  | 2.49                     | 0.48              |
| 1:Q:208:SER:OG   | 1:Q:209:ASN:N   | 2.46                     | 0.48              |
| 2:P:199:GLN:OE1  | 2:P:199:GLN:N   | 2.46                     | 0.48              |
| 1:E:127:PHE:CE1  | 2:F:124:GLN:HG2 | 2.48                     | 0.48              |
| 1:G:29:ILE:H     | 1:G:29:ILE:HG13 | 1.45                     | 0.48              |
| 2:H:2:ILE:HD12   | 2:H:90:GLN:OE1  | 2.14                     | 0.48              |
| 1:M:159:TRP:CD1  | 1:M:201:CYS:HA  | 2.49                     | 0.48              |
| 1:G:96:CYS:O     | 1:G:109:GLY:N   | 2.47                     | 0.48              |
| 2:N:7:SER:HB2    | 2:P:13:VAL:HG23 | 1.96                     | 0.48              |
| 2:P:13:VAL:HG21  | 2:P:19:VAL:HG22 | 1.95                     | 0.48              |
| 2:B:48:ILE:HG22  | 2:B:49:LYS:O    | 2.13                     | 0.47              |
| 1:E:41:PRO:HB2   | 1:E:44:LYS:HB2  | 1.96                     | 0.47              |
| 1:I:104:TYR:CG   | 2:J:49:LYS:HD2  | 2.49                     | 0.47              |
| 2:J:34:HIS:CE1   | 2:J:49:LYS:HZ3  | 2.32                     | 0.47              |
| 1:O:18:LEU:HD22  | 1:O:19:SER:N    | 2.29                     | 0.47              |
| 2:R:36:TYR:HE1   | 2:R:89:GLN:HG2  | 1.78                     | 0.47              |
| 1:S:33:TYR:HB2   | 1:S:98:ARG:HG3  | 1.96                     | 0.47              |
| 2:H:149:LYS:HB2  | 2:H:193:ALA:HB3 | 1.97                     | 0.47              |
| 2:J:90:GLN:OE1   | 2:J:97:THR:N    | 2.41                     | 0.47              |
| 2:N:63:SER:OG    | 2:N:64:GLY:N    | 2.46                     | 0.47              |
| 1:E:27:TYR:CE2   | 1:E:32:GLY:HA3  | 2.37                     | 0.47              |
| 2:N:35:TRP:CE2   | 2:N:73:LEU:HB2  | 2.50                     | 0.47              |
| 2:P:49:LYS:O     | 2:P:53:HIS:HB2  | 2.13                     | 0.47              |
| 2:P:136:LEU:HD22 | 2:P:139:PHE:CE1 | 2.50                     | 0.47              |
| 2:R:96:LEU:HD23  | 2:R:97:THR:H    | 1.78                     | 0.47              |
| 2:T:63:SER:OG    | 2:T:64:GLY:N    | 2.46                     | 0.47              |
| 2:B:37:GLN:HB2   | 2:B:47:LEU:HD11 | 1.94                     | 0.47              |
| 1:E:129:LEU:HG   | 1:E:130:ALA:N   | 2.27                     | 0.47              |
| 2:H:21:ILE:HD12  | 2:H:73:LEU:HD23 | 1.97                     | 0.47              |
| 1:K:124:PRO:CB   | 1:K:150:TYR:HB3 | 2.33                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:33:TYR:CD2   | 1:O:100:ASP:HA   | 2.49                     | 0.47              |
| 2:P:63:SER:OG    | 2:P:64:GLY:N     | 2.47                     | 0.47              |
| 1:Q:61:ASN:CG    | 1:Q:62:PRO:HD2   | 2.38                     | 0.47              |
| 1:S:36:HIS:CG    | 1:S:105:PHE:HE2  | 2.31                     | 0.47              |
| 1:I:2:VAL:HG22   | 1:I:27:TYR:HB2   | 1.95                     | 0.47              |
| 1:I:72:ARG:HA    | 1:I:79:PHE:HA    | 1.96                     | 0.47              |
| 2:J:36:TYR:HE2   | 2:J:89:GLN:HG2   | 1.79                     | 0.47              |
| 1:O:100:ASP:OD1  | 1:O:101:SER:N    | 2.46                     | 0.47              |
| 2:F:33:LEU:HG    | 2:F:71:PHE:CD2   | 2.50                     | 0.47              |
| 1:O:18:LEU:O     | 1:O:83:LEU:N     | 2.40                     | 0.47              |
| 2:J:47:LEU:HB3   | 2:J:48:ILE:HG12  | 1.96                     | 0.47              |
| 1:S:52:ILE:HG12  | 1:S:53:HIS:O     | 2.14                     | 0.47              |
| 2:T:7:SER:HG     | 2:T:22:THR:HG1   | 1.62                     | 0.47              |
| 1:A:135:SER:HA   | 1:A:191:SER:OG   | 2.14                     | 0.47              |
| 1:A:173:ALA:HB2  | 1:A:183:LEU:HD23 | 1.96                     | 0.47              |
| 2:B:145:LYS:HB3  | 2:B:197:THR:HB   | 1.96                     | 0.47              |
| 2:F:2:ILE:O      | 2:F:97:THR:HG21  | 2.15                     | 0.47              |
| 1:G:104:TYR:HB3  | 2:H:34:HIS:CE1   | 2.49                     | 0.47              |
| 1:K:131:PRO:HG3  | 1:K:143:LEU:HB3  | 1.95                     | 0.47              |
| 2:N:29:ILE:HA    | 2:N:92:TYR:CD2   | 2.50                     | 0.47              |
| 2:P:186:TYR:CE2  | 2:P:187:GLU:HG2  | 2.49                     | 0.47              |
| 1:Q:18:LEU:HB2   | 1:Q:86:VAL:HG11  | 1.96                     | 0.47              |
| 2:R:13:VAL:HG21  | 2:R:19:VAL:HG22  | 1.95                     | 0.47              |
| 2:T:199:GLN:OE1  | 2:T:199:GLN:N    | 2.45                     | 0.47              |
| 1:E:71:SER:O     | 1:E:80:SER:N     | 2.42                     | 0.47              |
| 1:E:142:ALA:HB2  | 1:E:188:THR:HG22 | 1.96                     | 0.47              |
| 2:L:46:LEU:HD22  | 2:L:55:ILE:HG12  | 1.96                     | 0.47              |
| 2:N:80:ALA:HA    | 2:N:106:ILE:HD13 | 1.97                     | 0.47              |
| 2:B:33:LEU:O     | 2:B:50:TYR:HA    | 2.15                     | 0.47              |
| 2:J:13:VAL:HG21  | 2:J:19:VAL:HG22  | 1.97                     | 0.47              |
| 1:K:153:GLU:HG2  | 1:K:154:PRO:HA   | 1.96                     | 0.47              |
| 1:C:35:TRP:CZ3   | 1:C:98:ARG:HD2   | 2.50                     | 0.46              |
| 2:J:23:CYS:HB2   | 2:J:35:TRP:CH2   | 2.51                     | 0.46              |
| 2:J:47:LEU:O     | 2:J:55:ILE:HG12  | 2.14                     | 0.46              |
| 1:O:189:VAL:HG22 | 1:O:190:PRO:HD2  | 1.97                     | 0.46              |
| 2:T:13:VAL:HG21  | 2:T:19:VAL:HG22  | 1.97                     | 0.46              |
| 1:A:31:PHE:N     | 1:A:31:PHE:CD1   | 2.82                     | 0.46              |
| 2:J:113:PRO:HD3  | 2:J:198:HIS:ND1  | 2.29                     | 0.46              |
| 1:O:70:ILE:HG23  | 1:O:80:SER:O     | 2.15                     | 0.46              |
| 2:D:35:TRP:CZ3   | 2:D:88:CYS:HB3   | 2.49                     | 0.46              |
| 1:E:48:TRP:HZ2   | 1:E:51:TYR:CD2   | 2.33                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:128:GLY:HA2  | 2:H:183:LYS:HE2  | 1.96                     | 0.46              |
| 2:J:61:ARG:NH2   | 2:J:79:GLU:HG3   | 2.31                     | 0.46              |
| 2:L:13:VAL:HG21  | 2:L:19:VAL:HG22  | 1.96                     | 0.46              |
| 1:M:32:GLY:O     | 1:M:54:TYR:CD2   | 2.67                     | 0.46              |
| 2:P:182:SER:O    | 2:P:186:TYR:HB3  | 2.16                     | 0.46              |
| 1:S:62:PRO:O     | 1:S:65:LYS:HB2   | 2.14                     | 0.46              |
| 2:H:190:LYS:HE3  | 2:H:210:ASN:HB3  | 1.97                     | 0.46              |
| 2:N:13:VAL:HG21  | 2:N:19:VAL:HG22  | 1.98                     | 0.46              |
| 1:O:18:LEU:N     | 1:O:83:LEU:O     | 2.36                     | 0.46              |
| 2:D:13:VAL:HG21  | 2:D:19:VAL:HG22  | 1.97                     | 0.46              |
| 1:M:131:PRO:HG3  | 1:M:143:LEU:HB3  | 1.97                     | 0.46              |
| 2:P:136:LEU:N    | 2:P:175:LEU:O    | 2.35                     | 0.46              |
| 1:C:88:ALA:O     | 1:C:91:THR:HG22  | 2.16                     | 0.46              |
| 1:Q:72:ARG:HA    | 1:Q:79:PHE:HA    | 1.97                     | 0.46              |
| 1:E:129:LEU:HD23 | 1:E:143:LEU:HB2  | 1.97                     | 0.46              |
| 1:K:6:GLU:CD     | 1:K:111:GLY:H    | 2.22                     | 0.46              |
| 1:S:142:ALA:HB2  | 1:S:188:THR:HG22 | 1.98                     | 0.46              |
| 2:F:47:LEU:O     | 2:F:55:ILE:HG12  | 2.15                     | 0.46              |
| 1:G:18:LEU:N     | 1:G:83:LEU:O     | 2.37                     | 0.46              |
| 2:L:149:LYS:HG2  | 2:L:154:LEU:HD23 | 1.97                     | 0.46              |
| 2:P:49:LYS:HG3   | 2:P:55:ILE:HD11  | 1.98                     | 0.46              |
| 1:C:48:TRP:CE3   | 1:C:61:ASN:HB2   | 2.51                     | 0.46              |
| 1:C:102:GLY:HA3  | 2:D:50:TYR:OH    | 2.15                     | 0.46              |
| 2:J:34:HIS:CE1   | 2:J:49:LYS:NZ    | 2.83                     | 0.46              |
| 2:L:37:GLN:HB2   | 2:L:47:LEU:HD11  | 1.98                     | 0.46              |
| 2:P:154:LEU:H    | 2:P:154:LEU:HD23 | 1.80                     | 0.46              |
| 1:S:61:ASN:OD1   | 1:S:63:SER:N     | 2.48                     | 0.46              |
| 1:I:148:LYS:NZ   | 1:I:176:GLN:OE1  | 2.37                     | 0.45              |
| 1:K:142:ALA:HB2  | 1:K:188:THR:HG22 | 1.99                     | 0.45              |
| 1:K:151:PHE:HA   | 1:K:152:PRO:HA   | 1.77                     | 0.45              |
| 1:M:158:SER:O    | 1:M:159:TRP:HD1  | 1.99                     | 0.45              |
| 1:O:48:TRP:HZ2   | 1:O:51:TYR:CD2   | 2.29                     | 0.45              |
| 1:O:179:GLY:O    | 1:O:180:LEU:HD13 | 2.15                     | 0.45              |
| 1:Q:29:ILE:HD12  | 1:Q:30:ARG:N     | 2.31                     | 0.45              |
| 1:S:135:SER:HA   | 1:S:191:SER:OG   | 2.16                     | 0.45              |
| 1:A:29:ILE:HG23  | 1:A:35:TRP:NE1   | 2.31                     | 0.45              |
| 1:A:53:HIS:HE1   | 1:A:54:TYR:CE2   | 2.34                     | 0.45              |
| 2:D:39:LYS:HG2   | 2:D:84:ALA:HB2   | 1.98                     | 0.45              |
| 1:G:71:SER:O     | 1:G:80:SER:N     | 2.45                     | 0.45              |
| 1:G:173:ALA:HB2  | 1:G:183:LEU:HD23 | 1.97                     | 0.45              |
| 1:K:30:ARG:O     | 1:K:54:TYR:HB2   | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:78:LEU:HD11  | 2:L:106:ILE:HG12 | 1.98                     | 0.45              |
| 1:M:100:ASP:OD1  | 1:M:101:SER:N    | 2.48                     | 0.45              |
| 1:Q:27:TYR:HE1   | 1:Q:31:PHE:O     | 1.99                     | 0.45              |
| 2:B:199:GLN:OE1  | 2:B:199:GLN:N    | 2.44                     | 0.45              |
| 2:L:35:TRP:CZ3   | 2:L:88:CYS:HB3   | 2.52                     | 0.45              |
| 2:N:157:GLY:HA3  | 2:P:154:LEU:HD11 | 1.97                     | 0.45              |
| 1:Q:29:ILE:H     | 1:Q:29:ILE:HG13  | 1.57                     | 0.45              |
| 2:D:158:ASN:OD1  | 2:D:158:ASN:N    | 2.49                     | 0.45              |
| 1:E:33:TYR:CD1   | 1:E:33:TYR:N     | 2.84                     | 0.45              |
| 1:K:36:HIS:HD2   | 1:K:48:TRP:NE1   | 2.10                     | 0.45              |
| 2:P:37:GLN:HB2   | 2:P:47:LEU:HD11  | 1.99                     | 0.45              |
| 2:B:35:TRP:CG    | 2:B:73:LEU:HD12  | 2.52                     | 0.45              |
| 2:D:35:TRP:CG    | 2:D:73:LEU:HD12  | 2.51                     | 0.45              |
| 2:D:149:LYS:HG2  | 2:D:154:LEU:HD23 | 1.99                     | 0.45              |
| 1:K:103:ASN:HB3  | 2:L:96:LEU:CD2   | 2.47                     | 0.45              |
| 1:O:123:GLY:HA2  | 1:O:124:PRO:HD3  | 1.69                     | 0.45              |
| 2:P:108:ARG:NH1  | 2:P:142:ARG:H    | 2.14                     | 0.45              |
| 1:Q:63:SER:C     | 1:Q:64:LEU:HG    | 2.42                     | 0.45              |
| 2:R:33:LEU:HG    | 2:R:71:PHE:CG    | 2.52                     | 0.45              |
| 1:G:36:HIS:CD2   | 1:G:99:LYS:HB2   | 2.52                     | 0.45              |
| 2:L:32:HIS:HD1   | 2:L:50:TYR:HE1   | 1.64                     | 0.45              |
| 1:Q:18:LEU:N     | 1:Q:83:LEU:O     | 2.38                     | 0.45              |
| 2:T:88:CYS:O     | 2:T:99:GLY:N     | 2.48                     | 0.45              |
| 2:T:90:GLN:OE1   | 2:T:90:GLN:N     | 2.45                     | 0.45              |
| 2:J:49:LYS:HG2   | 2:J:50:TYR:CD2   | 2.52                     | 0.45              |
| 1:K:28:PRO:HG2   | 1:K:31:PHE:CD2   | 2.52                     | 0.45              |
| 2:N:93:ASP:OD1   | 2:N:94:PHE:N     | 2.50                     | 0.45              |
| 1:O:171:PHE:HA   | 1:O:172:PRO:HD3  | 1.83                     | 0.45              |
| 2:P:105:GLU:CG   | 2:P:106:ILE:H    | 2.30                     | 0.45              |
| 1:K:28:PRO:HG2   | 1:K:31:PHE:CG    | 2.52                     | 0.45              |
| 1:M:72:ARG:HA    | 1:M:79:PHE:HA    | 1.99                     | 0.45              |
| 2:P:47:LEU:O     | 2:P:55:ILE:HG12  | 2.17                     | 0.45              |
| 1:A:113:LEU:HD12 | 1:A:114:VAL:H    | 1.82                     | 0.45              |
| 2:N:33:LEU:HG    | 2:N:34:HIS:N     | 2.31                     | 0.45              |
| 1:O:144:GLY:HA3  | 1:O:186:VAL:HG12 | 1.98                     | 0.45              |
| 1:S:31:PHE:N     | 1:S:31:PHE:CD1   | 2.83                     | 0.45              |
| 1:A:53:HIS:HB2   | 1:A:57:TYR:HB3   | 1.99                     | 0.44              |
| 1:A:168:VAL:HG22 | 1:A:187:VAL:HB   | 1.98                     | 0.44              |
| 2:D:12:SER:HB3   | 2:F:10:PHE:HB3   | 1.99                     | 0.44              |
| 1:E:143:LEU:O    | 1:E:187:VAL:N    | 2.36                     | 0.44              |
| 1:G:29:ILE:HG13  | 1:G:77:ASN:OD1   | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:200:ILE:HG22 | 1:O:215:ARG:HA   | 1.99                     | 0.44              |
| 1:E:34:SER:HB2   | 1:E:36:HIS:CE1   | 2.45                     | 0.44              |
| 2:F:147:GLN:HB3  | 2:F:195:GLU:HB3  | 1.99                     | 0.44              |
| 1:K:104:TYR:O    | 1:K:106:PRO:HD3  | 2.17                     | 0.44              |
| 1:A:27:TYR:OH    | 1:A:32:GLY:HA3   | 2.17                     | 0.44              |
| 2:D:158:ASN:HD22 | 2:D:181:LEU:HD21 | 1.82                     | 0.44              |
| 2:J:61:ARG:HH22  | 2:J:79:GLU:HG3   | 1.82                     | 0.44              |
| 1:K:33:TYR:CD2   | 1:K:100:ASP:HA   | 2.52                     | 0.44              |
| 2:F:61:ARG:HH21  | 2:F:82:ASP:CG    | 2.22                     | 0.44              |
| 2:H:112:ALA:HA   | 2:H:113:PRO:HD3  | 1.83                     | 0.44              |
| 1:I:104:TYR:O    | 1:I:106:PRO:HD3  | 2.17                     | 0.44              |
| 2:L:88:CYS:O     | 2:L:99:GLY:N     | 2.49                     | 0.44              |
| 1:A:48:TRP:HZ2   | 1:A:51:TYR:HD1   | 1.66                     | 0.44              |
| 2:N:150:VAL:HG13 | 2:N:192:TYR:CE1  | 2.53                     | 0.44              |
| 1:O:138:GLY:O    | 1:Q:65:LYS:NZ    | 2.41                     | 0.44              |
| 1:S:190:PRO:O    | 1:S:193:SER:OG   | 2.30                     | 0.44              |
| 1:I:36:HIS:CD2   | 1:I:51:TYR:HB2   | 2.52                     | 0.44              |
| 2:J:30:SER:O     | 2:J:32:HIS:N     | 2.44                     | 0.44              |
| 2:J:188:LYS:HB3  | 2:J:188:LYS:HE2  | 1.83                     | 0.44              |
| 1:O:35:TRP:CG    | 1:O:79:PHE:CE1   | 3.06                     | 0.44              |
| 1:O:52:ILE:HA    | 1:O:58:THR:HG22  | 2.00                     | 0.44              |
| 2:R:55:ILE:HG22  | 2:R:56:SER:N     | 2.33                     | 0.44              |
| 1:S:71:SER:O     | 1:S:80:SER:N     | 2.36                     | 0.44              |
| 1:S:131:PRO:HB3  | 1:S:143:LEU:HB3  | 2.00                     | 0.44              |
| 2:B:46:LEU:O     | 2:B:55:ILE:HG21  | 2.18                     | 0.44              |
| 2:F:166:GLN:HE21 | 2:F:171:SER:HB3  | 1.83                     | 0.44              |
| 2:H:150:VAL:HG13 | 2:H:192:TYR:CE1  | 2.52                     | 0.44              |
| 1:K:41:PRO:HB2   | 1:K:44:LYS:HB2   | 2.00                     | 0.44              |
| 1:O:104:TYR:HB3  | 2:P:34:HIS:CE1   | 2.53                     | 0.44              |
| 2:P:35:TRP:CE2   | 2:P:73:LEU:HB2   | 2.52                     | 0.44              |
| 2:P:89:GLN:HE21  | 2:P:90:GLN:C     | 2.26                     | 0.44              |
| 2:P:185:ASP:O    | 2:P:188:LYS:HG2  | 2.18                     | 0.44              |
| 1:Q:67:ARG:NH2   | 1:Q:86:VAL:HA    | 2.32                     | 0.44              |
| 2:R:33:LEU:HD13  | 2:R:34:HIS:N     | 2.33                     | 0.44              |
| 2:R:210:ASN:OD1  | 2:R:210:ASN:N    | 2.51                     | 0.44              |
| 1:A:98:ARG:NH2   | 1:A:100:ASP:OD2  | 2.51                     | 0.43              |
| 2:R:6:GLN:NE2    | 2:R:88:CYS:SG    | 2.90                     | 0.43              |
| 2:T:23:CYS:HB2   | 2:T:35:TRP:CH2   | 2.53                     | 0.43              |
| 1:E:54:TYR:HD1   | 1:E:55:SER:N     | 2.16                     | 0.43              |
| 1:E:164:LEU:HD11 | 1:E:187:VAL:HG21 | 1.99                     | 0.43              |
| 1:E:204:ASN:HB2  | 1:E:211:LYS:HE2  | 1.99                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:63:SER:O     | 2:H:73:LEU:HD12  | 2.18                     | 0.43              |
| 2:P:107:LYS:HD3  | 2:P:109:THR:CB   | 2.48                     | 0.43              |
| 1:Q:173:ALA:HB2  | 1:Q:183:LEU:HD23 | 2.00                     | 0.43              |
| 2:T:78:LEU:HD11  | 2:T:106:ILE:HG12 | 2.01                     | 0.43              |
| 1:G:29:ILE:HG22  | 1:G:35:TRP:NE1   | 2.32                     | 0.43              |
| 2:H:33:LEU:HD22  | 2:H:89:GLN:O     | 2.18                     | 0.43              |
| 1:K:72:ARG:HA    | 1:K:79:PHE:HA    | 2.00                     | 0.43              |
| 1:O:192:SER:HA   | 1:Q:66:THR:HA    | 1.99                     | 0.43              |
| 1:I:18:LEU:N     | 1:I:83:LEU:O     | 2.42                     | 0.43              |
| 1:K:54:TYR:CD1   | 1:K:55:SER:N     | 2.87                     | 0.43              |
| 2:L:33:LEU:HG    | 2:L:34:HIS:N     | 2.33                     | 0.43              |
| 1:O:27:TYR:HA    | 1:O:28:PRO:HD3   | 1.74                     | 0.43              |
| 2:P:21:ILE:HG23  | 2:P:102:THR:HG21 | 2.00                     | 0.43              |
| 2:R:85:THR:HG22  | 2:R:103:LYS:HG3  | 2.00                     | 0.43              |
| 1:C:33:TYR:CD2   | 1:C:33:TYR:N     | 2.85                     | 0.43              |
| 1:E:10:GLY:HA3   | 1:E:207:PRO:HG3  | 2.01                     | 0.43              |
| 1:I:6:GLU:CD     | 1:I:111:GLY:H    | 2.26                     | 0.43              |
| 2:J:129:THR:HG23 | 1:Q:76:LYS:HE2   | 1.99                     | 0.43              |
| 2:N:33:LEU:HD12  | 2:N:89:GLN:O     | 2.18                     | 0.43              |
| 2:T:142:ARG:HE   | 2:T:163:VAL:HG11 | 1.83                     | 0.43              |
| 2:B:112:ALA:HA   | 2:B:113:PRO:HD3  | 1.86                     | 0.43              |
| 2:B:142:ARG:HE   | 2:B:163:VAL:HG11 | 1.84                     | 0.43              |
| 1:C:53:HIS:HB2   | 1:C:57:TYR:CB    | 2.49                     | 0.43              |
| 1:I:33:TYR:N     | 1:I:33:TYR:CD1   | 2.87                     | 0.43              |
| 2:J:145:LYS:HB3  | 2:J:197:THR:OG1  | 2.19                     | 0.43              |
| 1:M:98:ARG:HH21  | 1:M:107:TYR:HE2  | 1.64                     | 0.43              |
| 1:O:129:LEU:HB3  | 1:O:144:GLY:O    | 2.18                     | 0.43              |
| 2:B:39:LYS:HG2   | 2:B:84:ALA:HB2   | 2.01                     | 0.43              |
| 2:D:32:HIS:CE1   | 2:D:50:TYR:HE1   | 2.36                     | 0.43              |
| 2:H:13:VAL:HG13  | 2:L:7:SER:HB2    | 2.01                     | 0.43              |
| 1:O:168:VAL:HG13 | 1:O:187:VAL:HG22 | 2.00                     | 0.43              |
| 2:D:7:SER:HB2    | 2:F:13:VAL:HG13  | 2.00                     | 0.43              |
| 2:F:21:ILE:HB    | 2:F:73:LEU:HB3   | 2.00                     | 0.43              |
| 2:F:36:TYR:HE1   | 2:F:89:GLN:CG    | 2.32                     | 0.43              |
| 2:H:158:ASN:OD1  | 2:H:158:ASN:N    | 2.51                     | 0.43              |
| 2:L:49:LYS:HZ2   | 2:L:50:TYR:HE2   | 1.64                     | 0.43              |
| 1:M:36:HIS:HE2   | 1:M:99:LYS:HB2   | 1.77                     | 0.43              |
| 2:P:136:LEU:HB3  | 2:P:139:PHE:CE1  | 2.53                     | 0.43              |
| 1:A:205:HIS:CD2  | 1:A:207:PRO:HD2  | 2.54                     | 0.43              |
| 2:J:155:GLN:OE1  | 2:J:158:ASN:ND2  | 2.41                     | 0.43              |
| 1:Q:173:ALA:HA   | 1:Q:183:LEU:HB3  | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:T:32:HIS:HB3   | 2:T:91:GLY:HA3   | 2.01                     | 0.43              |
| 1:A:8:GLY:HA3    | 1:A:20:LEU:HD23  | 2.01                     | 0.43              |
| 1:C:64:LEU:O     | 1:C:67:ARG:N     | 2.52                     | 0.43              |
| 1:G:61:ASN:HA    | 1:G:62:PRO:HD3   | 1.92                     | 0.43              |
| 1:S:48:TRP:HZ2   | 1:S:51:TYR:HD2   | 1.66                     | 0.43              |
| 2:J:7:SER:OG     | 2:J:22:THR:OG1   | 2.28                     | 0.42              |
| 2:J:25:ALA:O     | 2:J:69:THR:HG23  | 2.19                     | 0.42              |
| 2:J:33:LEU:O     | 2:J:34:HIS:ND1   | 2.52                     | 0.42              |
| 1:O:61:ASN:HA    | 1:O:62:PRO:HD3   | 1.86                     | 0.42              |
| 2:R:166:GLN:HE21 | 2:R:171:SER:HB3  | 1.83                     | 0.42              |
| 1:A:20:LEU:HD23  | 1:A:20:LEU:HA    | 1.89                     | 0.42              |
| 2:D:60:SER:O     | 2:R:24:ARG:NH1   | 2.35                     | 0.42              |
| 2:F:144:ALA:C    | 2:F:145:LYS:HD2  | 2.44                     | 0.42              |
| 2:H:23:CYS:HB2   | 2:H:35:TRP:CH2   | 2.54                     | 0.42              |
| 2:L:19:VAL:HB    | 2:L:75:ILE:HB    | 2.01                     | 0.42              |
| 2:N:88:CYS:O     | 2:N:99:GLY:N     | 2.53                     | 0.42              |
| 1:O:29:ILE:HD13  | 1:O:29:ILE:N     | 2.34                     | 0.42              |
| 2:P:147:GLN:HB3  | 2:P:195:GLU:HB2  | 2.00                     | 0.42              |
| 2:J:29:ILE:HD13  | 2:J:90:GLN:HB3   | 2.00                     | 0.42              |
| 2:L:59:PRO:HG2   | 2:L:62:PHE:HD2   | 1.85                     | 0.42              |
| 1:M:151:PHE:HA   | 1:M:152:PRO:HA   | 1.81                     | 0.42              |
| 2:P:35:TRP:CZ3   | 2:P:88:CYS:HB3   | 2.55                     | 0.42              |
| 2:P:121:SER:O    | 2:P:124:GLN:HG2  | 2.19                     | 0.42              |
| 2:P:123:GLU:O    | 2:P:126:LYS:HG2  | 2.19                     | 0.42              |
| 1:A:201:CYS:SG   | 1:A:214:LYS:HB2  | 2.59                     | 0.42              |
| 1:E:32:GLY:O     | 1:E:54:TYR:CD2   | 2.73                     | 0.42              |
| 2:F:21:ILE:HG23  | 2:F:102:THR:HG21 | 2.01                     | 0.42              |
| 2:F:150:VAL:HG13 | 2:F:192:TYR:CE1  | 2.55                     | 0.42              |
| 1:I:54:TYR:O     | 1:I:72:ARG:NH2   | 2.45                     | 0.42              |
| 1:G:36:HIS:HE2   | 1:G:99:LYS:HB2   | 1.82                     | 0.42              |
| 2:R:55:ILE:HG22  | 2:R:56:SER:H     | 1.85                     | 0.42              |
| 1:A:191:SER:HA   | 1:A:194:LEU:HD13 | 2.02                     | 0.42              |
| 2:F:186:TYR:O    | 2:F:192:TYR:OH   | 2.37                     | 0.42              |
| 1:I:98:ARG:NH1   | 1:I:100:ASP:HA   | 2.35                     | 0.42              |
| 1:I:206:LYS:HA   | 1:I:206:LYS:HD2  | 1.86                     | 0.42              |
| 2:L:49:LYS:HG2   | 2:L:50:TYR:CD2   | 2.51                     | 0.42              |
| 1:C:149:ASP:HA   | 1:C:180:LEU:HB3  | 2.02                     | 0.42              |
| 2:D:33:LEU:HD13  | 2:D:34:HIS:N     | 2.34                     | 0.42              |
| 1:G:31:PHE:CD1   | 1:G:31:PHE:N     | 2.86                     | 0.42              |
| 2:H:2:ILE:O      | 2:H:97:THR:HG21  | 2.20                     | 0.42              |
| 2:H:125:LEU:HD13 | 2:H:125:LEU:HA   | 1.93                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:150:VAL:HG13 | 2:H:192:TYR:HE1  | 1.85                     | 0.42              |
| 1:M:54:TYR:CD1   | 1:M:55:SER:N     | 2.82                     | 0.42              |
| 1:M:205:HIS:ND1  | 1:M:208:SER:HB3  | 2.34                     | 0.42              |
| 1:Q:124:PRO:HB3  | 1:Q:150:TYR:HB3  | 2.00                     | 0.42              |
| 1:S:122:LYS:HB3  | 1:S:123:GLY:HA3  | 2.01                     | 0.42              |
| 1:A:143:LEU:HB2  | 1:A:216:VAL:HG11 | 2.01                     | 0.42              |
| 2:B:35:TRP:CD2   | 2:B:73:LEU:HD12  | 2.54                     | 0.42              |
| 2:D:34:HIS:HB2   | 2:D:89:GLN:HG3   | 2.02                     | 0.42              |
| 2:R:36:TYR:CE1   | 2:R:89:GLN:HG2   | 2.54                     | 0.42              |
| 1:S:104:TYR:HB3  | 2:T:34:HIS:CD2   | 2.55                     | 0.42              |
| 1:C:122:LYS:HD2  | 1:C:149:ASP:O    | 2.18                     | 0.42              |
| 1:K:60:PHE:HE1   | 1:K:70:ILE:HG13  | 1.84                     | 0.42              |
| 2:L:2:ILE:O      | 2:L:97:THR:HG21  | 2.19                     | 0.42              |
| 2:L:23:CYS:HB2   | 2:L:35:TRP:CH2   | 2.55                     | 0.42              |
| 2:L:192:TYR:HB2  | 2:L:209:PHE:CE1  | 2.55                     | 0.42              |
| 2:B:13:VAL:HG21  | 2:B:19:VAL:HG22  | 2.01                     | 0.42              |
| 1:O:151:PHE:HA   | 1:O:152:PRO:HA   | 1.82                     | 0.42              |
| 1:Q:67:ARG:HH22  | 1:Q:86:VAL:HA    | 1.85                     | 0.42              |
| 2:R:29:ILE:HB    | 2:R:71:PHE:HE2   | 1.85                     | 0.42              |
| 1:A:151:PHE:HA   | 1:A:152:PRO:HA   | 1.83                     | 0.41              |
| 2:D:18:LYS:HB3   | 2:D:18:LYS:HE2   | 1.81                     | 0.41              |
| 2:D:49:LYS:C     | 2:D:51:ALA:HA    | 2.44                     | 0.41              |
| 1:E:60:PHE:O     | 1:E:65:LYS:NZ    | 2.53                     | 0.41              |
| 2:H:89:GLN:HG2   | 2:H:90:GLN:N     | 2.34                     | 0.41              |
| 2:J:14:THR:OG1   | 2:J:17:GLU:HG3   | 2.20                     | 0.41              |
| 2:J:108:ARG:HG2  | 2:J:140:TYR:CD2  | 2.55                     | 0.41              |
| 1:K:31:PHE:N     | 1:K:31:PHE:HD1   | 2.17                     | 0.41              |
| 2:L:61:ARG:NH1   | 2:L:79:GLU:HB2   | 2.35                     | 0.41              |
| 2:N:17:GLU:OE2   | 2:P:24:ARG:NH2   | 2.28                     | 0.41              |
| 2:N:47:LEU:HD23  | 2:N:47:LEU:HA    | 1.93                     | 0.41              |
| 1:Q:62:PRO:HD3   | 2:R:95:PRO:CG    | 2.50                     | 0.41              |
| 2:R:6:GLN:HE21   | 2:R:99:GLY:HA3   | 1.86                     | 0.41              |
| 1:E:54:TYR:CD1   | 1:E:55:SER:N     | 2.88                     | 0.41              |
| 1:I:124:PRO:CB   | 1:I:150:TYR:HB3  | 2.45                     | 0.41              |
| 2:L:24:ARG:HG2   | 2:L:69:THR:HG22  | 2.01                     | 0.41              |
| 2:R:29:ILE:O     | 2:R:29:ILE:HG22  | 2.20                     | 0.41              |
| 2:T:175:LEU:HD23 | 2:T:176:SER:N    | 2.35                     | 0.41              |
| 1:C:123:GLY:HA2  | 1:C:124:PRO:HD3  | 1.84                     | 0.41              |
| 1:G:32:GLY:O     | 1:G:54:TYR:CD2   | 2.73                     | 0.41              |
| 2:H:124:GLN:HG2  | 2:H:129:THR:O    | 2.20                     | 0.41              |
| 2:H:140:TYR:CG   | 2:H:141:PRO:HA   | 2.55                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:100:ASP:OD1  | 1:K:101:SER:N    | 2.50                     | 0.41              |
| 1:K:106:PRO:HG2  | 1:K:107:TYR:CD2  | 2.55                     | 0.41              |
| 1:A:122:LYS:O    | 1:A:205:HIS:HE1  | 2.04                     | 0.41              |
| 2:F:134:CYS:HB2  | 2:F:148:TRP:CH2  | 2.56                     | 0.41              |
| 2:H:157:GLY:HA3  | 2:L:154:LEU:HD13 | 2.03                     | 0.41              |
| 1:I:100:ASP:OD1  | 1:I:101:SER:N    | 2.49                     | 0.41              |
| 1:K:134:LYS:HB3  | 1:K:137:SER:HB2  | 2.02                     | 0.41              |
| 1:O:104:TYR:O    | 1:O:106:PRO:HD3  | 2.21                     | 0.41              |
| 1:Q:104:TYR:HB3  | 2:R:34:HIS:NE2   | 2.35                     | 0.41              |
| 2:H:47:LEU:HD23  | 2:H:47:LEU:HA    | 1.94                     | 0.41              |
| 1:I:29:ILE:HG23  | 1:I:35:TRP:NE1   | 2.36                     | 0.41              |
| 1:C:173:ALA:HA   | 1:C:183:LEU:HB3  | 2.02                     | 0.41              |
| 2:D:35:TRP:CD2   | 2:D:73:LEU:HD12  | 2.56                     | 0.41              |
| 2:D:186:TYR:O    | 2:D:192:TYR:OH   | 2.31                     | 0.41              |
| 1:E:51:TYR:CE2   | 2:F:94:PHE:HE2   | 2.39                     | 0.41              |
| 1:E:104:TYR:O    | 1:E:106:PRO:HD3  | 2.21                     | 0.41              |
| 2:F:63:SER:OG    | 2:F:64:GLY:N     | 2.52                     | 0.41              |
| 1:G:104:TYR:O    | 1:G:106:PRO:HD3  | 2.21                     | 0.41              |
| 1:K:104:TYR:CZ   | 2:L:49:LYS:HE2   | 2.56                     | 0.41              |
| 1:O:176:GLN:HG2  | 1:O:179:GLY:H    | 1.86                     | 0.41              |
| 1:E:48:TRP:CE3   | 1:E:61:ASN:HB2   | 2.56                     | 0.41              |
| 1:G:18:LEU:HB3   | 1:G:83:LEU:HB3   | 2.03                     | 0.41              |
| 2:D:47:LEU:O     | 2:D:55:ILE:HG12  | 2.21                     | 0.41              |
| 2:F:33:LEU:HG    | 2:F:71:PHE:CG    | 2.56                     | 0.41              |
| 2:F:134:CYS:HB2  | 2:F:148:TRP:CZ2  | 2.54                     | 0.41              |
| 1:G:65:LYS:HE3   | 1:G:65:LYS:HB2   | 1.86                     | 0.41              |
| 1:G:212:VAL:HA   | 1:Q:211:LYS:O    | 2.21                     | 0.41              |
| 1:I:168:VAL:HG12 | 1:I:187:VAL:HB   | 2.02                     | 0.41              |
| 2:J:34:HIS:ND1   | 2:J:49:LYS:HG3   | 2.36                     | 0.41              |
| 1:K:48:TRP:CZ2   | 1:K:50:GLY:HA2   | 2.56                     | 0.41              |
| 1:M:48:TRP:CE3   | 1:M:61:ASN:HB2   | 2.56                     | 0.41              |
| 2:N:158:ASN:OD1  | 2:N:158:ASN:N    | 2.54                     | 0.41              |
| 1:O:20:LEU:HB2   | 1:O:81:LEU:CD2   | 2.50                     | 0.41              |
| 1:O:81:LEU:O     | 1:O:82:LYS:HG2   | 2.20                     | 0.41              |
| 1:Q:217:GLU:HA   | 1:Q:218:PRO:HD3  | 1.92                     | 0.41              |
| 1:S:34:SER:HB2   | 1:S:53:HIS:HA    | 2.02                     | 0.41              |
| 2:T:29:ILE:HG22  | 2:T:92:TYR:HD2   | 1.85                     | 0.41              |
| 1:A:29:ILE:HG23  | 1:A:35:TRP:CD1   | 2.55                     | 0.41              |
| 1:A:32:GLY:O     | 1:A:54:TYR:HB3   | 2.21                     | 0.41              |
| 2:D:107:LYS:HD3  | 2:F:9:ASP:OD2    | 2.21                     | 0.41              |
| 1:E:129:LEU:HD11 | 2:F:118:PHE:CG   | 2.56                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:146:LEU:HD12 | 1:E:183:LEU:O    | 2.21                     | 0.41              |
| 2:N:90:GLN:OE1   | 2:N:92:TYR:N     | 2.54                     | 0.41              |
| 2:T:210:ASN:HB3  | 2:T:211:ARG:H    | 1.78                     | 0.41              |
| 2:F:35:TRP:CE2   | 2:F:73:LEU:HB2   | 2.56                     | 0.40              |
| 1:M:104:TYR:O    | 1:M:106:PRO:HD3  | 2.21                     | 0.40              |
| 1:M:158:SER:C    | 1:M:159:TRP:CD1  | 2.99                     | 0.40              |
| 1:Q:104:TYR:HB3  | 2:R:34:HIS:CE1   | 2.55                     | 0.40              |
| 1:I:53:HIS:CB    | 1:I:57:TYR:HB3   | 2.51                     | 0.40              |
| 1:O:35:TRP:CG    | 1:O:79:PHE:HE1   | 2.39                     | 0.40              |
| 1:S:29:ILE:HG13  | 1:S:29:ILE:H     | 1.75                     | 0.40              |
| 1:E:146:LEU:HD21 | 1:E:148:LYS:NZ   | 2.36                     | 0.40              |
| 1:I:71:SER:O     | 1:I:80:SER:N     | 2.50                     | 0.40              |
| 2:L:4:LEU:HD12   | 2:L:23:CYS:SG    | 2.62                     | 0.40              |
| 2:N:89:GLN:O     | 2:N:89:GLN:HG3   | 2.21                     | 0.40              |
| 2:N:149:LYS:HG2  | 2:N:154:LEU:HD23 | 2.04                     | 0.40              |
| 2:P:105:GLU:CG   | 2:P:106:ILE:N    | 2.84                     | 0.40              |
| 2:P:192:TYR:HB2  | 2:P:209:PHE:CE1  | 2.55                     | 0.40              |
| 1:A:18:LEU:N     | 1:A:83:LEU:O     | 2.41                     | 0.40              |
| 1:A:49:MET:HE1   | 1:A:94:TYR:HE2   | 1.87                     | 0.40              |
| 1:C:104:TYR:HB3  | 2:D:34:HIS:CE1   | 2.56                     | 0.40              |
| 2:J:33:LEU:HD22  | 2:J:34:HIS:H     | 1.85                     | 0.40              |
| 2:N:37:GLN:HB2   | 2:N:47:LEU:HD11  | 2.02                     | 0.40              |
| 1:O:64:LEU:H     | 1:O:64:LEU:HG    | 1.63                     | 0.40              |
| 2:P:136:LEU:HD22 | 2:P:139:PHE:HE1  | 1.86                     | 0.40              |
| 1:S:191:SER:HA   | 1:S:194:LEU:HD13 | 2.03                     | 0.40              |
| 1:C:206:LYS:HD2  | 1:C:206:LYS:HA   | 1.88                     | 0.40              |
| 1:E:33:TYR:HB2   | 1:E:98:ARG:HD2   | 2.04                     | 0.40              |
| 2:H:149:LYS:HG2  | 2:H:154:LEU:HD23 | 2.04                     | 0.40              |
| 2:J:4:LEU:HD12   | 2:J:23:CYS:SG    | 2.62                     | 0.40              |
| 1:K:53:HIS:HD2   | 1:K:57:TYR:CD2   | 2.40                     | 0.40              |
| 1:M:31:PHE:N     | 1:M:31:PHE:CD1   | 2.89                     | 0.40              |
| 2:N:13:VAL:HG13  | 2:P:7:SER:HB2    | 2.03                     | 0.40              |
| 1:Q:104:TYR:HB3  | 2:R:34:HIS:CD2   | 2.56                     | 0.40              |
| 2:R:33:LEU:HG    | 2:R:71:PHE:CD2   | 2.56                     | 0.40              |
| 2:R:39:LYS:HG2   | 2:R:84:ALA:HB2   | 2.04                     | 0.40              |
| 2:T:39:LYS:HG2   | 2:T:84:ALA:HB2   | 2.03                     | 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     | 216/225 (96%)   | 206 (95%)  | 9 (4%)   | 1 (0%)   | 24          | 57  |
| 1   | C     | 216/225 (96%)   | 206 (95%)  | 10 (5%)  | 0        | 100         | 100 |
| 1   | E     | 216/225 (96%)   | 209 (97%)  | 6 (3%)   | 1 (0%)   | 24          | 57  |
| 1   | G     | 216/225 (96%)   | 210 (97%)  | 5 (2%)   | 1 (0%)   | 24          | 57  |
| 1   | I     | 216/225 (96%)   | 207 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 1   | K     | 216/225 (96%)   | 209 (97%)  | 6 (3%)   | 1 (0%)   | 24          | 57  |
| 1   | M     | 216/225 (96%)   | 210 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| 1   | O     | 216/225 (96%)   | 207 (96%)  | 8 (4%)   | 1 (0%)   | 24          | 57  |
| 1   | Q     | 216/225 (96%)   | 207 (96%)  | 8 (4%)   | 1 (0%)   | 24          | 57  |
| 1   | S     | 216/225 (96%)   | 206 (95%)  | 9 (4%)   | 1 (0%)   | 24          | 57  |
| 2   | B     | 209/214 (98%)   | 201 (96%)  | 7 (3%)   | 1 (0%)   | 24          | 57  |
| 2   | D     | 209/214 (98%)   | 202 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| 2   | F     | 209/214 (98%)   | 204 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 2   | H     | 209/214 (98%)   | 202 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| 2   | J     | 209/214 (98%)   | 201 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 2   | L     | 209/214 (98%)   | 202 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| 2   | N     | 209/214 (98%)   | 201 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 2   | P     | 209/214 (98%)   | 199 (95%)  | 10 (5%)  | 0        | 100         | 100 |
| 2   | R     | 211/214 (99%)   | 196 (93%)  | 15 (7%)  | 0        | 100         | 100 |
| 2   | T     | 209/214 (98%)   | 201 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| All | All   | 4252/4390 (97%) | 4086 (96%) | 158 (4%) | 8 (0%)   | 43          | 74  |

All (8) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 33  | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 209 | ASN  |
| 1   | G     | 33  | TYR  |
| 2   | B     | 137 | ASN  |
| 1   | K     | 65  | LYS  |
| 1   | S     | 207 | PRO  |
| 1   | Q     | 56  | GLY  |
| 1   | O     | 28  | PRO  |

### 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     | 189/196 (96%) | 180 (95%) | 9 (5%)   | 23          | 50 |
| 1   | C     | 189/196 (96%) | 178 (94%) | 11 (6%)  | 18          | 45 |
| 1   | E     | 189/196 (96%) | 176 (93%) | 13 (7%)  | 14          | 41 |
| 1   | G     | 189/196 (96%) | 182 (96%) | 7 (4%)   | 30          | 57 |
| 1   | I     | 189/196 (96%) | 179 (95%) | 10 (5%)  | 20          | 48 |
| 1   | K     | 189/196 (96%) | 181 (96%) | 8 (4%)   | 26          | 53 |
| 1   | M     | 189/196 (96%) | 183 (97%) | 6 (3%)   | 34          | 60 |
| 1   | O     | 189/196 (96%) | 171 (90%) | 18 (10%) | 8           | 31 |
| 1   | Q     | 189/196 (96%) | 182 (96%) | 7 (4%)   | 30          | 57 |
| 1   | S     | 189/196 (96%) | 177 (94%) | 12 (6%)  | 16          | 44 |
| 2   | B     | 187/189 (99%) | 180 (96%) | 7 (4%)   | 30          | 57 |
| 2   | D     | 187/189 (99%) | 183 (98%) | 4 (2%)   | 47          | 66 |
| 2   | F     | 187/189 (99%) | 183 (98%) | 4 (2%)   | 47          | 66 |
| 2   | H     | 187/189 (99%) | 182 (97%) | 5 (3%)   | 39          | 63 |
| 2   | J     | 187/189 (99%) | 177 (95%) | 10 (5%)  | 20          | 48 |
| 2   | L     | 187/189 (99%) | 181 (97%) | 6 (3%)   | 34          | 60 |
| 2   | N     | 187/189 (99%) | 179 (96%) | 8 (4%)   | 26          | 52 |
| 2   | P     | 187/189 (99%) | 176 (94%) | 11 (6%)  | 18          | 45 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 2   | R     | 188/189 (100%)  | 179 (95%)  | 9 (5%)   | 23          | 50 |
| 2   | T     | 187/189 (99%)   | 179 (96%)  | 8 (4%)   | 26          | 52 |
| All | All   | 3761/3850 (98%) | 3588 (95%) | 173 (5%) | 24          | 51 |

All (173) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 6   | GLU  |
| 1   | A     | 19  | SER  |
| 1   | A     | 31  | PHE  |
| 1   | A     | 33  | TYR  |
| 1   | A     | 64  | LEU  |
| 1   | A     | 115 | THR  |
| 1   | A     | 122 | LYS  |
| 1   | A     | 143 | LEU  |
| 1   | A     | 187 | VAL  |
| 2   | B     | 13  | VAL  |
| 2   | B     | 28  | SER  |
| 2   | B     | 50  | TYR  |
| 2   | B     | 53  | HIS  |
| 2   | B     | 55  | ILE  |
| 2   | B     | 78  | LEU  |
| 2   | B     | 89  | GLN  |
| 1   | C     | 6   | GLU  |
| 1   | C     | 20  | LEU  |
| 1   | C     | 53  | HIS  |
| 1   | C     | 54  | TYR  |
| 1   | C     | 55  | SER  |
| 1   | C     | 57  | TYR  |
| 1   | C     | 64  | LEU  |
| 1   | C     | 66  | THR  |
| 1   | C     | 83  | LEU  |
| 1   | C     | 122 | LYS  |
| 1   | C     | 164 | LEU  |
| 2   | D     | 13  | VAL  |
| 2   | D     | 27  | GLN  |
| 2   | D     | 30  | SER  |
| 2   | D     | 52  | SER  |
| 1   | E     | 11  | LEU  |
| 1   | E     | 20  | LEU  |
| 1   | E     | 25  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 30  | ARG  |
| 1   | E     | 31  | PHE  |
| 1   | E     | 34  | SER  |
| 1   | E     | 54  | TYR  |
| 1   | E     | 55  | SER  |
| 1   | E     | 57  | TYR  |
| 1   | E     | 110 | GLN  |
| 1   | E     | 134 | LYS  |
| 1   | E     | 164 | LEU  |
| 1   | E     | 197 | GLN  |
| 2   | F     | 13  | VAL  |
| 2   | F     | 27  | GLN  |
| 2   | F     | 31  | ASP  |
| 2   | F     | 109 | THR  |
| 1   | G     | 6   | GLU  |
| 1   | G     | 20  | LEU  |
| 1   | G     | 29  | ILE  |
| 1   | G     | 31  | PHE  |
| 1   | G     | 33  | TYR  |
| 1   | G     | 54  | TYR  |
| 1   | G     | 55  | SER  |
| 2   | H     | 13  | VAL  |
| 2   | H     | 50  | TYR  |
| 2   | H     | 90  | GLN  |
| 2   | H     | 108 | ARG  |
| 2   | H     | 147 | GLN  |
| 1   | I     | 6   | GLU  |
| 1   | I     | 30  | ARG  |
| 1   | I     | 51  | TYR  |
| 1   | I     | 53  | HIS  |
| 1   | I     | 54  | TYR  |
| 1   | I     | 58  | THR  |
| 1   | I     | 81  | LEU  |
| 1   | I     | 121 | THR  |
| 1   | I     | 122 | LYS  |
| 1   | I     | 175 | LEU  |
| 2   | J     | 13  | VAL  |
| 2   | J     | 27  | GLN  |
| 2   | J     | 29  | ILE  |
| 2   | J     | 33  | LEU  |
| 2   | J     | 48  | ILE  |
| 2   | J     | 89  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | J     | 90  | GLN  |
| 2   | J     | 97  | THR  |
| 2   | J     | 109 | THR  |
| 2   | J     | 136 | LEU  |
| 1   | K     | 6   | GLU  |
| 1   | K     | 20  | LEU  |
| 1   | K     | 31  | PHE  |
| 1   | K     | 33  | TYR  |
| 1   | K     | 34  | SER  |
| 1   | K     | 53  | HIS  |
| 1   | K     | 54  | TYR  |
| 1   | K     | 104 | TYR  |
| 2   | L     | 13  | VAL  |
| 2   | L     | 26  | SER  |
| 2   | L     | 46  | LEU  |
| 2   | L     | 78  | LEU  |
| 2   | L     | 96  | LEU  |
| 2   | L     | 109 | THR  |
| 1   | M     | 6   | GLU  |
| 1   | M     | 20  | LEU  |
| 1   | M     | 54  | TYR  |
| 1   | M     | 121 | THR  |
| 1   | M     | 202 | ASN  |
| 1   | M     | 209 | ASN  |
| 2   | N     | 13  | VAL  |
| 2   | N     | 32  | HIS  |
| 2   | N     | 48  | ILE  |
| 2   | N     | 50  | TYR  |
| 2   | N     | 61  | ARG  |
| 2   | N     | 78  | LEU  |
| 2   | N     | 179 | LEU  |
| 2   | N     | 183 | LYS  |
| 1   | O     | 18  | LEU  |
| 1   | O     | 29  | ILE  |
| 1   | O     | 30  | ARG  |
| 1   | O     | 33  | TYR  |
| 1   | O     | 55  | SER  |
| 1   | O     | 64  | LEU  |
| 1   | O     | 72  | ARG  |
| 1   | O     | 77  | ASN  |
| 1   | O     | 81  | LEU  |
| 1   | O     | 114 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 122 | LYS  |
| 1   | O     | 129 | LEU  |
| 1   | O     | 143 | LEU  |
| 1   | O     | 159 | TRP  |
| 1   | O     | 175 | LEU  |
| 1   | O     | 180 | LEU  |
| 1   | O     | 183 | LEU  |
| 1   | O     | 189 | VAL  |
| 2   | P     | 39  | LYS  |
| 2   | P     | 48  | ILE  |
| 2   | P     | 49  | LYS  |
| 2   | P     | 50  | TYR  |
| 2   | P     | 78  | LEU  |
| 2   | P     | 106 | ILE  |
| 2   | P     | 115 | VAL  |
| 2   | P     | 117 | ILE  |
| 2   | P     | 139 | PHE  |
| 2   | P     | 183 | LYS  |
| 2   | P     | 186 | TYR  |
| 1   | Q     | 6   | GLU  |
| 1   | Q     | 20  | LEU  |
| 1   | Q     | 29  | ILE  |
| 1   | Q     | 57  | TYR  |
| 1   | Q     | 63  | SER  |
| 1   | Q     | 64  | LEU  |
| 1   | Q     | 206 | LYS  |
| 2   | R     | 13  | VAL  |
| 2   | R     | 29  | ILE  |
| 2   | R     | 69  | THR  |
| 2   | R     | 70  | ASP  |
| 2   | R     | 78  | LEU  |
| 2   | R     | 92  | TYR  |
| 2   | R     | 96  | LEU  |
| 2   | R     | 209 | PHE  |
| 2   | R     | 210 | ASN  |
| 1   | S     | 6   | GLU  |
| 1   | S     | 20  | LEU  |
| 1   | S     | 29  | ILE  |
| 1   | S     | 31  | PHE  |
| 1   | S     | 53  | HIS  |
| 1   | S     | 60  | PHE  |
| 1   | S     | 63  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | S     | 64  | LEU  |
| 1   | S     | 66  | THR  |
| 1   | S     | 67  | ARG  |
| 1   | S     | 69  | THR  |
| 1   | S     | 153 | GLU  |
| 2   | T     | 13  | VAL  |
| 2   | T     | 47  | LEU  |
| 2   | T     | 78  | LEU  |
| 2   | T     | 89  | GLN  |
| 2   | T     | 109 | THR  |
| 2   | T     | 136 | LEU  |
| 2   | T     | 175 | LEU  |
| 2   | T     | 202 | SER  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 169 | HIS  |
| 2   | B     | 138 | ASN  |
| 1   | C     | 40  | GLN  |
| 2   | D     | 34  | HIS  |
| 2   | D     | 38  | GLN  |
| 2   | D     | 76  | ASN  |
| 2   | D     | 147 | GLN  |
| 1   | E     | 36  | HIS  |
| 1   | E     | 61  | ASN  |
| 1   | E     | 103 | ASN  |
| 2   | F     | 53  | HIS  |
| 2   | F     | 124 | GLN  |
| 2   | F     | 137 | ASN  |
| 2   | F     | 147 | GLN  |
| 1   | G     | 204 | ASN  |
| 2   | H     | 76  | ASN  |
| 2   | H     | 124 | GLN  |
| 2   | J     | 11  | GLN  |
| 2   | J     | 34  | HIS  |
| 2   | J     | 89  | GLN  |
| 2   | J     | 147 | GLN  |
| 1   | K     | 36  | HIS  |
| 1   | K     | 176 | GLN  |
| 2   | L     | 147 | GLN  |
| 1   | M     | 160 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 204 | ASN  |
| 2   | N     | 124 | GLN  |
| 1   | O     | 169 | HIS  |
| 2   | P     | 34  | HIS  |
| 2   | P     | 89  | GLN  |
| 2   | P     | 152 | ASN  |
| 2   | P     | 166 | GLN  |
| 2   | R     | 6   | GLN  |
| 2   | R     | 34  | HIS  |
| 2   | R     | 89  | GLN  |
| 2   | R     | 152 | ASN  |
| 1   | S     | 103 | ASN  |
| 1   | S     | 169 | HIS  |
| 2   | T     | 34  | HIS  |
| 2   | T     | 89  | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ > 2      | OWAB(Å <sup>2</sup> ) | Q < 0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|---------|
| 1   | A     | 218/225 (96%)   | 0.11   | 2 (0%) 81 58   | 78, 111, 160, 222     | 0       |
| 1   | C     | 218/225 (96%)   | 0.18   | 2 (0%) 81 58   | 91, 122, 177, 248     | 0       |
| 1   | E     | 218/225 (96%)   | 0.57   | 24 (11%) 10 8  | 102, 159, 254, 334    | 0       |
| 1   | G     | 218/225 (96%)   | 0.26   | 8 (3%) 45 27   | 84, 110, 166, 227     | 0       |
| 1   | I     | 218/225 (96%)   | 0.22   | 4 (1%) 67 43   | 105, 141, 196, 248    | 0       |
| 1   | K     | 218/225 (96%)   | 0.16   | 3 (1%) 73 49   | 111, 146, 197, 255    | 0       |
| 1   | M     | 218/225 (96%)   | 0.32   | 6 (2%) 55 33   | 86, 120, 200, 273     | 0       |
| 1   | O     | 218/225 (96%)   | 0.90   | 25 (11%) 9 7   | 120, 192, 301, 337    | 0       |
| 1   | Q     | 218/225 (96%)   | 0.24   | 6 (2%) 55 33   | 102, 138, 186, 228    | 0       |
| 1   | S     | 218/225 (96%)   | 0.59   | 5 (2%) 61 38   | 156, 224, 263, 304    | 0       |
| 2   | B     | 211/214 (98%)   | 0.11   | 3 (1%) 73 49   | 86, 120, 146, 170     | 0       |
| 2   | D     | 211/214 (98%)   | 0.24   | 2 (0%) 81 58   | 78, 123, 156, 173     | 0       |
| 2   | F     | 211/214 (98%)   | 0.35   | 6 (2%) 55 33   | 97, 139, 197, 224     | 0       |
| 2   | H     | 211/214 (98%)   | 0.05   | 1 (0%) 87 70   | 92, 122, 148, 171     | 0       |
| 2   | J     | 211/214 (98%)   | 0.21   | 3 (1%) 73 49   | 95, 131, 160, 193     | 0       |
| 2   | L     | 211/214 (98%)   | 0.13   | 6 (2%) 55 33   | 101, 133, 164, 184    | 0       |
| 2   | N     | 211/214 (98%)   | 0.33   | 3 (1%) 73 49   | 96, 142, 204, 251     | 0       |
| 2   | P     | 211/214 (98%)   | 0.89   | 20 (9%) 14 10  | 109, 191, 319, 344    | 0       |
| 2   | R     | 213/214 (99%)   | 0.20   | 5 (2%) 61 38   | 109, 152, 202, 223    | 0       |
| 2   | T     | 211/214 (98%)   | 0.76   | 12 (5%) 29 18  | 186, 255, 312, 338    | 0       |
| All | All   | 4292/4390 (97%) | 0.34   | 146 (3%) 48 29 | 78, 139, 262, 344     | 0       |

All (146) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | P     | 181 | LEU  | 7.8  |
| 1   | O     | 184 | SER  | 7.5  |
| 1   | I     | 1   | GLN  | 4.6  |
| 2   | P     | 151 | ASP  | 4.2  |
| 2   | T     | 104 | VAL  | 4.1  |
| 2   | P     | 206 | THR  | 4.0  |
| 1   | O     | 79  | PHE  | 3.9  |
| 1   | G     | 163 | ALA  | 3.9  |
| 2   | D     | 64  | GLY  | 3.8  |
| 1   | O     | 126 | VAL  | 3.7  |
| 1   | G     | 110 | GLN  | 3.7  |
| 2   | P     | 133 | VAL  | 3.7  |
| 1   | Q     | 209 | ASN  | 3.7  |
| 2   | L     | 181 | LEU  | 3.6  |
| 1   | K     | 184 | SER  | 3.6  |
| 1   | O     | 161 | SER  | 3.5  |
| 2   | P     | 191 | VAL  | 3.4  |
| 2   | P     | 150 | VAL  | 3.4  |
| 2   | F     | 65  | SER  | 3.4  |
| 2   | T     | 11  | GLN  | 3.3  |
| 2   | P     | 180 | THR  | 3.3  |
| 2   | L     | 187 | GLU  | 3.3  |
| 2   | P     | 192 | TYR  | 3.2  |
| 2   | P     | 176 | SER  | 3.2  |
| 1   | O     | 145 | CYS  | 3.2  |
| 1   | E     | 161 | SER  | 3.2  |
| 2   | T     | 193 | ALA  | 3.2  |
| 1   | O     | 131 | PRO  | 3.1  |
| 1   | E     | 99  | LYS  | 3.1  |
| 1   | K     | 101 | SER  | 3.1  |
| 2   | P     | 131 | SER  | 3.1  |
| 1   | G     | 197 | GLN  | 3.0  |
| 1   | C     | 30  | ARG  | 3.0  |
| 1   | E     | 26  | GLY  | 3.0  |
| 1   | E     | 129 | LEU  | 3.0  |
| 1   | I     | 2   | VAL  | 3.0  |
| 1   | I     | 101 | SER  | 2.9  |
| 2   | P     | 149 | LYS  | 2.9  |
| 2   | J     | 187 | GLU  | 2.8  |
| 1   | A     | 30  | ARG  | 2.8  |
| 1   | S     | 209 | ASN  | 2.8  |
| 1   | M     | 199 | TYR  | 2.7  |
| 1   | S     | 26  | GLY  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | B     | 64  | GLY  | 2.7  |
| 2   | J     | 56  | SER  | 2.7  |
| 2   | R     | 22  | THR  | 2.7  |
| 1   | G     | 99  | LYS  | 2.7  |
| 2   | T     | 26  | SER  | 2.7  |
| 1   | C     | 99  | LYS  | 2.6  |
| 2   | D     | 118 | PHE  | 2.6  |
| 1   | G     | 196 | THR  | 2.6  |
| 1   | O     | 143 | LEU  | 2.6  |
| 2   | P     | 106 | ILE  | 2.6  |
| 1   | G     | 120 | SER  | 2.5  |
| 1   | M     | 170 | THR  | 2.5  |
| 1   | O     | 165 | THR  | 2.5  |
| 1   | O     | 96  | CYS  | 2.5  |
| 1   | O     | 7   | SER  | 2.5  |
| 2   | P     | 64  | GLY  | 2.5  |
| 2   | P     | 135 | LEU  | 2.5  |
| 1   | M     | 130 | ALA  | 2.5  |
| 1   | E     | 144 | GLY  | 2.5  |
| 2   | F     | 67  | SER  | 2.4  |
| 2   | J     | 152 | ASN  | 2.4  |
| 1   | O     | 162 | GLY  | 2.4  |
| 1   | E     | 127 | PHE  | 2.4  |
| 1   | O     | 159 | TRP  | 2.4  |
| 2   | T     | 148 | TRP  | 2.4  |
| 1   | E     | 142 | ALA  | 2.4  |
| 1   | E     | 128 | PRO  | 2.4  |
| 1   | E     | 126 | VAL  | 2.4  |
| 1   | G     | 30  | ARG  | 2.4  |
| 1   | O     | 189 | VAL  | 2.4  |
| 1   | E     | 102 | GLY  | 2.4  |
| 1   | E     | 209 | ASN  | 2.4  |
| 1   | M     | 214 | LYS  | 2.4  |
| 2   | T     | 126 | LYS  | 2.4  |
| 1   | E     | 101 | SER  | 2.4  |
| 1   | O     | 193 | SER  | 2.3  |
| 1   | E     | 145 | CYS  | 2.3  |
| 2   | T     | 29  | ILE  | 2.3  |
| 2   | T     | 55  | ILE  | 2.3  |
| 2   | P     | 139 | PHE  | 2.3  |
| 1   | I     | 122 | LYS  | 2.3  |
| 1   | M     | 30  | ARG  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | Q     | 136 | THR  | 2.3  |
| 1   | K     | 64  | LEU  | 2.3  |
| 1   | M     | 99  | LYS  | 2.3  |
| 1   | O     | 188 | THR  | 2.3  |
| 1   | O     | 144 | GLY  | 2.3  |
| 2   | R     | 137 | ASN  | 2.3  |
| 2   | P     | 61  | ARG  | 2.3  |
| 1   | S     | 153 | GLU  | 2.2  |
| 1   | E     | 141 | ALA  | 2.2  |
| 2   | P     | 129 | THR  | 2.2  |
| 1   | A     | 132 | SER  | 2.2  |
| 1   | Q     | 135 | SER  | 2.2  |
| 2   | L     | 183 | LYS  | 2.2  |
| 1   | O     | 172 | PRO  | 2.2  |
| 1   | O     | 213 | ASP  | 2.2  |
| 1   | Q     | 218 | PRO  | 2.2  |
| 2   | L     | 64  | GLY  | 2.2  |
| 2   | R     | 10  | PHE  | 2.2  |
| 1   | E     | 216 | VAL  | 2.2  |
| 1   | O     | 185 | SER  | 2.2  |
| 1   | Q     | 137 | SER  | 2.2  |
| 2   | B     | 65  | SER  | 2.2  |
| 1   | E     | 204 | ASN  | 2.2  |
| 2   | H     | 184 | ALA  | 2.2  |
| 2   | T     | 204 | PRO  | 2.2  |
| 1   | G     | 193 | SER  | 2.1  |
| 2   | L     | 115 | VAL  | 2.1  |
| 1   | O     | 142 | ALA  | 2.1  |
| 1   | O     | 63  | SER  | 2.1  |
| 1   | Q     | 123 | GLY  | 2.1  |
| 2   | P     | 196 | VAL  | 2.1  |
| 1   | E     | 150 | TYR  | 2.1  |
| 2   | P     | 193 | ALA  | 2.1  |
| 1   | S     | 124 | PRO  | 2.1  |
| 2   | R     | 12  | SER  | 2.1  |
| 2   | T     | 177 | SER  | 2.1  |
| 2   | N     | 41  | ASP  | 2.1  |
| 2   | F     | 112 | ALA  | 2.1  |
| 2   | F     | 91  | GLY  | 2.1  |
| 1   | E     | 143 | LEU  | 2.1  |
| 1   | O     | 129 | LEU  | 2.1  |
| 1   | S     | 107 | TYR  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 132 | SER  | 2.0  |
| 1   | E     | 193 | SER  | 2.0  |
| 2   | L     | 65  | SER  | 2.0  |
| 2   | P     | 152 | ASN  | 2.0  |
| 1   | E     | 199 | TYR  | 2.0  |
| 2   | F     | 109 | THR  | 2.0  |
| 2   | F     | 184 | ALA  | 2.0  |
| 1   | O     | 31  | PHE  | 2.0  |
| 2   | B     | 139 | PHE  | 2.0  |
| 1   | O     | 6   | GLU  | 2.0  |
| 1   | E     | 98  | ARG  | 2.0  |
| 1   | O     | 166 | SER  | 2.0  |
| 1   | E     | 156 | THR  | 2.0  |
| 2   | N     | 164 | THR  | 2.0  |
| 2   | N     | 98  | PHE  | 2.0  |
| 2   | T     | 194 | CYS  | 2.0  |
| 1   | E     | 197 | GLN  | 2.0  |
| 2   | T     | 205 | VAL  | 2.0  |
| 2   | R     | 73  | LEU  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no 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.