



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:00 PM UTC

PDB ID : 5ORF / pdb\_00005orf  
Title : Structure of ovine serum albumin in P1 space group  
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Deposited on : 2017-08-16  
Resolution : 2.54 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

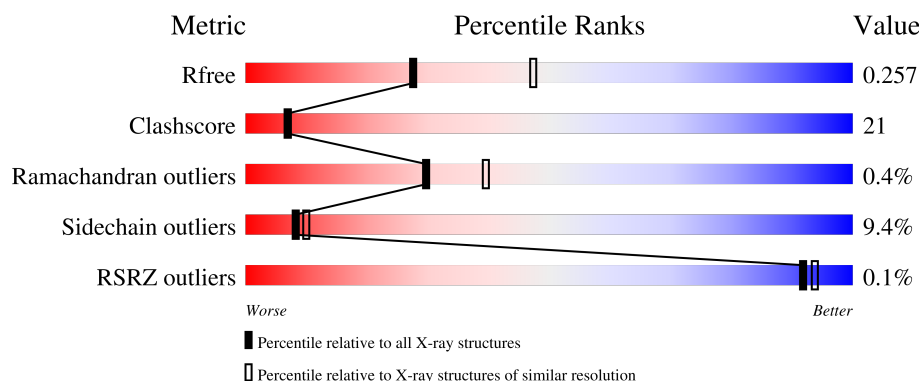
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.54 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                      | 1091 (2.54-2.54)                                      |
| Clashscore            | 190562                      | 1120 (2.54-2.54)                                      |
| Ramachandran outliers | 187476                      | 1106 (2.54-2.54)                                      |
| Sidechain outliers    | 187428                      | 1106 (2.54-2.54)                                      |
| RSRZ outliers         | 180081                      | 1091 (2.54-2.54)                                      |

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     | 583    | <div> <div>51%</div> <div>40%</div> <div>9%</div> </div>              |
| 1   | B     | 583    | <div> <div>57%</div> <div>37%</div> <div>6%</div> <div>•</div> </div> |
| 1   | C     | 583    | <div> <div>57%</div> <div>37%</div> <div>5%</div> <div>•</div> </div> |
| 1   | D     | 583    | <div> <div>51%</div> <div>39%</div> <div>9%</div> <div>•</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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 4   | PRO  | C     | 605 | -         | -        | X       | -                |
| 4   | PRO  | D     | 603 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

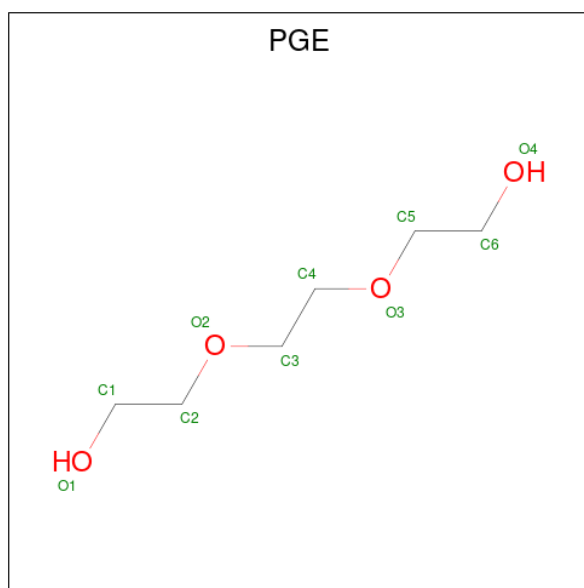
There are 5 unique types of molecules in this entry. The entry contains 19129 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Serum albumin.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 583      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4645  | 2933 | 780 | 893 | 39 |         |         |       |
| 1   | B     | 583      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4645  | 2933 | 780 | 893 | 39 |         |         |       |
| 1   | C     | 583      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4645  | 2933 | 780 | 893 | 39 |         |         |       |
| 1   | D     | 583      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4645  | 2933 | 780 | 893 | 39 |         |         |       |

- Molecule 2 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



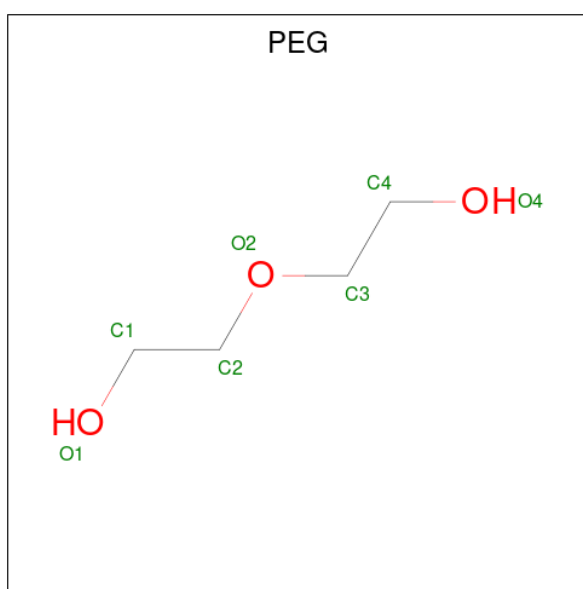
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 2   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |

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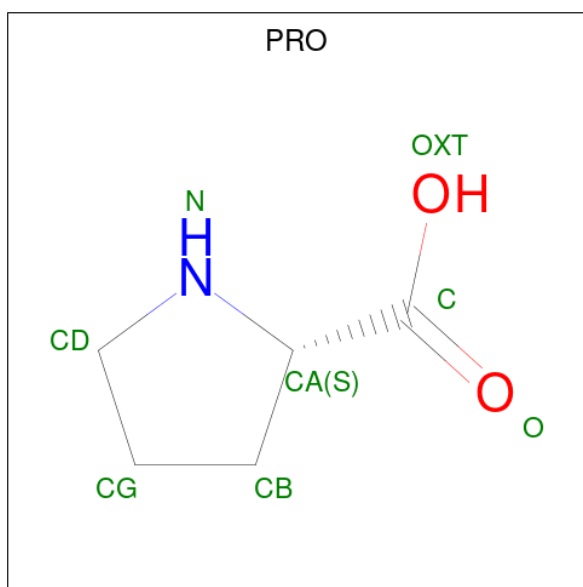
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 2   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 2   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 2   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 7     | 4 | 3 |         |         |
| 3   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 7     | 4 | 3 |         |         |

- Molecule 4 is PROLINE (CCD ID: PRO) (formula:  $C_5H_9NO_2$ ).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 4   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 5 | 1 | 2 |         |         |
| 4   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 5 | 1 | 2 |         |         |
| 4   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 5 | 1 | 2 |         |         |
| 4   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 5 | 1 | 2 |         |         |
| 4   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 5 | 1 | 2 |         |         |
| 4   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 5 | 1 | 2 |         |         |
| 4   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 5 | 1 | 2 |         |         |
| 4   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 5 | 1 | 2 |         |         |
| 4   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 5 | 1 | 2 |         |         |
| 4   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 5 | 1 | 2 |         |         |
| 4   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 5 | 1 | 2 |         |         |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5   | A     | 91       | Total | O  | 0       | 0       |
|     |       |          | 91    | 91 |         |         |

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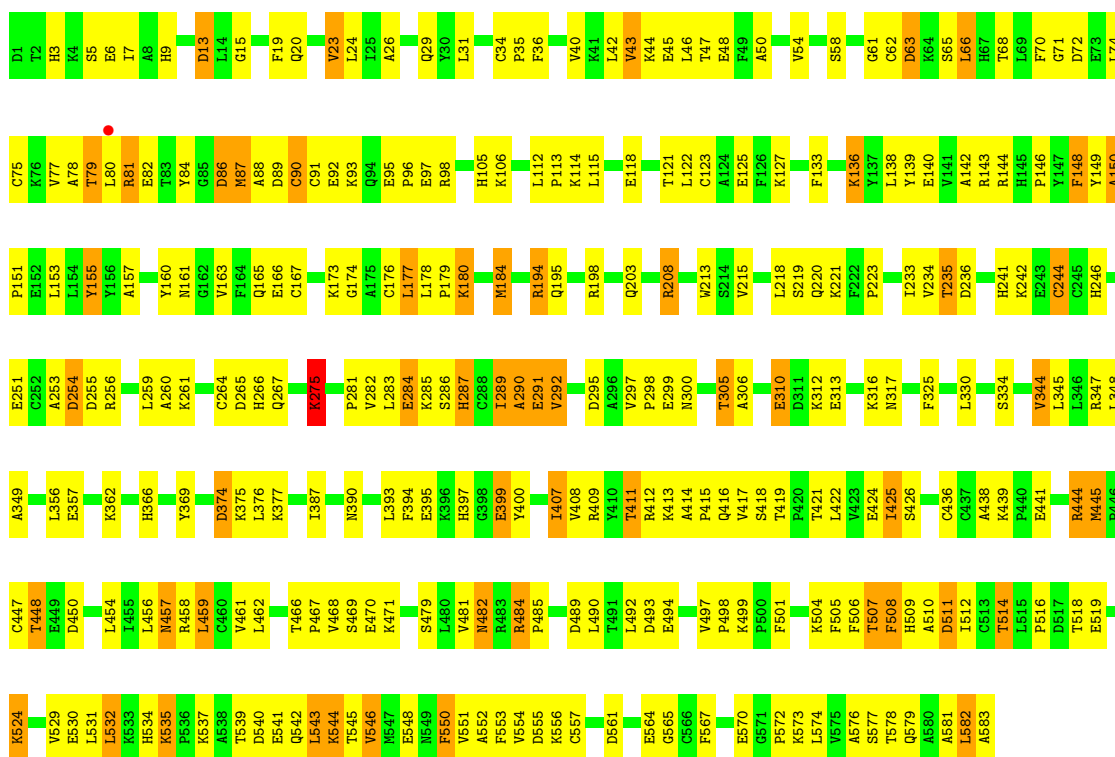
| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 5   | B     | 112      | Total<br>112 | O<br>112 | 0       | 0       |
| 5   | C     | 87       | Total<br>87  | O<br>87  | 0       | 0       |
| 5   | D     | 97       | Total<br>97  | O<br>97  | 0       | 0       |

### 3 Residue-property plots [i](#)

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: Serum albumin

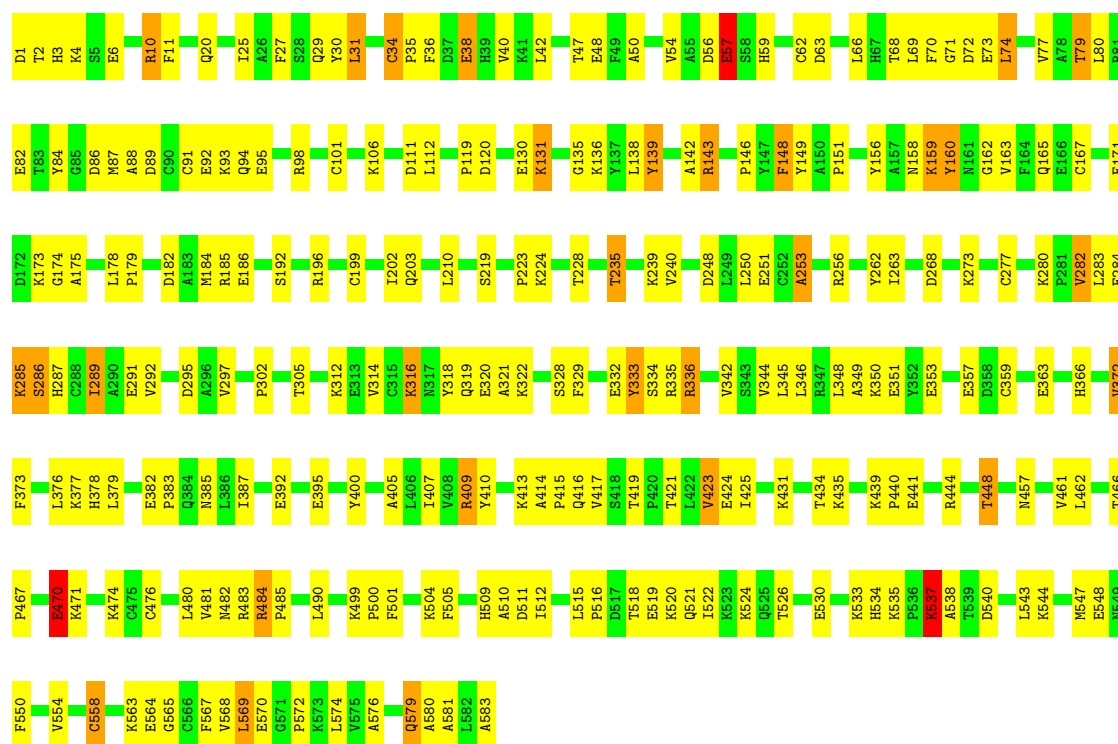
Chain A: 





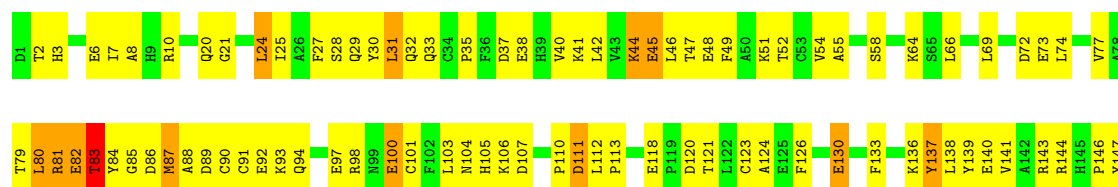
• Molecule 1: Serum albumin

Chain C: 57% 37% 5% •



• Molecule 1: Serum albumin

Chain D: 51% 39% 9% •



|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| H509 | A510 | D511 | I512 | C513 | T514 | L515 | P516 | E519 | S520 | K524 | Q525 | L528 | V529 | E530 | L531 | L532 | K533 | P536 | T539 | D540 | E541 | Q542 | L543 | K544 | T545 | V546 | M547 | E548 | N549 | F550 | F553 | V554 | D555 | K556 | C557 | C558 | D561 | D562 | K563 | E564 | G565 | C566 | L569 | E570 | G571 | P572 | K573 | L574 | A583 |      |      |
| R409 | Y410 | T411 | R412 | T419 | E424 | I425 | S426 | R427 | A438 | E441 | R444 | M445 | P446 | D450 | L454 | I455 | L456 | C460 | E464 | K465 | T466 | P467 | V468 | S469 | E470 | K471 | V472 | S479 | L480 | R484 | P485 | L490 | T491 | D493 | E494 | V497 | P498 | K499 | D502 | E503 | K504 | F505 | F508 |      |      |      |      |      |      |      |      |
| Y318 | D323 | V324 | F325 | L326 | F329 | S334 | A341 | K342 | S343 | V344 | L345 | R346 | R347 | L348 | A349 | K350 | C359 | K362 | E363 | D364 | F365 | H366 | A367 | C368 | F373 | L376 | K377 | H378 | E382 | P383 | Q384 | N385 | L386 | I387 | C391 | E392 | L393 | F394 | E395 | Y400 | G401 | F402 | Q403 | L406 | I407 | V408 |      |      |      |      |      |
| Q220 | P223 | K224 | T228 | D229 | V230 | T231 | T235 | D236 | K239 | K242 | E243 | C244 | C245 | H246 | G247 | D248 | L249 | L250 | E251 | R256 | L259 | A260 | Q267 | K275 | E276 | C277 | K280 | P281 | V282 | K285 | S286 | H287 | D293 | K294 | D295 | L301 | P302 | L303 | T305 | A306 | D307 | F308 | V314 | C315 |      |      |      |      |      |      |      |
| F148 | P151 | E152 | L153 | L154 | Y155 | Y156 | K159 | Y160 | Q165 | E166 | C167 | G168 | Q169 | K173 | G174 | A175 | C176 | L177 | L178 | P179 | K180 | M184 | K187 | V188 | L189 | A190 | S191 | A193 | R194 | Q195 | R196 | L197 | R198 | C199 | A200 | S201 | I202 | Q203 | K204 | F205 | G206 | E207 | K211 | A212 | W213 | S214 | V215 | A216 | R217 | L218 | S219 |

## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1                                                         | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 77.82Å 78.05Å 109.71Å<br>89.81° 74.54° 73.15°               | Depositor        |
| Resolution (Å)                                                          | 49.00 – 2.54<br>49.00 – 2.54                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 90.2 (49.00-2.54)<br>90.2 (49.00-2.54)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.09                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.85 (at 2.54Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.7.0032                                             | Depositor        |
| R, $R_{free}$                                                           | 0.196 , 0.258<br>0.194 , 0.257                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1414 reflections (1.81%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 48.1                                                        | Xtriage          |
| Anisotropy                                                              | 0.147                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 45.3                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                        | EDS              |
| Total number of atoms                                                   | 19129                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 54.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.15% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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     | 1.27         | 14/4742 (0.3%)  | 1.39        | 45/6402 (0.7%)   |
| 1   | B     | 1.26         | 10/4742 (0.2%)  | 1.40        | 41/6402 (0.6%)   |
| 1   | C     | 1.30         | 12/4742 (0.3%)  | 1.39        | 43/6402 (0.7%)   |
| 1   | D     | 1.33         | 20/4742 (0.4%)  | 1.44        | 48/6402 (0.7%)   |
| All | All   | 1.29         | 56/18968 (0.3%) | 1.41        | 177/25608 (0.7%) |

All (56) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | D     | 250 | LEU  | N-CA  | 7.98  | 1.55        | 1.46     |
| 1   | B     | 406 | LEU  | C-O   | -7.61 | 1.15        | 1.24     |
| 1   | D     | 219 | SER  | CA-C  | -7.33 | 1.42        | 1.52     |
| 1   | D     | 342 | VAL  | C-O   | -7.08 | 1.15        | 1.24     |
| 1   | C     | 31  | LEU  | CA-C  | -7.02 | 1.42        | 1.53     |
| 1   | C     | 409 | ARG  | CA-C  | -7.01 | 1.44        | 1.52     |
| 1   | A     | 148 | PHE  | C-O   | 6.70  | 1.31        | 1.23     |
| 1   | C     | 142 | ALA  | N-CA  | -6.68 | 1.37        | 1.46     |
| 1   | D     | 202 | ILE  | C-O   | -6.67 | 1.16        | 1.24     |
| 1   | A     | 26  | ALA  | N-CA  | 6.43  | 1.54        | 1.46     |
| 1   | C     | 139 | TYR  | CA-C  | 6.38  | 1.60        | 1.52     |
| 1   | D     | 235 | THR  | C-O   | -6.37 | 1.16        | 1.24     |
| 1   | A     | 161 | ASN  | C-O   | -6.33 | 1.16        | 1.24     |
| 1   | C     | 148 | PHE  | C-O   | 6.32  | 1.31        | 1.23     |
| 1   | B     | 142 | ALA  | C-O   | -6.32 | 1.16        | 1.24     |
| 1   | B     | 191 | SER  | C-O   | -6.27 | 1.16        | 1.24     |
| 1   | C     | 235 | THR  | C-O   | -5.93 | 1.17        | 1.24     |
| 1   | A     | 155 | TYR  | N-CA  | -5.84 | 1.39        | 1.46     |
| 1   | A     | 142 | ALA  | CA-C  | -5.82 | 1.45        | 1.52     |
| 1   | D     | 190 | ALA  | CA-C  | 5.74  | 1.59        | 1.52     |
| 1   | D     | 177 | LEU  | CA-C  | -5.74 | 1.46        | 1.53     |
| 1   | B     | 19  | PHE  | N-CA  | -5.72 | 1.39        | 1.46     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 150 | ALA  | N-CA  | 5.69  | 1.51        | 1.46     |
| 1   | B     | 340 | TYR  | CA-C  | -5.68 | 1.46        | 1.52     |
| 1   | D     | 325 | PHE  | N-CA  | -5.63 | 1.39        | 1.46     |
| 1   | A     | 194 | ARG  | CA-C  | 5.62  | 1.60        | 1.52     |
| 1   | D     | 191 | SER  | C-O   | -5.61 | 1.17        | 1.24     |
| 1   | D     | 554 | VAL  | N-CA  | -5.60 | 1.39        | 1.46     |
| 1   | B     | 157 | ALA  | CA-C  | 5.59  | 1.60        | 1.52     |
| 1   | A     | 136 | LYS  | C-O   | -5.55 | 1.16        | 1.24     |
| 1   | C     | 202 | ILE  | CA-C  | -5.53 | 1.46        | 1.52     |
| 1   | C     | 253 | ALA  | CA-C  | -5.53 | 1.45        | 1.52     |
| 1   | D     | 83  | THR  | CA-C  | 5.51  | 1.58        | 1.53     |
| 1   | C     | 467 | PRO  | C-O   | -5.50 | 1.17        | 1.23     |
| 1   | D     | 231 | THR  | C-O   | -5.44 | 1.17        | 1.24     |
| 1   | A     | 325 | PHE  | N-CA  | -5.42 | 1.39        | 1.46     |
| 1   | B     | 159 | LYS  | N-CA  | -5.42 | 1.39        | 1.46     |
| 1   | B     | 479 | SER  | C-O   | -5.38 | 1.17        | 1.24     |
| 1   | C     | 521 | GLN  | CA-C  | -5.33 | 1.46        | 1.52     |
| 1   | C     | 210 | LEU  | CA-C  | 5.33  | 1.59        | 1.52     |
| 1   | A     | 150 | ALA  | CA-CB | -5.32 | 1.46        | 1.53     |
| 1   | B     | 467 | PRO  | CA-C  | -5.32 | 1.46        | 1.52     |
| 1   | B     | 479 | SER  | CA-C  | -5.28 | 1.45        | 1.52     |
| 1   | A     | 46  | LEU  | CA-C  | -5.23 | 1.45        | 1.52     |
| 1   | D     | 193 | ALA  | N-CA  | -5.20 | 1.40        | 1.46     |
| 1   | D     | 236 | ASP  | N-CA  | -5.19 | 1.40        | 1.46     |
| 1   | A     | 457 | ASN  | N-CA  | -5.18 | 1.40        | 1.46     |
| 1   | D     | 546 | VAL  | N-CA  | -5.17 | 1.40        | 1.46     |
| 1   | A     | 177 | LEU  | CA-C  | -5.16 | 1.45        | 1.52     |
| 1   | D     | 147 | TYR  | N-CA  | 5.14  | 1.52        | 1.46     |
| 1   | D     | 256 | ARG  | CA-C  | 5.14  | 1.59        | 1.52     |
| 1   | A     | 543 | LEU  | N-CA  | 5.13  | 1.52        | 1.46     |
| 1   | D     | 424 | GLU  | N-CA  | -5.11 | 1.40        | 1.46     |
| 1   | D     | 530 | GLU  | CA-C  | -5.09 | 1.45        | 1.52     |
| 1   | C     | 160 | TYR  | CA-C  | 5.08  | 1.59        | 1.52     |
| 1   | D     | 513 | CYS  | CA-C  | -5.04 | 1.46        | 1.52     |

All (177) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | B     | 48  | GLU  | N-CA-C | -10.81 | 97.83       | 111.02   |
| 1   | D     | 497 | VAL  | CA-C-N | -10.49 | 108.70      | 119.92   |
| 1   | D     | 497 | VAL  | C-N-CA | -10.49 | 108.70      | 119.92   |
| 1   | A     | 118 | GLU  | CA-C-N | 9.86   | 129.49      | 119.24   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 118 | GLU  | C-N-CA | 9.86  | 129.49      | 119.24   |
| 1   | D     | 267 | GLN  | N-CA-C | 9.09  | 122.33      | 111.33   |
| 1   | C     | 302 | PRO  | CA-C-N | -8.77 | 111.00      | 119.85   |
| 1   | C     | 302 | PRO  | C-N-CA | -8.77 | 111.00      | 119.85   |
| 1   | B     | 381 | ASP  | N-CA-C | 8.52  | 120.64      | 111.36   |
| 1   | D     | 302 | PRO  | CA-C-N | -8.41 | 112.14      | 120.21   |
| 1   | D     | 302 | PRO  | C-N-CA | -8.41 | 112.14      | 120.21   |
| 1   | D     | 511 | ASP  | N-CA-C | -8.23 | 102.12      | 112.90   |
| 1   | D     | 133 | PHE  | N-CA-C | -8.18 | 102.34      | 111.82   |
| 1   | B     | 118 | GLU  | CA-C-N | 7.83  | 128.24      | 119.32   |
| 1   | B     | 118 | GLU  | C-N-CA | 7.83  | 128.24      | 119.32   |
| 1   | A     | 244 | CYS  | N-CA-C | -7.81 | 102.85      | 111.36   |
| 1   | D     | 445 | MET  | CA-C-N | -7.78 | 110.46      | 119.32   |
| 1   | D     | 445 | MET  | C-N-CA | -7.78 | 110.46      | 119.32   |
| 1   | C     | 484 | ARG  | CA-C-N | -7.77 | 110.95      | 119.19   |
| 1   | C     | 484 | ARG  | C-N-CA | -7.77 | 110.95      | 119.19   |
| 1   | C     | 10  | ARG  | N-CA-C | -7.77 | 102.72      | 112.90   |
| 1   | A     | 362 | LYS  | N-CA-C | -7.75 | 99.36       | 110.59   |
| 1   | D     | 178 | LEU  | CA-C-N | -7.70 | 111.02      | 119.19   |
| 1   | D     | 178 | LEU  | C-N-CA | -7.70 | 111.02      | 119.19   |
| 1   | B     | 178 | LEU  | CA-C-N | -7.70 | 110.45      | 118.85   |
| 1   | B     | 178 | LEU  | C-N-CA | -7.70 | 110.45      | 118.85   |
| 1   | C     | 228 | THR  | N-CA-C | -7.63 | 102.31      | 111.69   |
| 1   | C     | 400 | TYR  | N-CA-C | -7.57 | 102.72      | 110.97   |
| 1   | A     | 578 | THR  | N-CA-C | 7.43  | 119.03      | 111.07   |
| 1   | A     | 535 | LYS  | CA-C-N | 7.33  | 127.18      | 119.05   |
| 1   | A     | 535 | LYS  | C-N-CA | 7.33  | 127.18      | 119.05   |
| 1   | D     | 159 | LYS  | N-CA-C | -7.32 | 103.33      | 111.82   |
| 1   | D     | 174 | GLY  | N-CA-C | 7.31  | 121.74      | 112.83   |
| 1   | C     | 284 | GLU  | N-CA-C | -7.19 | 103.61      | 112.38   |
| 1   | D     | 364 | ASP  | CA-C-N | -7.08 | 112.41      | 119.56   |
| 1   | D     | 364 | ASP  | C-N-CA | -7.08 | 112.41      | 119.56   |
| 1   | D     | 444 | ARG  | N-CA-C | 7.02  | 118.72      | 111.14   |
| 1   | B     | 311 | ASP  | N-CA-C | 6.97  | 120.11      | 110.35   |
| 1   | B     | 425 | ILE  | N-CA-C | -6.81 | 103.84      | 110.72   |
| 1   | B     | 221 | LYS  | N-CA-C | -6.79 | 103.34      | 111.69   |
| 1   | B     | 41  | LYS  | N-CA-C | -6.76 | 103.84      | 111.14   |
| 1   | D     | 8   | ALA  | N-CA-C | -6.75 | 103.17      | 111.40   |
| 1   | B     | 284 | GLU  | N-CA-C | -6.65 | 104.42      | 112.54   |
| 1   | B     | 384 | GLN  | N-CA-C | -6.65 | 104.03      | 111.28   |
| 1   | C     | 143 | ARG  | N-CA-C | -6.58 | 104.18      | 111.82   |
| 1   | D     | 287 | HIS  | N-CA-C | 6.57  | 119.03      | 111.02   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | D     | 37  | ASP  | N-CA-C  | 6.55  | 118.07      | 111.07   |
| 1   | D     | 530 | GLU  | N-CA-C  | -6.50 | 104.83      | 112.89   |
| 1   | A     | 579 | GLN  | N-CA-C  | 6.47  | 118.21      | 111.03   |
| 1   | A     | 284 | GLU  | N-CA-C  | -6.46 | 104.23      | 111.28   |
| 1   | A     | 163 | VAL  | N-CA-C  | 6.46  | 116.62      | 110.42   |
| 1   | C     | 202 | ILE  | CB-CA-C | -6.46 | 103.71      | 111.97   |
| 1   | D     | 244 | CYS  | N-CA-C  | -6.46 | 103.75      | 111.69   |
| 1   | D     | 466 | THR  | CA-C-N  | -6.42 | 113.05      | 119.99   |
| 1   | D     | 466 | THR  | C-N-CA  | -6.42 | 113.05      | 119.99   |
| 1   | A     | 514 | THR  | N-CA-C  | 6.38  | 121.15      | 113.23   |
| 1   | D     | 301 | LEU  | N-CA-C  | -6.38 | 101.81      | 110.36   |
| 1   | C     | 101 | CYS  | N-CA-C  | 6.34  | 118.27      | 111.36   |
| 1   | B     | 87  | MET  | N-CA-C  | 6.34  | 117.78      | 107.32   |
| 1   | D     | 363 | GLU  | N-CA-C  | 6.33  | 118.19      | 111.28   |
| 1   | C     | 448 | THR  | CB-CA-C | -6.31 | 100.88      | 110.92   |
| 1   | D     | 525 | GLN  | N-CA-C  | -6.31 | 104.28      | 112.23   |
| 1   | C     | 569 | LEU  | N-CA-C  | 6.20  | 117.83      | 111.14   |
| 1   | C     | 79  | THR  | N-CA-C  | -6.19 | 105.59      | 113.02   |
| 1   | C     | 167 | CYS  | N-CA-C  | 6.14  | 121.70      | 113.72   |
| 1   | A     | 399 | GLU  | N-CA-C  | 6.09  | 117.61      | 110.97   |
| 1   | D     | 203 | GLN  | N-CA-C  | 6.04  | 117.67      | 111.14   |
| 1   | A     | 203 | GLN  | N-CA-C  | 6.03  | 119.02      | 111.24   |
| 1   | D     | 407 | ILE  | CB-CA-C | -6.03 | 104.16      | 111.88   |
| 1   | D     | 188 | VAL  | N-CA-C  | 6.00  | 116.78      | 110.72   |
| 1   | A     | 165 | GLN  | N-CA-C  | -5.99 | 104.33      | 111.69   |
| 1   | B     | 466 | THR  | CA-C-N  | -5.98 | 113.38      | 120.13   |
| 1   | B     | 466 | THR  | C-N-CA  | -5.98 | 113.38      | 120.13   |
| 1   | A     | 150 | ALA  | CA-C-N  | -5.96 | 113.04      | 119.24   |
| 1   | A     | 150 | ALA  | C-N-CA  | -5.96 | 113.04      | 119.24   |
| 1   | A     | 133 | PHE  | CA-C-N  | 5.94  | 128.16      | 120.44   |
| 1   | A     | 133 | PHE  | C-N-CA  | 5.94  | 128.16      | 120.44   |
| 1   | C     | 2   | THR  | N-CA-C  | 5.94  | 118.50      | 107.99   |
| 1   | D     | 137 | TYR  | N-CA-C  | -5.94 | 104.44      | 111.03   |
| 1   | B     | 332 | GLU  | N-CA-C  | -5.91 | 104.79      | 112.23   |
| 1   | D     | 100 | GLU  | N-CA-C  | -5.91 | 104.75      | 111.07   |
| 1   | A     | 275 | LYS  | N-CA-C  | 5.91  | 117.80      | 111.36   |
| 1   | A     | 511 | ASP  | N-CA-C  | -5.90 | 104.44      | 111.69   |
| 1   | D     | 199 | CYS  | N-CA-C  | 5.89  | 117.57      | 111.03   |
| 1   | C     | 537 | LYS  | N-CA-C  | -5.87 | 105.70      | 112.92   |
| 1   | B     | 275 | LYS  | N-CA-C  | 5.87  | 117.75      | 111.36   |
| 1   | C     | 377 | LYS  | N-CA-C  | 5.86  | 117.67      | 111.28   |
| 1   | A     | 255 | ASP  | N-CA-C  | 5.82  | 118.40      | 111.71   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | D     | 323 | ASP  | N-CA-C  | 5.73  | 117.53      | 111.28   |
| 1   | A     | 23  | VAL  | N-CA-C  | -5.73 | 105.14      | 110.53   |
| 1   | B     | 272 | SER  | N-CA-C  | -5.71 | 106.31      | 113.28   |
| 1   | D     | 141 | VAL  | CB-CA-C | -5.71 | 104.75      | 111.94   |
| 1   | D     | 282 | VAL  | N-CA-C  | 5.71  | 116.16      | 110.23   |
| 1   | C     | 372 | VAL  | N-CA-C  | 5.70  | 116.34      | 110.36   |
| 1   | C     | 359 | CYS  | N-CA-C  | 5.68  | 117.55      | 111.36   |
| 1   | B     | 28  | SER  | N-CA-C  | 5.67  | 118.19      | 111.33   |
| 1   | A     | 260 | ALA  | CA-C-N  | 5.66  | 128.13      | 120.65   |
| 1   | A     | 260 | ALA  | C-N-CA  | 5.66  | 128.13      | 120.65   |
| 1   | B     | 8   | ALA  | N-CA-C  | -5.63 | 105.15      | 111.28   |
| 1   | A     | 87  | MET  | N-CA-C  | 5.59  | 117.45      | 111.36   |
| 1   | B     | 84  | TYR  | N-CA-C  | 5.58  | 118.82      | 109.95   |
| 1   | C     | 48  | GLU  | N-CA-C  | -5.57 | 104.90      | 110.97   |
| 1   | C     | 235 | THR  | N-CA-C  | 5.55  | 117.77      | 111.11   |
| 1   | B     | 307 | ASP  | N-CA-C  | 5.55  | 120.17      | 112.90   |
| 1   | A     | 484 | ARG  | N-CA-C  | -5.54 | 104.92      | 112.35   |
| 1   | C     | 316 | LYS  | N-CA-C  | -5.52 | 105.27      | 112.23   |
| 1   | D     | 156 | TYR  | N-CA-C  | 5.51  | 117.36      | 111.36   |
| 1   | C     | 423 | VAL  | CB-CA-C | -5.50 | 104.82      | 112.02   |
| 1   | C     | 289 | ILE  | CB-CA-C | -5.49 | 104.95      | 111.81   |
| 1   | B     | 282 | VAL  | N-CA-C  | 5.48  | 120.73      | 109.34   |
| 1   | B     | 470 | GLU  | N-CA-C  | 5.47  | 116.92      | 111.07   |
| 1   | A     | 254 | ASP  | N-CA-C  | -5.46 | 104.55      | 111.11   |
| 1   | D     | 153 | LEU  | N-CA-C  | -5.46 | 105.40      | 111.36   |
| 1   | C     | 344 | VAL  | N-CA-C  | 5.45  | 115.65      | 110.42   |
| 1   | B     | 233 | ILE  | CB-CA-C | -5.44 | 104.72      | 112.22   |
| 1   | B     | 482 | ASN  | N-CA-C  | 5.43  | 119.90      | 113.16   |
| 1   | B     | 249 | LEU  | N-CA-C  | 5.41  | 116.86      | 111.07   |
| 1   | B     | 373 | PHE  | N-CA-C  | 5.40  | 117.86      | 111.33   |
| 1   | C     | 558 | CYS  | N-CA-C  | -5.39 | 106.20      | 112.89   |
| 1   | A     | 167 | CYS  | N-CA-C  | 5.39  | 119.91      | 113.23   |
| 1   | B     | 478 | GLU  | N-CA-C  | 5.37  | 117.21      | 111.36   |
| 1   | A     | 344 | VAL  | N-CA-CB | -5.35 | 104.29      | 110.55   |
| 1   | C     | 363 | GLU  | N-CA-C  | 5.35  | 116.92      | 111.14   |
| 1   | A     | 550 | PHE  | N-CA-C  | -5.34 | 105.54      | 111.36   |
| 1   | A     | 497 | VAL  | CA-C-N  | 5.32  | 125.32      | 119.89   |
| 1   | A     | 497 | VAL  | C-N-CA  | 5.32  | 125.32      | 119.89   |
| 1   | B     | 283 | LEU  | N-CA-C  | -5.29 | 106.33      | 112.89   |
| 1   | A     | 43  | VAL  | N-CA-C  | -5.29 | 105.24      | 111.00   |
| 1   | D     | 256 | ARG  | N-CA-C  | 5.28  | 116.72      | 111.07   |
| 1   | B     | 152 | GLU  | N-CA-C  | -5.28 | 105.69      | 111.82   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 565 | GLY  | N-CA-C  | -5.28 | 106.11      | 112.49   |
| 1   | C     | 297 | VAL  | N-CA-C  | 5.26  | 114.11      | 108.95   |
| 1   | D     | 87  | MET  | N-CA-C  | 5.26  | 117.02      | 111.28   |
| 1   | C     | 135 | GLY  | N-CA-C  | 5.24  | 119.01      | 112.73   |
| 1   | D     | 83  | THR  | CB-CA-C | -5.24 | 110.52      | 116.54   |
| 1   | A     | 567 | PHE  | N-CA-C  | -5.23 | 105.70      | 111.71   |
| 1   | D     | 499 | LYS  | N-CA-C  | -5.22 | 103.19      | 109.72   |
| 1   | C     | 185 | ARG  | N-CA-C  | -5.21 | 105.50      | 111.07   |
| 1   | C     | 253 | ALA  | N-CA-C  | -5.21 | 105.29      | 111.69   |
| 1   | B     | 86  | ASP  | N-CA-C  | 5.20  | 121.05      | 113.40   |
| 1   | B     | 497 | VAL  | CA-C-N  | 5.20  | 126.34      | 119.84   |
| 1   | B     | 497 | VAL  | C-N-CA  | 5.20  | 126.34      | 119.84   |
| 1   | C     | 470 | GLU  | N-CA-C  | -5.18 | 105.71      | 111.36   |
| 1   | B     | 469 | SER  | N-CA-C  | 5.18  | 117.40      | 109.07   |
| 1   | D     | 347 | ARG  | N-CA-C  | -5.17 | 105.56      | 111.14   |
| 1   | C     | 158 | ASN  | N-CA-C  | -5.17 | 105.73      | 111.36   |
| 1   | A     | 499 | LYS  | N-CA-C  | -5.17 | 103.27      | 109.83   |
| 1   | B     | 428 | SER  | N-CA-C  | 5.17  | 116.72      | 111.14   |
| 1   | C     | 353 | GLU  | N-CA-C  | -5.17 | 105.34      | 111.69   |
| 1   | C     | 68  | THR  | N-CA-CB | 5.16  | 117.80      | 110.16   |
| 1   | C     | 476 | CYS  | N-CA-C  | 5.16  | 118.68      | 112.38   |
| 1   | B     | 222 | PHE  | CA-C-N  | -5.16 | 114.51      | 119.87   |
| 1   | B     | 222 | PHE  | C-N-CA  | -5.16 | 114.51      | 119.87   |
| 1   | D     | 229 | ASP  | N-CA-C  | 5.15  | 116.58      | 111.07   |
| 1   | D     | 513 | CYS  | N-CA-C  | -5.14 | 107.18      | 113.50   |
| 1   | C     | 57  | GLU  | N-CA-C  | -5.14 | 106.27      | 112.54   |
| 1   | A     | 233 | ILE  | N-CA-C  | -5.14 | 105.59      | 110.42   |
| 1   | D     | 402 | PHE  | N-CA-C  | -5.13 | 106.18      | 112.90   |
| 1   | A     | 411 | THR  | N-CA-C  | -5.12 | 105.78      | 111.36   |
| 1   | B     | 305 | THR  | N-CA-C  | -5.12 | 105.39      | 111.69   |
| 1   | D     | 176 | CYS  | N-CA-CB | -5.12 | 102.57      | 110.20   |
| 1   | A     | 287 | HIS  | N-CA-C  | 5.12  | 117.25      | 111.11   |
| 1   | D     | 456 | LEU  | N-CA-C  | -5.08 | 105.93      | 111.82   |
| 1   | B     | 300 | ASN  | N-CA-C  | 5.08  | 118.25      | 111.24   |
| 1   | C     | 535 | LYS  | CA-C-N  | 5.08  | 126.19      | 119.84   |
| 1   | C     | 535 | LYS  | C-N-CA  | 5.08  | 126.19      | 119.84   |
| 1   | A     | 265 | ASP  | N-CA-C  | 5.07  | 117.47      | 111.33   |
| 1   | D     | 214 | SER  | N-CA-C  | -5.05 | 105.86      | 111.36   |
| 1   | C     | 171 | GLU  | CA-C-N  | -5.04 | 115.45      | 123.12   |
| 1   | C     | 171 | GLU  | C-N-CA  | -5.04 | 115.45      | 123.12   |
| 1   | C     | 149 | TYR  | N-CA-C  | -5.04 | 102.18      | 109.59   |
| 1   | A     | 184 | MET  | N-CA-C  | 5.03  | 116.58      | 111.14   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 235 | THR  | N-CA-C | 5.03  | 117.16      | 111.02   |
| 1   | A     | 66  | LEU  | N-CA-C | 5.03  | 116.76      | 111.28   |
| 1   | B     | 372 | VAL  | N-CA-C | 5.03  | 115.64      | 110.36   |
| 1   | A     | 259 | LEU  | N-CA-C | -5.02 | 105.90      | 112.23   |
| 1   | A     | 508 | PHE  | N-CA-C | 5.00  | 117.41      | 109.50   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 4645  | 0        | 4548     | 217     | 0            |
| 1   | B     | 4645  | 0        | 4548     | 169     | 0            |
| 1   | C     | 4645  | 0        | 4548     | 180     | 0            |
| 1   | D     | 4645  | 0        | 4552     | 223     | 0            |
| 2   | A     | 20    | 0        | 28       | 1       | 0            |
| 2   | B     | 10    | 0        | 14       | 3       | 0            |
| 2   | C     | 20    | 0        | 28       | 9       | 0            |
| 2   | D     | 10    | 0        | 14       | 3       | 0            |
| 3   | A     | 7     | 0        | 10       | 0       | 0            |
| 3   | C     | 7     | 0        | 10       | 0       | 0            |
| 4   | A     | 24    | 0        | 21       | 4       | 0            |
| 4   | B     | 24    | 0        | 21       | 1       | 0            |
| 4   | C     | 24    | 0        | 21       | 9       | 0            |
| 4   | D     | 16    | 0        | 14       | 6       | 0            |
| 5   | A     | 91    | 0        | 0        | 8       | 0            |
| 5   | B     | 112   | 0        | 0        | 14      | 0            |
| 5   | C     | 87    | 0        | 0        | 5       | 0            |
| 5   | D     | 97    | 0        | 0        | 4       | 0            |
| All | All   | 19129 | 0        | 18377    | 782     | 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 21.

All (782) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:33:GLN:N     | 1:D:84:TYR:OH    | 1.66                     | 1.25              |
| 1:C:174:GLY:H    | 4:C:605:PRO:HB3  | 1.12                     | 1.12              |
| 1:C:409:ARG:HH21 | 2:C:601:PGE:H22  | 1.11                     | 1.10              |
| 1:D:79:THR:HB    | 1:D:83:THR:CG2   | 1.82                     | 1.10              |
| 1:D:79:THR:HB    | 1:D:83:THR:HG23  | 1.17                     | 1.08              |
| 1:D:248:ASP:HB3  | 1:D:251:GLU:HG2  | 1.42                     | 0.99              |
| 1:D:46:LEU:HD21  | 1:D:73:GLU:HG3   | 1.43                     | 0.99              |
| 1:D:86:ASP:HB2   | 1:D:105:HIS:CD2  | 1.98                     | 0.99              |
| 1:C:174:GLY:N    | 4:C:605:PRO:HB3  | 1.79                     | 0.96              |
| 1:C:1:ASP:HB3    | 1:C:3:HIS:HE1    | 1.31                     | 0.96              |
| 1:C:409:ARG:NH2  | 2:C:601:PGE:H22  | 1.80                     | 0.95              |
| 1:C:547:MET:HE1  | 2:C:602:PGE:O4   | 1.68                     | 0.94              |
| 1:D:557:CYS:HG   | 1:D:566:CYS:HG   | 1.15                     | 0.94              |
| 1:D:86:ASP:HB2   | 1:D:105:HIS:HD2  | 1.31                     | 0.93              |
| 1:A:577:SER:O    | 1:A:581:ALA:HB3  | 1.67                     | 0.92              |
| 1:C:383:PRO:O    | 1:C:387:ILE:HG12 | 1.70                     | 0.92              |
| 1:D:409:ARG:HB2  | 4:D:603:PRO:HG3  | 1.53                     | 0.90              |
| 1:B:383:PRO:O    | 1:B:387:ILE:HG13 | 1.72                     | 0.90              |
| 1:D:79:THR:CB    | 1:D:83:THR:HG23  | 2.03                     | 0.87              |
| 1:A:387:ILE:HG12 | 1:A:448:THR:HG21 | 1.57                     | 0.87              |
| 1:D:77:VAL:O     | 1:D:79:THR:HG23  | 1.74                     | 0.87              |
| 1:C:289:ILE:O    | 1:C:292:VAL:HG12 | 1.75                     | 0.85              |
| 1:C:20:GLN:HE21  | 1:C:47:THR:HG21  | 1.41                     | 0.85              |
| 1:C:35:PRO:HG2   | 1:C:38:GLU:HG2   | 1.58                     | 0.85              |
| 1:D:100:GLU:HG3  | 1:D:101:CYS:N    | 1.91                     | 0.85              |
| 1:B:93:LYS:HG2   | 1:B:94:GLN:H     | 1.39                     | 0.85              |
| 1:A:289:ILE:O    | 1:A:292:VAL:HG12 | 1.77                     | 0.85              |
| 1:D:33:GLN:H     | 1:D:84:TYR:HH    | 0.89                     | 0.85              |
| 1:C:86:ASP:O     | 1:C:89:ASP:HB2   | 1.76                     | 0.84              |
| 1:C:564:GLU:O    | 1:C:568:VAL:HG23 | 1.76                     | 0.84              |
| 1:C:29:GLN:HG2   | 1:C:146:PRO:HA   | 1.60                     | 0.84              |
| 1:D:197:LEU:O    | 1:D:201:SER:OG   | 1.96                     | 0.83              |
| 1:A:74:LEU:C     | 1:A:74:LEU:HD23  | 2.04                     | 0.83              |
| 1:D:508:PHE:HE2  | 1:D:550:PHE:HE2  | 1.22                     | 0.83              |
| 1:A:544:LYS:O    | 1:A:548:GLU:HG3  | 1.79                     | 0.82              |
| 1:A:421:THR:HG23 | 1:A:462:LEU:HD13 | 1.62                     | 0.82              |
| 1:A:208:ARG:HG3  | 1:D:130:GLU:OE2  | 1.80                     | 0.82              |
| 1:C:50:ALA:O     | 1:C:54:VAL:HG23  | 1.80                     | 0.81              |
| 1:D:508:PHE:HE2  | 1:D:550:PHE:CE2  | 1.98                     | 0.81              |
| 1:D:508:PHE:CE2  | 1:D:550:PHE:CE2  | 2.69                     | 0.81              |
| 1:A:484:ARG:HB3  | 1:A:485:PRO:HD3  | 1.62                     | 0.81              |
| 1:D:86:ASP:CB    | 1:D:105:HIS:CD2  | 2.64                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:550:PHE:HD1  | 1:C:574:LEU:HD11 | 1.47                     | 0.80              |
| 1:D:74:LEU:O     | 1:D:77:VAL:HG12  | 1.81                     | 0.80              |
| 1:A:494:GLU:OE2  | 1:A:537:LYS:NZ   | 2.13                     | 0.80              |
| 1:C:470:GLU:CD   | 1:C:470:GLU:H    | 1.90                     | 0.80              |
| 1:C:1:ASP:HB3    | 1:C:3:HIS:CE1    | 2.17                     | 0.79              |
| 1:C:409:ARG:HG3  | 2:C:602:PGE:H1   | 1.65                     | 0.79              |
| 1:A:267:GLN:OE1  | 1:A:275:LYS:HD3  | 1.83                     | 0.79              |
| 1:D:275:LYS:HG2  | 1:D:276:GLU:H    | 1.47                     | 0.79              |
| 1:D:86:ASP:CB    | 1:D:105:HIS:HD2  | 1.96                     | 0.78              |
| 1:A:306:ALA:HB2  | 4:A:606:PRO:HD3  | 1.64                     | 0.77              |
| 1:D:275:LYS:HD3  | 1:D:275:LYS:H    | 1.49                     | 0.77              |
| 1:B:386:LEU:HD11 | 5:B:785:HOH:O    | 1.84                     | 0.76              |
| 1:B:251:GLU:CD   | 1:B:251:GLU:H    | 1.93                     | 0.76              |
| 1:C:174:GLY:H    | 4:C:605:PRO:CB   | 1.95                     | 0.76              |
| 1:B:140:GLU:OE1  | 1:B:143:ARG:HD3  | 1.85                     | 0.76              |
| 1:D:80:LEU:C     | 1:D:82:GLU:H     | 1.90                     | 0.76              |
| 1:A:411:THR:HG21 | 1:A:532:LEU:HB3  | 1.68                     | 0.75              |
| 1:D:31:LEU:HA    | 1:D:84:TYR:HE2   | 1.52                     | 0.74              |
| 1:B:315:CYS:O    | 1:B:319:GLN:HB2  | 1.87                     | 0.74              |
| 1:D:77:VAL:HG13  | 1:D:79:THR:CG2   | 2.17                     | 0.74              |
| 1:B:276:GLU:HG3  | 1:B:277:CYS:H    | 1.51                     | 0.74              |
| 1:D:386:LEU:HD21 | 2:D:601:PGE:H42  | 1.69                     | 0.74              |
| 1:B:471:LYS:O    | 1:B:474:LYS:HB3  | 1.87                     | 0.73              |
| 1:D:504:LYS:HE2  | 1:D:505:PHE:CE1  | 2.21                     | 0.73              |
| 1:B:126:PHE:CE1  | 1:B:130:GLU:HG3  | 2.24                     | 0.73              |
| 1:D:30:TYR:HE1   | 1:D:103:LEU:HD23 | 1.54                     | 0.73              |
| 1:C:547:MET:CE   | 2:C:602:PGE:O4   | 2.37                     | 0.73              |
| 1:C:515:LEU:HB3  | 1:C:519:GLU:HB2  | 1.71                     | 0.72              |
| 1:D:40:VAL:O     | 1:D:44:LYS:HG3   | 1.89                     | 0.72              |
| 1:B:289:ILE:HG22 | 1:B:290:ALA:N    | 2.02                     | 0.72              |
| 1:A:74:LEU:HD23  | 1:A:74:LEU:O     | 1.90                     | 0.72              |
| 1:B:101:CYS:SG   | 1:B:105:HIS:HE1  | 2.12                     | 0.72              |
| 1:A:72:ASP:HA    | 5:A:738:HOH:O    | 1.89                     | 0.72              |
| 1:B:90:CYS:HB2   | 1:B:102:PHE:CE1  | 2.25                     | 0.72              |
| 1:C:93:LYS:HG2   | 1:C:94:GLN:H     | 1.54                     | 0.71              |
| 1:D:41:LYS:O     | 1:D:45:GLU:HG2   | 1.90                     | 0.71              |
| 1:A:330:LEU:HD13 | 1:A:349:ALA:HB2  | 1.71                     | 0.71              |
| 1:B:267:GLN:OE1  | 1:B:275:LYS:HG3  | 1.90                     | 0.71              |
| 1:D:160:TYR:HA   | 1:D:184:MET:HE1  | 1.72                     | 0.71              |
| 1:A:48:GLU:OE1   | 1:A:48:GLU:HA    | 1.91                     | 0.70              |
| 1:B:90:CYS:SG    | 1:B:105:HIS:HE1  | 2.15                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:93:LYS:CG    | 1:B:94:GLN:H     | 2.03                     | 0.70              |
| 1:B:57:GLU:HG2   | 5:B:783:HOH:O    | 1.90                     | 0.70              |
| 1:B:16:GLU:O     | 1:B:20:GLN:HG3   | 1.91                     | 0.70              |
| 1:B:148:PHE:CD1  | 1:B:153:LEU:HB2  | 2.26                     | 0.70              |
| 1:A:550:PHE:CD1  | 1:A:574:LEU:HD21 | 2.26                     | 0.70              |
| 1:D:248:ASP:HB3  | 1:D:251:GLU:CG   | 2.18                     | 0.70              |
| 1:B:484:ARG:HB3  | 1:B:485:PRO:HD3  | 1.72                     | 0.69              |
| 1:D:33:GLN:HG3   | 1:D:84:TYR:HE1   | 1.56                     | 0.69              |
| 1:D:343:SER:OG   | 1:D:450:ASP:OD1  | 2.07                     | 0.69              |
| 1:A:357:GLU:OE1  | 1:A:357:GLU:HA   | 1.93                     | 0.69              |
| 1:B:267:GLN:OE1  | 1:B:275:LYS:HE3  | 1.92                     | 0.69              |
| 1:B:415:PRO:HD2  | 1:B:416:GLN:NE2  | 2.08                     | 0.69              |
| 1:A:576:ALA:HA   | 4:A:604:PRO:O    | 1.91                     | 0.69              |
| 1:C:66:LEU:HD13  | 1:C:250:LEU:HD12 | 1.74                     | 0.69              |
| 1:B:86:ASP:O     | 1:B:87:MET:HG2   | 1.93                     | 0.68              |
| 1:D:84:TYR:HB3   | 1:D:105:HIS:CE1  | 2.29                     | 0.68              |
| 1:C:84:TYR:HB3   | 1:C:87:MET:HE2   | 1.74                     | 0.68              |
| 1:C:405:ALA:HA   | 2:C:602:PGE:H32  | 1.74                     | 0.68              |
| 1:C:471:LYS:HE3  | 1:C:490:LEU:HD22 | 1.76                     | 0.68              |
| 1:C:550:PHE:CD1  | 1:C:574:LEU:HD11 | 2.29                     | 0.68              |
| 1:D:251:GLU:H    | 1:D:251:GLU:CD   | 2.02                     | 0.68              |
| 1:B:64:LYS:HD2   | 1:B:68:THR:HG21  | 1.75                     | 0.67              |
| 1:B:90:CYS:SG    | 1:B:105:HIS:CE1  | 2.88                     | 0.67              |
| 1:A:577:SER:O    | 1:A:581:ALA:CB   | 2.42                     | 0.67              |
| 1:B:302:PRO:HA   | 4:B:604:PRO:OXT  | 1.94                     | 0.67              |
| 1:C:439:LYS:O    | 1:C:444:ARG:NH2  | 2.26                     | 0.67              |
| 1:B:519:GLU:OE2  | 1:B:519:GLU:HA   | 1.93                     | 0.66              |
| 1:C:569:LEU:HB3  | 1:C:570:GLU:OE1  | 1.95                     | 0.66              |
| 1:A:42:LEU:HA    | 1:A:45:GLU:OE1   | 1.95                     | 0.66              |
| 1:A:531:LEU:HD21 | 1:A:546:VAL:HG11 | 1.76                     | 0.66              |
| 1:D:275:LYS:HG2  | 1:D:276:GLU:N    | 2.11                     | 0.66              |
| 1:D:411:THR:HG21 | 1:D:532:LEU:HB2  | 1.78                     | 0.66              |
| 1:D:471:LYS:HE2  | 1:D:490:LEU:HD22 | 1.76                     | 0.66              |
| 1:C:520:LYS:O    | 1:C:524:LYS:HG3  | 1.96                     | 0.65              |
| 1:D:409:ARG:CB   | 4:D:603:PRO:HG3  | 2.25                     | 0.65              |
| 1:A:413:LYS:HD3  | 1:A:490:LEU:HB2  | 1.78                     | 0.65              |
| 1:A:509:HIS:HB2  | 1:A:511:ASP:OD1  | 1.96                     | 0.65              |
| 1:C:174:GLY:CA   | 4:C:605:PRO:HB3  | 2.25                     | 0.65              |
| 1:A:484:ARG:HB3  | 1:A:485:PRO:CD   | 2.26                     | 0.65              |
| 1:B:507:THR:C    | 1:B:508:PHE:CD2  | 2.74                     | 0.65              |
| 1:B:318:TYR:OH   | 1:B:322:LYS:HE3  | 1.96                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:282:VAL:HG12 | 5:C:739:HOH:O    | 1.96                     | 0.64              |
| 1:A:31:LEU:CD2   | 1:A:87:MET:HE2   | 2.27                     | 0.64              |
| 1:D:508:PHE:CE2  | 1:D:550:PHE:HE2  | 2.07                     | 0.64              |
| 1:C:84:TYR:CB    | 1:C:87:MET:CE    | 2.75                     | 0.64              |
| 1:C:119:PRO:HB2  | 4:C:605:PRO:HD3  | 1.80                     | 0.64              |
| 1:C:30:TYR:CD2   | 1:C:74:LEU:HD11  | 2.32                     | 0.64              |
| 1:B:507:THR:C    | 1:B:508:PHE:HD2  | 2.06                     | 0.64              |
| 1:B:543:LEU:O    | 1:B:547:MET:HG3  | 1.97                     | 0.64              |
| 1:C:71:GLY:C     | 1:C:98:ARG:NH2   | 2.55                     | 0.64              |
| 1:D:30:TYR:C     | 1:D:31:LEU:HD23  | 2.23                     | 0.64              |
| 1:A:441:GLU:HA   | 1:A:444:ARG:HB2  | 1.78                     | 0.64              |
| 1:B:140:GLU:OE1  | 1:B:144:ARG:NH2  | 2.31                     | 0.64              |
| 1:D:33:GLN:N     | 1:D:84:TYR:HH    | 1.72                     | 0.64              |
| 1:B:36:PHE:HB2   | 1:B:139:TYR:CE2  | 2.33                     | 0.64              |
| 1:A:282:VAL:O    | 1:A:285:LYS:HB3  | 1.98                     | 0.63              |
| 1:C:71:GLY:HA3   | 1:C:98:ARG:CZ    | 2.28                     | 0.63              |
| 1:C:516:PRO:HG2  | 1:C:519:GLU:HG2  | 1.80                     | 0.63              |
| 1:A:149:TYR:OH   | 1:A:256:ARG:HD2  | 1.98                     | 0.63              |
| 1:A:148:PHE:CD1  | 1:A:153:LEU:HB2  | 2.34                     | 0.63              |
| 1:C:328:SER:O    | 1:C:332:GLU:HG2  | 1.99                     | 0.63              |
| 1:D:93:LYS:O     | 1:D:98:ARG:HD3   | 1.99                     | 0.63              |
| 1:B:160:TYR:HB2  | 1:B:184:MET:HE1  | 1.81                     | 0.62              |
| 1:D:77:VAL:HG13  | 1:D:79:THR:HG23  | 1.80                     | 0.62              |
| 1:D:203:GLN:HA   | 1:D:203:GLN:OE1  | 1.99                     | 0.62              |
| 1:A:5:SER:CB     | 1:A:62:CYS:O     | 2.47                     | 0.62              |
| 1:A:160:TYR:HB2  | 1:A:184:MET:HE1  | 1.81                     | 0.62              |
| 1:A:81:ARG:O     | 1:A:84:TYR:HD2   | 1.82                     | 0.62              |
| 1:A:223:PRO:HD2  | 1:A:295:ASP:HB3  | 1.82                     | 0.62              |
| 1:C:416:GLN:OE1  | 1:C:416:GLN:N    | 2.27                     | 0.62              |
| 1:C:151:PRO:HG3  | 1:C:253:ALA:HA   | 1.81                     | 0.62              |
| 1:C:34:CYS:H     | 1:C:84:TYR:HH    | 1.47                     | 0.62              |
| 1:C:120:ASP:OD1  | 4:C:605:PRO:N    | 2.33                     | 0.62              |
| 1:D:24:LEU:HD12  | 1:D:28:SER:OG    | 1.99                     | 0.62              |
| 1:A:20:GLN:HE21  | 1:A:47:THR:HG21  | 1.64                     | 0.61              |
| 1:C:382:GLU:OE1  | 1:C:383:PRO:HD3  | 2.00                     | 0.61              |
| 1:A:15:GLY:O     | 1:A:19:PHE:HB2   | 1.99                     | 0.61              |
| 1:A:264:CYS:O    | 1:A:267:GLN:HG2  | 2.00                     | 0.61              |
| 1:C:415:PRO:O    | 1:C:533:LYS:HE3  | 2.00                     | 0.61              |
| 1:D:277:CYS:O    | 1:D:285:LYS:HG3  | 2.00                     | 0.61              |
| 1:A:504:LYS:HE3  | 1:A:505:PHE:CE2  | 2.35                     | 0.61              |
| 1:C:414:ALA:O    | 1:C:417:VAL:HG23 | 2.00                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:374:ASP:N    | 1:A:374:ASP:OD1  | 2.33                     | 0.61              |
| 1:A:530:GLU:HA   | 1:A:530:GLU:OE1  | 1.99                     | 0.61              |
| 1:C:156:TYR:O    | 1:C:184:MET:HE1  | 2.00                     | 0.61              |
| 1:A:281:PRO:HG2  | 1:A:284:GLU:HG3  | 1.82                     | 0.61              |
| 1:C:38:GLU:OE1   | 1:C:38:GLU:HA    | 2.01                     | 0.61              |
| 1:B:332:GLU:OE1  | 1:B:336:ARG:NH2  | 2.34                     | 0.61              |
| 1:C:421:THR:O    | 1:C:425:ILE:HG12 | 2.01                     | 0.60              |
| 1:D:33:GLN:CA    | 1:D:84:TYR:OH    | 2.49                     | 0.60              |
| 1:D:79:THR:CB    | 1:D:83:THR:CG2   | 2.71                     | 0.60              |
| 1:A:375:LYS:HD3  | 1:A:375:LYS:C    | 2.27                     | 0.60              |
| 1:D:246:HIS:O    | 1:D:246:HIS:ND1  | 2.35                     | 0.60              |
| 1:A:31:LEU:HD21  | 1:A:87:MET:HE2   | 1.83                     | 0.60              |
| 1:A:471:LYS:HD2  | 1:A:493:ASP:OD2  | 2.01                     | 0.60              |
| 1:D:445:MET:O    | 1:D:446:PRO:C    | 2.40                     | 0.60              |
| 1:B:516:PRO:HB2  | 5:B:718:HOH:O    | 2.01                     | 0.60              |
| 1:D:409:ARG:HD3  | 2:D:601:PGE:H6   | 1.84                     | 0.60              |
| 1:B:351:GLU:HB3  | 1:B:376:LEU:HD22 | 1.83                     | 0.60              |
| 1:B:289:ILE:O    | 1:B:292:VAL:HG12 | 2.02                     | 0.60              |
| 1:B:56:ASP:HB3   | 5:B:790:HOH:O    | 2.00                     | 0.59              |
| 1:A:194:ARG:HA   | 1:A:454:LEU:HD22 | 1.84                     | 0.59              |
| 1:B:225:ALA:HB2  | 1:B:270:LEU:HD23 | 1.85                     | 0.59              |
| 1:D:382:GLU:OE1  | 1:D:383:PRO:HD3  | 2.01                     | 0.59              |
| 1:D:547:MET:HG2  | 5:D:780:HOH:O    | 2.01                     | 0.59              |
| 1:D:550:PHE:CE2  | 1:D:574:LEU:HD21 | 2.38                     | 0.59              |
| 1:A:140:GLU:HA   | 1:A:143:ARG:HD3  | 1.84                     | 0.59              |
| 1:B:276:GLU:HG3  | 1:B:277:CYS:N    | 2.17                     | 0.59              |
| 1:B:298:PRO:HB2  | 1:B:301:LEU:HD21 | 1.84                     | 0.59              |
| 1:B:421:THR:HG23 | 1:B:462:LEU:HD12 | 1.84                     | 0.59              |
| 1:C:84:TYR:CG    | 1:C:87:MET:CE    | 2.85                     | 0.59              |
| 1:C:395:GLU:OE1  | 1:C:395:GLU:HA   | 2.02                     | 0.59              |
| 1:D:148:PHE:CD1  | 1:D:153:LEU:HB2  | 2.37                     | 0.59              |
| 1:B:251:GLU:CD   | 1:B:251:GLU:N    | 2.60                     | 0.59              |
| 1:C:581:ALA:O    | 1:C:583:ALA:O    | 2.21                     | 0.59              |
| 1:A:289:ILE:HG22 | 1:A:290:ALA:N    | 2.18                     | 0.58              |
| 1:C:20:GLN:NE2   | 1:C:47:THR:HG21  | 2.17                     | 0.58              |
| 1:C:89:ASP:O     | 1:C:92:GLU:N     | 2.32                     | 0.58              |
| 1:D:304:LEU:O    | 1:D:306:ALA:N    | 2.37                     | 0.58              |
| 1:B:450:ASP:O    | 1:B:454:LEU:HG   | 2.03                     | 0.58              |
| 1:D:391:CYS:O    | 1:D:395:GLU:HG2  | 2.02                     | 0.58              |
| 1:B:90:CYS:CB    | 1:B:102:PHE:CE1  | 2.86                     | 0.58              |
| 1:C:173:LYS:HB2  | 4:C:605:PRO:HA   | 1.86                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:580:ALA:O    | 1:C:583:ALA:HB3  | 2.03                     | 0.58              |
| 1:B:46:LEU:O     | 1:B:50:ALA:N     | 2.34                     | 0.58              |
| 1:B:112:LEU:HB3  | 1:B:113:PRO:HD2  | 1.86                     | 0.58              |
| 1:C:84:TYR:CB    | 1:C:87:MET:HE2   | 2.33                     | 0.58              |
| 1:C:501:PHE:CD2  | 1:C:579:GLN:NE2  | 2.72                     | 0.58              |
| 1:B:90:CYS:HB2   | 1:B:102:PHE:HE1  | 1.66                     | 0.58              |
| 1:A:86:ASP:OD2   | 1:A:86:ASP:N     | 2.36                     | 0.58              |
| 1:A:253:ALA:O    | 1:A:254:ASP:C    | 2.45                     | 0.58              |
| 1:C:329:PHE:CE2  | 1:C:349:ALA:HA   | 2.39                     | 0.58              |
| 1:D:33:GLN:HG3   | 1:D:84:TYR:CE1   | 2.38                     | 0.58              |
| 1:D:33:GLN:CG    | 1:D:84:TYR:HE1   | 2.16                     | 0.58              |
| 1:D:69:LEU:O     | 1:D:73:GLU:HG2   | 2.04                     | 0.58              |
| 1:A:539:THR:HG22 | 1:A:541:GLU:H    | 1.68                     | 0.57              |
| 1:D:572:PRO:O    | 1:D:573:LYS:C    | 2.46                     | 0.57              |
| 1:C:316:LYS:O    | 1:C:320:GLU:HG2  | 2.04                     | 0.57              |
| 1:A:61:GLY:C     | 1:A:63:ASP:H     | 2.10                     | 0.57              |
| 1:C:84:TYR:CG    | 1:C:87:MET:HE1   | 2.38                     | 0.57              |
| 1:C:219:SER:HB2  | 1:C:334:SER:HB2  | 1.87                     | 0.57              |
| 1:D:38:GLU:O     | 1:D:42:LEU:HG    | 2.05                     | 0.57              |
| 1:D:173:LYS:O    | 1:D:177:LEU:HD13 | 2.02                     | 0.57              |
| 1:A:471:LYS:HE2  | 1:A:490:LEU:HD22 | 1.84                     | 0.57              |
| 1:D:419:THR:HG23 | 1:D:529:VAL:HG11 | 1.85                     | 0.57              |
| 1:B:44:LYS:HG3   | 1:B:45:GLU:HG3   | 1.86                     | 0.57              |
| 1:C:273:LYS:HD2  | 1:C:295:ASP:HA   | 1.85                     | 0.57              |
| 1:B:508:PHE:CD2  | 1:B:508:PHE:N    | 2.71                     | 0.57              |
| 1:B:470:GLU:CD   | 1:B:470:GLU:H    | 2.12                     | 0.56              |
| 1:D:259:LEU:HD12 | 1:D:259:LEU:O    | 2.05                     | 0.56              |
| 1:D:33:GLN:CG    | 1:D:84:TYR:CE1   | 2.88                     | 0.56              |
| 1:D:167:CYS:HB3  | 1:D:177:LEU:HD12 | 1.87                     | 0.56              |
| 1:A:138:LEU:HD21 | 1:A:157:ALA:HB2  | 1.87                     | 0.56              |
| 1:B:81:ARG:HA    | 1:B:88:ALA:HB2   | 1.88                     | 0.56              |
| 1:C:31:LEU:HD22  | 1:C:80:LEU:HD22  | 1.86                     | 0.56              |
| 1:D:25:ILE:HD11  | 1:D:138:LEU:HD22 | 1.87                     | 0.56              |
| 1:D:450:ASP:O    | 1:D:454:LEU:HG   | 2.05                     | 0.56              |
| 1:D:228:THR:O    | 1:D:231:THR:HB   | 2.05                     | 0.56              |
| 1:C:84:TYR:CD1   | 1:C:87:MET:HE1   | 2.41                     | 0.56              |
| 1:D:86:ASP:O     | 1:D:89:ASP:OD2   | 2.22                     | 0.56              |
| 1:C:466:THR:O    | 1:C:466:THR:HG23 | 2.05                     | 0.56              |
| 1:D:531:LEU:HD11 | 1:D:546:VAL:HG11 | 1.87                     | 0.56              |
| 1:C:484:ARG:HB3  | 1:C:485:PRO:HD3  | 1.86                     | 0.56              |
| 1:A:82:GLU:HA    | 1:A:88:ALA:HB2   | 1.88                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:415:PRO:O    | 1:B:533:LYS:HE2  | 2.06                     | 0.56              |
| 1:C:554:VAL:O    | 1:C:558:CYS:HB2  | 2.06                     | 0.56              |
| 1:A:150:ALA:O    | 1:A:151:PRO:C    | 2.47                     | 0.55              |
| 1:D:77:VAL:O     | 1:D:77:VAL:HG13  | 2.06                     | 0.55              |
| 1:A:79:THR:HG23  | 1:A:91:CYS:SG    | 2.46                     | 0.55              |
| 1:A:407:ILE:HG12 | 1:A:426:SER:HB3  | 1.88                     | 0.55              |
| 1:D:293:ASP:OD1  | 1:D:294:LYS:N    | 2.39                     | 0.55              |
| 1:D:304:LEU:O    | 1:D:305:THR:C    | 2.49                     | 0.55              |
| 1:A:139:TYR:O    | 1:A:143:ARG:HG2  | 2.05                     | 0.55              |
| 1:B:366:HIS:HA   | 1:B:369:TYR:CZ   | 2.41                     | 0.55              |
| 1:C:4:LYS:HZ3    | 1:C:57:GLU:HB3   | 1.72                     | 0.55              |
| 1:B:106:LYS:HG2  | 1:B:146:PRO:HB2  | 1.87                     | 0.55              |
| 1:A:299:GLU:OE1  | 1:A:299:GLU:HA   | 2.05                     | 0.55              |
| 1:A:400:TYR:OH   | 1:A:524:LYS:NZ   | 2.35                     | 0.55              |
| 1:D:239:LYS:O    | 1:D:243:GLU:HG3  | 2.06                     | 0.55              |
| 1:C:434:THR:O    | 1:D:561:ASP:HB2  | 2.06                     | 0.55              |
| 1:D:97:GLU:O     | 1:D:100:GLU:HG2  | 2.07                     | 0.55              |
| 1:B:531:LEU:HD11 | 1:B:582:LEU:HD11 | 1.87                     | 0.54              |
| 1:C:80:LEU:HB2   | 1:C:88:ALA:HB2   | 1.89                     | 0.54              |
| 1:D:47:THR:O     | 1:D:51:LYS:HG3   | 2.06                     | 0.54              |
| 1:A:84:TYR:CD1   | 1:A:87:MET:HG3   | 2.42                     | 0.54              |
| 1:B:139:TYR:O    | 1:B:143:ARG:HG2  | 2.06                     | 0.54              |
| 1:B:216:ALA:O    | 1:B:220:GLN:HG3  | 2.07                     | 0.54              |
| 1:C:256:ARG:CZ   | 1:C:286:SER:HB2  | 2.38                     | 0.54              |
| 1:D:350:LYS:NZ   | 1:D:479:SER:OG   | 2.40                     | 0.54              |
| 1:B:59:HIS:HB2   | 5:B:790:HOH:O    | 2.06                     | 0.54              |
| 1:B:470:GLU:CD   | 1:B:470:GLU:N    | 2.65                     | 0.54              |
| 1:A:261:LYS:O    | 1:A:264:CYS:N    | 2.40                     | 0.54              |
| 1:B:147:TYR:O    | 1:B:148:PHE:C    | 2.48                     | 0.54              |
| 1:A:306:ALA:HA   | 1:A:310:GLU:CD   | 2.33                     | 0.54              |
| 1:A:177:LEU:O    | 1:A:180:LYS:N    | 2.41                     | 0.54              |
| 1:B:184:MET:O    | 1:B:188:VAL:HG23 | 2.08                     | 0.54              |
| 1:D:386:LEU:HG   | 2:D:601:PGE:H3   | 1.88                     | 0.54              |
| 1:D:406:LEU:HD23 | 1:D:409:ARG:HD2  | 1.90                     | 0.54              |
| 1:A:24:LEU:HB2   | 1:A:43:VAL:HG21  | 1.89                     | 0.54              |
| 1:B:112:LEU:CD1  | 1:B:143:ARG:HE   | 2.21                     | 0.54              |
| 1:B:415:PRO:HD2  | 1:B:416:GLN:HE22 | 1.72                     | 0.54              |
| 1:D:223:PRO:HD2  | 1:D:295:ASP:HB3  | 1.89                     | 0.54              |
| 1:B:84:TYR:O     | 1:B:86:ASP:N     | 2.39                     | 0.53              |
| 1:B:508:PHE:HD2  | 1:B:508:PHE:N    | 2.07                     | 0.53              |
| 1:D:412:ARG:NH1  | 4:D:603:PRO:OXT  | 2.41                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:408:VAL:HG12 | 5:B:772:HOH:O    | 2.09                     | 0.53              |
| 1:B:501:PHE:HB2  | 1:B:534:HIS:CE1  | 2.44                     | 0.53              |
| 1:C:130:GLU:OE1  | 1:C:165:GLN:NE2  | 2.41                     | 0.53              |
| 1:C:348:LEU:HD23 | 1:C:379:LEU:HD12 | 1.91                     | 0.53              |
| 1:B:542:GLN:NE2  | 1:B:581:ALA:O    | 2.41                     | 0.53              |
| 1:D:304:LEU:C    | 1:D:306:ALA:N    | 2.64                     | 0.53              |
| 1:A:424:GLU:HG2  | 1:A:425:ILE:HD13 | 1.88                     | 0.53              |
| 1:A:582:LEU:N    | 1:A:582:LEU:HD12 | 2.24                     | 0.53              |
| 1:B:112:LEU:HD13 | 1:B:143:ARG:NH2  | 2.23                     | 0.53              |
| 1:B:414:ALA:O    | 1:B:417:VAL:HG23 | 2.08                     | 0.53              |
| 1:C:378:HIS:CE1  | 1:C:379:LEU:HG   | 2.43                     | 0.53              |
| 1:D:54:VAL:HG12  | 1:D:54:VAL:O     | 2.09                     | 0.53              |
| 1:A:471:LYS:HE2  | 1:A:490:LEU:CD2  | 2.38                     | 0.53              |
| 1:B:400:TYR:CE1  | 1:B:521:GLN:HG2  | 2.43                     | 0.53              |
| 1:B:428:SER:HB3  | 1:B:455:ILE:HG12 | 1.90                     | 0.53              |
| 1:C:419:THR:O    | 1:C:423:VAL:HG23 | 2.09                     | 0.53              |
| 1:D:112:LEU:HB3  | 1:D:113:PRO:HD2  | 1.91                     | 0.53              |
| 1:B:260:ALA:HB1  | 1:B:285:LYS:HD2  | 1.91                     | 0.53              |
| 1:A:86:ASP:HB3   | 1:A:105:HIS:CD2  | 2.44                     | 0.53              |
| 1:B:281:PRO:HG2  | 1:B:284:GLU:HB2  | 1.90                     | 0.53              |
| 1:C:94:GLN:O     | 1:C:98:ARG:N     | 2.40                     | 0.53              |
| 1:D:156:TYR:HE1  | 1:D:187:LYS:HD2  | 1.74                     | 0.53              |
| 1:A:45:GLU:O     | 1:A:48:GLU:HB2   | 2.09                     | 0.53              |
| 1:A:256:ARG:NH1  | 5:A:709:HOH:O    | 2.39                     | 0.53              |
| 1:C:148:PHE:CE2  | 1:C:192:SER:HB2  | 2.44                     | 0.53              |
| 1:D:106:LYS:HG2  | 1:D:146:PRO:HB2  | 1.91                     | 0.53              |
| 1:C:71:GLY:C     | 1:C:98:ARG:HH22  | 2.17                     | 0.52              |
| 1:C:409:ARG:O    | 1:C:413:LYS:HG3  | 2.10                     | 0.52              |
| 1:D:24:LEU:HD11  | 1:D:139:TYR:HB2  | 1.90                     | 0.52              |
| 1:D:194:ARG:HA   | 1:D:454:LEU:HD22 | 1.90                     | 0.52              |
| 1:C:256:ARG:NH2  | 5:C:705:HOH:O    | 2.41                     | 0.52              |
| 1:A:5:SER:HB3    | 1:A:62:CYS:O     | 2.08                     | 0.52              |
| 1:C:174:GLY:HA3  | 4:C:605:PRO:HB3  | 1.91                     | 0.52              |
| 1:D:438:ALA:HB3  | 5:D:732:HOH:O    | 2.10                     | 0.52              |
| 1:A:377:LYS:HE2  | 5:A:780:HOH:O    | 2.08                     | 0.52              |
| 1:C:329:PHE:HE2  | 1:C:349:ALA:HA   | 1.75                     | 0.52              |
| 1:A:3:HIS:ND1    | 1:A:6:GLU:OE2    | 2.43                     | 0.52              |
| 1:C:511:ASP:O    | 1:C:515:LEU:HG   | 2.10                     | 0.52              |
| 1:C:576:ALA:HA   | 5:C:716:HOH:O    | 2.09                     | 0.52              |
| 1:B:416:GLN:CD   | 1:B:416:GLN:H    | 2.17                     | 0.52              |
| 1:C:159:LYS:O    | 1:C:160:TYR:C    | 2.53                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:376:LEU:O    | 1:C:379:LEU:HB2  | 2.09                     | 0.52              |
| 1:D:304:LEU:C    | 1:D:306:ALA:H    | 2.18                     | 0.52              |
| 1:A:112:LEU:HB3  | 1:A:113:PRO:HD2  | 1.92                     | 0.52              |
| 1:D:82:GLU:C     | 1:D:83:THR:OG1   | 2.53                     | 0.52              |
| 1:B:402:PHE:CZ   | 2:B:601:PGE:H6   | 2.45                     | 0.52              |
| 1:D:213:TRP:CE2  | 1:D:342:VAL:HG11 | 2.45                     | 0.52              |
| 1:D:528:LEU:O    | 1:D:532:LEU:CD2  | 2.57                     | 0.52              |
| 1:A:412:ARG:O    | 1:A:492:LEU:HA   | 2.10                     | 0.52              |
| 1:B:501:PHE:CG   | 1:B:502:ASP:N    | 2.78                     | 0.52              |
| 1:D:318:TYR:HE1  | 1:D:326:LEU:HD11 | 1.74                     | 0.52              |
| 1:A:282:VAL:HG13 | 1:A:283:LEU:N    | 2.24                     | 0.51              |
| 1:A:106:LYS:HG2  | 1:A:146:PRO:HB2  | 1.91                     | 0.51              |
| 1:A:555:ASP:O    | 1:A:557:CYS:N    | 2.43                     | 0.51              |
| 1:B:221:LYS:NZ   | 1:B:290:ALA:O    | 2.44                     | 0.51              |
| 1:B:484:ARG:HB3  | 1:B:485:PRO:CD   | 2.41                     | 0.51              |
| 1:C:84:TYR:HB3   | 1:C:87:MET:CE    | 2.40                     | 0.51              |
| 1:C:174:GLY:O    | 1:C:178:LEU:HB2  | 2.11                     | 0.51              |
| 1:A:50:ALA:O     | 1:A:54:VAL:HG23  | 2.10                     | 0.51              |
| 1:A:93:LYS:HE2   | 1:A:97:GLU:CD    | 2.35                     | 0.51              |
| 1:C:251:GLU:OE1  | 1:C:251:GLU:N    | 2.35                     | 0.51              |
| 1:A:539:THR:HG22 | 1:A:541:GLU:N    | 2.26                     | 0.51              |
| 1:A:511:ASP:CG   | 1:B:175:ALA:HA   | 2.35                     | 0.51              |
| 1:D:359:CYS:HA   | 1:D:362:LYS:HG3  | 1.93                     | 0.51              |
| 1:A:219:SER:HB2  | 1:A:334:SER:HB2  | 1.93                     | 0.51              |
| 1:B:71:GLY:O     | 1:B:75:CYS:N     | 2.41                     | 0.51              |
| 1:B:220:GLN:O    | 1:B:223:PRO:HD3  | 2.10                     | 0.51              |
| 1:A:438:ALA:HB3  | 5:B:768:HOH:O    | 2.09                     | 0.51              |
| 1:C:224:LYS:NZ   | 1:C:268:ASP:O    | 2.33                     | 0.51              |
| 1:C:277:CYS:HA   | 1:C:280:LYS:HD2  | 1.92                     | 0.51              |
| 1:A:540:ASP:HA   | 1:A:543:LEU:HD12 | 1.93                     | 0.51              |
| 1:D:148:PHE:CE1  | 1:D:153:LEU:HB2  | 2.46                     | 0.50              |
| 1:B:33:GLN:OE1   | 1:B:112:LEU:HD21 | 2.11                     | 0.50              |
| 1:A:572:PRO:O    | 1:A:573:LYS:C    | 2.54                     | 0.50              |
| 1:A:489:ASP:O    | 1:A:490:LEU:C    | 2.53                     | 0.50              |
| 1:C:4:LYS:NZ     | 1:C:57:GLU:HB3   | 2.27                     | 0.50              |
| 1:C:38:GLU:OE1   | 1:C:38:GLU:CA    | 2.59                     | 0.50              |
| 1:D:528:LEU:O    | 1:D:532:LEU:HD22 | 2.11                     | 0.50              |
| 1:A:507:THR:CG2  | 1:A:509:HIS:CE1  | 2.95                     | 0.50              |
| 1:D:556:LYS:NZ   | 1:D:570:GLU:HG3  | 2.26                     | 0.50              |
| 1:B:314:VAL:HG12 | 1:B:315:CYS:N    | 2.25                     | 0.50              |
| 1:C:482:ASN:C    | 1:C:485:PRO:HD2  | 2.37                     | 0.50              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:61:GLY:C    | 1:A:63:ASP:N     | 2.70                     | 0.50              |
| 1:D:42:LEU:HA   | 1:D:45:GLU:CG    | 2.42                     | 0.50              |
| 1:D:469:SER:OG  | 1:D:472:VAL:HG23 | 2.11                     | 0.50              |
| 1:A:444:ARG:O   | 1:A:447:CYS:HB3  | 2.12                     | 0.50              |
| 1:B:451:TYR:O   | 1:B:455:ILE:HD12 | 2.11                     | 0.50              |
| 1:C:63:ASP:OD2  | 1:C:63:ASP:N     | 2.36                     | 0.49              |
| 1:A:256:ARG:CZ  | 1:A:286:SER:HB3  | 2.41                     | 0.49              |
| 1:B:517:ASP:O   | 1:B:518:THR:C    | 2.54                     | 0.49              |
| 1:C:199:CYS:O   | 1:C:203:GLN:HB2  | 2.12                     | 0.49              |
| 1:A:140:GLU:O   | 1:A:144:ARG:NH1  | 2.44                     | 0.49              |
| 1:B:166:GLU:O   | 1:B:169:GLN:HG3  | 2.12                     | 0.49              |
| 1:B:413:LYS:HB3 | 1:B:490:LEU:HB3  | 1.95                     | 0.49              |
| 1:C:470:GLU:CD  | 1:C:470:GLU:N    | 2.66                     | 0.49              |
| 1:D:69:LEU:O    | 1:D:73:GLU:CG    | 2.60                     | 0.49              |
| 1:D:72:ASP:OD1  | 1:D:73:GLU:HG2   | 2.13                     | 0.49              |
| 1:A:195:GLN:O   | 1:A:195:GLN:HG3  | 2.10                     | 0.49              |
| 1:A:458:ARG:O   | 1:A:459:LEU:C    | 2.55                     | 0.49              |
| 1:A:545:THR:CG2 | 1:A:582:LEU:HD21 | 2.42                     | 0.49              |
| 1:B:195:GLN:O   | 1:B:195:GLN:HG3  | 2.12                     | 0.49              |
| 1:B:535:LYS:HD2 | 5:B:801:HOH:O    | 2.12                     | 0.49              |
| 1:B:562:ASP:OD2 | 1:B:565:GLY:HA3  | 2.13                     | 0.49              |
| 1:C:70:PHE:O    | 1:C:74:LEU:HG    | 2.13                     | 0.49              |
| 1:D:27:PHE:HE1  | 1:D:42:LEU:HB3   | 1.78                     | 0.49              |
| 1:D:539:THR:OG1 | 1:D:542:GLN:HG3  | 2.12                     | 0.49              |
| 1:B:22:LEU:HG   | 1:B:154:LEU:HD11 | 1.94                     | 0.49              |
| 1:B:24:LEU:HD21 | 1:B:36:PHE:HE1   | 1.77                     | 0.49              |
| 1:C:36:PHE:HB2  | 1:C:139:TYR:CE2  | 2.47                     | 0.49              |
| 1:C:160:TYR:O   | 1:C:163:VAL:HB   | 2.11                     | 0.49              |
| 1:C:544:LYS:HA  | 1:C:547:MET:CE   | 2.41                     | 0.49              |
| 1:A:84:TYR:CG   | 1:A:87:MET:HG3   | 2.47                     | 0.49              |
| 1:A:95:GLU:HA   | 1:A:96:PRO:HA    | 1.59                     | 0.49              |
| 1:A:390:ASN:OD1 | 1:A:409:ARG:NH1  | 2.44                     | 0.49              |
| 1:A:138:LEU:CD2 | 1:A:157:ALA:HB2  | 2.43                     | 0.49              |
| 1:D:100:GLU:HG3 | 1:D:101:CYS:H    | 1.69                     | 0.49              |
| 1:B:230:VAL:O   | 1:B:234:VAL:HG23 | 2.12                     | 0.49              |
| 1:C:56:ASP:HB3  | 5:C:776:HOH:O    | 2.13                     | 0.49              |
| 1:C:540:ASP:O   | 1:C:543:LEU:HB2  | 2.12                     | 0.49              |
| 1:D:126:PHE:HZ  | 1:D:165:GLN:HG3  | 1.77                     | 0.49              |
| 1:A:20:GLN:NE2  | 1:A:47:THR:HG21  | 2.27                     | 0.49              |
| 1:A:77:VAL:HG13 | 1:A:78:ALA:H     | 1.78                     | 0.49              |
| 1:B:101:CYS:SG  | 1:B:105:HIS:CE1  | 3.01                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:141:VAL:O    | 1:B:145:HIS:HD2  | 1.95                     | 0.49              |
| 1:D:213:TRP:CD1  | 1:D:213:TRP:C    | 2.90                     | 0.49              |
| 1:C:162:GLY:O    | 1:C:165:GLN:HB2  | 2.13                     | 0.48              |
| 1:A:345:LEU:HA   | 1:A:348:LEU:HD12 | 1.95                     | 0.48              |
| 1:A:82:GLU:CA    | 1:A:88:ALA:HB2   | 2.43                     | 0.48              |
| 1:A:421:THR:O    | 1:A:422:LEU:C    | 2.54                     | 0.48              |
| 1:C:11:PHE:CD1   | 1:C:54:VAL:HG21  | 2.48                     | 0.48              |
| 1:C:160:TYR:HB2  | 1:C:184:MET:HE1  | 1.94                     | 0.48              |
| 1:D:403:GLN:HG2  | 1:D:427:ARG:HA   | 1.95                     | 0.48              |
| 1:A:419:THR:HG23 | 1:A:529:VAL:HG11 | 1.96                     | 0.48              |
| 1:A:516:PRO:HG2  | 1:A:519:GLU:CG   | 2.44                     | 0.48              |
| 1:A:235:THR:HG22 | 1:A:236:ASP:OD1  | 2.13                     | 0.48              |
| 1:A:501:PHE:HD2  | 1:A:534:HIS:CD2  | 2.31                     | 0.48              |
| 1:A:550:PHE:O    | 1:A:554:VAL:HG23 | 2.13                     | 0.48              |
| 4:A:606:PRO:HD2  | 5:A:747:HOH:O    | 2.13                     | 0.48              |
| 1:B:553:PHE:CZ   | 1:B:567:PHE:CD1  | 3.01                     | 0.48              |
| 1:D:3:HIS:N      | 1:D:6:GLU:OE2    | 2.46                     | 0.48              |
| 1:D:156:TYR:CE1  | 1:D:187:LYS:HD2  | 2.47                     | 0.48              |
| 1:A:347:ARG:HG2  | 1:A:481:VAL:CG1  | 2.44                     | 0.48              |
| 1:C:66:LEU:CD1   | 1:C:250:LEU:HD12 | 2.42                     | 0.48              |
| 1:C:182:ASP:O    | 1:C:186:GLU:HG2  | 2.14                     | 0.48              |
| 1:D:81:ARG:HB3   | 1:D:81:ARG:CZ    | 2.43                     | 0.48              |
| 1:D:204:LYS:NZ   | 1:D:464:GLU:HG3  | 2.28                     | 0.48              |
| 1:A:555:ASP:O    | 1:A:556:LYS:C    | 2.57                     | 0.48              |
| 1:C:131:LYS:HD2  | 1:C:131:LYS:C    | 2.39                     | 0.48              |
| 1:A:347:ARG:HG2  | 1:A:481:VAL:HG12 | 1.95                     | 0.48              |
| 1:C:510:ALA:HA   | 1:C:567:PHE:CE2  | 2.48                     | 0.48              |
| 1:D:498:PRO:HG3  | 1:D:536:PRO:HG2  | 1.94                     | 0.48              |
| 1:A:507:THR:HG22 | 1:A:509:HIS:CE1  | 2.49                     | 0.48              |
| 1:A:510:ALA:HB3  | 1:B:179:PRO:HB3  | 1.96                     | 0.48              |
| 1:B:561:ASP:OD1  | 1:B:561:ASP:N    | 2.45                     | 0.48              |
| 1:D:387:ILE:HD11 | 1:D:445:MET:HG3  | 1.95                     | 0.48              |
| 1:C:289:ILE:O    | 1:C:292:VAL:CG1  | 2.55                     | 0.48              |
| 1:A:393:LEU:HD12 | 1:A:397:HIS:ND1  | 2.29                     | 0.47              |
| 1:C:6:GLU:OE2    | 1:C:10:ARG:NE    | 2.47                     | 0.47              |
| 1:D:100:GLU:CG   | 1:D:101:CYS:N    | 2.71                     | 0.47              |
| 1:D:348:LEU:CD2  | 1:D:376:LEU:HB3  | 2.44                     | 0.47              |
| 1:A:74:LEU:C     | 1:A:74:LEU:CD2   | 2.76                     | 0.47              |
| 1:A:127:LYS:HD2  | 1:A:127:LYS:O    | 2.14                     | 0.47              |
| 1:B:139:TYR:OH   | 1:B:143:ARG:NH1  | 2.47                     | 0.47              |
| 1:B:367:ALA:O    | 1:B:368:CYS:C    | 2.56                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:25:ILE:HD11  | 1:C:138:LEU:HD22 | 1.95                     | 0.47              |
| 1:C:372:VAL:HG13 | 1:C:373:PHE:N    | 2.28                     | 0.47              |
| 1:D:549:ASN:HB3  | 5:D:758:HOH:O    | 2.14                     | 0.47              |
| 1:B:504:LYS:HE2  | 5:B:775:HOH:O    | 2.14                     | 0.47              |
| 1:C:42:LEU:HD22  | 1:C:73:GLU:HB3   | 1.95                     | 0.47              |
| 1:D:25:ILE:HD13  | 1:D:153:LEU:HD23 | 1.97                     | 0.47              |
| 1:D:348:LEU:HD22 | 1:D:376:LEU:HB3  | 1.96                     | 0.47              |
| 1:A:155:TYR:CD2  | 1:A:155:TYR:C    | 2.92                     | 0.47              |
| 1:B:113:PRO:O    | 1:B:144:ARG:NH1  | 2.48                     | 0.47              |
| 1:C:457:ASN:O    | 1:C:461:VAL:HG13 | 2.13                     | 0.47              |
| 1:D:558:CYS:O    | 1:D:563:LYS:HE3  | 2.14                     | 0.47              |
| 1:A:289:ILE:O    | 1:A:290:ALA:C    | 2.57                     | 0.47              |
| 1:B:409:ARG:NH2  | 2:B:601:PGE:H22  | 2.30                     | 0.47              |
| 1:C:59:HIS:HB3   | 1:C:62:CYS:SG    | 2.54                     | 0.47              |
| 1:C:289:ILE:C    | 1:C:291:GLU:H    | 2.22                     | 0.47              |
| 1:C:36:PHE:HB2   | 1:C:139:TYR:CD2  | 2.50                     | 0.47              |
| 1:A:29:GLN:HG2   | 1:A:146:PRO:HA   | 1.97                     | 0.47              |
| 1:A:35:PRO:HA    | 1:A:139:TYR:OH   | 2.15                     | 0.47              |
| 1:A:44:LYS:O     | 1:A:48:GLU:N     | 2.48                     | 0.47              |
| 1:A:531:LEU:HD21 | 1:A:546:VAL:CG1  | 2.45                     | 0.47              |
| 1:B:22:LEU:CD2   | 1:B:150:ALA:HB1  | 2.45                     | 0.47              |
| 1:C:175:ALA:HA   | 1:D:511:ASP:CG   | 2.39                     | 0.47              |
| 1:C:395:GLU:OE1  | 1:C:395:GLU:CA   | 2.62                     | 0.47              |
| 1:B:519:GLU:OE2  | 1:B:519:GLU:CA   | 2.61                     | 0.47              |
| 1:D:219:SER:HB2  | 1:D:334:SER:HB2  | 1.96                     | 0.47              |
| 1:D:52:THR:O     | 1:D:55:ALA:N     | 2.45                     | 0.47              |
| 1:D:382:GLU:OE1  | 1:D:383:PRO:CD   | 2.63                     | 0.47              |
| 1:B:482:ASN:O    | 1:B:483:ARG:C    | 2.58                     | 0.47              |
| 1:C:79:THR:HG22  | 1:C:82:GLU:HB3   | 1.96                     | 0.47              |
| 1:C:544:LYS:HA   | 1:C:547:MET:HE2  | 1.96                     | 0.46              |
| 1:D:219:SER:HB2  | 1:D:334:SER:CB   | 2.45                     | 0.46              |
| 1:D:553:PHE:HE1  | 1:D:570:GLU:HB2  | 1.80                     | 0.46              |
| 1:A:82:GLU:OE2   | 1:A:88:ALA:HB1   | 2.14                     | 0.46              |
| 1:B:414:ALA:HB1  | 1:B:417:VAL:CG2  | 2.45                     | 0.46              |
| 1:D:66:LEU:HD13  | 1:D:250:LEU:HD12 | 1.97                     | 0.46              |
| 1:A:86:ASP:HB2   | 1:A:105:HIS:ND1  | 2.29                     | 0.46              |
| 1:A:466:THR:O    | 1:A:467:PRO:C    | 2.56                     | 0.46              |
| 1:B:264:CYS:O    | 1:B:267:GLN:HB3  | 2.16                     | 0.46              |
| 1:B:415:PRO:HD2  | 1:B:416:GLN:CD   | 2.41                     | 0.46              |
| 1:C:421:THR:HG23 | 1:C:462:LEU:CD1  | 2.44                     | 0.46              |
| 1:D:110:PRO:O    | 1:D:111:ASP:C    | 2.58                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:386:LEU:HD12 | 1:D:386:LEU:HA   | 1.78                     | 0.46              |
| 1:A:40:VAL:O     | 1:A:44:LYS:HG2   | 2.15                     | 0.46              |
| 1:A:256:ARG:CZ   | 1:A:286:SER:CB   | 2.93                     | 0.46              |
| 1:A:282:VAL:HG13 | 1:A:283:LEU:HG   | 1.98                     | 0.46              |
| 1:B:406:LEU:O    | 1:B:407:ILE:C    | 2.58                     | 0.46              |
| 1:C:223:PRO:HD2  | 1:C:295:ASP:HB3  | 1.97                     | 0.46              |
| 1:D:151:PRO:HB2  | 1:D:256:ARG:NH1  | 2.31                     | 0.46              |
| 1:A:66:LEU:HA    | 1:A:66:LEU:HD23  | 1.57                     | 0.46              |
| 1:A:138:LEU:HD21 | 1:A:157:ALA:CB   | 2.45                     | 0.46              |
| 1:B:501:PHE:CD2  | 1:B:502:ASP:N    | 2.83                     | 0.46              |
| 1:D:528:LEU:O    | 1:D:528:LEU:HD12 | 2.15                     | 0.46              |
| 1:A:122:LEU:HD23 | 1:A:125:GLU:OE1  | 2.15                     | 0.46              |
| 1:A:414:ALA:O    | 1:A:416:GLN:N    | 2.48                     | 0.46              |
| 1:A:506:PHE:O    | 1:A:508:PHE:CD2  | 2.68                     | 0.46              |
| 1:B:35:PRO:O     | 1:B:38:GLU:HG2   | 2.15                     | 0.46              |
| 1:D:511:ASP:C    | 1:D:513:CYS:H    | 2.24                     | 0.46              |
| 1:A:139:TYR:O    | 1:A:143:ARG:CG   | 2.64                     | 0.46              |
| 1:A:531:LEU:CD2  | 1:A:546:VAL:HG11 | 2.45                     | 0.46              |
| 1:B:224:LYS:HG2  | 5:B:717:HOH:O    | 2.16                     | 0.46              |
| 1:C:69:LEU:O     | 1:C:73:GLU:HG2   | 2.16                     | 0.46              |
| 1:C:332:GLU:OE1  | 1:C:332:GLU:HA   | 2.15                     | 0.46              |
| 1:C:421:THR:HG23 | 1:C:462:LEU:HD12 | 1.98                     | 0.46              |
| 1:C:439:LYS:HB3  | 1:C:440:PRO:HD2  | 1.96                     | 0.46              |
| 2:C:602:PGE:H6   | 2:C:602:PGE:H42  | 1.70                     | 0.46              |
| 1:D:29:GLN:HG2   | 1:D:146:PRO:HA   | 1.97                     | 0.46              |
| 1:D:177:LEU:O    | 1:D:178:LEU:C    | 2.59                     | 0.46              |
| 1:A:177:LEU:O    | 1:A:178:LEU:C    | 2.58                     | 0.46              |
| 1:A:504:LYS:HE3  | 1:A:505:PHE:CZ   | 2.51                     | 0.46              |
| 2:A:601:PGE:H4   | 2:A:601:PGE:O4   | 2.15                     | 0.46              |
| 1:B:395:GLU:HG3  | 5:B:789:HOH:O    | 2.16                     | 0.46              |
| 1:C:501:PHE:HB2  | 1:C:534:HIS:CE1  | 2.50                     | 0.46              |
| 1:A:564:GLU:HG2  | 5:B:786:HOH:O    | 2.15                     | 0.46              |
| 1:B:318:TYR:OH   | 1:B:357:GLU:OE1  | 2.34                     | 0.46              |
| 1:C:219:SER:O    | 1:C:335:ARG:HA   | 2.15                     | 0.46              |
| 1:C:173:LYS:O    | 1:C:174:GLY:C    | 2.59                     | 0.45              |
| 1:D:80:LEU:HG    | 1:D:81:ARG:N     | 2.31                     | 0.45              |
| 1:D:123:CYS:O    | 1:D:124:ALA:C    | 2.58                     | 0.45              |
| 1:C:179:PRO:HB3  | 1:D:510:ALA:HB3  | 1.98                     | 0.45              |
| 1:C:572:PRO:HB2  | 5:C:722:HOH:O    | 2.16                     | 0.45              |
| 1:D:393:LEU:HD23 | 1:D:402:PHE:CD1  | 2.51                     | 0.45              |
| 1:D:409:ARG:HB2  | 4:D:603:PRO:CG   | 2.37                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:509:HIS:HB2  | 1:D:511:ASP:OD1  | 2.16                     | 0.45              |
| 1:A:36:PHE:CD2   | 1:A:136:LYS:HG3  | 2.51                     | 0.45              |
| 1:B:242:LYS:O    | 1:B:242:LYS:HG2  | 2.16                     | 0.45              |
| 1:C:1:ASP:C      | 1:C:3:HIS:CE1    | 2.94                     | 0.45              |
| 1:C:175:ALA:HA   | 1:D:511:ASP:OD1  | 2.15                     | 0.45              |
| 1:C:510:ALA:HB3  | 1:D:179:PRO:HB3  | 1.97                     | 0.45              |
| 1:A:408:VAL:HG12 | 1:A:412:ARG:HD2  | 1.98                     | 0.45              |
| 1:C:283:LEU:C    | 1:C:285:LYS:N    | 2.73                     | 0.45              |
| 1:D:24:LEU:HD12  | 1:D:24:LEU:O     | 2.17                     | 0.45              |
| 1:D:46:LEU:HD23  | 1:D:46:LEU:HA    | 1.67                     | 0.45              |
| 1:A:416:GLN:N    | 1:A:416:GLN:OE1  | 2.39                     | 0.45              |
| 1:B:93:LYS:HG2   | 1:B:94:GLN:N     | 2.19                     | 0.45              |
| 1:D:528:LEU:HD22 | 1:D:547:MET:SD   | 2.55                     | 0.45              |
| 1:B:87:MET:HB2   | 1:B:105:HIS:CE1  | 2.51                     | 0.45              |
| 1:B:487:PHE:O    | 1:B:490:LEU:HB2  | 2.17                     | 0.45              |
| 1:A:375:LYS:HD3  | 1:A:376:LEU:N    | 2.32                     | 0.45              |
| 1:A:417:VAL:HG12 | 1:A:418:SER:O    | 2.17                     | 0.45              |
| 1:A:516:PRO:HG2  | 1:A:519:GLU:HG3  | 1.98                     | 0.45              |
| 1:A:553:PHE:HA   | 1:A:556:LYS:HG2  | 1.98                     | 0.45              |
| 1:B:390:ASN:OD1  | 1:B:409:ARG:NH1  | 2.28                     | 0.45              |
| 1:D:509:HIS:O    | 1:D:512:ILE:HG22 | 2.17                     | 0.45              |
| 1:D:516:PRO:HG2  | 1:D:519:GLU:HG3  | 1.98                     | 0.45              |
| 1:A:198:ARG:HD3  | 1:A:241:HIS:CD2  | 2.52                     | 0.45              |
| 1:A:215:VAL:HG23 | 1:A:234:VAL:HG11 | 1.99                     | 0.45              |
| 1:C:4:LYS:NZ     | 1:C:57:GLU:CB    | 2.80                     | 0.45              |
| 1:A:36:PHE:HB2   | 1:A:139:TYR:CD2  | 2.51                     | 0.45              |
| 1:A:71:GLY:O     | 1:A:75:CYS:HB2   | 2.17                     | 0.45              |
| 1:B:93:LYS:CG    | 1:B:94:GLN:N     | 2.74                     | 0.45              |
| 1:C:88:ALA:O     | 1:C:91:CYS:HB3   | 2.17                     | 0.45              |
| 1:D:101:CYS:O    | 1:D:104:ASN:HB2  | 2.16                     | 0.45              |
| 1:A:456:LEU:O    | 1:A:459:LEU:HB3  | 2.17                     | 0.45              |
| 1:D:27:PHE:CE1   | 1:D:42:LEU:HB3   | 2.51                     | 0.45              |
| 1:A:344:VAL:HG11 | 1:A:445:MET:HE1  | 2.00                     | 0.44              |
| 1:A:546:VAL:HG23 | 1:A:582:LEU:HD22 | 1.99                     | 0.44              |
| 1:C:470:GLU:N    | 1:C:470:GLU:OE1  | 2.29                     | 0.44              |
| 1:A:177:LEU:HD12 | 1:A:178:LEU:N    | 2.32                     | 0.44              |
| 1:B:44:LYS:HG3   | 1:B:45:GLU:N     | 2.31                     | 0.44              |
| 1:C:332:GLU:OE1  | 1:C:336:ARG:NH2  | 2.50                     | 0.44              |
| 1:C:413:LYS:HD3  | 1:C:490:LEU:HB2  | 2.00                     | 0.44              |
| 1:A:275:LYS:HD2  | 1:A:275:LYS:HA   | 1.60                     | 0.44              |
| 1:B:402:PHE:HZ   | 2:B:601:PGE:H6   | 1.82                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:514:THR:O    | 1:D:514:THR:CG2  | 2.65                     | 0.44              |
| 1:B:11:PHE:CD1   | 1:B:54:VAL:HG21  | 2.52                     | 0.44              |
| 1:B:399:GLU:O    | 1:B:403:GLN:HG3  | 2.18                     | 0.44              |
| 1:D:84:TYR:O     | 1:D:85:GLY:C     | 2.61                     | 0.44              |
| 1:D:387:ILE:HG22 | 1:D:444:ARG:HD3  | 1.98                     | 0.44              |
| 1:A:66:LEU:O     | 1:A:70:PHE:HD2   | 2.00                     | 0.44              |
| 1:A:399:GLU:HG2  | 5:A:729:HOH:O    | 2.18                     | 0.44              |
| 1:B:457:ASN:O    | 1:B:461:VAL:HG13 | 2.17                     | 0.44              |
| 1:B:512:ILE:O    | 1:B:520:LYS:HE3  | 2.17                     | 0.44              |
| 1:B:402:PHE:CE1  | 1:B:406:LEU:HD21 | 2.53                     | 0.44              |
| 1:B:416:GLN:CD   | 1:B:416:GLN:N    | 2.75                     | 0.44              |
| 1:D:341:ALA:HA   | 1:D:446:PRO:HA   | 1.99                     | 0.44              |
| 1:D:347:ARG:CZ   | 1:D:485:PRO:HD3  | 2.48                     | 0.44              |
| 1:A:84:TYR:CD1   | 1:A:87:MET:CG    | 3.01                     | 0.44              |
| 1:B:511:ASP:OD1  | 1:B:511:ASP:N    | 2.49                     | 0.44              |
| 1:C:287:HIS:CD2  | 1:C:287:HIS:C    | 2.96                     | 0.44              |
| 1:D:42:LEU:HA    | 1:D:45:GLU:HG2   | 2.00                     | 0.44              |
| 1:D:167:CYS:HB3  | 1:D:177:LEU:CD1  | 2.48                     | 0.44              |
| 1:D:329:PHE:CD2  | 1:D:329:PHE:C    | 2.96                     | 0.44              |
| 1:D:514:THR:O    | 1:D:514:THR:HG23 | 2.18                     | 0.44              |
| 1:A:23:VAL:HG12  | 1:A:43:VAL:HG22  | 2.00                     | 0.44              |
| 1:A:66:LEU:HD12  | 1:A:251:GLU:OE2  | 2.18                     | 0.44              |
| 1:C:480:LEU:O    | 1:C:483:ARG:HG3  | 2.17                     | 0.44              |
| 1:D:35:PRO:HA    | 1:D:139:TYR:OH   | 2.17                     | 0.44              |
| 1:D:195:GLN:NE2  | 1:D:245:CYS:SG   | 2.91                     | 0.44              |
| 1:D:341:ALA:HB3  | 1:D:344:VAL:HG23 | 1.99                     | 0.44              |
| 1:A:148:PHE:HD1  | 1:A:153:LEU:HB2  | 1.81                     | 0.43              |
| 1:A:457:ASN:HB3  | 5:A:717:HOH:O    | 2.18                     | 0.43              |
| 1:C:505:PHE:HB3  | 1:C:530:GLU:HG3  | 2.00                     | 0.43              |
| 1:D:33:GLN:CB    | 1:D:84:TYR:OH    | 2.66                     | 0.43              |
| 1:D:81:ARG:HD2   | 1:D:81:ARG:O     | 2.17                     | 0.43              |
| 1:D:211:LYS:O    | 1:D:215:VAL:HG23 | 2.17                     | 0.43              |
| 1:B:267:GLN:NE2  | 1:B:278:CYS:SG   | 2.91                     | 0.43              |
| 1:B:289:ILE:O    | 1:B:292:VAL:CG1  | 2.66                     | 0.43              |
| 1:B:564:GLU:O    | 1:B:568:VAL:HG23 | 2.18                     | 0.43              |
| 1:C:262:TYR:C    | 1:C:262:TYR:CD2  | 2.96                     | 0.43              |
| 1:D:90:CYS:O     | 1:D:91:CYS:C     | 2.61                     | 0.43              |
| 1:A:140:GLU:OE1  | 1:A:143:ARG:NH1  | 2.43                     | 0.43              |
| 1:A:537:LYS:HA   | 1:A:537:LYS:HD2  | 1.78                     | 0.43              |
| 1:C:31:LEU:HD13  | 1:C:80:LEU:HD21  | 2.00                     | 0.43              |
| 1:C:318:TYR:OH   | 1:C:357:GLU:OE1  | 2.35                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:440:PRO:O    | 1:C:441:GLU:C    | 2.62                     | 0.43              |
| 1:D:101:CYS:O    | 1:D:104:ASN:N    | 2.51                     | 0.43              |
| 1:D:151:PRO:O    | 1:D:154:LEU:HB2  | 2.18                     | 0.43              |
| 1:D:152:GLU:O    | 1:D:152:GLU:HG3  | 2.17                     | 0.43              |
| 1:D:173:LYS:O    | 1:D:177:LEU:CD1  | 2.66                     | 0.43              |
| 1:D:502:ASP:HB2  | 5:D:764:HOH:O    | 2.17                     | 0.43              |
| 1:B:90:CYS:C     | 1:B:92:GLU:N     | 2.75                     | 0.43              |
| 1:D:21:GLY:O     | 1:D:25:ILE:HG13  | 2.19                     | 0.43              |
| 1:A:223:PRO:HB2  | 1:A:298:PRO:HD3  | 2.00                     | 0.43              |
| 1:A:316:LYS:O    | 1:A:317:ASN:C    | 2.57                     | 0.43              |
| 1:B:404:ASN:OD1  | 1:B:525:GLN:HG2  | 2.18                     | 0.43              |
| 1:C:95:GLU:OE2   | 1:C:98:ARG:NE    | 2.52                     | 0.43              |
| 1:D:6:GLU:O      | 1:D:10:ARG:HG2   | 2.19                     | 0.43              |
| 1:A:444:ARG:O    | 1:A:445:MET:C    | 2.62                     | 0.43              |
| 1:B:222:PHE:CE1  | 1:B:274:LEU:HD11 | 2.54                     | 0.43              |
| 1:D:87:MET:O     | 1:D:88:ALA:C     | 2.59                     | 0.43              |
| 1:D:118:GLU:HB3  | 1:D:121:THR:OG1  | 2.19                     | 0.43              |
| 1:D:403:GLN:O    | 1:D:407:ILE:HG12 | 2.18                     | 0.43              |
| 1:B:239:LYS:HA   | 1:B:242:LYS:HE2  | 2.00                     | 0.43              |
| 1:C:112:LEU:HD13 | 1:C:143:ARG:CZ   | 2.48                     | 0.43              |
| 1:C:119:PRO:CB   | 4:C:605:PRO:HD3  | 2.47                     | 0.43              |
| 1:D:220:GLN:HG2  | 1:D:334:SER:O    | 2.19                     | 0.43              |
| 1:D:407:ILE:HD13 | 1:D:426:SER:CB   | 2.49                     | 0.43              |
| 1:A:86:ASP:CB    | 1:A:105:HIS:CE1  | 3.02                     | 0.43              |
| 1:A:150:ALA:HB3  | 1:A:151:PRO:CD   | 2.48                     | 0.43              |
| 1:A:555:ASP:C    | 1:A:557:CYS:N    | 2.76                     | 0.43              |
| 1:C:537:LYS:O    | 1:C:538:ALA:C    | 2.62                     | 0.43              |
| 1:D:82:GLU:HA    | 1:D:88:ALA:HB2   | 2.01                     | 0.43              |
| 1:D:409:ARG:CA   | 4:D:603:PRO:HG3  | 2.48                     | 0.43              |
| 1:D:512:ILE:HD12 | 1:D:512:ILE:HA   | 1.76                     | 0.43              |
| 1:A:479:SER:OG   | 1:A:482:ASN:HB2  | 2.19                     | 0.43              |
| 1:B:126:PHE:HD1  | 1:B:133:PHE:CD2  | 2.36                     | 0.43              |
| 1:B:507:THR:O    | 1:B:508:PHE:CD2  | 2.71                     | 0.43              |
| 1:D:90:CYS:C     | 1:D:92:GLU:N     | 2.74                     | 0.43              |
| 1:D:400:TYR:OH   | 1:D:524:LYS:HD2  | 2.19                     | 0.43              |
| 1:B:118:GLU:HA   | 1:B:119:PRO:HD3  | 1.75                     | 0.42              |
| 1:B:515:LEU:HB3  | 1:B:519:GLU:HB2  | 2.00                     | 0.42              |
| 1:C:1:ASP:N      | 1:C:10:ARG:HH22  | 2.18                     | 0.42              |
| 1:C:106:LYS:HD3  | 1:C:146:PRO:O    | 2.19                     | 0.42              |
| 1:D:224:LYS:O    | 1:D:224:LYS:HG2  | 2.19                     | 0.42              |
| 1:A:174:GLY:C    | 1:A:176:CYS:H    | 2.27                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:350:LYS:NZ   | 1:B:479:SER:OG   | 2.52                     | 0.42              |
| 1:D:80:LEU:C     | 1:D:82:GLU:N     | 2.62                     | 0.42              |
| 1:D:308:PHE:HB2  | 1:D:373:PHE:HZ   | 1.84                     | 0.42              |
| 1:A:221:LYS:HE3  | 1:A:290:ALA:O    | 2.19                     | 0.42              |
| 1:B:46:LEU:HA    | 1:B:49:PHE:HB3   | 2.01                     | 0.42              |
| 1:C:509:HIS:O    | 1:C:512:ILE:HG22 | 2.19                     | 0.42              |
| 1:D:207:GLU:CD   | 1:D:242:LYS:HD3  | 2.44                     | 0.42              |
| 1:A:441:GLU:OE2  | 1:A:444:ARG:HD3  | 2.19                     | 0.42              |
| 1:B:35:PRO:HB2   | 1:B:38:GLU:OE1   | 2.19                     | 0.42              |
| 1:C:72:ASP:N     | 1:C:98:ARG:HH22  | 2.18                     | 0.42              |
| 1:D:79:THR:O     | 1:D:83:THR:N     | 2.53                     | 0.42              |
| 1:D:159:LYS:HA   | 1:D:159:LYS:HD3  | 1.81                     | 0.42              |
| 1:D:177:LEU:O    | 1:D:180:LYS:N    | 2.53                     | 0.42              |
| 1:D:512:ILE:CD1  | 1:D:520:LYS:HA   | 2.49                     | 0.42              |
| 1:B:528:LEU:HD12 | 1:B:528:LEU:HA   | 1.77                     | 0.42              |
| 1:D:42:LEU:HA    | 1:D:45:GLU:HG3   | 2.00                     | 0.42              |
| 1:A:282:VAL:HG13 | 1:A:283:LEU:H    | 1.82                     | 0.42              |
| 1:B:372:VAL:O    | 1:B:376:LEU:HG   | 2.20                     | 0.42              |
| 1:B:414:ALA:HB1  | 1:B:417:VAL:HG23 | 2.02                     | 0.42              |
| 1:B:472:VAL:O    | 1:B:473:THR:C    | 2.63                     | 0.42              |
| 1:B:535:LYS:HG3  | 1:B:582:LEU:HB3  | 2.02                     | 0.42              |
| 1:C:558:CYS:O    | 1:C:563:LYS:HE3  | 2.19                     | 0.42              |
| 1:D:205:PHE:CE2  | 1:D:480:LEU:HD13 | 2.54                     | 0.42              |
| 1:A:289:ILE:O    | 1:A:291:GLU:N    | 2.52                     | 0.42              |
| 1:A:289:ILE:C    | 1:A:291:GLU:N    | 2.77                     | 0.42              |
| 1:A:305:THR:O    | 1:A:310:GLU:HG3  | 2.20                     | 0.42              |
| 1:A:456:LEU:HD23 | 1:A:456:LEU:HA   | 1.86                     | 0.42              |
| 1:C:178:LEU:HD23 | 1:C:178:LEU:HA   | 1.78                     | 0.42              |
| 1:C:410:TYR:HE1  | 2:C:601:PGE:H2   | 1.85                     | 0.42              |
| 1:C:410:TYR:OH   | 2:C:601:PGE:H1   | 2.19                     | 0.42              |
| 1:D:160:TYR:CA   | 1:D:184:MET:HE1  | 2.47                     | 0.42              |
| 1:A:179:PRO:HB3  | 1:B:510:ALA:HB3  | 2.01                     | 0.42              |
| 1:A:220:GLN:O    | 1:A:223:PRO:HD3  | 2.20                     | 0.42              |
| 1:B:112:LEU:HD13 | 1:B:143:ARG:CZ   | 2.49                     | 0.42              |
| 1:C:248:ASP:OD1  | 1:C:248:ASP:N    | 2.52                     | 0.42              |
| 1:A:545:THR:HG21 | 1:A:582:LEU:HD21 | 2.01                     | 0.42              |
| 1:A:570:GLU:O    | 1:A:573:LYS:HB3  | 2.20                     | 0.42              |
| 1:B:306:ALA:HA   | 1:B:310:GLU:OE1  | 2.19                     | 0.42              |
| 1:C:27:PHE:CD2   | 1:C:74:LEU:HD21  | 2.55                     | 0.42              |
| 1:D:203:GLN:OE1  | 1:D:203:GLN:CA   | 2.67                     | 0.42              |
| 1:D:334:SER:HA   | 1:D:345:LEU:HD13 | 2.02                     | 0.42              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:65:SER:O    | 1:A:68:THR:HB    | 2.20                     | 0.42              |
| 1:A:412:ARG:HB3 | 1:A:492:LEU:HD12 | 2.02                     | 0.42              |
| 1:B:112:LEU:CD1 | 1:B:143:ARG:NE   | 2.82                     | 0.42              |
| 1:B:208:ARG:NH2 | 5:B:719:HOH:O    | 2.52                     | 0.42              |
| 1:C:36:PHE:CZ   | 1:C:40:VAL:HG21  | 2.54                     | 0.42              |
| 1:C:333:TYR:O   | 1:C:334:SER:C    | 2.62                     | 0.42              |
| 1:D:32:GLN:NE2  | 1:D:107:ASP:O    | 2.53                     | 0.42              |
| 1:D:260:ALA:HB1 | 1:D:285:LYS:HD3  | 2.02                     | 0.42              |
| 1:A:287:HIS:CD2 | 1:A:287:HIS:C    | 2.97                     | 0.41              |
| 1:A:422:LEU:O   | 1:A:426:SER:HB2  | 2.20                     | 0.41              |
| 1:A:509:HIS:N   | 5:A:716:HOH:O    | 2.45                     | 0.41              |
| 1:A:582:LEU:O   | 1:A:583:ALA:OXT  | 2.37                     | 0.41              |
| 1:C:321:ALA:O   | 1:C:322:LYS:C    | 2.63                     | 0.41              |
| 1:A:78:ALA:O    | 1:A:80:LEU:HG    | 2.20                     | 0.41              |
| 1:A:82:GLU:O    | 1:A:84:TYR:O     | 2.38                     | 0.41              |
| 1:A:89:ASP:O    | 1:A:90:CYS:C     | 2.63                     | 0.41              |
| 1:A:544:LYS:HG2 | 1:A:548:GLU:CD   | 2.45                     | 0.41              |
| 1:B:2:THR:O     | 1:B:3:HIS:ND1    | 2.53                     | 0.41              |
| 1:C:312:LYS:HE3 | 1:C:366:HIS:CG   | 2.55                     | 0.41              |
| 1:D:140:GLU:OE1 | 1:D:144:ARG:NH1  | 2.45                     | 0.41              |
| 1:A:317:ASN:HA  | 5:A:774:HOH:O    | 2.20                     | 0.41              |
| 1:C:499:LYS:HA  | 1:C:500:PRO:HD3  | 1.91                     | 0.41              |
| 1:A:581:ALA:HB3 | 1:A:582:LEU:HD12 | 2.03                     | 0.41              |
| 1:C:345:LEU:HA  | 1:C:348:LEU:HD12 | 2.01                     | 0.41              |
| 1:A:123:CYS:SG  | 1:A:173:LYS:HD3  | 2.60                     | 0.41              |
| 1:A:366:HIS:HA  | 1:A:369:TYR:CZ   | 2.56                     | 0.41              |
| 1:A:551:VAL:O   | 1:A:552:ALA:C    | 2.63                     | 0.41              |
| 1:B:36:PHE:CD2  | 1:B:136:LYS:HD2  | 2.56                     | 0.41              |
| 1:C:280:LYS:H   | 1:C:280:LYS:HG3  | 1.53                     | 0.41              |
| 1:C:522:ILE:O   | 1:C:526:THR:N    | 2.42                     | 0.41              |
| 1:C:543:LEU:O   | 1:C:547:MET:HG3  | 2.20                     | 0.41              |
| 1:A:3:HIS:NE2   | 4:A:605:PRO:HA   | 2.35                     | 0.41              |
| 1:A:412:ARG:HG2 | 1:A:492:LEU:HD12 | 2.03                     | 0.41              |
| 1:B:32:GLN:NE2  | 1:B:146:PRO:HG3  | 2.36                     | 0.41              |
| 1:B:80:LEU:HD23 | 1:B:91:CYS:HB2   | 2.02                     | 0.41              |
| 1:B:395:GLU:CG  | 5:B:789:HOH:O    | 2.68                     | 0.41              |
| 1:D:137:TYR:O   | 1:D:138:LEU:C    | 2.63                     | 0.41              |
| 1:D:564:GLU:O   | 1:D:564:GLU:HG3  | 2.20                     | 0.41              |
| 1:A:539:THR:N   | 1:A:542:GLN:OE1  | 2.51                     | 0.41              |
| 1:B:341:ALA:CB  | 1:B:449:GLU:HB2  | 2.51                     | 0.41              |
| 1:D:251:GLU:CD  | 1:D:251:GLU:N    | 2.75                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:532:LEU:HD22 | 1:D:532:LEU:N    | 2.35                     | 0.41              |
| 1:A:9:HIS:O      | 1:A:13:ASP:HB2   | 2.21                     | 0.41              |
| 1:A:242:LYS:NZ   | 1:D:169:GLN:OE1  | 2.54                     | 0.41              |
| 1:D:484:ARG:HB3  | 1:D:485:PRO:HD3  | 2.02                     | 0.41              |
| 1:A:36:PHE:HB2   | 1:A:139:TYR:CE2  | 2.56                     | 0.41              |
| 1:A:173:LYS:O    | 1:A:176:CYS:HB3  | 2.21                     | 0.41              |
| 1:A:356:LEU:O    | 1:A:357:GLU:C    | 2.63                     | 0.41              |
| 1:A:561:ASP:OD1  | 1:A:561:ASP:C    | 2.64                     | 0.41              |
| 1:B:505:PHE:HB3  | 1:B:530:GLU:HG3  | 2.03                     | 0.41              |
| 1:C:71:GLY:HA3   | 1:C:98:ARG:NH2   | 2.36                     | 0.41              |
| 1:C:387:ILE:HD12 | 1:C:448:THR:HG21 | 2.03                     | 0.41              |
| 1:D:49:PHE:CE2   | 1:D:69:LEU:HD11  | 2.55                     | 0.41              |
| 1:D:460:CYS:O    | 1:D:464:GLU:HB3  | 2.21                     | 0.41              |
| 1:A:394:PHE:O    | 1:A:395:GLU:C    | 2.64                     | 0.41              |
| 1:C:565:GLY:O    | 1:C:569:LEU:HD13 | 2.20                     | 0.41              |
| 1:A:90:CYS:O     | 1:A:91:CYS:C     | 2.64                     | 0.40              |
| 1:A:297:VAL:HA   | 1:A:298:PRO:HD3  | 1.91                     | 0.40              |
| 1:B:270:LEU:HD23 | 1:B:270:LEU:HA   | 1.97                     | 0.40              |
| 1:D:314:VAL:HG12 | 1:D:315:CYS:N    | 2.36                     | 0.40              |
| 1:A:93:LYS:O     | 1:A:98:ARG:HB2   | 2.20                     | 0.40              |
| 1:A:266:HIS:ND1  | 1:A:266:HIS:N    | 2.69                     | 0.40              |
| 1:B:81:ARG:CA    | 1:B:88:ALA:HB2   | 2.51                     | 0.40              |
| 1:B:259:LEU:O    | 1:B:259:LEU:HD12 | 2.21                     | 0.40              |
| 1:B:561:ASP:O    | 1:B:563:LYS:NZ   | 2.54                     | 0.40              |
| 1:D:31:LEU:HD23  | 1:D:31:LEU:N     | 2.35                     | 0.40              |
| 1:D:94:GLN:OE1   | 1:D:98:ARG:NH1   | 2.54                     | 0.40              |
| 1:D:140:GLU:HA   | 1:D:143:ARG:HD3  | 2.03                     | 0.40              |
| 1:A:5:SER:HB2    | 1:A:62:CYS:O     | 2.21                     | 0.40              |
| 1:C:305:THR:HG22 | 1:C:373:PHE:CD1  | 2.57                     | 0.40              |
| 1:D:93:LYS:O     | 1:D:94:GLN:OE1   | 2.39                     | 0.40              |
| 1:D:293:ASP:O    | 1:D:294:LYS:C    | 2.63                     | 0.40              |
| 1:D:408:VAL:HG12 | 4:D:603:PRO:HG2  | 2.04                     | 0.40              |
| 1:A:213:TRP:CD1  | 1:A:213:TRP:C    | 2.99                     | 0.40              |
| 1:B:80:LEU:HD12  | 1:B:84:TYR:HD2   | 1.87                     | 0.40              |
| 1:B:225:ALA:CB   | 1:B:270:LEU:HD23 | 2.50                     | 0.40              |
| 1:D:366:HIS:C    | 1:D:368:CYS:N    | 2.79                     | 0.40              |
| 1:D:499:LYS:HD3  | 1:D:533:LYS:HB3  | 2.04                     | 0.40              |
| 1:A:19:PHE:CD1   | 1:A:19:PHE:C     | 2.99                     | 0.40              |
| 1:A:436:CYS:HA   | 1:A:439:LYS:HG2  | 2.02                     | 0.40              |
| 1:C:30:TYR:CE2   | 1:C:74:LEU:HD11  | 2.57                     | 0.40              |
| 1:C:196:ARG:HA   | 1:C:196:ARG:HD2  | 1.82                     | 0.40              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:280:LYS:HB3 | 1:D:281:PRO:CD   | 2.51                     | 0.40              |
| 1:D:543:LEU:HA  | 1:D:543:LEU:HD23 | 1.88                     | 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     | 581/583 (100%)   | 502 (86%)  | 76 (13%)  | 3 (0%)   | 24          | 34 |
| 1   | B     | 581/583 (100%)   | 524 (90%)  | 55 (10%)  | 2 (0%)   | 36          | 45 |
| 1   | C     | 581/583 (100%)   | 527 (91%)  | 51 (9%)   | 3 (0%)   | 24          | 34 |
| 1   | D     | 581/583 (100%)   | 529 (91%)  | 51 (9%)   | 1 (0%)   | 43          | 56 |
| All | All   | 2324/2332 (100%) | 2082 (90%) | 233 (10%) | 9 (0%)   | 30          | 39 |

All (9) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 74  | LEU  |
| 1   | A     | 415 | PRO  |
| 1   | A     | 290 | ALA  |
| 1   | D     | 494 | GLU  |
| 1   | B     | 282 | VAL  |
| 1   | B     | 289 | ILE  |
| 1   | C     | 240 | VAL  |
| 1   | C     | 342 | VAL  |
| 1   | A     | 289 | 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     | 516/516 (100%)   | 465 (90%)  | 51 (10%)  | 7           | 9  |
| 1   | B     | 516/516 (100%)   | 461 (89%)  | 55 (11%)  | 6           | 7  |
| 1   | C     | 516/516 (100%)   | 481 (93%)  | 35 (7%)   | 14          | 20 |
| 1   | D     | 516/516 (100%)   | 461 (89%)  | 55 (11%)  | 6           | 7  |
| All | All   | 2064/2064 (100%) | 1868 (90%) | 196 (10%) | 8           | 9  |

All (196) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 7   | ILE  |
| 1   | A     | 13  | ASP  |
| 1   | A     | 34  | CYS  |
| 1   | A     | 58  | SER  |
| 1   | A     | 63  | ASP  |
| 1   | A     | 79  | THR  |
| 1   | A     | 81  | ARG  |
| 1   | A     | 86  | ASP  |
| 1   | A     | 90  | CYS  |
| 1   | A     | 92  | GLU  |
| 1   | A     | 114 | LYS  |
| 1   | A     | 115 | LEU  |
| 1   | A     | 121 | THR  |
| 1   | A     | 166 | GLU  |
| 1   | A     | 180 | LYS  |
| 1   | A     | 208 | ARG  |
| 1   | A     | 218 | LEU  |
| 1   | A     | 244 | CYS  |
| 1   | A     | 246 | HIS  |
| 1   | A     | 275 | LYS  |
| 1   | A     | 291 | GLU  |
| 1   | A     | 292 | VAL  |
| 1   | A     | 300 | ASN  |
| 1   | A     | 305 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 310 | GLU  |
| 1   | A     | 312 | LYS  |
| 1   | A     | 313 | GLU  |
| 1   | A     | 374 | ASP  |
| 1   | A     | 407 | ILE  |
| 1   | A     | 425 | ILE  |
| 1   | A     | 444 | ARG  |
| 1   | A     | 445 | MET  |
| 1   | A     | 448 | THR  |
| 1   | A     | 450 | ASP  |
| 1   | A     | 459 | LEU  |
| 1   | A     | 461 | VAL  |
| 1   | A     | 468 | VAL  |
| 1   | A     | 469 | SER  |
| 1   | A     | 470 | GLU  |
| 1   | A     | 482 | ASN  |
| 1   | A     | 498 | PRO  |
| 1   | A     | 507 | THR  |
| 1   | A     | 512 | ILE  |
| 1   | A     | 514 | THR  |
| 1   | A     | 518 | THR  |
| 1   | A     | 524 | LYS  |
| 1   | A     | 532 | LEU  |
| 1   | A     | 535 | LYS  |
| 1   | A     | 544 | LYS  |
| 1   | A     | 546 | VAL  |
| 1   | A     | 582 | LEU  |
| 1   | B     | 16  | GLU  |
| 1   | B     | 31  | LEU  |
| 1   | B     | 34  | CYS  |
| 1   | B     | 44  | LYS  |
| 1   | B     | 58  | SER  |
| 1   | B     | 73  | GLU  |
| 1   | B     | 76  | LYS  |
| 1   | B     | 89  | ASP  |
| 1   | B     | 104 | ASN  |
| 1   | B     | 111 | ASP  |
| 1   | B     | 131 | LYS  |
| 1   | B     | 144 | ARG  |
| 1   | B     | 159 | LYS  |
| 1   | B     | 169 | GLN  |
| 1   | B     | 171 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 173 | LYS  |
| 1   | B     | 221 | LYS  |
| 1   | B     | 239 | LYS  |
| 1   | B     | 251 | GLU  |
| 1   | B     | 267 | GLN  |
| 1   | B     | 268 | ASP  |
| 1   | B     | 282 | VAL  |
| 1   | B     | 284 | GLU  |
| 1   | B     | 289 | ILE  |
| 1   | B     | 310 | GLU  |
| 1   | B     | 319 | GLN  |
| 1   | B     | 324 | VAL  |
| 1   | B     | 336 | ARG  |
| 1   | B     | 342 | VAL  |
| 1   | B     | 343 | SER  |
| 1   | B     | 377 | LYS  |
| 1   | B     | 382 | GLU  |
| 1   | B     | 386 | LEU  |
| 1   | B     | 413 | LYS  |
| 1   | B     | 435 | LYS  |
| 1   | B     | 445 | MET  |
| 1   | B     | 450 | ASP  |
| 1   | B     | 455 | ILE  |
| 1   | B     | 464 | GLU  |
| 1   | B     | 466 | THR  |
| 1   | B     | 468 | VAL  |
| 1   | B     | 470 | GLU  |
| 1   | B     | 484 | ARG  |
| 1   | B     | 490 | LEU  |
| 1   | B     | 508 | PHE  |
| 1   | B     | 517 | ASP  |
| 1   | B     | 522 | ILE  |
| 1   | B     | 532 | LEU  |
| 1   | B     | 547 | MET  |
| 1   | B     | 550 | PHE  |
| 1   | B     | 553 | PHE  |
| 1   | B     | 554 | VAL  |
| 1   | B     | 561 | ASP  |
| 1   | B     | 569 | LEU  |
| 1   | B     | 574 | LEU  |
| 1   | C     | 34  | CYS  |
| 1   | C     | 38  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 57  | GLU  |
| 1   | C     | 77  | VAL  |
| 1   | C     | 111 | ASP  |
| 1   | C     | 131 | LYS  |
| 1   | C     | 136 | LYS  |
| 1   | C     | 159 | LYS  |
| 1   | C     | 235 | THR  |
| 1   | C     | 239 | LYS  |
| 1   | C     | 263 | ILE  |
| 1   | C     | 282 | VAL  |
| 1   | C     | 285 | LYS  |
| 1   | C     | 286 | SER  |
| 1   | C     | 314 | VAL  |
| 1   | C     | 319 | GLN  |
| 1   | C     | 333 | TYR  |
| 1   | C     | 336 | ARG  |
| 1   | C     | 346 | LEU  |
| 1   | C     | 350 | LYS  |
| 1   | C     | 351 | GLU  |
| 1   | C     | 385 | ASN  |
| 1   | C     | 392 | GLU  |
| 1   | C     | 407 | ILE  |
| 1   | C     | 424 | GLU  |
| 1   | C     | 431 | LYS  |
| 1   | C     | 435 | LYS  |
| 1   | C     | 470 | GLU  |
| 1   | C     | 474 | LYS  |
| 1   | C     | 481 | VAL  |
| 1   | C     | 504 | LYS  |
| 1   | C     | 518 | THR  |
| 1   | C     | 537 | LYS  |
| 1   | C     | 548 | GLU  |
| 1   | C     | 579 | GLN  |
| 1   | D     | 2   | THR  |
| 1   | D     | 7   | ILE  |
| 1   | D     | 20  | GLN  |
| 1   | D     | 24  | LEU  |
| 1   | D     | 31  | LEU  |
| 1   | D     | 44  | LYS  |
| 1   | D     | 45  | GLU  |
| 1   | D     | 48  | GLU  |
| 1   | D     | 58  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 64  | LYS  |
| 1   | D     | 80  | LEU  |
| 1   | D     | 81  | ARG  |
| 1   | D     | 82  | GLU  |
| 1   | D     | 83  | THR  |
| 1   | D     | 111 | ASP  |
| 1   | D     | 120 | ASP  |
| 1   | D     | 130 | GLU  |
| 1   | D     | 136 | LYS  |
| 1   | D     | 165 | GLN  |
| 1   | D     | 169 | GLN  |
| 1   | D     | 187 | LYS  |
| 1   | D     | 191 | SER  |
| 1   | D     | 201 | SER  |
| 1   | D     | 217 | ARG  |
| 1   | D     | 224 | LYS  |
| 1   | D     | 235 | THR  |
| 1   | D     | 239 | LYS  |
| 1   | D     | 244 | CYS  |
| 1   | D     | 251 | GLU  |
| 1   | D     | 267 | GLN  |
| 1   | D     | 275 | LYS  |
| 1   | D     | 286 | SER  |
| 1   | D     | 342 | VAL  |
| 1   | D     | 362 | LYS  |
| 1   | D     | 378 | HIS  |
| 1   | D     | 382 | GLU  |
| 1   | D     | 384 | GLN  |
| 1   | D     | 393 | LEU  |
| 1   | D     | 441 | GLU  |
| 1   | D     | 444 | ARG  |
| 1   | D     | 465 | LYS  |
| 1   | D     | 468 | VAL  |
| 1   | D     | 471 | LYS  |
| 1   | D     | 492 | LEU  |
| 1   | D     | 504 | LYS  |
| 1   | D     | 511 | ASP  |
| 1   | D     | 514 | THR  |
| 1   | D     | 519 | GLU  |
| 1   | D     | 531 | LEU  |
| 1   | D     | 539 | THR  |
| 1   | D     | 540 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 544 | LYS  |
| 1   | D     | 569 | LEU  |
| 1   | D     | 573 | LYS  |
| 1   | D     | 574 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 20  | GLN  |
| 1   | A     | 246 | HIS  |
| 1   | A     | 384 | GLN  |
| 1   | A     | 509 | HIS  |
| 1   | B     | 32  | GLN  |
| 1   | B     | 105 | HIS  |
| 1   | B     | 534 | HIS  |
| 1   | C     | 20  | GLN  |
| 1   | C     | 67  | HIS  |
| 1   | C     | 105 | HIS  |
| 1   | C     | 161 | ASN  |
| 1   | C     | 317 | ASN  |
| 1   | C     | 509 | HIS  |
| 1   | D     | 105 | HIS  |
| 1   | D     | 300 | ASN  |
| 1   | D     | 337 | HIS  |
| 1   | D     | 482 | ASN  |
| 1   | D     | 579 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

19 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 |
| 4   | PRO  | B     | 604 | -    | 8,8,8        | 0.69 | 0        | 10,10,10    | 1.41 | 2 (20%)  |
| 4   | PRO  | C     | 605 | -    | 8,8,8        | 1.00 | 1 (12%)  | 10,10,10    | 1.35 | 1 (10%)  |
| 4   | PRO  | B     | 602 | -    | 8,8,8        | 0.98 | 1 (12%)  | 10,10,10    | 2.13 | 3 (30%)  |
| 4   | PRO  | A     | 606 | -    | 8,8,8        | 0.81 | 0        | 10,10,10    | 1.29 | 1 (10%)  |
| 2   | PGE  | A     | 602 | -    | 9,9,9        | 0.63 | 0        | 8,8,8       | 0.46 | 0        |
| 2   | PGE  | D     | 601 | -    | 9,9,9        | 0.67 | 0        | 8,8,8       | 1.59 | 2 (25%)  |
| 2   | PGE  | A     | 601 | -    | 9,9,9        | 0.74 | 0        | 8,8,8       | 0.63 | 0        |
| 4   | PRO  | D     | 603 | -    | 8,8,8        | 1.14 | 1 (12%)  | 10,10,10    | 1.66 | 1 (10%)  |
| 2   | PGE  | B     | 601 | -    | 9,9,9        | 0.49 | 0        | 8,8,8       | 0.91 | 0        |
| 3   | PEG  | A     | 603 | -    | 6,6,6        | 0.64 | 0        | 5,5,5       | 0.49 | 0        |
| 4   | PRO  | D     | 602 | -    | 8,8,8        | 0.90 | 0        | 10,10,10    | 1.25 | 1 (10%)  |
| 4   | PRO  | B     | 603 | -    | 8,8,8        | 0.84 | 0        | 10,10,10    | 1.27 | 1 (10%)  |
| 4   | PRO  | A     | 605 | -    | 8,8,8        | 0.92 | 1 (12%)  | 10,10,10    | 1.45 | 2 (20%)  |
| 3   | PEG  | C     | 603 | -    | 6,6,6        | 1.91 | 1 (16%)  | 5,5,5       | 1.10 | 0        |
| 2   | PGE  | C     | 601 | -    | 9,9,9        | 0.46 | 0        | 8,8,8       | 1.05 | 1 (12%)  |
| 4   | PRO  | C     | 604 | -    | 8,8,8        | 0.85 | 1 (12%)  | 10,10,10    | 1.41 | 2 (20%)  |
| 4   | PRO  | C     | 606 | -    | 8,8,8        | 0.97 | 1 (12%)  | 10,10,10    | 1.17 | 1 (10%)  |
| 2   | PGE  | C     | 602 | -    | 9,9,9        | 0.81 | 0        | 8,8,8       | 0.71 | 0        |
| 4   | PRO  | A     | 604 | -    | 8,8,8        | 0.81 | 0        | 10,10,10    | 1.64 | 2 (20%)  |

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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 4   | PRO  | B     | 604 | -    | -       | 2/4/11/11 | 0/1/1/1 |
| 4   | PRO  | C     | 605 | -    | -       | 0/4/11/11 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 4   | PRO  | B     | 602 | -    | -       | 0/4/11/11 | 0/1/1/1 |
| 4   | PRO  | A     | 606 | -    | -       | 0/4/11/11 | 0/1/1/1 |
| 2   | PGE  | A     | 602 | -    | -       | 7/7/7/7   | -       |
| 2   | PGE  | D     | 601 | -    | -       | 5/7/7/7   | -       |
| 2   | PGE  | A     | 601 | -    | -       | 3/7/7/7   | -       |
| 4   | PRO  | D     | 603 | -    | -       | 4/4/11/11 | 0/1/1/1 |
| 2   | PGE  | B     | 601 | -    | -       | 4/7/7/7   | -       |
| 3   | PEG  | A     | 603 | -    | -       | 2/4/4/4   | -       |
| 4   | PRO  | D     | 602 | -    | -       | 4/4/11/11 | 0/1/1/1 |
| 4   | PRO  | B     | 603 | -    | -       | 4/4/11/11 | 0/1/1/1 |
| 4   | PRO  | A     | 605 | -    | -       | 4/4/11/11 | 0/1/1/1 |
| 3   | PEG  | C     | 603 | -    | -       | 3/4/4/4   | -       |
| 2   | PGE  | C     | 601 | -    | -       | 4/7/7/7   | -       |
| 4   | PRO  | C     | 604 | -    | -       | 2/4/11/11 | 0/1/1/1 |
| 4   | PRO  | C     | 606 | -    | -       | 4/4/11/11 | 0/1/1/1 |
| 2   | PGE  | C     | 602 | -    | -       | 4/7/7/7   | -       |
| 4   | PRO  | A     | 604 | -    | -       | 0/4/11/11 | 0/1/1/1 |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | C     | 603 | PEG  | O2-C3 | 3.26  | 1.56        | 1.42     |
| 4   | B     | 602 | PRO  | OXT-C | -2.36 | 1.23        | 1.30     |
| 4   | A     | 605 | PRO  | OXT-C | -2.30 | 1.23        | 1.30     |
| 4   | C     | 606 | PRO  | OXT-C | -2.10 | 1.23        | 1.30     |
| 4   | C     | 604 | PRO  | OXT-C | -2.09 | 1.24        | 1.30     |
| 4   | C     | 605 | PRO  | OXT-C | -2.05 | 1.24        | 1.30     |
| 4   | D     | 603 | PRO  | OXT-C | -2.04 | 1.24        | 1.30     |

All (20) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 4   | B     | 602 | PRO  | OXT-C-O  | -4.97 | 112.81      | 124.08   |
| 4   | D     | 603 | PRO  | OXT-C-O  | -3.58 | 115.97      | 124.08   |
| 4   | B     | 602 | PRO  | C-CA-N   | 3.08  | 118.88      | 106.84   |
| 2   | D     | 601 | PGE  | O4-C6-C5 | -3.04 | 93.90       | 111.82   |
| 2   | D     | 601 | PGE  | O3-C5-C6 | -3.03 | 96.76       | 110.11   |
| 4   | A     | 604 | PRO  | OXT-C-CA | 3.01  | 123.69      | 113.51   |
| 4   | B     | 604 | PRO  | OXT-C-O  | -2.83 | 117.65      | 124.08   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 4   | A     | 605 | PRO  | OXT-C-O  | -2.76 | 117.83      | 124.08   |
| 4   | A     | 604 | PRO  | OXT-C-O  | -2.72 | 117.90      | 124.08   |
| 4   | A     | 606 | PRO  | OXT-C-CA | 2.56  | 122.19      | 113.51   |
| 4   | A     | 605 | PRO  | OXT-C-CA | 2.50  | 121.96      | 113.51   |
| 4   | C     | 605 | PRO  | OXT-C-CA | 2.45  | 121.80      | 113.51   |
| 4   | C     | 604 | PRO  | OXT-C-CA | 2.43  | 121.75      | 113.51   |
| 4   | C     | 604 | PRO  | OXT-C-O  | -2.35 | 118.76      | 124.08   |
| 4   | D     | 602 | PRO  | OXT-C-O  | -2.32 | 118.81      | 124.08   |
| 4   | B     | 603 | PRO  | CD-N-CA  | 2.25  | 113.03      | 107.22   |
| 4   | B     | 604 | PRO  | OXT-C-CA | 2.21  | 120.98      | 113.51   |
| 2   | C     | 601 | PGE  | O1-C1-C2 | -2.20 | 98.90       | 111.82   |
| 4   | C     | 606 | PRO  | OXT-C-O  | -2.16 | 119.19      | 124.08   |
| 4   | B     | 602 | PRO  | OXT-C-CA | 2.15  | 120.80      | 113.51   |

There are no chirality outliers.

All (56) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 4   | A     | 605 | PRO  | O-C-CA-N    |
| 4   | A     | 605 | PRO  | OXT-C-CA-N  |
| 4   | A     | 605 | PRO  | O-C-CA-CB   |
| 4   | A     | 605 | PRO  | OXT-C-CA-CB |
| 4   | B     | 603 | PRO  | O-C-CA-N    |
| 4   | B     | 603 | PRO  | OXT-C-CA-N  |
| 4   | B     | 603 | PRO  | O-C-CA-CB   |
| 4   | B     | 603 | PRO  | OXT-C-CA-CB |
| 4   | C     | 604 | PRO  | O-C-CA-N    |
| 4   | C     | 604 | PRO  | OXT-C-CA-N  |
| 4   | D     | 602 | PRO  | O-C-CA-N    |
| 4   | D     | 602 | PRO  | OXT-C-CA-N  |
| 4   | D     | 603 | PRO  | O-C-CA-N    |
| 4   | D     | 603 | PRO  | OXT-C-CA-N  |
| 4   | D     | 603 | PRO  | O-C-CA-CB   |
| 4   | D     | 603 | PRO  | OXT-C-CA-CB |
| 2   | A     | 601 | PGE  | O1-C1-C2-O2 |
| 3   | C     | 603 | PEG  | O2-C3-C4-O4 |
| 2   | B     | 601 | PGE  | O3-C5-C6-O4 |
| 2   | D     | 601 | PGE  | O1-C1-C2-O2 |
| 2   | C     | 602 | PGE  | O3-C5-C6-O4 |
| 2   | C     | 602 | PGE  | C6-C5-O3-C4 |
| 2   | C     | 602 | PGE  | O1-C1-C2-O2 |
| 3   | A     | 603 | PEG  | O2-C3-C4-O4 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 3   | C     | 603 | PEG  | O1-C1-C2-O2 |
| 2   | C     | 601 | PGE  | O3-C5-C6-O4 |
| 3   | C     | 603 | PEG  | C1-C2-O2-C3 |
| 2   | A     | 601 | PGE  | O2-C3-C4-O3 |
| 2   | A     | 602 | PGE  | O3-C5-C6-O4 |
| 2   | C     | 601 | PGE  | C4-C3-O2-C2 |
| 2   | A     | 602 | PGE  | C3-C4-O3-C5 |
| 2   | C     | 602 | PGE  | C4-C3-O2-C2 |
| 2   | B     | 601 | PGE  | C6-C5-O3-C4 |
| 2   | C     | 601 | PGE  | O1-C1-C2-O2 |
| 2   | D     | 601 | PGE  | O3-C5-C6-O4 |
| 3   | A     | 603 | PEG  | C4-C3-O2-C2 |
| 2   | A     | 602 | PGE  | C4-C3-O2-C2 |
| 2   | A     | 602 | PGE  | O1-C1-C2-O2 |
| 2   | D     | 601 | PGE  | O2-C3-C4-O3 |
| 2   | A     | 601 | PGE  | C4-C3-O2-C2 |
| 2   | D     | 601 | PGE  | C4-C3-O2-C2 |
| 2   | A     | 602 | PGE  | C1-C2-O2-C3 |
| 2   | A     | 602 | PGE  | O2-C3-C4-O3 |
| 4   | B     | 604 | PRO  | OXT-C-CA-CB |
| 4   | C     | 606 | PRO  | O-C-CA-CB   |
| 4   | C     | 606 | PRO  | OXT-C-CA-CB |
| 4   | D     | 602 | PRO  | OXT-C-CA-CB |
| 2   | B     | 601 | PGE  | C3-C4-O3-C5 |
| 4   | C     | 606 | PRO  | O-C-CA-N    |
| 4   | B     | 604 | PRO  | O-C-CA-CB   |
| 2   | B     | 601 | PGE  | O2-C3-C4-O3 |
| 2   | D     | 601 | PGE  | C3-C4-O3-C5 |
| 4   | C     | 606 | PRO  | OXT-C-CA-N  |
| 4   | D     | 602 | PRO  | O-C-CA-CB   |
| 2   | C     | 601 | PGE  | O2-C3-C4-O3 |
| 2   | A     | 602 | PGE  | C6-C5-O3-C4 |

There are no ring outliers.

11 monomers are involved in 36 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | B     | 604 | PRO  | 1       | 0            |
| 4   | C     | 605 | PRO  | 9       | 0            |
| 4   | A     | 606 | PRO  | 2       | 0            |
| 2   | D     | 601 | PGE  | 3       | 0            |
| 2   | A     | 601 | PGE  | 1       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | D     | 603 | PRO  | 6       | 0            |
| 2   | B     | 601 | PGE  | 3       | 0            |
| 4   | A     | 605 | PRO  | 1       | 0            |
| 2   | C     | 601 | PGE  | 4       | 0            |
| 2   | C     | 602 | PGE  | 5       | 0            |
| 4   | A     | 604 | PRO  | 1       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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     | 583/583 (100%)   | -0.33  | 1 (0%) 91 93 | 31, 54, 87, 140       | 0     |
| 1   | B     | 583/583 (100%)   | -0.42  | 1 (0%) 91 93 | 28, 50, 83, 110       | 0     |
| 1   | C     | 583/583 (100%)   | -0.43  | 0 100 100    | 27, 50, 79, 129       | 0     |
| 1   | D     | 583/583 (100%)   | -0.38  | 0 100 100    | 31, 50, 84, 121       | 0     |
| All | All   | 2332/2332 (100%) | -0.39  | 2 (0%) 92 94 | 27, 51, 84, 140       | 0     |

All (2) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 77  | VAL  | 2.7  |
| 1   | A     | 80  | LEU  | 2.3  |

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 4   | PRO  | C     | 605 | 8/8   | 0.80 | 0.11 | 70,71,77,80                 | 0     |
| 4   | PRO  | B     | 602 | 8/8   | 0.82 | 0.09 | 48,62,72,79                 | 0     |
| 4   | PRO  | D     | 603 | 8/8   | 0.82 | 0.12 | 59,68,72,74                 | 0     |
| 4   | PRO  | A     | 606 | 8/8   | 0.84 | 0.10 | 58,81,91,91                 | 0     |
| 4   | PRO  | B     | 604 | 8/8   | 0.84 | 0.08 | 58,69,74,75                 | 0     |
| 4   | PRO  | D     | 602 | 8/8   | 0.85 | 0.07 | 71,78,87,91                 | 0     |
| 3   | PEG  | C     | 603 | 7/7   | 0.86 | 0.10 | 32,34,37,37                 | 0     |
| 4   | PRO  | C     | 606 | 8/8   | 0.86 | 0.08 | 56,61,66,70                 | 0     |
| 4   | PRO  | A     | 605 | 8/8   | 0.87 | 0.08 | 71,79,81,82                 | 0     |
| 4   | PRO  | B     | 603 | 8/8   | 0.88 | 0.08 | 61,67,70,73                 | 0     |
| 2   | PGE  | C     | 602 | 10/10 | 0.88 | 0.09 | 46,59,67,67                 | 0     |
| 3   | PEG  | A     | 603 | 7/7   | 0.89 | 0.09 | 52,58,65,68                 | 0     |
| 2   | PGE  | A     | 602 | 10/10 | 0.90 | 0.07 | 55,65,71,72                 | 0     |
| 4   | PRO  | A     | 604 | 8/8   | 0.92 | 0.08 | 63,74,81,83                 | 0     |
| 4   | PRO  | C     | 604 | 8/8   | 0.92 | 0.09 | 69,73,80,88                 | 0     |
| 2   | PGE  | D     | 601 | 10/10 | 0.93 | 0.09 | 50,60,76,78                 | 0     |
| 2   | PGE  | B     | 601 | 10/10 | 0.94 | 0.12 | 44,60,68,72                 | 0     |
| 2   | PGE  | A     | 601 | 10/10 | 0.94 | 0.10 | 52,60,67,72                 | 0     |
| 2   | PGE  | C     | 601 | 10/10 | 0.95 | 0.10 | 48,62,70,71                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.