



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:41 PM UTC

PDB ID : 1PMO / pdb\_00001pmo  
Title : Crystal structure of Escherichia coli GadB (neutral pH)  
Authors : Capitani, G.; De Biase, D.; Aurizi, C.; Gut, H.; Bossa, F.; Grutter, M.G.  
Deposited on : 2003-06-11  
Resolution : 2.30 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                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| 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                                                             |

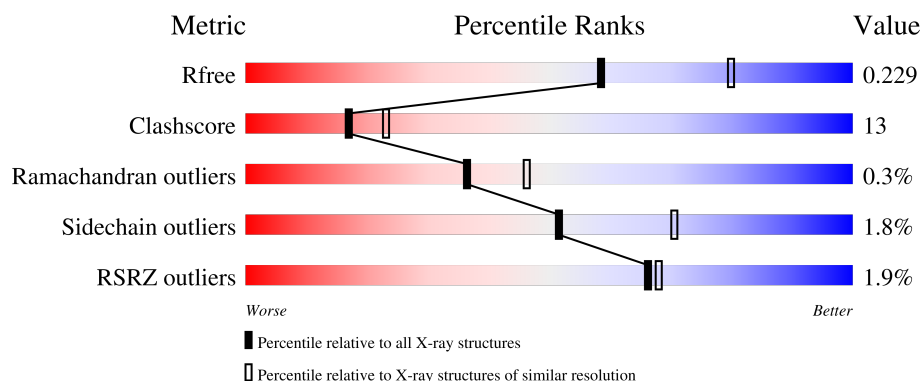
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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                      | 6319 (2.30-2.30)                                      |
| Clashscore            | 190562                      | 6919 (2.30-2.30)                                      |
| Ramachandran outliers | 187476                      | 6854 (2.30-2.30)                                      |
| Sidechain outliers    | 187428                      | 6854 (2.30-2.30)                                      |
| RSRZ outliers         | 180081                      | 6325 (2.30-2.30)                                      |

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     | 466    | <div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>67%</span> <span>28%</span> <span>..</span> </div> </div> |
| 1   | B     | 466    | <div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>73%</span> <span>24%</span> <span>..</span> </div> </div> |
| 1   | C     | 466    | <div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>72%</span> <span>24%</span> <span>..</span> </div> </div> |
| 1   | D     | 466    | <div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>73%</span> <span>23%</span> <span>..</span> </div> </div> |
| 1   | E     | 466    | <div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>75%</span> <span>22%</span> <span>..</span> </div> </div> |

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| Mol | Chain | Length | Quality of chain                                                                                                                               |
|-----|-------|--------|------------------------------------------------------------------------------------------------------------------------------------------------|
| 1   | F     | 466    | <div> <div>%</div> <div>  </div> <div>77%19% ..</div> </div> |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 3   | TRS  | A     | 3251 | -         | -        | X       | -                |
| 3   | TRS  | C     | 3250 | -         | -        | X       | -                |
| 3   | TRS  | C     | 3252 | -         | -        | X       | -                |
| 3   | TRS  | E     | 3246 | -         | -        | X       | -                |
| 3   | TRS  | F     | 3248 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

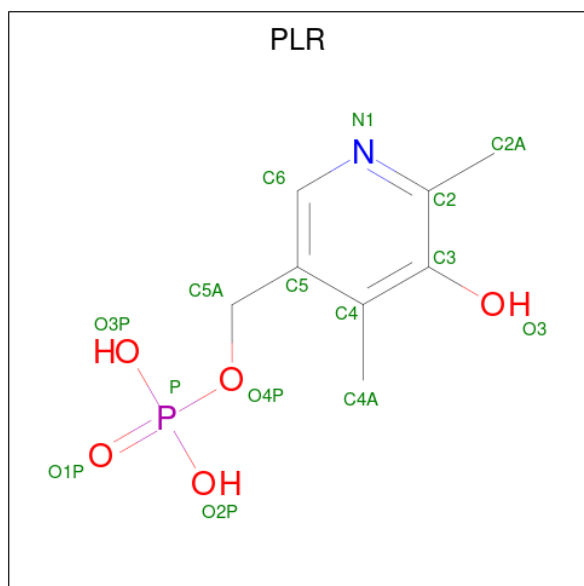
There are 4 unique types of molecules in this entry. The entry contains 23202 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glutamate decarboxylase beta.

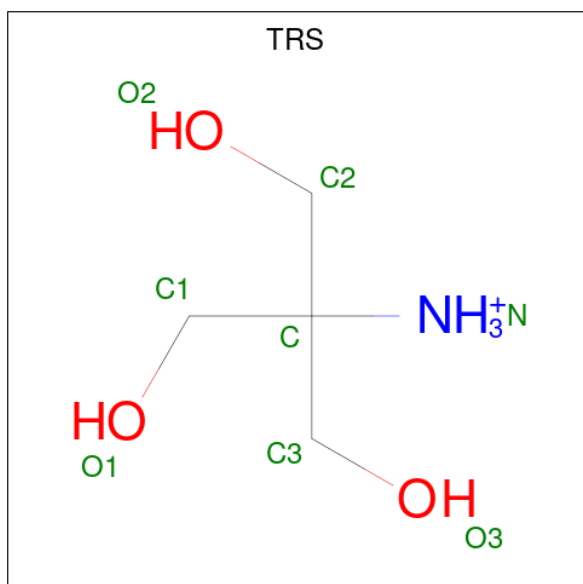
| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 455      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3616  | 2308 | 617 | 667 | 24 |         |         |       |
| 1   | B     | 463      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3681  | 2347 | 630 | 680 | 24 |         |         |       |
| 1   | C     | 454      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3607  | 2303 | 616 | 664 | 24 |         |         |       |
| 1   | D     | 454      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3607  | 2303 | 616 | 664 | 24 |         |         |       |
| 1   | E     | 463      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3681  | 2347 | 630 | 680 | 24 |         |         |       |
| 1   | F     | 454      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3607  | 2303 | 616 | 664 | 24 |         |         |       |

- Molecule 2 is (5-HYDROXY-4,6-DIMETHYLPYRIDIN-3-YL)METHYL DIHYDROGEN PHOSPHATE (CCD ID: PLR) (formula: C<sub>8</sub>H<sub>12</sub>NO<sub>5</sub>P).



| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 2   | A     | 1        | Total | C | N | O | P | 0       | 0       |
|     |       |          | 15    | 8 | 1 | 5 | 1 |         |         |
| 2   | B     | 1        | Total | C | N | O | P | 0       | 0       |
|     |       |          | 15    | 8 | 1 | 5 | 1 |         |         |
| 2   | C     | 1        | Total | C | N | O | P | 0       | 0       |
|     |       |          | 15    | 8 | 1 | 5 | 1 |         |         |
| 2   | D     | 1        | Total | C | N | O | P | 0       | 0       |
|     |       |          | 15    | 8 | 1 | 5 | 1 |         |         |
| 2   | E     | 1        | Total | C | N | O | P | 0       | 0       |
|     |       |          | 15    | 8 | 1 | 5 | 1 |         |         |
| 2   | F     | 1        | Total | C | N | O | P | 0       | 0       |
|     |       |          | 15    | 8 | 1 | 5 | 1 |         |         |

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula:  $C_4H_{12}NO_3$ ).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 3   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 4 | 1 | 3 |         |         |
| 3   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 4 | 1 | 3 |         |         |
| 3   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 4 | 1 | 3 |         |         |
| 3   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 4 | 1 | 3 |         |         |
| 3   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 4 | 1 | 3 |         |         |

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| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 3   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 4 | 1 | 3 |         |         |
| 3   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 4 | 1 | 3 |         |         |
| 3   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 4 | 1 | 3 |         |         |
| 3   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 4 | 1 | 3 |         |         |
| 3   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 4 | 1 | 3 |         |         |
| 3   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 4 | 1 | 3 |         |         |
| 3   | E     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 4 | 1 | 3 |         |         |
| 3   | E     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 4 | 1 | 3 |         |         |
| 3   | E     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 4 | 1 | 3 |         |         |
| 3   | E     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 4 | 1 | 3 |         |         |
| 3   | F     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 4 | 1 | 3 |         |         |
| 3   | F     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 4 | 1 | 3 |         |         |
| 3   | F     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 4 | 1 | 3 |         |         |

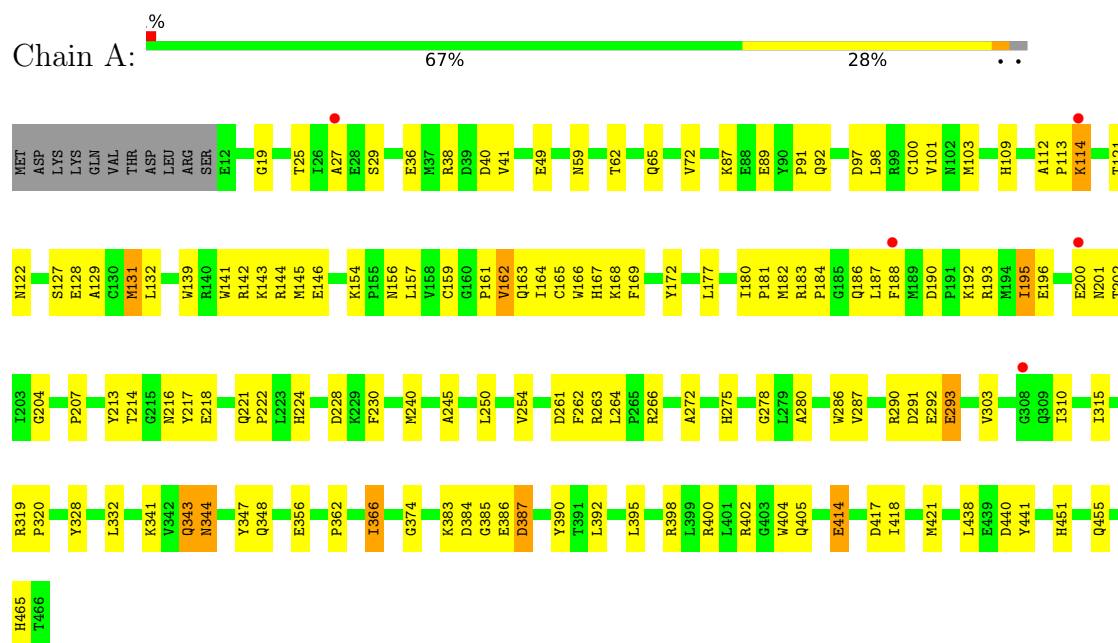
- Molecule 4 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 4   | A     | 188      | Total | O   | 0       | 0       |
|     |       |          | 188   | 188 |         |         |
| 4   | B     | 190      | Total | O   | 0       | 0       |
|     |       |          | 190   | 190 |         |         |
| 4   | C     | 207      | Total | O   | 0       | 0       |
|     |       |          | 207   | 207 |         |         |
| 4   | D     | 187      | Total | O   | 0       | 0       |
|     |       |          | 187   | 187 |         |         |
| 4   | E     | 208      | Total | O   | 0       | 0       |
|     |       |          | 208   | 208 |         |         |
| 4   | F     | 189      | Total | O   | 0       | 0       |
|     |       |          | 189   | 189 |         |         |

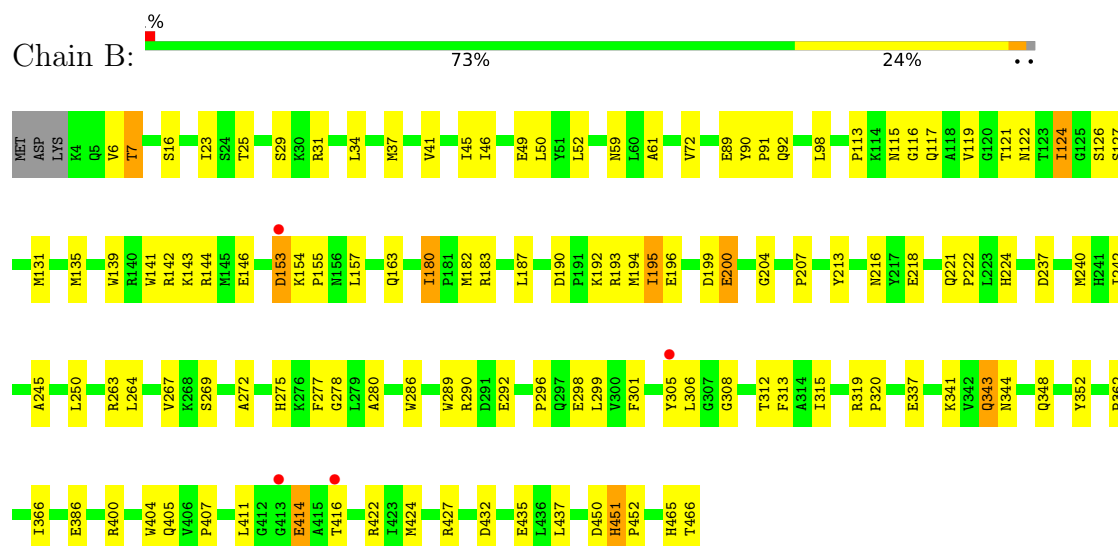
### 3 Residue-property plots

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.

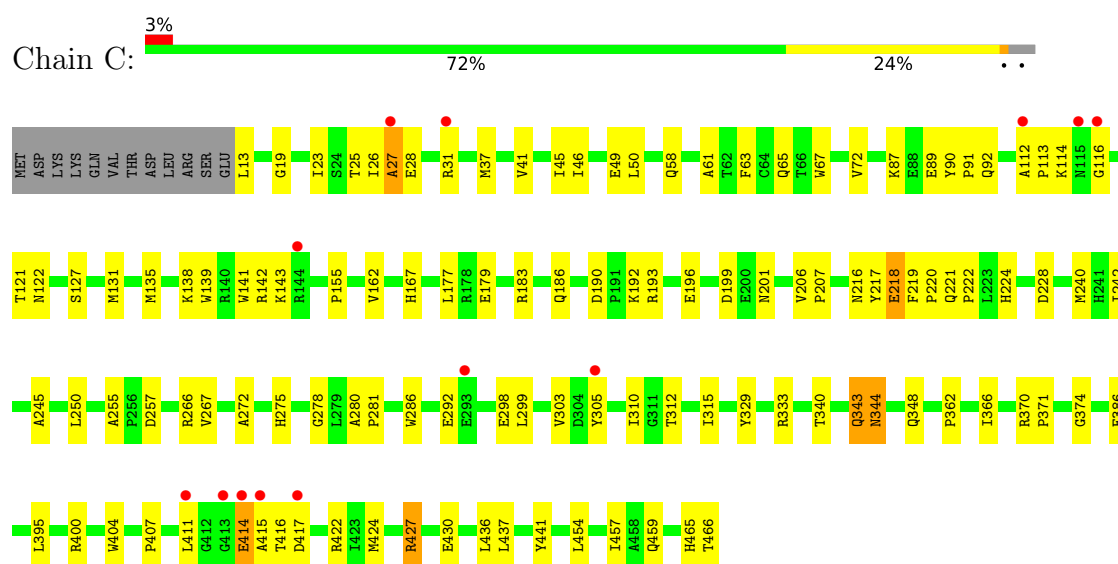
#### • Molecule 1: Glutamate decarboxylase beta



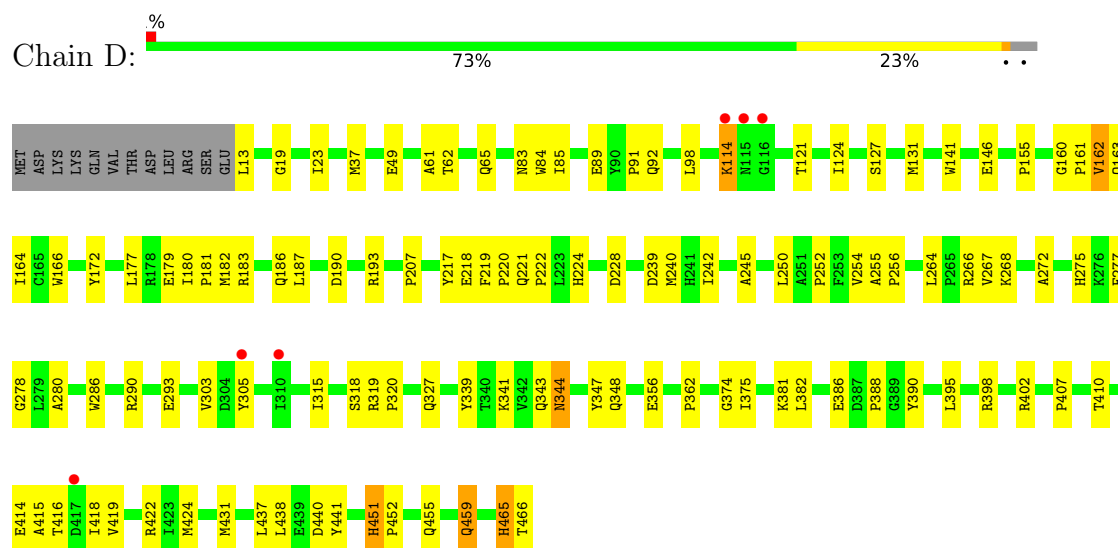
#### • Molecule 1: Glutamate decarboxylase beta



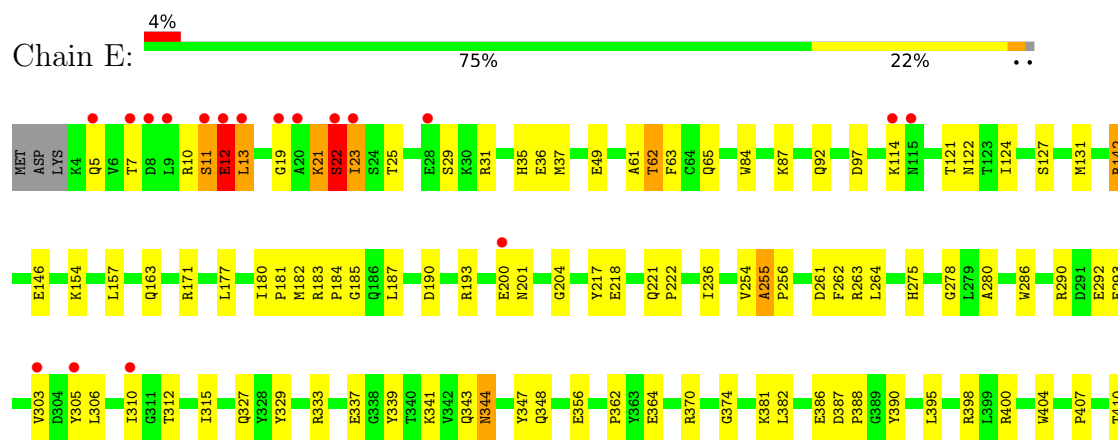
#### • Molecule 1: Glutamate decarboxylase beta



• Molecule 1: Glutamate decarboxylase beta

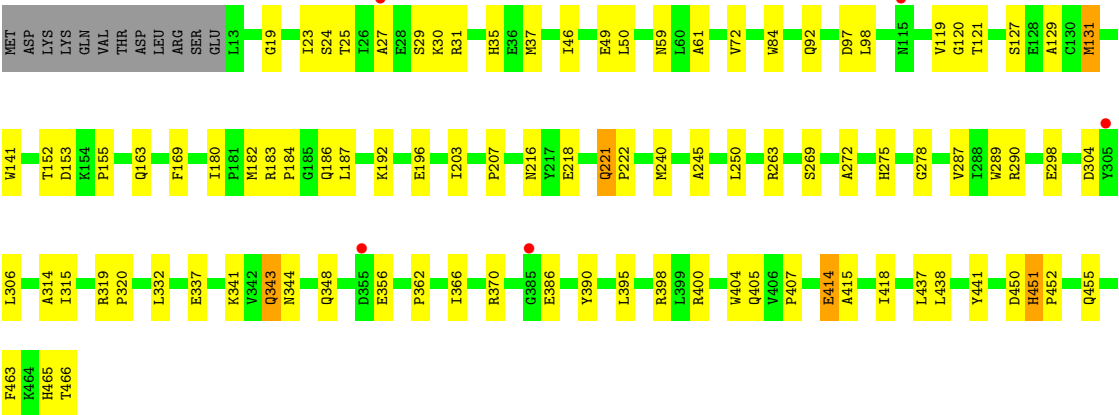
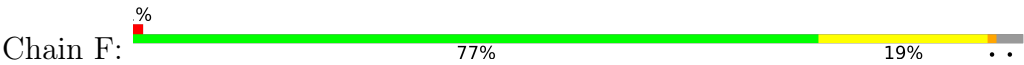


• Molecule 1: Glutamate decarboxylase beta





● Molecule 1: Glutamate decarboxylase beta



## 4 Data and refinement statistics

| Property                                                                | Value                                                          | Source           |
|-------------------------------------------------------------------------|----------------------------------------------------------------|------------------|
| Space group                                                             | P 32                                                           | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 116.00Å 116.00Å 207.35Å<br>90.00° 90.00° 120.00°               | Depositor        |
| Resolution (Å)                                                          | 20.00 – 2.30<br>20.00 – 2.30                                   | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.9 (20.00-2.30)<br>98.7 (20.00-2.30)                         | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.10                                                           | Depositor        |
| $R_{sym}$                                                               | (Not available)                                                | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.32 (at 2.30Å)                                                | Xtriage          |
| Refinement program                                                      | CNS                                                            | Depositor        |
| R, $R_{free}$                                                           | 0.200 , 0.233<br>0.196 , 0.229                                 | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2749 reflections (2.02%)                                       | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 26.7                                                           | Xtriage          |
| Anisotropy                                                              | 0.079                                                          | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.41 , 53.2                                                    | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$    | Xtriage          |
| Estimated twinning fraction                                             | 0.003 for -h,-k,l<br>0.025 for h,-h-k,-l<br>0.016 for -k,-h,-l | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.94                                                           | EDS              |
| Total number of atoms                                                   | 23202                                                          | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 28.0                                                           | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% 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: PLR, TRS

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     | 0.41         | 0/3710      | 0.94        | 13/5028 (0.3%)  |
| 1   | B     | 0.41         | 0/3775      | 0.92        | 11/5115 (0.2%)  |
| 1   | C     | 0.44         | 0/3701      | 0.92        | 10/5016 (0.2%)  |
| 1   | D     | 0.41         | 0/3701      | 0.91        | 8/5016 (0.2%)   |
| 1   | E     | 0.43         | 0/3775      | 0.95        | 21/5115 (0.4%)  |
| 1   | F     | 0.44         | 0/3701      | 0.93        | 11/5016 (0.2%)  |
| All | All   | 0.42         | 0/22363     | 0.93        | 74/30306 (0.2%) |

There are no bond length outliers.

All (74) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 278 | GLY  | N-CA-C | -7.65 | 106.25      | 114.67   |
| 1   | D     | 218 | GLU  | N-CA-C | -7.51 | 96.49       | 108.73   |
| 1   | F     | 218 | GLU  | N-CA-C | -7.49 | 96.53       | 108.73   |
| 1   | C     | 218 | GLU  | N-CA-C | -7.38 | 96.70       | 108.73   |
| 1   | B     | 218 | GLU  | N-CA-C | -7.33 | 96.78       | 108.73   |
| 1   | F     | 278 | GLY  | N-CA-C | -7.33 | 106.61      | 114.67   |
| 1   | E     | 218 | GLU  | N-CA-C | -7.29 | 96.86       | 108.73   |
| 1   | C     | 278 | GLY  | N-CA-C | -7.24 | 106.71      | 114.67   |
| 1   | E     | 278 | GLY  | N-CA-C | -7.21 | 106.74      | 114.67   |
| 1   | A     | 218 | GLU  | N-CA-C | -7.12 | 97.12       | 108.73   |
| 1   | A     | 418 | ILE  | N-CA-C | 6.89  | 117.98      | 108.89   |
| 1   | D     | 451 | HIS  | CA-C-N | 6.73  | 127.27      | 119.47   |
| 1   | D     | 451 | HIS  | C-N-CA | 6.73  | 127.27      | 119.47   |
| 1   | A     | 278 | GLY  | N-CA-C | -6.59 | 106.69      | 115.32   |
| 1   | E     | 387 | ASP  | CA-C-N | 6.59  | 126.72      | 119.87   |
| 1   | E     | 387 | ASP  | C-N-CA | 6.59  | 126.72      | 119.87   |
| 1   | D     | 278 | GLY  | N-CA-C | -6.49 | 106.82      | 115.32   |
| 1   | E     | 11  | SER  | N-CA-C | -6.44 | 103.96      | 112.72   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | E     | 180 | ILE  | CA-C-N  | 6.33  | 126.28      | 119.76   |
| 1   | E     | 180 | ILE  | C-N-CA  | 6.33  | 126.28      | 119.76   |
| 1   | F     | 152 | THR  | N-CA-C  | -6.30 | 105.54      | 112.72   |
| 1   | F     | 153 | ASP  | N-CA-C  | 6.23  | 118.59      | 111.11   |
| 1   | A     | 180 | ILE  | CA-C-N  | 6.18  | 126.12      | 119.76   |
| 1   | A     | 180 | ILE  | C-N-CA  | 6.18  | 126.12      | 119.76   |
| 1   | A     | 465 | HIS  | N-CA-C  | 6.17  | 118.80      | 111.71   |
| 1   | D     | 180 | ILE  | CA-C-N  | 6.13  | 126.07      | 119.76   |
| 1   | D     | 180 | ILE  | C-N-CA  | 6.13  | 126.07      | 119.76   |
| 1   | E     | 22  | SER  | CB-CA-C | -6.09 | 108.55      | 115.79   |
| 1   | E     | 451 | HIS  | CA-C-N  | 6.02  | 126.45      | 119.47   |
| 1   | E     | 451 | HIS  | C-N-CA  | 6.02  | 126.45      | 119.47   |
| 1   | A     | 451 | HIS  | CA-C-N  | 6.01  | 126.44      | 119.47   |
| 1   | A     | 451 | HIS  | C-N-CA  | 6.01  | 126.44      | 119.47   |
| 1   | E     | 21  | LYS  | N-CA-C  | 5.99  | 118.51      | 109.41   |
| 1   | E     | 415 | ALA  | N-CA-C  | -5.89 | 104.64      | 112.94   |
| 1   | B     | 451 | HIS  | CA-C-N  | 5.88  | 126.28      | 119.47   |
| 1   | B     | 451 | HIS  | C-N-CA  | 5.88  | 126.28      | 119.47   |
| 1   | C     | 90  | TYR  | CA-C-N  | 5.71  | 125.39      | 119.05   |
| 1   | C     | 90  | TYR  | C-N-CA  | 5.71  | 125.39      | 119.05   |
| 1   | B     | 7   | THR  | N-CA-C  | 5.50  | 118.61      | 110.46   |
| 1   | E     | 465 | HIS  | N-CA-C  | 5.50  | 119.61      | 113.01   |
| 1   | B     | 180 | ILE  | CA-C-N  | 5.46  | 125.39      | 119.76   |
| 1   | B     | 180 | ILE  | C-N-CA  | 5.46  | 125.39      | 119.76   |
| 1   | C     | 206 | VAL  | N-CA-C  | 5.46  | 113.56      | 108.15   |
| 1   | E     | 35  | HIS  | N-CA-C  | 5.43  | 118.49      | 110.46   |
| 1   | C     | 415 | ALA  | N-CA-C  | -5.41 | 106.53      | 113.02   |
| 1   | A     | 144 | ARG  | N-CA-C  | -5.34 | 105.57      | 111.71   |
| 1   | D     | 465 | HIS  | N-CA-C  | 5.30  | 119.38      | 113.01   |
| 1   | F     | 465 | HIS  | N-CA-C  | 5.28  | 118.98      | 112.54   |
| 1   | E     | 22  | SER  | N-CA-C  | 5.24  | 118.97      | 109.32   |
| 1   | B     | 213 | TYR  | N-CA-C  | 5.22  | 117.87      | 111.82   |
| 1   | E     | 263 | ARG  | N-CA-C  | -5.21 | 106.18      | 112.54   |
| 1   | D     | 62  | THR  | N-CA-C  | 5.21  | 117.58      | 110.55   |
| 1   | B     | 90  | TYR  | CA-C-N  | 5.20  | 124.82      | 119.05   |
| 1   | B     | 90  | TYR  | C-N-CA  | 5.20  | 124.82      | 119.05   |
| 1   | C     | 162 | VAL  | CB-CA-C | -5.19 | 105.64      | 111.45   |
| 1   | A     | 62  | THR  | N-CA-C  | 5.15  | 117.50      | 110.55   |
| 1   | E     | 255 | ALA  | CA-C-N  | 5.15  | 124.94      | 119.28   |
| 1   | E     | 255 | ALA  | C-N-CA  | 5.15  | 124.94      | 119.28   |
| 1   | B     | 263 | ARG  | N-CA-C  | -5.14 | 106.27      | 112.54   |
| 1   | C     | 167 | HIS  | N-CA-C  | -5.14 | 105.76      | 111.36   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 263 | ARG  | N-CA-C | -5.13 | 106.28      | 112.54   |
| 1   | A     | 167 | HIS  | N-CA-C | -5.13 | 105.77      | 111.36   |
| 1   | A     | 213 | TYR  | N-CA-C | 5.13  | 117.77      | 111.82   |
| 1   | F     | 263 | ARG  | N-CA-C | -5.11 | 106.30      | 112.54   |
| 1   | F     | 35  | HIS  | N-CA-C | 5.11  | 117.65      | 110.14   |
| 1   | F     | 451 | HIS  | CA-C-N | 5.10  | 125.38      | 119.47   |
| 1   | F     | 451 | HIS  | C-N-CA | 5.10  | 125.38      | 119.47   |
| 1   | C     | 25  | THR  | N-CA-C | -5.06 | 107.11      | 113.28   |
| 1   | E     | 370 | ARG  | CA-C-N | 5.04  | 125.06      | 119.32   |
| 1   | E     | 370 | ARG  | C-N-CA | 5.04  | 125.06      | 119.32   |
| 1   | F     | 370 | ARG  | CA-C-N | 5.03  | 125.05      | 119.32   |
| 1   | F     | 370 | ARG  | C-N-CA | 5.03  | 125.05      | 119.32   |
| 1   | C     | 414 | GLU  | N-CA-C | -5.03 | 106.93      | 113.16   |
| 1   | E     | 62  | THR  | N-CA-C | 5.03  | 117.33      | 110.55   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3616  | 0        | 3516     | 126     | 0            |
| 1   | B     | 3681  | 0        | 3586     | 94      | 0            |
| 1   | C     | 3607  | 0        | 3510     | 97      | 0            |
| 1   | D     | 3607  | 0        | 3510     | 93      | 0            |
| 1   | E     | 3681  | 0        | 3586     | 99      | 0            |
| 1   | F     | 3607  | 0        | 3510     | 80      | 0            |
| 2   | A     | 15    | 0        | 9        | 0       | 0            |
| 2   | B     | 15    | 0        | 9        | 1       | 0            |
| 2   | C     | 15    | 0        | 9        | 1       | 0            |
| 2   | D     | 15    | 0        | 9        | 0       | 0            |
| 2   | E     | 15    | 0        | 9        | 0       | 0            |
| 2   | F     | 15    | 0        | 9        | 1       | 0            |
| 3   | A     | 24    | 0        | 36       | 11      | 0            |
| 3   | B     | 16    | 0        | 24       | 7       | 0            |
| 3   | C     | 24    | 0        | 36       | 18      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | D     | 24    | 0        | 36       | 9       | 0            |
| 3   | E     | 32    | 0        | 48       | 14      | 0            |
| 3   | F     | 24    | 0        | 36       | 17      | 0            |
| 4   | A     | 188   | 0        | 0        | 6       | 0            |
| 4   | B     | 190   | 0        | 0        | 2       | 0            |
| 4   | C     | 207   | 0        | 0        | 5       | 0            |
| 4   | D     | 187   | 0        | 0        | 6       | 0            |
| 4   | E     | 208   | 0        | 0        | 5       | 0            |
| 4   | F     | 189   | 0        | 0        | 5       | 0            |
| All | All   | 23202 | 0        | 21488    | 552     | 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 13.

All (552) 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:A:65:GLN:HB3   | 3:A:3236:TRS:H31 | 1.20                     | 1.11              |
| 1:F:250:LEU:HD23 | 1:F:343:GLN:HG3  | 1.42                     | 1.01              |
| 1:A:250:LEU:HD23 | 1:A:343:GLN:HG3  | 1.44                     | 0.98              |
| 1:B:250:LEU:HD23 | 1:B:343:GLN:HG3  | 1.46                     | 0.97              |
| 1:C:436:LEU:HD11 | 3:C:3252:TRS:H21 | 1.47                     | 0.96              |
| 1:A:183:ARG:HG2  | 1:A:414:GLU:HB2  | 1.47                     | 0.94              |
| 1:F:72:VAL:HG21  | 3:F:3240:TRS:H12 | 1.54                     | 0.88              |
| 1:B:190:ASP:OD1  | 1:B:193:ARG:HD3  | 1.76                     | 0.85              |
| 1:D:121:THR:OG1  | 3:D:3244:TRS:H11 | 1.76                     | 0.85              |
| 1:C:250:LEU:HD23 | 1:C:343:GLN:HG3  | 1.57                     | 0.84              |
| 1:C:183:ARG:HD2  | 1:C:186:GLN:HE21 | 1.40                     | 0.84              |
| 1:B:183:ARG:HG2  | 1:B:414:GLU:HB2  | 1.59                     | 0.84              |
| 1:A:91:PRO:HB2   | 3:C:3252:TRS:H12 | 1.60                     | 0.82              |
| 1:C:281:PRO:HB3  | 3:C:3250:TRS:H22 | 1.62                     | 0.82              |
| 1:C:362:PRO:HB2  | 1:C:386:GLU:HG2  | 1.64                     | 0.81              |
| 1:E:49:GLU:O     | 1:F:92:GLN:HG2   | 1.83                     | 0.79              |
| 1:E:427:ARG:HH21 | 3:E:3239:TRS:H12 | 1.47                     | 0.78              |
| 1:A:114:LYS:H    | 1:A:114:LYS:HD2  | 1.49                     | 0.78              |
| 1:D:190:ASP:OD1  | 1:D:193:ARG:HD3  | 1.82                     | 0.78              |
| 1:A:190:ASP:OD1  | 1:A:193:ARG:HD3  | 1.84                     | 0.77              |
| 1:D:114:LYS:H    | 1:D:114:LYS:HD2  | 1.48                     | 0.77              |
| 1:A:65:GLN:HB3   | 3:A:3236:TRS:C3  | 2.09                     | 0.77              |
| 1:C:72:VAL:HG11  | 3:C:3250:TRS:H12 | 1.66                     | 0.77              |
| 1:D:362:PRO:HB2  | 1:D:386:GLU:HG2  | 1.67                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:65:GLN:HB3   | 3:D:3238:TRS:N   | 2.00                     | 0.76              |
| 1:D:277:PHE:HZ   | 1:D:424:MET:HE1  | 1.50                     | 0.75              |
| 1:E:92:GLN:HG2   | 1:F:49:GLU:O     | 1.87                     | 0.74              |
| 1:D:221:GLN:HB3  | 1:D:222:PRO:HD3  | 1.69                     | 0.74              |
| 1:E:362:PRO:HB2  | 1:E:386:GLU:HG2  | 1.70                     | 0.73              |
| 1:E:411:LEU:O    | 1:E:416:THR:HA   | 1.89                     | 0.73              |
| 1:C:183:ARG:HB2  | 1:C:186:GLN:HG3  | 1.69                     | 0.73              |
| 1:E:127:SER:O    | 1:E:131:MET:HG2  | 1.88                     | 0.73              |
| 1:E:5:GLN:HG3    | 1:E:10:ARG:HD2   | 1.70                     | 0.73              |
| 1:A:214:THR:CG2  | 1:A:366:ILE:HD11 | 2.18                     | 0.73              |
| 1:F:183:ARG:HE   | 1:F:414:GLU:HG2  | 1.54                     | 0.73              |
| 1:E:427:ARG:NH2  | 3:E:3239:TRS:H12 | 2.04                     | 0.72              |
| 1:A:221:GLN:HB3  | 1:A:222:PRO:HD3  | 1.70                     | 0.72              |
| 1:B:341:LYS:HE2  | 1:C:19:GLY:O     | 1.88                     | 0.72              |
| 1:C:183:ARG:HD2  | 1:C:186:GLN:NE2  | 2.02                     | 0.72              |
| 1:B:124:ILE:CD1  | 1:B:319:ARG:HD2  | 2.19                     | 0.72              |
| 1:E:200:GLU:H    | 1:E:200:GLU:CD   | 1.97                     | 0.72              |
| 1:D:390:TYR:HA   | 1:D:455:GLN:HG3  | 1.72                     | 0.72              |
| 1:C:114:LYS:HZ2  | 1:C:292:GLU:HG2  | 1.55                     | 0.71              |
| 1:F:356:GLU:HG2  | 1:F:438:LEU:HD13 | 1.71                     | 0.71              |
| 1:A:65:GLN:CB    | 3:A:3236:TRS:H31 | 2.11                     | 0.71              |
| 1:C:121:THR:HA   | 3:C:3243:TRS:H12 | 1.72                     | 0.71              |
| 1:E:190:ASP:OD1  | 1:E:193:ARG:HD3  | 1.91                     | 0.71              |
| 1:A:91:PRO:CB    | 3:C:3252:TRS:H12 | 2.20                     | 0.71              |
| 1:D:242:ILE:HD11 | 1:D:267:VAL:HG22 | 1.73                     | 0.71              |
| 1:E:7:THR:HA     | 1:E:10:ARG:HD3   | 1.71                     | 0.71              |
| 1:D:277:PHE:CZ   | 1:D:424:MET:HE1  | 2.25                     | 0.71              |
| 1:E:315:ILE:HG21 | 1:F:315:ILE:HD13 | 1.73                     | 0.70              |
| 1:C:207:PRO:HG2  | 1:C:240:MET:HE2  | 1.74                     | 0.70              |
| 1:E:183:ARG:HH21 | 1:E:414:GLU:HG2  | 1.56                     | 0.70              |
| 1:D:84:TRP:HZ2   | 3:D:3244:TRS:H12 | 1.57                     | 0.69              |
| 1:A:341:LYS:HE2  | 1:F:19:GLY:O     | 1.91                     | 0.69              |
| 1:F:121:THR:OG1  | 3:F:3248:TRS:H31 | 1.92                     | 0.69              |
| 1:A:172:TYR:CD1  | 1:B:135:MET:HE1  | 2.27                     | 0.68              |
| 1:E:364:GLU:OE1  | 1:E:381:LYS:HE3  | 1.93                     | 0.68              |
| 1:B:362:PRO:HB2  | 1:B:386:GLU:HG2  | 1.75                     | 0.68              |
| 1:F:127:SER:O    | 1:F:131:MET:HG2  | 1.94                     | 0.68              |
| 1:F:72:VAL:HG21  | 3:F:3240:TRS:C1  | 2.24                     | 0.68              |
| 1:F:250:LEU:CD2  | 1:F:343:GLN:HG3  | 2.22                     | 0.68              |
| 1:C:92:GLN:HG2   | 1:D:49:GLU:O     | 1.93                     | 0.68              |
| 1:A:164:ILE:HD12 | 1:A:165:CYS:N    | 2.07                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:161:PRO:HB3  | 1:A:182:MET:HE3  | 1.77                     | 0.67              |
| 1:C:49:GLU:O     | 1:D:92:GLN:HG2   | 1.94                     | 0.67              |
| 1:D:422:ARG:HD2  | 4:D:3284:HOH:O   | 1.95                     | 0.67              |
| 1:A:291:ASP:OD1  | 1:A:293:GLU:HG2  | 1.95                     | 0.67              |
| 1:D:19:GLY:O     | 1:E:341:LYS:HE2  | 1.95                     | 0.66              |
| 1:C:242:ILE:HD13 | 1:C:267:VAL:HG13 | 1.77                     | 0.66              |
| 1:F:183:ARG:HG3  | 1:F:184:PRO:HD2  | 1.78                     | 0.66              |
| 1:D:84:TRP:CZ2   | 3:D:3244:TRS:H12 | 2.31                     | 0.66              |
| 1:A:114:LYS:HE2  | 1:A:292:GLU:HG2  | 1.77                     | 0.66              |
| 1:A:162:VAL:HG22 | 1:A:166:TRP:CD1  | 2.30                     | 0.66              |
| 1:A:100:CYS:HA   | 1:A:103:MET:HE3  | 1.78                     | 0.66              |
| 1:A:214:THR:HB   | 1:A:366:ILE:HD11 | 1.77                     | 0.65              |
| 1:B:250:LEU:HD23 | 1:B:343:GLN:CG   | 2.23                     | 0.65              |
| 1:D:303:VAL:HG23 | 1:D:305:TYR:CE1  | 2.31                     | 0.65              |
| 1:C:138:LYS:O    | 1:C:142:ARG:HG3  | 1.95                     | 0.65              |
| 1:A:127:SER:O    | 1:A:131:MET:HG2  | 1.96                     | 0.65              |
| 1:A:214:THR:HG21 | 1:A:366:ILE:HD11 | 1.79                     | 0.65              |
| 1:B:200:GLU:CD   | 1:B:200:GLU:H    | 2.05                     | 0.65              |
| 1:A:214:THR:CB   | 1:A:366:ILE:HD11 | 2.27                     | 0.65              |
| 1:C:250:LEU:CD2  | 1:C:343:GLN:HG3  | 2.25                     | 0.65              |
| 1:E:398:ARG:HD3  | 4:E:3343:HOH:O   | 1.97                     | 0.64              |
| 1:D:65:GLN:HB3   | 3:D:3238:TRS:HN2 | 1.61                     | 0.64              |
| 1:A:87:LYS:HG2   | 1:A:310:ILE:HD13 | 1.80                     | 0.64              |
| 1:E:37:MET:HE1   | 1:F:332:LEU:HD22 | 1.80                     | 0.64              |
| 1:D:183:ARG:HG2  | 1:D:414:GLU:HB3  | 1.80                     | 0.64              |
| 1:F:120:GLY:H    | 3:F:3249:TRS:H32 | 1.63                     | 0.64              |
| 1:A:392:LEU:HD13 | 1:A:421:MET:HB2  | 1.80                     | 0.63              |
| 1:C:207:PRO:CG   | 1:C:240:MET:HE2  | 2.28                     | 0.63              |
| 1:C:422:ARG:HG2  | 4:C:3329:HOH:O   | 1.98                     | 0.63              |
| 1:D:339:TYR:O    | 1:D:343:GLN:HG2  | 1.98                     | 0.63              |
| 1:E:131:MET:HE3  | 1:F:315:ILE:HG23 | 1.80                     | 0.63              |
| 1:F:119:VAL:HG13 | 3:F:3249:TRS:H31 | 1.80                     | 0.63              |
| 1:A:383:LYS:HB2  | 1:A:386:GLU:HG3  | 1.80                     | 0.63              |
| 1:A:356:GLU:HG2  | 1:A:438:LEU:HD13 | 1.81                     | 0.63              |
| 1:A:49:GLU:O     | 1:B:92:GLN:HG2   | 1.98                     | 0.63              |
| 1:E:121:THR:OG1  | 3:E:3246:TRS:H11 | 1.99                     | 0.63              |
| 1:F:207:PRO:HG2  | 1:F:240:MET:HE2  | 1.81                     | 0.62              |
| 1:A:192:LYS:O    | 1:A:196:GLU:HG3  | 1.99                     | 0.62              |
| 1:C:190:ASP:OD1  | 1:C:193:ARG:HD3  | 1.99                     | 0.62              |
| 1:B:31:ARG:NH1   | 1:B:34:LEU:HD11  | 2.15                     | 0.62              |
| 1:E:221:GLN:HB3  | 1:E:222:PRO:HD3  | 1.81                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:415:ALA:HB1  | 1:D:418:ILE:HD12 | 1.82                     | 0.62              |
| 1:C:121:THR:HA   | 3:C:3243:TRS:C1  | 2.30                     | 0.62              |
| 1:C:135:MET:HE1  | 1:D:172:TYR:CD1  | 2.34                     | 0.62              |
| 1:C:192:LYS:O    | 1:C:196:GLU:HG3  | 1.99                     | 0.62              |
| 1:E:131:MET:CE   | 1:F:315:ILE:HG23 | 2.30                     | 0.62              |
| 1:E:10:ARG:HE    | 1:E:12:GLU:HB3   | 1.63                     | 0.61              |
| 1:F:192:LYS:O    | 1:F:196:GLU:HG3  | 1.98                     | 0.61              |
| 1:F:390:TYR:HA   | 1:F:455:GLN:HG3  | 1.82                     | 0.61              |
| 1:D:23:ILE:HG21  | 1:D:37:MET:HE2   | 1.83                     | 0.61              |
| 3:E:3246:TRS:O1  | 3:E:3246:TRS:O2  | 2.16                     | 0.61              |
| 1:B:143:LYS:HE3  | 1:B:298:GLU:OE1  | 2.00                     | 0.61              |
| 1:A:182:MET:HG3  | 1:A:187:LEU:O    | 2.01                     | 0.60              |
| 1:A:92:GLN:HG2   | 1:B:49:GLU:O     | 2.01                     | 0.60              |
| 1:B:216:ASN:HD21 | 1:B:366:ILE:HG22 | 1.65                     | 0.60              |
| 1:B:250:LEU:CD2  | 1:B:343:GLN:HG3  | 2.27                     | 0.60              |
| 1:E:87:LYS:HG2   | 1:E:310:ILE:HD12 | 1.82                     | 0.60              |
| 1:A:142:ARG:O    | 1:A:146:GLU:HG3  | 2.01                     | 0.60              |
| 1:B:221:GLN:HB3  | 1:B:222:PRO:HD3  | 1.84                     | 0.60              |
| 1:F:72:VAL:HG11  | 3:F:3240:TRS:H22 | 1.82                     | 0.60              |
| 1:B:305:TYR:HB2  | 1:B:308:GLY:O    | 2.01                     | 0.60              |
| 1:E:183:ARG:HG2  | 1:E:414:GLU:HB2  | 1.82                     | 0.59              |
| 1:A:161:PRO:CB   | 1:A:182:MET:HE3  | 2.32                     | 0.59              |
| 1:C:362:PRO:CB   | 1:C:386:GLU:HG2  | 2.30                     | 0.59              |
| 1:D:162:VAL:HG11 | 1:D:166:TRP:HB2  | 1.84                     | 0.59              |
| 1:D:341:LYS:HE2  | 1:E:19:GLY:O     | 2.02                     | 0.59              |
| 1:D:362:PRO:CB   | 1:D:386:GLU:HG2  | 2.32                     | 0.59              |
| 1:A:250:LEU:CD2  | 1:A:343:GLN:HG3  | 2.27                     | 0.59              |
| 1:C:114:LYS:NZ   | 1:C:292:GLU:HG2  | 2.17                     | 0.59              |
| 1:E:142:ARG:O    | 1:E:146:GLU:HG3  | 2.02                     | 0.59              |
| 1:F:183:ARG:HD2  | 1:F:186:GLN:HE21 | 1.66                     | 0.59              |
| 1:F:84:TRP:HZ2   | 3:F:3248:TRS:H32 | 1.67                     | 0.59              |
| 1:F:131:MET:CE   | 1:F:169:PHE:HB2  | 2.33                     | 0.59              |
| 1:A:250:LEU:HD23 | 1:A:343:GLN:CG   | 2.27                     | 0.59              |
| 1:E:381:LYS:HD2  | 1:E:418:ILE:HG23 | 1.84                     | 0.59              |
| 1:A:87:LYS:HG2   | 1:A:310:ILE:CD1  | 2.32                     | 0.59              |
| 1:A:181:PRO:O    | 1:A:193:ARG:NH2  | 2.36                     | 0.59              |
| 1:A:101:VAL:HG21 | 3:A:3251:TRS:H12 | 1.84                     | 0.58              |
| 1:A:114:LYS:H    | 1:A:114:LYS:CD   | 2.15                     | 0.58              |
| 1:E:84:TRP:HZ2   | 3:E:3246:TRS:H12 | 1.67                     | 0.58              |
| 1:E:339:TYR:O    | 1:E:343:GLN:HG2  | 2.02                     | 0.58              |
| 1:C:127:SER:O    | 1:C:131:MET:HG2  | 2.03                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:298:GLU:H    | 1:C:298:GLU:CD   | 2.12                     | 0.58              |
| 1:B:127:SER:O    | 1:B:131:MET:HG2  | 2.04                     | 0.57              |
| 1:D:162:VAL:CG1  | 1:D:166:TRP:HB2  | 2.34                     | 0.57              |
| 1:C:121:THR:CA   | 3:C:3243:TRS:H12 | 2.35                     | 0.57              |
| 1:D:114:LYS:H    | 1:D:114:LYS:CD   | 2.15                     | 0.57              |
| 1:F:23:ILE:HG21  | 1:F:37:MET:HE2   | 1.86                     | 0.57              |
| 1:A:27:ALA:HA    | 4:A:3382:HOH:O   | 2.04                     | 0.57              |
| 1:C:303:VAL:HG23 | 1:C:305:TYR:CE1  | 2.40                     | 0.57              |
| 1:C:221:GLN:HB3  | 1:C:222:PRO:HD3  | 1.87                     | 0.57              |
| 1:D:356:GLU:HG2  | 1:D:438:LEU:HD13 | 1.86                     | 0.57              |
| 1:E:293:GLU:HG3  | 4:E:3369:HOH:O   | 2.04                     | 0.57              |
| 1:D:13:LEU:N     | 1:D:13:LEU:HD12  | 2.20                     | 0.56              |
| 1:E:181:PRO:O    | 1:E:193:ARG:NH2  | 2.32                     | 0.56              |
| 1:A:121:THR:OG1  | 3:A:3251:TRS:H21 | 2.05                     | 0.56              |
| 1:E:183:ARG:HE   | 1:E:414:GLU:HB2  | 1.69                     | 0.56              |
| 1:E:254:VAL:HG21 | 1:E:347:TYR:CE2  | 2.41                     | 0.56              |
| 1:B:362:PRO:CB   | 1:B:386:GLU:HG2  | 2.36                     | 0.56              |
| 1:F:398:ARG:HD3  | 4:F:3330:HOH:O   | 2.06                     | 0.56              |
| 1:A:92:GLN:HA    | 1:A:92:GLN:NE2   | 2.21                     | 0.56              |
| 1:E:182:MET:HG2  | 1:E:187:LEU:O    | 2.05                     | 0.56              |
| 1:B:144:ARG:NH1  | 1:B:237:ASP:O    | 2.37                     | 0.56              |
| 1:B:199:ASP:HB2  | 1:B:200:GLU:OE2  | 2.06                     | 0.56              |
| 1:B:6:VAL:HA     | 1:C:257:ASP:HB2  | 1.89                     | 0.55              |
| 1:C:411:LEU:O    | 1:C:416:THR:HA   | 2.06                     | 0.55              |
| 1:B:25:THR:O     | 1:B:29:SER:HB3   | 2.06                     | 0.55              |
| 1:C:114:LYS:NZ   | 1:C:292:GLU:H    | 2.04                     | 0.55              |
| 1:A:177:LEU:HD13 | 1:A:177:LEU:C    | 2.32                     | 0.55              |
| 1:C:250:LEU:HD23 | 1:C:343:GLN:CG   | 2.35                     | 0.54              |
| 1:B:23:ILE:HG21  | 1:B:37:MET:HE2   | 1.89                     | 0.54              |
| 1:A:395:LEU:HD21 | 1:A:441:TYR:CZ   | 2.43                     | 0.54              |
| 1:A:103:MET:HE1  | 1:A:328:TYR:CD1  | 2.43                     | 0.54              |
| 1:D:293:GLU:HG3  | 4:D:3371:HOH:O   | 2.07                     | 0.54              |
| 1:B:121:THR:HA   | 3:B:3242:TRS:C1  | 2.37                     | 0.54              |
| 1:C:422:ARG:HG2  | 1:C:422:ARG:HH11 | 1.72                     | 0.54              |
| 1:B:124:ILE:HD13 | 1:B:319:ARG:HD2  | 1.90                     | 0.54              |
| 1:D:13:LEU:N     | 4:D:3293:HOH:O   | 2.41                     | 0.54              |
| 1:D:162:VAL:HG22 | 1:D:166:TRP:CD1  | 2.43                     | 0.54              |
| 1:D:431:MET:HE3  | 1:E:13:LEU:HD22  | 1.90                     | 0.54              |
| 1:E:182:MET:HE2  | 1:E:187:LEU:HB3  | 1.89                     | 0.54              |
| 1:A:183:ARG:HG2  | 1:A:414:GLU:CB   | 2.30                     | 0.54              |
| 1:D:242:ILE:HD13 | 1:D:267:VAL:HG13 | 1.89                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:402:ARG:HD2  | 1:D:440:ASP:OD1  | 2.08                     | 0.54              |
| 1:D:362:PRO:CG   | 1:D:388:PRO:HG3  | 2.37                     | 0.53              |
| 1:C:65:GLN:HG3   | 3:C:3250:TRS:N   | 2.23                     | 0.53              |
| 1:C:87:LYS:HG2   | 1:C:310:ILE:HD12 | 1.88                     | 0.53              |
| 1:C:333:ARG:HH21 | 1:C:427:ARG:HH22 | 1.57                     | 0.53              |
| 1:F:207:PRO:CG   | 1:F:240:MET:HE2  | 2.39                     | 0.53              |
| 1:F:290:ARG:HD3  | 4:F:3329:HOH:O   | 2.08                     | 0.53              |
| 1:A:141:TRP:O    | 1:A:145:MET:HG2  | 2.08                     | 0.53              |
| 1:E:84:TRP:CZ2   | 3:E:3246:TRS:H12 | 2.44                     | 0.53              |
| 1:F:141:TRP:CZ3  | 1:F:155:PRO:HB3  | 2.44                     | 0.53              |
| 1:D:228:ASP:HA   | 1:D:266:ARG:HH21 | 1.73                     | 0.53              |
| 1:E:11:SER:O     | 1:E:22:SER:HB2   | 2.09                     | 0.53              |
| 1:F:121:THR:CB   | 3:F:3248:TRS:H31 | 2.39                     | 0.53              |
| 1:F:415:ALA:HB1  | 1:F:418:ILE:HD12 | 1.90                     | 0.53              |
| 1:A:164:ILE:HD13 | 1:A:168:LYS:HE3  | 1.90                     | 0.53              |
| 1:E:22:SER:OG    | 1:E:23:ILE:N     | 2.37                     | 0.53              |
| 1:E:184:PRO:HA   | 3:E:3253:TRS:H12 | 1.91                     | 0.53              |
| 1:A:97:ASP:OD2   | 3:A:3251:TRS:H11 | 2.09                     | 0.52              |
| 1:B:224:HIS:CD2  | 1:B:264:LEU:HB3  | 2.43                     | 0.52              |
| 1:C:121:THR:CB   | 3:C:3243:TRS:H12 | 2.39                     | 0.52              |
| 1:C:344:ASN:O    | 1:C:348:GLN:HG3  | 2.09                     | 0.52              |
| 1:D:362:PRO:HG3  | 1:D:388:PRO:HG3  | 1.91                     | 0.52              |
| 1:E:10:ARG:HG3   | 1:E:12:GLU:HG3   | 1.92                     | 0.52              |
| 1:E:344:ASN:O    | 1:E:348:GLN:HG3  | 2.10                     | 0.52              |
| 1:C:216:ASN:HD21 | 1:C:366:ILE:HG22 | 1.75                     | 0.52              |
| 1:D:127:SER:O    | 1:D:131:MET:HG2  | 2.10                     | 0.52              |
| 1:B:121:THR:OG1  | 3:B:3242:TRS:H12 | 2.10                     | 0.52              |
| 1:C:242:ILE:HD11 | 1:C:267:VAL:HG22 | 1.92                     | 0.52              |
| 1:E:36:GLU:HG3   | 1:F:337:GLU:HG2  | 1.92                     | 0.52              |
| 1:C:343:GLN:OE1  | 1:C:343:GLN:HA   | 2.09                     | 0.51              |
| 1:E:183:ARG:HE   | 1:E:414:GLU:CB   | 2.23                     | 0.51              |
| 1:F:84:TRP:CZ2   | 3:F:3248:TRS:H32 | 2.45                     | 0.51              |
| 1:A:162:VAL:CG1  | 1:A:166:TRP:HB2  | 2.40                     | 0.51              |
| 1:A:172:TYR:CG   | 1:B:135:MET:HE1  | 2.45                     | 0.51              |
| 1:E:163:GLN:HG2  | 4:E:3307:HOH:O   | 2.10                     | 0.51              |
| 1:E:312:THR:HG22 | 3:E:3246:TRS:O3  | 2.11                     | 0.51              |
| 1:E:65:GLN:HB3   | 3:E:3239:TRS:O1  | 2.11                     | 0.51              |
| 1:F:183:ARG:NE   | 1:F:414:GLU:HG2  | 2.24                     | 0.51              |
| 1:B:122:ASN:HB2  | 1:B:286:TRP:CZ3  | 2.46                     | 0.51              |
| 1:A:38:ARG:HH21  | 1:A:40:ASP:HB2   | 1.76                     | 0.51              |
| 3:E:3239:TRS:H21 | 4:E:3380:HOH:O   | 2.10                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:141:TRP:CD2  | 1:F:203:ILE:HG22 | 2.45                     | 0.51              |
| 1:C:281:PRO:HD3  | 3:C:3250:TRS:O1  | 2.10                     | 0.51              |
| 1:D:414:GLU:C    | 1:D:416:THR:H    | 2.19                     | 0.51              |
| 1:E:415:ALA:HB1  | 1:E:418:ILE:HD12 | 1.93                     | 0.51              |
| 1:B:344:ASN:O    | 1:B:348:GLN:HG3  | 2.11                     | 0.50              |
| 1:F:97:ASP:OD2   | 3:F:3248:TRS:O3  | 2.23                     | 0.50              |
| 1:F:356:GLU:HG2  | 1:F:438:LEU:CD1  | 2.41                     | 0.50              |
| 3:D:3238:TRS:O3  | 3:D:3238:TRS:O1  | 2.16                     | 0.50              |
| 1:F:120:GLY:N    | 3:F:3249:TRS:H32 | 2.26                     | 0.50              |
| 1:A:25:THR:O     | 1:A:29:SER:HB3   | 2.11                     | 0.50              |
| 1:A:224:HIS:CD2  | 1:A:264:LEU:HB3  | 2.47                     | 0.50              |
| 2:C:1502:PLR:O2P | 1:D:318:SER:HB2  | 2.11                     | 0.50              |
| 1:F:245:ALA:HA   | 1:F:272:ALA:HA   | 1.93                     | 0.50              |
| 1:A:400:ARG:CZ   | 1:B:306:LEU:HD21 | 2.42                     | 0.50              |
| 1:D:183:ARG:HG2  | 1:D:414:GLU:CB   | 2.42                     | 0.50              |
| 1:A:207:PRO:CG   | 1:A:240:MET:HE2  | 2.42                     | 0.50              |
| 1:A:38:ARG:HB2   | 1:A:41:VAL:HG23  | 1.93                     | 0.50              |
| 1:B:192:LYS:O    | 1:B:196:GLU:HG3  | 2.12                     | 0.50              |
| 1:B:41:VAL:O     | 1:B:45:ILE:HG13  | 2.12                     | 0.49              |
| 1:B:194:MET:HE3  | 1:B:195:ILE:CD1  | 2.43                     | 0.49              |
| 1:E:329:TYR:CZ   | 1:E:333:ARG:HD3  | 2.47                     | 0.49              |
| 1:A:38:ARG:HB2   | 1:A:41:VAL:CG2   | 2.42                     | 0.49              |
| 1:C:139:TRP:CE2  | 1:C:299:LEU:HD21 | 2.47                     | 0.49              |
| 1:D:65:GLN:HB3   | 3:D:3238:TRS:HN1 | 1.75                     | 0.49              |
| 1:D:395:LEU:HD21 | 1:D:441:TYR:CZ   | 2.47                     | 0.49              |
| 1:A:89:GLU:C     | 1:A:91:PRO:HD3   | 2.37                     | 0.49              |
| 1:E:171:ARG:NH1  | 1:F:298:GLU:O    | 2.44                     | 0.49              |
| 1:C:61:ALA:HB2   | 1:C:407:PRO:HD3  | 1.94                     | 0.49              |
| 1:D:250:LEU:HD12 | 1:D:375:ILE:HG22 | 1.94                     | 0.49              |
| 1:B:121:THR:HA   | 3:B:3242:TRS:H12 | 1.94                     | 0.49              |
| 1:E:264:LEU:O    | 1:E:290:ARG:NH2  | 2.46                     | 0.49              |
| 1:B:275:HIS:HA   | 1:B:280:ALA:O    | 2.13                     | 0.49              |
| 1:F:129:ALA:HB1  | 1:F:287:VAL:HB   | 1.95                     | 0.49              |
| 1:A:162:VAL:HG11 | 1:A:166:TRP:HB2  | 1.93                     | 0.49              |
| 1:A:128:GLU:HA   | 1:A:131:MET:HG3  | 1.94                     | 0.49              |
| 1:E:329:TYR:CE2  | 1:E:333:ARG:HD3  | 2.48                     | 0.49              |
| 1:F:30:LYS:C     | 1:F:31:ARG:HD2   | 2.37                     | 0.49              |
| 1:F:343:GLN:OE1  | 1:F:343:GLN:HA   | 2.13                     | 0.49              |
| 1:C:217:TYR:CD2  | 1:C:374:GLY:HA2  | 2.48                     | 0.49              |
| 1:B:183:ARG:NE   | 1:B:414:GLU:OE2  | 2.46                     | 0.48              |
| 1:B:72:VAL:HG11  | 3:B:3237:TRS:H32 | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:362:PRO:CB   | 1:E:386:GLU:HG2  | 2.42                     | 0.48              |
| 1:D:124:ILE:HD11 | 1:D:319:ARG:HD2  | 1.95                     | 0.48              |
| 1:A:344:ASN:O    | 1:A:348:GLN:HG3  | 2.13                     | 0.48              |
| 1:C:333:ARG:HH22 | 1:C:427:ARG:HH12 | 1.60                     | 0.48              |
| 1:C:340:THR:O    | 1:C:344:ASN:HB2  | 2.13                     | 0.48              |
| 1:C:28:GLU:HG2   | 1:C:31:ARG:HH21  | 1.79                     | 0.48              |
| 1:B:142:ARG:O    | 1:B:146:GLU:HG3  | 2.13                     | 0.48              |
| 1:A:19:GLY:O     | 1:F:341:LYS:HE2  | 2.14                     | 0.47              |
| 1:A:122:ASN:HB2  | 1:A:286:TRP:CZ3  | 2.49                     | 0.47              |
| 1:A:154:LYS:O    | 1:A:201:ASN:HB3  | 2.13                     | 0.47              |
| 1:C:141:TRP:CZ3  | 1:C:155:PRO:HG3  | 2.49                     | 0.47              |
| 1:D:162:VAL:HG13 | 1:D:163:GLN:O    | 2.15                     | 0.47              |
| 1:E:382:LEU:HD22 | 1:E:388:PRO:HG2  | 1.95                     | 0.47              |
| 1:D:319:ARG:HB2  | 1:D:320:PRO:HD2  | 1.96                     | 0.47              |
| 1:D:303:VAL:HG23 | 1:D:305:TYR:HE1  | 1.77                     | 0.47              |
| 1:E:25:THR:O     | 1:E:29:SER:HB3   | 2.14                     | 0.47              |
| 1:E:183:ARG:CG   | 1:E:414:GLU:HB2  | 2.43                     | 0.47              |
| 1:A:164:ILE:HD12 | 1:A:164:ILE:C    | 2.38                     | 0.47              |
| 1:D:356:GLU:HG2  | 1:D:438:LEU:CD1  | 2.44                     | 0.47              |
| 1:A:254:VAL:HG21 | 1:A:347:TYR:CE2  | 2.49                     | 0.47              |
| 1:C:414:GLU:HG2  | 1:C:414:GLU:O    | 2.14                     | 0.47              |
| 1:B:121:THR:CB   | 3:B:3242:TRS:H12 | 2.44                     | 0.47              |
| 1:A:163:GLN:HG2  | 4:A:3293:HOH:O   | 2.14                     | 0.47              |
| 1:B:7:THR:HA     | 1:C:255:ALA:HA   | 1.95                     | 0.47              |
| 1:B:46:ILE:O     | 1:B:50:LEU:HG    | 2.14                     | 0.47              |
| 1:B:411:LEU:O    | 1:B:416:THR:HA   | 2.15                     | 0.47              |
| 1:B:422:ARG:HG2  | 1:B:422:ARG:HH11 | 1.80                     | 0.47              |
| 1:C:114:LYS:HZ2  | 1:C:292:GLU:CG   | 2.26                     | 0.47              |
| 1:C:315:ILE:HD13 | 1:D:315:ILE:HD13 | 1.96                     | 0.47              |
| 1:D:61:ALA:HB2   | 1:D:407:PRO:HD3  | 1.96                     | 0.47              |
| 1:A:402:ARG:HD2  | 1:A:440:ASP:OD1  | 2.15                     | 0.47              |
| 1:E:306:LEU:HD21 | 1:F:400:ARG:CZ   | 2.45                     | 0.47              |
| 1:E:362:PRO:CG   | 1:E:388:PRO:HG3  | 2.45                     | 0.47              |
| 1:A:398:ARG:HD3  | 4:A:3318:HOH:O   | 2.15                     | 0.47              |
| 1:B:89:GLU:C     | 1:B:91:PRO:HD3   | 2.40                     | 0.47              |
| 1:B:269:SER:HB3  | 1:B:289:TRP:CD1  | 2.50                     | 0.47              |
| 1:D:224:HIS:CD2  | 1:D:264:LEU:HB3  | 2.50                     | 0.47              |
| 1:D:275:HIS:HA   | 1:D:280:ALA:O    | 2.14                     | 0.47              |
| 1:B:31:ARG:HH11  | 1:B:34:LEU:HD11  | 1.80                     | 0.47              |
| 1:B:182:MET:HG3  | 1:B:187:LEU:O    | 2.15                     | 0.47              |
| 1:C:41:VAL:O     | 1:C:45:ILE:HG13  | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:38:ARG:HE    | 1:A:38:ARG:HB3   | 1.52                     | 0.46              |
| 1:D:242:ILE:CD1  | 1:D:267:VAL:HG22 | 2.42                     | 0.46              |
| 1:E:337:GLU:HB2  | 4:F:3399:HOH:O   | 2.15                     | 0.46              |
| 1:E:356:GLU:HG2  | 1:E:438:LEU:HD13 | 1.97                     | 0.46              |
| 1:D:239:ASP:OD2  | 1:D:268:LYS:NZ   | 2.47                     | 0.46              |
| 1:A:188:PHE:HZ   | 1:A:216:ASN:HD22 | 1.64                     | 0.46              |
| 1:C:143:LYS:HE3  | 1:C:298:GLU:OE1  | 2.16                     | 0.46              |
| 1:C:224:HIS:CD2  | 1:C:266:ARG:HB2  | 2.51                     | 0.46              |
| 1:A:109:HIS:HD2  | 1:A:261:ASP:OD2  | 1.98                     | 0.46              |
| 1:A:356:GLU:HG2  | 1:A:438:LEU:CD1  | 2.46                     | 0.46              |
| 1:D:163:GLN:HG2  | 4:D:3356:HOH:O   | 2.16                     | 0.46              |
| 1:D:186:GLN:O    | 1:D:186:GLN:HG3  | 2.15                     | 0.46              |
| 1:F:121:THR:HA   | 3:F:3248:TRS:H31 | 1.97                     | 0.46              |
| 1:B:52:LEU:HB3   | 3:C:3252:TRS:H32 | 1.98                     | 0.46              |
| 1:B:194:MET:HE3  | 1:B:195:ILE:HD13 | 1.98                     | 0.46              |
| 1:E:10:ARG:C     | 1:E:12:GLU:H     | 2.23                     | 0.46              |
| 1:A:103:MET:HE1  | 1:A:328:TYR:HD1  | 1.80                     | 0.46              |
| 1:A:195:ILE:HD11 | 1:A:230:PHE:HB2  | 1.98                     | 0.46              |
| 1:B:113:PRO:C    | 1:B:115:ASN:H    | 2.23                     | 0.46              |
| 1:D:181:PRO:O    | 1:D:193:ARG:NH2  | 2.45                     | 0.46              |
| 1:A:343:GLN:OE1  | 1:A:343:GLN:HA   | 2.15                     | 0.46              |
| 1:F:23:ILE:HG21  | 1:F:37:MET:CE    | 2.46                     | 0.46              |
| 1:D:381:LYS:HE2  | 4:D:3386:HOH:O   | 2.16                     | 0.46              |
| 1:F:344:ASN:O    | 1:F:348:GLN:HG3  | 2.17                     | 0.45              |
| 1:A:91:PRO:HB2   | 3:C:3252:TRS:C1  | 2.39                     | 0.45              |
| 1:A:293:GLU:CD   | 1:A:293:GLU:H    | 2.23                     | 0.45              |
| 1:B:16:SER:O     | 1:C:427:ARG:HD2  | 2.16                     | 0.45              |
| 1:B:180:ILE:HD12 | 1:B:180:ILE:N    | 2.31                     | 0.45              |
| 1:E:182:MET:CE   | 1:E:187:LEU:HB3  | 2.45                     | 0.45              |
| 1:E:183:ARG:HE   | 1:E:414:GLU:CG   | 2.29                     | 0.45              |
| 1:C:245:ALA:HA   | 1:C:272:ALA:HA   | 1.97                     | 0.45              |
| 1:B:124:ILE:HD11 | 1:B:319:ARG:HD2  | 1.97                     | 0.45              |
| 1:E:122:ASN:HB2  | 1:E:286:TRP:CZ3  | 2.51                     | 0.45              |
| 1:F:216:ASN:HD21 | 1:F:366:ILE:HG22 | 1.82                     | 0.45              |
| 1:B:245:ALA:HA   | 1:B:272:ALA:HA   | 1.99                     | 0.45              |
| 1:A:139:TRP:O    | 1:A:143:LYS:HG3  | 2.16                     | 0.45              |
| 1:B:157:LEU:HD13 | 1:B:157:LEU:C    | 2.42                     | 0.45              |
| 1:B:157:LEU:HD22 | 1:B:204:GLY:O    | 2.17                     | 0.45              |
| 1:C:13:LEU:N     | 4:C:3318:HOH:O   | 2.50                     | 0.45              |
| 1:E:217:TYR:CD2  | 1:E:374:GLY:HA2  | 2.51                     | 0.45              |
| 1:F:72:VAL:HG11  | 3:F:3240:TRS:H12 | 1.99                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:163:GLN:HG2  | 4:B:3339:HOH:O   | 2.16                     | 0.45              |
| 1:D:245:ALA:HA   | 1:D:272:ALA:HA   | 1.98                     | 0.45              |
| 1:F:25:THR:O     | 1:F:29:SER:HB3   | 2.17                     | 0.45              |
| 1:F:46:ILE:O     | 1:F:50:LEU:HG    | 2.16                     | 0.45              |
| 1:F:182:MET:HG3  | 1:F:187:LEU:O    | 2.16                     | 0.45              |
| 1:B:301:PHE:O    | 1:B:312:THR:HG22 | 2.17                     | 0.45              |
| 1:D:163:GLN:NE2  | 1:D:164:ILE:HG22 | 2.31                     | 0.45              |
| 1:D:390:TYR:CA   | 1:D:455:GLN:HG3  | 2.45                     | 0.45              |
| 1:E:97:ASP:OD2   | 3:E:3246:TRS:O1  | 2.33                     | 0.45              |
| 1:F:98:LEU:HD23  | 3:F:3248:TRS:O1  | 2.17                     | 0.45              |
| 1:F:121:THR:HB   | 3:F:3249:TRS:O2  | 2.17                     | 0.45              |
| 1:B:119:VAL:HG22 | 1:B:292:GLU:OE2  | 2.17                     | 0.45              |
| 1:C:312:THR:HG22 | 3:C:3243:TRS:O2  | 2.16                     | 0.45              |
| 1:A:207:PRO:HG2  | 1:A:240:MET:HE2  | 1.98                     | 0.44              |
| 1:C:65:GLN:HG3   | 3:C:3250:TRS:HN1 | 1.80                     | 0.44              |
| 1:C:135:MET:HE1  | 1:D:172:TYR:CG   | 2.52                     | 0.44              |
| 1:D:89:GLU:C     | 1:D:91:PRO:HD3   | 2.42                     | 0.44              |
| 1:F:221:GLN:CB   | 1:F:222:PRO:HD3  | 2.45                     | 0.44              |
| 1:A:315:ILE:HD13 | 1:B:315:ILE:HD13 | 1.98                     | 0.44              |
| 1:C:122:ASN:HB2  | 1:C:286:TRP:CZ3  | 2.53                     | 0.44              |
| 1:D:83:ASN:OD1   | 1:D:85:ILE:HG22  | 2.17                     | 0.44              |
| 1:E:124:ILE:HD13 | 1:E:124:ILE:HA   | 1.87                     | 0.44              |
| 1:E:154:LYS:HB3  | 1:E:154:LYS:HE2  | 1.76                     | 0.44              |
| 1:E:62:THR:HA    | 1:E:466:THR:OXT  | 2.18                     | 0.44              |
| 1:A:156:ASN:OD1  | 1:A:202:THR:HA   | 2.16                     | 0.44              |
| 1:A:186:GLN:O    | 1:A:186:GLN:HG3  | 2.17                     | 0.44              |
| 1:B:16:SER:OG    | 1:C:430:GLU:OE2  | 2.33                     | 0.44              |
| 1:E:61:ALA:HB2   | 1:E:407:PRO:HD3  | 2.00                     | 0.44              |
| 1:E:183:ARG:HE   | 1:E:414:GLU:HG2  | 1.82                     | 0.44              |
| 1:A:59:ASN:HA    | 1:A:405:GLN:HB3  | 1.98                     | 0.44              |
| 1:A:228:ASP:HA   | 1:A:266:ARG:HH21 | 1.82                     | 0.44              |
| 1:F:463:PHE:CE2  | 1:F:466:THR:HG22 | 2.52                     | 0.44              |
| 1:B:135:MET:HE2  | 1:B:135:MET:HB3  | 1.88                     | 0.44              |
| 1:C:26:ILE:O     | 1:C:27:ALA:C     | 2.60                     | 0.44              |
| 1:E:395:LEU:HD21 | 1:E:441:TYR:CZ   | 2.52                     | 0.44              |
| 1:A:114:LYS:CE   | 1:A:292:GLU:HG2  | 2.47                     | 0.44              |
| 1:A:400:ARG:HA   | 1:A:404:TRP:O    | 2.17                     | 0.44              |
| 1:D:382:LEU:HD22 | 1:D:388:PRO:HG2  | 2.00                     | 0.44              |
| 1:E:400:ARG:HA   | 1:E:404:TRP:O    | 2.18                     | 0.44              |
| 1:F:59:ASN:HA    | 1:F:405:GLN:HB3  | 1.99                     | 0.44              |
| 1:F:398:ARG:HD2  | 1:F:398:ARG:N    | 2.31                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:101:VAL:CG2  | 3:A:3251:TRS:H12 | 2.47                     | 0.44              |
| 1:F:61:ALA:HB2   | 1:F:407:PRO:HD3  | 2.00                     | 0.44              |
| 1:F:163:GLN:HG2  | 4:F:3308:HOH:O   | 2.18                     | 0.44              |
| 1:A:98:LEU:CD2   | 3:A:3251:TRS:O3  | 2.65                     | 0.44              |
| 1:A:362:PRO:C    | 1:A:383:LYS:HG3  | 2.42                     | 0.44              |
| 1:C:135:MET:HE1  | 1:D:172:TYR:CB   | 2.48                     | 0.44              |
| 1:B:264:LEU:O    | 1:B:290:ARG:NH2  | 2.51                     | 0.43              |
| 1:E:275:HIS:HA   | 1:E:280:ALA:O    | 2.17                     | 0.43              |
| 1:F:24:SER:HB3   | 1:F:27:ALA:HB3   | 2.00                     | 0.43              |
| 1:B:277:PHE:CE1  | 1:B:424:MET:HE1  | 2.53                     | 0.43              |
| 1:C:58:GLN:HE22  | 3:C:3252:TRS:H31 | 1.83                     | 0.43              |
| 1:C:454:LEU:HA   | 1:C:457:ILE:HD12 | 2.00                     | 0.43              |
| 1:D:161:PRO:HB3  | 1:D:182:MET:HE3  | 2.00                     | 0.43              |
| 1:D:459:GLN:HE21 | 1:D:459:GLN:HB3  | 1.49                     | 0.43              |
| 1:E:410:THR:HA   | 1:E:418:ILE:O    | 2.18                     | 0.43              |
| 1:A:162:VAL:HG13 | 1:A:163:GLN:O    | 2.18                     | 0.43              |
| 1:A:217:TYR:CD2  | 1:A:374:GLY:HA2  | 2.53                     | 0.43              |
| 1:B:277:PHE:CZ   | 1:B:424:MET:HE1  | 2.53                     | 0.43              |
| 1:A:190:ASP:HA   | 4:A:3322:HOH:O   | 2.18                     | 0.43              |
| 1:A:319:ARG:HB2  | 1:A:320:PRO:HD2  | 2.00                     | 0.43              |
| 1:B:207:PRO:HG2  | 1:B:240:MET:HE2  | 1.99                     | 0.43              |
| 1:C:23:ILE:HG21  | 1:C:37:MET:HE2   | 2.00                     | 0.43              |
| 1:C:177:LEU:HD13 | 1:C:177:LEU:C    | 2.44                     | 0.43              |
| 1:F:269:SER:HB3  | 1:F:289:TRP:CD1  | 2.53                     | 0.43              |
| 1:C:329:TYR:CE2  | 1:C:333:ARG:HD3  | 2.54                     | 0.43              |
| 1:C:400:ARG:HA   | 1:C:404:TRP:O    | 2.19                     | 0.43              |
| 1:F:121:THR:CA   | 3:F:3248:TRS:H31 | 2.48                     | 0.43              |
| 1:B:450:ASP:C    | 1:B:452:PRO:HD3  | 2.44                     | 0.43              |
| 1:D:160:GLY:O    | 1:D:179:GLU:HG3  | 2.18                     | 0.43              |
| 1:A:36:GLU:HG2   | 1:B:337:GLU:OE2  | 2.19                     | 0.43              |
| 1:D:410:THR:HG22 | 1:D:419:VAL:HG22 | 2.00                     | 0.43              |
| 1:F:362:PRO:HB2  | 1:F:386:GLU:HG2  | 2.01                     | 0.43              |
| 1:A:172:TYR:CB   | 1:B:135:MET:HE1  | 2.49                     | 0.43              |
| 1:B:242:ILE:CD1  | 1:B:267:VAL:HG22 | 2.49                     | 0.43              |
| 1:B:343:GLN:HA   | 1:B:343:GLN:OE1  | 2.19                     | 0.43              |
| 1:B:432:ASP:HA   | 1:C:26:ILE:HD12  | 2.01                     | 0.43              |
| 1:C:89:GLU:C     | 1:C:91:PRO:HD3   | 2.44                     | 0.43              |
| 1:A:162:VAL:CG2  | 1:A:166:TRP:CD1  | 3.01                     | 0.42              |
| 1:C:183:ARG:HH11 | 1:C:183:ARG:HG2  | 1.84                     | 0.42              |
| 1:D:255:ALA:N    | 1:D:256:PRO:HD3  | 2.34                     | 0.42              |
| 1:E:114:LYS:HE2  | 4:E:3369:HOH:O   | 2.18                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:185:GLY:H    | 3:E:3253:TRS:C1  | 2.32                     | 0.42              |
| 1:A:262:PHE:O    | 1:A:290:ARG:NH2  | 2.51                     | 0.42              |
| 1:A:417:ASP:HB2  | 4:A:3419:HOH:O   | 2.18                     | 0.42              |
| 1:D:242:ILE:HD13 | 1:D:267:VAL:CG1  | 2.50                     | 0.42              |
| 1:A:162:VAL:HG22 | 1:A:166:TRP:HD1  | 1.81                     | 0.42              |
| 1:A:216:ASN:HD21 | 1:A:366:ILE:HG13 | 1.83                     | 0.42              |
| 3:A:3236:TRS:H12 | 4:A:3437:HOH:O   | 2.18                     | 0.42              |
| 1:D:252:PRO:HG3  | 4:D:3282:HOH:O   | 2.18                     | 0.42              |
| 1:D:254:VAL:HG21 | 1:D:347:TYR:CE2  | 2.54                     | 0.42              |
| 1:E:460:GLN:HG2  | 1:F:306:LEU:O    | 2.18                     | 0.42              |
| 1:D:217:TYR:CD2  | 1:D:374:GLY:HA2  | 2.54                     | 0.42              |
| 1:D:219:PHE:HA   | 1:D:220:PRO:HD3  | 1.85                     | 0.42              |
| 1:E:343:GLN:OE1  | 1:E:343:GLN:HA   | 2.19                     | 0.42              |
| 1:B:299:LEU:HB3  | 1:B:313:PHE:CE1  | 2.54                     | 0.42              |
| 1:D:177:LEU:CD1  | 1:D:179:GLU:HB2  | 2.49                     | 0.42              |
| 1:D:242:ILE:N    | 1:D:242:ILE:HD12 | 2.34                     | 0.42              |
| 1:E:10:ARG:HG3   | 1:E:12:GLU:CG    | 2.50                     | 0.42              |
| 1:E:131:MET:HE2  | 1:F:315:ILE:HG23 | 2.02                     | 0.42              |
| 1:E:154:LYS:O    | 1:E:201:ASN:HB3  | 2.19                     | 0.42              |
| 1:E:261:ASP:HB2  | 1:E:262:PHE:H    | 1.59                     | 0.42              |
| 1:F:314:ALA:HB2  | 4:F:3340:HOH:O   | 2.20                     | 0.42              |
| 1:A:264:LEU:O    | 1:A:290:ARG:NH2  | 2.52                     | 0.42              |
| 1:A:303:VAL:HB   | 1:B:465:HIS:CD2  | 2.55                     | 0.42              |
| 1:B:59:ASN:HA    | 1:B:405:GLN:HB3  | 2.02                     | 0.42              |
| 1:E:12:GLU:HB2   | 1:E:13:LEU:H     | 1.65                     | 0.42              |
| 1:E:121:THR:HA   | 3:E:3246:TRS:H11 | 2.00                     | 0.42              |
| 1:A:128:GLU:O    | 1:A:132:LEU:HG   | 2.19                     | 0.42              |
| 1:A:129:ALA:HB1  | 1:A:287:VAL:HB   | 2.01                     | 0.42              |
| 1:A:390:TYR:N    | 1:A:455:GLN:NE2  | 2.67                     | 0.42              |
| 1:D:207:PRO:CG   | 1:D:240:MET:HE2  | 2.49                     | 0.42              |
| 1:D:264:LEU:O    | 1:D:290:ARG:NH2  | 2.53                     | 0.42              |
| 1:E:303:VAL:HG23 | 1:E:305:TYR:CE2  | 2.55                     | 0.42              |
| 1:A:245:ALA:HA   | 1:A:272:ALA:HA   | 2.02                     | 0.42              |
| 1:D:451:HIS:N    | 1:D:452:PRO:HD3  | 2.35                     | 0.42              |
| 1:F:250:LEU:HD23 | 1:F:343:GLN:CG   | 2.29                     | 0.42              |
| 1:C:199:ASP:OD1  | 1:C:201:ASN:N    | 2.43                     | 0.42              |
| 1:E:114:LYS:HZ3  | 1:E:292:GLU:HG2  | 1.84                     | 0.42              |
| 1:B:319:ARG:HB2  | 1:B:320:PRO:CD   | 2.50                     | 0.42              |
| 1:D:465:HIS:O    | 1:D:466:THR:HB   | 2.20                     | 0.42              |
| 1:E:200:GLU:HG3  | 1:E:236:ILE:HD11 | 2.02                     | 0.42              |
| 1:F:72:VAL:CG2   | 3:F:3240:TRS:H12 | 2.38                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:450:ASP:C    | 1:F:452:PRO:HD3  | 2.45                     | 0.42              |
| 1:A:275:HIS:HA   | 1:A:280:ALA:O    | 2.20                     | 0.41              |
| 1:B:117:GLN:HB2  | 4:B:3389:HOH:O   | 2.20                     | 0.41              |
| 1:B:427:ARG:HH21 | 3:B:3237:TRS:H21 | 1.84                     | 0.41              |
| 1:E:157:LEU:HD12 | 1:E:204:GLY:O    | 2.20                     | 0.41              |
| 1:A:386:GLU:O    | 1:A:387:ASP:C    | 2.62                     | 0.41              |
| 1:B:465:HIS:O    | 1:B:466:THR:HB   | 2.20                     | 0.41              |
| 1:D:98:LEU:HD23  | 3:D:3244:TRS:O3  | 2.21                     | 0.41              |
| 1:F:395:LEU:HD21 | 1:F:441:TYR:CZ   | 2.55                     | 0.41              |
| 1:A:383:LYS:O    | 1:A:384:ASP:C    | 2.63                     | 0.41              |
| 1:B:6:VAL:CA     | 1:C:257:ASP:HB2  | 2.49                     | 0.41              |
| 1:B:126:SER:HB2  | 2:B:1501:PLR:O4P | 2.20                     | 0.41              |
| 1:E:388:PRO:HB2  | 1:E:390:TYR:CE2  | 2.55                     | 0.41              |
| 1:A:142:ARG:O    | 1:A:145:MET:HB2  | 2.21                     | 0.41              |
| 1:A:159:CYS:SG   | 1:A:177:LEU:HD11 | 2.60                     | 0.41              |
| 1:A:332:LEU:HD22 | 1:B:37:MET:HE1   | 2.03                     | 0.41              |
| 1:C:46:ILE:O     | 1:C:50:LEU:HG    | 2.20                     | 0.41              |
| 1:C:67:TRP:O     | 3:C:3250:TRS:H32 | 2.21                     | 0.41              |
| 1:C:465:HIS:O    | 1:C:466:THR:HB   | 2.19                     | 0.41              |
| 1:F:180:ILE:N    | 1:F:180:ILE:HD12 | 2.35                     | 0.41              |
| 1:F:319:ARG:HB2  | 1:F:320:PRO:HD2  | 2.01                     | 0.41              |
| 1:B:153:ASP:OD2  | 1:B:154:LYS:HG3  | 2.21                     | 0.41              |
| 1:B:400:ARG:HA   | 1:B:404:TRP:O    | 2.21                     | 0.41              |
| 1:B:451:HIS:N    | 1:B:452:PRO:HD3  | 2.35                     | 0.41              |
| 1:C:275:HIS:HA   | 1:C:280:ALA:O    | 2.20                     | 0.41              |
| 1:D:344:ASN:HD22 | 1:D:344:ASN:HA   | 1.66                     | 0.41              |
| 1:E:362:PRO:HG3  | 1:E:388:PRO:HG3  | 2.01                     | 0.41              |
| 1:A:98:LEU:HD21  | 3:A:3251:TRS:O3  | 2.21                     | 0.41              |
| 1:A:177:LEU:C    | 1:A:177:LEU:CD1  | 2.93                     | 0.41              |
| 1:C:183:ARG:HH12 | 1:C:414:GLU:HB2  | 1.86                     | 0.41              |
| 1:C:371:PRO:HD2  | 4:C:3367:HOH:O   | 2.20                     | 0.41              |
| 1:E:114:LYS:NZ   | 1:E:292:GLU:HG2  | 2.34                     | 0.41              |
| 1:A:157:LEU:HD22 | 1:A:204:GLY:O    | 2.21                     | 0.41              |
| 1:A:161:PRO:CG   | 1:A:182:MET:HE3  | 2.51                     | 0.41              |
| 1:B:352:TYR:OH   | 1:B:435:GLU:OE2  | 2.26                     | 0.41              |
| 1:D:344:ASN:O    | 1:D:348:GLN:HG3  | 2.21                     | 0.41              |
| 1:E:114:LYS:H    | 1:E:114:LYS:HG3  | 1.61                     | 0.41              |
| 1:E:255:ALA:N    | 1:E:256:PRO:HD3  | 2.36                     | 0.41              |
| 1:F:451:HIS:N    | 1:F:452:PRO:HD3  | 2.36                     | 0.41              |
| 1:A:131:MET:CE   | 1:A:169:PHE:HB2  | 2.51                     | 0.41              |
| 1:B:139:TRP:HB3  | 1:B:296:PRO:HG2  | 2.01                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:63:PHE:CG    | 1:C:424:MET:HE2  | 2.56                     | 0.41              |
| 1:D:141:TRP:CZ3  | 1:D:155:PRO:HB3  | 2.56                     | 0.41              |
| 1:A:112:ALA:HA   | 1:A:113:PRO:HD3  | 1.97                     | 0.41              |
| 1:A:187:LEU:HD12 | 1:A:366:ILE:HD12 | 2.02                     | 0.41              |
| 1:A:400:ARG:NE   | 1:B:306:LEU:HD21 | 2.36                     | 0.41              |
| 1:B:98:LEU:HD23  | 3:B:3242:TRS:O3  | 2.21                     | 0.41              |
| 1:C:177:LEU:HD11 | 1:C:179:GLU:HB2  | 2.03                     | 0.41              |
| 1:C:218:GLU:O    | 1:C:220:PRO:HD3  | 2.21                     | 0.41              |
| 1:C:228:ASP:HA   | 1:C:266:ARG:HH21 | 1.85                     | 0.41              |
| 1:C:395:LEU:HD21 | 1:C:441:TYR:CZ   | 2.56                     | 0.41              |
| 1:D:182:MET:HG2  | 1:D:187:LEU:HD22 | 2.03                     | 0.41              |
| 1:E:185:GLY:N    | 3:E:3253:TRS:O1  | 2.49                     | 0.41              |
| 1:F:186:GLN:O    | 1:F:186:GLN:HG3  | 2.21                     | 0.41              |
| 1:A:182:MET:HG2  | 1:A:187:LEU:HD22 | 2.03                     | 0.41              |
| 1:B:61:ALA:HB2   | 1:B:407:PRO:HD3  | 2.02                     | 0.41              |
| 1:C:58:GLN:NE2   | 3:C:3252:TRS:H31 | 2.35                     | 0.41              |
| 1:C:114:LYS:HE2  | 4:C:3389:HOH:O   | 2.21                     | 0.41              |
| 1:C:417:ASP:HB3  | 4:C:3311:HOH:O   | 2.21                     | 0.41              |
| 1:F:275:HIS:NE2  | 2:F:1505:PLR:O1P | 2.48                     | 0.41              |
| 1:A:72:VAL:HG11  | 3:A:3236:TRS:H22 | 2.03                     | 0.40              |
| 1:C:112:ALA:HA   | 1:C:113:PRO:HD3  | 1.93                     | 0.40              |
| 1:C:219:PHE:HA   | 1:C:220:PRO:HD3  | 1.87                     | 0.40              |
| 3:D:3244:TRS:H21 | 3:D:3245:TRS:O3  | 2.20                     | 0.40              |
| 1:C:135:MET:HE1  | 1:D:172:TYR:HA   | 2.02                     | 0.40              |
| 1:D:23:ILE:HG21  | 1:D:37:MET:CE    | 2.49                     | 0.40              |
| 1:E:63:PHE:CD1   | 1:E:63:PHE:N     | 2.89                     | 0.40              |
| 1:E:306:LEU:HD21 | 1:F:400:ARG:NE   | 2.36                     | 0.40              |
| 1:E:183:ARG:NH2  | 1:E:414:GLU:HG2  | 2.29                     | 0.40              |
| 1:E:286:TRP:HZ2  | 1:E:327:GLN:HG2  | 1.86                     | 0.40              |
| 1:A:154:LYS:HB3  | 1:A:154:LYS:HE2  | 1.85                     | 0.40              |
| 1:B:141:TRP:CZ3  | 1:B:155:PRO:HG3  | 2.57                     | 0.40              |
| 1:B:242:ILE:HD11 | 1:B:267:VAL:HG22 | 2.02                     | 0.40              |
| 1:D:286:TRP:HZ2  | 1:D:327:GLN:HG2  | 1.85                     | 0.40              |
| 1:A:183:ARG:O    | 1:A:184:PRO:C    | 2.65                     | 0.40              |
| 1:C:370:ARG:HA   | 1:C:371:PRO:HD3  | 1.88                     | 0.40              |
| 1:F:400:ARG:HA   | 1:F:404:TRP:O    | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 1   | A     | 453/466 (97%)   | 436 (96%)  | 15 (3%) | 2 (0%)   | 30          | 38  |
| 1   | B     | 461/466 (99%)   | 446 (97%)  | 14 (3%) | 1 (0%)   | 43          | 55  |
| 1   | C     | 452/466 (97%)   | 436 (96%)  | 14 (3%) | 2 (0%)   | 30          | 38  |
| 1   | D     | 452/466 (97%)   | 437 (97%)  | 15 (3%) | 0        | 100         | 100 |
| 1   | E     | 461/466 (99%)   | 437 (95%)  | 20 (4%) | 4 (1%)   | 14          | 17  |
| 1   | F     | 452/466 (97%)   | 440 (97%)  | 12 (3%) | 0        | 100         | 100 |
| All | All   | 2731/2796 (98%) | 2632 (96%) | 90 (3%) | 9 (0%)   | 36          | 46  |

All (9) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 27  | ALA  |
| 1   | E     | 12  | GLU  |
| 1   | A     | 385 | GLY  |
| 1   | B     | 116 | GLY  |
| 1   | C     | 116 | GLY  |
| 1   | E     | 13  | LEU  |
| 1   | E     | 22  | SER  |
| 1   | A     | 387 | ASP  |
| 1   | E     | 23  | ILE  |

### 5.3.2 Protein sidechains

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 379/390 (97%)   | 369 (97%)  | 10 (3%)  | 40          | 59 |
| 1   | B     | 387/390 (99%)   | 380 (98%)  | 7 (2%)   | 51          | 70 |
| 1   | C     | 378/390 (97%)   | 373 (99%)  | 5 (1%)   | 61          | 77 |
| 1   | D     | 378/390 (97%)   | 371 (98%)  | 7 (2%)   | 50          | 69 |
| 1   | E     | 387/390 (99%)   | 381 (98%)  | 6 (2%)   | 55          | 73 |
| 1   | F     | 378/390 (97%)   | 372 (98%)  | 6 (2%)   | 55          | 73 |
| All | All   | 2287/2340 (98%) | 2246 (98%) | 41 (2%)  | 51          | 70 |

All (41) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 114 | LYS  |
| 1   | A     | 131 | MET  |
| 1   | A     | 162 | VAL  |
| 1   | A     | 195 | ILE  |
| 1   | A     | 200 | GLU  |
| 1   | A     | 293 | GLU  |
| 1   | A     | 343 | GLN  |
| 1   | A     | 344 | ASN  |
| 1   | A     | 366 | ILE  |
| 1   | A     | 414 | GLU  |
| 1   | B     | 124 | ILE  |
| 1   | B     | 153 | ASP  |
| 1   | B     | 195 | ILE  |
| 1   | B     | 200 | GLU  |
| 1   | B     | 343 | GLN  |
| 1   | B     | 414 | GLU  |
| 1   | B     | 437 | LEU  |
| 1   | C     | 343 | GLN  |
| 1   | C     | 344 | ASN  |
| 1   | C     | 427 | ARG  |
| 1   | C     | 437 | LEU  |
| 1   | C     | 459 | GLN  |
| 1   | D     | 114 | LYS  |
| 1   | D     | 146 | GLU  |
| 1   | D     | 162 | VAL  |
| 1   | D     | 344 | ASN  |
| 1   | D     | 398 | ARG  |
| 1   | D     | 437 | LEU  |
| 1   | D     | 459 | GLN  |
| 1   | E     | 12  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 21  | LYS  |
| 1   | E     | 31  | ARG  |
| 1   | E     | 142 | ARG  |
| 1   | E     | 177 | LEU  |
| 1   | E     | 344 | ASN  |
| 1   | F     | 131 | MET  |
| 1   | F     | 221 | GLN  |
| 1   | F     | 304 | ASP  |
| 1   | F     | 343 | GLN  |
| 1   | F     | 414 | GLU  |
| 1   | F     | 437 | LEU  |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 47  | ASN  |
| 1   | A     | 71  | ASN  |
| 1   | A     | 92  | GLN  |
| 1   | A     | 109 | HIS  |
| 1   | A     | 117 | GLN  |
| 1   | A     | 186 | GLN  |
| 1   | A     | 216 | ASN  |
| 1   | A     | 309 | GLN  |
| 1   | A     | 344 | ASN  |
| 1   | A     | 405 | GLN  |
| 1   | A     | 455 | GLN  |
| 1   | A     | 459 | GLN  |
| 1   | B     | 5   | GLN  |
| 1   | B     | 109 | HIS  |
| 1   | B     | 216 | ASN  |
| 1   | B     | 309 | GLN  |
| 1   | B     | 459 | GLN  |
| 1   | C     | 58  | GLN  |
| 1   | C     | 109 | HIS  |
| 1   | C     | 186 | GLN  |
| 1   | C     | 309 | GLN  |
| 1   | C     | 459 | GLN  |
| 1   | D     | 47  | ASN  |
| 1   | D     | 167 | HIS  |
| 1   | D     | 186 | GLN  |
| 1   | D     | 201 | ASN  |
| 1   | D     | 309 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 344 | ASN  |
| 1   | D     | 459 | GLN  |
| 1   | E     | 216 | ASN  |
| 1   | E     | 302 | ASN  |
| 1   | E     | 309 | GLN  |
| 1   | E     | 344 | ASN  |
| 1   | E     | 455 | GLN  |
| 1   | F     | 35  | HIS  |
| 1   | F     | 58  | GLN  |
| 1   | F     | 186 | GLN  |
| 1   | F     | 216 | ASN  |
| 1   | F     | 309 | GLN  |
| 1   | F     | 344 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 3   | TRS  | E     | 3246 | -    | 7,7,7        | 0.56 | 0           | 9,9,9       | 0.30 | 0           |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | PLR  | E     | 1504 | -    | 15,15,15     | 0.86 | 0        | 21,22,22    | 1.48 | 5 (23%)  |
| 3   | TRS  | F     | 3240 | -    | 7,7,7        | 0.40 | 0        | 9,9,9       | 0.44 | 0        |
| 3   | TRS  | F     | 3249 | -    | 7,7,7        | 0.48 | 0        | 9,9,9       | 0.33 | 0        |
| 3   | TRS  | D     | 3238 | -    | 7,7,7        | 0.50 | 0        | 9,9,9       | 0.35 | 0        |
| 3   | TRS  | E     | 3247 | -    | 7,7,7        | 0.35 | 0        | 9,9,9       | 0.53 | 0        |
| 3   | TRS  | D     | 3245 | -    | 7,7,7        | 0.38 | 0        | 9,9,9       | 0.47 | 0        |
| 3   | TRS  | D     | 3244 | -    | 7,7,7        | 0.44 | 0        | 9,9,9       | 0.38 | 0        |
| 3   | TRS  | A     | 3251 | -    | 7,7,7        | 0.32 | 0        | 9,9,9       | 0.42 | 0        |
| 3   | TRS  | B     | 3242 | -    | 7,7,7        | 0.46 | 0        | 9,9,9       | 0.36 | 0        |
| 3   | TRS  | E     | 3253 | -    | 7,7,7        | 0.46 | 0        | 9,9,9       | 0.35 | 0        |
| 3   | TRS  | B     | 3237 | -    | 7,7,7        | 0.49 | 0        | 9,9,9       | 0.36 | 0        |
| 2   | PLR  | B     | 1501 | -    | 15,15,15     | 0.95 | 1 (6%)   | 21,22,22    | 1.50 | 5 (23%)  |
| 3   | TRS  | E     | 3239 | -    | 7,7,7        | 0.50 | 0        | 9,9,9       | 0.23 | 0        |
| 3   | TRS  | C     | 3243 | -    | 7,7,7        | 0.40 | 0        | 9,9,9       | 0.43 | 0        |
| 3   | TRS  | F     | 3248 | -    | 7,7,7        | 0.41 | 0        | 9,9,9       | 0.30 | 0        |
| 2   | PLR  | A     | 1500 | -    | 15,15,15     | 0.74 | 0        | 21,22,22    | 1.44 | 5 (23%)  |
| 2   | PLR  | C     | 1502 | -    | 15,15,15     | 0.91 | 0        | 21,22,22    | 1.45 | 4 (19%)  |
| 3   | TRS  | C     | 3252 | -    | 7,7,7        | 0.42 | 0        | 9,9,9       | 0.39 | 0        |
| 2   | PLR  | D     | 1503 | -    | 15,15,15     | 0.92 | 0        | 21,22,22    | 1.50 | 5 (23%)  |
| 2   | PLR  | F     | 1505 | -    | 15,15,15     | 0.91 | 0        | 21,22,22    | 1.49 | 5 (23%)  |
| 3   | TRS  | A     | 3241 | -    | 7,7,7        | 0.44 | 0        | 9,9,9       | 0.37 | 0        |
| 3   | TRS  | A     | 3236 | -    | 7,7,7        | 0.46 | 0        | 9,9,9       | 0.27 | 0        |
| 3   | TRS  | C     | 3250 | -    | 7,7,7        | 0.51 | 0        | 9,9,9       | 0.22 | 0        |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 3   | TRS  | E     | 3246 | -    | -       | 9/9/9/9  | -       |
| 2   | PLR  | E     | 1504 | -    | -       | 0/6/6/6  | 0/1/1/1 |
| 3   | TRS  | F     | 3240 | -    | -       | 9/9/9/9  | -       |
| 3   | TRS  | F     | 3249 | -    | -       | 9/9/9/9  | -       |
| 3   | TRS  | D     | 3238 | -    | -       | 9/9/9/9  | -       |
| 3   | TRS  | E     | 3247 | -    | -       | 9/9/9/9  | -       |
| 3   | TRS  | D     | 3245 | -    | -       | 9/9/9/9  | -       |
| 3   | TRS  | D     | 3244 | -    | -       | 9/9/9/9  | -       |
| 3   | TRS  | A     | 3251 | -    | -       | 9/9/9/9  | -       |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 3   | TRS  | B     | 3242 | -    | -       | 9/9/9/9  | -       |
| 3   | TRS  | E     | 3253 | -    | -       | 9/9/9/9  | -       |
| 3   | TRS  | B     | 3237 | -    | -       | 9/9/9/9  | -       |
| 2   | PLR  | B     | 1501 | -    | -       | 0/6/6/6  | 0/1/1/1 |
| 3   | TRS  | E     | 3239 | -    | -       | 9/9/9/9  | -       |
| 3   | TRS  | C     | 3243 | -    | -       | 9/9/9/9  | -       |
| 3   | TRS  | F     | 3248 | -    | -       | 9/9/9/9  | -       |
| 2   | PLR  | A     | 1500 | -    | -       | 0/6/6/6  | 0/1/1/1 |
| 2   | PLR  | C     | 1502 | -    | -       | 0/6/6/6  | 0/1/1/1 |
| 3   | TRS  | C     | 3252 | -    | -       | 9/9/9/9  | -       |
| 2   | PLR  | D     | 1503 | -    | -       | 0/6/6/6  | 0/1/1/1 |
| 2   | PLR  | F     | 1505 | -    | -       | 0/6/6/6  | 0/1/1/1 |
| 3   | TRS  | A     | 3241 | -    | -       | 9/9/9/9  | -       |
| 3   | TRS  | A     | 3236 | -    | -       | 9/9/9/9  | -       |
| 3   | TRS  | C     | 3250 | -    | -       | 9/9/9/9  | -       |

All (1) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 2   | B     | 1501 | PLR  | C5-C4 | 2.36 | 1.43        | 1.40     |

All (29) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2   | B     | 1501 | PLR  | C4A-C4-C5 | 2.97  | 124.00      | 120.94   |
| 2   | F     | 1505 | PLR  | C4A-C4-C5 | 2.83  | 123.86      | 120.94   |
| 2   | D     | 1503 | PLR  | C3-C2-N1  | -2.78 | 117.45      | 120.96   |
| 2   | E     | 1504 | PLR  | C3-C2-N1  | -2.77 | 117.47      | 120.96   |
| 2   | F     | 1505 | PLR  | C3-C2-N1  | -2.75 | 117.50      | 120.96   |
| 2   | D     | 1503 | PLR  | C4A-C4-C5 | 2.73  | 123.75      | 120.94   |
| 2   | D     | 1503 | PLR  | C6-N1-C2  | 2.72  | 124.14      | 119.20   |
| 2   | C     | 1502 | PLR  | C4A-C4-C5 | 2.72  | 123.74      | 120.94   |
| 2   | B     | 1501 | PLR  | C3-C2-N1  | -2.70 | 117.55      | 120.96   |
| 2   | A     | 1500 | PLR  | C4A-C4-C5 | 2.70  | 123.72      | 120.94   |
| 2   | C     | 1502 | PLR  | C3-C2-N1  | -2.69 | 117.57      | 120.96   |
| 2   | B     | 1501 | PLR  | C6-N1-C2  | 2.68  | 124.06      | 119.20   |
| 2   | A     | 1500 | PLR  | C3-C2-N1  | -2.67 | 117.60      | 120.96   |
| 2   | E     | 1504 | PLR  | C2A-C2-C3 | 2.64  | 123.89      | 120.80   |
| 2   | A     | 1500 | PLR  | C6-N1-C2  | 2.60  | 123.92      | 119.20   |
| 2   | C     | 1502 | PLR  | C6-N1-C2  | 2.60  | 123.91      | 119.20   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2   | F     | 1505 | PLR  | C6-N1-C2  | 2.57  | 123.87      | 119.20   |
| 2   | E     | 1504 | PLR  | C4A-C4-C5 | 2.57  | 123.58      | 120.94   |
| 2   | C     | 1502 | PLR  | C2A-C2-C3 | 2.56  | 123.80      | 120.80   |
| 2   | D     | 1503 | PLR  | C2A-C2-C3 | 2.56  | 123.80      | 120.80   |
| 2   | E     | 1504 | PLR  | C6-N1-C2  | 2.56  | 123.84      | 119.20   |
| 2   | F     | 1505 | PLR  | C2A-C2-C3 | 2.52  | 123.75      | 120.80   |
| 2   | B     | 1501 | PLR  | C2A-C2-C3 | 2.32  | 123.51      | 120.80   |
| 2   | A     | 1500 | PLR  | C2A-C2-C3 | 2.25  | 123.43      | 120.80   |
| 2   | B     | 1501 | PLR  | C4A-C4-C3 | -2.17 | 116.91      | 120.52   |
| 2   | F     | 1505 | PLR  | C4A-C4-C3 | -2.06 | 117.10      | 120.52   |
| 2   | E     | 1504 | PLR  | O3P-P-O1P | 2.02  | 118.70      | 110.83   |
| 2   | D     | 1503 | PLR  | C4A-C4-C3 | -2.01 | 117.17      | 120.52   |
| 2   | A     | 1500 | PLR  | O3P-P-O1P | 2.01  | 118.68      | 110.83   |

There are no chirality outliers.

All (162) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      |
|-----|-------|------|------|------------|
| 3   | A     | 3236 | TRS  | N-C-C3-O3  |
| 3   | A     | 3241 | TRS  | N-C-C2-O2  |
| 3   | A     | 3241 | TRS  | N-C-C3-O3  |
| 3   | A     | 3251 | TRS  | N-C-C1-O1  |
| 3   | B     | 3237 | TRS  | N-C-C1-O1  |
| 3   | B     | 3237 | TRS  | N-C-C3-O3  |
| 3   | B     | 3242 | TRS  | N-C-C3-O3  |
| 3   | C     | 3243 | TRS  | N-C-C3-O3  |
| 3   | D     | 3238 | TRS  | C3-C-C2-O2 |
| 3   | D     | 3238 | TRS  | N-C-C2-O2  |
| 3   | D     | 3244 | TRS  | N-C-C1-O1  |
| 3   | D     | 3244 | TRS  | N-C-C2-O2  |
| 3   | D     | 3245 | TRS  | N-C-C3-O3  |
| 3   | E     | 3239 | TRS  | N-C-C1-O1  |
| 3   | E     | 3239 | TRS  | N-C-C2-O2  |
| 3   | E     | 3246 | TRS  | N-C-C1-O1  |
| 3   | E     | 3246 | TRS  | N-C-C2-O2  |
| 3   | E     | 3253 | TRS  | N-C-C3-O3  |
| 3   | F     | 3240 | TRS  | N-C-C2-O2  |
| 3   | F     | 3248 | TRS  | N-C-C2-O2  |
| 3   | F     | 3248 | TRS  | N-C-C3-O3  |
| 3   | F     | 3249 | TRS  | N-C-C1-O1  |
| 3   | F     | 3249 | TRS  | N-C-C3-O3  |
| 3   | A     | 3236 | TRS  | C3-C-C2-O2 |

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| Mol | Chain | Res  | Type | Atoms      |
|-----|-------|------|------|------------|
| 3   | A     | 3236 | TRS  | C1-C-C3-O3 |
| 3   | A     | 3241 | TRS  | C3-C-C2-O2 |
| 3   | A     | 3241 | TRS  | C1-C-C3-O3 |
| 3   | A     | 3251 | TRS  | C2-C-C1-O1 |
| 3   | B     | 3237 | TRS  | C3-C-C1-O1 |
| 3   | B     | 3237 | TRS  | C3-C-C2-O2 |
| 3   | B     | 3237 | TRS  | C2-C-C3-O3 |
| 3   | B     | 3242 | TRS  | C3-C-C2-O2 |
| 3   | B     | 3242 | TRS  | C1-C-C3-O3 |
| 3   | C     | 3243 | TRS  | C1-C-C3-O3 |
| 3   | C     | 3250 | TRS  | C3-C-C2-O2 |
| 3   | C     | 3250 | TRS  | C1-C-C3-O3 |
| 3   | C     | 3252 | TRS  | C3-C-C1-O1 |
| 3   | D     | 3238 | TRS  | C3-C-C1-O1 |
| 3   | D     | 3238 | TRS  | C1-C-C3-O3 |
| 3   | D     | 3244 | TRS  | C3-C-C1-O1 |
| 3   | D     | 3244 | TRS  | C1-C-C2-O2 |
| 3   | D     | 3245 | TRS  | C2-C-C3-O3 |
| 3   | E     | 3239 | TRS  | C3-C-C1-O1 |
| 3   | E     | 3239 | TRS  | C1-C-C2-O2 |
| 3   | E     | 3239 | TRS  | C2-C-C3-O3 |
| 3   | E     | 3246 | TRS  | C2-C-C1-O1 |
| 3   | E     | 3246 | TRS  | C1-C-C2-O2 |
| 3   | E     | 3246 | TRS  | C2-C-C3-O3 |
| 3   | E     | 3253 | TRS  | C2-C-C1-O1 |
| 3   | E     | 3253 | TRS  | C2-C-C3-O3 |
| 3   | F     | 3240 | TRS  | C3-C-C2-O2 |
| 3   | F     | 3248 | TRS  | C1-C-C2-O2 |
| 3   | F     | 3248 | TRS  | C1-C-C3-O3 |
| 3   | F     | 3249 | TRS  | C2-C-C1-O1 |
| 3   | F     | 3249 | TRS  | C1-C-C2-O2 |
| 3   | F     | 3249 | TRS  | C1-C-C3-O3 |
| 3   | A     | 3236 | TRS  | C3-C-C1-O1 |
| 3   | A     | 3236 | TRS  | N-C-C2-O2  |
| 3   | A     | 3236 | TRS  | C2-C-C3-O3 |
| 3   | A     | 3241 | TRS  | C3-C-C1-O1 |
| 3   | A     | 3241 | TRS  | C1-C-C2-O2 |
| 3   | A     | 3241 | TRS  | C2-C-C3-O3 |
| 3   | A     | 3251 | TRS  | C3-C-C1-O1 |
| 3   | A     | 3251 | TRS  | C1-C-C2-O2 |
| 3   | A     | 3251 | TRS  | N-C-C2-O2  |
| 3   | A     | 3251 | TRS  | C1-C-C3-O3 |

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| Mol | Chain | Res  | Type | Atoms      |
|-----|-------|------|------|------------|
| 3   | A     | 3251 | TRS  | N-C-C3-O3  |
| 3   | B     | 3237 | TRS  | C2-C-C1-O1 |
| 3   | B     | 3237 | TRS  | N-C-C2-O2  |
| 3   | B     | 3237 | TRS  | C1-C-C3-O3 |
| 3   | B     | 3242 | TRS  | C2-C-C1-O1 |
| 3   | B     | 3242 | TRS  | N-C-C1-O1  |
| 3   | B     | 3242 | TRS  | N-C-C2-O2  |
| 3   | B     | 3242 | TRS  | C2-C-C3-O3 |
| 3   | C     | 3243 | TRS  | C3-C-C1-O1 |
| 3   | C     | 3243 | TRS  | N-C-C1-O1  |
| 3   | C     | 3243 | TRS  | C1-C-C2-O2 |
| 3   | C     | 3243 | TRS  | N-C-C2-O2  |
| 3   | C     | 3243 | TRS  | C2-C-C3-O3 |
| 3   | C     | 3250 | TRS  | C3-C-C1-O1 |
| 3   | C     | 3250 | TRS  | N-C-C2-O2  |
| 3   | C     | 3250 | TRS  | N-C-C3-O3  |
| 3   | C     | 3252 | TRS  | N-C-C1-O1  |
| 3   | C     | 3252 | TRS  | C3-C-C2-O2 |
| 3   | C     | 3252 | TRS  | C2-C-C3-O3 |
| 3   | C     | 3252 | TRS  | N-C-C3-O3  |
| 3   | D     | 3238 | TRS  | N-C-C1-O1  |
| 3   | D     | 3238 | TRS  | C1-C-C2-O2 |
| 3   | D     | 3238 | TRS  | N-C-C3-O3  |
| 3   | D     | 3244 | TRS  | C2-C-C1-O1 |
| 3   | D     | 3244 | TRS  | C3-C-C2-O2 |
| 3   | D     | 3244 | TRS  | C1-C-C3-O3 |
| 3   | D     | 3244 | TRS  | N-C-C3-O3  |
| 3   | D     | 3245 | TRS  | C2-C-C1-O1 |
| 3   | D     | 3245 | TRS  | N-C-C1-O1  |
| 3   | D     | 3245 | TRS  | C3-C-C2-O2 |
| 3   | D     | 3245 | TRS  | N-C-C2-O2  |
| 3   | D     | 3245 | TRS  | C1-C-C3-O3 |
| 3   | E     | 3239 | TRS  | C2-C-C1-O1 |
| 3   | E     | 3239 | TRS  | N-C-C3-O3  |
| 3   | E     | 3246 | TRS  | N-C-C3-O3  |
| 3   | E     | 3247 | TRS  | C3-C-C1-O1 |
| 3   | E     | 3247 | TRS  | N-C-C1-O1  |
| 3   | E     | 3247 | TRS  | C1-C-C2-O2 |
| 3   | E     | 3247 | TRS  | N-C-C2-O2  |
| 3   | E     | 3247 | TRS  | C2-C-C3-O3 |
| 3   | E     | 3247 | TRS  | N-C-C3-O3  |
| 3   | E     | 3253 | TRS  | N-C-C1-O1  |

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| Mol | Chain | Res  | Type | Atoms      |
|-----|-------|------|------|------------|
| 3   | E     | 3253 | TRS  | C3-C-C2-O2 |
| 3   | E     | 3253 | TRS  | N-C-C2-O2  |
| 3   | E     | 3253 | TRS  | C1-C-C3-O3 |
| 3   | F     | 3240 | TRS  | C3-C-C1-O1 |
| 3   | F     | 3240 | TRS  | N-C-C1-O1  |
| 3   | F     | 3240 | TRS  | C1-C-C2-O2 |
| 3   | F     | 3240 | TRS  | C1-C-C3-O3 |
| 3   | F     | 3240 | TRS  | N-C-C3-O3  |
| 3   | F     | 3248 | TRS  | C2-C-C1-O1 |
| 3   | F     | 3248 | TRS  | N-C-C1-O1  |
| 3   | F     | 3249 | TRS  | C3-C-C1-O1 |
| 3   | F     | 3249 | TRS  | N-C-C2-O2  |
| 3   | A     | 3236 | TRS  | C2-C-C1-O1 |
| 3   | A     | 3236 | TRS  | C1-C-C2-O2 |
| 3   | A     | 3241 | TRS  | C2-C-C1-O1 |
| 3   | A     | 3251 | TRS  | C3-C-C2-O2 |
| 3   | A     | 3251 | TRS  | C2-C-C3-O3 |
| 3   | B     | 3237 | TRS  | C1-C-C2-O2 |
| 3   | B     | 3242 | TRS  | C3-C-C1-O1 |
| 3   | B     | 3242 | TRS  | C1-C-C2-O2 |
| 3   | C     | 3243 | TRS  | C2-C-C1-O1 |
| 3   | C     | 3243 | TRS  | C3-C-C2-O2 |
| 3   | C     | 3250 | TRS  | C2-C-C1-O1 |
| 3   | C     | 3250 | TRS  | C1-C-C2-O2 |
| 3   | C     | 3250 | TRS  | C2-C-C3-O3 |
| 3   | C     | 3252 | TRS  | C2-C-C1-O1 |
| 3   | C     | 3252 | TRS  | C1-C-C2-O2 |
| 3   | C     | 3252 | TRS  | C1-C-C3-O3 |
| 3   | D     | 3238 | TRS  | C2-C-C1-O1 |
| 3   | D     | 3238 | TRS  | C2-C-C3-O3 |
| 3   | D     | 3244 | TRS  | C2-C-C3-O3 |
| 3   | D     | 3245 | TRS  | C3-C-C1-O1 |
| 3   | D     | 3245 | TRS  | C1-C-C2-O2 |
| 3   | E     | 3239 | TRS  | C3-C-C2-O2 |
| 3   | E     | 3239 | TRS  | C1-C-C3-O3 |
| 3   | E     | 3246 | TRS  | C3-C-C1-O1 |
| 3   | E     | 3246 | TRS  | C3-C-C2-O2 |
| 3   | E     | 3246 | TRS  | C1-C-C3-O3 |
| 3   | E     | 3247 | TRS  | C2-C-C1-O1 |
| 3   | E     | 3247 | TRS  | C3-C-C2-O2 |
| 3   | E     | 3247 | TRS  | C1-C-C3-O3 |
| 3   | E     | 3253 | TRS  | C3-C-C1-O1 |

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| Mol | Chain | Res  | Type | Atoms      |
|-----|-------|------|------|------------|
| 3   | E     | 3253 | TRS  | C1-C-C2-O2 |
| 3   | F     | 3240 | TRS  | C2-C-C1-O1 |
| 3   | F     | 3240 | TRS  | C2-C-C3-O3 |
| 3   | F     | 3248 | TRS  | C3-C-C1-O1 |
| 3   | F     | 3248 | TRS  | C3-C-C2-O2 |
| 3   | F     | 3248 | TRS  | C2-C-C3-O3 |
| 3   | F     | 3249 | TRS  | C3-C-C2-O2 |
| 3   | F     | 3249 | TRS  | C2-C-C3-O3 |
| 3   | A     | 3236 | TRS  | N-C-C1-O1  |
| 3   | A     | 3241 | TRS  | N-C-C1-O1  |
| 3   | C     | 3250 | TRS  | N-C-C1-O1  |
| 3   | C     | 3252 | TRS  | N-C-C2-O2  |

There are no ring outliers.

19 monomers are involved in 79 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | E     | 3246 | TRS  | 7       | 0            |
| 3   | F     | 3240 | TRS  | 5       | 0            |
| 3   | F     | 3249 | TRS  | 4       | 0            |
| 3   | D     | 3238 | TRS  | 4       | 0            |
| 3   | D     | 3245 | TRS  | 1       | 0            |
| 3   | D     | 3244 | TRS  | 5       | 0            |
| 3   | A     | 3251 | TRS  | 6       | 0            |
| 3   | B     | 3242 | TRS  | 5       | 0            |
| 3   | E     | 3253 | TRS  | 3       | 0            |
| 3   | B     | 3237 | TRS  | 2       | 0            |
| 2   | B     | 1501 | PLR  | 1       | 0            |
| 3   | E     | 3239 | TRS  | 4       | 0            |
| 3   | C     | 3243 | TRS  | 5       | 0            |
| 3   | F     | 3248 | TRS  | 8       | 0            |
| 2   | C     | 1502 | PLR  | 1       | 0            |
| 3   | C     | 3252 | TRS  | 7       | 0            |
| 2   | F     | 1505 | PLR  | 1       | 0            |
| 3   | A     | 3236 | TRS  | 5       | 0            |
| 3   | C     | 3250 | TRS  | 6       | 0            |

## 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     | 455/466 (97%)   | 0.04   | 5 (1%) 78 79  | 16, 26, 46, 58        | 0     |
| 1   | B     | 463/466 (99%)   | -0.03  | 4 (0%) 81 82  | 16, 27, 47, 56        | 0     |
| 1   | C     | 454/466 (97%)   | -0.01  | 13 (2%) 53 56 | 13, 25, 47, 59        | 0     |
| 1   | D     | 454/466 (97%)   | -0.01  | 6 (1%) 75 76  | 16, 26, 45, 53        | 0     |
| 1   | E     | 463/466 (99%)   | -0.01  | 18 (3%) 43 45 | 14, 24, 51, 64        | 0     |
| 1   | F     | 454/466 (97%)   | -0.00  | 5 (1%) 78 79  | 14, 25, 45, 55        | 0     |
| All | All   | 2743/2796 (98%) | -0.00  | 51 (1%) 66 68 | 13, 26, 47, 64        | 0     |

All (51) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 13  | LEU  | 4.1  |
| 1   | E     | 12  | GLU  | 4.1  |
| 1   | C     | 415 | ALA  | 3.8  |
| 1   | E     | 28  | GLU  | 3.6  |
| 1   | C     | 115 | ASN  | 3.4  |
| 1   | F     | 115 | ASN  | 3.4  |
| 1   | E     | 310 | ILE  | 3.2  |
| 1   | E     | 115 | ASN  | 3.2  |
| 1   | D     | 305 | TYR  | 3.0  |
| 1   | C     | 414 | GLU  | 3.0  |
| 1   | E     | 23  | ILE  | 2.9  |
| 1   | F     | 27  | ALA  | 2.8  |
| 1   | E     | 305 | TYR  | 2.8  |
| 1   | E     | 11  | SER  | 2.8  |
| 1   | F     | 305 | TYR  | 2.8  |
| 1   | A     | 114 | LYS  | 2.7  |
| 1   | C     | 27  | ALA  | 2.7  |
| 1   | C     | 112 | ALA  | 2.6  |
| 1   | C     | 31  | ARG  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 7   | THR  | 2.6  |
| 1   | E     | 9   | LEU  | 2.6  |
| 1   | C     | 417 | ASP  | 2.5  |
| 1   | E     | 114 | LYS  | 2.5  |
| 1   | D     | 114 | LYS  | 2.5  |
| 1   | D     | 310 | ILE  | 2.5  |
| 1   | F     | 385 | GLY  | 2.5  |
| 1   | D     | 417 | ASP  | 2.4  |
| 1   | F     | 355 | ASP  | 2.4  |
| 1   | A     | 200 | GLU  | 2.4  |
| 1   | E     | 22  | SER  | 2.4  |
| 1   | E     | 200 | GLU  | 2.4  |
| 1   | C     | 413 | GLY  | 2.3  |
| 1   | A     | 27  | ALA  | 2.3  |
| 1   | C     | 144 | ARG  | 2.3  |
| 1   | D     | 115 | ASN  | 2.3  |
| 1   | E     | 303 | VAL  | 2.3  |
| 1   | D     | 116 | GLY  | 2.3  |
| 1   | B     | 413 | GLY  | 2.2  |
| 1   | B     | 416 | THR  | 2.2  |
| 1   | E     | 19  | GLY  | 2.2  |
| 1   | E     | 20  | ALA  | 2.2  |
| 1   | C     | 305 | TYR  | 2.2  |
| 1   | C     | 411 | LEU  | 2.2  |
| 1   | A     | 188 | PHE  | 2.2  |
| 1   | C     | 293 | GLU  | 2.2  |
| 1   | B     | 153 | ASP  | 2.1  |
| 1   | A     | 308 | GLY  | 2.1  |
| 1   | E     | 5   | GLN  | 2.1  |
| 1   | E     | 8   | ASP  | 2.1  |
| 1   | B     | 305 | TYR  | 2.0  |
| 1   | C     | 116 | GLY  | 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 ⓘ

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(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 3   | TRS  | B     | 3242 | 8/8   | 0.71 | 0.18 | 63,65,66,67                | 0     |
| 3   | TRS  | C     | 3252 | 8/8   | 0.73 | 0.23 | 54,54,54,55                | 0     |
| 3   | TRS  | E     | 3253 | 8/8   | 0.75 | 0.17 | 62,62,62,62                | 0     |
| 3   | TRS  | D     | 3244 | 8/8   | 0.78 | 0.20 | 58,58,59,59                | 0     |
| 3   | TRS  | C     | 3250 | 8/8   | 0.79 | 0.26 | 55,56,57,57                | 0     |
| 3   | TRS  | C     | 3243 | 8/8   | 0.79 | 0.19 | 58,60,60,60                | 0     |
| 3   | TRS  | F     | 3240 | 8/8   | 0.79 | 0.20 | 60,61,61,61                | 0     |
| 3   | TRS  | E     | 3246 | 8/8   | 0.82 | 0.15 | 48,51,51,53                | 0     |
| 3   | TRS  | F     | 3248 | 8/8   | 0.82 | 0.17 | 56,58,59,59                | 0     |
| 3   | TRS  | A     | 3251 | 8/8   | 0.83 | 0.20 | 48,49,50,51                | 0     |
| 3   | TRS  | A     | 3241 | 8/8   | 0.83 | 0.19 | 65,66,66,66                | 0     |
| 3   | TRS  | F     | 3249 | 8/8   | 0.84 | 0.18 | 60,60,60,61                | 0     |
| 3   | TRS  | D     | 3245 | 8/8   | 0.85 | 0.16 | 65,65,65,66                | 0     |
| 3   | TRS  | A     | 3236 | 8/8   | 0.85 | 0.20 | 64,64,65,65                | 0     |
| 3   | TRS  | E     | 3239 | 8/8   | 0.86 | 0.18 | 47,48,49,49                | 0     |
| 3   | TRS  | D     | 3238 | 8/8   | 0.86 | 0.17 | 54,55,55,56                | 0     |
| 3   | TRS  | E     | 3247 | 8/8   | 0.88 | 0.15 | 47,47,48,49                | 0     |
| 3   | TRS  | B     | 3237 | 8/8   | 0.90 | 0.21 | 73,73,74,74                | 0     |
| 2   | PLR  | F     | 1505 | 15/15 | 0.96 | 0.08 | 20,24,25,27                | 0     |
| 2   | PLR  | E     | 1504 | 15/15 | 0.97 | 0.07 | 17,21,22,22                | 0     |
| 2   | PLR  | A     | 1500 | 15/15 | 0.97 | 0.08 | 26,27,27,28                | 0     |
| 2   | PLR  | B     | 1501 | 15/15 | 0.97 | 0.07 | 23,24,26,26                | 0     |
| 2   | PLR  | D     | 1503 | 15/15 | 0.97 | 0.07 | 23,27,29,30                | 0     |
| 2   | PLR  | C     | 1502 | 15/15 | 0.98 | 0.06 | 18,22,22,23                | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.