



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:32 AM UTC

PDB ID : 3KCF / pdb\_00003kcf  
Title : Crystal structure of TGFbRI complexed with a pyrazolone inhibitor  
Authors : Boriack-Sjodin, P.A.  
Deposited on : 2009-10-21  
Resolution : 2.80 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  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

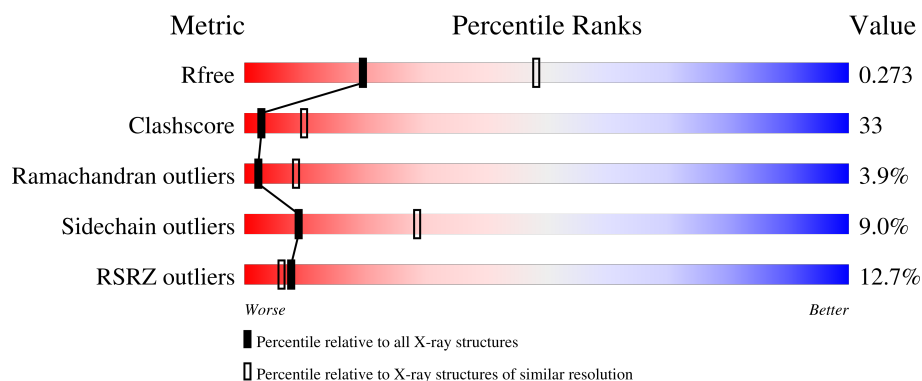
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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                      | 3866 (2.80-2.80)                                      |
| Clashscore            | 190562                      | 4276 (2.80-2.80)                                      |
| Ramachandran outliers | 187476                      | 4196 (2.80-2.80)                                      |
| Sidechain outliers    | 187428                      | 4198 (2.80-2.80)                                      |
| RSRZ outliers         | 180081                      | 3869 (2.80-2.80)                                      |

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     | 342    | <div> <div>16%</div> <div>43%</div> <div>45%</div> <div>8%</div> <div>••</div> </div> |
| 1   | B     | 342    | <div> <div>4%</div> <div>48%</div> <div>39%</div> <div>7%</div> <div>5%</div> </div>  |
| 1   | C     | 342    | <div> <div>26%</div> <div>35%</div> <div>54%</div> <div>8%</div> <div>•</div> </div>  |
| 1   | D     | 342    | <div> <div>7%</div> <div>48%</div> <div>38%</div> <div>10%</div> <div>•</div> </div>  |
| 1   | E     | 342    | <div> <div>8%</div> <div>50%</div> <div>38%</div> <div>8%</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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3   | PO4  | B     | 11  | -         | -        | X       | -                |
| 3   | PO4  | E     | 3   | -         | -        | X       | -                |

## 2 Entry composition [i](#)

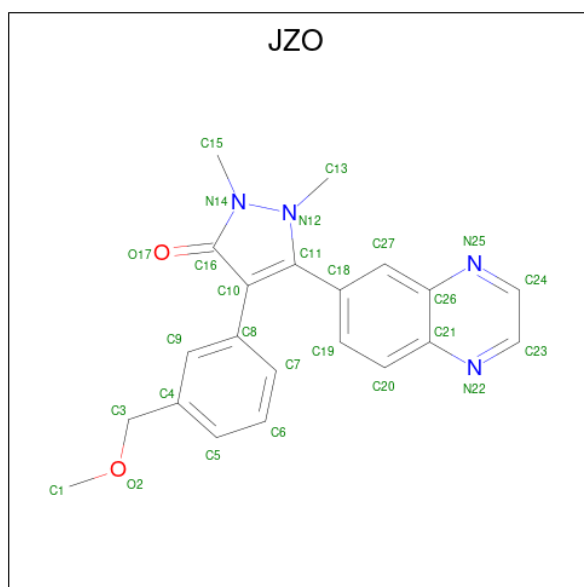
There are 4 unique types of molecules in this entry. The entry contains 13297 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TGF-beta receptor type-1.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 328      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2617  | 1650 | 469 | 482 | 16 |         |         |       |
| 1   | B     | 324      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2590  | 1636 | 463 | 475 | 16 |         |         |       |
| 1   | C     | 330      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2629  | 1658 | 471 | 484 | 16 |         |         |       |
| 1   | D     | 330      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2629  | 1658 | 471 | 484 | 16 |         |         |       |
| 1   | E     | 330      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2629  | 1658 | 471 | 484 | 16 |         |         |       |

- Molecule 2 is 4-[3-(methoxymethyl)phenyl]-1,2-dimethyl-5-quinoxalin-6-yl-1,2-dihydro-3H-pyrazol-3-one (CCD ID: JZO) (formula: C<sub>21</sub>H<sub>20</sub>N<sub>4</sub>O<sub>2</sub>).



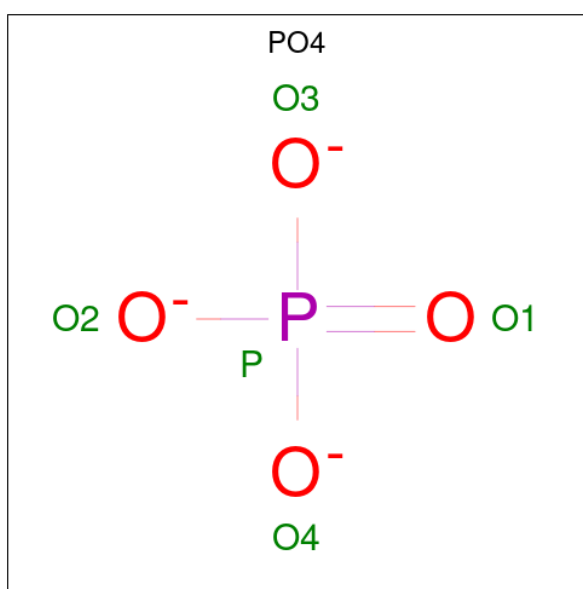
| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 2   | A     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 27    | 21 | 4 | 2 |         |         |

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| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 2   | B     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 27    | 21 | 4 | 2 |         |         |
| 2   | C     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 27    | 21 | 4 | 2 |         |         |
| 2   | D     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 27    | 21 | 4 | 2 |         |         |
| 2   | E     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 27    | 21 | 4 | 2 |         |         |

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | A     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | A     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | A     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | B     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | B     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | B     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | C     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | D     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | D     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | D     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | E     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | E     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | E     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

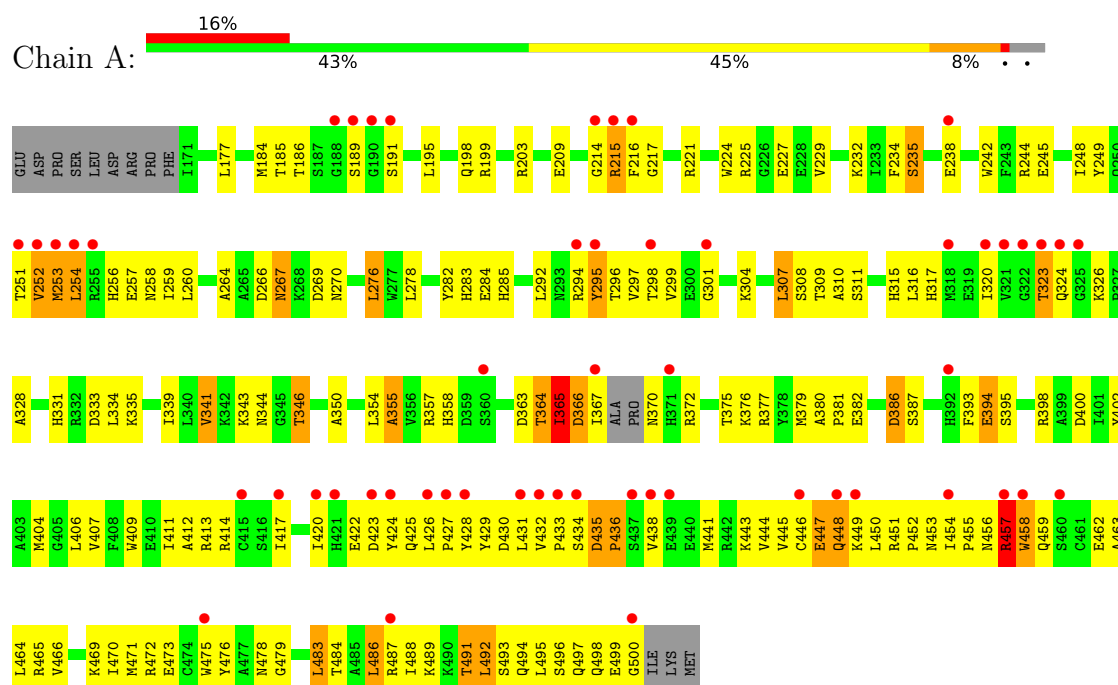
- Molecule 4 is water.

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

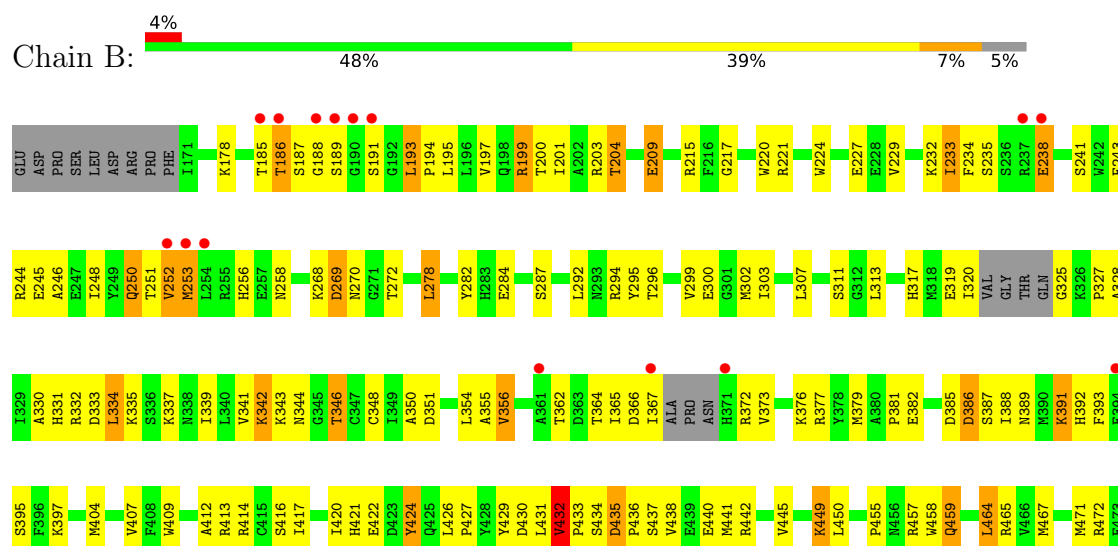
### 3 Residue-property plots

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

#### • Molecule 1: TGF-beta receptor type-1



#### • Molecule 1: TGF-beta receptor type-1

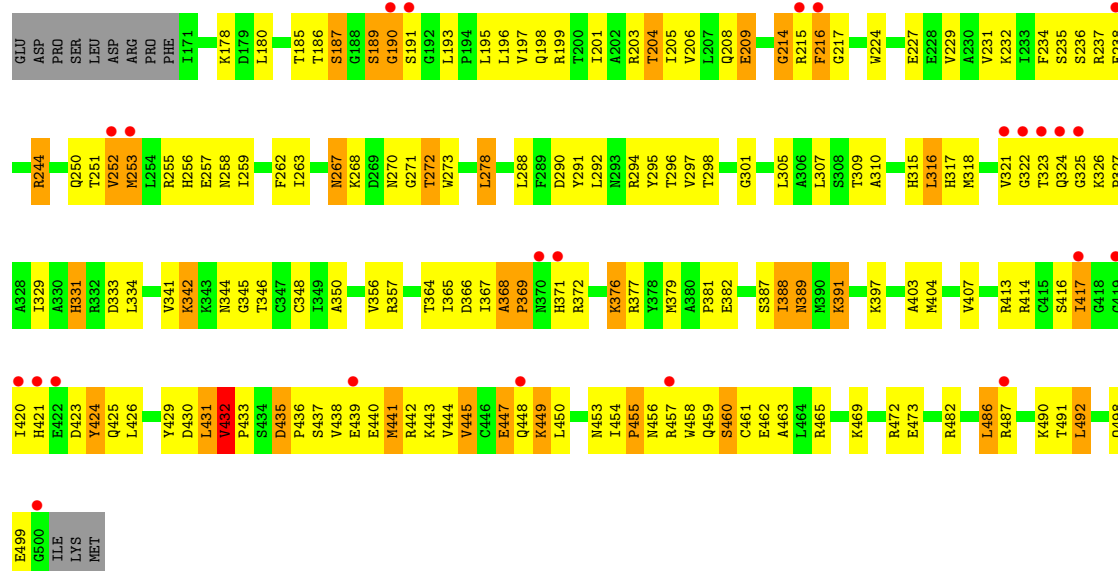




• Molecule 1: TGF-beta receptor type-1

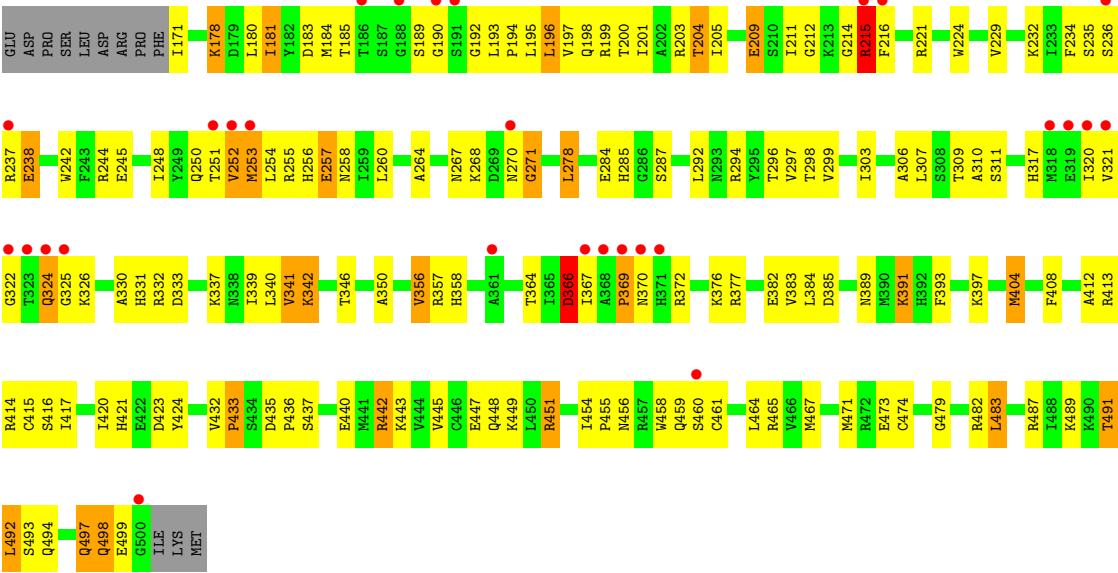


• Molecule 1: TGF-beta receptor type-1



• Molecule 1: TGF-beta receptor type-1





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 2 2 21                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 174.03Å 249.08Å 138.01Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 34.86 – 2.80<br>34.86 – 2.80                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.6 (34.86-2.80)<br>99.6 (34.86-2.80)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.10                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.12 (at 2.81Å)                                             | Xtriage          |
| Refinement program                                                      | CNX 2005                                                    | Depositor        |
| R, $R_{free}$                                                           | 0.235 , 0.278<br>0.232 , 0.273                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 3747 reflections (5.10%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 50.2                                                        | Xtriage          |
| Anisotropy                                                              | 0.249                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.36 , 62.7                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.91                                                        | EDS              |
| Total number of atoms                                                   | 13297                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 52.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: JZO, PO4

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

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # $ Z  > 5$    | RMSZ        | # $ Z  > 5$     |
| 1   | A     | 0.47         | 2/2668 (0.1%)  | 0.89        | 7/3600 (0.2%)   |
| 1   | B     | 0.49         | 0/2640         | 0.98        | 11/3560 (0.3%)  |
| 1   | C     | 0.42         | 0/2682         | 0.92        | 5/3622 (0.1%)   |
| 1   | D     | 0.49         | 0/2682         | 1.08        | 19/3622 (0.5%)  |
| 1   | E     | 0.51         | 0/2682         | 1.00        | 12/3622 (0.3%)  |
| All | All   | 0.48         | 2/13354 (0.0%) | 0.98        | 54/18026 (0.3%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | B     | 0                   | 1                   |
| 1   | D     | 0                   | 1                   |
| 1   | E     | 0                   | 1                   |
| All | All   | 0                   | 3                   |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 245 | GLU  | CA-C  | -9.75 | 1.40        | 1.52     |
| 1   | A     | 245 | GLU  | N-CA  | 9.30  | 1.57        | 1.46     |

All (54) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | D     | 296 | THR  | N-CA-C | -7.70 | 98.03       | 109.81   |
| 1   | B     | 296 | THR  | N-CA-C | -7.68 | 97.72       | 109.85   |
| 1   | B     | 268 | LYS  | N-CA-C | 7.31  | 122.64      | 113.43   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | D     | 432 | VAL  | CA-C-N  | 7.15  | 127.57      | 119.92   |
| 1   | D     | 432 | VAL  | C-N-CA  | 7.15  | 127.57      | 119.92   |
| 1   | D     | 368 | ALA  | CA-C-N  | 7.10  | 128.72      | 119.84   |
| 1   | D     | 368 | ALA  | C-N-CA  | 7.10  | 128.72      | 119.84   |
| 1   | E     | 296 | THR  | N-CA-C  | -6.92 | 99.99       | 109.95   |
| 1   | D     | 435 | ASP  | CA-C-N  | 6.74  | 126.77      | 119.89   |
| 1   | D     | 435 | ASP  | C-N-CA  | 6.74  | 126.77      | 119.89   |
| 1   | A     | 254 | LEU  | N-CA-C  | -6.49 | 105.18      | 113.23   |
| 1   | D     | 268 | LYS  | N-CA-C  | 6.39  | 124.41      | 110.80   |
| 1   | E     | 321 | VAL  | N-CA-C  | 6.38  | 119.02      | 111.05   |
| 1   | B     | 435 | ASP  | CA-C-N  | 6.22  | 126.19      | 120.03   |
| 1   | B     | 435 | ASP  | C-N-CA  | 6.22  | 126.19      | 120.03   |
| 1   | E     | 268 | LYS  | N-CA-C  | 6.14  | 123.89      | 110.80   |
| 1   | E     | 251 | THR  | N-CA-C  | -5.93 | 98.73       | 108.76   |
| 1   | D     | 237 | ARG  | N-CA-C  | 5.93  | 119.62      | 112.38   |
| 1   | B     | 241 | SER  | N-CA-C  | -5.82 | 104.86      | 111.14   |
| 1   | A     | 295 | TYR  | N-CA-C  | 5.80  | 117.06      | 108.60   |
| 1   | C     | 466 | VAL  | N-CA-C  | -5.78 | 106.65      | 113.42   |
| 1   | D     | 255 | ARG  | N-CA-C  | -5.68 | 97.60       | 107.49   |
| 1   | B     | 459 | GLN  | N-CA-C  | -5.67 | 106.52      | 113.50   |
| 1   | D     | 288 | LEU  | N-CA-C  | -5.67 | 105.10      | 111.28   |
| 1   | D     | 193 | LEU  | CA-C-N  | 5.64  | 125.59      | 119.78   |
| 1   | D     | 193 | LEU  | C-N-CA  | 5.64  | 125.59      | 119.78   |
| 1   | C     | 184 | MET  | N-CA-C  | -5.59 | 103.99      | 112.04   |
| 1   | E     | 474 | CYS  | N-CA-C  | -5.56 | 106.39      | 114.12   |
| 1   | E     | 212 | GLY  | N-CA-C  | 5.52  | 118.95      | 111.72   |
| 1   | B     | 373 | VAL  | N-CA-C  | 5.51  | 115.55      | 108.82   |
| 1   | E     | 264 | ALA  | N-CA-C  | 5.50  | 116.63      | 108.60   |
| 1   | E     | 181 | ILE  | N-CA-C  | -5.42 | 104.59      | 110.23   |
| 1   | A     | 380 | ALA  | CA-C-N  | 5.40  | 124.86      | 119.24   |
| 1   | A     | 380 | ALA  | C-N-CA  | 5.40  | 124.86      | 119.24   |
| 1   | B     | 432 | VAL  | CA-C-N  | 5.38  | 125.36      | 120.03   |
| 1   | B     | 432 | VAL  | C-N-CA  | 5.38  | 125.36      | 120.03   |
| 1   | D     | 445 | VAL  | N-CA-C  | 5.38  | 118.65      | 111.44   |
| 1   | E     | 391 | LYS  | N-CA-C  | -5.33 | 106.62      | 113.23   |
| 1   | A     | 435 | ASP  | CA-C-N  | 5.29  | 126.45      | 119.84   |
| 1   | A     | 435 | ASP  | C-N-CA  | 5.29  | 126.45      | 119.84   |
| 1   | D     | 437 | SER  | N-CA-C  | -5.28 | 102.37      | 110.14   |
| 1   | D     | 263 | ILE  | CB-CA-C | -5.27 | 106.36      | 111.05   |
| 1   | B     | 243 | PHE  | N-CA-C  | 5.26  | 116.70      | 111.07   |
| 1   | E     | 183 | ASP  | N-CA-C  | 5.24  | 116.99      | 111.28   |
| 1   | D     | 391 | LYS  | N-CA-C  | -5.23 | 106.90      | 113.28   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | E     | 366 | ASP  | N-CA-C | 5.22  | 121.92      | 110.80   |
| 1   | E     | 370 | ASN  | N-CA-C | -5.20 | 106.02      | 114.09   |
| 1   | D     | 331 | HIS  | N-CA-C | 5.16  | 116.59      | 111.07   |
| 1   | C     | 494 | GLN  | N-CA-C | -5.14 | 106.51      | 112.89   |
| 1   | C     | 235 | SER  | N-CA-C | -5.13 | 103.76      | 110.53   |
| 1   | C     | 453 | ASN  | N-CA-C | 5.12  | 117.52      | 109.39   |
| 1   | A     | 235 | SER  | N-CA-C | -5.10 | 102.14      | 110.20   |
| 1   | B     | 253 | MET  | N-CA-C | 5.07  | 117.37      | 110.88   |
| 1   | D     | 214 | GLY  | N-CA-C | 5.07  | 117.94      | 110.80   |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | B     | 424 | TYR  | Sidechain |
| 1   | D     | 424 | TYR  | Sidechain |
| 1   | E     | 424 | TYR  | Sidechain |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2617  | 0        | 2618     | 184     | 0            |
| 1   | B     | 2590  | 0        | 2595     | 128     | 0            |
| 1   | C     | 2629  | 0        | 2631     | 257     | 0            |
| 1   | D     | 2629  | 0        | 2631     | 166     | 0            |
| 1   | E     | 2629  | 0        | 2631     | 141     | 0            |
| 2   | A     | 27    | 0        | 20       | 1       | 0            |
| 2   | B     | 27    | 0        | 20       | 0       | 0            |
| 2   | C     | 27    | 0        | 20       | 3       | 0            |
| 2   | D     | 27    | 0        | 20       | 3       | 0            |
| 2   | E     | 27    | 0        | 20       | 1       | 0            |
| 3   | A     | 15    | 0        | 0        | 0       | 0            |
| 3   | B     | 15    | 0        | 0        | 4       | 0            |
| 3   | C     | 5     | 0        | 0        | 1       | 0            |
| 3   | D     | 15    | 0        | 0        | 1       | 0            |
| 3   | E     | 15    | 0        | 0        | 3       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | A     | 1     | 0        | 0        | 1       | 0            |
| 4   | C     | 1     | 0        | 0        | 0       | 0            |
| 4   | E     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 13297 | 0        | 13206    | 874     | 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 33.

All (874) 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:B:376:LYS:HA   | 1:B:379:MET:HE3  | 1.28                     | 1.14              |
| 1:E:216:PHE:HB3  | 1:E:238:GLU:HG2  | 1.22                     | 1.10              |
| 1:A:443:LYS:HG2  | 1:A:448:GLN:HE21 | 1.19                     | 1.08              |
| 1:C:461:CYS:HB2  | 1:C:464:LEU:HD23 | 1.35                     | 1.05              |
| 1:D:367:ILE:HG13 | 1:D:369:PRO:HD3  | 1.40                     | 1.04              |
| 1:E:253:MET:HB2  | 1:E:326:LYS:HB3  | 1.41                     | 1.01              |
| 1:E:367:ILE:HG13 | 1:E:369:PRO:HD3  | 1.40                     | 1.01              |
| 1:C:253:MET:HB3  | 1:C:326:LYS:HB3  | 1.49                     | 0.95              |
| 1:A:309:THR:HG22 | 1:A:404:MET:HE2  | 1.46                     | 0.94              |
| 1:E:256:HIS:HD2  | 1:E:258:ASN:H    | 1.11                     | 0.94              |
| 1:C:244:ARG:HH11 | 1:C:367:ILE:HG12 | 1.33                     | 0.93              |
| 1:B:331:HIS:HD2  | 1:B:333:ASP:H    | 1.17                     | 0.92              |
| 1:C:215:ARG:HH11 | 1:C:215:ARG:HB3  | 1.33                     | 0.91              |
| 1:D:417:ILE:HG13 | 1:D:420:ILE:HG13 | 1.49                     | 0.91              |
| 1:A:372:ARG:HH11 | 1:A:438:VAL:HG11 | 1.33                     | 0.91              |
| 1:B:317:HIS:HB3  | 1:B:397:LYS:HE3  | 1.53                     | 0.88              |
| 1:C:376:LYS:HA   | 1:C:379:MET:HG3  | 1.56                     | 0.87              |
| 1:C:417:ILE:HB   | 1:C:420:ILE:HD11 | 1.57                     | 0.86              |
| 1:D:310:ALA:HA   | 1:D:404:MET:HE1  | 1.56                     | 0.86              |
| 1:A:443:LYS:HG2  | 1:A:448:GLN:NE2  | 1.88                     | 0.86              |
| 1:C:406:LEU:HD12 | 1:C:427:PRO:HB3  | 1.58                     | 0.86              |
| 1:E:487:ARG:O    | 1:E:491:THR:HG22 | 1.76                     | 0.86              |
| 1:E:216:PHE:HB3  | 1:E:238:GLU:CG   | 2.06                     | 0.86              |
| 1:A:267:ASN:HD22 | 1:A:267:ASN:H    | 1.20                     | 0.86              |
| 1:A:372:ARG:HH21 | 1:A:386:ASP:HB2  | 1.39                     | 0.85              |
| 1:C:302:MET:HE3  | 1:C:467:MET:HG3  | 1.59                     | 0.85              |
| 1:B:458:TRP:HZ3  | 1:B:471:MET:HE1  | 1.42                     | 0.84              |
| 1:A:267:ASN:HD22 | 1:A:267:ASN:N    | 1.74                     | 0.84              |
| 1:D:487:ARG:NH2  | 1:D:490:LYS:HD2  | 1.92                     | 0.84              |
| 1:C:409:TRP:HD1  | 1:C:471:MET:HE1  | 1.41                     | 0.84              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:215:ARG:HG3  | 1:C:216:PHE:H    | 1.41                     | 0.83              |
| 1:A:498:GLN:HG3  | 1:A:499:GLU:H    | 1.44                     | 0.81              |
| 1:E:204:THR:HG22 | 1:E:224:TRP:NE1  | 1.96                     | 0.80              |
| 1:B:244:ARG:HG2  | 1:B:244:ARG:HH11 | 1.46                     | 0.80              |
| 1:D:251:THR:O    | 1:D:252:VAL:HG22 | 1.81                     | 0.80              |
| 1:C:181:ILE:HA   | 1:C:184:MET:HE3  | 1.62                     | 0.79              |
| 1:D:389:ASN:ND2  | 1:D:391:LYS:H    | 1.79                     | 0.79              |
| 1:C:244:ARG:NH1  | 1:C:367:ILE:HG12 | 1.97                     | 0.78              |
| 1:D:309:THR:HG22 | 1:D:404:MET:HE2  | 1.64                     | 0.78              |
| 1:A:259:ILE:HD11 | 1:A:316:LEU:HG   | 1.66                     | 0.78              |
| 1:C:199:ARG:HD2  | 1:C:203:ARG:CZ   | 2.14                     | 0.78              |
| 1:A:372:ARG:NH2  | 1:A:386:ASP:HB2  | 1.97                     | 0.78              |
| 1:A:457:ARG:HB2  | 1:A:457:ARG:HH11 | 1.49                     | 0.78              |
| 1:E:256:HIS:CD2  | 1:E:258:ASN:H    | 1.98                     | 0.77              |
| 1:D:469:LYS:O    | 1:D:473:GLU:HG3  | 1.85                     | 0.77              |
| 1:D:487:ARG:HH22 | 1:D:490:LYS:HD2  | 1.48                     | 0.76              |
| 1:A:417:ILE:HG13 | 1:A:420:ILE:HD11 | 1.66                     | 0.76              |
| 1:D:252:VAL:HG21 | 1:D:327:PRO:HD2  | 1.66                     | 0.75              |
| 1:D:253:MET:HE2  | 1:D:324:GLN:O    | 1.85                     | 0.75              |
| 1:E:204:THR:HG22 | 1:E:224:TRP:HE1  | 1.47                     | 0.75              |
| 1:A:301:GLY:HA2  | 1:A:304:LYS:NZ   | 2.02                     | 0.75              |
| 1:A:376:LYS:HA   | 1:A:379:MET:SD   | 2.27                     | 0.74              |
| 1:D:389:ASN:HD21 | 1:D:391:LYS:HB3  | 1.51                     | 0.74              |
| 1:C:479:GLY:HA2  | 1:C:482:ARG:HD2  | 1.69                     | 0.74              |
| 1:D:317:HIS:HB3  | 1:D:397:LYS:HE3  | 1.70                     | 0.74              |
| 1:E:357:ARG:HB2  | 1:E:366:ASP:HB2  | 1.68                     | 0.74              |
| 1:A:455:PRO:O    | 1:A:458:TRP:HB2  | 1.87                     | 0.74              |
| 1:C:297:VAL:HG22 | 1:C:298:THR:H    | 1.50                     | 0.74              |
| 1:C:310:ALA:HA   | 1:C:404:MET:HE1  | 1.70                     | 0.74              |
| 1:E:199:ARG:HD2  | 1:E:203:ARG:CZ   | 2.19                     | 0.73              |
| 1:C:309:THR:HG22 | 1:C:404:MET:HE2  | 1.68                     | 0.73              |
| 1:B:256:HIS:CD2  | 1:B:258:ASN:H    | 2.05                     | 0.73              |
| 1:D:389:ASN:C    | 1:D:389:ASN:HD22 | 1.97                     | 0.73              |
| 1:B:344:ASN:OD1  | 1:B:346:THR:HB   | 1.88                     | 0.73              |
| 1:D:331:HIS:HD2  | 1:D:333:ASP:H    | 1.36                     | 0.73              |
| 1:C:432:VAL:HG21 | 1:C:436:PRO:HB3  | 1.71                     | 0.73              |
| 1:C:320:ILE:HG22 | 1:C:321:VAL:H    | 1.55                     | 0.72              |
| 1:D:198:GLN:HE22 | 1:D:250:GLN:HE21 | 1.38                     | 0.72              |
| 1:A:249:TYR:HA   | 1:A:254:LEU:HD23 | 1.71                     | 0.72              |
| 1:C:249:TYR:HA   | 1:C:254:LEU:HD23 | 1.72                     | 0.72              |
| 1:E:309:THR:HG22 | 1:E:404:MET:HE3  | 1.72                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:284:GLU:HB3  | 1:A:343:LYS:HE2  | 1.73                     | 0.71              |
| 1:E:253:MET:HE2  | 1:E:325:GLY:HA2  | 1.70                     | 0.71              |
| 1:D:435:ASP:HA   | 3:D:15:PO4:O3    | 1.90                     | 0.71              |
| 1:E:256:HIS:HD2  | 1:E:258:ASN:N    | 1.89                     | 0.71              |
| 1:E:417:ILE:O    | 1:E:420:ILE:HG12 | 1.91                     | 0.71              |
| 1:C:473:GLU:HB3  | 1:C:483:LEU:HG   | 1.73                     | 0.71              |
| 1:C:406:LEU:HD12 | 1:C:427:PRO:CB   | 2.21                     | 0.70              |
| 1:C:199:ARG:HD2  | 1:C:203:ARG:NH2  | 2.07                     | 0.70              |
| 1:C:409:TRP:CD1  | 1:C:471:MET:HE1  | 2.26                     | 0.70              |
| 1:D:199:ARG:HD2  | 1:D:203:ARG:CZ   | 2.21                     | 0.70              |
| 1:D:256:HIS:CD2  | 1:D:258:ASN:H    | 2.09                     | 0.70              |
| 1:D:414:ARG:HH21 | 1:D:423:ASP:HA   | 1.55                     | 0.70              |
| 1:A:301:GLY:HA2  | 1:A:304:LYS:HZ3  | 1.57                     | 0.70              |
| 1:A:498:GLN:HG3  | 1:A:499:GLU:N    | 2.06                     | 0.70              |
| 1:A:307:LEU:HD23 | 1:A:492:LEU:HB3  | 1.74                     | 0.69              |
| 1:C:461:CYS:CB   | 1:C:464:LEU:HD23 | 2.17                     | 0.69              |
| 1:C:483:LEU:HD13 | 1:C:488:ILE:HD11 | 1.74                     | 0.69              |
| 1:E:356:VAL:HG22 | 1:E:393:PHE:HE1  | 1.57                     | 0.69              |
| 1:C:240:ARG:HH11 | 1:C:240:ARG:HB2  | 1.57                     | 0.69              |
| 1:C:444:VAL:HG13 | 1:C:450:LEU:HD12 | 1.74                     | 0.69              |
| 1:C:253:MET:HB3  | 1:C:326:LYS:CB   | 2.20                     | 0.69              |
| 1:D:357:ARG:HB2  | 1:D:366:ASP:HB2  | 1.74                     | 0.69              |
| 1:C:320:ILE:HG22 | 1:C:321:VAL:N    | 2.07                     | 0.69              |
| 1:C:414:ARG:HH11 | 1:C:414:ARG:HB3  | 1.57                     | 0.69              |
| 1:C:376:LYS:HA   | 1:C:379:MET:CG   | 2.20                     | 0.69              |
| 1:E:310:ALA:CA   | 1:E:404:MET:HE1  | 2.23                     | 0.69              |
| 1:B:252:VAL:HG12 | 1:B:253:MET:HG3  | 1.75                     | 0.69              |
| 1:E:252:VAL:HG12 | 1:E:253:MET:H    | 1.58                     | 0.68              |
| 1:E:467:MET:O    | 1:E:471:MET:HG3  | 1.93                     | 0.68              |
| 1:A:469:LYS:O    | 1:A:473:GLU:HG3  | 1.94                     | 0.68              |
| 1:E:253:MET:HG3  | 1:E:326:LYS:N    | 2.09                     | 0.68              |
| 1:C:459:GLN:NE2  | 1:C:465:ARG:HG3  | 2.09                     | 0.68              |
| 1:C:381:PRO:HD2  | 1:C:482:ARG:HH22 | 1.58                     | 0.68              |
| 1:C:470:ILE:HD13 | 1:C:488:ILE:HG23 | 1.76                     | 0.67              |
| 1:A:367:ILE:O    | 1:A:370:ASN:HB2  | 1.94                     | 0.67              |
| 1:E:331:HIS:HD2  | 1:E:333:ASP:H    | 1.42                     | 0.67              |
| 1:A:267:ASN:N    | 1:A:267:ASN:ND2  | 2.42                     | 0.67              |
| 1:C:428:TYR:HD1  | 1:C:441:MET:HE1  | 1.60                     | 0.67              |
| 1:A:443:LYS:HE2  | 1:A:448:GLN:NE2  | 2.11                     | 0.66              |
| 1:C:414:ARG:HH11 | 1:C:414:ARG:CB   | 2.09                     | 0.66              |
| 1:C:215:ARG:HG3  | 1:C:216:PHE:N    | 2.11                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:178:LYS:HD3  | 1:D:178:LYS:N    | 2.08                     | 0.66              |
| 1:C:215:ARG:HH11 | 1:C:215:ARG:CB   | 2.07                     | 0.66              |
| 1:A:235:SER:HB2  | 1:A:238:GLU:HG2  | 1.78                     | 0.66              |
| 1:B:431:LEU:O    | 1:B:432:VAL:HG23 | 1.96                     | 0.66              |
| 1:A:372:ARG:NH1  | 1:A:438:VAL:HG11 | 2.10                     | 0.66              |
| 1:B:385:ASP:HA   | 1:B:442:ARG:CZ   | 2.26                     | 0.66              |
| 1:E:189:SER:O    | 1:E:252:VAL:HG13 | 1.96                     | 0.65              |
| 1:E:260:LEU:HD13 | 1:E:340:LEU:HD13 | 1.78                     | 0.65              |
| 1:C:471:MET:HE2  | 1:C:475:TRP:CH2  | 2.32                     | 0.65              |
| 1:A:284:GLU:OE2  | 1:A:343:LYS:HE2  | 1.96                     | 0.65              |
| 1:C:414:ARG:HB3  | 1:C:414:ARG:NH1  | 2.11                     | 0.65              |
| 1:D:389:ASN:HD22 | 1:D:391:LYS:H    | 1.43                     | 0.65              |
| 1:E:258:ASN:ND2  | 1:E:311:SER:HB2  | 2.12                     | 0.65              |
| 1:A:458:TRP:O    | 1:A:464:LEU:HD12 | 1.97                     | 0.65              |
| 1:C:357:ARG:NE   | 1:C:366:ASP:OD1  | 2.28                     | 0.65              |
| 1:C:430:ASP:OD1  | 1:C:431:LEU:HG   | 1.95                     | 0.65              |
| 1:C:372:ARG:NH1  | 1:C:438:VAL:HG11 | 2.11                     | 0.65              |
| 1:A:394:GLU:O    | 1:A:398:ARG:HG2  | 1.97                     | 0.65              |
| 1:D:251:THR:HG22 | 1:D:252:VAL:HG13 | 1.79                     | 0.65              |
| 1:A:310:ALA:HA   | 1:A:404:MET:HE1  | 1.79                     | 0.64              |
| 1:E:181:ILE:HA   | 1:E:184:MET:HE3  | 1.78                     | 0.64              |
| 1:E:297:VAL:HG12 | 1:E:298:THR:O    | 1.97                     | 0.64              |
| 1:D:443:LYS:HA   | 1:D:447:GLU:CG   | 2.27                     | 0.64              |
| 1:D:235:SER:O    | 1:D:238:GLU:HG2  | 1.97                     | 0.64              |
| 1:E:204:THR:CG2  | 1:E:224:TRP:HE1  | 2.09                     | 0.64              |
| 1:A:217:GLY:N    | 1:A:238:GLU:OE2  | 2.31                     | 0.64              |
| 1:A:298:THR:HG22 | 1:A:299:VAL:N    | 2.11                     | 0.64              |
| 1:A:309:THR:HG22 | 1:A:404:MET:CE   | 2.23                     | 0.64              |
| 1:A:463:ALA:HB1  | 1:A:495:LEU:HD21 | 1.79                     | 0.64              |
| 1:D:262:PHE:HD1  | 2:D:4:JZO:H1     | 1.63                     | 0.64              |
| 1:E:253:MET:HB2  | 1:E:326:LYS:CB   | 2.25                     | 0.64              |
| 1:C:331:HIS:HD2  | 1:C:333:ASP:H    | 1.44                     | 0.64              |
| 1:E:244:ARG:NH2  | 1:E:366:ASP:OD2  | 2.30                     | 0.64              |
| 1:E:322:GLY:HA3  | 1:E:324:GLN:NE2  | 2.13                     | 0.64              |
| 1:B:244:ARG:HG2  | 1:B:244:ARG:NH1  | 2.11                     | 0.64              |
| 1:C:490:LYS:O    | 1:C:494:GLN:HB2  | 1.98                     | 0.64              |
| 1:A:445:VAL:O    | 1:A:449:LYS:HA   | 1.98                     | 0.64              |
| 1:C:237:ARG:HD3  | 1:C:238:GLU:OE2  | 1.98                     | 0.63              |
| 1:C:467:MET:O    | 1:C:471:MET:HG3  | 1.99                     | 0.63              |
| 1:E:404:MET:HE2  | 1:E:408:PHE:CE2  | 2.33                     | 0.63              |
| 1:D:367:ILE:CG1  | 1:D:369:PRO:HD3  | 2.23                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:381:PRO:HG3  | 1:B:445:VAL:CG1  | 2.28                     | 0.63              |
| 1:C:418:GLY:O    | 1:C:420:ILE:N    | 2.31                     | 0.63              |
| 1:B:204:THR:CG2  | 1:B:224:TRP:HE1  | 2.12                     | 0.63              |
| 1:E:357:ARG:H    | 1:E:366:ASP:HB3  | 1.63                     | 0.63              |
| 1:C:368:ALA:N    | 1:C:369:PRO:HD2  | 2.14                     | 0.62              |
| 1:C:418:GLY:O    | 1:C:420:ILE:HG23 | 1.99                     | 0.62              |
| 1:D:185:THR:C    | 1:D:187:SER:H    | 2.07                     | 0.62              |
| 1:E:445:VAL:HG13 | 1:E:451:ARG:NH1  | 2.14                     | 0.62              |
| 1:A:454:ILE:HG23 | 1:A:458:TRP:CE3  | 2.34                     | 0.62              |
| 1:B:215:ARG:HD2  | 1:B:351:ASP:OD2  | 2.00                     | 0.62              |
| 1:C:478:ASN:C    | 1:C:478:ASN:HD22 | 2.06                     | 0.62              |
| 1:E:199:ARG:HD2  | 1:E:203:ARG:NH2  | 2.15                     | 0.62              |
| 1:A:298:THR:HG22 | 1:A:299:VAL:H    | 1.63                     | 0.62              |
| 1:C:459:GLN:HE21 | 1:C:459:GLN:HA   | 1.63                     | 0.62              |
| 1:C:285:HIS:HB2  | 1:C:341:VAL:HG13 | 1.81                     | 0.62              |
| 1:D:244:ARG:NH2  | 1:D:367:ILE:HG22 | 2.14                     | 0.62              |
| 1:E:310:ALA:HA   | 1:E:404:MET:HE1  | 1.81                     | 0.62              |
| 1:C:297:VAL:HG12 | 1:C:415:CYS:HA   | 1.81                     | 0.62              |
| 1:E:184:MET:HB3  | 1:E:193:LEU:HD23 | 1.82                     | 0.62              |
| 1:D:416:SER:HA   | 1:D:421:HIS:HB3  | 1.81                     | 0.61              |
| 1:C:382:GLU:HB2  | 1:C:388:ILE:HB   | 1.82                     | 0.61              |
| 1:E:432:VAL:HG22 | 1:E:433:PRO:HD2  | 1.82                     | 0.61              |
| 1:C:428:TYR:CD1  | 1:C:441:MET:HE1  | 2.35                     | 0.61              |
| 1:E:331:HIS:CD2  | 1:E:333:ASP:H    | 2.19                     | 0.61              |
| 1:D:178:LYS:HG2  | 1:D:227:GLU:OE2  | 2.01                     | 0.61              |
| 1:A:284:GLU:HB3  | 1:A:343:LYS:CE   | 2.30                     | 0.61              |
| 1:C:420:ILE:HG13 | 1:C:420:ILE:O    | 2.00                     | 0.61              |
| 1:D:198:GLN:HE22 | 1:D:250:GLN:NE2  | 1.98                     | 0.61              |
| 1:C:443:LYS:HG3  | 1:C:447:GLU:OE1  | 2.01                     | 0.61              |
| 1:C:458:TRP:HZ3  | 1:C:471:MET:SD   | 2.23                     | 0.61              |
| 1:B:377:ARG:NH1  | 3:B:11:PO4:O1    | 2.33                     | 0.61              |
| 1:B:302:MET:HE1  | 1:B:464:LEU:HD13 | 1.83                     | 0.61              |
| 1:D:216:PHE:HA   | 1:D:238:GLU:OE2  | 2.01                     | 0.60              |
| 1:E:357:ARG:HB2  | 1:E:366:ASP:CB   | 2.30                     | 0.60              |
| 1:C:466:VAL:O    | 1:C:470:ILE:HG13 | 2.01                     | 0.60              |
| 1:D:318:MET:HE1  | 1:D:486:LEU:HG   | 1.82                     | 0.60              |
| 1:C:302:MET:HG3  | 1:C:411:ILE:HG22 | 1.82                     | 0.60              |
| 1:E:214:GLY:O    | 1:E:215:ARG:C    | 2.44                     | 0.60              |
| 1:B:432:VAL:HG11 | 1:B:436:PRO:HG3  | 1.84                     | 0.60              |
| 1:C:377:ARG:HG3  | 1:C:436:PRO:HG2  | 1.83                     | 0.60              |
| 1:A:428:TYR:HD1  | 1:A:441:MET:HE1  | 1.66                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:381:PRO:HG3  | 1:A:445:VAL:CG1  | 2.31                     | 0.60              |
| 1:C:425:GLN:HE21 | 1:C:425:GLN:HA   | 1.67                     | 0.60              |
| 1:C:284:GLU:HB3  | 1:C:343:LYS:HZ2  | 1.65                     | 0.59              |
| 1:D:459:GLN:NE2  | 1:D:465:ARG:HG3  | 2.17                     | 0.59              |
| 1:A:464:LEU:HD13 | 1:A:464:LEU:O    | 2.01                     | 0.59              |
| 1:D:331:HIS:HE1  | 1:D:350:ALA:O    | 1.85                     | 0.59              |
| 1:A:428:TYR:CD1  | 1:A:441:MET:HE1  | 2.36                     | 0.59              |
| 1:C:287:SER:HA   | 1:C:339:ILE:O    | 2.02                     | 0.59              |
| 1:A:331:HIS:HD2  | 1:A:333:ASP:H    | 1.49                     | 0.59              |
| 1:A:413:ARG:HH12 | 1:A:422:GLU:HB3  | 1.67                     | 0.59              |
| 1:D:294:ARG:HG2  | 1:D:294:ARG:HH11 | 1.68                     | 0.59              |
| 1:E:331:HIS:HD2  | 1:E:333:ASP:N    | 1.99                     | 0.59              |
| 1:A:377:ARG:NH1  | 1:A:426:LEU:HD13 | 2.18                     | 0.59              |
| 1:B:432:VAL:CG1  | 1:B:436:PRO:HG3  | 2.32                     | 0.59              |
| 1:C:459:GLN:NE2  | 1:C:459:GLN:HA   | 2.16                     | 0.59              |
| 1:E:498:GLN:O    | 1:E:499:GLU:HG3  | 2.03                     | 0.59              |
| 1:B:458:TRP:CZ3  | 1:B:471:MET:HE1  | 2.32                     | 0.59              |
| 1:D:256:HIS:HD2  | 1:D:258:ASN:H    | 1.51                     | 0.59              |
| 1:C:285:HIS:CB   | 1:C:341:VAL:HG13 | 2.33                     | 0.58              |
| 1:D:204:THR:CG2  | 1:D:224:TRP:HE1  | 2.15                     | 0.58              |
| 1:A:398:ARG:HD2  | 1:A:479:GLY:O    | 2.03                     | 0.58              |
| 1:C:248:ILE:O    | 1:C:251:THR:HG23 | 2.03                     | 0.58              |
| 1:A:409:TRP:HA   | 1:A:471:MET:HE3  | 1.83                     | 0.58              |
| 1:A:443:LYS:HE2  | 1:A:448:GLN:HE22 | 1.68                     | 0.58              |
| 1:D:294:ARG:HD3  | 1:D:295:TYR:CE2  | 2.38                     | 0.58              |
| 1:E:322:GLY:HA3  | 1:E:324:GLN:HE22 | 1.68                     | 0.58              |
| 1:E:389:ASN:HD21 | 1:E:391:LYS:HB3  | 1.68                     | 0.58              |
| 1:C:215:ARG:CG   | 1:C:216:PHE:H    | 2.15                     | 0.58              |
| 1:C:493:SER:O    | 1:C:497:GLN:HG3  | 2.02                     | 0.58              |
| 1:A:221:ARG:HD2  | 1:A:282:TYR:OH   | 2.03                     | 0.58              |
| 1:A:413:ARG:HG2  | 1:A:413:ARG:HH11 | 1.68                     | 0.58              |
| 1:B:362:THR:O    | 1:B:364:THR:HG23 | 2.03                     | 0.58              |
| 1:C:442:ARG:HA   | 1:C:446:CYS:SG   | 2.43                     | 0.58              |
| 1:C:487:ARG:NH1  | 1:C:490:LYS:HD3  | 2.18                     | 0.58              |
| 1:D:178:LYS:HE2  | 1:D:227:GLU:OE2  | 2.04                     | 0.58              |
| 1:D:262:PHE:CD1  | 2:D:4:JZO:H1     | 2.38                     | 0.58              |
| 1:D:377:ARG:HE   | 1:D:426:LEU:HB3  | 1.69                     | 0.58              |
| 1:C:313:LEU:HD22 | 1:C:334:LEU:CD1  | 2.34                     | 0.58              |
| 1:E:330:ALA:HB3  | 1:E:356:VAL:HG13 | 1.86                     | 0.58              |
| 1:A:459:GLN:HB3  | 1:A:465:ARG:HD3  | 1.86                     | 0.58              |
| 1:C:260:LEU:HD13 | 1:C:340:LEU:CD1  | 2.34                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:315:HIS:O    | 1:D:326:LYS:HE3  | 2.05                     | 0.57              |
| 1:D:310:ALA:HA   | 1:D:404:MET:CE   | 2.31                     | 0.57              |
| 1:B:331:HIS:CD2  | 1:B:333:ASP:H    | 2.09                     | 0.57              |
| 1:C:313:LEU:HD22 | 1:C:334:LEU:HD12 | 1.85                     | 0.57              |
| 1:B:365:ILE:HD11 | 1:B:367:ILE:HD13 | 1.86                     | 0.57              |
| 1:C:183:ASP:O    | 1:C:187:SER:HB2  | 2.04                     | 0.57              |
| 1:C:451:ARG:HE   | 1:C:475:TRP:HB3  | 1.69                     | 0.57              |
| 1:D:487:ARG:HA   | 1:D:487:ARG:NE   | 2.19                     | 0.57              |
| 1:A:364:THR:O    | 1:A:365:ILE:HG23 | 2.04                     | 0.57              |
| 1:B:437:SER:OG   | 1:B:440:GLU:HG3  | 2.03                     | 0.57              |
| 1:C:232:LYS:HE3  | 1:C:234:PHE:CZ   | 2.39                     | 0.57              |
| 1:E:204:THR:CG2  | 1:E:224:TRP:NE1  | 2.65                     | 0.57              |
| 1:A:466:VAL:O    | 1:A:470:ILE:HG13 | 2.04                     | 0.57              |
| 1:C:244:ARG:NH2  | 1:C:366:ASP:OD1  | 2.38                     | 0.57              |
| 1:A:214:GLY:O    | 1:A:215:ARG:C    | 2.48                     | 0.57              |
| 1:C:472:ARG:C    | 1:C:474:CYS:H    | 2.12                     | 0.57              |
| 1:B:215:ARG:NH1  | 1:B:215:ARG:HB3  | 2.19                     | 0.57              |
| 1:D:368:ALA:HB2  | 1:E:178:LYS:HD3  | 1.87                     | 0.56              |
| 1:A:463:ALA:HB2  | 1:A:495:LEU:HD11 | 1.86                     | 0.56              |
| 1:C:331:HIS:CD2  | 1:C:333:ASP:H    | 2.23                     | 0.56              |
| 1:D:215:ARG:HG2  | 1:D:215:ARG:HH11 | 1.69                     | 0.56              |
| 1:A:297:VAL:HG22 | 1:A:298:THR:N    | 2.20                     | 0.56              |
| 1:C:494:GLN:HA   | 1:C:497:GLN:NE2  | 2.20                     | 0.56              |
| 1:D:342:LYS:HD3  | 1:D:346:THR:HG23 | 1.86                     | 0.56              |
| 1:D:389:ASN:ND2  | 1:D:389:ASN:C    | 2.59                     | 0.56              |
| 1:E:209:GLU:OE2  | 1:E:221:ARG:HD3  | 2.06                     | 0.56              |
| 1:E:317:HIS:HB3  | 1:E:397:LYS:HE3  | 1.87                     | 0.56              |
| 1:D:456:ASN:C    | 1:D:458:TRP:H    | 2.12                     | 0.56              |
| 1:C:256:HIS:CD2  | 1:C:258:ASN:H    | 2.24                     | 0.56              |
| 1:C:426:LEU:O    | 1:C:429:TYR:HB3  | 2.06                     | 0.56              |
| 1:D:178:LYS:HE2  | 1:D:227:GLU:CD   | 2.31                     | 0.56              |
| 1:E:245:GLU:HB3  | 1:E:278:LEU:HD21 | 1.86                     | 0.56              |
| 1:A:487:ARG:HE   | 1:A:491:THR:HG22 | 1.70                     | 0.56              |
| 1:A:195:LEU:HD12 | 1:A:195:LEU:H    | 1.70                     | 0.56              |
| 1:B:217:GLY:N    | 1:B:238:GLU:OE2  | 2.39                     | 0.56              |
| 1:D:425:GLN:HB3  | 1:D:429:TYR:CD2  | 2.41                     | 0.56              |
| 1:E:404:MET:HE2  | 1:E:408:PHE:CZ   | 2.41                     | 0.56              |
| 1:B:199:ARG:HH11 | 1:B:203:ARG:NH2  | 2.04                     | 0.55              |
| 1:C:232:LYS:HE3  | 1:C:234:PHE:HZ   | 1.71                     | 0.55              |
| 1:D:344:ASN:OD1  | 1:D:346:THR:HG22 | 2.07                     | 0.55              |
| 1:D:432:VAL:CG1  | 1:D:436:PRO:HG3  | 2.37                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:435:ASP:N    | 1:E:436:PRO:HD3  | 2.21                     | 0.55              |
| 1:A:177:LEU:H    | 1:A:227:GLU:CD   | 2.15                     | 0.55              |
| 1:E:389:ASN:ND2  | 1:E:391:LYS:HB3  | 2.21                     | 0.55              |
| 1:A:456:ASN:C    | 1:A:458:TRP:H    | 2.15                     | 0.55              |
| 1:C:283:HIS:ND1  | 3:C:10:PO4:O4    | 2.39                     | 0.55              |
| 1:C:313:LEU:HD11 | 1:C:317:HIS:NE2  | 2.21                     | 0.55              |
| 1:C:379:MET:HE2  | 1:C:383:VAL:HG11 | 1.89                     | 0.55              |
| 1:D:189:SER:O    | 1:D:191:SER:N    | 2.39                     | 0.55              |
| 1:E:256:HIS:CD2  | 1:E:257:GLU:N    | 2.74                     | 0.55              |
| 1:B:331:HIS:HD2  | 1:B:333:ASP:N    | 1.97                     | 0.55              |
| 1:C:487:ARG:HH21 | 1:C:491:THR:HG22 | 1.71                     | 0.55              |
| 1:D:272:THR:HG22 | 1:D:273:TRP:CD1  | 2.42                     | 0.55              |
| 1:D:217:GLY:N    | 1:D:238:GLU:OE1  | 2.40                     | 0.55              |
| 1:C:478:ASN:HD21 | 1:C:480:ALA:HB3  | 1.72                     | 0.55              |
| 1:D:459:GLN:HE22 | 1:D:465:ARG:HG3  | 1.72                     | 0.55              |
| 1:E:190:GLY:C    | 1:E:192:GLY:H    | 2.15                     | 0.55              |
| 1:E:310:ALA:HB2  | 1:E:404:MET:HE1  | 1.89                     | 0.55              |
| 1:D:234:PHE:HA   | 1:D:238:GLU:OE1  | 2.06                     | 0.55              |
| 1:A:177:LEU:N    | 1:A:227:GLU:OE2  | 2.40                     | 0.55              |
| 1:B:253:MET:HE3  | 1:B:325:GLY:O    | 2.07                     | 0.54              |
| 1:E:244:ARG:O    | 1:E:248:ILE:HG12 | 2.08                     | 0.54              |
| 1:A:447:GLU:O    | 1:A:449:LYS:N    | 2.40                     | 0.54              |
| 1:C:362:THR:HG22 | 1:C:364:THR:HG23 | 1.87                     | 0.54              |
| 1:C:458:TRP:HE3  | 1:C:468:ALA:HB2  | 1.73                     | 0.54              |
| 1:C:258:ASN:O    | 1:C:348:CYS:HA   | 2.08                     | 0.54              |
| 1:A:457:ARG:HH11 | 1:A:457:ARG:CB   | 2.20                     | 0.54              |
| 1:B:434:SER:O    | 1:B:435:ASP:HB3  | 2.07                     | 0.54              |
| 1:C:438:VAL:O    | 1:C:442:ARG:HB2  | 2.07                     | 0.54              |
| 1:C:435:ASP:N    | 1:C:436:PRO:HD3  | 2.21                     | 0.54              |
| 1:D:417:ILE:O    | 1:D:420:ILE:HG12 | 2.08                     | 0.54              |
| 1:C:240:ARG:HH11 | 1:C:240:ARG:CB   | 2.20                     | 0.54              |
| 1:B:197:VAL:O    | 1:B:201:ILE:HG12 | 2.08                     | 0.54              |
| 1:C:293:ASN:HD22 | 1:C:424:TYR:HD2  | 1.55                     | 0.54              |
| 1:C:417:ILE:HG12 | 1:C:461:CYS:SG   | 2.47                     | 0.54              |
| 1:C:487:ARG:O    | 1:C:491:THR:HG23 | 2.08                     | 0.54              |
| 1:D:432:VAL:HG13 | 1:D:436:PRO:HG3  | 1.90                     | 0.54              |
| 1:E:331:HIS:HE1  | 1:E:350:ALA:O    | 1.90                     | 0.54              |
| 1:E:331:HIS:O    | 1:E:332:ARG:HB2  | 2.07                     | 0.54              |
| 1:E:473:GLU:HB3  | 1:E:483:LEU:HG   | 1.90                     | 0.53              |
| 1:A:251:THR:O    | 1:A:252:VAL:HG22 | 2.08                     | 0.53              |
| 1:E:389:ASN:HD21 | 1:E:391:LYS:CB   | 2.21                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:356:VAL:HG23 | 1:C:365:ILE:HG23 | 1.91                     | 0.53              |
| 1:D:417:ILE:HD11 | 1:D:457:ARG:HH11 | 1.74                     | 0.53              |
| 1:D:441:MET:O    | 1:D:442:ARG:C    | 2.51                     | 0.53              |
| 1:B:409:TRP:HD1  | 1:B:471:MET:CE   | 2.22                     | 0.53              |
| 1:D:372:ARG:NH1  | 1:D:438:VAL:HG11 | 2.24                     | 0.53              |
| 1:D:376:LYS:HA   | 1:D:379:MET:HE3  | 1.89                     | 0.53              |
| 1:E:372:ARG:NH1  | 1:E:383:VAL:O    | 2.42                     | 0.53              |
| 1:A:486:LEU:O    | 1:A:489:LYS:HB3  | 2.09                     | 0.53              |
| 1:B:246:ALA:O    | 1:B:250:GLN:HG3  | 2.08                     | 0.53              |
| 1:B:331:HIS:HE1  | 1:B:350:ALA:O    | 1.92                     | 0.53              |
| 1:E:184:MET:HB3  | 1:E:193:LEU:CD2  | 2.39                     | 0.53              |
| 1:A:498:GLN:CG   | 1:A:499:GLU:H    | 2.17                     | 0.53              |
| 1:B:333:ASP:HB2  | 1:B:354:LEU:HD12 | 1.91                     | 0.53              |
| 1:B:413:ARG:NH1  | 1:B:422:GLU:HB3  | 2.24                     | 0.53              |
| 1:D:251:THR:O    | 1:D:252:VAL:CG2  | 2.54                     | 0.53              |
| 1:D:294:ARG:HG2  | 1:D:294:ARG:O    | 2.08                     | 0.53              |
| 1:E:252:VAL:HG12 | 1:E:253:MET:N    | 2.21                     | 0.53              |
| 1:C:232:LYS:HG2  | 1:C:234:PHE:CE1  | 2.43                     | 0.53              |
| 1:D:331:HIS:CD2  | 1:D:333:ASP:H    | 2.22                     | 0.53              |
| 1:C:256:HIS:HD2  | 1:C:258:ASN:HB2  | 1.74                     | 0.52              |
| 1:C:372:ARG:HH12 | 1:C:438:VAL:HG11 | 1.73                     | 0.52              |
| 1:B:430:ASP:O    | 1:B:431:LEU:HD23 | 2.08                     | 0.52              |
| 1:C:288:LEU:HD12 | 1:C:292:LEU:HD13 | 1.92                     | 0.52              |
| 1:C:483:LEU:HD12 | 1:C:483:LEU:H    | 1.73                     | 0.52              |
| 1:E:198:GLN:HE22 | 1:E:250:GLN:NE2  | 2.07                     | 0.52              |
| 1:C:382:GLU:H    | 1:C:382:GLU:CD   | 2.16                     | 0.52              |
| 1:D:259:ILE:CD1  | 1:D:316:LEU:HD13 | 2.39                     | 0.52              |
| 1:D:456:ASN:C    | 1:D:458:TRP:N    | 2.63                     | 0.52              |
| 1:C:253:MET:HB3  | 1:C:326:LYS:CG   | 2.38                     | 0.52              |
| 1:C:403:ALA:O    | 1:C:407:VAL:HG23 | 2.09                     | 0.52              |
| 1:C:408:PHE:O    | 1:C:411:ILE:HB   | 2.09                     | 0.52              |
| 1:E:204:THR:HG22 | 1:E:224:TRP:CD1  | 2.45                     | 0.52              |
| 1:A:459:GLN:O    | 1:A:465:ARG:NH1  | 2.43                     | 0.52              |
| 1:A:487:ARG:HH21 | 1:A:491:THR:N    | 2.08                     | 0.52              |
| 1:B:248:ILE:HD12 | 1:B:355:ALA:HB3  | 1.92                     | 0.52              |
| 1:C:244:ARG:HH12 | 1:C:366:ASP:HB3  | 1.74                     | 0.52              |
| 1:D:469:LYS:HE2  | 1:D:473:GLU:OE2  | 2.10                     | 0.52              |
| 1:C:221:ARG:HD2  | 1:C:282:TYR:OH   | 2.09                     | 0.52              |
| 1:C:278:LEU:HG   | 2:C:3:JZO:H1B    | 1.92                     | 0.52              |
| 1:C:317:HIS:HB3  | 1:C:397:LYS:HE2  | 1.92                     | 0.52              |
| 1:E:200:THR:O    | 1:E:204:THR:HB   | 2.09                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:377:ARG:NH1  | 3:E:3:PO4:O3     | 2.43                     | 0.52              |
| 1:A:253:MET:HG2  | 1:A:324:GLN:O    | 2.10                     | 0.52              |
| 1:A:296:THR:HG22 | 1:A:414:ARG:HH11 | 1.73                     | 0.52              |
| 1:A:447:GLU:C    | 1:A:449:LYS:H    | 2.17                     | 0.52              |
| 1:A:459:GLN:C    | 1:A:465:ARG:HH11 | 2.18                     | 0.52              |
| 1:C:471:MET:HE2  | 1:C:475:TRP:HH2  | 1.73                     | 0.52              |
| 1:D:244:ARG:HH21 | 1:D:367:ILE:CG2  | 2.22                     | 0.52              |
| 1:C:459:GLN:HE22 | 1:C:465:ARG:HG3  | 1.72                     | 0.52              |
| 1:C:372:ARG:CZ   | 1:C:438:VAL:HG11 | 2.40                     | 0.51              |
| 1:C:425:GLN:HA   | 1:C:425:GLN:NE2  | 2.25                     | 0.51              |
| 1:A:216:PHE:HA   | 1:A:238:GLU:OE1  | 2.10                     | 0.51              |
| 1:A:260:LEU:HD23 | 4:A:504:HOH:O    | 2.11                     | 0.51              |
| 1:A:488:ILE:O    | 1:A:492:LEU:HB2  | 2.11                     | 0.51              |
| 1:B:471:MET:O    | 1:B:474:CYS:HB2  | 2.10                     | 0.51              |
| 1:C:209:GLU:OE1  | 1:C:221:ARG:NH1  | 2.43                     | 0.51              |
| 1:E:310:ALA:CB   | 1:E:404:MET:HE1  | 2.40                     | 0.51              |
| 1:A:462:GLU:O    | 1:A:466:VAL:HG23 | 2.09                     | 0.51              |
| 1:C:478:ASN:C    | 1:C:478:ASN:ND2  | 2.69                     | 0.51              |
| 1:E:417:ILE:HD11 | 1:E:464:LEU:HD21 | 1.91                     | 0.51              |
| 1:B:248:ILE:CD1  | 1:B:355:ALA:HB3  | 2.40                     | 0.51              |
| 1:C:189:SER:C    | 1:C:191:SER:H    | 2.17                     | 0.51              |
| 1:C:284:GLU:HB3  | 1:C:343:LYS:NZ   | 2.26                     | 0.51              |
| 1:C:479:GLY:HA2  | 1:C:482:ARG:CD   | 2.40                     | 0.51              |
| 1:C:483:LEU:HD12 | 1:C:483:LEU:N    | 2.25                     | 0.51              |
| 1:D:448:GLN:O    | 1:D:450:LEU:N    | 2.43                     | 0.51              |
| 1:A:184:MET:C    | 1:A:186:THR:H    | 2.18                     | 0.51              |
| 1:C:332:ARG:NH2  | 1:C:367:ILE:HG21 | 2.26                     | 0.51              |
| 1:A:195:LEU:H    | 1:A:195:LEU:CD1  | 2.24                     | 0.51              |
| 1:A:344:ASN:OD1  | 1:A:346:THR:OG1  | 2.28                     | 0.51              |
| 1:A:412:ALA:C    | 1:A:414:ARG:H    | 2.18                     | 0.51              |
| 1:D:433:PRO:HG2  | 1:D:440:GLU:OE1  | 2.11                     | 0.51              |
| 1:A:309:THR:CG2  | 1:A:404:MET:HE2  | 2.30                     | 0.51              |
| 1:B:220:TRP:NE1  | 1:B:233:ILE:HD11 | 2.26                     | 0.51              |
| 1:B:313:LEU:HD11 | 1:B:317:HIS:NE2  | 2.25                     | 0.51              |
| 1:C:462:GLU:O    | 1:C:466:VAL:HG23 | 2.11                     | 0.51              |
| 1:A:407:VAL:O    | 1:A:411:ILE:HG13 | 2.11                     | 0.50              |
| 1:A:413:ARG:NH1  | 1:A:422:GLU:HB3  | 2.26                     | 0.50              |
| 1:A:417:ILE:HG13 | 1:A:420:ILE:CD1  | 2.38                     | 0.50              |
| 1:A:417:ILE:CG1  | 1:A:420:ILE:HD11 | 2.38                     | 0.50              |
| 1:C:343:LYS:C    | 1:C:345:GLY:H    | 2.18                     | 0.50              |
| 1:C:376:LYS:O    | 1:C:378:TYR:N    | 2.44                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:381:PRO:HD2  | 1:C:482:ARG:NH2  | 2.25                     | 0.50              |
| 1:D:267:ASN:OD1  | 1:D:267:ASN:N    | 2.45                     | 0.50              |
| 1:E:297:VAL:N    | 1:E:414:ARG:O    | 2.44                     | 0.50              |
| 1:C:256:HIS:HB2  | 1:C:315:HIS:ND1  | 2.27                     | 0.50              |
| 1:D:342:LYS:HD3  | 1:D:346:THR:CG2  | 2.42                     | 0.50              |
| 1:A:420:ILE:HG13 | 1:A:420:ILE:O    | 2.10                     | 0.50              |
| 1:C:368:ALA:H    | 1:C:369:PRO:HD2  | 1.75                     | 0.50              |
| 1:D:244:ARG:HG2  | 1:D:244:ARG:HH11 | 1.77                     | 0.50              |
| 1:A:431:LEU:HD13 | 1:A:444:VAL:CG1  | 2.41                     | 0.50              |
| 1:B:377:ARG:HD3  | 1:B:427:PRO:HD2  | 1.92                     | 0.50              |
| 1:B:472:ARG:C    | 1:B:474:CYS:H    | 2.20                     | 0.50              |
| 1:C:288:LEU:HB3  | 1:C:339:ILE:HB   | 1.93                     | 0.50              |
| 1:C:335:LYS:HG2  | 1:C:337:LYS:H    | 1.77                     | 0.50              |
| 1:D:417:ILE:HD11 | 1:D:457:ARG:NH1  | 2.26                     | 0.50              |
| 1:B:376:LYS:CA   | 1:B:379:MET:HE3  | 2.20                     | 0.50              |
| 1:C:418:GLY:C    | 1:C:420:ILE:H    | 2.20                     | 0.50              |
| 1:D:205:ILE:CG2  | 1:D:206:VAL:N    | 2.75                     | 0.50              |
| 1:E:385:ASP:C    | 1:E:385:ASP:OD2  | 2.54                     | 0.50              |
| 1:A:471:MET:HE2  | 1:A:475:TRP:CH2  | 2.47                     | 0.49              |
| 1:B:311:SER:HA   | 1:B:489:LYS:HG3  | 1.94                     | 0.49              |
| 1:C:468:ALA:HA   | 1:C:471:MET:SD   | 2.52                     | 0.49              |
| 1:A:328:ALA:HB1  | 1:A:393:PHE:CE2  | 2.47                     | 0.49              |
| 1:A:366:ASP:O    | 1:A:367:ILE:HB   | 2.10                     | 0.49              |
| 1:C:198:GLN:HB3  | 1:C:264:ALA:HB1  | 1.93                     | 0.49              |
| 1:C:407:VAL:O    | 1:C:408:PHE:C    | 2.54                     | 0.49              |
| 1:D:199:ARG:HD2  | 1:D:203:ARG:NH2  | 2.28                     | 0.49              |
| 1:D:443:LYS:O    | 1:D:447:GLU:HB2  | 2.12                     | 0.49              |
| 1:A:215:ARG:HG2  | 1:A:215:ARG:HH11 | 1.78                     | 0.49              |
| 1:A:470:ILE:HG23 | 1:A:483:LEU:CD1  | 2.42                     | 0.49              |
| 1:B:385:ASP:HA   | 1:B:442:ARG:NH2  | 2.27                     | 0.49              |
| 1:C:177:LEU:HB2  | 1:C:227:GLU:OE1  | 2.12                     | 0.49              |
| 1:C:288:LEU:HD12 | 1:C:288:LEU:O    | 2.12                     | 0.49              |
| 1:C:406:LEU:HD22 | 1:C:406:LEU:H    | 1.78                     | 0.49              |
| 1:D:205:ILE:HG22 | 1:D:206:VAL:N    | 2.26                     | 0.49              |
| 1:A:375:THR:O    | 1:A:379:MET:HG3  | 2.13                     | 0.49              |
| 1:B:317:HIS:HB3  | 1:B:397:LYS:CE   | 2.36                     | 0.49              |
| 1:C:448:GLN:HB2  | 1:C:450:LEU:HG   | 1.94                     | 0.49              |
| 1:C:476:TYR:O    | 1:C:478:ASN:N    | 2.45                     | 0.49              |
| 1:D:381:PRO:HG3  | 1:D:445:VAL:CG1  | 2.42                     | 0.49              |
| 1:E:320:ILE:HD13 | 1:E:326:LYS:HG2  | 1.95                     | 0.49              |
| 1:B:433:PRO:HG2  | 1:B:440:GLU:OE2  | 2.11                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:368:ALA:HB2  | 1:E:178:LYS:HG2  | 1.94                     | 0.49              |
| 1:A:304:LYS:HZ3  | 1:A:304:LYS:HB2  | 1.78                     | 0.49              |
| 1:B:195:LEU:H    | 1:B:195:LEU:CD1  | 2.25                     | 0.49              |
| 1:B:199:ARG:HD3  | 1:B:203:ARG:CZ   | 2.42                     | 0.49              |
| 1:B:377:ARG:HA   | 1:B:441:MET:HE2  | 1.95                     | 0.49              |
| 1:D:459:GLN:O    | 1:D:465:ARG:NH1  | 2.46                     | 0.49              |
| 1:E:412:ALA:C    | 1:E:414:ARG:H    | 2.21                     | 0.49              |
| 1:B:337:LYS:HD2  | 3:B:12:PO4:O2    | 2.12                     | 0.49              |
| 1:C:260:LEU:HD13 | 1:C:340:LEU:HD13 | 1.94                     | 0.49              |
| 1:C:402:TYR:CE1  | 1:C:406:LEU:HD21 | 2.48                     | 0.49              |
| 1:D:426:LEU:O    | 1:D:429:TYR:HB3  | 2.13                     | 0.49              |
| 1:D:448:GLN:HB2  | 1:D:450:LEU:HD12 | 1.94                     | 0.49              |
| 1:E:253:MET:HG3  | 1:E:326:LYS:H    | 1.76                     | 0.49              |
| 1:E:385:ASP:HA   | 1:E:442:ARG:HD2  | 1.95                     | 0.49              |
| 1:B:409:TRP:HB2  | 1:B:471:MET:HE3  | 1.95                     | 0.49              |
| 1:C:258:ASN:OD1  | 1:C:308:SER:HB2  | 2.13                     | 0.49              |
| 1:C:406:LEU:HD22 | 1:C:406:LEU:N    | 2.28                     | 0.49              |
| 1:C:417:ILE:H    | 1:C:420:ILE:CG1  | 2.26                     | 0.49              |
| 1:D:259:ILE:HD13 | 1:D:316:LEU:HD13 | 1.94                     | 0.49              |
| 1:E:432:VAL:HG22 | 1:E:433:PRO:CD   | 2.43                     | 0.49              |
| 1:A:251:THR:O    | 1:A:251:THR:OG1  | 2.30                     | 0.48              |
| 1:C:197:VAL:O    | 1:C:201:ILE:HG13 | 2.12                     | 0.48              |
| 1:E:242:TRP:CD1  | 1:E:278:LEU:HD13 | 2.47                     | 0.48              |
| 1:A:393:PHE:O    | 1:A:394:GLU:C    | 2.56                     | 0.48              |
| 1:C:287:SER:C    | 1:C:289:PHE:N    | 2.69                     | 0.48              |
| 1:C:334:LEU:HD23 | 1:C:335:LYS:H    | 1.78                     | 0.48              |
| 1:B:282:TYR:HE2  | 1:B:284:GLU:HG2  | 1.78                     | 0.48              |
| 1:B:287:SER:HA   | 1:B:339:ILE:O    | 2.13                     | 0.48              |
| 1:D:417:ILE:HG13 | 1:D:420:ILE:CG1  | 2.34                     | 0.48              |
| 1:B:372:ARG:NH2  | 1:B:438:VAL:HG11 | 2.29                     | 0.48              |
| 1:B:392:HIS:O    | 1:B:395:SER:HB3  | 2.12                     | 0.48              |
| 1:C:303:ILE:HG21 | 1:C:496:SER:HB2  | 1.95                     | 0.48              |
| 1:E:237:ARG:O    | 1:E:237:ARG:HG2  | 2.13                     | 0.48              |
| 1:A:242:TRP:CD1  | 1:A:276:LEU:HB3  | 2.48                     | 0.48              |
| 1:C:199:ARG:HD2  | 1:C:203:ARG:NE   | 2.29                     | 0.48              |
| 1:C:320:ILE:CG2  | 1:C:321:VAL:N    | 2.76                     | 0.48              |
| 1:C:413:ARG:HG3  | 1:C:422:GLU:HB2  | 1.95                     | 0.48              |
| 1:A:195:LEU:HD12 | 1:A:195:LEU:N    | 2.28                     | 0.48              |
| 1:A:328:ALA:HB1  | 1:A:393:PHE:HE2  | 1.77                     | 0.48              |
| 1:C:307:LEU:HD22 | 1:C:493:SER:HA   | 1.95                     | 0.48              |
| 1:C:476:TYR:C    | 1:C:478:ASN:N    | 2.72                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:258:ASN:O    | 1:B:348:CYS:HA   | 2.13                     | 0.48              |
| 1:B:302:MET:HE3  | 1:B:467:MET:HG3  | 1.95                     | 0.48              |
| 1:C:414:ARG:HH11 | 1:C:414:ARG:CA   | 2.27                     | 0.48              |
| 1:E:447:GLU:O    | 1:E:449:LYS:HG3  | 2.13                     | 0.48              |
| 1:B:191:SER:HB2  | 1:B:250:GLN:HA   | 1.96                     | 0.48              |
| 1:C:406:LEU:H    | 1:C:406:LEU:CD2  | 2.27                     | 0.48              |
| 1:B:253:MET:CE   | 1:B:325:GLY:N    | 2.77                     | 0.48              |
| 1:C:183:ASP:O    | 1:C:187:SER:CB   | 2.62                     | 0.48              |
| 1:C:476:TYR:O    | 1:C:477:ALA:C    | 2.56                     | 0.48              |
| 1:D:459:GLN:NE2  | 1:D:459:GLN:HA   | 2.29                     | 0.48              |
| 1:E:215:ARG:NH1  | 1:E:215:ARG:HG3  | 2.29                     | 0.48              |
| 1:A:459:GLN:HA   | 1:A:465:ARG:CG   | 2.43                     | 0.48              |
| 1:D:454:ILE:HG23 | 1:D:458:TRP:CE3  | 2.49                     | 0.48              |
| 1:C:496:SER:C    | 1:C:498:GLN:H    | 2.21                     | 0.47              |
| 1:D:342:LYS:HE3  | 1:D:348:CYS:HB3  | 1.96                     | 0.47              |
| 1:D:431:LEU:CD1  | 1:D:450:LEU:HD13 | 2.44                     | 0.47              |
| 1:A:315:HIS:HE1  | 1:A:326:LYS:HD2  | 1.79                     | 0.47              |
| 1:A:232:LYS:HE3  | 1:A:234:PHE:CZ   | 2.49                     | 0.47              |
| 1:A:252:VAL:HG23 | 1:A:253:MET:N    | 2.29                     | 0.47              |
| 1:A:393:PHE:O    | 1:A:395:SER:N    | 2.47                     | 0.47              |
| 1:B:319:GLU:C    | 1:B:320:ILE:HG13 | 2.39                     | 0.47              |
| 1:C:211:ILE:HD12 | 2:C:3:JZO:C24    | 2.44                     | 0.47              |
| 1:C:256:HIS:CD2  | 1:C:258:ASN:HB2  | 2.49                     | 0.47              |
| 1:D:244:ARG:HH21 | 1:D:367:ILE:HG22 | 1.78                     | 0.47              |
| 1:B:186:THR:HG22 | 1:B:186:THR:O    | 2.13                     | 0.47              |
| 1:B:317:HIS:CB   | 1:B:397:LYS:HE3  | 2.36                     | 0.47              |
| 1:B:376:LYS:HD2  | 1:B:379:MET:CE   | 2.44                     | 0.47              |
| 1:B:412:ALA:C    | 1:B:414:ARG:N    | 2.71                     | 0.47              |
| 1:A:412:ALA:C    | 1:A:414:ARG:N    | 2.70                     | 0.47              |
| 1:C:365:ILE:CG2  | 1:C:366:ASP:N    | 2.77                     | 0.47              |
| 1:D:216:PHE:CA   | 1:D:238:GLU:OE2  | 2.62                     | 0.47              |
| 1:E:285:HIS:HB2  | 1:E:341:VAL:HG22 | 1.97                     | 0.47              |
| 1:C:464:LEU:HD22 | 1:C:464:LEU:H    | 1.79                     | 0.47              |
| 1:A:248:ILE:CD1  | 1:A:355:ALA:HB3  | 2.44                     | 0.47              |
| 1:A:331:HIS:HD2  | 1:A:333:ASP:N    | 2.12                     | 0.47              |
| 1:A:434:SER:O    | 1:A:435:ASP:HB3  | 2.14                     | 0.47              |
| 1:A:447:GLU:C    | 1:A:449:LYS:N    | 2.73                     | 0.47              |
| 1:B:187:SER:O    | 1:B:189:SER:N    | 2.47                     | 0.47              |
| 1:B:412:ALA:C    | 1:B:414:ARG:H    | 2.23                     | 0.47              |
| 1:C:287:SER:C    | 1:C:289:PHE:H    | 2.23                     | 0.47              |
| 1:C:402:TYR:CD1  | 1:C:402:TYR:C    | 2.93                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:415:CYS:SG   | 1:C:416:SER:N    | 2.88                     | 0.47              |
| 1:C:452:PRO:HD2  | 1:C:475:TRP:CZ3  | 2.49                     | 0.47              |
| 1:E:181:ILE:O    | 1:E:184:MET:HG2  | 2.15                     | 0.47              |
| 1:A:358:HIS:HB2  | 1:A:393:PHE:CD1  | 2.50                     | 0.47              |
| 1:A:409:TRP:CA   | 1:A:471:MET:HE3  | 2.44                     | 0.47              |
| 1:B:478:ASN:OD1  | 1:B:478:ASN:C    | 2.58                     | 0.47              |
| 1:D:208:GLN:C    | 1:D:209:GLU:HG3  | 2.40                     | 0.47              |
| 1:D:297:VAL:HG22 | 1:D:298:THR:O    | 2.15                     | 0.47              |
| 1:D:424:TYR:OH   | 1:D:426:LEU:HD23 | 2.15                     | 0.47              |
| 1:E:253:MET:CE   | 1:E:320:ILE:HG21 | 2.45                     | 0.47              |
| 1:E:270:ASN:O    | 1:E:271:GLY:C    | 2.57                     | 0.47              |
| 1:A:294:ARG:HH11 | 1:A:294:ARG:HG2  | 1.78                     | 0.47              |
| 1:A:372:ARG:HD3  | 1:A:379:MET:HE1  | 1.96                     | 0.47              |
| 1:B:215:ARG:HB3  | 1:B:215:ARG:CZ   | 2.44                     | 0.47              |
| 1:C:381:PRO:HD3  | 1:C:402:TYR:CE2  | 2.50                     | 0.47              |
| 1:C:418:GLY:C    | 1:C:420:ILE:N    | 2.73                     | 0.47              |
| 1:A:454:ILE:O    | 1:A:455:PRO:C    | 2.58                     | 0.47              |
| 1:C:259:ILE:O    | 1:C:260:LEU:C    | 2.57                     | 0.47              |
| 1:C:268:LYS:HG3  | 1:C:275:GLN:HB2  | 1.95                     | 0.47              |
| 1:D:244:ARG:HG2  | 1:D:244:ARG:NH1  | 2.30                     | 0.47              |
| 1:E:460:SER:O    | 1:E:465:ARG:NH1  | 2.48                     | 0.47              |
| 1:A:406:LEU:HD22 | 1:A:427:PRO:HB3  | 1.97                     | 0.46              |
| 1:B:303:ILE:CD1  | 1:B:499:GLU:HG3  | 2.45                     | 0.46              |
| 1:D:364:THR:C    | 1:D:365:ILE:HD12 | 2.39                     | 0.46              |
| 1:E:180:LEU:O    | 1:E:181:ILE:C    | 2.58                     | 0.46              |
| 1:E:199:ARG:O    | 1:E:203:ARG:HG3  | 2.14                     | 0.46              |
| 1:D:253:MET:HE2  | 1:D:324:GLN:C    | 2.40                     | 0.46              |
| 1:E:232:LYS:HG2  | 1:E:234:PHE:CE1  | 2.50                     | 0.46              |
| 1:A:450:LEU:O    | 1:A:451:ARG:HD2  | 2.14                     | 0.46              |
| 1:C:320:ILE:CG2  | 1:C:321:VAL:H    | 2.24                     | 0.46              |
| 1:C:457:ARG:HG3  | 1:C:458:TRP:HD1  | 1.80                     | 0.46              |
| 1:D:403:ALA:O    | 1:D:407:VAL:HG23 | 2.16                     | 0.46              |
| 1:D:460:SER:OG   | 1:D:461:CYS:N    | 2.49                     | 0.46              |
| 1:A:459:GLN:OE1  | 1:A:465:ARG:HG2  | 2.16                     | 0.46              |
| 1:B:251:THR:HG21 | 1:B:327:PRO:HD2  | 1.97                     | 0.46              |
| 1:C:244:ARG:NH1  | 1:C:366:ASP:HB3  | 2.31                     | 0.46              |
| 1:C:416:SER:C    | 1:C:417:ILE:HD12 | 2.41                     | 0.46              |
| 1:E:258:ASN:HD22 | 1:E:311:SER:HB2  | 1.79                     | 0.46              |
| 1:E:287:SER:HA   | 1:E:339:ILE:O    | 2.16                     | 0.46              |
| 1:E:294:ARG:HG2  | 1:E:294:ARG:HH11 | 1.80                     | 0.46              |
| 1:E:432:VAL:CG2  | 1:E:433:PRO:HD2  | 2.46                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:199:ARG:O    | 1:A:203:ARG:HG2  | 2.16                     | 0.46              |
| 1:D:389:ASN:HD21 | 1:D:391:LYS:CB   | 2.23                     | 0.46              |
| 1:B:432:VAL:HG13 | 1:B:433:PRO:HD2  | 1.97                     | 0.46              |
| 1:B:449:LYS:NZ   | 1:B:449:LYS:HB2  | 2.31                     | 0.46              |
| 1:D:214:GLY:O    | 1:D:215:ARG:C    | 2.59                     | 0.46              |
| 1:B:195:LEU:HD12 | 1:B:195:LEU:N    | 2.31                     | 0.46              |
| 1:B:334:LEU:O    | 1:B:335:LYS:HB3  | 2.16                     | 0.46              |
| 1:D:429:TYR:CZ   | 1:D:430:ASP:OD2  | 2.69                     | 0.46              |
| 1:C:365:ILE:HG22 | 1:C:366:ASP:N    | 2.30                     | 0.46              |
| 1:D:185:THR:O    | 1:D:187:SER:N    | 2.49                     | 0.46              |
| 1:A:365:ILE:O    | 1:A:367:ILE:N    | 2.49                     | 0.46              |
| 1:C:428:TYR:O    | 1:C:432:VAL:HG12 | 2.16                     | 0.46              |
| 1:D:431:LEU:HD13 | 1:D:450:LEU:HD13 | 1.98                     | 0.46              |
| 1:D:462:GLU:O    | 1:D:463:ALA:C    | 2.59                     | 0.46              |
| 1:A:417:ILE:O    | 1:A:420:ILE:HG12 | 2.17                     | 0.46              |
| 1:B:232:LYS:HZ1  | 1:B:245:GLU:CD   | 2.23                     | 0.46              |
| 1:B:365:ILE:O    | 1:B:365:ILE:HG13 | 2.13                     | 0.46              |
| 1:C:213:LYS:HG2  | 1:C:218:GLU:HG3  | 1.97                     | 0.46              |
| 1:D:431:LEU:HD11 | 1:D:450:LEU:HD22 | 1.97                     | 0.46              |
| 1:E:443:LYS:HG2  | 1:E:448:GLN:HE21 | 1.80                     | 0.46              |
| 1:A:471:MET:HE2  | 1:A:475:TRP:HH2  | 1.80                     | 0.45              |
| 1:C:181:ILE:HA   | 1:C:184:MET:CE   | 2.41                     | 0.45              |
| 1:C:398:ARG:HD3  | 1:C:479:GLY:C    | 2.42                     | 0.45              |
| 1:D:295:TYR:O    | 1:D:414:ARG:NH1  | 2.49                     | 0.45              |
| 1:E:454:ILE:HG23 | 1:E:458:TRP:CE3  | 2.51                     | 0.45              |
| 1:E:498:GLN:C    | 1:E:499:GLU:HG3  | 2.42                     | 0.45              |
| 1:A:320:ILE:HB   | 1:A:326:LYS:H    | 1.80                     | 0.45              |
| 1:A:413:ARG:NH1  | 1:A:423:ASP:O    | 2.49                     | 0.45              |
| 1:A:455:PRO:HB2  | 1:A:458:TRP:CD1  | 2.51                     | 0.45              |
| 1:C:406:LEU:O    | 1:C:410:GLU:HG3  | 2.16                     | 0.45              |
| 1:C:331:HIS:CD2  | 1:C:333:ASP:C    | 2.94                     | 0.45              |
| 1:E:342:LYS:HG2  | 1:E:346:THR:O    | 2.16                     | 0.45              |
| 1:C:302:MET:HG3  | 1:C:411:ILE:CG2  | 2.45                     | 0.45              |
| 1:C:324:GLN:HG3  | 1:C:325:GLY:N    | 2.32                     | 0.45              |
| 1:D:435:ASP:N    | 1:D:436:PRO:HD3  | 2.31                     | 0.45              |
| 1:E:285:HIS:CB   | 1:E:341:VAL:HG22 | 2.47                     | 0.45              |
| 1:E:413:ARG:NH1  | 1:E:423:ASP:O    | 2.48                     | 0.45              |
| 1:E:494:GLN:O    | 1:E:497:GLN:HB3  | 2.16                     | 0.45              |
| 1:A:426:LEU:O    | 1:A:429:TYR:HB3  | 2.17                     | 0.45              |
| 1:A:432:VAL:HG21 | 1:A:436:PRO:HB3  | 1.98                     | 0.45              |
| 1:B:479:GLY:HA2  | 1:B:482:ARG:HD2  | 1.99                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:443:LYS:HA   | 1:D:447:GLU:HG3  | 1.98                     | 0.45              |
| 1:A:294:ARG:HG2  | 1:A:294:ARG:NH1  | 2.32                     | 0.45              |
| 1:B:200:THR:O    | 1:B:204:THR:HB   | 2.17                     | 0.45              |
| 1:B:492:LEU:HD12 | 1:B:492:LEU:HA   | 1.65                     | 0.45              |
| 1:C:278:LEU:HD12 | 1:C:278:LEU:HA   | 1.81                     | 0.45              |
| 1:D:235:SER:O    | 1:D:236:SER:C    | 2.60                     | 0.45              |
| 1:B:424:TYR:CD2  | 1:B:424:TYR:C    | 2.95                     | 0.45              |
| 1:A:331:HIS:CD2  | 1:A:333:ASP:H    | 2.33                     | 0.45              |
| 1:A:409:TRP:HA   | 1:A:471:MET:CE   | 2.46                     | 0.45              |
| 1:A:476:TYR:C    | 1:A:478:ASN:N    | 2.74                     | 0.45              |
| 1:A:476:TYR:C    | 1:A:478:ASN:H    | 2.24                     | 0.45              |
| 1:B:342:LYS:HD3  | 1:B:346:THR:HG22 | 1.99                     | 0.45              |
| 1:B:393:PHE:C    | 1:B:395:SER:N    | 2.74                     | 0.45              |
| 1:B:412:ALA:O    | 1:B:414:ARG:N    | 2.50                     | 0.45              |
| 1:C:340:LEU:O    | 1:C:347:CYS:HA   | 2.17                     | 0.45              |
| 1:C:376:LYS:C    | 1:C:378:TYR:N    | 2.73                     | 0.45              |
| 1:E:459:GLN:HA   | 1:E:459:GLN:NE2  | 2.32                     | 0.45              |
| 1:E:461:CYS:HB3  | 1:E:464:LEU:HD23 | 1.98                     | 0.45              |
| 1:A:215:ARG:HH21 | 1:A:354:LEU:HD11 | 1.82                     | 0.45              |
| 1:A:251:THR:HG21 | 1:A:357:ARG:HD3  | 1.98                     | 0.45              |
| 1:A:301:GLY:HA2  | 1:A:304:LYS:HZ2  | 1.78                     | 0.45              |
| 1:B:409:TRP:CB   | 1:B:471:MET:HE3  | 2.47                     | 0.45              |
| 1:C:173:GLU:H    | 1:C:173:GLU:CD   | 2.24                     | 0.45              |
| 1:D:372:ARG:HH11 | 1:D:438:VAL:HG21 | 1.81                     | 0.45              |
| 1:A:458:TRP:CG   | 1:A:464:LEU:HD11 | 2.52                     | 0.45              |
| 1:B:404:MET:O    | 1:B:407:VAL:HB   | 2.17                     | 0.45              |
| 1:C:332:ARG:HG3  | 1:C:356:VAL:HG12 | 1.98                     | 0.45              |
| 1:D:424:TYR:CD2  | 1:D:424:TYR:C    | 2.95                     | 0.45              |
| 1:E:244:ARG:HH21 | 1:E:248:ILE:HD11 | 1.82                     | 0.45              |
| 1:E:299:VAL:O    | 1:E:303:ILE:HG13 | 2.16                     | 0.45              |
| 1:E:497:GLN:C    | 1:E:499:GLU:H    | 2.24                     | 0.45              |
| 1:A:292:LEU:HD21 | 1:A:411:ILE:HA   | 1.98                     | 0.44              |
| 1:A:294:ARG:O    | 1:A:295:TYR:CG   | 2.70                     | 0.44              |
| 1:B:204:THR:CG2  | 1:B:224:TRP:NE1  | 2.78                     | 0.44              |
| 1:B:431:LEU:HD13 | 1:B:450:LEU:HD13 | 1.99                     | 0.44              |
| 1:B:432:VAL:HG13 | 1:B:433:PRO:CD   | 2.47                     | 0.44              |
| 1:C:268:LYS:CG   | 1:C:275:GLN:HB2  | 2.46                     | 0.44              |
| 1:C:486:LEU:O    | 1:C:489:LYS:HB3  | 2.18                     | 0.44              |
| 1:D:256:HIS:O    | 1:D:257:GLU:C    | 2.60                     | 0.44              |
| 1:D:329:ILE:HA   | 1:D:356:VAL:O    | 2.17                     | 0.44              |
| 1:D:413:ARG:NH1  | 1:D:423:ASP:O    | 2.50                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:469:LYS:HD2  | 1:D:472:ARG:HH21 | 1.83                     | 0.44              |
| 1:E:198:GLN:HE22 | 1:E:250:GLN:HE22 | 1.64                     | 0.44              |
| 1:A:430:ASP:OD1  | 1:A:431:LEU:HG   | 2.18                     | 0.44              |
| 1:A:432:VAL:CG2  | 1:A:433:PRO:HD2  | 2.47                     | 0.44              |
| 1:A:435:ASP:N    | 1:A:436:PRO:HD3  | 2.32                     | 0.44              |
| 1:B:377:ARG:HH12 | 3:B:11:PO4:P     | 2.40                     | 0.44              |
| 1:C:487:ARG:C    | 1:C:489:LYS:N    | 2.74                     | 0.44              |
| 1:C:496:SER:C    | 1:C:498:GLN:N    | 2.75                     | 0.44              |
| 1:A:484:THR:O    | 1:A:488:ILE:HG13 | 2.17                     | 0.44              |
| 1:C:389:ASN:HD21 | 1:C:391:LYS:HB3  | 1.81                     | 0.44              |
| 1:E:237:ARG:O    | 1:E:237:ARG:CG   | 2.64                     | 0.44              |
| 1:E:358:HIS:HB2  | 1:E:393:PHE:CD1  | 2.52                     | 0.44              |
| 1:B:487:ARG:O    | 1:B:491:THR:HG23 | 2.18                     | 0.44              |
| 1:C:342:LYS:HB2  | 1:C:344:ASN:OD1  | 2.17                     | 0.44              |
| 1:D:294:ARG:HD3  | 1:D:295:TYR:CZ   | 2.52                     | 0.44              |
| 1:D:318:MET:HE3  | 1:D:318:MET:HB2  | 1.87                     | 0.44              |
| 1:B:178:LYS:HD3  | 1:B:227:GLU:OE2  | 2.17                     | 0.44              |
| 1:B:204:THR:HG22 | 1:B:224:TRP:HE1  | 1.81                     | 0.44              |
| 1:B:416:SER:HA   | 1:B:421:HIS:HB3  | 1.98                     | 0.44              |
| 1:E:237:ARG:NH1  | 1:E:238:GLU:OE2  | 2.51                     | 0.44              |
| 1:A:298:THR:CG2  | 1:A:299:VAL:N    | 2.80                     | 0.44              |
| 1:C:319:GLU:OE2  | 1:C:360:SER:HB3  | 2.17                     | 0.44              |
| 1:D:217:GLY:CA   | 1:D:238:GLU:OE1  | 2.66                     | 0.44              |
| 1:D:376:LYS:N    | 1:D:379:MET:HE3  | 2.32                     | 0.44              |
| 1:D:448:GLN:O    | 1:D:449:LYS:C    | 2.60                     | 0.44              |
| 1:B:457:ARG:C    | 1:B:459:GLN:H    | 2.26                     | 0.44              |
| 1:C:319:GLU:HG2  | 1:C:320:ILE:N    | 2.31                     | 0.44              |
| 1:C:405:GLY:HA3  | 1:C:475:TRP:HE1  | 1.83                     | 0.44              |
| 1:E:489:LYS:O    | 1:E:493:SER:HB2  | 2.18                     | 0.44              |
| 1:A:323:THR:OG1  | 1:A:324:GLN:N    | 2.51                     | 0.43              |
| 1:B:432:VAL:HG11 | 1:B:436:PRO:CG   | 2.48                     | 0.43              |
| 1:C:368:ALA:N    | 1:C:369:PRO:CD   | 2.80                     | 0.43              |
| 1:C:483:LEU:CD1  | 1:C:488:ILE:HD11 | 2.46                     | 0.43              |
| 1:E:184:MET:HG3  | 1:E:185:THR:N    | 2.33                     | 0.43              |
| 1:E:211:ILE:HD12 | 2:E:5:JZO:C24    | 2.49                     | 0.43              |
| 1:A:331:HIS:HE1  | 1:A:350:ALA:O    | 2.01                     | 0.43              |
| 1:B:385:ASP:O    | 1:B:387:SER:N    | 2.51                     | 0.43              |
| 1:D:232:LYS:HG2  | 1:D:234:PHE:CE1  | 2.54                     | 0.43              |
| 1:D:424:TYR:O    | 1:D:425:GLN:NE2  | 2.51                     | 0.43              |
| 1:E:181:ILE:HA   | 1:E:184:MET:CE   | 2.45                     | 0.43              |
| 1:A:381:PRO:HG3  | 1:A:445:VAL:HG12 | 1.99                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:425:GLN:HB3  | 1:A:429:TYR:CD2  | 2.52                     | 0.43              |
| 1:C:417:ILE:H    | 1:C:420:ILE:HG13 | 1.83                     | 0.43              |
| 1:C:425:GLN:HE21 | 1:C:425:GLN:CA   | 2.28                     | 0.43              |
| 1:C:478:ASN:ND2  | 1:C:480:ALA:H    | 2.16                     | 0.43              |
| 1:E:389:ASN:C    | 1:E:391:LYS:H    | 2.25                     | 0.43              |
| 1:A:402:TYR:CD1  | 1:A:402:TYR:C    | 2.96                     | 0.43              |
| 1:C:422:GLU:OE1  | 1:C:422:GLU:N    | 2.51                     | 0.43              |
| 1:B:209:GLU:OE2  | 1:B:221:ARG:NH1  | 2.51                     | 0.43              |
| 1:C:313:LEU:N    | 1:C:349:ILE:HD11 | 2.34                     | 0.43              |
| 1:C:334:LEU:HD23 | 1:C:335:LYS:N    | 2.34                     | 0.43              |
| 1:C:406:LEU:HB3  | 1:C:427:PRO:HG2  | 1.99                     | 0.43              |
| 1:A:358:HIS:HB2  | 1:A:393:PHE:CE1  | 2.53                     | 0.43              |
| 1:C:199:ARG:O    | 1:C:203:ARG:HG3  | 2.18                     | 0.43              |
| 1:C:217:GLY:HA3  | 1:C:234:PHE:HA   | 2.01                     | 0.43              |
| 1:C:262:PHE:CD1  | 2:C:3:JZO:H1     | 2.54                     | 0.43              |
| 1:C:297:VAL:HG13 | 1:C:298:THR:N    | 2.32                     | 0.43              |
| 1:B:269:ASP:HB3  | 1:B:270:ASN:H    | 1.63                     | 0.43              |
| 1:B:385:ASP:HB2  | 1:B:442:ARG:HH21 | 1.83                     | 0.43              |
| 1:D:498:GLN:C    | 1:D:499:GLU:HG3  | 2.44                     | 0.43              |
| 1:E:306:ALA:HB1  | 1:E:492:LEU:HD21 | 2.00                     | 0.43              |
| 1:E:461:CYS:SG   | 1:E:464:LEU:HD23 | 2.59                     | 0.43              |
| 1:B:300:GLU:HG3  | 1:B:501:ILE:HD13 | 2.01                     | 0.43              |
| 1:C:234:PHE:CE1  | 1:C:278:LEU:HD22 | 2.54                     | 0.43              |
| 1:D:234:PHE:CE1  | 1:D:278:LEU:HD22 | 2.53                     | 0.43              |
| 1:D:438:VAL:HG12 | 1:D:439:GLU:N    | 2.33                     | 0.43              |
| 1:E:297:VAL:O    | 1:E:415:CYS:HA   | 2.19                     | 0.43              |
| 1:E:492:LEU:HD12 | 1:E:492:LEU:HA   | 1.66                     | 0.43              |
| 1:A:499:GLU:HG3  | 1:A:500:GLY:H    | 1.84                     | 0.43              |
| 1:B:319:GLU:HB2  | 1:B:328:ALA:HB2  | 2.01                     | 0.43              |
| 1:D:331:HIS:HD2  | 1:D:333:ASP:N    | 2.12                     | 0.43              |
| 1:D:371:HIS:ND1  | 1:D:371:HIS:N    | 2.66                     | 0.43              |
| 1:E:416:SER:HA   | 1:E:421:HIS:HB3  | 2.00                     | 0.43              |
| 1:B:495:LEU:O    | 1:B:499:GLU:HG2  | 2.18                     | 0.43              |
| 1:C:414:ARG:HH11 | 1:C:414:ARG:HA   | 1.84                     | 0.43              |
| 1:C:484:THR:O    | 1:C:488:ILE:HG13 | 2.19                     | 0.43              |
| 1:D:376:LYS:CA   | 1:D:379:MET:HE3  | 2.48                     | 0.43              |
| 1:B:343:LYS:HG3  | 3:B:6:PO4:P      | 2.59                     | 0.42              |
| 1:C:372:ARG:NH2  | 1:C:438:VAL:HG11 | 2.34                     | 0.42              |
| 1:C:488:ILE:O    | 1:C:488:ILE:HG22 | 2.18                     | 0.42              |
| 1:E:254:LEU:HD12 | 1:E:254:LEU:HA   | 1.80                     | 0.42              |
| 1:A:215:ARG:NH2  | 1:A:354:LEU:HD11 | 2.33                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:409:TRP:CE2  | 1:A:452:PRO:HB3  | 2.54                     | 0.42              |
| 1:B:389:ASN:HD21 | 1:B:391:LYS:HB2  | 1.84                     | 0.42              |
| 1:C:432:VAL:HA   | 1:C:433:PRO:HD3  | 1.81                     | 0.42              |
| 1:C:472:ARG:C    | 1:C:474:CYS:N    | 2.75                     | 0.42              |
| 1:C:483:LEU:HD13 | 1:C:488:ILE:CD1  | 2.48                     | 0.42              |
| 1:A:315:HIS:CE1  | 1:A:326:LYS:CD   | 3.02                     | 0.42              |
| 1:C:297:VAL:CG1  | 1:C:415:CYS:HA   | 2.49                     | 0.42              |
| 1:C:492:LEU:HD12 | 1:C:495:LEU:HD23 | 2.01                     | 0.42              |
| 1:D:197:VAL:O    | 1:D:201:ILE:HG13 | 2.19                     | 0.42              |
| 1:D:262:PHE:HD1  | 2:D:4:JZO:C1     | 2.31                     | 0.42              |
| 1:D:429:TYR:CE1  | 1:D:430:ASP:HB3  | 2.53                     | 0.42              |
| 1:E:180:LEU:HD13 | 1:E:201:ILE:HD11 | 2.02                     | 0.42              |
| 1:E:199:ARG:HD2  | 1:E:203:ARG:NE   | 2.34                     | 0.42              |
| 1:E:479:GLY:HA2  | 1:E:482:ARG:CZ   | 2.49                     | 0.42              |
| 1:A:335:LYS:O    | 1:A:339:ILE:HG13 | 2.19                     | 0.42              |
| 1:C:237:ARG:CD   | 1:C:238:GLU:OE2  | 2.66                     | 0.42              |
| 1:D:189:SER:O    | 1:D:190:GLY:C    | 2.61                     | 0.42              |
| 1:D:234:PHE:HB3  | 1:D:238:GLU:HG3  | 2.01                     | 0.42              |
| 1:A:198:GLN:HB3  | 1:A:264:ALA:HB1  | 2.02                     | 0.42              |
| 1:A:456:ASN:C    | 1:A:458:TRP:N    | 2.77                     | 0.42              |
| 1:A:456:ASN:O    | 1:A:458:TRP:N    | 2.52                     | 0.42              |
| 1:B:388:ILE:HG13 | 1:B:395:SER:OG   | 2.19                     | 0.42              |
| 1:C:298:THR:O    | 1:C:301:GLY:N    | 2.52                     | 0.42              |
| 1:C:410:GLU:O    | 1:C:414:ARG:HG2  | 2.19                     | 0.42              |
| 1:E:377:ARG:NH1  | 3:E:3:PO4:O4     | 2.50                     | 0.42              |
| 1:A:184:MET:O    | 1:A:186:THR:N    | 2.52                     | 0.42              |
| 1:A:459:GLN:C    | 1:A:465:ARG:NH1  | 2.77                     | 0.42              |
| 1:B:342:LYS:HB2  | 1:B:346:THR:HG22 | 2.02                     | 0.42              |
| 1:C:367:ILE:O    | 1:C:367:ILE:HG22 | 2.19                     | 0.42              |
| 1:C:464:LEU:H    | 1:C:464:LEU:CD2  | 2.32                     | 0.42              |
| 1:D:443:LYS:HA   | 1:D:447:GLU:HG2  | 1.99                     | 0.42              |
| 1:D:444:VAL:O    | 1:D:450:LEU:HB2  | 2.20                     | 0.42              |
| 1:E:190:GLY:C    | 1:E:192:GLY:N    | 2.76                     | 0.42              |
| 1:E:389:ASN:ND2  | 1:E:391:LYS:CB   | 2.82                     | 0.42              |
| 1:A:189:SER:C    | 1:A:191:SER:H    | 2.26                     | 0.42              |
| 1:D:322:GLY:O    | 1:D:323:THR:C    | 2.63                     | 0.42              |
| 1:D:441:MET:HE3  | 1:D:441:MET:HA   | 2.00                     | 0.42              |
| 1:D:473:GLU:O    | 1:D:482:ARG:HA   | 2.19                     | 0.42              |
| 1:E:310:ALA:HA   | 1:E:404:MET:CE   | 2.47                     | 0.42              |
| 1:B:409:TRP:CD1  | 1:B:471:MET:CE   | 3.03                     | 0.42              |
| 1:C:216:PHE:HA   | 1:C:238:GLU:HG3  | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:470:ILE:HG21 | 1:C:488:ILE:HG23 | 2.01                     | 0.42              |
| 1:A:224:TRP:O    | 1:A:225:ARG:C    | 2.62                     | 0.42              |
| 1:A:315:HIS:O    | 1:A:315:HIS:ND1  | 2.52                     | 0.42              |
| 1:A:317:HIS:HE1  | 1:A:400:ASP:HB2  | 1.84                     | 0.42              |
| 1:A:493:SER:O    | 1:A:496:SER:HB3  | 2.19                     | 0.42              |
| 1:B:294:ARG:O    | 1:B:294:ARG:HD3  | 2.20                     | 0.42              |
| 1:B:366:ASP:O    | 1:B:367:ILE:C    | 2.62                     | 0.42              |
| 1:C:215:ARG:HH11 | 1:C:215:ARG:CG   | 2.32                     | 0.42              |
| 1:C:253:MET:HE2  | 1:C:324:GLN:O    | 2.19                     | 0.42              |
| 1:C:307:LEU:O    | 1:C:307:LEU:HD12 | 2.19                     | 0.42              |
| 1:C:334:LEU:HD21 | 1:C:339:ILE:HD11 | 2.02                     | 0.42              |
| 1:A:199:ARG:HD2  | 1:A:266:ASP:OD2  | 2.20                     | 0.42              |
| 1:C:177:LEU:HD23 | 1:C:177:LEU:HA   | 1.85                     | 0.42              |
| 1:C:319:GLU:CD   | 1:C:360:SER:HB3  | 2.45                     | 0.42              |
| 1:E:235:SER:O    | 1:E:236:SER:C    | 2.63                     | 0.42              |
| 1:E:254:LEU:O    | 1:E:255:ARG:C    | 2.62                     | 0.42              |
| 1:A:257:GLU:O    | 1:A:257:GLU:HG2  | 2.19                     | 0.41              |
| 1:B:331:HIS:O    | 1:B:332:ARG:HB2  | 2.20                     | 0.41              |
| 1:C:253:MET:HG3  | 1:C:253:MET:O    | 2.20                     | 0.41              |
| 1:C:333:ASP:HB2  | 1:C:354:LEU:HD12 | 2.02                     | 0.41              |
| 1:C:486:LEU:O    | 1:C:486:LEU:HD13 | 2.20                     | 0.41              |
| 1:A:308:SER:HB3  | 1:A:346:THR:HG22 | 2.02                     | 0.41              |
| 1:A:413:ARG:HH11 | 1:A:413:ARG:CG   | 2.32                     | 0.41              |
| 1:A:424:TYR:OH   | 1:A:426:LEU:HD23 | 2.21                     | 0.41              |
| 1:B:294:ARG:HD2  | 1:B:295:TYR:CZ   | 2.54                     | 0.41              |
| 1:B:490:LYS:HE3  | 1:B:490:LYS:HB2  | 1.86                     | 0.41              |
| 1:C:254:LEU:HD12 | 1:C:254:LEU:HA   | 1.88                     | 0.41              |
| 1:C:414:ARG:HA   | 1:C:414:ARG:HD2  | 1.78                     | 0.41              |
| 1:D:290:ASP:O    | 1:D:291:TYR:C    | 2.63                     | 0.41              |
| 1:D:391:LYS:O    | 1:D:391:LYS:HG2  | 2.20                     | 0.41              |
| 1:D:429:TYR:CD1  | 1:D:429:TYR:C    | 2.98                     | 0.41              |
| 1:A:297:VAL:CG2  | 1:A:298:THR:N    | 2.83                     | 0.41              |
| 1:B:195:LEU:H    | 1:B:195:LEU:HD12 | 1.85                     | 0.41              |
| 1:B:234:PHE:CE1  | 1:B:278:LEU:HD22 | 2.55                     | 0.41              |
| 1:B:393:PHE:O    | 1:B:395:SER:N    | 2.53                     | 0.41              |
| 1:B:459:GLN:O    | 1:B:465:ARG:HD3  | 2.20                     | 0.41              |
| 1:C:443:LYS:O    | 1:C:448:GLN:NE2  | 2.54                     | 0.41              |
| 1:D:251:THR:C    | 1:D:252:VAL:HG22 | 2.43                     | 0.41              |
| 1:D:344:ASN:OD1  | 1:D:346:THR:CG2  | 2.68                     | 0.41              |
| 1:D:357:ARG:HE   | 1:D:366:ASP:CG   | 2.27                     | 0.41              |
| 1:E:455:PRO:HD2  | 1:E:458:TRP:CE2  | 2.55                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:193:LEU:HB3  | 1:B:194:PRO:CD   | 2.50                     | 0.41              |
| 1:B:385:ASP:OD1  | 1:B:385:ASP:C    | 2.63                     | 0.41              |
| 1:D:278:LEU:HD12 | 1:D:278:LEU:HA   | 1.91                     | 0.41              |
| 1:E:201:ILE:O    | 1:E:205:ILE:HG13 | 2.21                     | 0.41              |
| 1:A:429:TYR:CG   | 1:A:430:ASP:N    | 2.88                     | 0.41              |
| 1:B:426:LEU:O    | 1:B:429:TYR:HB3  | 2.20                     | 0.41              |
| 1:B:330:ALA:HB3  | 1:B:356:VAL:HG22 | 2.02                     | 0.41              |
| 1:C:208:GLN:NE2  | 1:C:223:LYS:HD2  | 2.35                     | 0.41              |
| 1:D:180:LEU:HD13 | 1:D:201:ILE:HD11 | 2.03                     | 0.41              |
| 1:E:194:PRO:O    | 1:E:197:VAL:N    | 2.54                     | 0.41              |
| 1:A:244:ARG:HD2  | 1:A:244:ARG:HA   | 1.85                     | 0.41              |
| 1:A:285:HIS:HB3  | 1:A:341:VAL:HG22 | 2.03                     | 0.41              |
| 1:A:494:GLN:O    | 1:A:497:GLN:N    | 2.50                     | 0.41              |
| 1:C:240:ARG:HH11 | 1:C:240:ARG:CG   | 2.33                     | 0.41              |
| 1:C:443:LYS:HG3  | 1:C:447:GLU:CD   | 2.46                     | 0.41              |
| 1:D:455:PRO:HD2  | 1:D:458:TRP:CE3  | 2.56                     | 0.41              |
| 1:D:498:GLN:O    | 1:D:499:GLU:CG   | 2.69                     | 0.41              |
| 1:E:185:THR:O    | 1:E:185:THR:HG22 | 2.21                     | 0.41              |
| 1:E:337:LYS:NZ   | 3:E:2:PO4:O1     | 2.49                     | 0.41              |
| 1:A:317:HIS:NE2  | 1:A:400:ASP:OD2  | 2.53                     | 0.41              |
| 1:D:331:HIS:CE1  | 1:D:350:ALA:O    | 2.69                     | 0.41              |
| 1:A:256:HIS:CD2  | 1:A:258:ASN:H    | 2.38                     | 0.41              |
| 1:A:258:ASN:OD1  | 1:A:311:SER:HB2  | 2.21                     | 0.41              |
| 1:A:377:ARG:HA   | 1:A:441:MET:HE2  | 2.02                     | 0.41              |
| 1:B:417:ILE:O    | 1:B:420:ILE:HG12 | 2.20                     | 0.41              |
| 1:B:431:LEU:CD1  | 1:B:450:LEU:HD13 | 2.51                     | 0.41              |
| 1:B:455:PRO:HD2  | 1:B:458:TRP:CD2  | 2.56                     | 0.41              |
| 1:C:330:ALA:HB3  | 1:C:356:VAL:HG13 | 2.02                     | 0.41              |
| 1:C:370:ASN:O    | 1:C:390:MET:HE3  | 2.21                     | 0.41              |
| 1:C:458:TRP:HB3  | 1:C:464:LEU:HB3  | 2.02                     | 0.41              |
| 1:D:215:ARG:HG2  | 1:D:215:ARG:NH1  | 2.35                     | 0.41              |
| 1:D:270:ASN:O    | 1:D:271:GLY:C    | 2.64                     | 0.41              |
| 1:D:305:LEU:HD23 | 1:D:345:GLY:O    | 2.21                     | 0.41              |
| 1:E:215:ARG:HG3  | 1:E:215:ARG:HH11 | 1.84                     | 0.41              |
| 1:A:328:ALA:HB3  | 1:A:358:HIS:HB3  | 2.03                     | 0.41              |
| 1:E:194:PRO:O    | 1:E:195:LEU:C    | 2.64                     | 0.41              |
| 1:E:384:LEU:O    | 1:E:442:ARG:HG3  | 2.21                     | 0.41              |
| 1:A:278:LEU:HD23 | 1:A:278:LEU:HA   | 1.95                     | 0.40              |
| 1:A:393:PHE:C    | 1:A:395:SER:N    | 2.79                     | 0.40              |
| 1:B:385:ASP:O    | 1:B:386:ASP:C    | 2.64                     | 0.40              |
| 1:C:216:PHE:HB3  | 1:C:238:GLU:HB3  | 2.03                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:376:LYS:C    | 1:C:378:TYR:H    | 2.29                     | 0.40              |
| 1:C:478:ASN:ND2  | 1:C:480:ALA:HB3  | 2.37                     | 0.40              |
| 1:D:217:GLY:N    | 1:D:238:GLU:CD   | 2.80                     | 0.40              |
| 1:D:253:MET:HE3  | 1:D:326:LYS:H    | 1.84                     | 0.40              |
| 1:D:492:LEU:HD12 | 1:D:492:LEU:HA   | 1.76                     | 0.40              |
| 1:E:196:LEU:HD12 | 1:E:196:LEU:HA   | 1.93                     | 0.40              |
| 1:E:437:SER:OG   | 1:E:440:GLU:HG3  | 2.22                     | 0.40              |
| 1:E:459:GLN:NE2  | 1:E:465:ARG:HD2  | 2.35                     | 0.40              |
| 1:A:283:HIS:H    | 2:A:1:JZO:C23    | 2.35                     | 0.40              |
| 1:C:417:ILE:HD12 | 1:C:417:ILE:N    | 2.36                     | 0.40              |
| 1:D:453:ASN:O    | 1:D:455:PRO:HD3  | 2.20                     | 0.40              |
| 1:D:490:LYS:HB2  | 1:D:490:LYS:HE3  | 1.84                     | 0.40              |
| 1:A:428:TYR:CE2  | 1:A:452:PRO:HD3  | 2.56                     | 0.40              |
| 1:B:234:PHE:CD1  | 1:B:234:PHE:N    | 2.89                     | 0.40              |
| 1:B:409:TRP:CD1  | 1:B:471:MET:HE3  | 2.56                     | 0.40              |
| 1:C:286:GLY:O    | 1:C:340:LEU:HA   | 2.22                     | 0.40              |
| 1:C:189:SER:C    | 1:C:191:SER:N    | 2.80                     | 0.40              |
| 1:C:379:MET:CE   | 1:C:383:VAL:HG11 | 2.49                     | 0.40              |
| 1:D:297:VAL:CG2  | 1:D:301:GLY:HA3  | 2.51                     | 0.40              |
| 1:A:398:ARG:NH1  | 1:A:398:ARG:HG3  | 2.36                     | 0.40              |
| 1:A:453:ASN:O    | 1:A:455:PRO:HD3  | 2.21                     | 0.40              |
| 1:C:350:ALA:O    | 1:C:351:ASP:HB3  | 2.22                     | 0.40              |
| 1:C:494:GLN:HG3  | 1:C:497:GLN:NE2  | 2.36                     | 0.40              |
| 1:D:387:SER:O    | 1:D:388:ILE:C    | 2.65                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles       |
|-----|-------|---------------|-----------|----------|----------|-------------------|
| 1   | A     | 324/342 (95%) | 262 (81%) | 44 (14%) | 18 (6%)  | <b>1</b> <b>4</b> |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1   | B     | 318/342 (93%)   | 281 (88%)  | 31 (10%)  | 6 (2%)   | 6           | 22 |
| 1   | C     | 328/342 (96%)   | 251 (76%)  | 61 (19%)  | 16 (5%)  | 1           | 6  |
| 1   | D     | 328/342 (96%)   | 276 (84%)  | 38 (12%)  | 14 (4%)  | 2           | 7  |
| 1   | E     | 328/342 (96%)   | 291 (89%)  | 28 (8%)   | 9 (3%)   | 4           | 15 |
| All | All   | 1626/1710 (95%) | 1361 (84%) | 202 (12%) | 63 (4%)  | 2           | 8  |

All (63) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 215 | ARG  |
| 1   | A     | 252 | VAL  |
| 1   | A     | 366 | ASP  |
| 1   | A     | 447 | GLU  |
| 1   | B     | 235 | SER  |
| 1   | B     | 386 | ASP  |
| 1   | D     | 252 | VAL  |
| 1   | D     | 253 | MET  |
| 1   | D     | 449 | LYS  |
| 1   | E     | 215 | ARG  |
| 1   | E     | 366 | ASP  |
| 1   | A     | 185 | THR  |
| 1   | A     | 253 | MET  |
| 1   | A     | 323 | THR  |
| 1   | A     | 363 | ASP  |
| 1   | A     | 365 | ILE  |
| 1   | A     | 386 | ASP  |
| 1   | A     | 436 | PRO  |
| 1   | A     | 448 | GLN  |
| 1   | A     | 457 | ARG  |
| 1   | A     | 483 | LEU  |
| 1   | B     | 185 | THR  |
| 1   | B     | 188 | GLY  |
| 1   | C     | 252 | VAL  |
| 1   | C     | 318 | MET  |
| 1   | C     | 362 | THR  |
| 1   | C     | 377 | ARG  |
| 1   | C     | 419 | GLY  |
| 1   | D     | 186 | THR  |
| 1   | D     | 187 | SER  |
| 1   | D     | 190 | GLY  |
| 1   | E     | 271 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 498 | GLN  |
| 1   | A     | 387 | SER  |
| 1   | A     | 394 | GLU  |
| 1   | B     | 186 | THR  |
| 1   | C     | 386 | ASP  |
| 1   | C     | 389 | ASN  |
| 1   | C     | 460 | SER  |
| 1   | C     | 477 | ALA  |
| 1   | D     | 189 | SER  |
| 1   | D     | 369 | PRO  |
| 1   | E     | 483 | LEU  |
| 1   | A     | 355 | ALA  |
| 1   | B     | 252 | VAL  |
| 1   | C     | 367 | ILE  |
| 1   | D     | 325 | GLY  |
| 1   | D     | 431 | LEU  |
| 1   | D     | 455 | PRO  |
| 1   | D     | 460 | SER  |
| 1   | E     | 252 | VAL  |
| 1   | C     | 433 | PRO  |
| 1   | C     | 473 | GLU  |
| 1   | E     | 253 | MET  |
| 1   | A     | 446 | CYS  |
| 1   | C     | 332 | ARG  |
| 1   | D     | 447 | GLU  |
| 1   | E     | 369 | PRO  |
| 1   | C     | 436 | PRO  |
| 1   | E     | 433 | PRO  |
| 1   | C     | 444 | VAL  |
| 1   | D     | 388 | ILE  |
| 1   | C     | 188 | GLY  |

### 5.3.2 Protein sidechains ⓘ

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

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

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 281/294 (96%)   | 262 (93%)  | 19 (7%)  | 14          | 42 |
| 1   | B     | 278/294 (95%)   | 251 (90%)  | 27 (10%) | 8           | 25 |
| 1   | C     | 282/294 (96%)   | 257 (91%)  | 25 (9%)  | 9           | 29 |
| 1   | D     | 282/294 (96%)   | 255 (90%)  | 27 (10%) | 8           | 26 |
| 1   | E     | 282/294 (96%)   | 254 (90%)  | 28 (10%) | 7           | 24 |
| All | All   | 1405/1470 (96%) | 1279 (91%) | 126 (9%) | 9           | 28 |

All (126) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 209 | GLU  |
| 1   | A     | 229 | VAL  |
| 1   | A     | 267 | ASN  |
| 1   | A     | 269 | ASP  |
| 1   | A     | 270 | ASN  |
| 1   | A     | 276 | LEU  |
| 1   | A     | 307 | LEU  |
| 1   | A     | 334 | LEU  |
| 1   | A     | 341 | VAL  |
| 1   | A     | 346 | THR  |
| 1   | A     | 364 | THR  |
| 1   | A     | 365 | ILE  |
| 1   | A     | 382 | GLU  |
| 1   | A     | 457 | ARG  |
| 1   | A     | 458 | TRP  |
| 1   | A     | 472 | ARG  |
| 1   | A     | 486 | LEU  |
| 1   | A     | 491 | THR  |
| 1   | A     | 492 | LEU  |
| 1   | B     | 193 | LEU  |
| 1   | B     | 199 | ARG  |
| 1   | B     | 204 | THR  |
| 1   | B     | 209 | GLU  |
| 1   | B     | 229 | VAL  |
| 1   | B     | 233 | ILE  |
| 1   | B     | 238 | GLU  |
| 1   | B     | 250 | GLN  |
| 1   | B     | 269 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 272 | THR  |
| 1   | B     | 278 | LEU  |
| 1   | B     | 292 | LEU  |
| 1   | B     | 299 | VAL  |
| 1   | B     | 307 | LEU  |
| 1   | B     | 334 | LEU  |
| 1   | B     | 341 | VAL  |
| 1   | B     | 342 | LYS  |
| 1   | B     | 346 | THR  |
| 1   | B     | 356 | VAL  |
| 1   | B     | 382 | GLU  |
| 1   | B     | 391 | LYS  |
| 1   | B     | 432 | VAL  |
| 1   | B     | 449 | LYS  |
| 1   | B     | 464 | LEU  |
| 1   | B     | 486 | LEU  |
| 1   | B     | 491 | THR  |
| 1   | B     | 492 | LEU  |
| 1   | C     | 177 | LEU  |
| 1   | C     | 195 | LEU  |
| 1   | C     | 204 | THR  |
| 1   | C     | 209 | GLU  |
| 1   | C     | 215 | ARG  |
| 1   | C     | 229 | VAL  |
| 1   | C     | 240 | ARG  |
| 1   | C     | 241 | SER  |
| 1   | C     | 244 | ARG  |
| 1   | C     | 247 | GLU  |
| 1   | C     | 255 | ARG  |
| 1   | C     | 272 | THR  |
| 1   | C     | 278 | LEU  |
| 1   | C     | 296 | THR  |
| 1   | C     | 297 | VAL  |
| 1   | C     | 326 | LYS  |
| 1   | C     | 334 | LEU  |
| 1   | C     | 356 | VAL  |
| 1   | C     | 364 | THR  |
| 1   | C     | 382 | GLU  |
| 1   | C     | 392 | HIS  |
| 1   | C     | 414 | ARG  |
| 1   | C     | 446 | CYS  |
| 1   | C     | 478 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 483 | LEU  |
| 1   | D     | 195 | LEU  |
| 1   | D     | 196 | LEU  |
| 1   | D     | 204 | THR  |
| 1   | D     | 209 | GLU  |
| 1   | D     | 216 | PHE  |
| 1   | D     | 229 | VAL  |
| 1   | D     | 231 | VAL  |
| 1   | D     | 244 | ARG  |
| 1   | D     | 267 | ASN  |
| 1   | D     | 272 | THR  |
| 1   | D     | 278 | LEU  |
| 1   | D     | 292 | LEU  |
| 1   | D     | 307 | LEU  |
| 1   | D     | 316 | LEU  |
| 1   | D     | 321 | VAL  |
| 1   | D     | 334 | LEU  |
| 1   | D     | 341 | VAL  |
| 1   | D     | 342 | LYS  |
| 1   | D     | 376 | LYS  |
| 1   | D     | 382 | GLU  |
| 1   | D     | 389 | ASN  |
| 1   | D     | 417 | ILE  |
| 1   | D     | 432 | VAL  |
| 1   | D     | 441 | MET  |
| 1   | D     | 486 | LEU  |
| 1   | D     | 491 | THR  |
| 1   | D     | 492 | LEU  |
| 1   | E     | 171 | ILE  |
| 1   | E     | 178 | LYS  |
| 1   | E     | 196 | LEU  |
| 1   | E     | 204 | THR  |
| 1   | E     | 209 | GLU  |
| 1   | E     | 215 | ARG  |
| 1   | E     | 229 | VAL  |
| 1   | E     | 238 | GLU  |
| 1   | E     | 257 | GLU  |
| 1   | E     | 267 | ASN  |
| 1   | E     | 278 | LEU  |
| 1   | E     | 284 | GLU  |
| 1   | E     | 292 | LEU  |
| 1   | E     | 307 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 324 | GLN  |
| 1   | E     | 341 | VAL  |
| 1   | E     | 342 | LYS  |
| 1   | E     | 356 | VAL  |
| 1   | E     | 364 | THR  |
| 1   | E     | 376 | LYS  |
| 1   | E     | 382 | GLU  |
| 1   | E     | 404 | MET  |
| 1   | E     | 442 | ARG  |
| 1   | E     | 451 | ARG  |
| 1   | E     | 456 | ASN  |
| 1   | E     | 491 | THR  |
| 1   | E     | 492 | LEU  |
| 1   | E     | 497 | GLN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 250 | GLN  |
| 1   | A     | 267 | ASN  |
| 1   | A     | 270 | ASN  |
| 1   | A     | 324 | GLN  |
| 1   | A     | 331 | HIS  |
| 1   | A     | 448 | GLN  |
| 1   | B     | 250 | GLN  |
| 1   | B     | 256 | HIS  |
| 1   | B     | 258 | ASN  |
| 1   | B     | 315 | HIS  |
| 1   | B     | 331 | HIS  |
| 1   | B     | 389 | ASN  |
| 1   | B     | 421 | HIS  |
| 1   | C     | 208 | GLN  |
| 1   | C     | 250 | GLN  |
| 1   | C     | 256 | HIS  |
| 1   | C     | 258 | ASN  |
| 1   | C     | 331 | HIS  |
| 1   | C     | 370 | ASN  |
| 1   | C     | 389 | ASN  |
| 1   | C     | 425 | GLN  |
| 1   | C     | 453 | ASN  |
| 1   | C     | 459 | GLN  |
| 1   | C     | 478 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 497 | GLN  |
| 1   | C     | 498 | GLN  |
| 1   | D     | 250 | GLN  |
| 1   | D     | 256 | HIS  |
| 1   | D     | 315 | HIS  |
| 1   | D     | 324 | GLN  |
| 1   | D     | 331 | HIS  |
| 1   | D     | 358 | HIS  |
| 1   | D     | 370 | ASN  |
| 1   | D     | 389 | ASN  |
| 1   | D     | 392 | HIS  |
| 1   | D     | 459 | GLN  |
| 1   | D     | 497 | GLN  |
| 1   | E     | 250 | GLN  |
| 1   | E     | 256 | HIS  |
| 1   | E     | 258 | ASN  |
| 1   | E     | 315 | HIS  |
| 1   | E     | 324 | GLN  |
| 1   | E     | 331 | HIS  |
| 1   | E     | 370 | ASN  |
| 1   | E     | 389 | ASN  |
| 1   | E     | 421 | HIS  |
| 1   | E     | 448 | GLN  |
| 1   | E     | 459 | GLN  |
| 1   | E     | 478 | ASN  |
| 1   | E     | 497 | 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

18 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | PO4  | C     | 10  | -    | 4,4,4        | 1.64 | 1 (25%)  | 6,6,6       | 0.49 | 0        |
| 2   | JZO  | B     | 2   | -    | 28,30,30     | 1.68 | 8 (28%)  | 38,43,43    | 1.49 | 8 (21%)  |
| 3   | PO4  | D     | 14  | -    | 4,4,4        | 1.82 | 2 (50%)  | 6,6,6       | 0.45 | 0        |
| 3   | PO4  | D     | 15  | -    | 4,4,4        | 1.90 | 2 (50%)  | 6,6,6       | 0.42 | 0        |
| 2   | JZO  | D     | 4   | -    | 28,30,30     | 1.77 | 10 (35%) | 38,43,43    | 1.55 | 9 (23%)  |
| 3   | PO4  | E     | 2   | -    | 4,4,4        | 1.79 | 1 (25%)  | 6,6,6       | 0.46 | 0        |
| 2   | JZO  | C     | 3   | -    | 28,30,30     | 1.65 | 9 (32%)  | 38,43,43    | 1.56 | 9 (23%)  |
| 3   | PO4  | E     | 3   | -    | 4,4,4        | 1.84 | 2 (50%)  | 6,6,6       | 0.49 | 0        |
| 3   | PO4  | B     | 11  | -    | 4,4,4        | 1.72 | 0        | 6,6,6       | 0.44 | 0        |
| 2   | JZO  | E     | 5   | -    | 28,30,30     | 1.70 | 9 (32%)  | 38,43,43    | 1.57 | 9 (23%)  |
| 3   | PO4  | A     | 22  | -    | 4,4,4        | 1.72 | 1 (25%)  | 6,6,6       | 0.48 | 0        |
| 3   | PO4  | D     | 13  | -    | 4,4,4        | 1.71 | 0        | 6,6,6       | 0.47 | 0        |
| 3   | PO4  | A     | 21  | -    | 4,4,4        | 1.67 | 0        | 6,6,6       | 0.47 | 0        |
| 3   | PO4  | A     | 9   | -    | 4,4,4        | 1.75 | 2 (50%)  | 6,6,6       | 0.46 | 0        |
| 3   | PO4  | B     | 6   | -    | 4,4,4        | 1.56 | 1 (25%)  | 6,6,6       | 0.48 | 0        |
| 3   | PO4  | E     | 1   | -    | 4,4,4        | 1.72 | 1 (25%)  | 6,6,6       | 0.47 | 0        |
| 2   | JZO  | A     | 1   | -    | 28,30,30     | 1.72 | 9 (32%)  | 38,43,43    | 1.51 | 8 (21%)  |
| 3   | PO4  | B     | 12  | -    | 4,4,4        | 1.80 | 1 (25%)  | 6,6,6       | 0.46 | 0        |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 2   | JZO  | B     | 2   | -    | -       | 0/11/11/11 | 0/4/4/4 |
| 2   | JZO  | D     | 4   | -    | -       | 0/11/11/11 | 0/4/4/4 |
| 2   | JZO  | C     | 3   | -    | -       | 0/11/11/11 | 0/4/4/4 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 2   | JZO  | E     | 5   | -    | -       | 0/11/11/11 | 0/4/4/4 |
| 2   | JZO  | A     | 1   | -    | -       | 0/11/11/11 | 0/4/4/4 |

All (59) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | D     | 4   | JZO  | C27-C18 | 3.49  | 1.43        | 1.37     |
| 2   | E     | 5   | JZO  | C27-C18 | 3.38  | 1.43        | 1.37     |
| 2   | C     | 3   | JZO  | C27-C18 | 3.32  | 1.43        | 1.37     |
| 2   | D     | 4   | JZO  | C7-C8   | 3.27  | 1.44        | 1.39     |
| 2   | A     | 1   | JZO  | C27-C18 | 3.24  | 1.43        | 1.37     |
| 2   | B     | 2   | JZO  | C27-C18 | 3.22  | 1.43        | 1.37     |
| 2   | D     | 4   | JZO  | C20-C19 | 3.22  | 1.43        | 1.36     |
| 2   | B     | 2   | JZO  | C7-C8   | 3.11  | 1.44        | 1.39     |
| 2   | E     | 5   | JZO  | C7-C8   | 3.08  | 1.44        | 1.39     |
| 2   | A     | 1   | JZO  | C7-C8   | 2.99  | 1.44        | 1.39     |
| 2   | A     | 1   | JZO  | C20-C19 | 2.99  | 1.43        | 1.36     |
| 2   | E     | 5   | JZO  | C20-C19 | 2.89  | 1.42        | 1.36     |
| 2   | E     | 5   | JZO  | C19-C18 | 2.88  | 1.43        | 1.39     |
| 2   | B     | 2   | JZO  | C20-C19 | 2.86  | 1.42        | 1.36     |
| 2   | C     | 3   | JZO  | C20-C19 | 2.84  | 1.42        | 1.36     |
| 2   | C     | 3   | JZO  | C19-C18 | 2.83  | 1.43        | 1.39     |
| 2   | E     | 5   | JZO  | C23-N22 | 2.82  | 1.38        | 1.32     |
| 2   | B     | 2   | JZO  | C19-C18 | 2.81  | 1.43        | 1.39     |
| 2   | A     | 1   | JZO  | C19-C18 | 2.73  | 1.43        | 1.39     |
| 2   | D     | 4   | JZO  | C6-C7   | 2.70  | 1.43        | 1.38     |
| 2   | B     | 2   | JZO  | C6-C7   | 2.57  | 1.43        | 1.38     |
| 2   | D     | 4   | JZO  | C23-N22 | 2.56  | 1.37        | 1.32     |
| 2   | E     | 5   | JZO  | C18-C11 | 2.55  | 1.52        | 1.48     |
| 2   | C     | 3   | JZO  | C7-C8   | 2.52  | 1.43        | 1.39     |
| 2   | C     | 3   | JZO  | C23-N22 | 2.47  | 1.37        | 1.32     |
| 2   | B     | 2   | JZO  | C23-N22 | 2.47  | 1.37        | 1.32     |
| 2   | D     | 4   | JZO  | C9-C8   | 2.46  | 1.43        | 1.39     |
| 2   | A     | 1   | JZO  | C6-C7   | 2.45  | 1.43        | 1.38     |
| 2   | D     | 4   | JZO  | C6-C5   | 2.42  | 1.43        | 1.38     |
| 2   | E     | 5   | JZO  | C9-C8   | 2.40  | 1.43        | 1.39     |
| 2   | A     | 1   | JZO  | C5-C4   | 2.33  | 1.43        | 1.38     |
| 2   | A     | 1   | JZO  | C23-N22 | 2.32  | 1.37        | 1.32     |
| 3   | D     | 15  | PO4  | P-O3    | -2.31 | 1.47        | 1.54     |
| 2   | D     | 4   | JZO  | C18-C11 | 2.30  | 1.51        | 1.48     |
| 2   | D     | 4   | JZO  | C5-C4   | 2.29  | 1.43        | 1.38     |
| 2   | A     | 1   | JZO  | C9-C8   | 2.26  | 1.42        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | E     | 3   | PO4  | P-O2    | -2.25 | 1.48        | 1.54     |
| 2   | C     | 3   | JZO  | C18-C11 | 2.23  | 1.51        | 1.48     |
| 2   | E     | 5   | JZO  | C6-C7   | 2.21  | 1.42        | 1.38     |
| 2   | C     | 3   | JZO  | C9-C8   | 2.21  | 1.42        | 1.39     |
| 3   | D     | 14  | PO4  | P-O4    | -2.19 | 1.48        | 1.54     |
| 2   | D     | 4   | JZO  | C19-C18 | 2.18  | 1.42        | 1.39     |
| 2   | C     | 3   | JZO  | C6-C7   | 2.13  | 1.42        | 1.38     |
| 2   | C     | 3   | JZO  | C24-N25 | 2.13  | 1.36        | 1.32     |
| 3   | D     | 15  | PO4  | P-O4    | -2.12 | 1.48        | 1.54     |
| 3   | E     | 1   | PO4  | P-O3    | -2.11 | 1.48        | 1.54     |
| 2   | B     | 2   | JZO  | C18-C11 | 2.09  | 1.51        | 1.48     |
| 3   | E     | 2   | PO4  | P-O3    | -2.09 | 1.48        | 1.54     |
| 3   | B     | 6   | PO4  | P-O3    | -2.07 | 1.48        | 1.54     |
| 3   | A     | 22  | PO4  | P-O3    | -2.07 | 1.48        | 1.54     |
| 2   | E     | 5   | JZO  | C24-N25 | 2.06  | 1.36        | 1.32     |
| 2   | A     | 1   | JZO  | C6-C5   | 2.06  | 1.42        | 1.38     |
| 3   | B     | 12  | PO4  | P-O4    | -2.05 | 1.48        | 1.54     |
| 2   | B     | 2   | JZO  | C5-C4   | 2.04  | 1.43        | 1.38     |
| 3   | D     | 14  | PO4  | P-O3    | -2.03 | 1.48        | 1.54     |
| 3   | A     | 9   | PO4  | P-O2    | -2.02 | 1.48        | 1.54     |
| 3   | C     | 10  | PO4  | P-O4    | -2.02 | 1.48        | 1.54     |
| 3   | E     | 3   | PO4  | P-O4    | -2.01 | 1.48        | 1.54     |
| 3   | A     | 9   | PO4  | P-O3    | -2.01 | 1.48        | 1.54     |

All (43) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 2   | C     | 3   | JZO  | C10-C16-N14 | 3.72 | 108.00      | 104.41   |
| 2   | C     | 3   | JZO  | C23-N22-C21 | 3.68 | 122.50      | 116.93   |
| 2   | D     | 4   | JZO  | C23-N22-C21 | 3.60 | 122.38      | 116.93   |
| 2   | E     | 5   | JZO  | C23-N22-C21 | 3.54 | 122.28      | 116.93   |
| 2   | A     | 1   | JZO  | C23-N22-C21 | 3.53 | 122.27      | 116.93   |
| 2   | E     | 5   | JZO  | C10-C16-N14 | 3.44 | 107.73      | 104.41   |
| 2   | A     | 1   | JZO  | C10-C16-N14 | 3.41 | 107.70      | 104.41   |
| 2   | E     | 5   | JZO  | C24-N25-C26 | 3.40 | 122.07      | 116.93   |
| 2   | B     | 2   | JZO  | C10-C16-N14 | 3.35 | 107.64      | 104.41   |
| 2   | B     | 2   | JZO  | C23-N22-C21 | 3.34 | 121.98      | 116.93   |
| 2   | D     | 4   | JZO  | C10-C16-N14 | 3.29 | 107.59      | 104.41   |
| 2   | D     | 4   | JZO  | C24-N25-C26 | 3.25 | 121.85      | 116.93   |
| 2   | B     | 2   | JZO  | C24-N25-C26 | 3.16 | 121.72      | 116.93   |
| 2   | A     | 1   | JZO  | C24-N25-C26 | 3.11 | 121.64      | 116.93   |
| 2   | C     | 3   | JZO  | C24-N25-C26 | 2.96 | 121.41      | 116.93   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | E     | 5   | JZO  | C26-C21-N22 | -2.96 | 118.33      | 121.00   |
| 2   | A     | 1   | JZO  | C26-C21-N22 | -2.86 | 118.42      | 121.00   |
| 2   | D     | 4   | JZO  | C24-C23-N22 | -2.82 | 118.56      | 122.76   |
| 2   | C     | 3   | JZO  | C26-C21-N22 | -2.80 | 118.48      | 121.00   |
| 2   | D     | 4   | JZO  | C26-C21-N22 | -2.77 | 118.50      | 121.00   |
| 2   | B     | 2   | JZO  | C26-C21-N22 | -2.75 | 118.52      | 121.00   |
| 2   | E     | 5   | JZO  | C24-C23-N22 | -2.72 | 118.72      | 122.76   |
| 2   | C     | 3   | JZO  | C24-C23-N22 | -2.71 | 118.73      | 122.76   |
| 2   | A     | 1   | JZO  | C24-C23-N22 | -2.61 | 118.88      | 122.76   |
| 2   | C     | 3   | JZO  | C27-C26-N25 | 2.54  | 120.93      | 118.01   |
| 2   | B     | 2   | JZO  | C24-C23-N22 | -2.54 | 118.99      | 122.76   |
| 2   | D     | 4   | JZO  | C27-C26-N25 | 2.52  | 120.91      | 118.01   |
| 2   | E     | 5   | JZO  | C27-C26-N25 | 2.45  | 120.83      | 118.01   |
| 2   | A     | 1   | JZO  | C27-C26-N25 | 2.33  | 120.69      | 118.01   |
| 2   | B     | 2   | JZO  | C27-C26-N25 | 2.30  | 120.65      | 118.01   |
| 2   | E     | 5   | JZO  | C15-N14-N12 | 2.28  | 125.85      | 120.94   |
| 2   | C     | 3   | JZO  | C15-N14-N12 | 2.26  | 125.79      | 120.94   |
| 2   | E     | 5   | JZO  | C23-C24-N25 | -2.25 | 119.41      | 122.76   |
| 2   | A     | 1   | JZO  | C23-C24-N25 | -2.21 | 119.48      | 122.76   |
| 2   | D     | 4   | JZO  | C23-C24-N25 | -2.17 | 119.54      | 122.76   |
| 2   | B     | 2   | JZO  | C23-C24-N25 | -2.16 | 119.55      | 122.76   |
| 2   | A     | 1   | JZO  | C15-N14-N12 | 2.11  | 125.48      | 120.94   |
| 2   | B     | 2   | JZO  | C15-N14-N12 | 2.09  | 125.44      | 120.94   |
| 2   | C     | 3   | JZO  | C23-C24-N25 | -2.05 | 119.72      | 122.76   |
| 2   | C     | 3   | JZO  | C21-C26-N25 | -2.05 | 119.16      | 121.00   |
| 2   | D     | 4   | JZO  | C21-C26-N25 | -2.05 | 119.16      | 121.00   |
| 2   | E     | 5   | JZO  | C21-C26-N25 | -2.01 | 119.19      | 121.00   |
| 2   | D     | 4   | JZO  | C8-C10-C11  | 2.01  | 130.92      | 127.01   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 17 short contacts:

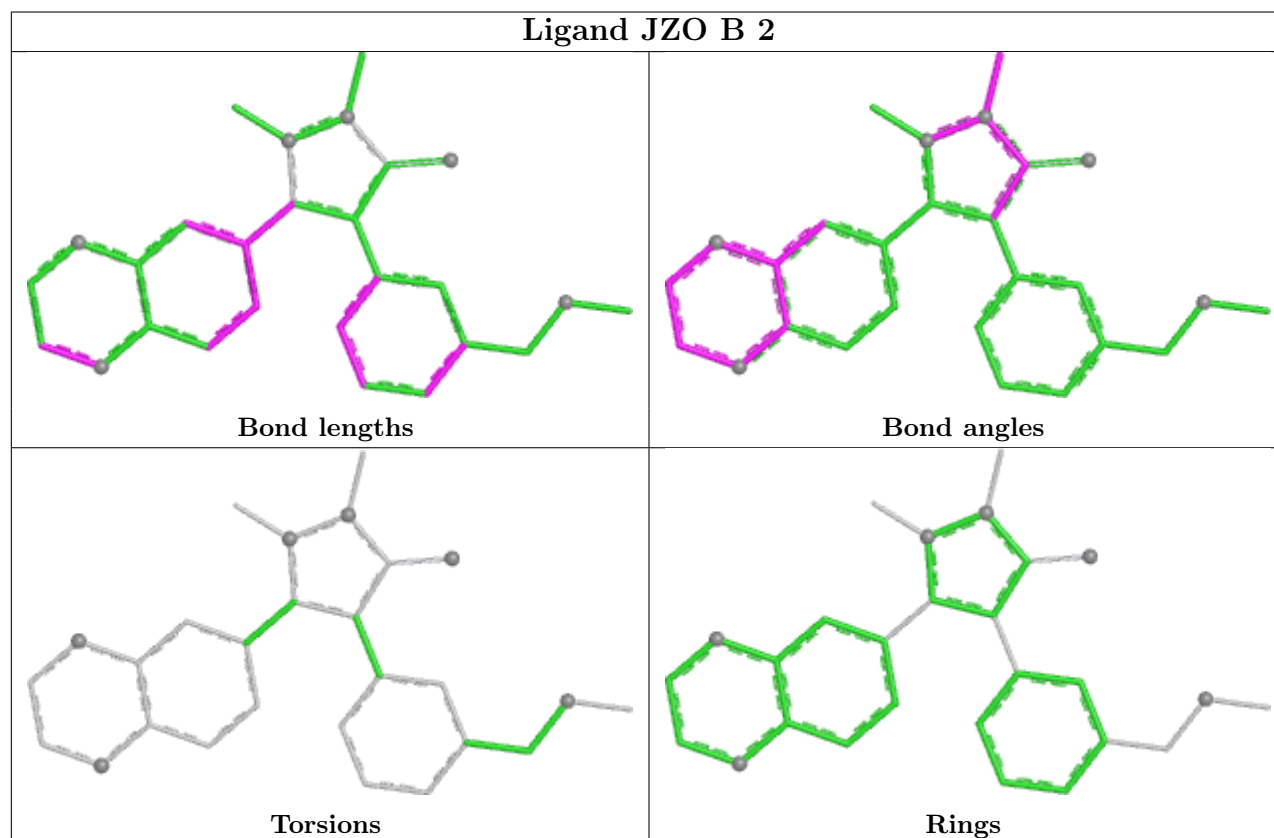
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | C     | 10  | PO4  | 1       | 0            |
| 3   | D     | 15  | PO4  | 1       | 0            |
| 2   | D     | 4   | JZO  | 3       | 0            |
| 3   | E     | 2   | PO4  | 1       | 0            |
| 2   | C     | 3   | JZO  | 3       | 0            |
| 3   | E     | 3   | PO4  | 2       | 0            |

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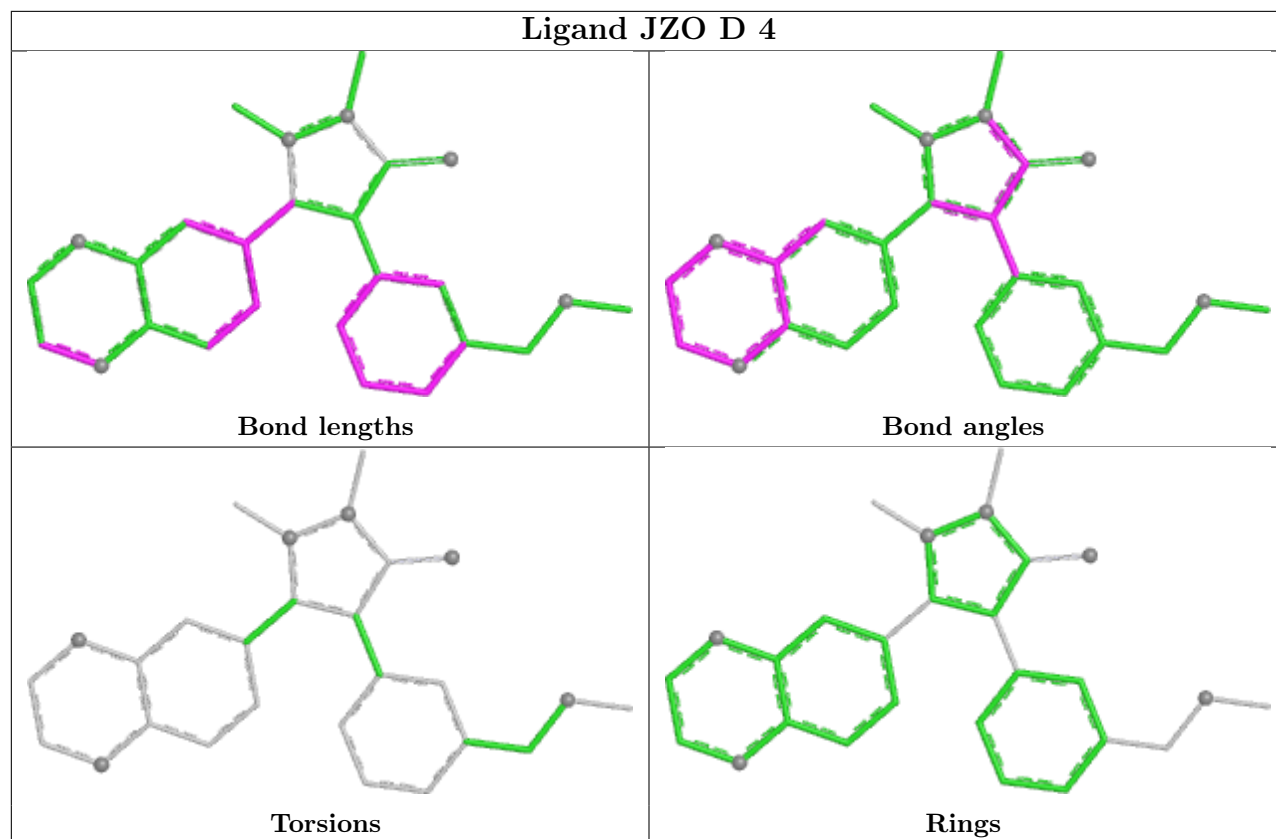
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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | B     | 11  | PO4  | 2       | 0            |
| 2   | E     | 5   | JZO  | 1       | 0            |
| 3   | B     | 6   | PO4  | 1       | 0            |
| 2   | A     | 1   | JZO  | 1       | 0            |
| 3   | B     | 12  | PO4  | 1       | 0            |

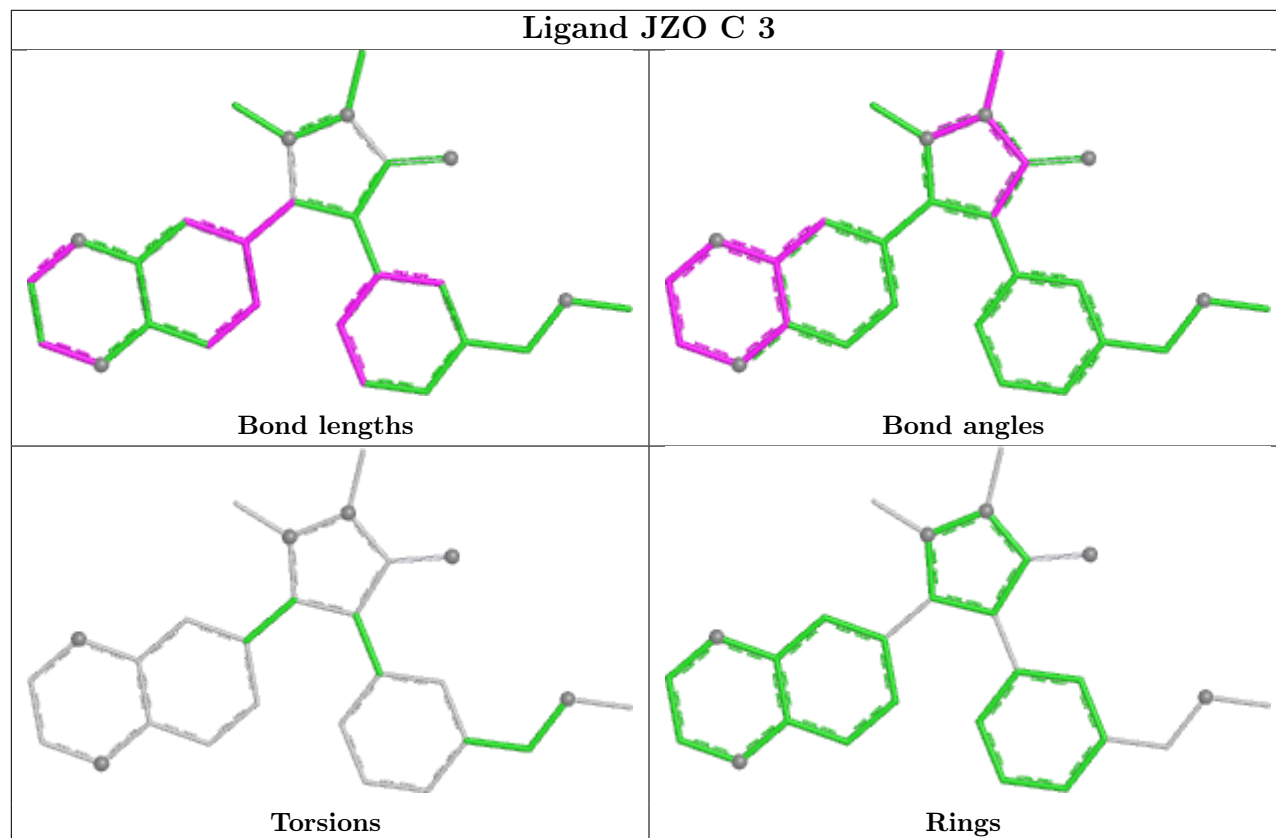
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## Ligand JZO D 4

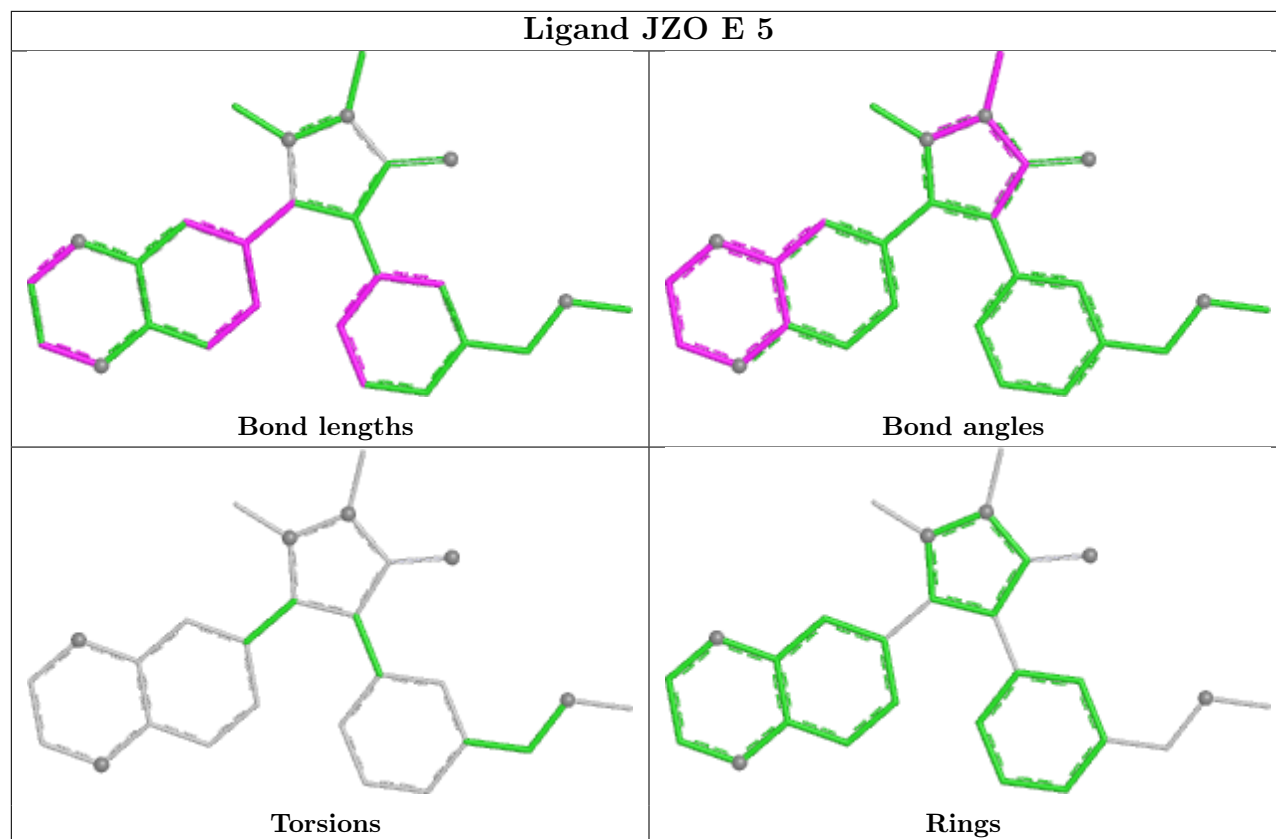


## Ligand JZO C 3

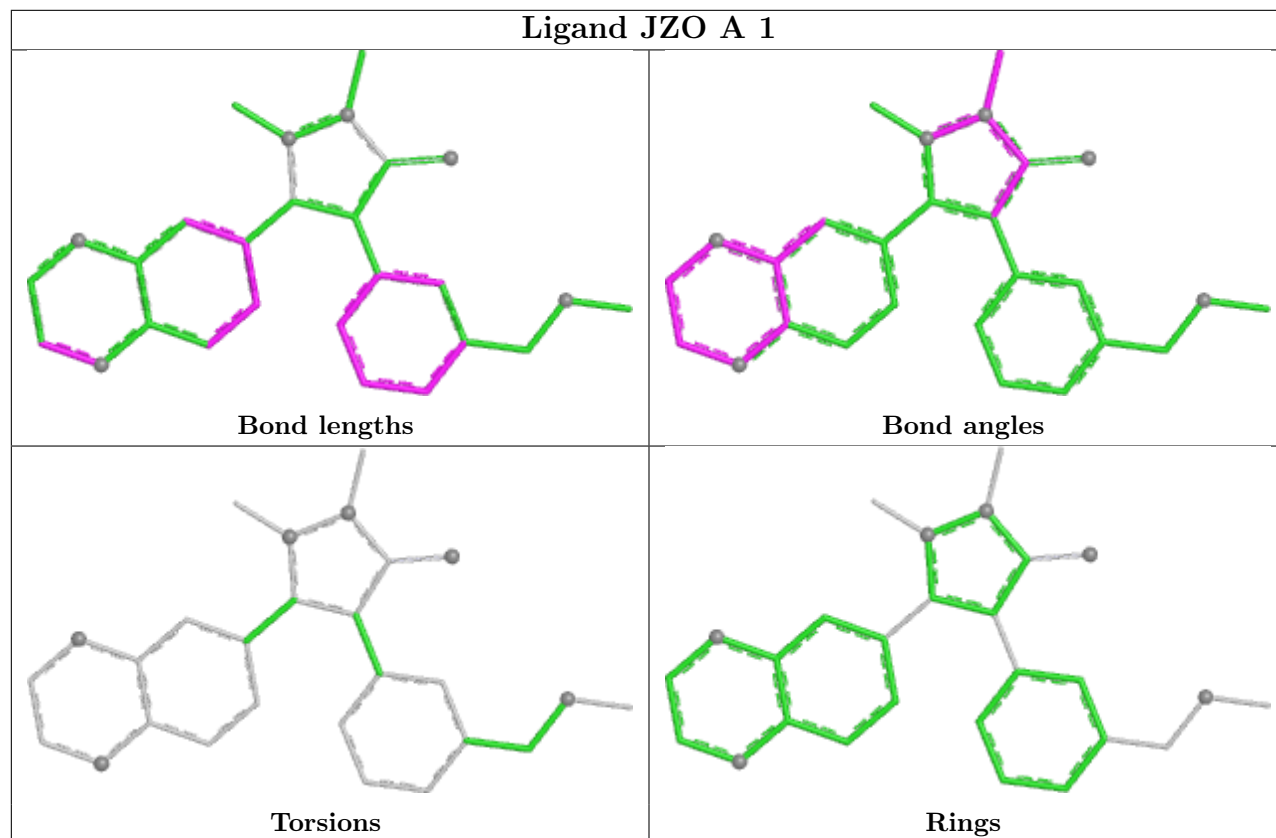




## Ligand JZO E 5



## Ligand JZO A 1



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 328/342 (95%)   | 0.85   | 54 (16%) 4 3  | 23, 67, 105, 113      | 0     |
| 1   | B     | 324/342 (94%)   | 0.06   | 15 (4%) 37 29 | 17, 38, 68, 98        | 0     |
| 1   | C     | 330/342 (96%)   | 1.26   | 88 (26%) 1 1  | 21, 71, 100, 110      | 0     |
| 1   | D     | 330/342 (96%)   | 0.32   | 24 (7%) 21 15 | 20, 43, 82, 93        | 0     |
| 1   | E     | 330/342 (96%)   | 0.08   | 28 (8%) 16 12 | 18, 37, 76, 93        | 0     |
| All | All   | 1642/1710 (96%) | 0.52   | 209 (12%) 8 6 | 17, 47, 96, 113       | 0     |

All (209) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 252 | VAL  | 6.5  |
| 1   | C     | 369 | PRO  | 5.8  |
| 1   | D     | 321 | VAL  | 5.2  |
| 1   | C     | 500 | GLY  | 5.2  |
| 1   | C     | 455 | PRO  | 5.1  |
| 1   | E     | 191 | SER  | 4.9  |
| 1   | C     | 367 | ILE  | 4.8  |
| 1   | D     | 252 | VAL  | 4.8  |
| 1   | A     | 190 | GLY  | 4.8  |
| 1   | D     | 500 | GLY  | 4.4  |
| 1   | A     | 253 | MET  | 4.4  |
| 1   | B     | 191 | SER  | 4.4  |
| 1   | B     | 252 | VAL  | 4.3  |
| 1   | D     | 323 | THR  | 4.3  |
| 1   | A     | 500 | GLY  | 4.3  |
| 1   | E     | 500 | GLY  | 4.2  |
| 1   | E     | 370 | ASN  | 4.1  |
| 1   | A     | 324 | GLN  | 4.1  |
| 1   | C     | 321 | VAL  | 4.0  |
| 1   | A     | 251 | THR  | 4.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 325 | GLY  | 4.0  |
| 1   | C     | 426 | LEU  | 3.9  |
| 1   | C     | 323 | THR  | 3.9  |
| 1   | E     | 371 | HIS  | 3.9  |
| 1   | D     | 420 | ILE  | 3.8  |
| 1   | A     | 323 | THR  | 3.8  |
| 1   | E     | 367 | ILE  | 3.8  |
| 1   | E     | 321 | VAL  | 3.7  |
| 1   | D     | 216 | PHE  | 3.7  |
| 1   | C     | 424 | TYR  | 3.7  |
| 1   | D     | 325 | GLY  | 3.7  |
| 1   | C     | 457 | ARG  | 3.6  |
| 1   | C     | 217 | GLY  | 3.6  |
| 1   | A     | 417 | ILE  | 3.6  |
| 1   | D     | 324 | GLN  | 3.5  |
| 1   | E     | 215 | ARG  | 3.5  |
| 1   | D     | 422 | GLU  | 3.5  |
| 1   | A     | 446 | CYS  | 3.5  |
| 1   | C     | 361 | ALA  | 3.4  |
| 1   | E     | 323 | THR  | 3.4  |
| 1   | C     | 477 | ALA  | 3.4  |
| 1   | C     | 419 | GLY  | 3.3  |
| 1   | B     | 367 | ILE  | 3.3  |
| 1   | C     | 454 | ILE  | 3.3  |
| 1   | A     | 252 | VAL  | 3.3  |
| 1   | C     | 377 | ARG  | 3.3  |
| 1   | E     | 252 | VAL  | 3.3  |
| 1   | D     | 190 | GLY  | 3.3  |
| 1   | D     | 370 | ASN  | 3.3  |
| 1   | C     | 472 | ARG  | 3.3  |
| 1   | E     | 322 | GLY  | 3.3  |
| 1   | C     | 443 | LYS  | 3.2  |
| 1   | D     | 238 | GLU  | 3.2  |
| 1   | C     | 450 | LEU  | 3.2  |
| 1   | E     | 324 | GLN  | 3.2  |
| 1   | C     | 318 | MET  | 3.2  |
| 1   | C     | 420 | ILE  | 3.2  |
| 1   | E     | 188 | GLY  | 3.2  |
| 1   | C     | 476 | TYR  | 3.2  |
| 1   | B     | 188 | GLY  | 3.2  |
| 1   | A     | 320 | ILE  | 3.2  |
| 1   | E     | 216 | PHE  | 3.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 321 | VAL  | 3.2  |
| 1   | A     | 431 | LEU  | 3.1  |
| 1   | C     | 434 | SER  | 3.1  |
| 1   | C     | 421 | HIS  | 3.1  |
| 1   | C     | 392 | HIS  | 3.1  |
| 1   | C     | 187 | SER  | 3.1  |
| 1   | C     | 371 | HIS  | 3.0  |
| 1   | A     | 367 | ILE  | 3.0  |
| 1   | C     | 431 | LEU  | 3.0  |
| 1   | C     | 253 | MET  | 3.0  |
| 1   | C     | 370 | ASN  | 2.9  |
| 1   | A     | 420 | ILE  | 2.9  |
| 1   | C     | 425 | GLN  | 2.9  |
| 1   | C     | 427 | PRO  | 2.9  |
| 1   | A     | 325 | GLY  | 2.9  |
| 1   | C     | 188 | GLY  | 2.9  |
| 1   | C     | 291 | TYR  | 2.9  |
| 1   | C     | 467 | MET  | 2.9  |
| 1   | A     | 438 | VAL  | 2.9  |
| 1   | C     | 438 | VAL  | 2.9  |
| 1   | C     | 365 | ILE  | 2.9  |
| 1   | C     | 463 | ALA  | 2.8  |
| 1   | D     | 417 | ILE  | 2.8  |
| 1   | D     | 448 | GLN  | 2.8  |
| 1   | A     | 216 | PHE  | 2.8  |
| 1   | A     | 392 | HIS  | 2.8  |
| 1   | C     | 496 | SER  | 2.8  |
| 1   | C     | 466 | VAL  | 2.8  |
| 1   | D     | 322 | GLY  | 2.8  |
| 1   | A     | 294 | ARG  | 2.8  |
| 1   | A     | 487 | ARG  | 2.8  |
| 1   | A     | 432 | VAL  | 2.8  |
| 1   | C     | 417 | ILE  | 2.8  |
| 1   | C     | 191 | SER  | 2.8  |
| 1   | C     | 448 | GLN  | 2.7  |
| 1   | A     | 458 | TRP  | 2.7  |
| 1   | C     | 411 | ILE  | 2.7  |
| 1   | C     | 364 | THR  | 2.7  |
| 1   | C     | 325 | GLY  | 2.7  |
| 1   | A     | 191 | SER  | 2.7  |
| 1   | A     | 215 | ARG  | 2.7  |
| 1   | B     | 189 | SER  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 499 | GLU  | 2.7  |
| 1   | A     | 415 | CYS  | 2.7  |
| 1   | A     | 457 | ARG  | 2.7  |
| 1   | C     | 462 | GLU  | 2.7  |
| 1   | C     | 407 | VAL  | 2.6  |
| 1   | A     | 475 | TRP  | 2.6  |
| 1   | D     | 191 | SER  | 2.6  |
| 1   | C     | 458 | TRP  | 2.6  |
| 1   | A     | 322 | GLY  | 2.6  |
| 1   | C     | 444 | VAL  | 2.6  |
| 1   | A     | 371 | HIS  | 2.5  |
| 1   | C     | 433 | PRO  | 2.5  |
| 1   | B     | 238 | GLU  | 2.5  |
| 1   | E     | 237 | ARG  | 2.5  |
| 1   | C     | 490 | LYS  | 2.5  |
| 1   | A     | 238 | GLU  | 2.5  |
| 1   | C     | 292 | LEU  | 2.5  |
| 1   | B     | 190 | GLY  | 2.5  |
| 1   | E     | 253 | MET  | 2.5  |
| 1   | D     | 371 | HIS  | 2.5  |
| 1   | C     | 423 | ASP  | 2.5  |
| 1   | E     | 190 | GLY  | 2.5  |
| 1   | B     | 237 | ARG  | 2.5  |
| 1   | B     | 371 | HIS  | 2.5  |
| 1   | A     | 318 | MET  | 2.4  |
| 1   | E     | 369 | PRO  | 2.4  |
| 1   | C     | 216 | PHE  | 2.4  |
| 1   | E     | 319 | GLU  | 2.4  |
| 1   | C     | 429 | TYR  | 2.4  |
| 1   | B     | 186 | THR  | 2.4  |
| 1   | A     | 448 | GLN  | 2.4  |
| 1   | E     | 318 | MET  | 2.4  |
| 1   | D     | 487 | ARG  | 2.4  |
| 1   | C     | 368 | ALA  | 2.4  |
| 1   | C     | 475 | TRP  | 2.4  |
| 1   | C     | 422 | GLU  | 2.4  |
| 1   | D     | 421 | HIS  | 2.4  |
| 1   | A     | 188 | GLY  | 2.3  |
| 1   | A     | 460 | SER  | 2.3  |
| 1   | E     | 236 | SER  | 2.3  |
| 1   | C     | 483 | LEU  | 2.3  |
| 1   | C     | 488 | ILE  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 485 | ALA  | 2.3  |
| 1   | A     | 295 | TYR  | 2.3  |
| 1   | C     | 251 | THR  | 2.3  |
| 1   | A     | 255 | ARG  | 2.3  |
| 1   | C     | 390 | MET  | 2.3  |
| 1   | C     | 324 | GLN  | 2.3  |
| 1   | B     | 185 | THR  | 2.3  |
| 1   | C     | 215 | ARG  | 2.3  |
| 1   | D     | 439 | GLU  | 2.3  |
| 1   | A     | 449 | LYS  | 2.3  |
| 1   | C     | 304 | LYS  | 2.3  |
| 1   | A     | 189 | SER  | 2.3  |
| 1   | E     | 460 | SER  | 2.3  |
| 1   | C     | 380 | ALA  | 2.2  |
| 1   | C     | 453 | ASN  | 2.2  |
| 1   | A     | 254 | LEU  | 2.2  |
| 1   | D     | 215 | ARG  | 2.2  |
| 1   | D     | 457 | ARG  | 2.2  |
| 1   | E     | 251 | THR  | 2.2  |
| 1   | C     | 416 | SER  | 2.2  |
| 1   | B     | 253 | MET  | 2.2  |
| 1   | C     | 459 | GLN  | 2.2  |
| 1   | C     | 296 | THR  | 2.2  |
| 1   | A     | 360 | SER  | 2.2  |
| 1   | A     | 424 | TYR  | 2.2  |
| 1   | A     | 426 | LEU  | 2.2  |
| 1   | B     | 361 | ALA  | 2.2  |
| 1   | C     | 464 | LEU  | 2.2  |
| 1   | C     | 468 | ALA  | 2.2  |
| 1   | E     | 361 | ALA  | 2.2  |
| 1   | A     | 421 | HIS  | 2.2  |
| 1   | C     | 393 | PHE  | 2.2  |
| 1   | C     | 465 | ARG  | 2.2  |
| 1   | C     | 432 | VAL  | 2.2  |
| 1   | C     | 378 | TYR  | 2.2  |
| 1   | E     | 320 | ILE  | 2.1  |
| 1   | A     | 427 | PRO  | 2.1  |
| 1   | A     | 423 | ASP  | 2.1  |
| 1   | A     | 214 | GLY  | 2.1  |
| 1   | C     | 486 | LEU  | 2.1  |
| 1   | A     | 428 | TYR  | 2.1  |
| 1   | C     | 412 | ALA  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 298 | THR  | 2.1  |
| 1   | D     | 419 | GLY  | 2.1  |
| 1   | E     | 186 | THR  | 2.1  |
| 1   | E     | 368 | ALA  | 2.1  |
| 1   | A     | 437 | SER  | 2.1  |
| 1   | B     | 394 | GLU  | 2.1  |
| 1   | C     | 189 | SER  | 2.1  |
| 1   | C     | 300 | GLU  | 2.1  |
| 1   | D     | 253 | MET  | 2.1  |
| 1   | A     | 433 | PRO  | 2.1  |
| 1   | B     | 254 | LEU  | 2.1  |
| 1   | C     | 410 | GLU  | 2.1  |
| 1   | C     | 470 | ILE  | 2.1  |
| 1   | A     | 434 | SER  | 2.1  |
| 1   | C     | 362 | THR  | 2.1  |
| 1   | A     | 454 | ILE  | 2.1  |
| 1   | A     | 439 | GLU  | 2.1  |
| 1   | C     | 381 | PRO  | 2.0  |
| 1   | E     | 270 | ASN  | 2.0  |
| 1   | C     | 384 | LEU  | 2.0  |
| 1   | A     | 301 | GLY  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | PO4  | A     | 21  | 5/5   | 0.87 | 0.29 | 35,36,36,37                 | 5     |
| 3   | PO4  | C     | 10  | 5/5   | 0.90 | 0.10 | 61,61,63,63                 | 0     |

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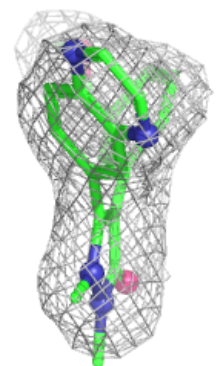
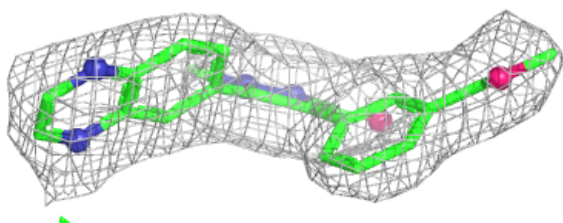
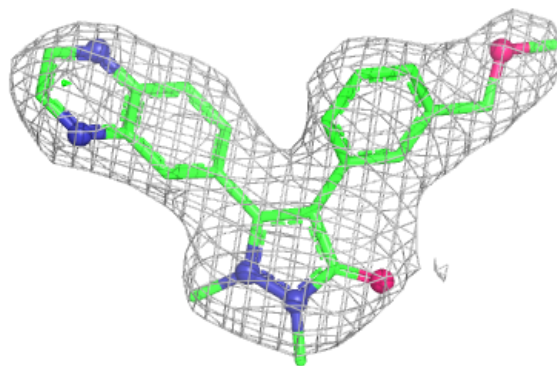
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | PO4  | A     | 9   | 5/5   | 0.92 | 0.10 | 69,70,70,71                 | 0     |
| 3   | PO4  | B     | 6   | 5/5   | 0.93 | 0.09 | 37,37,38,40                 | 0     |
| 3   | PO4  | A     | 22  | 5/5   | 0.93 | 0.20 | 19,20,22,23                 | 5     |
| 3   | PO4  | D     | 15  | 5/5   | 0.93 | 0.23 | 2,7,8,8                     | 5     |
| 3   | PO4  | D     | 13  | 5/5   | 0.94 | 0.08 | 54,54,55,56                 | 0     |
| 3   | PO4  | D     | 14  | 5/5   | 0.94 | 0.23 | 21,21,21,22                 | 5     |
| 2   | JZO  | C     | 3   | 27/27 | 0.95 | 0.10 | 41,47,49,50                 | 0     |
| 2   | JZO  | D     | 4   | 27/27 | 0.96 | 0.08 | 25,28,35,39                 | 0     |
| 2   | JZO  | E     | 5   | 27/27 | 0.96 | 0.09 | 25,28,32,32                 | 0     |
| 3   | PO4  | B     | 12  | 5/5   | 0.96 | 0.21 | 15,16,16,18                 | 5     |
| 3   | PO4  | B     | 11  | 5/5   | 0.96 | 0.17 | 1,2,6,6                     | 5     |
| 3   | PO4  | E     | 2   | 5/5   | 0.96 | 0.21 | 7,8,10,11                   | 5     |
| 3   | PO4  | E     | 1   | 5/5   | 0.97 | 0.10 | 44,44,46,46                 | 0     |
| 2   | JZO  | A     | 1   | 27/27 | 0.97 | 0.07 | 26,30,34,39                 | 0     |
| 3   | PO4  | E     | 3   | 5/5   | 0.97 | 0.18 | 1,1,2,3                     | 5     |
| 2   | JZO  | B     | 2   | 27/27 | 0.98 | 0.06 | 17,22,26,30                 | 0     |

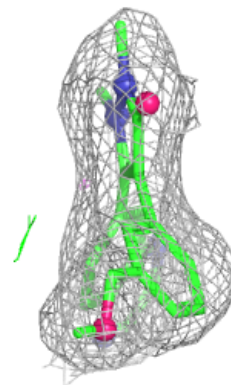
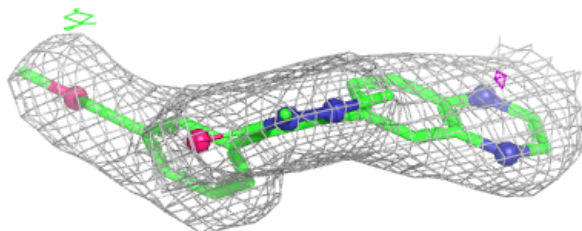
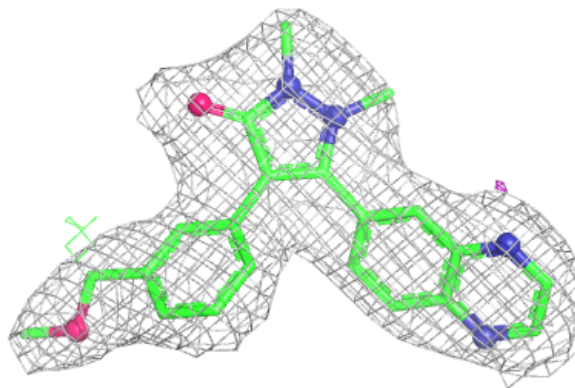
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around JZO C 3:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

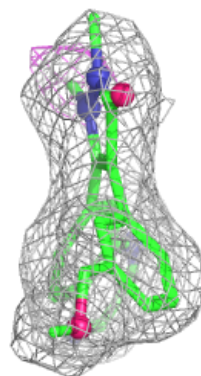
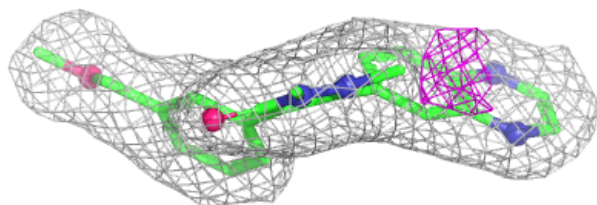
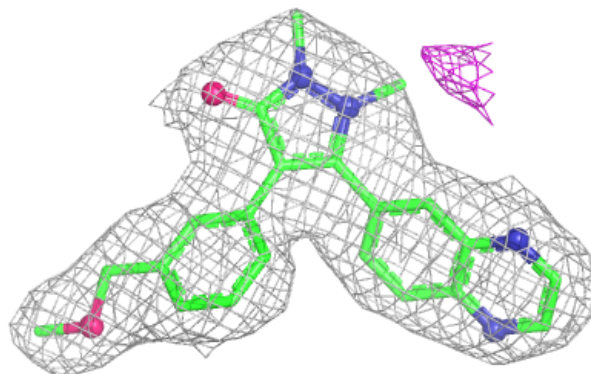
**Electron density around JZO D 4:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

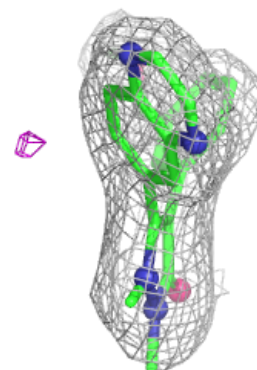
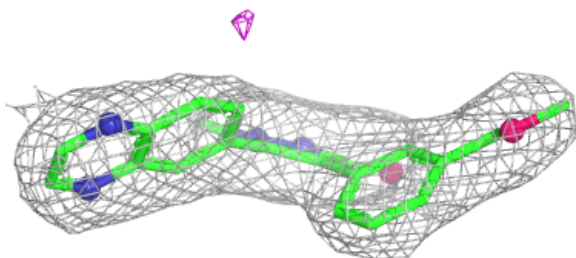
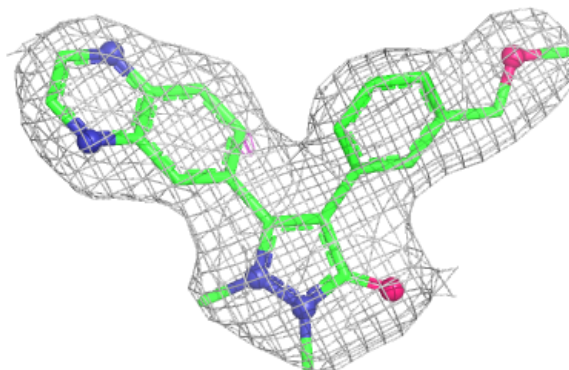


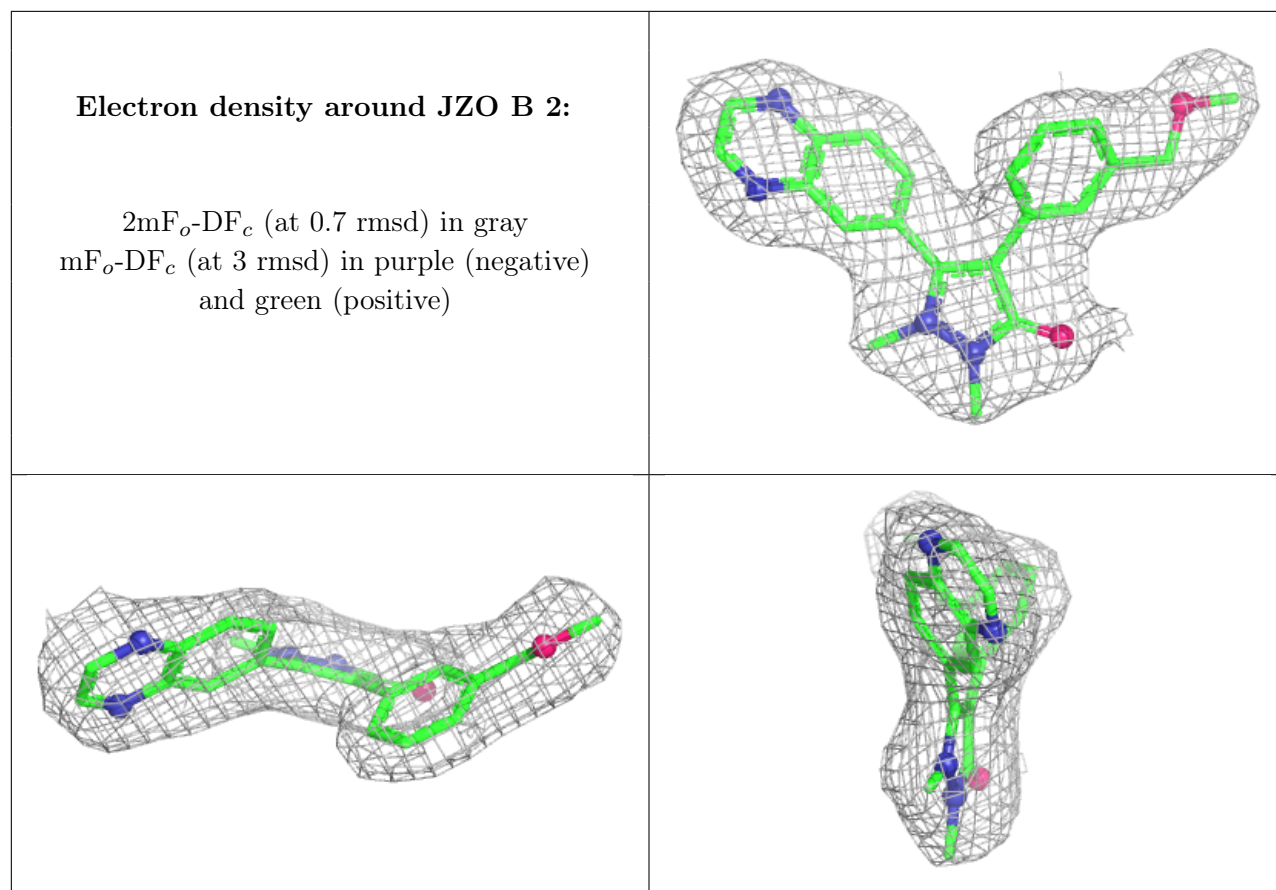
**Electron density around JZO E 5:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around JZO A 1:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers ⓘ

There are no such residues in this entry.