



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:29 PM UTC

PDB ID : 4Y97 / pdb\_00004y97  
Title : Crystal Structure of human Pol alpha B-subunit in complex with C-terminal domain of catalytic subunit  
Authors : Suwa, Y.; Gu, J.; Baranovskiy, A.G.; Babayeva, N.D.; Tahirov, T.H.  
Deposited on : 2015-02-17  
Resolution : 2.51 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

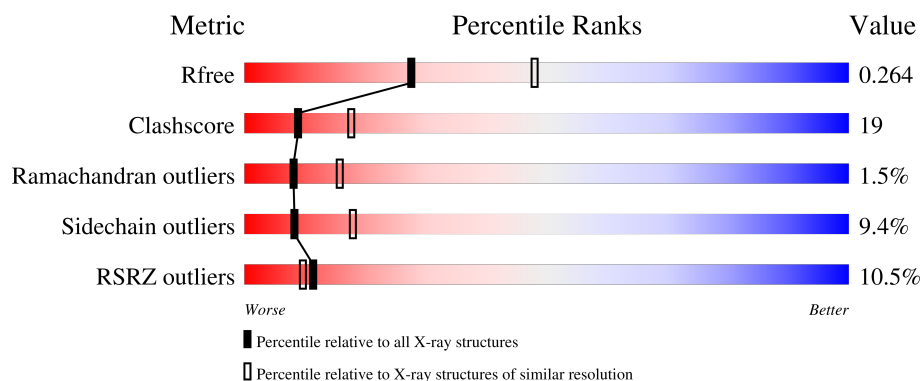
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.51 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 5829 (2.50-2.50)                                      |
| Clashscore            | 190562                      | 6492 (2.50-2.50)                                      |
| Ramachandran outliers | 187476                      | 6378 (2.50-2.50)                                      |
| Sidechain outliers    | 187428                      | 6380 (2.50-2.50)                                      |
| RSRZ outliers         | 180081                      | 5833 (2.50-2.50)                                      |

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     | 598    |                  |
| 1   | C     | 598    |                  |
| 1   | E     | 598    |                  |
| 1   | G     | 598    |                  |
| 2   | B     | 180    |                  |

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| Mol | Chain | Length | Quality of chain                                                                           |
|-----|-------|--------|--------------------------------------------------------------------------------------------|
| 2   | D     | 180    | <div><div></div><div>12%</div><div>64%</div><div>27%</div><div>7%</div><div>..</div></div> |
| 2   | F     | 180    | <div><div></div><div>10%</div><div>57%</div><div>37%</div><div>...</div></div>             |
| 2   | H     | 180    | <div><div></div><div>27%</div><div>52%</div><div>40%</div><div>7%</div><div>.</div></div>  |

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 19724 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 DNA polymerase alpha subunit B.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 442      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3439  | 2187 | 574 | 663 | 15 |         |         |       |
| 1   | C     | 441      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3435  | 2187 | 573 | 660 | 15 |         |         |       |
| 1   | E     | 439      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3422  | 2178 | 571 | 658 | 15 |         |         |       |
| 1   | G     | 436      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3400  | 2164 | 568 | 653 | 15 |         |         |       |

- Molecule 2 is a protein called DNA polymerase alpha catalytic subunit.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 2   | B     | 173      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1426  | 902 | 240 | 269 | 15 |         |         |       |
| 2   | D     | 178      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1466  | 926 | 248 | 277 | 15 |         |         |       |
| 2   | F     | 176      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1451  | 919 | 244 | 273 | 15 |         |         |       |
| 2   | H     | 179      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1475  | 931 | 250 | 279 | 15 |         |         |       |

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | B     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 3   | D     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 3   | F     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 3   | H     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

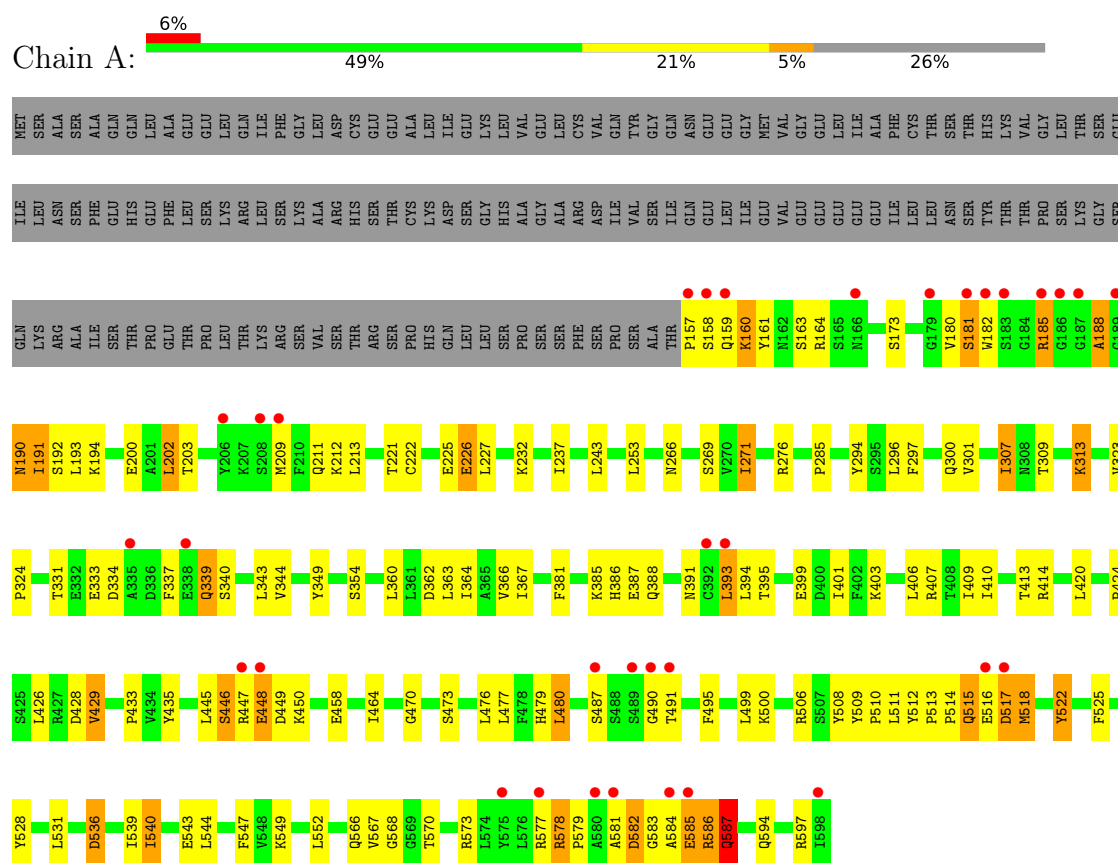
- Molecule 4 is water.

| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 4   | A     | 37       | Total<br>37 | O<br>37 | 0       | 0       |
| 4   | B     | 8        | Total<br>8  | O<br>8  | 0       | 0       |
| 4   | C     | 63       | Total<br>63 | O<br>63 | 0       | 0       |
| 4   | D     | 24       | Total<br>24 | O<br>24 | 0       | 0       |
| 4   | E     | 39       | Total<br>39 | O<br>39 | 0       | 0       |
| 4   | F     | 14       | Total<br>14 | O<br>14 | 0       | 0       |
| 4   | G     | 13       | Total<br>13 | O<br>13 | 0       | 0       |
| 4   | H     | 4        | Total<br>4  | O<br>4  | 0       | 0       |

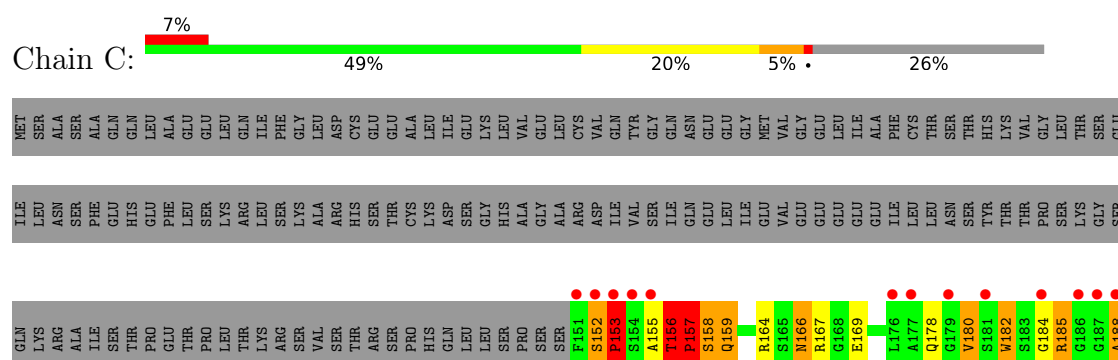
### 3 Residue-property plots

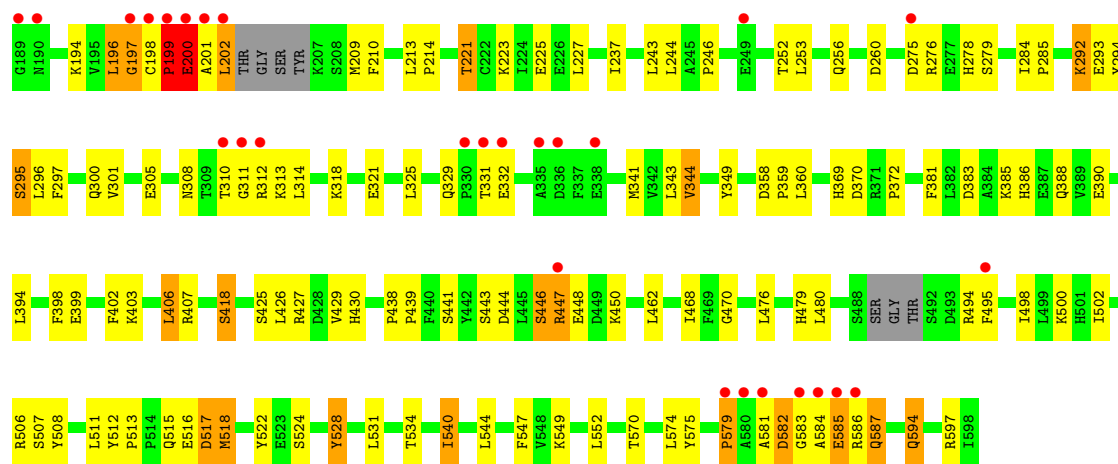
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

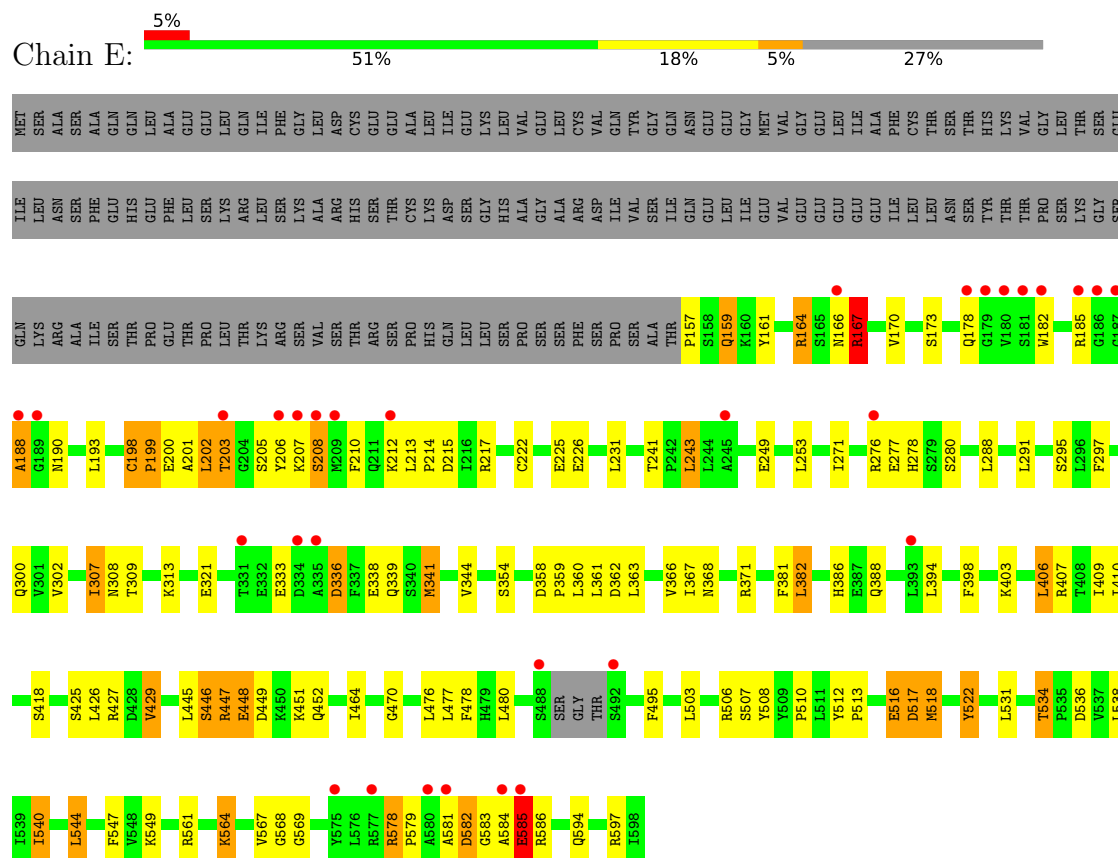


#### • Molecule 1: DNA polymerase alpha subunit B

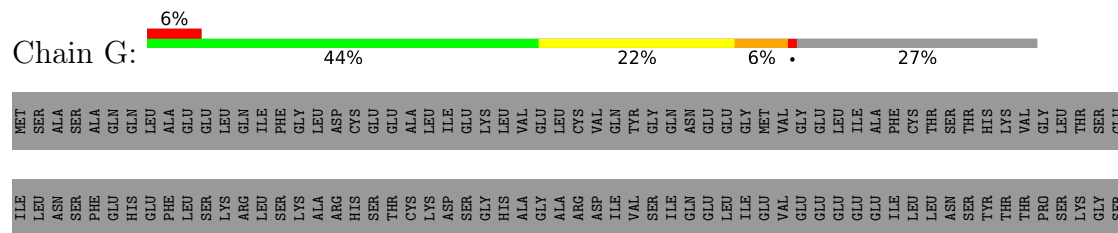


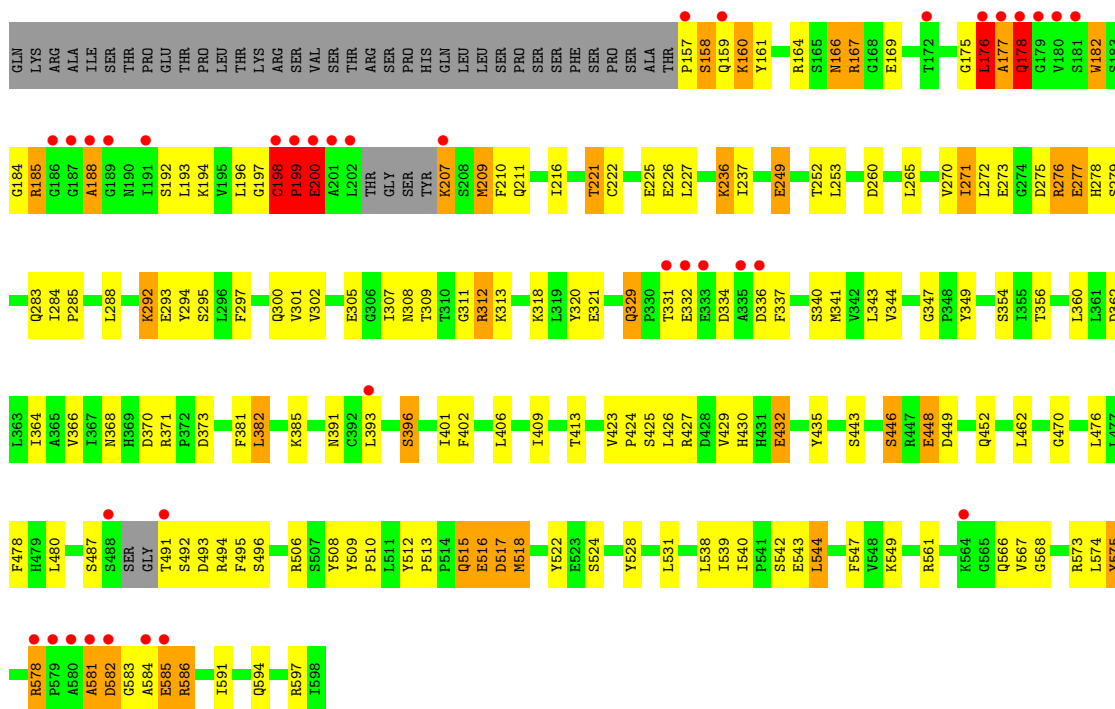


• Molecule 1: DNA polymerase alpha subunit B

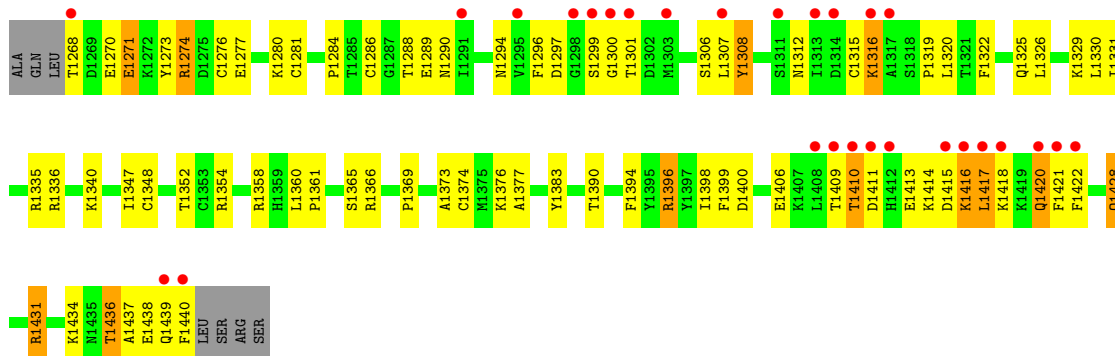


• Molecule 1: DNA polymerase alpha subunit B

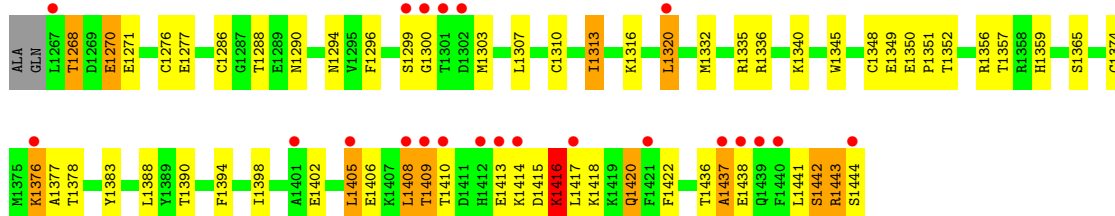




• Molecule 2: DNA polymerase alpha catalytic subunit



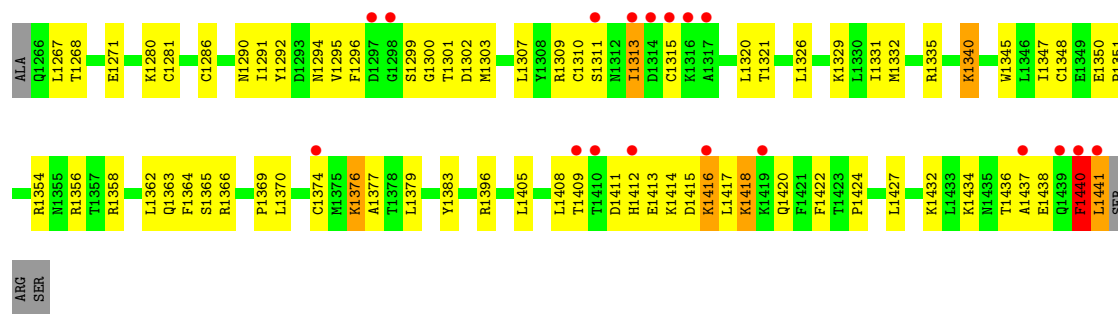
• Molecule 2: DNA polymerase alpha catalytic subunit



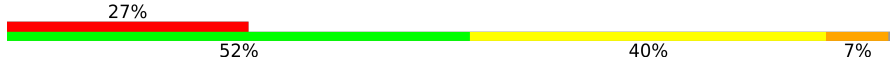
• Molecule 2: DNA polymerase alpha catalytic subunit

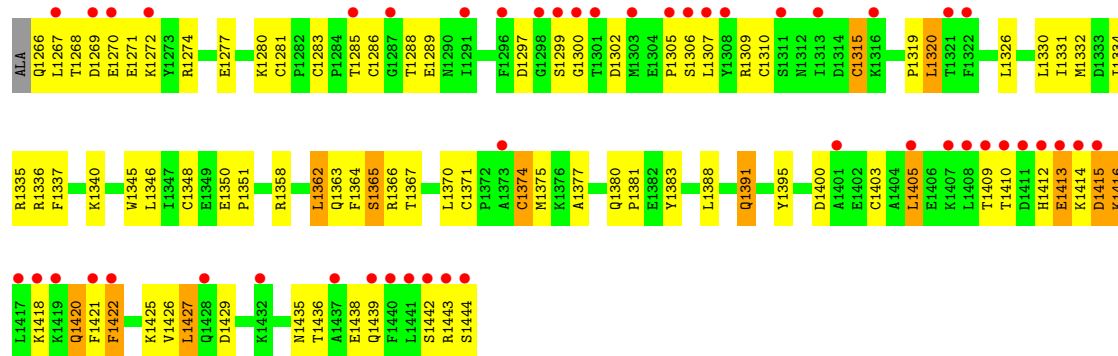


Chain F: 



• Molecule 2: DNA polymerase alpha catalytic subunit

Chain H: 



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 103.59Å 137.13Å 132.09Å<br>90.00° 100.97° 90.00°            | Depositor        |
| Resolution (Å)                                                          | 47.68 – 2.51<br>47.68 – 2.51                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 94.2 (47.68-2.51)<br>94.4 (47.68-2.51)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.08                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.07 (at 2.51Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.1                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.218 , 0.257<br>0.228 , 0.264                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 5894 reflections (5.04%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 31.2                                                        | Xtriage          |
| Anisotropy                                                              | 0.639                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 50.8                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.93                                                        | EDS              |
| Total number of atoms                                                   | 19724                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 50.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.52         | 0/3517  | 1.03        | 16/4777 (0.3%)   |
| 1   | C     | 0.58         | 0/3512  | 1.34        | 29/4769 (0.6%)   |
| 1   | E     | 0.54         | 0/3499  | 1.07        | 21/4751 (0.4%)   |
| 1   | G     | 0.47         | 0/3475  | 1.15        | 29/4717 (0.6%)   |
| 2   | B     | 0.48         | 0/1459  | 1.08        | 8/1967 (0.4%)    |
| 2   | D     | 0.49         | 0/1499  | 0.98        | 8/2019 (0.4%)    |
| 2   | F     | 0.47         | 0/1484  | 1.02        | 7/2001 (0.3%)    |
| 2   | H     | 0.42         | 0/1508  | 0.97        | 7/2031 (0.3%)    |
| All | All   | 0.51         | 0/19953 | 1.11        | 125/27032 (0.5%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | E     | 0                   | 1                   |

There are no bond length outliers.

All (125) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 1   | C     | 156  | THR  | CA-C-N | 35.00  | 163.59      | 119.84   |
| 1   | C     | 156  | THR  | C-N-CA | 35.00  | 163.59      | 119.84   |
| 1   | G     | 198  | CYS  | CA-C-N | 20.53  | 145.50      | 119.84   |
| 1   | G     | 198  | CYS  | C-N-CA | 20.53  | 145.50      | 119.84   |
| 2   | B     | 1439 | GLN  | N-CA-C | -17.60 | 92.21       | 114.56   |
| 1   | C     | 198  | CYS  | CA-C-N | 13.29  | 136.45      | 119.84   |
| 1   | C     | 198  | CYS  | C-N-CA | 13.29  | 136.45      | 119.84   |
| 1   | G     | 198  | CYS  | N-CA-C | -12.16 | 82.94       | 109.81   |

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| Mol | Chain | Res  | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1   | C     | 156  | THR  | C-N-CD   | -11.96 | 75.98       | 125.00   |
| 1   | G     | 197  | GLY  | N-CA-C   | 10.32  | 130.63      | 111.12   |
| 2   | F     | 1374 | CYS  | N-CA-C   | -9.90  | 95.83       | 110.48   |
| 1   | C     | 582  | ASP  | N-CA-C   | 9.83   | 125.95      | 110.32   |
| 2   | B     | 1374 | CYS  | N-CA-C   | -9.78  | 96.01       | 110.48   |
| 2   | H     | 1374 | CYS  | N-CA-C   | -9.75  | 96.04       | 110.48   |
| 1   | C     | 180  | VAL  | N-CA-C   | -9.68  | 103.71      | 113.10   |
| 1   | C     | 152  | SER  | CA-C-N   | 9.62   | 131.87      | 119.84   |
| 1   | C     | 152  | SER  | C-N-CA   | 9.62   | 131.87      | 119.84   |
| 2   | D     | 1374 | CYS  | N-CA-C   | -9.49  | 96.43       | 110.48   |
| 1   | G     | 582  | ASP  | N-CA-C   | 9.15   | 124.86      | 110.32   |
| 1   | E     | 582  | ASP  | N-CA-C   | 9.10   | 124.80      | 110.32   |
| 1   | A     | 582  | ASP  | N-CA-C   | 8.80   | 124.31      | 110.32   |
| 1   | E     | 205  | SER  | N-CA-C   | 8.75   | 120.89      | 111.36   |
| 1   | E     | 178  | GLN  | N-CA-C   | -8.45  | 97.33       | 110.42   |
| 1   | G     | 429  | VAL  | N-CA-C   | 7.78   | 119.49      | 110.62   |
| 1   | A     | 429  | VAL  | N-CA-C   | 7.75   | 119.46      | 110.62   |
| 1   | C     | 429  | VAL  | N-CA-C   | 7.66   | 119.35      | 110.62   |
| 1   | E     | 429  | VAL  | N-CA-C   | 7.55   | 119.23      | 110.62   |
| 1   | C     | 152  | SER  | N-CA-C   | 7.46   | 118.70      | 110.13   |
| 1   | E     | 210  | PHE  | N-CA-C   | -7.41  | 95.38       | 108.13   |
| 1   | C     | 182  | TRP  | N-CA-C   | -7.12  | 97.65       | 109.46   |
| 1   | G     | 200  | GLU  | N-CA-C   | 6.81   | 125.31      | 110.80   |
| 1   | G     | 381  | PHE  | N-CA-C   | -6.76  | 104.67      | 113.12   |
| 1   | C     | 390  | GLU  | CA-CB-CG | 6.76   | 127.62      | 114.10   |
| 2   | H     | 1416 | LYS  | N-CA-C   | -6.75  | 104.00      | 111.36   |
| 1   | A     | 181  | SER  | N-CA-C   | -6.74  | 99.05       | 109.76   |
| 1   | E     | 381  | PHE  | N-CA-C   | -6.68  | 104.77      | 113.12   |
| 1   | C     | 381  | PHE  | N-CA-C   | -6.47  | 105.03      | 113.12   |
| 1   | A     | 381  | PHE  | N-CA-C   | -6.39  | 105.13      | 113.12   |
| 1   | G     | 198  | CYS  | C-N-CD   | -6.29  | 99.21       | 125.00   |
| 1   | C     | 153  | PRO  | N-CA-C   | 6.24   | 125.33      | 112.47   |
| 2   | F     | 1422 | PHE  | N-CA-C   | 6.21   | 118.93      | 109.62   |
| 2   | D     | 1416 | LYS  | N-CA-C   | -6.21  | 104.59      | 111.36   |
| 1   | G     | 581  | ALA  | N-CA-C   | 6.17   | 123.93      | 110.80   |
| 2   | F     | 1409 | THR  | N-CA-C   | 6.11   | 117.63      | 110.97   |
| 2   | D     | 1422 | PHE  | N-CA-C   | 6.10   | 118.77      | 109.62   |
| 1   | A     | 581  | ALA  | N-CA-C   | 6.08   | 123.75      | 110.80   |
| 1   | A     | 491  | THR  | N-CA-C   | -6.06  | 105.47      | 112.92   |
| 1   | A     | 188  | ALA  | N-CA-C   | 6.04   | 118.81      | 110.35   |
| 1   | E     | 581  | ALA  | N-CA-C   | 6.03   | 123.65      | 110.80   |
| 1   | C     | 188  | ALA  | N-CA-C   | 5.99   | 118.74      | 110.35   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | B     | 1422 | PHE  | N-CA-C  | 5.97  | 118.58      | 109.62   |
| 2   | D     | 1442 | SER  | N-CA-C  | -5.94 | 106.17      | 113.41   |
| 1   | C     | 581  | ALA  | N-CA-C  | 5.89  | 123.35      | 110.80   |
| 2   | H     | 1409 | THR  | N-CA-C  | 5.89  | 117.39      | 110.97   |
| 1   | E     | 470  | GLY  | N-CA-C  | -5.87 | 100.73      | 110.95   |
| 1   | G     | 199  | PRO  | N-CA-C  | 5.86  | 124.54      | 112.47   |
| 1   | A     | 446  | SER  | N-CA-C  | -5.86 | 102.93      | 110.19   |
| 2   | H     | 1299 | SER  | N-CA-C  | 5.83  | 119.17      | 110.14   |
| 2   | H     | 1422 | PHE  | N-CA-C  | 5.81  | 118.34      | 109.62   |
| 1   | E     | 188  | ALA  | N-CA-C  | 5.81  | 118.48      | 110.35   |
| 1   | E     | 208  | SER  | N-CA-C  | -5.79 | 100.26      | 109.76   |
| 2   | F     | 1440 | PHE  | N-CA-C  | -5.78 | 98.49       | 110.80   |
| 1   | C     | 199  | PRO  | N-CA-C  | 5.76  | 124.34      | 112.47   |
| 1   | A     | 543  | GLU  | N-CA-C  | -5.76 | 105.75      | 112.89   |
| 2   | B     | 1409 | THR  | N-CA-C  | 5.76  | 117.25      | 110.97   |
| 1   | G     | 197  | GLY  | CA-C-N  | 5.75  | 135.84      | 121.80   |
| 1   | G     | 197  | GLY  | C-N-CA  | 5.75  | 135.84      | 121.80   |
| 2   | B     | 1416 | LYS  | N-CA-C  | -5.72 | 105.12      | 111.36   |
| 2   | D     | 1409 | THR  | N-CA-C  | 5.71  | 117.19      | 110.97   |
| 1   | G     | 188  | ALA  | N-CA-C  | 5.70  | 118.32      | 110.35   |
| 1   | G     | 522  | TYR  | N-CA-C  | 5.69  | 118.25      | 111.71   |
| 1   | C     | 446  | SER  | N-CA-C  | -5.62 | 103.22      | 110.19   |
| 1   | G     | 446  | SER  | N-CA-C  | -5.58 | 103.28      | 110.19   |
| 1   | E     | 446  | SER  | N-CA-C  | -5.57 | 103.28      | 110.19   |
| 2   | F     | 1436 | THR  | N-CA-C  | -5.55 | 105.33      | 111.71   |
| 2   | F     | 1299 | SER  | N-CA-C  | 5.53  | 118.59      | 109.85   |
| 1   | G     | 182  | TRP  | N-CA-C  | -5.52 | 100.98      | 109.76   |
| 1   | C     | 522  | TYR  | N-CA-C  | 5.51  | 118.22      | 111.82   |
| 1   | E     | 516  | GLU  | N-CA-C  | 5.49  | 118.57      | 108.58   |
| 1   | C     | 470  | GLY  | N-CA-C  | -5.49 | 101.40      | 110.95   |
| 1   | C     | 331  | THR  | N-CA-C  | -5.46 | 102.68      | 110.59   |
| 2   | F     | 1365 | SER  | N-CA-C  | -5.45 | 101.39      | 109.94   |
| 1   | G     | 578  | ARG  | CA-C-N  | 5.44  | 126.20      | 120.11   |
| 1   | G     | 578  | ARG  | C-N-CA  | 5.44  | 126.20      | 120.11   |
| 1   | C     | 157  | PRO  | CA-N-CD | -5.44 | 104.39      | 112.00   |
| 1   | C     | 184  | GLY  | N-CA-C  | -5.42 | 104.01      | 112.58   |
| 2   | B     | 1365 | SER  | N-CA-C  | -5.40 | 101.46      | 109.94   |
| 1   | G     | 331  | THR  | N-CA-C  | -5.34 | 102.85      | 110.59   |
| 1   | A     | 528  | TYR  | N-CA-C  | 5.33  | 120.44      | 113.30   |
| 1   | G     | 178  | GLN  | N-CA-C  | 5.29  | 118.05      | 109.79   |
| 2   | B     | 1299 | SER  | N-CA-C  | 5.27  | 118.18      | 109.85   |
| 1   | A     | 470  | GLY  | N-CA-C  | -5.27 | 101.78      | 110.95   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | E     | 536  | ASP  | N-CA-C | -5.26 | 105.22      | 111.69   |
| 1   | E     | 522  | TYR  | N-CA-C | 5.26  | 117.75      | 111.71   |
| 1   | E     | 295  | SER  | N-CA-C | -5.25 | 99.55       | 108.26   |
| 1   | C     | 587  | GLN  | N-CA-C | -5.24 | 96.75       | 107.70   |
| 1   | G     | 470  | GLY  | N-CA-C | -5.22 | 101.86      | 110.95   |
| 2   | D     | 1299 | SER  | N-CA-C | 5.19  | 118.05      | 109.85   |
| 1   | A     | 587  | GLN  | N-CA-C | -5.18 | 96.88       | 107.70   |
| 1   | G     | 184  | GLY  | N-CA-C | -5.17 | 103.67      | 112.51   |
| 1   | A     | 578  | ARG  | CA-C-N | 5.16  | 125.89      | 120.11   |
| 1   | A     | 578  | ARG  | C-N-CA | 5.16  | 125.89      | 120.11   |
| 1   | G     | 516  | GLU  | N-CA-C | 5.14  | 117.94      | 108.58   |
| 1   | A     | 522  | TYR  | N-CA-C | 5.14  | 117.62      | 111.71   |
| 2   | B     | 1436 | THR  | N-CA-C | -5.14 | 105.80      | 111.71   |
| 1   | E     | 198  | CYS  | CA-C-N | 5.12  | 126.24      | 119.84   |
| 1   | E     | 198  | CYS  | C-N-CA | 5.12  | 126.24      | 119.84   |
| 1   | E     | 578  | ARG  | CA-C-N | 5.11  | 125.84      | 120.11   |
| 1   | E     | 578  | ARG  | C-N-CA | 5.11  | 125.84      | 120.11   |
| 1   | C     | 295  | SER  | N-CA-C | -5.10 | 99.79       | 108.26   |
| 1   | C     | 534  | THR  | N-CA-C | -5.09 | 101.88      | 109.42   |
| 1   | E     | 585  | GLU  | N-CA-C | 5.09  | 121.65      | 110.80   |
| 1   | G     | 295  | SER  | N-CA-C | -5.09 | 99.81       | 108.26   |
| 1   | G     | 543  | GLU  | N-CA-C | -5.08 | 106.59      | 112.89   |
| 1   | G     | 528  | TYR  | N-CA-C | 5.07  | 120.10      | 113.30   |
| 1   | A     | 536  | ASP  | N-CA-C | -5.07 | 105.85      | 112.23   |
| 1   | C     | 528  | TYR  | N-CA-C | 5.07  | 120.09      | 113.30   |
| 2   | D     | 1365 | SER  | N-CA-C | -5.07 | 101.98      | 109.94   |
| 2   | H     | 1436 | THR  | N-CA-C | -5.06 | 105.89      | 111.71   |
| 2   | H     | 1365 | SER  | N-CA-C | -5.06 | 102.00      | 109.94   |
| 1   | G     | 197  | GLY  | CA-C-O | 5.05  | 125.89      | 120.94   |
| 1   | C     | 579  | PRO  | N-CA-C | 5.04  | 118.54      | 111.33   |
| 2   | D     | 1436 | THR  | N-CA-C | -5.04 | 105.92      | 111.71   |
| 1   | E     | 534  | THR  | N-CA-C | -5.03 | 101.98      | 109.42   |
| 1   | G     | 277  | GLU  | N-CA-C | 5.02  | 117.41      | 111.33   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | E     | 522 | TYR  | Sidechain |

## 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     | 3439  | 0        | 3414     | 137     | 0            |
| 1   | C     | 3435  | 0        | 3410     | 139     | 0            |
| 1   | E     | 3422  | 0        | 3398     | 85      | 0            |
| 1   | G     | 3400  | 0        | 3380     | 151     | 0            |
| 2   | B     | 1426  | 0        | 1389     | 53      | 0            |
| 2   | D     | 1466  | 0        | 1434     | 51      | 0            |
| 2   | F     | 1451  | 0        | 1419     | 64      | 0            |
| 2   | H     | 1475  | 0        | 1442     | 79      | 0            |
| 3   | B     | 2     | 0        | 0        | 0       | 0            |
| 3   | D     | 2     | 0        | 0        | 0       | 0            |
| 3   | F     | 2     | 0        | 0        | 0       | 0            |
| 3   | H     | 2     | 0        | 0        | 0       | 0            |
| 4   | A     | 37    | 0        | 0        | 3       | 0            |
| 4   | B     | 8     | 0        | 0        | 0       | 0            |
| 4   | C     | 63    | 0        | 0        | 3       | 0            |
| 4   | D     | 24    | 0        | 0        | 2       | 0            |
| 4   | E     | 39    | 0        | 0        | 4       | 0            |
| 4   | F     | 14    | 0        | 0        | 2       | 0            |
| 4   | G     | 13    | 0        | 0        | 2       | 0            |
| 4   | H     | 4     | 0        | 0        | 0       | 0            |
| All | All   | 19724 | 0        | 19286    | 722     | 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 19.

All (722) 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:E:161:TYR:O    | 1:E:164:ARG:HD2  | 1.42                     | 1.16              |
| 1:G:209:MET:HB2  | 2:H:1443:ARG:HB3 | 1.30                     | 1.11              |
| 1:C:185:ARG:HH11 | 1:C:185:ARG:HB3  | 1.06                     | 1.08              |
| 1:G:169:GLU:HB3  | 1:G:597:ARG:HD2  | 1.40                     | 1.03              |
| 1:C:166:ASN:HD22 | 1:C:166:ASN:N    | 1.54                     | 1.03              |
| 1:E:164:ARG:HG3  | 1:E:164:ARG:HH11 | 1.23                     | 1.01              |
| 2:H:1307:LEU:O   | 2:H:1319:PRO:HG2 | 1.62                     | 1.00              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:166:ASN:H     | 1:C:166:ASN:ND2   | 1.46                     | 0.99              |
| 1:C:152:SER:HB3   | 1:C:153:PRO:HD2   | 1.43                     | 0.98              |
| 1:A:157:PRO:O     | 1:A:159:GLN:N     | 1.97                     | 0.96              |
| 1:G:198:CYS:N     | 1:G:199:PRO:HD3   | 1.79                     | 0.95              |
| 2:F:1267:LEU:HD22 | 2:F:1271:GLU:HG3  | 1.48                     | 0.95              |
| 2:H:1412:HIS:O    | 2:H:1416:LYS:HG3  | 1.67                     | 0.94              |
| 2:F:1313:ILE:HD13 | 2:F:1313:ILE:H    | 1.34                     | 0.92              |
| 1:C:246:PRO:HG3   | 1:C:311:GLY:HA3   | 1.49                     | 0.91              |
| 1:A:160:LYS:HE3   | 1:A:160:LYS:H     | 1.32                     | 0.91              |
| 2:D:1376:LYS:HE2  | 2:D:1376:LYS:HA   | 1.52                     | 0.91              |
| 2:B:1288:THR:HG21 | 2:B:1312:ASN:HB2  | 1.50                     | 0.90              |
| 1:C:495:PHE:HB2   | 1:C:549:LYS:HE3   | 1.54                     | 0.90              |
| 2:F:1268:THR:HG22 | 2:F:1271:GLU:HG2  | 1.54                     | 0.89              |
| 1:G:198:CYS:N     | 1:G:199:PRO:CD    | 2.28                     | 0.89              |
| 2:D:1313:ILE:HD12 | 2:D:1313:ILE:H    | 1.35                     | 0.88              |
| 1:G:426:LEU:HD11  | 1:G:518:MET:HE3   | 1.53                     | 0.88              |
| 1:G:209:MET:HB2   | 2:H:1443:ARG:CB   | 2.04                     | 0.87              |
| 1:A:160:LYS:H     | 1:A:160:LYS:CE    | 1.86                     | 0.87              |
| 1:A:506:ARG:HG2   | 1:A:506:ARG:HH11  | 1.40                     | 0.87              |
| 1:C:185:ARG:HB3   | 1:C:185:ARG:NH1   | 1.90                     | 0.86              |
| 1:G:185:ARG:CG    | 1:G:188:ALA:HB3   | 2.07                     | 0.85              |
| 2:B:1286:CYS:SG   | 2:B:1288:THR:HG22 | 2.15                     | 0.85              |
| 2:D:1409:THR:HG23 | 2:D:1410:THR:HG23 | 1.58                     | 0.82              |
| 1:G:432:GLU:HG2   | 2:H:1442:SER:H    | 1.46                     | 0.81              |
| 1:C:185:ARG:HH11  | 1:C:185:ARG:CB    | 1.92                     | 0.81              |
| 1:A:227:LEU:HD23  | 1:A:301:VAL:HB    | 1.63                     | 0.80              |
| 1:A:393:LEU:HD23  | 1:A:394:LEU:N     | 1.96                     | 0.80              |
| 1:C:244:LEU:O     | 1:C:246:PRO:HD3   | 1.80                     | 0.80              |
| 1:G:432:GLU:HG3   | 2:H:1442:SER:HB2  | 1.62                     | 0.80              |
| 1:C:166:ASN:HD22  | 1:C:166:ASN:H     | 0.81                     | 0.79              |
| 2:B:1414:LYS:HG3  | 2:B:1415:ASP:N    | 1.96                     | 0.79              |
| 1:C:185:ARG:HB2   | 1:C:188:ALA:HB3   | 1.63                     | 0.79              |
| 2:H:1331:ILE:O    | 2:H:1335:ARG:HG3  | 1.82                     | 0.79              |
| 1:G:198:CYS:H     | 1:G:199:PRO:CD    | 1.71                     | 0.79              |
| 2:H:1414:LYS:HG3  | 2:H:1415:ASP:N    | 1.97                     | 0.79              |
| 1:A:516:GLU:O     | 1:A:517:ASP:HB2   | 1.83                     | 0.79              |
| 1:C:516:GLU:O     | 1:C:517:ASP:HB2   | 1.82                     | 0.78              |
| 1:A:271:ILE:HD12  | 1:A:271:ILE:C     | 2.08                     | 0.78              |
| 2:H:1271:GLU:HG2  | 2:H:1274:ARG:HH21 | 1.49                     | 0.78              |
| 1:C:156:THR:HG22  | 1:C:157:PRO:N     | 1.97                     | 0.78              |
| 2:F:1376:LYS:O    | 2:F:1376:LYS:HD3  | 1.82                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:1331:ILE:O    | 2:F:1335:ARG:HG3  | 1.83                     | 0.78              |
| 1:G:292:LYS:H     | 1:G:292:LYS:HD3   | 1.47                     | 0.78              |
| 1:G:199:PRO:HG2   | 1:G:200:GLU:H     | 1.49                     | 0.77              |
| 1:C:407:ARG:HH22  | 1:C:444:ASP:CG    | 1.92                     | 0.77              |
| 1:A:339:GLN:HG2   | 1:A:577:ARG:NH2   | 1.98                     | 0.76              |
| 1:G:185:ARG:HD2   | 1:G:373:ASP:OD2   | 1.85                     | 0.76              |
| 2:F:1412:HIS:HD2  | 2:F:1413:GLU:H    | 1.32                     | 0.76              |
| 1:E:516:GLU:O     | 1:E:517:ASP:HB2   | 1.86                     | 0.76              |
| 2:H:1410:THR:HG22 | 2:H:1412:HIS:H    | 1.51                     | 0.76              |
| 1:C:407:ARG:HH11  | 1:C:407:ARG:HG3   | 1.51                     | 0.75              |
| 2:D:1414:LYS:NZ   | 2:D:1418:LYS:HD3  | 2.00                     | 0.75              |
| 2:B:1268:THR:HB   | 2:B:1271:GLU:CD   | 2.10                     | 0.75              |
| 1:G:516:GLU:O     | 1:G:517:ASP:HB2   | 1.84                     | 0.75              |
| 1:E:386:HIS:HD2   | 1:E:388:GLN:H     | 1.34                     | 0.75              |
| 1:G:209:MET:O     | 1:G:209:MET:HG2   | 1.86                     | 0.75              |
| 1:G:175:GLY:C     | 1:G:177:ALA:H     | 1.95                     | 0.74              |
| 1:A:160:LYS:H     | 1:A:160:LYS:CD    | 2.00                     | 0.73              |
| 2:D:1402:GLU:O    | 2:D:1406:GLU:HG2  | 1.86                     | 0.73              |
| 2:F:1313:ILE:HD13 | 2:F:1313:ILE:N    | 2.03                     | 0.73              |
| 1:A:313:LYS:HB2   | 1:A:313:LYS:NZ    | 2.03                     | 0.73              |
| 2:B:1307:LEU:HD11 | 2:B:1326:LEU:HD11 | 1.71                     | 0.73              |
| 2:B:1411:ASP:HA   | 2:B:1414:LYS:HG2  | 1.69                     | 0.73              |
| 1:G:292:LYS:HD3   | 1:G:292:LYS:N     | 2.03                     | 0.73              |
| 1:G:300:GLN:HG2   | 1:G:302:VAL:HG13  | 1.69                     | 0.73              |
| 1:E:276:ARG:HD2   | 1:G:277:GLU:O     | 1.89                     | 0.73              |
| 1:C:246:PRO:HG3   | 1:C:311:GLY:CA    | 2.19                     | 0.72              |
| 2:B:1414:LYS:HG3  | 2:B:1415:ASP:H    | 1.50                     | 0.72              |
| 1:E:164:ARG:HG3   | 1:E:164:ARG:NH1   | 1.94                     | 0.72              |
| 1:G:284:ILE:HD12  | 1:G:285:PRO:O     | 1.90                     | 0.71              |
| 1:A:157:PRO:C     | 1:A:159:GLN:H     | 1.96                     | 0.71              |
| 2:H:1280:LYS:HB3  | 2:H:1289:GLU:OE1  | 1.90                     | 0.71              |
| 2:B:1360:LEU:HD12 | 2:B:1361:PRO:HD2  | 1.71                     | 0.71              |
| 1:C:152:SER:HB3   | 1:C:153:PRO:CD    | 2.19                     | 0.71              |
| 2:H:1307:LEU:HD11 | 2:H:1326:LEU:HD11 | 1.72                     | 0.71              |
| 1:C:426:LEU:CD1   | 1:C:518:MET:HE3   | 2.20                     | 0.70              |
| 2:F:1396:ARG:NH1  | 2:F:1434:LYS:HE2  | 2.05                     | 0.70              |
| 1:G:271:ILE:HD12  | 1:G:272:LEU:N     | 2.07                     | 0.70              |
| 1:G:506:ARG:HG2   | 1:G:506:ARG:HH11  | 1.56                     | 0.70              |
| 1:C:312:ARG:NH1   | 1:C:313:LYS:HD2   | 2.06                     | 0.70              |
| 1:G:185:ARG:HG2   | 1:G:188:ALA:HB3   | 1.73                     | 0.70              |
| 2:F:1416:LYS:NZ   | 2:F:1416:LYS:HB3  | 2.07                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:1294:ASN:HD22 | 2:F:1296:PHE:H    | 1.38                     | 0.69              |
| 2:B:1268:THR:HB   | 2:B:1271:GLU:CG   | 2.23                     | 0.69              |
| 2:H:1268:THR:HB   | 2:H:1271:GLU:OE1  | 1.92                     | 0.69              |
| 1:C:166:ASN:N     | 1:C:166:ASN:ND2   | 2.22                     | 0.69              |
| 2:F:1268:THR:HG22 | 2:F:1271:GLU:CG   | 2.22                     | 0.69              |
| 2:B:1271:GLU:O    | 2:B:1274:ARG:HG2  | 1.93                     | 0.68              |
| 1:A:409:ILE:O     | 1:A:413:THR:HG22  | 1.93                     | 0.68              |
| 2:F:1412:HIS:HD2  | 2:F:1413:GLU:N    | 1.92                     | 0.68              |
| 1:C:369:HIS:HD2   | 1:C:370:ASP:OD1   | 1.76                     | 0.68              |
| 1:C:156:THR:HG23  | 1:C:159:GLN:CB    | 2.24                     | 0.68              |
| 1:C:332:GLU:OE2   | 1:C:332:GLU:HA    | 1.94                     | 0.68              |
| 1:C:292:LYS:H     | 1:C:292:LYS:HD2   | 1.58                     | 0.68              |
| 2:F:1280:LYS:HG2  | 2:F:1291:ILE:HG12 | 1.76                     | 0.68              |
| 1:A:160:LYS:HE3   | 1:A:160:LYS:N     | 2.06                     | 0.68              |
| 1:A:446:SER:O     | 1:A:450:LYS:HG3   | 1.94                     | 0.68              |
| 1:G:207:LYS:HB2   | 1:G:207:LYS:NZ    | 2.08                     | 0.67              |
| 2:D:1349:GLU:HG2  | 2:D:1378:THR:O    | 1.94                     | 0.67              |
| 1:C:196:LEU:HD23  | 1:C:197:GLY:H     | 1.58                     | 0.67              |
| 2:D:1376:LYS:O    | 2:D:1376:LYS:HD3  | 1.95                     | 0.67              |
| 1:C:200:GLU:HG2   | 1:C:528:TYR:CG    | 2.28                     | 0.67              |
| 1:A:313:LYS:HE2   | 2:F:1313:ILE:HB   | 1.75                     | 0.67              |
| 1:A:386:HIS:HD2   | 1:A:388:GLN:H     | 1.42                     | 0.67              |
| 1:A:477:LEU:HD11  | 1:A:540:ILE:HD13  | 1.77                     | 0.67              |
| 2:F:1292:TYR:CE2  | 2:F:1307:LEU:HD12 | 2.29                     | 0.67              |
| 2:F:1441:LEU:O    | 2:F:1441:LEU:HG   | 1.95                     | 0.67              |
| 1:G:160:LYS:NZ    | 1:G:566:GLN:NE2   | 2.43                     | 0.66              |
| 1:C:196:LEU:CD2   | 1:C:197:GLY:H     | 2.08                     | 0.66              |
| 2:F:1294:ASN:ND2  | 2:F:1296:PHE:H    | 1.93                     | 0.66              |
| 1:C:275:ASP:OD2   | 1:C:278:HIS:ND1   | 2.26                     | 0.66              |
| 1:C:403:LYS:NZ    | 1:E:407:ARG:HH22  | 1.94                     | 0.66              |
| 1:A:185:ARG:HB3   | 1:A:188:ALA:HB3   | 1.78                     | 0.66              |
| 1:A:477:LEU:HD21  | 1:A:499:LEU:HD21  | 1.78                     | 0.66              |
| 1:G:178:GLN:HG3   | 1:G:575:TYR:CE2   | 2.30                     | 0.66              |
| 1:G:175:GLY:O     | 1:G:177:ALA:N     | 2.29                     | 0.66              |
| 1:A:160:LYS:HZ2   | 1:A:566:GLN:HB3   | 1.60                     | 0.66              |
| 1:A:388:GLN:HB3   | 1:A:393:LEU:CD2   | 2.26                     | 0.66              |
| 2:F:1268:THR:CG2  | 2:F:1271:GLU:HG2  | 2.24                     | 0.66              |
| 1:E:477:LEU:HD11  | 1:E:540:ILE:HD13  | 1.78                     | 0.65              |
| 1:C:194:LYS:HE3   | 4:C:618:HOH:O     | 1.96                     | 0.65              |
| 1:G:207:LYS:HE2   | 1:G:524:SER:OG    | 1.97                     | 0.65              |
| 2:H:1307:LEU:C    | 2:H:1319:PRO:HG2  | 2.21                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1331:ILE:HG23 | 2:B:1440:PHE:HZ   | 1.60                     | 0.65              |
| 2:B:1417:LEU:HD13 | 2:B:1421:PHE:CD1  | 2.30                     | 0.65              |
| 1:C:292:LYS:HD2   | 1:C:292:LYS:N     | 2.11                     | 0.65              |
| 1:E:446:SER:HB2   | 1:E:448:GLU:HG2   | 1.77                     | 0.65              |
| 1:G:164:ARG:HG2   | 1:G:164:ARG:HH11  | 1.61                     | 0.65              |
| 1:G:185:ARG:HG3   | 1:G:185:ARG:HH11  | 1.61                     | 0.65              |
| 2:D:1294:ASN:HD22 | 2:D:1296:PHE:H    | 1.42                     | 0.65              |
| 2:B:1307:LEU:HD23 | 2:B:1320:LEU:HD23 | 1.78                     | 0.65              |
| 1:A:506:ARG:HG2   | 1:A:506:ARG:NH1   | 2.06                     | 0.65              |
| 1:G:178:GLN:HG3   | 1:G:575:TYR:HE2   | 1.60                     | 0.65              |
| 2:H:1413:GLU:HA   | 2:H:1416:LYS:HE3  | 1.78                     | 0.64              |
| 1:C:446:SER:O     | 1:C:450:LYS:HG3   | 1.96                     | 0.64              |
| 1:G:446:SER:HB2   | 1:G:448:GLU:HG2   | 1.77                     | 0.64              |
| 1:E:297:PHE:CD1   | 1:E:480:LEU:HD11  | 2.32                     | 0.64              |
| 2:F:1345:TRP:CE3  | 2:F:1358:ARG:HG3  | 2.33                     | 0.64              |
| 1:A:386:HIS:CD2   | 1:A:388:GLN:H     | 2.16                     | 0.64              |
| 2:D:1313:ILE:HD12 | 2:D:1313:ILE:N    | 2.10                     | 0.64              |
| 1:C:480:LEU:HD23  | 1:C:498:ILE:HG23  | 1.80                     | 0.64              |
| 2:F:1412:HIS:CD2  | 2:F:1413:GLU:H    | 2.16                     | 0.64              |
| 2:H:1391:GLN:CA   | 2:H:1391:GLN:HE21 | 2.11                     | 0.64              |
| 1:C:386:HIS:HD2   | 1:C:388:GLN:H     | 1.46                     | 0.63              |
| 1:G:432:GLU:HG3   | 2:H:1442:SER:CB   | 2.28                     | 0.63              |
| 2:D:1303:MET:HE3  | 2:D:1417:LEU:HD21 | 1.81                     | 0.63              |
| 1:A:313:LYS:HE2   | 2:F:1313:ILE:CG2  | 2.28                     | 0.63              |
| 1:C:227:LEU:HD23  | 1:C:301:VAL:HB    | 1.80                     | 0.63              |
| 1:C:169:GLU:HB3   | 1:C:597:ARG:HD2   | 1.79                     | 0.63              |
| 1:E:185:ARG:HB3   | 1:E:188:ALA:HB3   | 1.81                     | 0.62              |
| 1:C:308:ASN:HD21  | 1:C:311:GLY:HA2   | 1.62                     | 0.62              |
| 2:D:1409:THR:HG23 | 2:D:1410:THR:N    | 2.14                     | 0.62              |
| 2:H:1307:LEU:HD11 | 2:H:1326:LEU:CD1  | 2.29                     | 0.62              |
| 1:C:476:LEU:HD21  | 1:C:502:ILE:HG12  | 1.82                     | 0.62              |
| 1:C:223:LYS:HE3   | 4:C:641:HOH:O     | 1.99                     | 0.62              |
| 2:B:1331:ILE:HG23 | 2:B:1440:PHE:CZ   | 2.35                     | 0.62              |
| 1:C:156:THR:CG2   | 1:C:159:GLN:HB3   | 2.29                     | 0.62              |
| 1:C:221:THR:HG21  | 1:C:276:ARG:HB3   | 1.81                     | 0.62              |
| 1:G:506:ARG:HG2   | 1:G:506:ARG:NH1   | 2.14                     | 0.62              |
| 1:C:358:ASP:OD1   | 2:F:1424:PRO:HD2  | 1.99                     | 0.62              |
| 1:A:285:PRO:HG2   | 1:A:313:LYS:HZ2   | 1.65                     | 0.62              |
| 1:A:495:PHE:HB2   | 1:A:549:LYS:HE3   | 1.80                     | 0.62              |
| 1:C:372:PRO:O     | 1:C:418:SER:HB3   | 2.00                     | 0.62              |
| 2:D:1268:THR:HG23 | 2:D:1271:GLU:CD   | 2.25                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:586:ARG:HG3  | 1:G:586:ARG:HH11 | 1.63                     | 0.62              |
| 1:A:313:LYS:HB2  | 1:A:313:LYS:HZ3  | 1.63                     | 0.61              |
| 1:A:476:LEU:HD11 | 1:A:510:PRO:HD2  | 1.82                     | 0.61              |
| 1:C:308:ASN:ND2  | 1:C:311:GLY:HA2  | 2.15                     | 0.61              |
| 1:A:587:GLN:HE21 | 1:A:587:GLN:HA   | 1.64                     | 0.61              |
| 1:C:157:PRO:O    | 1:C:158:SER:HB2  | 1.98                     | 0.61              |
| 2:F:1348:CYS:SG  | 2:F:1377:ALA:HB3 | 2.41                     | 0.61              |
| 1:G:185:ARG:HG3  | 1:G:188:ALA:HB3  | 1.81                     | 0.61              |
| 1:G:275:ASP:OD2  | 1:G:278:HIS:ND1  | 2.29                     | 0.61              |
| 1:C:407:ARG:HG3  | 1:C:407:ARG:NH1  | 2.15                     | 0.61              |
| 2:B:1316:LYS:HE3 | 2:B:1316:LYS:O   | 2.00                     | 0.61              |
| 1:C:209:MET:HA   | 2:D:1443:ARG:HG3 | 1.82                     | 0.61              |
| 2:H:1340:LYS:HG2 | 2:H:1383:TYR:CD2 | 2.36                     | 0.61              |
| 2:F:1307:LEU:HB3 | 2:F:1320:LEU:CD2 | 2.31                     | 0.61              |
| 1:G:292:LYS:H    | 1:G:292:LYS:CD   | 2.07                     | 0.61              |
| 1:G:495:PHE:HB2  | 1:G:549:LYS:HE3  | 1.82                     | 0.61              |
| 1:C:182:TRP:HE1  | 1:C:594:GLN:NE2  | 1.99                     | 0.61              |
| 2:B:1280:LYS:HD3 | 2:B:1289:GLU:OE2 | 1.99                     | 0.60              |
| 1:G:347:GLY:O    | 1:G:561:ARG:HG3  | 2.01                     | 0.60              |
| 1:G:216:ILE:HG21 | 4:G:613:HOH:O    | 2.00                     | 0.60              |
| 1:A:424:PRO:O    | 1:A:458:GLU:HG3  | 2.01                     | 0.60              |
| 1:C:209:MET:HA   | 2:D:1443:ARG:CG  | 2.32                     | 0.60              |
| 2:B:1270:GLU:CD  | 2:B:1270:GLU:C   | 2.69                     | 0.60              |
| 1:G:426:LEU:CD1  | 1:G:518:MET:HE3  | 2.29                     | 0.60              |
| 2:F:1340:LYS:HD2 | 2:F:1383:TYR:CD2 | 2.37                     | 0.60              |
| 2:F:1412:HIS:CD2 | 2:F:1413:GLU:N   | 2.69                     | 0.60              |
| 1:A:394:LEU:HD13 | 1:A:401:ILE:CD1  | 2.32                     | 0.59              |
| 1:G:586:ARG:HG3  | 1:G:586:ARG:NH1  | 2.17                     | 0.59              |
| 1:A:500:LYS:HE3  | 1:A:552:LEU:HD21 | 1.83                     | 0.59              |
| 1:C:312:ARG:HH11 | 1:C:313:LYS:HB3  | 1.66                     | 0.59              |
| 1:E:164:ARG:HE   | 1:E:167:ARG:NH2  | 2.00                     | 0.59              |
| 1:A:182:TRP:CE3  | 1:A:573:ARG:HD3  | 2.37                     | 0.59              |
| 1:E:308:ASN:ND2  | 1:E:313:LYS:O    | 2.34                     | 0.59              |
| 1:G:209:MET:CB   | 2:H:1443:ARG:HB3 | 2.20                     | 0.59              |
| 1:C:156:THR:HG23 | 1:C:159:GLN:HB2  | 1.84                     | 0.59              |
| 1:C:500:LYS:HE3  | 1:C:552:LEU:HD21 | 1.85                     | 0.59              |
| 2:D:1313:ILE:H   | 2:D:1313:ILE:CD1 | 2.12                     | 0.59              |
| 1:C:156:THR:HG23 | 1:C:159:GLN:HB3  | 1.83                     | 0.59              |
| 1:C:200:GLU:HG2  | 1:C:528:TYR:CD1  | 2.38                     | 0.59              |
| 1:G:164:ARG:HG2  | 1:G:164:ARG:NH1  | 2.18                     | 0.59              |
| 1:G:311:GLY:O    | 1:G:312:ARG:HD2  | 2.02                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:1414:LYS:CG   | 2:H:1415:ASP:N    | 2.65                     | 0.59              |
| 1:E:307:ILE:CG2   | 1:E:309:THR:HG23  | 2.32                     | 0.59              |
| 2:B:1286:CYS:HB3  | 2:B:1315:CYS:SG   | 2.43                     | 0.58              |
| 1:C:156:THR:N     | 1:C:157:PRO:CD    | 2.66                     | 0.58              |
| 2:D:1268:THR:HG23 | 2:D:1271:GLU:HG2  | 1.85                     | 0.58              |
| 1:A:202:LEU:C     | 1:A:202:LEU:HD23  | 2.28                     | 0.58              |
| 1:A:394:LEU:HD13  | 1:A:401:ILE:HD12  | 1.85                     | 0.58              |
| 1:E:212:LYS:HB2   | 1:E:215:ASP:OD2   | 2.03                     | 0.58              |
| 1:G:207:LYS:HB2   | 1:G:207:LYS:HZ2   | 1.66                     | 0.58              |
| 1:C:495:PHE:CE1   | 1:C:544:LEU:HD13  | 2.38                     | 0.58              |
| 2:B:1277:GLU:OE2  | 2:B:1336:ARG:NH2  | 2.37                     | 0.58              |
| 1:E:386:HIS:CD2   | 1:E:388:GLN:H     | 2.18                     | 0.58              |
| 2:H:1366:ARG:HG3  | 2:H:1366:ARG:HH11 | 1.69                     | 0.58              |
| 1:A:495:PHE:CE1   | 1:A:544:LEU:HD13  | 2.39                     | 0.58              |
| 2:F:1307:LEU:HB3  | 2:F:1320:LEU:HD21 | 1.86                     | 0.58              |
| 1:E:564:LYS:HD3   | 1:E:569:GLY:HA2   | 1.86                     | 0.58              |
| 2:B:1340:LYS:HD3  | 2:B:1383:TYR:CG   | 2.39                     | 0.57              |
| 1:C:223:LYS:NZ    | 1:C:256:GLN:HE21  | 2.02                     | 0.57              |
| 1:C:321:GLU:HA    | 4:C:661:HOH:O     | 2.04                     | 0.57              |
| 1:G:334:ASP:HA    | 1:G:337:PHE:CE2   | 2.38                     | 0.57              |
| 1:G:275:ASP:CG    | 1:G:278:HIS:HD1   | 2.12                     | 0.57              |
| 1:A:243:LEU:HD22  | 1:A:253:LEU:HD13  | 1.87                     | 0.57              |
| 1:G:271:ILE:HD13  | 1:G:283:GLN:HB3   | 1.85                     | 0.57              |
| 2:B:1308:TYR:CD1  | 2:B:1308:TYR:C    | 2.82                     | 0.57              |
| 1:G:396:SER:OG    | 1:G:401:ILE:HD11  | 2.04                     | 0.57              |
| 1:A:307:ILE:HA    | 4:A:614:HOH:O     | 2.03                     | 0.57              |
| 1:C:579:PRO:HG3   | 1:C:587:GLN:HB3   | 1.87                     | 0.57              |
| 1:C:209:MET:HE3   | 2:D:1444:SER:HB2  | 1.86                     | 0.57              |
| 2:H:1320:LEU:HD21 | 2:H:1426:VAL:HG22 | 1.85                     | 0.57              |
| 1:A:313:LYS:HE2   | 2:F:1313:ILE:CB   | 2.34                     | 0.57              |
| 1:A:426:LEU:HD11  | 1:A:518:MET:HE3   | 1.87                     | 0.57              |
| 2:D:1277:GLU:OE2  | 2:D:1336:ARG:NH2  | 2.37                     | 0.56              |
| 1:C:447:ARG:O     | 1:C:447:ARG:NE    | 2.38                     | 0.56              |
| 1:C:292:LYS:HG2   | 1:C:293:GLU:N     | 2.20                     | 0.56              |
| 2:D:1416:LYS:HD2  | 2:D:1416:LYS:C    | 2.31                     | 0.56              |
| 1:C:292:LYS:H     | 1:C:292:LYS:CD    | 2.18                     | 0.56              |
| 1:E:170:VAL:HG13  | 1:E:594:GLN:HG2   | 1.87                     | 0.56              |
| 1:E:508:TYR:CE2   | 1:E:531:LEU:HD23  | 2.41                     | 0.56              |
| 1:C:297:PHE:CD1   | 1:C:480:LEU:HD11  | 2.41                     | 0.56              |
| 2:D:1340:LYS:HD3  | 2:D:1383:TYR:CD2  | 2.41                     | 0.56              |
| 1:E:157:PRO:HB3   | 1:E:354:SER:HB3   | 1.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:343:LEU:C     | 1:A:343:LEU:HD23  | 2.30                     | 0.56              |
| 1:A:579:PRO:HG3   | 1:A:587:GLN:HB3   | 1.88                     | 0.56              |
| 1:G:308:ASN:ND2   | 1:G:311:GLY:HA2   | 2.21                     | 0.56              |
| 1:A:393:LEU:HD23  | 1:A:393:LEU:C     | 2.30                     | 0.56              |
| 2:B:1294:ASN:HD22 | 2:B:1296:PHE:H    | 1.53                     | 0.56              |
| 1:G:292:LYS:HE2   | 1:G:293:GLU:H     | 1.70                     | 0.55              |
| 1:E:338:GLU:HG2   | 1:E:339:GLN:N     | 2.21                     | 0.55              |
| 2:H:1350:GLU:OE2  | 2:H:1351:PRO:HD2  | 2.05                     | 0.55              |
| 2:H:1391:GLN:HE21 | 2:H:1391:GLN:C    | 2.13                     | 0.55              |
| 1:C:343:LEU:HD23  | 1:C:344:VAL:N     | 2.21                     | 0.55              |
| 1:A:448:GLU:HA    | 1:A:448:GLU:OE1   | 2.06                     | 0.55              |
| 1:G:221:THR:O     | 1:G:225:GLU:HG3   | 2.06                     | 0.55              |
| 1:G:237:ILE:HD12  | 1:G:252:THR:HG21  | 1.89                     | 0.55              |
| 1:G:271:ILE:HD12  | 1:G:271:ILE:C     | 2.32                     | 0.55              |
| 1:G:426:LEU:HD21  | 1:G:435:TYR:HB2   | 1.88                     | 0.55              |
| 1:C:386:HIS:CD2   | 1:C:388:GLN:H     | 2.23                     | 0.55              |
| 1:E:394:LEU:HD12  | 1:E:398:PHE:HE1   | 1.72                     | 0.55              |
| 1:A:160:LYS:CD    | 1:A:160:LYS:N     | 2.70                     | 0.55              |
| 1:A:313:LYS:CE    | 2:F:1313:ILE:HB   | 2.36                     | 0.55              |
| 1:E:495:PHE:HB2   | 1:E:549:LYS:HE3   | 1.89                     | 0.55              |
| 2:B:1281:CYS:SG   | 2:B:1326:LEU:HD23 | 2.47                     | 0.54              |
| 1:G:157:PRO:O     | 1:G:158:SER:HB2   | 2.05                     | 0.54              |
| 1:G:297:PHE:CE1   | 1:G:300:GLN:HB2   | 2.42                     | 0.54              |
| 2:H:1330:LEU:O    | 2:H:1334:ILE:HG13 | 2.06                     | 0.54              |
| 1:A:426:LEU:CD1   | 1:A:518:MET:HE3   | 2.37                     | 0.54              |
| 1:G:160:LYS:HZ2   | 1:G:566:GLN:HE21  | 1.55                     | 0.54              |
| 1:G:185:ARG:CD    | 1:G:373:ASP:OD2   | 2.55                     | 0.54              |
| 1:C:540:ILE:HD12  | 1:C:540:ILE:H     | 1.72                     | 0.54              |
| 1:A:407:ARG:HG3   | 1:A:407:ARG:HH11  | 1.72                     | 0.54              |
| 1:A:344:VAL:HG11  | 1:A:539:ILE:HG21  | 1.90                     | 0.54              |
| 1:A:388:GLN:HB3   | 1:A:393:LEU:HD21  | 1.90                     | 0.54              |
| 1:C:312:ARG:HH11  | 1:C:313:LYS:HD2   | 1.71                     | 0.54              |
| 1:E:582:ASP:OD1   | 1:E:583:GLY:N     | 2.40                     | 0.54              |
| 1:G:175:GLY:C     | 1:G:177:ALA:N     | 2.64                     | 0.54              |
| 1:G:209:MET:HE2   | 2:H:1444:SER:HB2  | 1.90                     | 0.54              |
| 1:C:325:LEU:HD21  | 1:C:506:ARG:HD3   | 1.90                     | 0.54              |
| 1:G:341:MET:HG3   | 1:G:575:TYR:CE1   | 2.42                     | 0.54              |
| 2:B:1331:ILE:O    | 2:B:1335:ARG:HG3  | 2.07                     | 0.54              |
| 2:D:1409:THR:HG23 | 2:D:1410:THR:H    | 1.71                     | 0.54              |
| 2:F:1345:TRP:CZ3  | 2:F:1358:ARG:HG3  | 2.43                     | 0.54              |
| 1:E:217:ARG:HD2   | 2:F:1364:PHE:CE1  | 2.43                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:182:TRP:CZ2   | 1:A:594:GLN:HG3   | 2.43                     | 0.54              |
| 1:A:445:LEU:HD22  | 1:A:449:ASP:HB3   | 1.90                     | 0.54              |
| 1:C:341:MET:HE1   | 1:C:370:ASP:HB3   | 1.88                     | 0.54              |
| 1:E:426:LEU:CD1   | 1:E:518:MET:HE3   | 2.37                     | 0.54              |
| 1:E:547:PHE:CD1   | 1:E:547:PHE:C     | 2.86                     | 0.54              |
| 1:A:388:GLN:HB3   | 1:A:393:LEU:HD22  | 1.88                     | 0.53              |
| 1:C:223:LYS:HZ3   | 1:C:256:GLN:NE2   | 2.06                     | 0.53              |
| 2:H:1337:PHE:HE2  | 2:H:1395:TYR:CE2  | 2.26                     | 0.53              |
| 2:H:1413:GLU:HA   | 2:H:1416:LYS:CE   | 2.37                     | 0.53              |
| 2:F:1307:LEU:O    | 2:F:1320:LEU:HG   | 2.08                     | 0.53              |
| 1:C:194:LYS:O     | 1:C:462:LEU:HD12  | 2.08                     | 0.53              |
| 1:C:275:ASP:CG    | 1:C:278:HIS:HD1   | 2.15                     | 0.53              |
| 1:C:343:LEU:HD23  | 1:C:343:LEU:C     | 2.33                     | 0.53              |
| 2:D:1268:THR:HG23 | 2:D:1271:GLU:CG   | 2.38                     | 0.53              |
| 2:B:1415:ASP:HA   | 2:B:1418:LYS:HB3  | 1.90                     | 0.53              |
| 1:E:222:CYS:O     | 1:E:226:GLU:HB2   | 2.09                     | 0.53              |
| 1:G:221:THR:HG22  | 1:G:225:GLU:CD    | 2.34                     | 0.53              |
| 1:C:180:VAL:HG12  | 1:C:180:VAL:O     | 2.09                     | 0.53              |
| 1:C:213:LEU:HB2   | 1:C:214:PRO:HD3   | 1.91                     | 0.53              |
| 1:E:512:TYR:HA    | 1:E:513:PRO:C     | 2.33                     | 0.53              |
| 2:F:1281:CYS:SG   | 2:F:1326:LEU:HD23 | 2.49                     | 0.53              |
| 1:A:182:TRP:CD2   | 1:A:573:ARG:HD3   | 2.43                     | 0.53              |
| 1:C:221:THR:HG22  | 1:C:225:GLU:OE2   | 2.09                     | 0.53              |
| 1:G:199:PRO:CG    | 1:G:200:GLU:H     | 2.19                     | 0.53              |
| 2:B:1438:GLU:OE1  | 2:B:1438:GLU:N    | 2.42                     | 0.53              |
| 2:B:1308:TYR:C    | 2:B:1308:TYR:HD1  | 2.17                     | 0.52              |
| 2:F:1268:THR:HG22 | 2:F:1271:GLU:CD   | 2.34                     | 0.52              |
| 1:G:185:ARG:HB3   | 1:G:185:ARG:CZ    | 2.39                     | 0.52              |
| 1:G:311:GLY:C     | 1:G:312:ARG:HD2   | 2.34                     | 0.52              |
| 1:G:354:SER:HB2   | 1:G:356:THR:HG23  | 1.91                     | 0.52              |
| 1:C:201:ALA:HA    | 1:C:439:PRO:CD    | 2.39                     | 0.52              |
| 2:F:1415:ASP:HA   | 2:F:1418:LYS:HB3  | 1.89                     | 0.52              |
| 1:A:477:LEU:HD21  | 1:A:499:LEU:CD2   | 2.40                     | 0.52              |
| 1:E:427:ARG:HD3   | 4:E:616:HOH:O     | 2.08                     | 0.52              |
| 1:G:300:GLN:HG2   | 1:G:302:VAL:CG1   | 2.38                     | 0.52              |
| 1:C:182:TRP:HE1   | 1:C:594:GLN:HE22  | 1.58                     | 0.52              |
| 1:G:586:ARG:HH11  | 1:G:586:ARG:CG    | 2.23                     | 0.52              |
| 2:B:1410:THR:HG23 | 2:B:1413:GLU:HB3  | 1.92                     | 0.52              |
| 1:C:295:SER:O     | 1:C:296:LEU:HD23  | 2.09                     | 0.52              |
| 2:D:1376:LYS:HE2  | 2:D:1376:LYS:CA   | 2.33                     | 0.52              |
| 2:F:1307:LEU:HD23 | 2:F:1320:LEU:HD23 | 1.92                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:294:TYR:CD1   | 1:G:487:SER:HB3   | 2.44                     | 0.52              |
| 1:A:333:GLU:H     | 1:A:333:GLU:CD    | 2.17                     | 0.52              |
| 1:C:196:LEU:CD1   | 1:C:468:ILE:HD12  | 2.39                     | 0.52              |
| 1:A:222:CYS:O     | 1:A:226:GLU:HB2   | 2.09                     | 0.52              |
| 1:A:285:PRO:HG2   | 1:A:313:LYS:NZ    | 2.25                     | 0.52              |
| 1:A:512:TYR:HA    | 1:A:513:PRO:C     | 2.35                     | 0.52              |
| 1:C:426:LEU:HD11  | 1:C:518:MET:HE3   | 1.92                     | 0.52              |
| 1:G:271:ILE:HD12  | 1:G:272:LEU:C     | 2.35                     | 0.52              |
| 2:B:1307:LEU:HD11 | 2:B:1326:LEU:CD1  | 2.37                     | 0.51              |
| 1:A:570:THR:HG22  | 1:A:597:ARG:HA    | 1.92                     | 0.51              |
| 2:B:1276:CYS:SG   | 2:B:1390:THR:HG22 | 2.49                     | 0.51              |
| 2:F:1347:ILE:CD1  | 2:F:1356:ARG:HB2  | 2.40                     | 0.51              |
| 2:H:1307:LEU:HD12 | 2:H:1319:PRO:HB2  | 1.92                     | 0.51              |
| 2:H:1420:GLN:HE21 | 2:H:1420:GLN:C    | 2.17                     | 0.51              |
| 1:A:192:SER:OG    | 1:A:194:LYS:HE3   | 2.09                     | 0.51              |
| 2:B:1400:ASP:HA   | 2:B:1434:LYS:HD2  | 1.93                     | 0.51              |
| 1:G:478:PHE:CD1   | 1:G:544:LEU:HD11  | 2.45                     | 0.51              |
| 2:H:1413:GLU:CA   | 2:H:1416:LYS:HE3  | 2.41                     | 0.51              |
| 2:B:1394:PHE:O    | 2:B:1398:ILE:HG23 | 2.11                     | 0.51              |
| 1:G:574:LEU:HD12  | 1:G:574:LEU:N     | 2.25                     | 0.51              |
| 1:A:509:TYR:CE2   | 1:A:518:MET:SD    | 3.04                     | 0.51              |
| 2:H:1363:GLN:OE1  | 2:H:1375:MET:HE1  | 2.11                     | 0.51              |
| 2:B:1330:LEU:HD11 | 2:B:1399:PHE:CE2  | 2.46                     | 0.51              |
| 1:E:447:ARG:HH11  | 1:E:447:ARG:HB3   | 1.75                     | 0.51              |
| 1:A:362:ASP:O     | 1:A:366:VAL:HG23  | 2.11                     | 0.51              |
| 1:G:160:LYS:NZ    | 1:G:566:GLN:HE21  | 2.09                     | 0.51              |
| 1:G:494:ARG:NH1   | 1:G:494:ARG:HG3   | 2.25                     | 0.51              |
| 1:A:160:LYS:NZ    | 1:A:566:GLN:HB3   | 2.26                     | 0.51              |
| 2:D:1408:LEU:HD12 | 2:D:1413:GLU:OE1  | 2.10                     | 0.51              |
| 1:G:307:ILE:HG23  | 1:G:309:THR:HG23  | 1.93                     | 0.51              |
| 1:G:510:PRO:HA    | 4:G:607:HOH:O     | 2.11                     | 0.51              |
| 1:A:339:GLN:HG2   | 1:A:577:ARG:CZ    | 2.41                     | 0.50              |
| 1:C:402:PHE:CD1   | 1:C:430:HIS:CE1   | 2.99                     | 0.50              |
| 2:D:1414:LYS:HZ1  | 2:D:1418:LYS:HD3  | 1.74                     | 0.50              |
| 2:F:1363:GLN:NE2  | 2:F:1370:LEU:HD23 | 2.26                     | 0.50              |
| 1:A:360:LEU:HD11  | 1:A:409:ILE:HD11  | 1.93                     | 0.50              |
| 1:C:494:ARG:HG3   | 1:C:494:ARG:NH1   | 2.26                     | 0.50              |
| 1:E:202:LEU:HD12  | 2:H:1364:PHE:HB3  | 1.92                     | 0.50              |
| 1:E:583:GLY:O     | 1:E:585:GLU:N     | 2.45                     | 0.50              |
| 1:G:368:ASN:O     | 1:G:371:ARG:HG2   | 2.11                     | 0.50              |
| 1:A:211:GLN:HG2   | 4:A:611:HOH:O     | 2.10                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:207:LYS:HD3   | 2:H:1443:ARG:NH1  | 2.26                     | 0.50              |
| 1:G:578:ARG:HG3   | 1:G:578:ARG:HH11  | 1.76                     | 0.50              |
| 2:D:1270:GLU:OE1  | 2:D:1270:GLU:C    | 2.55                     | 0.50              |
| 1:E:308:ASN:HD21  | 1:E:313:LYS:H     | 1.58                     | 0.50              |
| 1:E:368:ASN:O     | 1:E:371:ARG:HG2   | 2.11                     | 0.50              |
| 2:H:1435:ASN:O    | 2:H:1439:GLN:HB2  | 2.11                     | 0.50              |
| 1:G:334:ASP:HA    | 1:G:337:PHE:CD2   | 2.47                     | 0.50              |
| 2:D:1359:HIS:C    | 2:D:1359:HIS:CD2  | 2.90                     | 0.50              |
| 1:E:170:VAL:CG1   | 1:E:594:GLN:HG2   | 2.42                     | 0.50              |
| 1:G:210:PHE:HE1   | 2:H:1388:LEU:HD23 | 1.76                     | 0.50              |
| 1:C:583:GLY:O     | 1:C:585:GLU:N     | 2.44                     | 0.50              |
| 1:E:363:LEU:O     | 1:E:367:ILE:HG13  | 2.11                     | 0.50              |
| 1:G:446:SER:HB3   | 1:G:448:GLU:OE2   | 2.12                     | 0.50              |
| 1:G:512:TYR:HA    | 1:G:513:PRO:C     | 2.36                     | 0.50              |
| 2:D:1320:LEU:HD13 | 2:D:1320:LEU:O    | 2.12                     | 0.50              |
| 1:G:305:GLU:HB3   | 1:G:318:LYS:HB3   | 1.93                     | 0.50              |
| 1:G:542:SER:C     | 1:G:561:ARG:NH1   | 2.70                     | 0.50              |
| 1:G:391:ASN:HB2   | 1:G:393:LEU:HG    | 1.94                     | 0.49              |
| 2:H:1414:LYS:NZ   | 2:H:1418:LYS:NZ   | 2.60                     | 0.49              |
| 1:A:157:PRO:C     | 1:A:159:GLN:N     | 2.64                     | 0.49              |
| 1:A:157:PRO:HB3   | 1:A:354:SER:HB3   | 1.94                     | 0.49              |
| 1:A:200:GLU:OE2   | 1:A:203:THR:HG22  | 2.12                     | 0.49              |
| 1:E:307:ILE:HG22  | 4:E:602:HOH:O     | 2.11                     | 0.49              |
| 1:G:432:GLU:CG    | 2:H:1442:SER:H    | 2.22                     | 0.49              |
| 2:H:1366:ARG:HG3  | 2:H:1366:ARG:NH1  | 2.27                     | 0.49              |
| 1:C:407:ARG:NH2   | 1:C:444:ASP:OD2   | 2.45                     | 0.49              |
| 1:E:503:LEU:HD22  | 1:E:534:THR:HG23  | 1.94                     | 0.49              |
| 1:G:221:THR:HG21  | 1:G:276:ARG:HB2   | 1.94                     | 0.49              |
| 1:G:448:GLU:HG2   | 1:G:449:ASP:H     | 1.77                     | 0.49              |
| 1:A:191:ILE:HD13  | 1:A:191:ILE:O     | 2.11                     | 0.49              |
| 1:C:253:LEU:HD12  | 1:C:314:LEU:HD22  | 1.95                     | 0.49              |
| 1:G:185:ARG:CG    | 1:G:185:ARG:HH11  | 2.24                     | 0.49              |
| 1:G:583:GLY:O     | 1:G:585:GLU:N     | 2.45                     | 0.49              |
| 1:G:547:PHE:CD1   | 1:G:547:PHE:C     | 2.91                     | 0.49              |
| 2:H:1346:LEU:HD23 | 2:H:1381:PRO:HA   | 1.94                     | 0.49              |
| 2:H:1414:LYS:HZ2  | 2:H:1418:LYS:HZ1  | 1.61                     | 0.49              |
| 1:G:494:ARG:HG3   | 1:G:494:ARG:HH11  | 1.77                     | 0.49              |
| 1:A:586:ARG:HG3   | 1:A:586:ARG:NH1   | 2.28                     | 0.49              |
| 1:E:358:ASP:HB2   | 1:E:359:PRO:HD3   | 1.95                     | 0.49              |
| 2:H:1281:CYS:SG   | 2:H:1326:LEU:HD23 | 2.53                     | 0.49              |
| 1:A:339:GLN:HG2   | 1:A:577:ARG:HH21  | 1.77                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:237:ILE:HD13  | 1:C:252:THR:HG21  | 1.95                     | 0.49              |
| 1:E:338:GLU:HG2   | 1:E:339:GLN:H     | 1.75                     | 0.49              |
| 2:H:1420:GLN:HB3  | 2:H:1421:PHE:CD1  | 2.47                     | 0.49              |
| 1:C:426:LEU:HD13  | 1:C:518:MET:HE3   | 1.91                     | 0.49              |
| 1:C:547:PHE:CD1   | 1:C:547:PHE:C     | 2.91                     | 0.49              |
| 2:F:1294:ASN:HD22 | 2:F:1296:PHE:N    | 2.10                     | 0.49              |
| 1:G:308:ASN:HD21  | 1:G:311:GLY:HA2   | 1.78                     | 0.49              |
| 1:G:385:LYS:HE2   | 1:G:427:ARG:HD2   | 1.94                     | 0.49              |
| 1:A:213:LEU:HG    | 4:A:627:HOH:O     | 2.13                     | 0.48              |
| 2:B:1437:ALA:HB3  | 2:B:1438:GLU:OE1  | 2.13                     | 0.48              |
| 1:C:512:TYR:HA    | 1:C:513:PRO:C     | 2.38                     | 0.48              |
| 2:H:1297:ASP:HB2  | 2:H:1306:SER:OG   | 2.13                     | 0.48              |
| 1:A:313:LYS:HE2   | 2:F:1313:ILE:HG21 | 1.94                     | 0.48              |
| 1:C:285:PRO:HD2   | 1:C:312:ARG:O     | 2.13                     | 0.48              |
| 1:C:296:LEU:HA    | 1:C:300:GLN:OE1   | 2.14                     | 0.48              |
| 2:H:1345:TRP:CE3  | 2:H:1358:ARG:HG3  | 2.49                     | 0.48              |
| 2:D:1415:ASP:HA   | 2:D:1418:LYS:HB3  | 1.95                     | 0.48              |
| 1:A:586:ARG:HG3   | 1:A:586:ARG:HH11  | 1.77                     | 0.48              |
| 1:C:201:ALA:HA    | 1:C:439:PRO:HD3   | 1.94                     | 0.48              |
| 2:F:1416:LYS:HB3  | 2:F:1416:LYS:HZ2  | 1.78                     | 0.48              |
| 2:D:1416:LYS:HG3  | 2:D:1417:LEU:N    | 2.27                     | 0.48              |
| 2:H:1413:GLU:N    | 2:H:1416:LYS:HE3  | 2.28                     | 0.48              |
| 1:C:152:SER:CB    | 1:C:153:PRO:CD    | 2.87                     | 0.48              |
| 1:G:236:LYS:HD3   | 1:G:236:LYS:N     | 2.28                     | 0.48              |
| 1:G:221:THR:HG22  | 1:G:225:GLU:OE2   | 2.13                     | 0.48              |
| 2:H:1412:HIS:O    | 2:H:1416:LYS:CG   | 2.51                     | 0.48              |
| 1:A:227:LEU:HD23  | 1:A:301:VAL:CB    | 2.37                     | 0.48              |
| 1:E:360:LEU:HD11  | 1:E:409:ILE:HD11  | 1.96                     | 0.48              |
| 1:E:447:ARG:HG2   | 1:E:448:GLU:N     | 2.28                     | 0.48              |
| 1:A:307:ILE:CG2   | 1:A:309:THR:HG23  | 2.44                     | 0.47              |
| 2:D:1286:CYS:SG   | 2:D:1288:THR:HG23 | 2.54                     | 0.47              |
| 1:A:297:PHE:CG    | 1:A:480:LEU:HD11  | 2.49                     | 0.47              |
| 1:A:583:GLY:O     | 1:A:585:GLU:N     | 2.47                     | 0.47              |
| 1:E:164:ARG:NE    | 1:E:167:ARG:NH2   | 2.62                     | 0.47              |
| 1:E:321:GLU:HB2   | 4:E:635:HOH:O     | 2.12                     | 0.47              |
| 1:C:152:SER:CB    | 1:C:153:PRO:HD2   | 2.29                     | 0.47              |
| 1:C:199:PRO:O     | 1:C:200:GLU:HB2   | 2.14                     | 0.47              |
| 1:C:313:LYS:HG2   | 1:C:314:LEU:N     | 2.29                     | 0.47              |
| 1:E:243:LEU:HD22  | 1:E:253:LEU:HD13  | 1.96                     | 0.47              |
| 1:E:182:TRP:HE1   | 1:E:594:GLN:HE22  | 1.63                     | 0.47              |
| 2:H:1286:CYS:HB3  | 2:H:1315:CYS:HB2  | 1.95                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:426:LEU:HD11  | 1:A:435:TYR:HB2   | 1.96                     | 0.47              |
| 2:B:1348:CYS:SG   | 2:B:1377:ALA:HB3  | 2.55                     | 0.47              |
| 1:C:402:PHE:CE2   | 1:C:406:LEU:HD22  | 2.49                     | 0.47              |
| 1:E:164:ARG:NH1   | 1:E:164:ARG:CG    | 2.67                     | 0.47              |
| 1:E:201:ALA:HB3   | 2:H:1367:THR:C    | 2.39                     | 0.47              |
| 2:F:1405:LEU:O    | 2:F:1414:LYS:HE2  | 2.14                     | 0.47              |
| 1:G:160:LYS:NZ    | 1:G:566:GLN:HB2   | 2.30                     | 0.47              |
| 1:G:382:LEU:HD23  | 1:G:382:LEU:HA    | 1.72                     | 0.47              |
| 2:B:1428:GLN:HG2  | 2:B:1431:ARG:HH21 | 1.80                     | 0.47              |
| 1:C:221:THR:CG2   | 1:C:276:ARG:H     | 2.28                     | 0.47              |
| 1:C:260:ASP:OD1   | 1:C:260:ASP:C     | 2.57                     | 0.47              |
| 2:F:1408:LEU:O    | 2:F:1414:LYS:HE3  | 2.15                     | 0.47              |
| 1:G:341:MET:HE1   | 1:G:370:ASP:HB3   | 1.96                     | 0.47              |
| 1:A:266:ASN:HD22  | 2:F:1302:ASP:HA   | 1.80                     | 0.46              |
| 1:A:363:LEU:O     | 1:A:367:ILE:HG13  | 2.15                     | 0.46              |
| 1:E:157:PRO:N     | 1:E:159:GLN:OE1   | 2.48                     | 0.46              |
| 1:E:445:LEU:HD22  | 1:E:449:ASP:HB3   | 1.95                     | 0.46              |
| 1:G:237:ILE:HD11  | 1:G:320:TYR:CZ    | 2.50                     | 0.46              |
| 1:A:191:ILE:HD11  | 1:A:193:LEU:HG    | 1.96                     | 0.46              |
| 2:F:1408:LEU:HB2  | 2:F:1414:LYS:HG2  | 1.96                     | 0.46              |
| 1:A:331:THR:HB    | 1:A:333:GLU:OE2   | 2.16                     | 0.46              |
| 1:A:567:VAL:HG12  | 1:A:568:GLY:N     | 2.30                     | 0.46              |
| 1:C:516:GLU:O     | 1:C:517:ASP:CB    | 2.56                     | 0.46              |
| 1:E:476:LEU:HD21  | 1:E:510:PRO:HD2   | 1.97                     | 0.46              |
| 1:A:307:ILE:HG23  | 1:A:309:THR:HG23  | 1.97                     | 0.46              |
| 1:A:395:THR:HA    | 2:B:1325:GLN:NE2  | 2.31                     | 0.46              |
| 1:A:514:PRO:O     | 2:B:1358:ARG:NH2  | 2.34                     | 0.46              |
| 1:G:362:ASP:O     | 1:G:366:VAL:HG23  | 2.16                     | 0.46              |
| 1:A:586:ARG:HH11  | 1:A:586:ARG:CG    | 2.29                     | 0.46              |
| 1:G:249:GLU:H     | 1:G:249:GLU:CD    | 2.22                     | 0.46              |
| 1:C:223:LYS:NZ    | 1:C:256:GLN:NE2   | 2.64                     | 0.46              |
| 1:E:202:LEU:HD12  | 2:H:1364:PHE:CB   | 2.46                     | 0.46              |
| 1:E:297:PHE:CG    | 1:E:480:LEU:HD11  | 2.50                     | 0.46              |
| 2:F:1416:LYS:HB3  | 2:F:1416:LYS:HZ3  | 1.81                     | 0.46              |
| 2:H:1405:LEU:HD11 | 2:H:1422:PHE:CD2  | 2.51                     | 0.46              |
| 1:C:157:PRO:O     | 1:C:158:SER:CB    | 2.64                     | 0.46              |
| 1:E:182:TRP:C     | 1:E:341:MET:HE2   | 2.41                     | 0.46              |
| 1:G:343:LEU:HD23  | 1:G:344:VAL:N     | 2.30                     | 0.46              |
| 2:H:1271:GLU:HG2  | 2:H:1274:ARG:NH2  | 2.25                     | 0.46              |
| 2:B:1352:THR:O    | 2:B:1352:THR:HG22 | 2.14                     | 0.46              |
| 2:D:1349:GLU:O    | 2:D:1351:PRO:HD3  | 2.16                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:1335:ARG:NH2  | 4:F:1607:HOH:O    | 2.49                     | 0.46              |
| 1:C:305:GLU:HB3   | 1:C:318:LYS:HB3   | 1.97                     | 0.46              |
| 2:H:1414:LYS:NZ   | 2:H:1418:LYS:HZ1  | 2.13                     | 0.46              |
| 1:A:232:LYS:HG3   | 1:A:237:ILE:HB    | 1.98                     | 0.45              |
| 1:A:296:LEU:HA    | 1:A:300:GLN:OE1   | 2.16                     | 0.45              |
| 2:B:1373:ALA:HB1  | 1:C:155:ALA:HB2   | 1.98                     | 0.45              |
| 2:B:1307:LEU:HD23 | 2:B:1320:LEU:CD2  | 2.46                     | 0.45              |
| 1:E:445:LEU:CD2   | 1:E:449:ASP:HB3   | 2.46                     | 0.45              |
| 1:E:476:LEU:HD22  | 1:E:508:TYR:O     | 2.16                     | 0.45              |
| 1:C:292:LYS:CG    | 1:C:293:GLU:N     | 2.79                     | 0.45              |
| 1:C:480:LEU:HD12  | 1:C:511:LEU:HD13  | 1.98                     | 0.45              |
| 1:E:382:LEU:HD13  | 1:E:429:VAL:CG1   | 2.47                     | 0.45              |
| 1:E:426:LEU:HD11  | 1:E:518:MET:HE3   | 1.98                     | 0.45              |
| 1:G:476:LEU:HD22  | 1:G:508:TYR:O     | 2.16                     | 0.45              |
| 1:A:446:SER:O     | 1:A:450:LYS:CG    | 2.63                     | 0.45              |
| 2:D:1345:TRP:CE3  | 2:D:1356:ARG:HG2  | 2.52                     | 0.45              |
| 1:E:166:ASN:HB3   | 1:E:597:ARG:HD2   | 1.98                     | 0.45              |
| 1:E:213:LEU:HB2   | 1:E:214:PRO:HD3   | 1.99                     | 0.45              |
| 1:G:182:TRP:HE1   | 1:G:594:GLN:NE2   | 2.15                     | 0.45              |
| 1:G:192:SER:C     | 1:G:193:LEU:HD23  | 2.42                     | 0.45              |
| 2:H:1365:SER:HB3  | 2:H:1370:LEU:HD13 | 1.98                     | 0.45              |
| 1:C:196:LEU:O     | 1:C:197:GLY:O     | 2.35                     | 0.45              |
| 2:D:1348:CYS:SG   | 2:D:1377:ALA:HB3  | 2.56                     | 0.45              |
| 1:E:406:LEU:O     | 1:E:410:ILE:HG13  | 2.16                     | 0.45              |
| 1:G:161:TYR:O     | 1:G:164:ARG:NH1   | 2.49                     | 0.45              |
| 1:G:194:LYS:O     | 1:G:462:LEU:HD12  | 2.16                     | 0.45              |
| 2:H:1277:GLU:CD   | 2:H:1336:ARG:HH22 | 2.23                     | 0.45              |
| 2:H:1310:CYS:CB   | 2:H:1315:CYS:SG   | 3.04                     | 0.45              |
| 1:G:329:GLN:HE21  | 1:G:329:GLN:CA    | 2.29                     | 0.45              |
| 1:A:161:TYR:O     | 1:A:164:ARG:HG2   | 2.17                     | 0.45              |
| 2:D:1290:ASN:HD21 | 2:D:1310:CYS:HA   | 1.81                     | 0.45              |
| 1:E:280:SER:O     | 2:F:1363:GLN:HG3  | 2.16                     | 0.45              |
| 1:G:491:THR:HG23  | 1:G:492:SER:N     | 2.32                     | 0.45              |
| 2:H:1410:THR:HG22 | 2:H:1412:HIS:HB2  | 1.98                     | 0.45              |
| 1:C:182:TRP:CZ3   | 1:C:575:TYR:CD2   | 3.05                     | 0.45              |
| 1:A:160:LYS:N     | 1:A:160:LYS:HD3   | 2.32                     | 0.45              |
| 1:A:271:ILE:C     | 1:A:271:ILE:CD1   | 2.80                     | 0.45              |
| 1:A:586:ARG:HD2   | 1:A:586:ARG:HA    | 1.28                     | 0.45              |
| 1:G:493:ASP:OD2   | 1:G:496:SER:OG    | 2.33                     | 0.45              |
| 1:A:160:LYS:H     | 1:A:160:LYS:HD3   | 1.78                     | 0.44              |
| 1:C:156:THR:N     | 1:C:157:PRO:HD2   | 2.31                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:166:ASN:HB2   | 1:C:597:ARG:CD    | 2.47                     | 0.44              |
| 1:E:333:GLU:O     | 1:E:336:ASP:HB2   | 2.17                     | 0.44              |
| 1:G:515:GLN:HE21  | 1:G:515:GLN:HB3   | 1.59                     | 0.44              |
| 1:A:476:LEU:HD22  | 1:A:508:TYR:O     | 2.17                     | 0.44              |
| 2:F:1440:PHE:HD1  | 2:F:1440:PHE:HA   | 1.66                     | 0.44              |
| 1:G:222:CYS:O     | 1:G:226:GLU:HB2   | 2.17                     | 0.44              |
| 2:H:1283:CYS:SG   | 2:H:1285:THR:OG1  | 2.75                     | 0.44              |
| 2:H:1400:ASP:OD1  | 2:H:1403:CYS:HB2  | 2.17                     | 0.44              |
| 1:A:547:PHE:CD1   | 1:A:547:PHE:C     | 2.96                     | 0.44              |
| 2:B:1307:LEU:O    | 2:B:1319:PRO:HD2  | 2.17                     | 0.44              |
| 1:C:164:ARG:HH11  | 1:C:167:ARG:HB2   | 1.81                     | 0.44              |
| 2:F:1290:ASN:HD21 | 2:F:1310:CYS:HA   | 1.82                     | 0.44              |
| 1:G:508:TYR:CE2   | 1:G:531:LEU:HD23  | 2.53                     | 0.44              |
| 1:A:294:TYR:CD1   | 1:A:294:TYR:C     | 2.95                     | 0.44              |
| 1:A:399:GLU:OE2   | 1:A:403:LYS:HE2   | 2.17                     | 0.44              |
| 2:B:1396:ARG:NH1  | 2:B:1434:LYS:HE2  | 2.32                     | 0.44              |
| 2:H:1348:CYS:SG   | 2:H:1377:ALA:HB3  | 2.57                     | 0.44              |
| 2:H:1425:LYS:HD3  | 2:H:1429:ASP:OD2  | 2.17                     | 0.44              |
| 1:A:212:LYS:HA    | 1:A:212:LYS:HD2   | 1.88                     | 0.44              |
| 1:C:223:LYS:HZ1   | 1:C:256:GLN:HE21  | 1.65                     | 0.44              |
| 1:C:403:LYS:NZ    | 1:E:407:ARG:NH2   | 2.62                     | 0.44              |
| 2:F:1369:PRO:HG2  | 2:F:1379:LEU:HB2  | 1.99                     | 0.44              |
| 2:H:1380:GLN:OE1  | 2:H:1380:GLN:HA   | 2.18                     | 0.44              |
| 1:E:249:GLU:CD    | 1:E:249:GLU:N     | 2.76                     | 0.44              |
| 1:G:273:GLU:CD    | 2:H:1362:LEU:HD23 | 2.43                     | 0.44              |
| 1:C:312:ARG:HD2   | 1:C:313:LYS:HB3   | 2.00                     | 0.44              |
| 1:G:160:LYS:HZ1   | 1:G:566:GLN:NE2   | 2.14                     | 0.44              |
| 1:G:297:PHE:CG    | 1:G:480:LEU:HD11  | 2.53                     | 0.44              |
| 1:C:202:LEU:HD23  | 1:C:202:LEU:O     | 2.17                     | 0.44              |
| 1:C:383:ASP:OD2   | 1:C:427:ARG:NH2   | 2.37                     | 0.44              |
| 2:D:1316:LYS:HE2  | 2:D:1316:LYS:HB3  | 1.82                     | 0.44              |
| 1:G:210:PHE:CE1   | 2:H:1388:LEU:HD23 | 2.51                     | 0.44              |
| 1:G:476:LEU:HD13  | 1:G:509:TYR:CD1   | 2.52                     | 0.44              |
| 1:G:476:LEU:HD13  | 1:G:509:TYR:HA    | 1.99                     | 0.44              |
| 2:H:1280:LYS:HD3  | 2:H:1289:GLU:OE1  | 2.17                     | 0.44              |
| 1:C:349:TYR:HB3   | 1:C:360:LEU:HB2   | 2.00                     | 0.44              |
| 1:E:506:ARG:HG2   | 1:E:506:ARG:HH11  | 1.83                     | 0.44              |
| 2:H:1286:CYS:SG   | 2:H:1288:THR:HG23 | 2.58                     | 0.44              |
| 1:A:509:TYR:CE1   | 1:A:511:LEU:HB3   | 2.53                     | 0.43              |
| 1:E:159:GLN:H     | 1:E:159:GLN:HG2   | 1.46                     | 0.43              |
| 1:G:176:LEU:HG    | 1:G:176:LEU:O     | 2.17                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:180:VAL:HG23  | 1:A:180:VAL:O     | 2.17                     | 0.43              |
| 2:B:1417:LEU:HD13 | 2:B:1421:PHE:HD1  | 1.78                     | 0.43              |
| 1:C:494:ARG:HG3   | 1:C:494:ARG:HH11  | 1.83                     | 0.43              |
| 2:F:1362:LEU:N    | 2:F:1362:LEU:CD1  | 2.81                     | 0.43              |
| 2:H:1422:PHE:HB3  | 2:H:1427:LEU:HD21 | 1.99                     | 0.43              |
| 1:A:193:LEU:CD2   | 1:A:464:ILE:HG12  | 2.48                     | 0.43              |
| 1:A:445:LEU:HD22  | 1:A:449:ASP:CB    | 2.47                     | 0.43              |
| 1:E:193:LEU:HD22  | 1:E:464:ILE:HG12  | 2.00                     | 0.43              |
| 1:E:200:GLU:OE2   | 1:E:203:THR:HG22  | 2.18                     | 0.43              |
| 2:H:1320:LEU:HD12 | 2:H:1320:LEU:O    | 2.17                     | 0.43              |
| 1:C:166:ASN:HB2   | 1:C:597:ARG:HD3   | 2.01                     | 0.43              |
| 1:C:221:THR:HG23  | 1:C:276:ARG:H     | 1.83                     | 0.43              |
| 1:E:512:TYR:CD1   | 1:E:513:PRO:HA    | 2.53                     | 0.43              |
| 2:H:1425:LYS:HD3  | 2:H:1425:LYS:C    | 2.43                     | 0.43              |
| 1:A:221:THR:HG21  | 1:A:276:ARG:HB3   | 1.99                     | 0.43              |
| 2:F:1286:CYS:HB3  | 2:F:1315:CYS:HB2  | 2.00                     | 0.43              |
| 2:F:1313:ILE:H    | 2:F:1313:ILE:CD1  | 2.01                     | 0.43              |
| 1:A:271:ILE:HD12  | 1:A:271:ILE:O     | 2.18                     | 0.43              |
| 1:A:413:THR:HG21  | 1:A:420:LEU:HD11  | 2.01                     | 0.43              |
| 2:B:1297:ASP:HB2  | 2:B:1306:SER:HA   | 2.00                     | 0.43              |
| 1:C:284:ILE:O     | 1:C:284:ILE:HG13  | 2.19                     | 0.43              |
| 2:D:1296:PHE:HZ   | 2:D:1405:LEU:CD1  | 2.32                     | 0.43              |
| 2:F:1295:VAL:HG23 | 4:F:1603:HOH:O    | 2.18                     | 0.43              |
| 1:G:227:LEU:HD23  | 1:G:301:VAL:HB    | 2.01                     | 0.43              |
| 1:G:292:LYS:N     | 1:G:292:LYS:CD    | 2.72                     | 0.43              |
| 1:C:210:PHE:HE1   | 2:D:1388:LEU:HD23 | 1.83                     | 0.43              |
| 1:C:294:TYR:CD1   | 1:C:294:TYR:C     | 2.97                     | 0.43              |
| 1:C:574:LEU:N     | 1:C:574:LEU:HD12  | 2.33                     | 0.43              |
| 2:D:1394:PHE:O    | 2:D:1398:ILE:HG23 | 2.19                     | 0.43              |
| 2:B:1268:THR:CG2  | 2:B:1271:GLU:HG2  | 2.50                     | 0.42              |
| 1:C:394:LEU:HD12  | 1:C:398:PHE:HE1   | 1.83                     | 0.42              |
| 2:D:1276:CYS:SG   | 2:D:1390:THR:HG22 | 2.58                     | 0.42              |
| 1:G:586:ARG:HA    | 1:G:586:ARG:HD2   | 1.31                     | 0.42              |
| 1:A:190:ASN:HD22  | 1:A:190:ASN:HA    | 1.56                     | 0.42              |
| 1:A:578:ARG:HA    | 1:A:579:PRO:HD2   | 1.87                     | 0.42              |
| 2:B:1284:PRO:HG2  | 2:B:1322:PHE:CG   | 2.54                     | 0.42              |
| 1:G:176:LEU:O     | 1:G:177:ALA:O     | 2.38                     | 0.42              |
| 1:G:402:PHE:CD1   | 1:G:430:HIS:CE1   | 3.07                     | 0.42              |
| 2:H:1412:HIS:C    | 2:H:1416:LYS:HE3  | 2.45                     | 0.42              |
| 1:G:285:PRO:HD2   | 1:G:312:ARG:O     | 2.20                     | 0.42              |
| 1:A:388:GLN:CB    | 1:A:393:LEU:HD22  | 2.49                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:478:PHE:HD1   | 1:E:544:LEU:HD11  | 1.85                     | 0.42              |
| 2:F:1427:LEU:HD23 | 2:F:1427:LEU:HA   | 1.84                     | 0.42              |
| 1:G:292:LYS:HE2   | 1:G:293:GLU:N     | 2.34                     | 0.42              |
| 1:A:458:GLU:HG3   | 1:A:473:SER:OG    | 2.20                     | 0.42              |
| 1:C:202:LEU:HG    | 2:D:1442:SER:HB3  | 2.01                     | 0.42              |
| 1:E:534:THR:O     | 4:E:637:HOH:O     | 2.21                     | 0.42              |
| 2:F:1362:LEU:N    | 2:F:1362:LEU:HD12 | 2.34                     | 0.42              |
| 2:H:1371:CYS:O    | 2:H:1374:CYS:O    | 2.38                     | 0.42              |
| 1:A:495:PHE:O     | 1:A:499:LEU:HG    | 2.20                     | 0.42              |
| 1:G:292:LYS:CE    | 1:G:293:GLU:H     | 2.31                     | 0.42              |
| 2:H:1268:THR:HG22 | 2:H:1270:GLU:H    | 1.85                     | 0.42              |
| 1:A:221:THR:HG22  | 1:A:225:GLU:CD    | 2.45                     | 0.42              |
| 1:C:508:TYR:CZ    | 1:C:531:LEU:HD23  | 2.55                     | 0.42              |
| 2:D:1335:ARG:HD3  | 4:D:1606:HOH:O    | 2.20                     | 0.42              |
| 2:D:1350:GLU:OE2  | 2:D:1352:THR:HG23 | 2.20                     | 0.42              |
| 1:E:243:LEU:HD23  | 1:E:243:LEU:N     | 2.35                     | 0.42              |
| 1:G:385:LYS:HE2   | 1:G:427:ARG:CD    | 2.50                     | 0.42              |
| 1:A:479:HIS:CG    | 1:A:515:GLN:HG3   | 2.54                     | 0.42              |
| 1:A:508:TYR:CZ    | 1:A:531:LEU:HD23  | 2.55                     | 0.42              |
| 1:A:516:GLU:O     | 1:A:517:ASP:CB    | 2.55                     | 0.42              |
| 2:B:1316:LYS:HA   | 2:B:1316:LYS:HD2  | 1.64                     | 0.42              |
| 1:G:260:ASP:C     | 1:G:260:ASP:OD1   | 2.63                     | 0.42              |
| 2:B:1290:ASN:N    | 2:B:1290:ASN:HD22 | 2.18                     | 0.42              |
| 2:D:1409:THR:CG2  | 2:D:1410:THR:N    | 2.82                     | 0.42              |
| 2:F:1441:LEU:O    | 2:F:1441:LEU:CG   | 2.64                     | 0.42              |
| 1:A:388:GLN:O     | 1:A:393:LEU:HD22  | 2.20                     | 0.41              |
| 1:E:564:LYS:CD    | 1:E:569:GLY:HA2   | 2.49                     | 0.41              |
| 1:G:360:LEU:HD11  | 1:G:409:ILE:HG12  | 2.00                     | 0.41              |
| 1:G:364:ILE:HG23  | 1:G:413:THR:HG22  | 2.02                     | 0.41              |
| 2:H:1391:GLN:HE21 | 2:H:1391:GLN:HA   | 1.85                     | 0.41              |
| 1:A:410:ILE:HD13  | 1:A:445:LEU:HD21  | 2.01                     | 0.41              |
| 1:C:479:HIS:CD2   | 1:C:515:GLN:NE2   | 2.88                     | 0.41              |
| 1:E:567:VAL:HG12  | 1:E:568:GLY:N     | 2.35                     | 0.41              |
| 1:A:360:LEU:O     | 1:A:364:ILE:HG13  | 2.19                     | 0.41              |
| 1:A:522:TYR:HA    | 1:A:525:PHE:HB3   | 2.02                     | 0.41              |
| 2:B:1360:LEU:HD11 | 2:B:1369:PRO:HG3  | 2.02                     | 0.41              |
| 1:C:196:LEU:HD11  | 1:C:468:ILE:HD12  | 2.00                     | 0.41              |
| 1:C:476:LEU:CD2   | 1:C:502:ILE:HG12  | 2.50                     | 0.41              |
| 1:C:570:THR:HG22  | 1:C:597:ARG:HA    | 2.02                     | 0.41              |
| 1:E:166:ASN:O     | 1:E:167:ARG:C     | 2.63                     | 0.41              |
| 1:E:217:ARG:HD2   | 2:F:1364:PHE:CD1  | 2.54                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:349:TYR:HB3   | 1:A:360:LEU:HB2   | 2.03                     | 0.41              |
| 1:C:358:ASP:N     | 1:C:359:PRO:CD    | 2.83                     | 0.41              |
| 2:D:1438:GLU:OE2  | 2:D:1441:LEU:HD12 | 2.20                     | 0.41              |
| 1:G:349:TYR:HB3   | 1:G:360:LEU:HB2   | 2.02                     | 0.41              |
| 1:G:542:SER:C     | 1:G:561:ARG:HH11  | 2.28                     | 0.41              |
| 1:G:567:VAL:HG12  | 1:G:568:GLY:N     | 2.35                     | 0.41              |
| 2:H:1400:ASP:CG   | 2:H:1403:CYS:HB2  | 2.45                     | 0.41              |
| 1:A:386:HIS:HD2   | 1:A:388:GLN:N     | 2.12                     | 0.41              |
| 1:C:166:ASN:O     | 1:C:167:ARG:C     | 2.62                     | 0.41              |
| 1:E:288:LEU:HD22  | 1:E:291:LEU:HD12  | 2.02                     | 0.41              |
| 1:E:300:GLN:NE2   | 1:E:302:VAL:HG12  | 2.35                     | 0.41              |
| 2:H:1415:ASP:HA   | 2:H:1418:LYS:HB3  | 2.02                     | 0.41              |
| 1:A:182:TRP:CD2   | 1:A:573:ARG:CD    | 3.03                     | 0.41              |
| 1:A:323:VAL:HA    | 1:A:324:PRO:HD3   | 1.87                     | 0.41              |
| 1:A:343:LEU:HD23  | 1:A:344:VAL:N     | 2.35                     | 0.41              |
| 1:C:200:GLU:OE1   | 1:C:438:PRO:HA    | 2.20                     | 0.41              |
| 1:E:225:GLU:CD    | 1:E:277:GLU:HB3   | 2.46                     | 0.41              |
| 1:G:166:ASN:O     | 1:G:167:ARG:C     | 2.63                     | 0.41              |
| 2:H:1345:TRP:CZ3  | 2:H:1358:ARG:HG3  | 2.56                     | 0.41              |
| 2:F:1354:ARG:HG2  | 2:F:1354:ARG:HH11 | 1.86                     | 0.41              |
| 2:F:1396:ARG:HH12 | 2:F:1434:LYS:HE2  | 1.84                     | 0.41              |
| 1:G:166:ASN:HB2   | 1:G:597:ARG:HD3   | 2.03                     | 0.41              |
| 1:A:331:THR:CB    | 1:A:333:GLU:OE2   | 2.69                     | 0.41              |
| 1:A:331:THR:OG1   | 1:A:334:ASP:OD1   | 2.38                     | 0.41              |
| 1:A:426:LEU:HD22  | 1:A:433:PRO:O     | 2.21                     | 0.41              |
| 1:C:209:MET:CA    | 2:D:1443:ARG:HG3  | 2.49                     | 0.41              |
| 1:E:578:ARG:HA    | 1:E:579:PRO:HD3   | 1.85                     | 0.41              |
| 1:A:164:ARG:HG2   | 1:A:164:ARG:HH11  | 1.86                     | 0.41              |
| 1:A:334:ASP:HA    | 1:A:337:PHE:CD2   | 2.56                     | 0.41              |
| 2:B:1416:LYS:O    | 2:B:1420:GLN:HB2  | 2.21                     | 0.41              |
| 1:C:399:GLU:OE2   | 1:C:403:LYS:HE3   | 2.21                     | 0.41              |
| 2:F:1348:CYS:SG   | 2:F:1377:ALA:CB   | 3.08                     | 0.41              |
| 2:F:1351:PRO:HA   | 2:F:1354:ARG:HH11 | 1.86                     | 0.41              |
| 1:G:270:VAL:HG21  | 1:G:288:LEU:HD11  | 2.01                     | 0.41              |
| 2:H:1269:ASP:HA   | 2:H:1272:LYS:HG2  | 2.01                     | 0.41              |
| 1:C:156:THR:N     | 1:C:157:PRO:HD3   | 2.36                     | 0.41              |
| 2:D:1437:ALA:N    | 4:D:1601:HOH:O    | 2.52                     | 0.41              |
| 1:E:585:GLU:C     | 1:E:585:GLU:OE2   | 2.64                     | 0.41              |
| 2:F:1303:MET:HE3  | 2:F:1417:LEU:HD21 | 2.03                     | 0.41              |
| 2:B:1273:TYR:HB3  | 2:B:1394:PHE:CD1  | 2.56                     | 0.40              |
| 2:D:1416:LYS:O    | 2:D:1420:GLN:HB2  | 2.21                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:344:VAL:HG11 | 1:G:539:ILE:HG21  | 2.03                     | 0.40              |
| 1:A:387:GLU:O    | 1:A:391:ASN:ND2   | 2.54                     | 0.40              |
| 1:A:536:ASP:OD1  | 1:A:586:ARG:NH2   | 2.54                     | 0.40              |
| 2:D:1340:LYS:HD3 | 2:D:1383:TYR:CG   | 2.57                     | 0.40              |
| 1:E:207:LYS:HG2  | 1:E:208:SER:N     | 2.36                     | 0.40              |
| 1:G:423:VAL:HA   | 1:G:424:PRO:HD3   | 1.91                     | 0.40              |
| 2:H:1268:THR:O   | 2:H:1269:ASP:C    | 2.64                     | 0.40              |
| 1:G:160:LYS:HZ2  | 1:G:566:GLN:HB2   | 1.85                     | 0.40              |
| 2:D:1405:LEU:HA  | 2:D:1408:LEU:HD23 | 2.03                     | 0.40              |
| 2:D:1414:LYS:HZ3 | 2:D:1418:LYS:HD3  | 1.81                     | 0.40              |
| 1:E:362:ASP:O    | 1:E:366:VAL:HG23  | 2.21                     | 0.40              |
| 1:G:199:PRO:CG   | 1:G:200:GLU:N     | 2.85                     | 0.40              |
| 1:G:252:THR:C    | 1:G:253:LEU:HD23  | 2.46                     | 0.40              |
| 1:G:308:ASN:OD1  | 1:G:313:LYS:O     | 2.40                     | 0.40              |
| 1:G:573:ARG:C    | 1:G:574:LEU:HD12  | 2.46                     | 0.40              |
| 1:A:506:ARG:HD2  | 1:A:506:ARG:N     | 2.37                     | 0.40              |
| 2:B:1354:ARG:HA  | 2:B:1354:ARG:HD3  | 1.91                     | 0.40              |
| 1:G:185:ARG:CG   | 1:G:185:ARG:NH1   | 2.81                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|---------|----------|-------------|----|
| 1   | A     | 440/598 (74%) | 412 (94%) | 22 (5%) | 6 (1%)   | 9           | 17 |
| 1   | C     | 435/598 (73%) | 409 (94%) | 18 (4%) | 8 (2%)   | 6           | 12 |
| 1   | E     | 435/598 (73%) | 414 (95%) | 16 (4%) | 5 (1%)   | 11          | 22 |
| 1   | G     | 430/598 (72%) | 400 (93%) | 19 (4%) | 11 (3%)  | 4           | 7  |
| 2   | B     | 171/180 (95%) | 163 (95%) | 7 (4%)  | 1 (1%)   | 21          | 38 |
| 2   | D     | 176/180 (98%) | 166 (94%) | 8 (4%)  | 2 (1%)   | 11          | 22 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 2   | F     | 174/180 (97%)   | 164 (94%)  | 7 (4%)   | 3 (2%)   | 7           | 13 |
| 2   | H     | 177/180 (98%)   | 168 (95%)  | 8 (4%)   | 1 (1%)   | 21          | 38 |
| All | All   | 2438/3112 (78%) | 2296 (94%) | 105 (4%) | 37 (2%)  | 8           | 16 |

All (37) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 158  | SER  |
| 1   | A     | 517  | ASP  |
| 1   | A     | 585  | GLU  |
| 1   | C     | 157  | PRO  |
| 1   | C     | 199  | PRO  |
| 1   | C     | 517  | ASP  |
| 1   | C     | 585  | GLU  |
| 1   | E     | 517  | ASP  |
| 1   | E     | 585  | GLU  |
| 2   | F     | 1438 | GLU  |
| 1   | G     | 177  | ALA  |
| 1   | G     | 198  | CYS  |
| 1   | G     | 200  | GLU  |
| 1   | G     | 517  | ASP  |
| 1   | G     | 585  | GLU  |
| 1   | A     | 584  | ALA  |
| 2   | B     | 1300 | GLY  |
| 1   | C     | 153  | PRO  |
| 1   | C     | 197  | GLY  |
| 1   | C     | 200  | GLU  |
| 1   | C     | 584  | ALA  |
| 2   | D     | 1300 | GLY  |
| 1   | E     | 584  | ALA  |
| 2   | F     | 1300 | GLY  |
| 1   | G     | 584  | ALA  |
| 2   | H     | 1300 | GLY  |
| 1   | E     | 199  | PRO  |
| 1   | G     | 176  | LEU  |
| 1   | G     | 199  | PRO  |
| 2   | D     | 1437 | ALA  |
| 2   | F     | 1437 | ALA  |
| 1   | A     | 487  | SER  |
| 1   | G     | 167  | ARG  |
| 1   | G     | 581  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 490 | GLY  |
| 1   | E     | 167 | ARG  |
| 1   | G     | 158 | SER  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 389/527 (74%)   | 358 (92%)  | 31 (8%)  | 11          | 24 |
| 1   | C     | 389/527 (74%)   | 356 (92%)  | 33 (8%)  | 10          | 22 |
| 1   | E     | 387/527 (73%)   | 349 (90%)  | 38 (10%) | 7           | 16 |
| 1   | G     | 385/527 (73%)   | 343 (89%)  | 42 (11%) | 6           | 13 |
| 2   | B     | 162/168 (96%)   | 145 (90%)  | 17 (10%) | 6           | 14 |
| 2   | D     | 167/168 (99%)   | 154 (92%)  | 13 (8%)  | 11          | 24 |
| 2   | F     | 165/168 (98%)   | 147 (89%)  | 18 (11%) | 6           | 13 |
| 2   | H     | 168/168 (100%)  | 152 (90%)  | 16 (10%) | 8           | 17 |
| All | All   | 2212/2780 (80%) | 2004 (91%) | 208 (9%) | 8           | 18 |

All (208) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 160 | LYS  |
| 1   | A     | 163 | SER  |
| 1   | A     | 173 | SER  |
| 1   | A     | 181 | SER  |
| 1   | A     | 185 | ARG  |
| 1   | A     | 190 | ASN  |
| 1   | A     | 191 | ILE  |
| 1   | A     | 202 | LEU  |
| 1   | A     | 209 | MET  |
| 1   | A     | 226 | GLU  |
| 1   | A     | 269 | SER  |
| 1   | A     | 271 | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 307  | ILE  |
| 1   | A     | 313  | LYS  |
| 1   | A     | 339  | GLN  |
| 1   | A     | 340  | SER  |
| 1   | A     | 385  | LYS  |
| 1   | A     | 393  | LEU  |
| 1   | A     | 406  | LEU  |
| 1   | A     | 414  | ARG  |
| 1   | A     | 428  | ASP  |
| 1   | A     | 429  | VAL  |
| 1   | A     | 447  | ARG  |
| 1   | A     | 448  | GLU  |
| 1   | A     | 480  | LEU  |
| 1   | A     | 515  | GLN  |
| 1   | A     | 518  | MET  |
| 1   | A     | 540  | ILE  |
| 1   | A     | 582  | ASP  |
| 1   | A     | 586  | ARG  |
| 1   | A     | 587  | GLN  |
| 2   | B     | 1271 | GLU  |
| 2   | B     | 1274 | ARG  |
| 2   | B     | 1301 | THR  |
| 2   | B     | 1308 | TYR  |
| 2   | B     | 1316 | LYS  |
| 2   | B     | 1329 | LYS  |
| 2   | B     | 1347 | ILE  |
| 2   | B     | 1366 | ARG  |
| 2   | B     | 1376 | LYS  |
| 2   | B     | 1396 | ARG  |
| 2   | B     | 1406 | GLU  |
| 2   | B     | 1410 | THR  |
| 2   | B     | 1417 | LEU  |
| 2   | B     | 1420 | GLN  |
| 2   | B     | 1428 | GLN  |
| 2   | B     | 1431 | ARG  |
| 2   | B     | 1436 | THR  |
| 1   | C     | 153  | PRO  |
| 1   | C     | 156  | THR  |
| 1   | C     | 158  | SER  |
| 1   | C     | 159  | GLN  |
| 1   | C     | 166  | ASN  |
| 1   | C     | 178  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 185  | ARG  |
| 1   | C     | 196  | LEU  |
| 1   | C     | 199  | PRO  |
| 1   | C     | 200  | GLU  |
| 1   | C     | 202  | LEU  |
| 1   | C     | 221  | THR  |
| 1   | C     | 243  | LEU  |
| 1   | C     | 279  | SER  |
| 1   | C     | 292  | LYS  |
| 1   | C     | 310  | THR  |
| 1   | C     | 329  | GLN  |
| 1   | C     | 344  | VAL  |
| 1   | C     | 385  | LYS  |
| 1   | C     | 406  | LEU  |
| 1   | C     | 418  | SER  |
| 1   | C     | 425  | SER  |
| 1   | C     | 441  | SER  |
| 1   | C     | 443  | SER  |
| 1   | C     | 447  | ARG  |
| 1   | C     | 448  | GLU  |
| 1   | C     | 507  | SER  |
| 1   | C     | 518  | MET  |
| 1   | C     | 524  | SER  |
| 1   | C     | 540  | ILE  |
| 1   | C     | 582  | ASP  |
| 1   | C     | 586  | ARG  |
| 1   | C     | 594  | GLN  |
| 2   | D     | 1268 | THR  |
| 2   | D     | 1270 | GLU  |
| 2   | D     | 1307 | LEU  |
| 2   | D     | 1313 | ILE  |
| 2   | D     | 1320 | LEU  |
| 2   | D     | 1332 | MET  |
| 2   | D     | 1357 | THR  |
| 2   | D     | 1376 | LYS  |
| 2   | D     | 1405 | LEU  |
| 2   | D     | 1408 | LEU  |
| 2   | D     | 1416 | LYS  |
| 2   | D     | 1420 | GLN  |
| 2   | D     | 1443 | ARG  |
| 1   | E     | 159  | GLN  |
| 1   | E     | 164  | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | E     | 167  | ARG  |
| 1   | E     | 173  | SER  |
| 1   | E     | 190  | ASN  |
| 1   | E     | 198  | CYS  |
| 1   | E     | 199  | PRO  |
| 1   | E     | 202  | LEU  |
| 1   | E     | 203  | THR  |
| 1   | E     | 206  | TYR  |
| 1   | E     | 231  | LEU  |
| 1   | E     | 241  | THR  |
| 1   | E     | 243  | LEU  |
| 1   | E     | 271  | ILE  |
| 1   | E     | 278  | HIS  |
| 1   | E     | 307  | ILE  |
| 1   | E     | 336  | ASP  |
| 1   | E     | 341  | MET  |
| 1   | E     | 344  | VAL  |
| 1   | E     | 361  | LEU  |
| 1   | E     | 382  | LEU  |
| 1   | E     | 403  | LYS  |
| 1   | E     | 406  | LEU  |
| 1   | E     | 418  | SER  |
| 1   | E     | 425  | SER  |
| 1   | E     | 447  | ARG  |
| 1   | E     | 448  | GLU  |
| 1   | E     | 451  | LYS  |
| 1   | E     | 452  | GLN  |
| 1   | E     | 507  | SER  |
| 1   | E     | 518  | MET  |
| 1   | E     | 538  | LEU  |
| 1   | E     | 540  | ILE  |
| 1   | E     | 544  | LEU  |
| 1   | E     | 561  | ARG  |
| 1   | E     | 564  | LYS  |
| 1   | E     | 585  | GLU  |
| 1   | E     | 586  | ARG  |
| 2   | F     | 1301 | THR  |
| 2   | F     | 1309 | ARG  |
| 2   | F     | 1311 | SER  |
| 2   | F     | 1313 | ILE  |
| 2   | F     | 1321 | THR  |
| 2   | F     | 1329 | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | F     | 1332 | MET  |
| 2   | F     | 1340 | LYS  |
| 2   | F     | 1350 | GLU  |
| 2   | F     | 1366 | ARG  |
| 2   | F     | 1376 | LYS  |
| 2   | F     | 1411 | ASP  |
| 2   | F     | 1416 | LYS  |
| 2   | F     | 1418 | LYS  |
| 2   | F     | 1420 | GLN  |
| 2   | F     | 1432 | LYS  |
| 2   | F     | 1440 | PHE  |
| 2   | F     | 1441 | LEU  |
| 1   | G     | 159  | GLN  |
| 1   | G     | 160  | LYS  |
| 1   | G     | 166  | ASN  |
| 1   | G     | 176  | LEU  |
| 1   | G     | 178  | GLN  |
| 1   | G     | 185  | ARG  |
| 1   | G     | 196  | LEU  |
| 1   | G     | 199  | PRO  |
| 1   | G     | 207  | LYS  |
| 1   | G     | 209  | MET  |
| 1   | G     | 211  | GLN  |
| 1   | G     | 221  | THR  |
| 1   | G     | 236  | LYS  |
| 1   | G     | 249  | GLU  |
| 1   | G     | 265  | LEU  |
| 1   | G     | 271  | ILE  |
| 1   | G     | 276  | ARG  |
| 1   | G     | 279  | SER  |
| 1   | G     | 292  | LYS  |
| 1   | G     | 312  | ARG  |
| 1   | G     | 321  | GLU  |
| 1   | G     | 329  | GLN  |
| 1   | G     | 332  | GLU  |
| 1   | G     | 336  | ASP  |
| 1   | G     | 340  | SER  |
| 1   | G     | 382  | LEU  |
| 1   | G     | 396  | SER  |
| 1   | G     | 406  | LEU  |
| 1   | G     | 425  | SER  |
| 1   | G     | 432  | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | G     | 443  | SER  |
| 1   | G     | 448  | GLU  |
| 1   | G     | 452  | GLN  |
| 1   | G     | 515  | GLN  |
| 1   | G     | 518  | MET  |
| 1   | G     | 538  | LEU  |
| 1   | G     | 540  | ILE  |
| 1   | G     | 544  | LEU  |
| 1   | G     | 575  | TYR  |
| 1   | G     | 582  | ASP  |
| 1   | G     | 586  | ARG  |
| 1   | G     | 591  | ILE  |
| 2   | H     | 1266 | GLN  |
| 2   | H     | 1267 | LEU  |
| 2   | H     | 1302 | ASP  |
| 2   | H     | 1305 | PRO  |
| 2   | H     | 1309 | ARG  |
| 2   | H     | 1315 | CYS  |
| 2   | H     | 1320 | LEU  |
| 2   | H     | 1332 | MET  |
| 2   | H     | 1362 | LEU  |
| 2   | H     | 1391 | GLN  |
| 2   | H     | 1405 | LEU  |
| 2   | H     | 1413 | GLU  |
| 2   | H     | 1415 | ASP  |
| 2   | H     | 1420 | GLN  |
| 2   | H     | 1427 | LEU  |
| 2   | H     | 1438 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 190  | ASN  |
| 1   | A     | 256  | GLN  |
| 1   | A     | 283  | GLN  |
| 1   | A     | 369  | HIS  |
| 1   | A     | 386  | HIS  |
| 1   | A     | 454  | GLN  |
| 1   | A     | 530  | GLN  |
| 1   | A     | 566  | GLN  |
| 1   | A     | 587  | GLN  |
| 2   | B     | 1294 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 1363 | GLN  |
| 2   | B     | 1420 | GLN  |
| 2   | B     | 1435 | ASN  |
| 1   | C     | 166  | ASN  |
| 1   | C     | 178  | GLN  |
| 1   | C     | 234  | HIS  |
| 1   | C     | 248  | GLN  |
| 1   | C     | 256  | GLN  |
| 1   | C     | 283  | GLN  |
| 1   | C     | 369  | HIS  |
| 1   | C     | 386  | HIS  |
| 1   | C     | 391  | ASN  |
| 1   | C     | 452  | GLN  |
| 1   | C     | 454  | GLN  |
| 1   | C     | 515  | GLN  |
| 1   | C     | 587  | GLN  |
| 2   | D     | 1290 | ASN  |
| 2   | D     | 1294 | ASN  |
| 2   | D     | 1439 | GLN  |
| 1   | E     | 159  | GLN  |
| 1   | E     | 178  | GLN  |
| 1   | E     | 190  | ASN  |
| 1   | E     | 256  | GLN  |
| 1   | E     | 283  | GLN  |
| 1   | E     | 300  | GLN  |
| 1   | E     | 308  | ASN  |
| 1   | E     | 329  | GLN  |
| 1   | E     | 369  | HIS  |
| 1   | E     | 386  | HIS  |
| 1   | E     | 388  | GLN  |
| 1   | E     | 391  | ASN  |
| 1   | E     | 419  | HIS  |
| 1   | E     | 452  | GLN  |
| 1   | E     | 566  | GLN  |
| 2   | F     | 1290 | ASN  |
| 2   | F     | 1294 | ASN  |
| 2   | F     | 1363 | GLN  |
| 2   | F     | 1412 | HIS  |
| 1   | G     | 190  | ASN  |
| 1   | G     | 256  | GLN  |
| 1   | G     | 283  | GLN  |
| 1   | G     | 329  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | G     | 339  | GLN  |
| 1   | G     | 369  | HIS  |
| 1   | G     | 386  | HIS  |
| 1   | G     | 419  | HIS  |
| 1   | G     | 454  | GLN  |
| 1   | G     | 515  | GLN  |
| 1   | G     | 566  | GLN  |
| 1   | G     | 594  | GLN  |
| 2   | H     | 1290 | ASN  |
| 2   | H     | 1312 | ASN  |
| 2   | H     | 1420 | GLN  |
| 2   | H     | 1439 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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     | 442/598 (73%)   | 0.35   | 34 (7%)   | 19 17 | 18, 42, 87, 110       | 0       |
| 1   | C     | 441/598 (73%)   | 0.21   | 41 (9%)   | 14 12 | 16, 35, 86, 106       | 0       |
| 1   | E     | 439/598 (73%)   | 0.27   | 31 (7%)   | 22 19 | 20, 38, 86, 105       | 0       |
| 1   | G     | 436/598 (72%)   | 0.70   | 36 (8%)   | 17 15 | 31, 53, 91, 115       | 0       |
| 2   | B     | 173/180 (96%)   | 0.85   | 28 (16%)  | 4 3   | 15, 55, 104, 116      | 0       |
| 2   | D     | 178/180 (98%)   | 0.51   | 22 (12%)  | 8 6   | 17, 50, 96, 110       | 0       |
| 2   | F     | 176/180 (97%)   | 0.57   | 18 (10%)  | 12 10 | 26, 48, 89, 104       | 0       |
| 2   | H     | 179/180 (99%)   | 1.37   | 48 (26%)  | 1 1   | 39, 71, 105, 118      | 0       |
| All | All   | 2464/3112 (79%) | 0.51   | 258 (10%) | 11 10 | 15, 46, 94, 118       | 0       |

All (258) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | C     | 311  | GLY  | 7.7  |
| 1   | G     | 202  | LEU  | 6.8  |
| 1   | C     | 202  | LEU  | 6.3  |
| 1   | G     | 580  | ALA  | 6.0  |
| 2   | F     | 1441 | LEU  | 5.5  |
| 1   | C     | 201  | ALA  | 5.3  |
| 1   | C     | 151  | PHE  | 5.2  |
| 1   | C     | 580  | ALA  | 5.1  |
| 1   | C     | 153  | PRO  | 5.1  |
| 2   | D     | 1267 | LEU  | 5.0  |
| 2   | F     | 1313 | ILE  | 4.9  |
| 2   | B     | 1300 | GLY  | 4.8  |
| 1   | C     | 312  | ARG  | 4.8  |
| 1   | C     | 152  | SER  | 4.7  |
| 1   | G     | 581  | ALA  | 4.6  |
| 1   | C     | 199  | PRO  | 4.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | C     | 198  | CYS  | 4.6  |
| 1   | C     | 584  | ALA  | 4.5  |
| 1   | C     | 187  | GLY  | 4.4  |
| 1   | G     | 199  | PRO  | 4.4  |
| 1   | A     | 581  | ALA  | 4.4  |
| 1   | G     | 201  | ALA  | 4.4  |
| 2   | H     | 1437 | ALA  | 4.4  |
| 2   | B     | 1298 | GLY  | 4.4  |
| 1   | C     | 177  | ALA  | 4.3  |
| 1   | E     | 209  | MET  | 4.3  |
| 2   | H     | 1313 | ILE  | 4.3  |
| 2   | F     | 1440 | PHE  | 4.3  |
| 1   | G     | 393  | LEU  | 4.2  |
| 2   | B     | 1440 | PHE  | 4.2  |
| 2   | F     | 1439 | GLN  | 4.2  |
| 1   | G     | 491  | THR  | 4.1  |
| 2   | H     | 1440 | PHE  | 4.0  |
| 2   | F     | 1314 | ASP  | 4.0  |
| 1   | A     | 584  | ALA  | 4.0  |
| 1   | C     | 179  | GLY  | 4.0  |
| 1   | A     | 209  | MET  | 3.9  |
| 2   | H     | 1307 | LEU  | 3.9  |
| 1   | E     | 206  | TYR  | 3.8  |
| 1   | E     | 581  | ALA  | 3.8  |
| 1   | G     | 187  | GLY  | 3.8  |
| 2   | B     | 1311 | SER  | 3.8  |
| 2   | D     | 1300 | GLY  | 3.8  |
| 2   | H     | 1441 | LEU  | 3.8  |
| 1   | E     | 186  | GLY  | 3.8  |
| 2   | H     | 1421 | PHE  | 3.7  |
| 1   | A     | 187  | GLY  | 3.7  |
| 2   | B     | 1417 | LEU  | 3.7  |
| 2   | D     | 1409 | THR  | 3.7  |
| 1   | E     | 187  | GLY  | 3.7  |
| 1   | C     | 581  | ALA  | 3.6  |
| 1   | C     | 335  | ALA  | 3.6  |
| 2   | D     | 1301 | THR  | 3.6  |
| 2   | B     | 1316 | LYS  | 3.5  |
| 1   | G     | 198  | CYS  | 3.5  |
| 1   | G     | 180  | VAL  | 3.5  |
| 1   | G     | 584  | ALA  | 3.5  |
| 1   | C     | 154  | SER  | 3.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | D     | 1437 | ALA  | 3.4  |
| 2   | B     | 1439 | GLN  | 3.4  |
| 2   | B     | 1317 | ALA  | 3.4  |
| 2   | H     | 1443 | ARG  | 3.4  |
| 1   | E     | 492  | SER  | 3.3  |
| 1   | G     | 336  | ASP  | 3.3  |
| 2   | F     | 1412 | HIS  | 3.3  |
| 2   | H     | 1410 | THR  | 3.3  |
| 2   | H     | 1412 | HIS  | 3.2  |
| 1   | E     | 584  | ALA  | 3.2  |
| 2   | H     | 1308 | TYR  | 3.2  |
| 2   | B     | 1299 | SER  | 3.2  |
| 1   | A     | 393  | LEU  | 3.2  |
| 1   | G     | 332  | GLU  | 3.1  |
| 2   | B     | 1412 | HIS  | 3.1  |
| 1   | E     | 585  | GLU  | 3.1  |
| 2   | D     | 1376 | LYS  | 3.1  |
| 1   | G     | 335  | ALA  | 3.1  |
| 1   | A     | 157  | PRO  | 3.1  |
| 2   | B     | 1421 | PHE  | 3.1  |
| 2   | B     | 1409 | THR  | 3.0  |
| 1   | G     | 188  | ALA  | 3.0  |
| 2   | F     | 1416 | LYS  | 3.0  |
| 2   | D     | 1413 | GLU  | 3.0  |
| 2   | B     | 1301 | THR  | 3.0  |
| 2   | D     | 1438 | GLU  | 3.0  |
| 2   | D     | 1408 | LEU  | 3.0  |
| 2   | D     | 1440 | PHE  | 3.0  |
| 1   | A     | 179  | GLY  | 3.0  |
| 1   | C     | 188  | ALA  | 2.9  |
| 2   | F     | 1437 | ALA  | 2.9  |
| 2   | H     | 1306 | SER  | 2.9  |
| 1   | A     | 186  | GLY  | 2.9  |
| 2   | H     | 1303 | MET  | 2.9  |
| 1   | E     | 580  | ALA  | 2.9  |
| 2   | H     | 1422 | PHE  | 2.9  |
| 2   | H     | 1300 | GLY  | 2.9  |
| 1   | A     | 491  | THR  | 2.9  |
| 1   | G     | 579  | PRO  | 2.9  |
| 2   | H     | 1408 | LEU  | 2.9  |
| 1   | C     | 200  | GLU  | 2.9  |
| 1   | G     | 488  | SER  | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | E     | 393  | LEU  | 2.9  |
| 2   | H     | 1442 | SER  | 2.8  |
| 2   | H     | 1305 | PRO  | 2.8  |
| 1   | E     | 335  | ALA  | 2.8  |
| 2   | H     | 1407 | LYS  | 2.8  |
| 1   | E     | 488  | SER  | 2.8  |
| 1   | C     | 336  | ASP  | 2.8  |
| 2   | H     | 1287 | GLY  | 2.8  |
| 1   | C     | 310  | THR  | 2.8  |
| 2   | D     | 1417 | LEU  | 2.8  |
| 1   | A     | 189  | GLY  | 2.8  |
| 2   | H     | 1413 | GLU  | 2.8  |
| 2   | D     | 1444 | SER  | 2.7  |
| 2   | H     | 1444 | SER  | 2.7  |
| 2   | B     | 1268 | THR  | 2.7  |
| 2   | F     | 1317 | ALA  | 2.7  |
| 1   | G     | 179  | GLY  | 2.7  |
| 2   | H     | 1298 | GLY  | 2.7  |
| 2   | D     | 1401 | ALA  | 2.7  |
| 2   | H     | 1409 | THR  | 2.7  |
| 1   | C     | 447  | ARG  | 2.7  |
| 2   | H     | 1299 | SER  | 2.7  |
| 1   | A     | 392  | CYS  | 2.7  |
| 2   | D     | 1421 | PHE  | 2.7  |
| 1   | A     | 158  | SER  | 2.7  |
| 1   | A     | 185  | ARG  | 2.7  |
| 2   | B     | 1415 | ASP  | 2.6  |
| 1   | C     | 585  | GLU  | 2.6  |
| 1   | E     | 208  | SER  | 2.6  |
| 2   | B     | 1410 | THR  | 2.6  |
| 1   | A     | 516  | GLU  | 2.6  |
| 2   | F     | 1410 | THR  | 2.6  |
| 2   | H     | 1419 | LYS  | 2.6  |
| 2   | H     | 1417 | LEU  | 2.6  |
| 1   | G     | 181  | SER  | 2.6  |
| 1   | C     | 197  | GLY  | 2.6  |
| 1   | G     | 585  | GLU  | 2.6  |
| 1   | A     | 166  | ASN  | 2.6  |
| 1   | G     | 177  | ALA  | 2.6  |
| 1   | A     | 338  | GLU  | 2.5  |
| 2   | B     | 1408 | LEU  | 2.5  |
| 2   | H     | 1267 | LEU  | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | E     | 166  | ASN  | 2.5  |
| 1   | G     | 178  | GLN  | 2.5  |
| 2   | H     | 1373 | ALA  | 2.5  |
| 1   | C     | 331  | THR  | 2.5  |
| 2   | H     | 1405 | LEU  | 2.5  |
| 1   | E     | 188  | ALA  | 2.5  |
| 1   | A     | 577  | ARG  | 2.5  |
| 2   | D     | 1302 | ASP  | 2.5  |
| 2   | B     | 1291 | ILE  | 2.5  |
| 2   | H     | 1296 | PHE  | 2.5  |
| 1   | A     | 335  | ALA  | 2.5  |
| 2   | B     | 1303 | MET  | 2.5  |
| 2   | F     | 1315 | CYS  | 2.5  |
| 1   | E     | 179  | GLY  | 2.5  |
| 2   | H     | 1414 | LYS  | 2.5  |
| 2   | F     | 1409 | THR  | 2.5  |
| 1   | G     | 157  | PRO  | 2.4  |
| 1   | G     | 200  | GLU  | 2.4  |
| 2   | H     | 1415 | ASP  | 2.4  |
| 1   | G     | 176  | LEU  | 2.4  |
| 2   | D     | 1410 | THR  | 2.4  |
| 1   | C     | 181  | SER  | 2.4  |
| 1   | C     | 186  | GLY  | 2.4  |
| 1   | G     | 582  | ASP  | 2.4  |
| 1   | C     | 176  | LEU  | 2.4  |
| 1   | C     | 586  | ARG  | 2.4  |
| 1   | C     | 579  | PRO  | 2.4  |
| 2   | D     | 1414 | LYS  | 2.4  |
| 1   | C     | 189  | GLY  | 2.4  |
| 1   | E     | 189  | GLY  | 2.4  |
| 1   | C     | 275  | ASP  | 2.4  |
| 2   | F     | 1297 | ASP  | 2.4  |
| 1   | A     | 206  | TYR  | 2.4  |
| 2   | B     | 1422 | PHE  | 2.4  |
| 1   | E     | 245  | ALA  | 2.4  |
| 2   | H     | 1401 | ALA  | 2.4  |
| 1   | E     | 207  | LYS  | 2.4  |
| 2   | H     | 1285 | THR  | 2.4  |
| 2   | B     | 1420 | GLN  | 2.4  |
| 2   | H     | 1411 | ASP  | 2.4  |
| 1   | C     | 338  | GLU  | 2.4  |
| 1   | G     | 333  | GLU  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | G     | 331  | THR  | 2.3  |
| 1   | C     | 495  | PHE  | 2.3  |
| 1   | E     | 575  | TYR  | 2.3  |
| 1   | E     | 182  | TRP  | 2.3  |
| 1   | A     | 208  | SER  | 2.3  |
| 1   | A     | 487  | SER  | 2.3  |
| 2   | B     | 1295 | VAL  | 2.3  |
| 1   | A     | 585  | GLU  | 2.3  |
| 1   | A     | 490  | GLY  | 2.3  |
| 1   | E     | 212  | LYS  | 2.3  |
| 2   | H     | 1270 | GLU  | 2.3  |
| 1   | E     | 203  | THR  | 2.3  |
| 1   | E     | 178  | GLN  | 2.3  |
| 2   | D     | 1299 | SER  | 2.3  |
| 2   | B     | 1418 | LYS  | 2.3  |
| 2   | H     | 1269 | ASP  | 2.3  |
| 2   | F     | 1374 | CYS  | 2.3  |
| 2   | H     | 1311 | SER  | 2.2  |
| 2   | H     | 1418 | LYS  | 2.2  |
| 1   | C     | 249  | GLU  | 2.2  |
| 1   | E     | 331  | THR  | 2.2  |
| 2   | D     | 1412 | HIS  | 2.2  |
| 2   | H     | 1321 | THR  | 2.2  |
| 1   | G     | 207  | LYS  | 2.2  |
| 2   | F     | 1316 | LYS  | 2.2  |
| 1   | A     | 489  | SER  | 2.2  |
| 1   | E     | 180  | VAL  | 2.2  |
| 1   | E     | 181  | SER  | 2.2  |
| 2   | H     | 1322 | PHE  | 2.2  |
| 1   | A     | 181  | SER  | 2.2  |
| 2   | F     | 1311 | SER  | 2.2  |
| 1   | E     | 276  | ARG  | 2.2  |
| 1   | G     | 564  | LYS  | 2.2  |
| 1   | G     | 186  | GLY  | 2.1  |
| 2   | D     | 1320 | LEU  | 2.1  |
| 2   | B     | 1313 | ILE  | 2.1  |
| 1   | G     | 578  | ARG  | 2.1  |
| 2   | D     | 1439 | GLN  | 2.1  |
| 1   | C     | 184  | GLY  | 2.1  |
| 1   | G     | 191  | ILE  | 2.1  |
| 2   | H     | 1291 | ILE  | 2.1  |
| 1   | A     | 447  | ARG  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 575  | TYR  | 2.1  |
| 1   | E     | 577  | ARG  | 2.1  |
| 1   | A     | 183  | SER  | 2.1  |
| 2   | H     | 1432 | LYS  | 2.1  |
| 1   | A     | 159  | GLN  | 2.1  |
| 1   | A     | 182  | TRP  | 2.1  |
| 1   | C     | 332  | GLU  | 2.1  |
| 2   | B     | 1411 | ASP  | 2.1  |
| 2   | F     | 1419 | LYS  | 2.1  |
| 1   | C     | 330  | PRO  | 2.1  |
| 1   | G     | 159  | GLN  | 2.1  |
| 2   | H     | 1428 | GLN  | 2.1  |
| 1   | A     | 580  | ALA  | 2.1  |
| 1   | C     | 155  | ALA  | 2.1  |
| 2   | B     | 1307 | LEU  | 2.1  |
| 2   | D     | 1405 | LEU  | 2.1  |
| 1   | G     | 189  | GLY  | 2.1  |
| 1   | A     | 448  | GLU  | 2.1  |
| 2   | H     | 1272 | LYS  | 2.1  |
| 1   | E     | 334  | ASP  | 2.1  |
| 2   | B     | 1314 | ASP  | 2.1  |
| 2   | H     | 1439 | GLN  | 2.0  |
| 1   | C     | 190  | ASN  | 2.0  |
| 1   | C     | 583  | GLY  | 2.0  |
| 2   | F     | 1298 | GLY  | 2.0  |
| 1   | A     | 598  | ILE  | 2.0  |
| 1   | A     | 517  | ASP  | 2.0  |
| 1   | E     | 185  | ARG  | 2.0  |
| 2   | B     | 1416 | LYS  | 2.0  |
| 2   | H     | 1316 | LYS  | 2.0  |
| 1   | G     | 172  | THR  | 2.0  |
| 2   | H     | 1301 | THR  | 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](#)

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 3   | ZN   | B     | 1501 | 1/1   | 0.98 | 0.05 | 82,82,82,82                 | 0     |
| 3   | ZN   | F     | 1502 | 1/1   | 0.98 | 0.04 | 62,62,62,62                 | 0     |
| 3   | ZN   | H     | 1501 | 1/1   | 0.98 | 0.04 | 88,88,88,88                 | 0     |
| 3   | ZN   | F     | 1501 | 1/1   | 0.99 | 0.03 | 53,53,53,53                 | 0     |
| 3   | ZN   | B     | 1502 | 1/1   | 0.99 | 0.04 | 37,37,37,37                 | 0     |
| 3   | ZN   | D     | 1501 | 1/1   | 0.99 | 0.02 | 66,66,66,66                 | 0     |
| 3   | ZN   | H     | 1502 | 1/1   | 0.99 | 0.03 | 64,64,64,64                 | 0     |
| 3   | ZN   | D     | 1502 | 1/1   | 1.00 | 0.01 | 43,43,43,43                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.