



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:55 PM UTC

PDB ID : 2VGF / pdb\_00002vgf  
Title : HUMAN ERYTHROCYTE PYRUVATE KINASE: T384M mutant  
Authors : Valentini, G.; Chiarelli, L.R.; Fortin, R.; Dolzan, M.; Galizzi, A.; Abraham, D.J.; Wang, C.; Bianchi, P.; Zanella, A.; Mattevi, A.  
Deposited on : 2007-11-12  
Resolution : 2.75 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

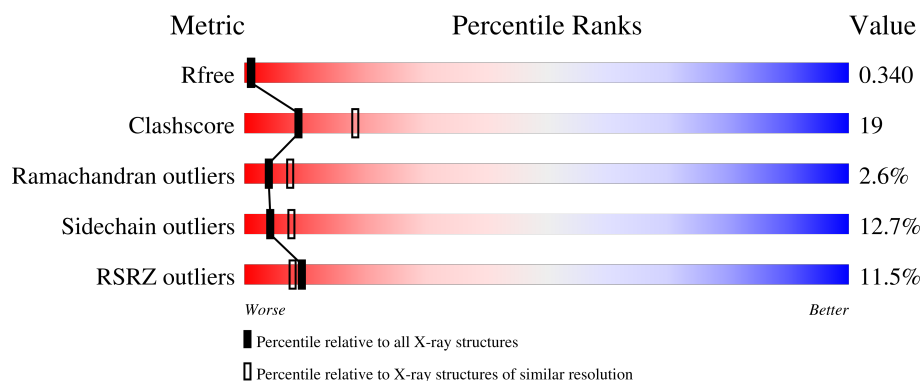
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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                      | 1009 (2.76-2.76)                                      |
| Clashscore            | 190562                      | 1044 (2.76-2.76)                                      |
| Ramachandran outliers | 187476                      | 1024 (2.76-2.76)                                      |
| Sidechain outliers    | 187428                      | 1024 (2.76-2.76)                                      |
| RSRZ outliers         | 180081                      | 1009 (2.76-2.76)                                      |

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     | 528    |                  |
| 1   | B     | 528    |                  |
| 1   | C     | 528    |                  |
| 1   | D     | 528    |                  |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15550 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.

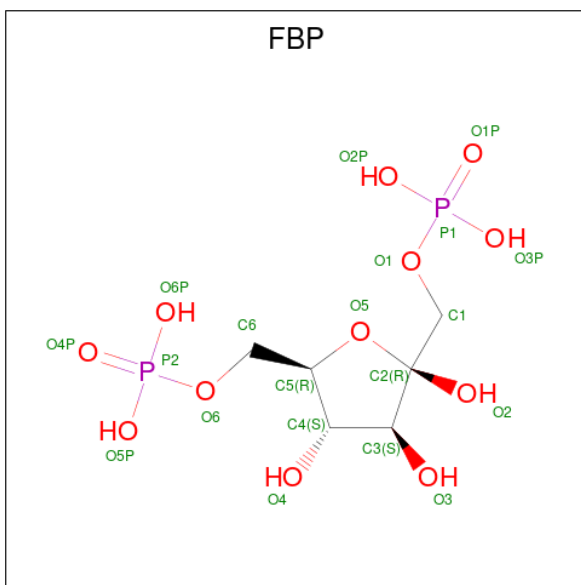
- Molecule 1 is a protein called PYRUVATE KINASE ISOZYMES R/L.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 517      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3913  | 2458 | 709 | 727 | 19 |         |         |       |
| 1   | B     | 491      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3720  | 2340 | 673 | 688 | 19 |         |         |       |
| 1   | C     | 517      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3913  | 2458 | 709 | 727 | 19 |         |         |       |
| 1   | D     | 512      | Total | C    | N   | O   | S  | 7       | 0       | 0     |
|     |       |          | 3880  | 2437 | 703 | 721 | 19 |         |         |       |

There are 4 discrepancies between the modelled and reference sequences:

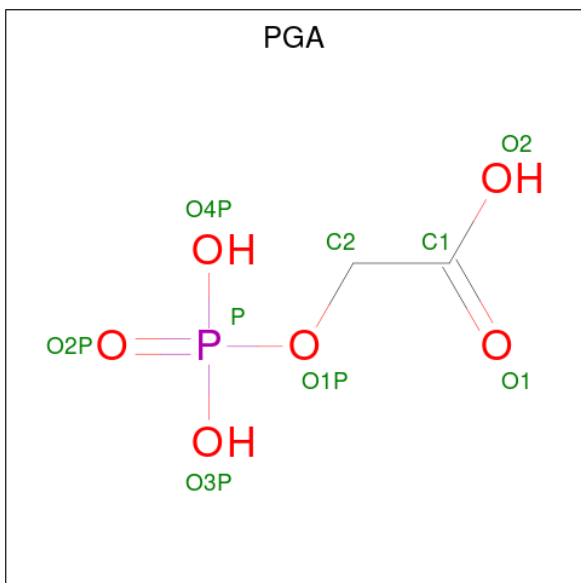
| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 384     | MET      | THR    | engineered mutation | UNP P30613 |
| B     | 384     | MET      | THR    | engineered mutation | UNP P30613 |
| C     | 384     | MET      | THR    | engineered mutation | UNP P30613 |
| D     | 384     | MET      | THR    | engineered mutation | UNP P30613 |

- Molecule 2 is 1,6-di-O-phosphono-beta-D-fructofuranose (CCD ID: FBP) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>12</sub>P<sub>2</sub>).



| Mol | Chain | Residues | Atoms |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---|---------|---------|
| 2   | A     | 1        | Total | C | O  | P | 0       | 0       |
|     |       |          | 20    | 6 | 12 | 2 |         |         |
| 2   | B     | 1        | Total | C | O  | P | 0       | 0       |
|     |       |          | 20    | 6 | 12 | 2 |         |         |
| 2   | C     | 1        | Total | C | O  | P | 0       | 0       |
|     |       |          | 20    | 6 | 12 | 2 |         |         |
| 2   | D     | 1        | Total | C | O  | P | 0       | 0       |
|     |       |          | 20    | 6 | 12 | 2 |         |         |

- Molecule 3 is 2-PHOSPHOGLYCOLIC ACID (CCD ID: PGA) (formula:  $C_2H_5O_6P$ ).



| Mol | Chain | Residues | Atoms                  | ZeroOcc | AltConf |
|-----|-------|----------|------------------------|---------|---------|
| 3   | A     | 1        | Total C O P<br>9 2 6 1 | 0       | 0       |
| 3   | B     | 1        | Total C O P<br>9 2 6 1 | 0       | 0       |
| 3   | C     | 1        | Total C O P<br>9 2 6 1 | 0       | 0       |
| 3   | D     | 1        | Total C O P<br>9 2 6 1 | 0       | 0       |

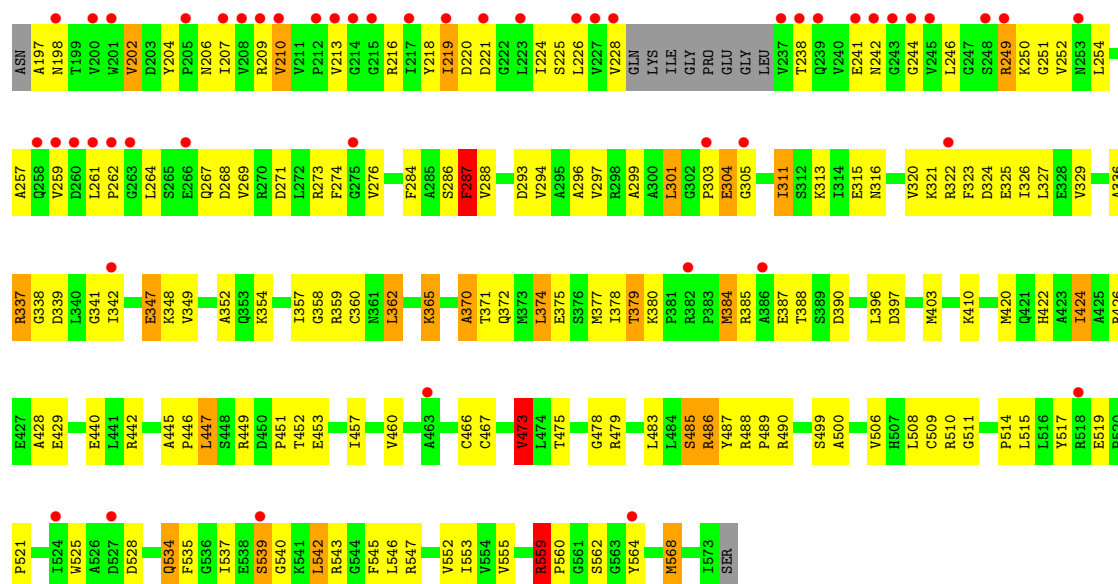
- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms          | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 4   | A     | 1        | Total K<br>1 1 | 0       | 0       |
| 4   | B     | 1        | Total K<br>1 1 | 0       | 0       |
| 4   | C     | 1        | Total K<br>1 1 | 0       | 0       |
| 4   | D     | 1        | Total K<br>1 1 | 0       | 0       |

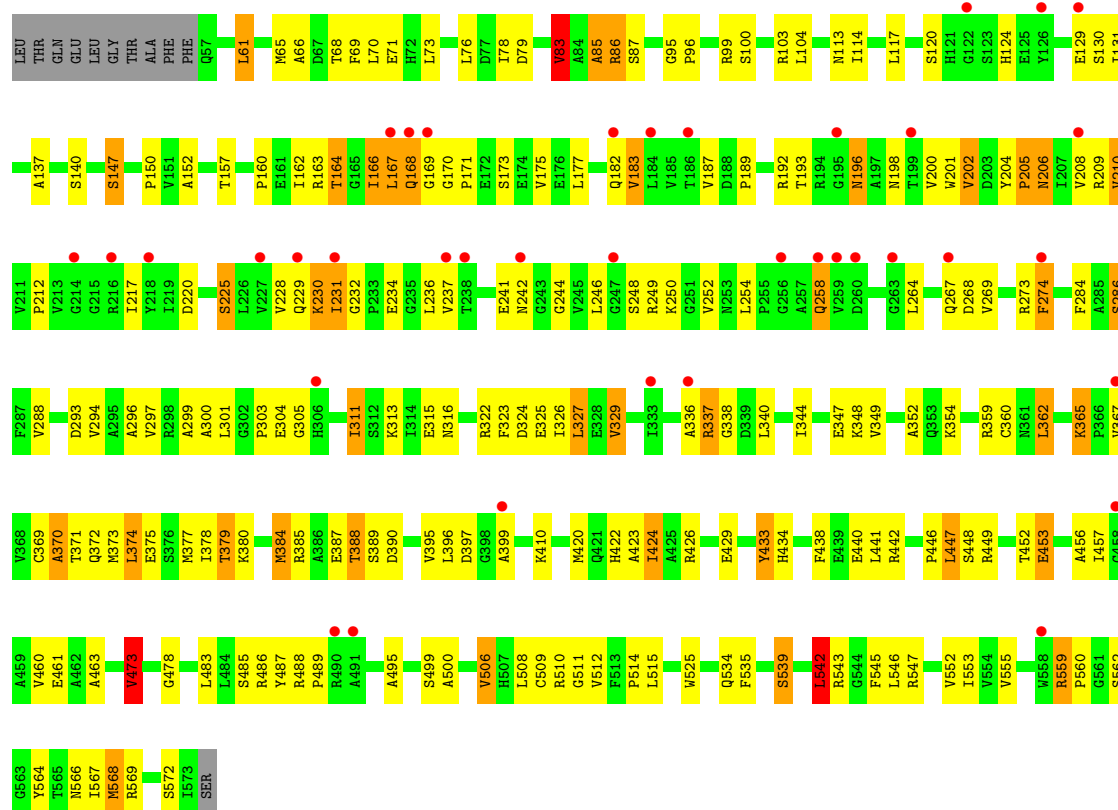
- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 5   | A     | 1        | Total Mn<br>1 1 | 0       | 0       |
| 5   | B     | 1        | Total Mn<br>1 1 | 0       | 0       |
| 5   | C     | 1        | Total Mn<br>1 1 | 0       | 0       |
| 5   | D     | 1        | Total Mn<br>1 1 | 0       | 0       |



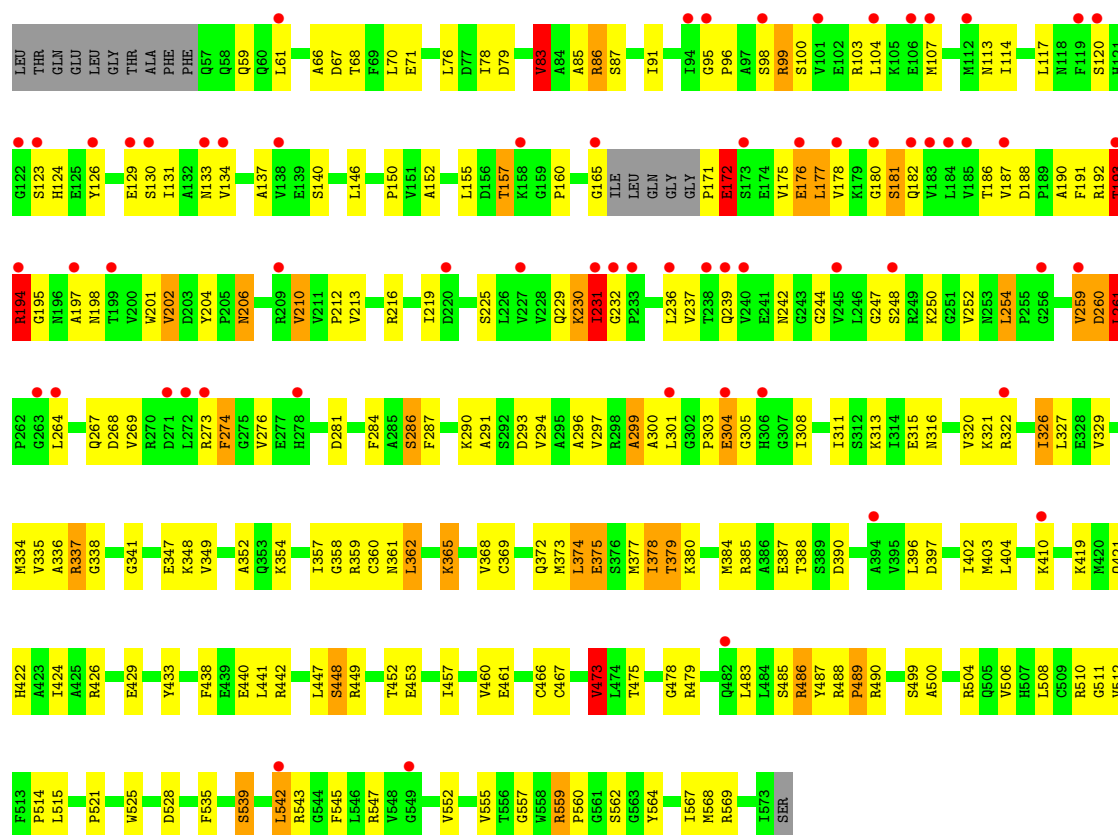


• Molecule 1: PYRUVATE KINASE ISOZYMES R/L



• Molecule 1: PYRUVATE KINASE ISOZYMES R/L





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 76.30Å 172.98Å 85.78Å<br>90.00° 93.12° 90.00°               | Depositor        |
| Resolution (Å)                                                          | 20.00 – 2.75<br>20.00 – 2.75                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 93.7 (20.00-2.75)<br>93.5 (20.00-2.75)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.08                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.51 (at 2.75Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.2.0019                                             | Depositor        |
| R, $R_{free}$                                                           | 0.268 , 0.303<br>0.319 , 0.340                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1103 reflections (2.03%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 57.8                                                        | Xtriage          |
| Anisotropy                                                              | 0.106                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 6.7                                                  | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.86                                                        | EDS              |
| Total number of atoms                                                   | 15550                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 14.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: PGA, MN, K, FBP

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

| Mol | Chain | Bond lengths |                 | Bond angles |                 |
|-----|-------|--------------|-----------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 5$     | RMSZ        | $\# Z  > 5$     |
| 1   | A     | 1.14         | 13/3977 (0.3%)  | 1.22        | 26/5390 (0.5%)  |
| 1   | B     | 1.20         | 10/3777 (0.3%)  | 1.21        | 21/5115 (0.4%)  |
| 1   | C     | 1.18         | 15/3977 (0.4%)  | 1.19        | 20/5390 (0.4%)  |
| 1   | D     | 1.76         | 28/3943 (0.7%)  | 1.34        | 26/5342 (0.5%)  |
| All | All   | 1.35         | 66/15674 (0.4%) | 1.24        | 93/21237 (0.4%) |

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   | A     | 0                   | 1                   |
| 1   | D     | 0                   | 3                   |
| All | All   | 0                   | 4                   |

All (66) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | D     | 172 | GLU  | CD-OE1 | 46.24 | 2.13        | 1.25     |
| 1   | D     | 171 | PRO  | C-N    | 43.80 | 1.95        | 1.33     |
| 1   | D     | 194 | ARG  | CZ-NH1 | 36.09 | 1.83        | 1.32     |
| 1   | D     | 230 | LYS  | CE-NZ  | 27.32 | 2.31        | 1.49     |
| 1   | A     | 382 | ARG  | CZ-NH2 | 22.12 | 1.62        | 1.33     |
| 1   | C     | 230 | LYS  | CE-NZ  | 17.79 | 2.02        | 1.49     |
| 1   | D     | 176 | GLU  | CD-OE1 | 16.10 | 1.55        | 1.25     |
| 1   | A     | 168 | GLN  | CD-NE2 | 14.75 | 1.64        | 1.33     |
| 1   | B     | 144 | SER  | CB-OG  | 14.17 | 1.70        | 1.42     |
| 1   | D     | 192 | ARG  | CZ-NH1 | 13.51 | 1.51        | 1.32     |
| 1   | A     | 410 | LYS  | CE-NZ  | 13.14 | 1.88        | 1.49     |
| 1   | D     | 260 | ASP  | CG-OD1 | 12.61 | 1.49        | 1.25     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | D     | 176 | GLU  | CD-OE2 | 11.30 | 1.46        | 1.25     |
| 1   | D     | 172 | GLU  | CG-CD  | 11.16 | 1.79        | 1.52     |
| 1   | C     | 241 | GLU  | CD-OE2 | 10.55 | 1.45        | 1.25     |
| 1   | B     | 176 | GLU  | CD-OE1 | 10.31 | 1.45        | 1.25     |
| 1   | C     | 241 | GLU  | CD-OE1 | 9.90  | 1.44        | 1.25     |
| 1   | B     | 176 | GLU  | CD-OE2 | 9.79  | 1.44        | 1.25     |
| 1   | A     | 260 | ASP  | C-O    | 9.67  | 1.36        | 1.24     |
| 1   | D     | 181 | SER  | C-O    | 9.49  | 1.34        | 1.23     |
| 1   | D     | 180 | GLY  | C-O    | -9.45 | 1.10        | 1.23     |
| 1   | B     | 182 | GLN  | CD-OE1 | 9.30  | 1.41        | 1.23     |
| 1   | B     | 249 | ARG  | CZ-NH2 | 9.21  | 1.45        | 1.33     |
| 1   | D     | 230 | LYS  | CG-CD  | 8.86  | 1.79        | 1.52     |
| 1   | D     | 194 | ARG  | NE-CZ  | 8.12  | 1.42        | 1.33     |
| 1   | D     | 67  | ASP  | CG-OD2 | 7.86  | 1.40        | 1.25     |
| 1   | D     | 231 | ILE  | CA-CB  | 7.61  | 1.61        | 1.53     |
| 1   | D     | 180 | GLY  | C-N    | 7.43  | 1.45        | 1.33     |
| 1   | B     | 209 | ARG  | CZ-NH1 | 7.32  | 1.43        | 1.32     |
| 1   | D     | 192 | ARG  | CD-NE  | 7.26  | 1.56        | 1.46     |
| 1   | D     | 326 | ILE  | CA-CB  | -7.11 | 1.45        | 1.54     |
| 1   | D     | 181 | SER  | C-N    | 7.04  | 1.42        | 1.33     |
| 1   | D     | 165 | GLY  | C-O    | 6.90  | 1.37        | 1.23     |
| 1   | A     | 153 | ILE  | CA-CB  | -6.69 | 1.45        | 1.54     |
| 1   | C     | 209 | ARG  | CZ-NH1 | 6.60  | 1.42        | 1.32     |
| 1   | A     | 102 | GLU  | CD-OE2 | 6.60  | 1.37        | 1.25     |
| 1   | D     | 195 | GLY  | C-O    | 6.55  | 1.32        | 1.23     |
| 1   | A     | 243 | GLY  | C-O    | 6.50  | 1.30        | 1.23     |
| 1   | D     | 335 | VAL  | CA-C   | -6.46 | 1.46        | 1.53     |
| 1   | D     | 247 | GLY  | C-O    | 6.37  | 1.33        | 1.24     |
| 1   | C     | 463 | ALA  | CA-CB  | -6.09 | 1.43        | 1.53     |
| 1   | A     | 209 | ARG  | CZ-NH1 | 6.07  | 1.41        | 1.32     |
| 1   | C     | 495 | ALA  | CA-CB  | -6.03 | 1.45        | 1.53     |
| 1   | C     | 367 | VAL  | C-O    | -5.94 | 1.18        | 1.24     |
| 1   | A     | 154 | ALA  | CA-CB  | -5.84 | 1.45        | 1.53     |
| 1   | A     | 230 | LYS  | CE-NZ  | 5.66  | 1.66        | 1.49     |
| 1   | C     | 85  | ALA  | CA-CB  | -5.65 | 1.44        | 1.53     |
| 1   | D     | 448 | SER  | CA-C   | -5.62 | 1.45        | 1.52     |
| 1   | B     | 485 | SER  | N-CA   | -5.60 | 1.39        | 1.46     |
| 1   | B     | 428 | ALA  | CA-CB  | -5.55 | 1.44        | 1.53     |
| 1   | D     | 99  | ARG  | CZ-NH1 | 5.50  | 1.40        | 1.32     |
| 1   | C     | 456 | ALA  | CA-CB  | -5.48 | 1.44        | 1.53     |
| 1   | D     | 172 | GLU  | C-O    | 5.45  | 1.30        | 1.24     |
| 1   | A     | 368 | VAL  | CA-CB  | -5.44 | 1.47        | 1.54     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | D     | 198 | ASN  | CG-OD1 | 5.42  | 1.33        | 1.23     |
| 1   | C     | 230 | LYS  | CD-CE  | 5.39  | 1.68        | 1.52     |
| 1   | C     | 399 | ALA  | CA-C   | -5.33 | 1.45        | 1.52     |
| 1   | A     | 229 | GLN  | CD-NE2 | 5.32  | 1.44        | 1.33     |
| 1   | D     | 172 | GLU  | CA-CB  | 5.24  | 1.62        | 1.53     |
| 1   | A     | 168 | GLN  | CD-OE1 | 5.18  | 1.33        | 1.23     |
| 1   | B     | 311 | ILE  | CA-C   | -5.12 | 1.46        | 1.52     |
| 1   | B     | 249 | ARG  | NE-CZ  | 5.08  | 1.38        | 1.33     |
| 1   | C     | 424 | ILE  | CA-CB  | -5.07 | 1.47        | 1.54     |
| 1   | C     | 209 | ARG  | CD-NE  | 5.05  | 1.53        | 1.46     |
| 1   | C     | 209 | ARG  | CZ-NH2 | 5.04  | 1.40        | 1.33     |
| 1   | C     | 311 | ILE  | CA-CB  | 5.03  | 1.60        | 1.54     |

All (93) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | D     | 171 | PRO  | O-C-N      | -24.76 | 83.38       | 123.00   |
| 1   | D     | 194 | ARG  | NE-CZ-NH1  | -23.12 | 98.38       | 121.50   |
| 1   | D     | 171 | PRO  | CA-C-N     | 12.26  | 144.95      | 121.54   |
| 1   | D     | 171 | PRO  | C-N-CA     | 12.26  | 144.95      | 121.54   |
| 1   | D     | 260 | ASP  | CB-CG-OD1  | -9.43  | 96.71       | 118.40   |
| 1   | B     | 184 | LEU  | O-C-N      | 9.07   | 133.22      | 123.06   |
| 1   | A     | 382 | ARG  | NE-CZ-NH2  | -9.03  | 111.08      | 119.20   |
| 1   | D     | 261 | LEU  | CA-C-N     | 8.71   | 129.37      | 120.14   |
| 1   | D     | 261 | LEU  | C-N-CA     | 8.71   | 129.37      | 120.14   |
| 1   | A     | 410 | LYS  | CD-CE-NZ   | 8.33   | 138.55      | 111.90   |
| 1   | D     | 473 | VAL  | CB-CA-C    | -8.15  | 98.48       | 110.62   |
| 1   | C     | 244 | GLY  | N-CA-C     | 7.92   | 120.39      | 110.96   |
| 1   | B     | 142 | ALA  | N-CA-C     | -7.90  | 103.62      | 113.18   |
| 1   | A     | 368 | VAL  | CB-CA-C    | -7.85  | 100.17      | 110.84   |
| 1   | D     | 194 | ARG  | NH1-CZ-NH2 | 7.45   | 128.98      | 119.30   |
| 1   | D     | 347 | GLU  | CB-CA-C    | -7.29  | 95.90       | 110.42   |
| 1   | D     | 192 | ARG  | NE-CZ-NH2  | -7.19  | 112.73      | 119.20   |
| 1   | B     | 473 | VAL  | CB-CA-C    | -7.17  | 99.94       | 110.62   |
| 1   | A     | 204 | TYR  | CA-C-N     | 6.89   | 128.45      | 119.84   |
| 1   | A     | 204 | TYR  | C-N-CA     | 6.89   | 128.45      | 119.84   |
| 1   | C     | 258 | GLN  | OE1-CD-NE2 | -6.87  | 115.73      | 122.60   |
| 1   | C     | 274 | PHE  | N-CA-C     | -6.80  | 103.79      | 111.07   |
| 1   | B     | 184 | LEU  | CA-C-O     | -6.53  | 113.53      | 121.36   |
| 1   | A     | 410 | LYS  | CG-CD-CE   | -6.49  | 96.38       | 111.30   |
| 1   | C     | 473 | VAL  | CB-CA-C    | -6.47  | 100.98      | 110.62   |
| 1   | D     | 490 | ARG  | N-CA-C     | -6.39  | 105.61      | 113.41   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 182 | GLN  | OE1-CD-NE2 | -6.36 | 116.24      | 122.60   |
| 1   | C     | 196 | ASN  | N-CA-C     | 6.34  | 117.50      | 108.74   |
| 1   | C     | 230 | LYS  | CD-CE-NZ   | -6.29 | 91.79       | 111.90   |
| 1   | D     | 489 | PRO  | N-CA-C     | -6.22 | 102.44      | 111.33   |
| 1   | C     | 229 | GLN  | N-CA-C     | -6.08 | 107.09      | 114.75   |
| 1   | A     | 274 | PHE  | N-CA-C     | -6.05 | 104.68      | 111.28   |
| 1   | D     | 172 | GLU  | CG-CD-OE1  | -6.00 | 104.61      | 118.40   |
| 1   | D     | 378 | ILE  | N-CA-C     | -5.93 | 105.29      | 113.00   |
| 1   | D     | 286 | SER  | N-CA-C     | 5.92  | 117.94      | 110.24   |
| 1   | A     | 196 | ASN  | N-CA-C     | 5.90  | 116.03      | 108.24   |
| 1   | A     | 347 | GLU  | CB-CA-C    | -5.86 | 98.75       | 110.42   |
| 1   | A     | 361 | ASN  | N-CA-C     | -5.77 | 104.89      | 111.07   |
| 1   | B     | 287 | PHE  | N-CA-C     | 5.74  | 123.02      | 110.80   |
| 1   | A     | 478 | GLY  | N-CA-C     | -5.71 | 107.89      | 114.69   |
| 1   | A     | 473 | VAL  | CB-CA-C    | -5.70 | 102.12      | 110.62   |
| 1   | B     | 109 | LYS  | N-CA-CB    | 5.67  | 118.45      | 110.12   |
| 1   | A     | 442 | ARG  | N-CA-C     | -5.65 | 104.33      | 111.11   |
| 1   | B     | 370 | ALA  | N-CA-C     | 5.64  | 117.75      | 109.24   |
| 1   | D     | 365 | LYS  | CA-C-N     | 5.61  | 125.56      | 119.78   |
| 1   | D     | 365 | LYS  | C-N-CA     | 5.61  | 125.56      | 119.78   |
| 1   | A     | 286 | SER  | N-CA-C     | 5.61  | 117.53      | 110.24   |
| 1   | C     | 183 | VAL  | N-CA-C     | 5.61  | 116.19      | 108.12   |
| 1   | D     | 375 | GLU  | N-CA-C     | 5.58  | 118.08      | 111.33   |
| 1   | A     | 211 | VAL  | N-CA-C     | 5.57  | 113.07      | 107.55   |
| 1   | C     | 378 | ILE  | N-CA-C     | -5.54 | 105.79      | 113.00   |
| 1   | C     | 509 | CYS  | N-CA-C     | 5.53  | 117.75      | 108.73   |
| 1   | B     | 365 | LYS  | CA-C-N     | 5.50  | 125.51      | 119.90   |
| 1   | B     | 365 | LYS  | C-N-CA     | 5.50  | 125.51      | 119.90   |
| 1   | A     | 438 | PHE  | N-CA-C     | -5.49 | 105.37      | 111.36   |
| 1   | A     | 144 | SER  | CA-C-N     | 5.39  | 125.21      | 119.28   |
| 1   | A     | 144 | SER  | C-N-CA     | 5.39  | 125.21      | 119.28   |
| 1   | C     | 370 | ALA  | N-CA-C     | 5.39  | 117.38      | 109.24   |
| 1   | B     | 144 | SER  | O-C-N      | 5.38  | 124.50      | 121.27   |
| 1   | B     | 378 | ILE  | N-CA-C     | -5.36 | 106.03      | 113.00   |
| 1   | C     | 365 | LYS  | CA-C-N     | 5.34  | 125.33      | 119.89   |
| 1   | C     | 365 | LYS  | C-N-CA     | 5.34  | 125.33      | 119.89   |
| 1   | C     | 347 | GLU  | CB-CA-C    | -5.33 | 98.53       | 110.21   |
| 1   | B     | 424 | ILE  | CB-CA-C    | -5.32 | 104.96      | 112.14   |
| 1   | D     | 181 | SER  | O-C-N      | 5.28  | 128.58      | 121.83   |
| 1   | D     | 232 | GLY  | CA-C-N     | 5.25  | 125.31      | 119.32   |
| 1   | D     | 232 | GLY  | C-N-CA     | 5.25  | 125.31      | 119.32   |
| 1   | A     | 183 | VAL  | N-CA-C     | 5.25  | 116.28      | 108.46   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 274 | PHE  | N-CA-C     | -5.24 | 105.46      | 111.07   |
| 1   | A     | 251 | GLY  | N-CA-C     | 5.22  | 119.68      | 112.37   |
| 1   | A     | 489 | PRO  | N-CA-C     | -5.21 | 103.27      | 111.34   |
| 1   | C     | 478 | GLY  | N-CA-C     | -5.18 | 108.47      | 115.21   |
| 1   | B     | 347 | GLU  | CB-CA-C    | -5.17 | 98.89       | 110.21   |
| 1   | D     | 316 | ASN  | N-CA-C     | 5.17  | 115.99      | 108.14   |
| 1   | A     | 541 | LYS  | N-CA-C     | -5.16 | 105.34      | 110.97   |
| 1   | C     | 316 | ASN  | N-CA-C     | 5.14  | 115.96      | 108.14   |
| 1   | A     | 102 | GLU  | OE1-CD-OE2 | -5.14 | 110.57      | 122.90   |
| 1   | C     | 286 | SER  | N-CA-C     | 5.12  | 116.89      | 110.24   |
| 1   | C     | 69  | PHE  | N-CA-C     | -5.12 | 105.40      | 111.69   |
| 1   | D     | 424 | ILE  | CB-CA-C    | -5.11 | 105.16      | 112.22   |
| 1   | B     | 316 | ASN  | N-CA-C     | 5.11  | 115.91      | 108.14   |
| 1   | B     | 144 | SER  | CA-C-N     | 5.09  | 124.88      | 119.28   |
| 1   | B     | 144 | SER  | C-N-CA     | 5.09  | 124.88      | 119.28   |
| 1   | B     | 490 | ARG  | N-CA-C     | -5.07 | 107.23      | 113.41   |
| 1   | A     | 99  | ARG  | N-CA-C     | -5.06 | 107.77      | 114.04   |
| 1   | A     | 126 | TYR  | OH-CZ-CE2  | -5.04 | 104.78      | 119.90   |
| 1   | D     | 244 | GLY  | N-CA-C     | 5.04  | 116.96      | 110.96   |
| 1   | B     | 445 | ALA  | CA-C-N     | 5.03  | 125.47      | 120.14   |
| 1   | B     | 445 | ALA  | C-N-CA     | 5.03  | 125.47      | 120.14   |
| 1   | B     | 559 | ARG  | N-CA-C     | 5.03  | 112.74      | 108.22   |
| 1   | A     | 187 | VAL  | N-CA-C     | -5.02 | 107.81      | 112.43   |
| 1   | C     | 542 | LEU  | N-CA-C     | 5.01  | 118.16      | 111.75   |
| 1   | C     | 147 | SER  | N-CA-C     | 5.00  | 119.65      | 113.50   |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 382 | ARG  | Sidechain |
| 1   | D     | 172 | GLU  | Sidechain |
| 1   | D     | 194 | ARG  | Sidechain |
| 1   | D     | 260 | ASP  | 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     | 3913  | 0        | 3994     | 168     | 0            |
| 1   | B     | 3720  | 0        | 3804     | 159     | 0            |
| 1   | C     | 3913  | 0        | 3994     | 145     | 0            |
| 1   | D     | 3880  | 0        | 3957     | 150     | 0            |
| 2   | A     | 20    | 0        | 10       | 1       | 0            |
| 2   | B     | 20    | 0        | 10       | 1       | 0            |
| 2   | C     | 20    | 0        | 10       | 0       | 0            |
| 2   | D     | 20    | 0        | 10       | 2       | 0            |
| 3   | A     | 9     | 0        | 2        | 1       | 0            |
| 3   | B     | 9     | 0        | 2        | 0       | 0            |
| 3   | C     | 9     | 0        | 2        | 0       | 0            |
| 3   | D     | 9     | 0        | 2        | 1       | 0            |
| 4   | A     | 1     | 0        | 0        | 0       | 0            |
| 4   | B     | 1     | 0        | 0        | 0       | 0            |
| 4   | C     | 1     | 0        | 0        | 0       | 0            |
| 4   | D     | 1     | 0        | 0        | 0       | 0            |
| 5   | A     | 1     | 0        | 0        | 0       | 0            |
| 5   | B     | 1     | 0        | 0        | 0       | 0            |
| 5   | C     | 1     | 0        | 0        | 0       | 0            |
| 5   | D     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 15550 | 0        | 15797    | 579     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (579) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:172:GLU:CD   | 1:D:172:GLU:CG   | 1.80                     | 1.55              |
| 1:D:230:LYS:CD   | 1:D:230:LYS:CG   | 1.79                     | 1.55              |
| 1:D:194:ARG:NH1  | 1:D:194:ARG:CZ   | 1.83                     | 1.42              |
| 1:B:144:SER:CB   | 1:B:144:SER:OG   | 1.70                     | 1.39              |
| 1:A:410:LYS:CE   | 1:A:410:LYS:NZ   | 1.88                     | 1.36              |
| 1:C:230:LYS:CE   | 1:C:230:LYS:NZ   | 2.02                     | 1.20              |
| 1:B:315:GLU:OE2  | 1:B:339:ASP:OD2  | 1.78                     | 1.00              |
| 1:D:86:ARG:HB3   | 1:D:426:ARG:HG2  | 1.44                     | 0.98              |
| 1:B:379:THR:HG22 | 1:B:380:LYS:HG3  | 1.45                     | 0.97              |
| 1:D:379:THR:HG22 | 1:D:380:LYS:HG3  | 1.44                     | 0.96              |
| 1:A:86:ARG:HB3   | 1:A:426:ARG:HG2  | 1.45                     | 0.96              |
| 1:A:442:ARG:HH21 | 1:B:442:ARG:HH21 | 1.06                     | 0.95              |
| 1:A:442:ARG:HH21 | 1:B:442:ARG:NH2  | 1.65                     | 0.94              |
| 1:C:379:THR:HG22 | 1:C:380:LYS:HG3  | 1.48                     | 0.94              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:379:THR:HG22 | 1:A:380:LYS:HG3  | 1.49                     | 0.94              |
| 1:D:230:LYS:CE   | 1:D:230:LYS:NZ   | 2.31                     | 0.93              |
| 1:A:384:MET:HE1  | 1:C:375:GLU:HB2  | 1.51                     | 0.92              |
| 1:B:86:ARG:HB3   | 1:B:426:ARG:HG2  | 1.48                     | 0.92              |
| 1:B:261:LEU:HD12 | 1:B:262:PRO:HD2  | 1.51                     | 0.91              |
| 1:D:172:GLU:CD   | 1:D:172:GLU:OE1  | 2.13                     | 0.90              |
| 1:B:162:ILE:HB   | 1:B:252:VAL:HB   | 1.50                     | 0.90              |
| 1:C:86:ARG:HB3   | 1:C:426:ARG:HG2  | 1.53                     | 0.90              |
| 1:C:452:THR:HG22 | 1:C:483:LEU:HD12 | 1.54                     | 0.89              |
| 1:A:375:GLU:HB2  | 1:C:384:MET:HE1  | 1.54                     | 0.87              |
| 1:B:452:THR:HG22 | 1:B:483:LEU:HD12 | 1.56                     | 0.86              |
| 1:D:114:ILE:HG12 | 1:D:152:ALA:HB3  | 1.58                     | 0.85              |
| 1:A:369:CYS:SG   | 1:A:373:MET:HE3  | 2.17                     | 0.84              |
| 1:C:208:VAL:HA   | 1:C:236:LEU:HD11 | 1.60                     | 0.83              |
| 1:A:442:ARG:NH2  | 1:B:442:ARG:HH21 | 1.76                     | 0.83              |
| 1:C:453:GLU:HG2  | 1:C:483:LEU:HD13 | 1.62                     | 0.82              |
| 1:B:175:VAL:HG13 | 1:B:197:ALA:HA   | 1.62                     | 0.81              |
| 1:C:269:VAL:O    | 1:C:273:ARG:HG2  | 1.80                     | 0.81              |
| 1:D:452:THR:HG22 | 1:D:483:LEU:HD12 | 1.63                     | 0.81              |
| 1:C:535:PHE:O    | 1:C:539:SER:OG   | 1.99                     | 0.81              |
| 1:C:374:LEU:HD12 | 1:C:387:GLU:HB3  | 1.64                     | 0.80              |
| 1:C:442:ARG:HH21 | 1:D:442:ARG:HH21 | 1.27                     | 0.80              |
| 1:A:191:PHE:C    | 1:A:193:THR:H    | 1.90                     | 0.79              |
| 1:A:374:LEU:HD12 | 1:A:387:GLU:HB3  | 1.63                     | 0.78              |
| 1:A:86:ARG:HD3   | 1:A:422:HIS:ND1  | 1.98                     | 0.78              |
| 1:C:114:ILE:HG12 | 1:C:152:ALA:HB3  | 1.66                     | 0.78              |
| 1:D:204:TYR:CE1  | 1:D:261:LEU:HD13 | 2.19                     | 0.77              |
| 1:A:453:GLU:HG2  | 1:A:483:LEU:HD13 | 1.66                     | 0.76              |
| 1:B:535:PHE:O    | 1:B:539:SER:OG   | 2.04                     | 0.76              |
| 1:B:374:LEU:HD12 | 1:B:387:GLU:HB3  | 1.68                     | 0.76              |
| 1:C:177:LEU:HD12 | 1:C:183:VAL:HG21 | 1.68                     | 0.76              |
| 1:A:535:PHE:O    | 1:A:539:SER:OG   | 2.05                     | 0.75              |
| 1:D:453:GLU:HG2  | 1:D:483:LEU:HD13 | 1.67                     | 0.75              |
| 1:A:163:ARG:NH1  | 1:A:249:ARG:O    | 2.21                     | 0.74              |
| 1:A:191:PHE:O    | 1:A:193:THR:N    | 2.21                     | 0.74              |
| 1:A:321:LYS:HE3  | 1:C:79:ASP:OD2   | 1.86                     | 0.74              |
| 1:D:374:LEU:HD12 | 1:D:387:GLU:HB3  | 1.68                     | 0.74              |
| 1:A:452:THR:HG22 | 1:A:483:LEU:HD12 | 1.70                     | 0.72              |
| 1:C:85:ALA:HB2   | 1:C:545:PHE:CE2  | 2.25                     | 0.72              |
| 1:D:86:ARG:HD3   | 1:D:422:HIS:ND1  | 2.05                     | 0.71              |
| 1:B:114:ILE:HG12 | 1:B:152:ALA:HB3  | 1.71                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:269:VAL:O    | 1:B:273:ARG:HG2  | 1.91                     | 0.71              |
| 1:A:83:VAL:O     | 1:A:83:VAL:CG1   | 2.39                     | 0.70              |
| 1:B:202:VAL:HG13 | 1:B:204:TYR:H    | 1.56                     | 0.70              |
| 1:D:535:PHE:O    | 1:D:539:SER:OG   | 2.10                     | 0.70              |
| 1:B:539:SER:O    | 1:B:543:ARG:HG3  | 1.91                     | 0.70              |
| 1:B:375:GLU:HB2  | 1:D:384:MET:HE1  | 1.73                     | 0.70              |
| 1:D:204:TYR:HE1  | 1:D:261:LEU:HD13 | 1.57                     | 0.70              |
| 1:B:384:MET:HE1  | 1:D:375:GLU:HB2  | 1.73                     | 0.70              |
| 1:D:187:VAL:HG12 | 1:D:202:VAL:HG12 | 1.74                     | 0.70              |
| 1:B:514:PRO:O    | 1:B:515:LEU:HD23 | 1.91                     | 0.69              |
| 1:B:83:VAL:CG1   | 1:B:83:VAL:O     | 2.40                     | 0.69              |
| 1:D:488:ARG:NH1  | 1:D:510:ARG:HB3  | 2.07                     | 0.69              |
| 1:B:453:GLU:HG2  | 1:B:483:LEU:HD13 | 1.74                     | 0.69              |
| 1:D:204:TYR:CZ   | 1:D:206:ASN:HB2  | 2.28                     | 0.69              |
| 1:D:269:VAL:O    | 1:D:273:ARG:HG2  | 1.91                     | 0.69              |
| 1:B:66:ALA:HB1   | 1:B:71:GLU:HB3   | 1.75                     | 0.69              |
| 1:B:146:LEU:HB2  | 1:B:542:LEU:HD12 | 1.73                     | 0.69              |
| 1:C:372:GLN:HG2  | 1:C:375:GLU:HG3  | 1.73                     | 0.69              |
| 1:C:442:ARG:NH2  | 1:D:442:ARG:HH21 | 1.91                     | 0.69              |
| 1:D:225:SER:HB3  | 1:D:242:ASN:H    | 1.58                     | 0.69              |
| 1:A:114:ILE:HG12 | 1:A:152:ALA:HB3  | 1.75                     | 0.68              |
| 1:A:315:GLU:HG2  | 1:A:336:ALA:CB   | 2.22                     | 0.68              |
| 1:D:487:TYR:O    | 1:D:488:ARG:HB2  | 1.92                     | 0.68              |
| 1:C:354:LYS:NZ   | 1:C:397:ASP:OD1  | 2.26                     | 0.68              |
| 1:A:87:SER:HB3   | 1:A:511:GLY:HA2  | 1.75                     | 0.68              |
| 1:B:86:ARG:HD3   | 1:B:422:HIS:ND1  | 2.10                     | 0.67              |
| 1:A:360:CYS:SG   | 1:A:367:VAL:HB   | 2.35                     | 0.67              |
| 1:C:177:LEU:HD21 | 1:C:246:LEU:HD22 | 1.76                     | 0.67              |
| 1:C:337:ARG:HH22 | 1:C:390:ASP:CG   | 2.02                     | 0.67              |
| 1:B:559:ARG:HD2  | 1:B:564:TYR:CD1  | 2.28                     | 0.67              |
| 1:A:85:ALA:HB2   | 1:A:545:PHE:CE2  | 2.30                     | 0.66              |
| 1:D:146:LEU:HB2  | 1:D:542:LEU:HD12 | 1.77                     | 0.66              |
| 1:A:166:ILE:HD12 | 1:A:166:ILE:H    | 1.60                     | 0.66              |
| 1:B:204:TYR:CE1  | 1:B:261:LEU:HB2  | 2.30                     | 0.66              |
| 1:C:337:ARG:NH2  | 1:C:390:ASP:OD1  | 2.28                     | 0.66              |
| 1:C:83:VAL:O     | 1:C:83:VAL:CG1   | 2.42                     | 0.66              |
| 1:D:230:LYS:CG   | 1:D:230:LYS:CE   | 2.73                     | 0.65              |
| 1:A:216:ARG:HA   | 1:A:226:LEU:O    | 1.97                     | 0.65              |
| 1:A:322:ARG:O    | 1:A:326:ILE:HG13 | 1.97                     | 0.65              |
| 1:B:475:THR:HA   | 2:B:580:FBP:H61  | 1.78                     | 0.65              |
| 1:A:442:ARG:NH2  | 1:B:442:ARG:NH2  | 2.40                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:514:PRO:O    | 1:A:515:LEU:HD23 | 1.97                     | 0.65              |
| 1:A:68:THR:HB    | 1:C:440:GLU:OE2  | 1.97                     | 0.64              |
| 1:A:372:GLN:HG2  | 1:A:375:GLU:HG3  | 1.80                     | 0.64              |
| 1:D:337:ARG:HH22 | 1:D:390:ASP:CG   | 2.04                     | 0.64              |
| 1:C:86:ARG:HD3   | 1:C:422:HIS:ND1  | 2.12                     | 0.64              |
| 1:D:402:ILE:HG13 | 1:D:421:GLN:NE2  | 2.12                     | 0.64              |
| 1:D:542:LEU:O    | 1:D:542:LEU:HD22 | 1.96                     | 0.64              |
| 1:B:175:VAL:CG1  | 1:B:197:ALA:HA   | 2.26                     | 0.64              |
| 1:C:442:ARG:HH21 | 1:D:442:ARG:NH2  | 1.95                     | 0.64              |
| 1:A:191:PHE:C    | 1:A:193:THR:N    | 2.55                     | 0.64              |
| 1:D:83:VAL:O     | 1:D:83:VAL:CG1   | 2.45                     | 0.64              |
| 1:A:384:MET:HE1  | 1:C:375:GLU:CB   | 2.25                     | 0.64              |
| 1:B:321:LYS:HE3  | 1:D:79:ASP:OD2   | 1.98                     | 0.64              |
| 1:A:384:MET:CE   | 1:C:375:GLU:HB2  | 2.27                     | 0.64              |
| 1:B:210:VAL:HG12 | 1:B:257:ALA:HB1  | 1.78                     | 0.63              |
| 1:C:210:VAL:O    | 1:C:212:PRO:HD3  | 1.98                     | 0.63              |
| 1:A:375:GLU:CB   | 1:C:384:MET:HE1  | 2.28                     | 0.63              |
| 1:B:146:LEU:CB   | 1:B:542:LEU:HD12 | 2.29                     | 0.63              |
| 1:A:402:ILE:HG13 | 1:A:421:GLN:NE2  | 2.14                     | 0.63              |
| 1:A:488:ARG:NH1  | 1:A:510:ARG:HB3  | 2.14                     | 0.62              |
| 1:C:559:ARG:HD2  | 1:C:564:TYR:CD1  | 2.33                     | 0.62              |
| 1:A:354:LYS:NZ   | 1:A:397:ASP:OD1  | 2.33                     | 0.62              |
| 1:A:83:VAL:O     | 1:A:83:VAL:HG12  | 1.98                     | 0.62              |
| 1:A:559:ARG:HD2  | 1:A:564:TYR:CD1  | 2.35                     | 0.62              |
| 1:D:453:GLU:CG   | 1:D:483:LEU:HD13 | 2.30                     | 0.62              |
| 1:B:117:LEU:HD11 | 1:B:131:ILE:HG13 | 1.82                     | 0.62              |
| 1:D:322:ARG:O    | 1:D:326:ILE:HG13 | 2.00                     | 0.62              |
| 1:A:204:TYR:CZ   | 1:A:206:ASN:HB2  | 2.35                     | 0.61              |
| 1:C:210:VAL:O    | 1:C:212:PRO:CD   | 2.48                     | 0.61              |
| 1:D:441:LEU:O    | 1:D:442:ARG:C    | 2.39                     | 0.61              |
| 1:A:506:VAL:HG13 | 1:A:512:VAL:HG11 | 1.82                     | 0.61              |
| 1:B:542:LEU:HD22 | 1:B:542:LEU:O    | 2.00                     | 0.61              |
| 1:D:315:GLU:HG2  | 1:D:336:ALA:CB   | 2.31                     | 0.61              |
| 1:C:473:VAL:HG13 | 1:C:555:VAL:HB   | 1.82                     | 0.61              |
| 1:D:172:GLU:CD   | 1:D:172:GLU:CB   | 2.74                     | 0.61              |
| 1:A:155:LEU:HD23 | 1:A:155:LEU:C    | 2.26                     | 0.60              |
| 1:A:539:SER:O    | 1:A:543:ARG:HG3  | 2.01                     | 0.60              |
| 1:B:372:GLN:HG2  | 1:B:375:GLU:HG3  | 1.83                     | 0.60              |
| 1:D:349:VAL:O    | 1:D:352:ALA:N    | 2.34                     | 0.60              |
| 1:A:375:GLU:HB2  | 1:C:384:MET:CE   | 2.29                     | 0.60              |
| 1:D:230:LYS:CD   | 1:D:230:LYS:CB   | 2.75                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:194:ARG:NH1  | 1:D:194:ARG:NE   | 2.47                     | 0.60              |
| 1:B:177:LEU:HD12 | 1:B:183:VAL:HG21 | 1.82                     | 0.60              |
| 1:D:85:ALA:HB2   | 1:D:545:PHE:CE2  | 2.36                     | 0.60              |
| 1:D:86:ARG:HB3   | 1:D:426:ARG:CG   | 2.24                     | 0.60              |
| 1:C:460:VAL:HG22 | 1:C:489:PRO:HG3  | 1.82                     | 0.60              |
| 1:C:66:ALA:HB1   | 1:C:71:GLU:HB3   | 1.83                     | 0.59              |
| 1:B:99:ARG:NH2   | 1:B:129:GLU:OE1  | 2.33                     | 0.59              |
| 1:A:337:ARG:HH22 | 1:A:390:ASP:CG   | 2.11                     | 0.59              |
| 1:B:79:ASP:OD2   | 1:D:321:LYS:HE3  | 2.02                     | 0.59              |
| 1:D:557:GLY:HA3  | 2:D:580:FBP:O3   | 2.02                     | 0.59              |
| 1:A:320:VAL:HG11 | 1:C:78:ILE:HD13  | 1.84                     | 0.59              |
| 1:D:315:GLU:HG2  | 1:D:336:ALA:HB3  | 1.83                     | 0.59              |
| 1:D:514:PRO:O    | 1:D:515:LEU:HD23 | 2.02                     | 0.59              |
| 1:B:225:SER:HB3  | 1:B:242:ASN:HB2  | 1.83                     | 0.59              |
| 1:C:225:SER:HB3  | 1:C:242:ASN:HB2  | 1.84                     | 0.59              |
| 1:D:506:VAL:CG1  | 1:D:512:VAL:HG11 | 2.32                     | 0.59              |
| 1:A:192:ARG:O    | 1:A:192:ARG:HG2  | 2.02                     | 0.59              |
| 1:A:117:LEU:HD11 | 1:A:131:ILE:HG13 | 1.84                     | 0.58              |
| 1:B:420:MET:O    | 1:B:424:ILE:HG13 | 2.04                     | 0.58              |
| 1:D:460:VAL:HG22 | 1:D:489:PRO:HG3  | 1.86                     | 0.58              |
| 1:B:183:VAL:O    | 1:B:238:THR:OG1  | 2.18                     | 0.58              |
| 1:D:137:ALA:O    | 1:D:140:SER:OG   | 2.15                     | 0.58              |
| 1:C:177:LEU:CD1  | 1:C:183:VAL:HG21 | 2.34                     | 0.58              |
| 1:D:506:VAL:CG1  | 1:D:512:VAL:CG1  | 2.82                     | 0.58              |
| 1:A:215:GLY:O    | 1:A:227:VAL:HA   | 2.04                     | 0.58              |
| 1:C:230:LYS:NZ   | 1:C:230:LYS:CD   | 2.67                     | 0.58              |
| 1:D:506:VAL:HG13 | 1:D:512:VAL:HG11 | 1.85                     | 0.57              |
| 1:C:539:SER:O    | 1:C:543:ARG:HG3  | 2.05                     | 0.57              |
| 1:A:85:ALA:HB2   | 1:A:545:PHE:HE2  | 1.70                     | 0.57              |
| 1:D:559:ARG:HD2  | 1:D:564:TYR:CD1  | 2.39                     | 0.57              |
| 1:B:86:ARG:HB3   | 1:B:426:ARG:CG   | 2.29                     | 0.57              |
| 1:B:213:VAL:HA   | 1:B:228:VAL:HG12 | 1.87                     | 0.57              |
| 1:D:83:VAL:O     | 1:D:83:VAL:HG12  | 2.03                     | 0.56              |
| 1:B:85:ALA:HB2   | 1:B:545:PHE:CE2  | 2.39                     | 0.56              |
| 1:D:499:SER:O    | 1:D:500:ALA:C    | 2.48                     | 0.56              |
| 1:A:204:TYR:CE2  | 1:A:206:ASN:HB2  | 2.39                     | 0.56              |
| 1:C:167:LEU:O    | 1:C:170:GLY:N    | 2.33                     | 0.56              |
| 1:C:230:LYS:HB2  | 1:C:237:VAL:HB   | 1.88                     | 0.56              |
| 1:D:539:SER:O    | 1:D:543:ARG:HG3  | 2.05                     | 0.56              |
| 1:B:219:ILE:HA   | 1:B:251:GLY:O    | 2.05                     | 0.56              |
| 1:D:281:ASP:OD2  | 1:D:504:ARG:NE   | 2.32                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:157:THR:HG22 | 1:D:286:SER:HB2  | 1.87                     | 0.56              |
| 1:A:440:GLU:OE2  | 1:C:68:THR:HB    | 2.05                     | 0.56              |
| 1:A:303:PRO:C    | 1:A:305:GLY:H    | 2.13                     | 0.56              |
| 1:A:506:VAL:CG1  | 1:A:512:VAL:CG1  | 2.83                     | 0.56              |
| 1:C:86:ARG:HG2   | 1:C:422:HIS:CE1  | 2.41                     | 0.55              |
| 1:C:488:ARG:NH1  | 1:C:510:ARG:HB3  | 2.22                     | 0.55              |
| 1:A:487:TYR:O    | 1:A:488:ARG:HB2  | 2.06                     | 0.55              |
| 1:B:286:SER:HA   | 1:B:313:LYS:HE2  | 1.89                     | 0.55              |
| 1:A:506:VAL:CG1  | 1:A:512:VAL:HG11 | 2.36                     | 0.55              |
| 1:C:162:ILE:HG22 | 1:C:252:VAL:HB   | 1.86                     | 0.55              |
| 1:C:446:PRO:C    | 1:C:447:LEU:O    | 2.48                     | 0.55              |
| 1:D:175:VAL:HG12 | 1:D:177:LEU:CD2  | 2.37                     | 0.55              |
| 1:A:228:VAL:HG22 | 1:A:238:THR:HG22 | 1.89                     | 0.55              |
| 1:C:117:LEU:HD11 | 1:C:131:ILE:HG13 | 1.88                     | 0.55              |
| 1:B:159:GLY:O    | 1:B:161:GLU:N    | 2.36                     | 0.55              |
| 1:B:288:VAL:HG12 | 1:B:326:ILE:HD13 | 1.89                     | 0.55              |
| 1:B:86:ARG:NH2   | 1:B:113:ASN:OD1  | 2.40                     | 0.55              |
| 1:C:453:GLU:CG   | 1:C:483:LEU:HD13 | 2.35                     | 0.55              |
| 1:A:473:VAL:HG13 | 1:A:555:VAL:HB   | 1.90                     | 0.54              |
| 1:D:230:LYS:HB2  | 1:D:237:VAL:HB   | 1.89                     | 0.54              |
| 1:D:337:ARG:NH2  | 1:D:390:ASP:OD1  | 2.39                     | 0.54              |
| 1:C:86:ARG:NH2   | 1:C:113:ASN:OD1  | 2.40                     | 0.54              |
| 1:A:453:GLU:CG   | 1:A:483:LEU:HD13 | 2.38                     | 0.54              |
| 1:B:87:SER:HB2   | 1:B:511:GLY:CA   | 2.37                     | 0.54              |
| 1:C:204:TYR:O    | 1:C:205:PRO:C    | 2.50                     | 0.54              |
| 1:D:150:PRO:HG2  | 1:D:514:PRO:HG2  | 1.88                     | 0.54              |
| 1:A:228:VAL:HA   | 1:A:238:THR:HG22 | 1.89                     | 0.54              |
| 1:B:460:VAL:HG22 | 1:B:489:PRO:HG3  | 1.90                     | 0.54              |
| 1:A:158:LYS:HG2  | 1:A:161:GLU:HG3  | 1.89                     | 0.54              |
| 1:A:475:THR:HA   | 2:A:580:FBP:H61  | 1.89                     | 0.54              |
| 1:C:349:VAL:O    | 1:C:352:ALA:N    | 2.41                     | 0.54              |
| 1:B:87:SER:CB    | 1:B:511:GLY:HA2  | 2.38                     | 0.54              |
| 1:B:322:ARG:O    | 1:B:326:ILE:HG13 | 2.07                     | 0.54              |
| 1:C:514:PRO:O    | 1:C:515:LEU:HD23 | 2.08                     | 0.54              |
| 1:C:446:PRO:O    | 1:C:447:LEU:O    | 2.25                     | 0.54              |
| 1:D:194:ARG:NH1  | 1:D:194:ARG:CD   | 2.70                     | 0.54              |
| 1:A:293:ASP:O    | 1:A:297:VAL:HG23 | 2.07                     | 0.53              |
| 1:B:259:VAL:HG12 | 1:B:261:LEU:HB3  | 1.90                     | 0.53              |
| 1:C:542:LEU:O    | 1:C:542:LEU:HD22 | 2.08                     | 0.53              |
| 1:A:288:VAL:HG12 | 1:A:326:ILE:HD13 | 1.89                     | 0.53              |
| 1:B:337:ARG:HH22 | 1:B:390:ASP:CG   | 2.14                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:86:ARG:NH2   | 1:D:113:ASN:OD1  | 2.42                     | 0.53              |
| 1:D:372:GLN:HG2  | 1:D:375:GLU:HG3  | 1.89                     | 0.53              |
| 1:D:473:VAL:HG13 | 1:D:555:VAL:HB   | 1.89                     | 0.53              |
| 1:A:71:GLU:O     | 1:A:72:HIS:C     | 2.50                     | 0.53              |
| 1:B:183:VAL:HG22 | 1:B:198:ASN:HA   | 1.90                     | 0.53              |
| 1:D:117:LEU:HD11 | 1:D:131:ILE:HG13 | 1.91                     | 0.53              |
| 1:A:137:ALA:O    | 1:A:140:SER:OG   | 2.17                     | 0.53              |
| 1:A:271:ASP:O    | 1:A:274:PHE:HB3  | 2.08                     | 0.53              |
| 1:B:488:ARG:NH1  | 1:B:510:ARG:HB3  | 2.22                     | 0.53              |
| 1:C:322:ARG:O    | 1:C:326:ILE:HG13 | 2.09                     | 0.53              |
| 1:D:181:SER:O    | 1:D:239:GLN:HG3  | 2.08                     | 0.53              |
| 1:D:485:SER:O    | 1:D:486:ARG:C    | 2.52                     | 0.53              |
| 1:B:85:ALA:HB2   | 1:B:545:PHE:HE2  | 1.73                     | 0.53              |
| 1:D:354:LYS:NZ   | 1:D:397:ASP:OD1  | 2.42                     | 0.53              |
| 1:A:184:LEU:HG   | 1:A:186:THR:HG22 | 1.91                     | 0.53              |
| 1:A:542:LEU:O    | 1:A:542:LEU:HD22 | 2.09                     | 0.53              |
| 1:C:499:SER:O    | 1:C:500:ALA:C    | 2.52                     | 0.53              |
| 1:C:461:GLU:OE1  | 1:D:461:GLU:OE1  | 2.27                     | 0.53              |
| 1:A:87:SER:CB    | 1:A:511:GLY:HA2  | 2.37                     | 0.52              |
| 1:C:196:ASN:OD1  | 1:C:196:ASN:C    | 2.51                     | 0.52              |
| 1:C:395:VAL:O    | 1:C:510:ARG:NH1  | 2.33                     | 0.52              |
| 1:D:438:PHE:CZ   | 1:D:442:ARG:HD3  | 2.45                     | 0.52              |
| 1:D:348:LYS:O    | 1:D:349:VAL:C    | 2.52                     | 0.52              |
| 1:A:447:LEU:HD13 | 1:B:467:CYS:SG   | 2.49                     | 0.52              |
| 1:D:191:PHE:O    | 1:D:201:TRP:HB2  | 2.09                     | 0.52              |
| 1:C:208:VAL:HA   | 1:C:236:LEU:CD1  | 2.36                     | 0.52              |
| 1:A:66:ALA:HB1   | 1:A:71:GLU:HB3   | 1.90                     | 0.52              |
| 1:B:163:ARG:HA   | 1:B:250:LYS:O    | 2.10                     | 0.52              |
| 1:A:129:GLU:O    | 1:A:130:SER:C    | 2.53                     | 0.52              |
| 1:B:83:VAL:O     | 1:B:83:VAL:HG13  | 2.10                     | 0.52              |
| 1:B:375:GLU:CB   | 1:D:384:MET:HE1  | 2.38                     | 0.52              |
| 1:C:567:ILE:HG12 | 1:D:569:ARG:HG2  | 1.92                     | 0.52              |
| 1:B:159:GLY:C    | 1:B:161:GLU:H    | 2.17                     | 0.52              |
| 1:B:164:THR:HG23 | 1:B:250:LYS:H    | 1.75                     | 0.52              |
| 1:B:202:VAL:HG11 | 1:B:207:ILE:HD12 | 1.91                     | 0.51              |
| 1:A:357:ILE:O    | 1:A:358:GLY:C    | 2.50                     | 0.51              |
| 1:C:288:VAL:HG12 | 1:C:326:ILE:HD13 | 1.92                     | 0.51              |
| 1:C:315:GLU:HG2  | 1:C:336:ALA:CB   | 2.41                     | 0.51              |
| 1:B:78:ILE:HD13  | 1:D:320:VAL:HG11 | 1.93                     | 0.51              |
| 1:C:87:SER:CB    | 1:C:511:GLY:HA2  | 2.41                     | 0.51              |
| 1:D:377:MET:C    | 1:D:379:THR:H    | 2.18                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:506:VAL:HG13 | 1:A:512:VAL:CG1  | 2.41                     | 0.51              |
| 1:C:168:GLN:C    | 1:C:170:GLY:H    | 2.17                     | 0.51              |
| 1:A:206:ASN:O    | 1:A:210:VAL:HG23 | 2.11                     | 0.51              |
| 1:A:284:PHE:HD1  | 1:A:311:ILE:HB   | 1.75                     | 0.51              |
| 1:B:377:MET:C    | 1:B:379:THR:H    | 2.18                     | 0.51              |
| 1:D:66:ALA:HB1   | 1:D:71:GLU:HB3   | 1.92                     | 0.51              |
| 1:D:87:SER:CB    | 1:D:511:GLY:HA2  | 2.41                     | 0.51              |
| 1:A:369:CYS:SG   | 1:A:373:MET:CE   | 2.97                     | 0.51              |
| 1:B:487:TYR:O    | 1:B:488:ARG:HB2  | 2.10                     | 0.50              |
| 1:D:296:ALA:O    | 1:D:299:ALA:HB3  | 2.11                     | 0.50              |
| 1:B:68:THR:HB    | 1:D:440:GLU:OE2  | 2.11                     | 0.50              |
| 1:C:360:CYS:HB3  | 1:C:365:LYS:O    | 2.10                     | 0.50              |
| 1:B:224:ILE:CD1  | 1:B:244:GLY:HA3  | 2.41                     | 0.50              |
| 1:C:150:PRO:HG2  | 1:C:514:PRO:HG2  | 1.93                     | 0.50              |
| 1:B:144:SER:OG   | 1:B:144:SER:CA   | 2.53                     | 0.50              |
| 1:B:453:GLU:CG   | 1:B:483:LEU:HD13 | 2.40                     | 0.50              |
| 1:B:87:SER:HB2   | 1:B:511:GLY:N    | 2.26                     | 0.50              |
| 1:A:349:VAL:O    | 1:A:352:ALA:N    | 2.45                     | 0.50              |
| 1:B:183:VAL:HG13 | 1:B:198:ASN:O    | 2.11                     | 0.50              |
| 1:D:87:SER:HB3   | 1:D:511:GLY:HA2  | 1.93                     | 0.50              |
| 1:A:286:SER:HA   | 1:A:313:LYS:HE2  | 1.93                     | 0.50              |
| 1:B:228:VAL:CG2  | 1:B:238:THR:HG22 | 2.42                     | 0.50              |
| 1:D:293:ASP:O    | 1:D:297:VAL:HG23 | 2.12                     | 0.50              |
| 1:A:91:ILE:HB    | 1:A:403:MET:HG3  | 1.94                     | 0.49              |
| 1:B:349:VAL:O    | 1:B:352:ALA:N    | 2.45                     | 0.49              |
| 1:D:213:VAL:HG13 | 1:D:229:GLN:HA   | 1.93                     | 0.49              |
| 1:D:378:ILE:O    | 1:D:378:ILE:HG22 | 2.12                     | 0.49              |
| 1:A:485:SER:O    | 1:A:486:ARG:C    | 2.55                     | 0.49              |
| 1:B:164:THR:HG21 | 1:B:246:LEU:HD11 | 1.94                     | 0.49              |
| 1:C:163:ARG:HD2  | 1:C:249:ARG:HH21 | 1.77                     | 0.49              |
| 1:D:286:SER:HA   | 1:D:313:LYS:HE2  | 1.93                     | 0.49              |
| 1:A:70:LEU:CD2   | 1:C:362:LEU:HD12 | 2.43                     | 0.49              |
| 1:A:91:ILE:HG23  | 1:A:114:ILE:HG22 | 1.95                     | 0.49              |
| 1:B:440:GLU:OE2  | 1:D:68:THR:HB    | 2.13                     | 0.49              |
| 1:B:473:VAL:HG13 | 1:B:555:VAL:HB   | 1.93                     | 0.49              |
| 1:C:323:PHE:O    | 1:C:324:ASP:C    | 2.55                     | 0.49              |
| 1:D:219:ILE:HG12 | 1:D:252:VAL:HG22 | 1.95                     | 0.49              |
| 1:D:403:MET:HG2  | 1:D:404:LEU:N    | 2.27                     | 0.49              |
| 1:A:377:MET:C    | 1:A:379:THR:H    | 2.20                     | 0.49              |
| 1:A:210:VAL:HG11 | 1:A:258:GLN:O    | 2.13                     | 0.49              |
| 1:B:102:GLU:OE1  | 1:B:105:LYS:HD2  | 2.13                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:217:ILE:HG12 | 1:C:254:LEU:CD2  | 2.42                     | 0.49              |
| 1:A:269:VAL:O    | 1:A:273:ARG:HG2  | 2.11                     | 0.49              |
| 1:B:446:PRO:O    | 1:B:447:LEU:O    | 2.30                     | 0.49              |
| 1:C:448:SER:OG   | 1:C:449:ARG:N    | 2.46                     | 0.49              |
| 1:C:168:GLN:C    | 1:C:170:GLY:N    | 2.70                     | 0.49              |
| 1:B:315:GLU:HG2  | 1:B:336:ALA:CB   | 2.43                     | 0.49              |
| 1:A:70:LEU:HD21  | 1:C:362:LEU:HD12 | 1.95                     | 0.49              |
| 1:A:294:VAL:O    | 1:A:295:ALA:C    | 2.56                     | 0.49              |
| 1:C:87:SER:HB2   | 1:C:511:GLY:CA   | 2.43                     | 0.49              |
| 1:C:438:PHE:CZ   | 1:C:442:ARG:HD3  | 2.48                     | 0.49              |
| 1:C:264:LEU:HD12 | 1:C:268:ASP:CB   | 2.43                     | 0.48              |
| 1:B:158:LYS:O    | 1:B:161:GLU:HG3  | 2.13                     | 0.48              |
| 1:B:537:ILE:O    | 1:B:540:GLY:N    | 2.47                     | 0.48              |
| 1:D:210:VAL:O    | 1:D:212:PRO:HD3  | 2.12                     | 0.48              |
| 1:D:448:SER:OG   | 1:D:449:ARG:N    | 2.45                     | 0.48              |
| 1:A:87:SER:HB2   | 1:A:511:GLY:N    | 2.28                     | 0.48              |
| 1:A:441:LEU:O    | 1:A:442:ARG:C    | 2.53                     | 0.48              |
| 1:A:157:THR:HG22 | 1:A:286:SER:H    | 1.77                     | 0.48              |
| 1:B:219:ILE:HG23 | 1:B:251:GLY:O    | 2.13                     | 0.48              |
| 1:B:221:ASP:HA   | 1:B:342:ILE:HD11 | 1.94                     | 0.48              |
| 1:C:325:GLU:HG3  | 1:C:326:ILE:N    | 2.29                     | 0.48              |
| 1:D:155:LEU:C    | 1:D:155:LEU:HD23 | 2.39                     | 0.48              |
| 1:D:194:ARG:HD2  | 1:D:194:ARG:HH11 | 1.77                     | 0.48              |
| 1:B:216:ARG:HD2  | 1:B:218:TYR:CZ   | 2.48                     | 0.48              |
| 1:C:293:ASP:O    | 1:C:297:VAL:HG23 | 2.14                     | 0.48              |
| 1:B:271:ASP:O    | 1:B:274:PHE:HB3  | 2.14                     | 0.48              |
| 1:C:315:GLU:HG2  | 1:C:336:ALA:HB3  | 1.95                     | 0.48              |
| 1:A:521:PRO:HA   | 1:A:528:ASP:OD1  | 2.13                     | 0.48              |
| 1:C:202:VAL:HG13 | 1:C:204:TYR:H    | 1.78                     | 0.48              |
| 1:D:76:LEU:HD23  | 1:D:76:LEU:HA    | 1.69                     | 0.48              |
| 1:D:360:CYS:HB3  | 1:D:365:LYS:O    | 2.13                     | 0.48              |
| 1:A:315:GLU:HG2  | 1:A:336:ALA:HB3  | 1.94                     | 0.48              |
| 1:A:434:HIS:O    | 1:A:435:ARG:C    | 2.57                     | 0.48              |
| 1:B:144:SER:CB   | 1:B:144:SER:HG   | 2.13                     | 0.48              |
| 1:B:499:SER:O    | 1:B:500:ALA:C    | 2.56                     | 0.47              |
| 1:C:348:LYS:O    | 1:C:349:VAL:C    | 2.57                     | 0.47              |
| 1:B:218:TYR:C    | 1:B:219:ILE:HG13 | 2.39                     | 0.47              |
| 1:C:83:VAL:O     | 1:C:83:VAL:HG12  | 2.14                     | 0.47              |
| 1:B:264:LEU:HD12 | 1:B:264:LEU:HA   | 1.73                     | 0.47              |
| 1:D:188:ASP:OD2  | 1:D:190:ALA:HB3  | 2.14                     | 0.47              |
| 1:A:303:PRO:C    | 1:A:305:GLY:N    | 2.72                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:83:VAL:O     | 1:B:83:VAL:HG12  | 2.14                     | 0.47              |
| 1:D:254:LEU:HD12 | 1:D:259:VAL:HG22 | 1.96                     | 0.47              |
| 1:A:167:LEU:O    | 1:A:168:GLN:C    | 2.57                     | 0.47              |
| 1:B:104:LEU:O    | 1:B:108:ILE:HG13 | 2.14                     | 0.47              |
| 1:A:315:GLU:HB3  | 1:A:339:ASP:HB2  | 1.96                     | 0.47              |
| 1:A:208:VAL:HG12 | 1:A:236:LEU:HG   | 1.97                     | 0.47              |
| 1:A:478:GLY:O    | 1:A:479:ARG:C    | 2.57                     | 0.47              |
| 1:B:323:PHE:O    | 1:B:324:ASP:C    | 2.58                     | 0.47              |
| 1:B:362:LEU:HD12 | 1:D:70:LEU:CD2   | 2.44                     | 0.47              |
| 1:A:347:GLU:OE2  | 1:A:347:GLU:N    | 2.27                     | 0.47              |
| 1:A:367:VAL:O    | 1:A:367:VAL:HG13 | 2.13                     | 0.47              |
| 1:A:460:VAL:HG22 | 1:A:489:PRO:HG3  | 1.96                     | 0.47              |
| 1:C:559:ARG:HD3  | 1:C:560:PRO:O    | 2.15                     | 0.47              |
| 1:D:231:ILE:HG12 | 1:D:236:LEU:HD23 | 1.96                     | 0.47              |
| 1:A:446:PRO:C    | 1:A:447:LEU:O    | 2.57                     | 0.47              |
| 1:A:403:MET:HG2  | 1:A:404:LEU:N    | 2.30                     | 0.47              |
| 1:D:358:GLY:O    | 1:D:361:ASN:HB2  | 2.15                     | 0.47              |
| 1:A:164:THR:HA   | 1:A:201:TRP:O    | 2.14                     | 0.46              |
| 1:B:337:ARG:NH2  | 1:B:390:ASP:OD1  | 2.44                     | 0.46              |
| 1:B:514:PRO:C    | 1:B:515:LEU:HD23 | 2.40                     | 0.46              |
| 1:B:141:PHE:CD1  | 1:B:141:PHE:N    | 2.83                     | 0.46              |
| 1:A:323:PHE:CE1  | 1:A:333:ILE:HG13 | 2.50                     | 0.46              |
| 1:B:466:CYS:O    | 1:B:467:CYS:C    | 2.56                     | 0.46              |
| 1:B:284:PHE:HD1  | 1:B:311:ILE:HB   | 1.79                     | 0.46              |
| 1:B:341:GLY:HA3  | 1:D:385:ARG:HE   | 1.80                     | 0.46              |
| 1:B:559:ARG:HD2  | 1:B:564:TYR:CE1  | 2.50                     | 0.46              |
| 1:A:146:LEU:HB2  | 1:A:542:LEU:HD12 | 1.98                     | 0.46              |
| 1:A:207:ILE:C    | 1:A:209:ARG:H    | 2.24                     | 0.46              |
| 1:B:303:PRO:C    | 1:B:305:GLY:H    | 2.23                     | 0.46              |
| 1:D:303:PRO:C    | 1:D:305:GLY:H    | 2.23                     | 0.46              |
| 1:D:369:CYS:SG   | 1:D:373:MET:HE3  | 2.56                     | 0.46              |
| 1:A:97:ALA:O     | 1:A:103:ARG:HD3  | 2.16                     | 0.46              |
| 1:B:449:ARG:O    | 1:B:451:PRO:HD3  | 2.16                     | 0.46              |
| 1:B:483:LEU:O    | 1:B:486:ARG:HB2  | 2.16                     | 0.46              |
| 1:D:87:SER:H     | 1:D:429:GLU:CD   | 2.23                     | 0.46              |
| 1:D:129:GLU:O    | 1:D:130:SER:C    | 2.58                     | 0.46              |
| 1:B:301:LEU:HD12 | 1:B:301:LEU:HA   | 1.70                     | 0.46              |
| 1:D:172:GLU:OE1  | 1:D:172:GLU:N    | 2.49                     | 0.46              |
| 1:D:281:ASP:CG   | 1:D:504:ARG:HE   | 2.19                     | 0.46              |
| 1:B:86:ARG:HA    | 1:B:429:GLU:OE1  | 2.14                     | 0.46              |
| 1:B:478:GLY:O    | 1:B:479:ARG:C    | 2.58                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:393:ASN:O    | 1:A:397:ASP:N    | 2.47                     | 0.46              |
| 1:B:225:SER:OG   | 1:B:241:GLU:HB3  | 2.15                     | 0.46              |
| 1:C:166:ILE:CG2  | 1:C:167:LEU:N    | 2.79                     | 0.46              |
| 1:C:370:ALA:O    | 1:C:371:THR:HB   | 2.15                     | 0.46              |
| 1:C:525:TRP:CE2  | 1:C:560:PRO:HG3  | 2.50                     | 0.46              |
| 1:D:357:ILE:O    | 1:D:358:GLY:C    | 2.57                     | 0.46              |
| 1:B:446:PRO:C    | 1:B:447:LEU:O    | 2.58                     | 0.46              |
| 1:C:274:PHE:C    | 1:C:274:PHE:CD2  | 2.94                     | 0.46              |
| 1:D:466:CYS:O    | 1:D:467:CYS:C    | 2.56                     | 0.46              |
| 1:A:274:PHE:C    | 1:A:274:PHE:CD2  | 2.94                     | 0.45              |
| 1:A:276:VAL:HG11 | 1:A:304:GLU:HB2  | 1.98                     | 0.45              |
| 1:A:188:ASP:C    | 1:A:188:ASP:OD1  | 2.60                     | 0.45              |
| 1:B:76:LEU:HD23  | 1:B:76:LEU:HA    | 1.82                     | 0.45              |
| 1:B:320:VAL:HG11 | 1:D:78:ILE:HD13  | 1.98                     | 0.45              |
| 1:B:377:MET:C    | 1:B:379:THR:N    | 2.74                     | 0.45              |
| 1:B:452:THR:CG2  | 1:B:483:LEU:HD12 | 2.37                     | 0.45              |
| 1:C:129:GLU:O    | 1:C:130:SER:C    | 2.57                     | 0.45              |
| 1:D:475:THR:HA   | 2:D:580:FBP:H61  | 1.98                     | 0.45              |
| 1:A:191:PHE:N    | 1:A:191:PHE:CD1  | 2.84                     | 0.45              |
| 1:B:296:ALA:O    | 1:B:299:ALA:HB3  | 2.17                     | 0.45              |
| 1:B:315:GLU:HG2  | 1:B:336:ALA:HB3  | 1.97                     | 0.45              |
| 1:B:525:TRP:CE2  | 1:B:560:PRO:HG3  | 2.51                     | 0.45              |
| 1:C:85:ALA:HB2   | 1:C:545:PHE:HE2  | 1.79                     | 0.45              |
| 1:C:487:TYR:O    | 1:C:488:ARG:HB2  | 2.15                     | 0.45              |
| 1:D:403:MET:HG2  | 1:D:404:LEU:H    | 1.82                     | 0.45              |
| 1:B:276:VAL:HG11 | 1:B:304:GLU:HB2  | 1.99                     | 0.45              |
| 1:B:360:CYS:HB3  | 1:B:365:LYS:O    | 2.16                     | 0.45              |
| 1:C:369:CYS:SG   | 1:C:373:MET:HE3  | 2.57                     | 0.45              |
| 1:B:375:GLU:HB2  | 1:D:384:MET:CE   | 2.43                     | 0.45              |
| 1:D:204:TYR:CE1  | 1:D:206:ASN:HB2  | 2.51                     | 0.45              |
| 1:A:210:VAL:HG12 | 1:A:257:ALA:HB1  | 1.98                     | 0.45              |
| 1:B:304:GLU:H    | 1:B:304:GLU:HG2  | 1.59                     | 0.45              |
| 1:C:83:VAL:O     | 1:C:83:VAL:HG13  | 2.17                     | 0.45              |
| 1:C:87:SER:HB2   | 1:C:511:GLY:N    | 2.32                     | 0.45              |
| 1:C:299:ALA:O    | 1:C:300:ALA:C    | 2.57                     | 0.45              |
| 1:A:385:ARG:HG2  | 1:C:372:GLN:OE1  | 2.17                     | 0.45              |
| 1:A:87:SER:CB    | 1:A:511:GLY:CA   | 2.96                     | 0.44              |
| 1:A:372:GLN:HB2  | 1:C:385:ARG:HB2  | 1.99                     | 0.44              |
| 1:B:157:THR:HG22 | 1:B:286:SER:HB2  | 1.98                     | 0.44              |
| 1:C:284:PHE:HD1  | 1:C:311:ILE:HB   | 1.82                     | 0.44              |
| 1:D:336:ALA:HB1  | 3:D:581:PGA:C1   | 2.47                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:354:LYS:NZ   | 1:B:397:ASP:OD1  | 2.45                     | 0.44              |
| 1:C:267:GLN:O    | 1:C:268:ASP:C    | 2.60                     | 0.44              |
| 1:B:225:SER:O    | 1:B:226:LEU:HD23 | 2.18                     | 0.44              |
| 1:C:168:GLN:O    | 1:C:170:GLY:N    | 2.51                     | 0.44              |
| 1:C:377:MET:C    | 1:C:379:THR:H    | 2.25                     | 0.44              |
| 1:C:420:MET:O    | 1:C:424:ILE:HG13 | 2.16                     | 0.44              |
| 1:A:58:GLN:O     | 1:A:59:GLN:C     | 2.61                     | 0.44              |
| 1:B:293:ASP:O    | 1:B:297:VAL:HG23 | 2.18                     | 0.44              |
| 1:C:506:VAL:CG1  | 1:C:512:VAL:CG1  | 2.95                     | 0.44              |
| 1:B:58:GLN:O     | 1:B:59:GLN:C     | 2.61                     | 0.44              |
| 1:B:372:GLN:HA   | 1:B:375:GLU:HG3  | 1.99                     | 0.44              |
| 1:C:137:ALA:O    | 1:C:140:SER:OG   | 2.28                     | 0.44              |
| 1:D:181:SER:O    | 1:D:239:GLN:CG   | 2.65                     | 0.44              |
| 1:A:175:VAL:HG11 | 1:A:196:ASN:C    | 2.43                     | 0.44              |
| 1:B:337:ARG:HD3  | 1:B:370:ALA:O    | 2.17                     | 0.44              |
| 1:C:86:ARG:HB3   | 1:C:426:ARG:CG   | 2.37                     | 0.44              |
| 1:C:286:SER:HA   | 1:C:313:LYS:HE2  | 1.99                     | 0.44              |
| 1:D:264:LEU:HA   | 1:D:264:LEU:HD12 | 1.79                     | 0.44              |
| 1:A:86:ARG:HG2   | 1:A:422:HIS:CE1  | 2.52                     | 0.44              |
| 1:A:370:ALA:O    | 1:A:371:THR:HB   | 2.17                     | 0.44              |
| 1:A:479:ARG:HG3  | 1:A:479:ARG:HH11 | 1.83                     | 0.44              |
| 1:C:95:GLY:O     | 1:C:96:PRO:C     | 2.60                     | 0.44              |
| 1:C:162:ILE:HG12 | 1:C:204:TYR:HB2  | 2.00                     | 0.44              |
| 1:C:340:LEU:O    | 1:C:344:ILE:HG12 | 2.17                     | 0.44              |
| 1:D:299:ALA:O    | 1:D:300:ALA:C    | 2.61                     | 0.44              |
| 1:A:396:LEU:HD12 | 1:A:396:LEU:HA   | 1.88                     | 0.43              |
| 1:D:86:ARG:HA    | 1:D:429:GLU:OE1  | 2.18                     | 0.43              |
| 1:D:187:VAL:CG1  | 1:D:202:VAL:HG12 | 2.46                     | 0.43              |
| 1:D:276:VAL:HG11 | 1:D:304:GLU:HB2  | 1.99                     | 0.43              |
| 1:B:100:SER:O    | 1:B:101:VAL:C    | 2.60                     | 0.43              |
| 1:C:231:ILE:HD13 | 1:C:231:ILE:C    | 2.43                     | 0.43              |
| 1:C:441:LEU:O    | 1:C:442:ARG:C    | 2.60                     | 0.43              |
| 1:D:521:PRO:HA   | 1:D:528:ASP:OD1  | 2.18                     | 0.43              |
| 1:A:102:GLU:OE1  | 1:A:105:LYS:HD2  | 2.19                     | 0.43              |
| 1:C:192:ARG:HA   | 1:C:201:TRP:CD2  | 2.54                     | 0.43              |
| 1:D:133:ASN:O    | 1:D:134:VAL:C    | 2.61                     | 0.43              |
| 1:A:202:VAL:HG13 | 1:A:204:TYR:H    | 1.83                     | 0.43              |
| 1:B:228:VAL:HG23 | 1:B:238:THR:HG22 | 1.99                     | 0.43              |
| 1:C:327:LEU:C    | 1:C:329:VAL:H    | 2.25                     | 0.43              |
| 1:C:506:VAL:HG13 | 1:C:512:VAL:HG11 | 2.00                     | 0.43              |
| 1:B:87:SER:HB2   | 1:B:511:GLY:HA2  | 1.95                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:89:SER:HA    | 1:B:113:ASN:OD1  | 2.18                     | 0.43              |
| 1:B:162:ILE:CB   | 1:B:252:VAL:HB   | 2.35                     | 0.43              |
| 1:D:87:SER:HB2   | 1:D:511:GLY:N    | 2.34                     | 0.43              |
| 1:C:87:SER:CB    | 1:C:511:GLY:CA   | 2.96                     | 0.43              |
| 1:C:162:ILE:HG22 | 1:C:162:ILE:O    | 2.18                     | 0.43              |
| 1:D:123:SER:O    | 1:D:126:TYR:HB3  | 2.18                     | 0.43              |
| 1:D:362:LEU:O    | 1:D:486:ARG:NH2  | 2.51                     | 0.43              |
| 1:B:553:ILE:HG23 | 1:B:568:MET:HE3  | 2.00                     | 0.43              |
| 1:C:446:PRO:O    | 1:C:447:LEU:C    | 2.61                     | 0.43              |
| 1:A:258:GLN:H    | 1:A:258:GLN:HG2  | 1.70                     | 0.43              |
| 1:B:87:SER:H     | 1:B:429:GLU:CD   | 2.26                     | 0.43              |
| 1:B:97:ALA:O     | 1:B:103:ARG:HD3  | 2.18                     | 0.43              |
| 1:B:509:CYS:O    | 1:B:510:ARG:C    | 2.61                     | 0.43              |
| 1:D:204:TYR:CE1  | 1:D:261:LEU:CD1  | 2.95                     | 0.43              |
| 1:D:303:PRO:C    | 1:D:305:GLY:N    | 2.77                     | 0.43              |
| 1:A:281:ASP:C    | 1:A:282:ILE:HG13 | 2.44                     | 0.43              |
| 1:A:347:GLU:HG2  | 1:C:423:ALA:HB1  | 2.01                     | 0.43              |
| 1:A:559:ARG:HD3  | 1:A:560:PRO:O    | 2.19                     | 0.43              |
| 1:B:515:LEU:HD11 | 1:B:539:SER:HB2  | 2.00                     | 0.43              |
| 1:C:177:LEU:HD21 | 1:C:246:LEU:CD2  | 2.48                     | 0.43              |
| 1:A:317:HIS:HE2  | 1:C:79:ASP:CG    | 2.27                     | 0.42              |
| 1:C:177:LEU:HD23 | 1:C:246:LEU:HB2  | 2.01                     | 0.42              |
| 1:C:388:THR:HG22 | 1:C:389:SER:N    | 2.34                     | 0.42              |
| 1:D:201:TRP:CG   | 1:D:202:VAL:H    | 2.37                     | 0.42              |
| 1:D:284:PHE:HD1  | 1:D:311:ILE:HB   | 1.84                     | 0.42              |
| 1:D:525:TRP:CE2  | 1:D:560:PRO:HG3  | 2.54                     | 0.42              |
| 1:A:150:PRO:HG2  | 1:A:514:PRO:HG2  | 2.01                     | 0.42              |
| 1:A:475:THR:OG1  | 1:A:478:GLY:N    | 2.48                     | 0.42              |
| 1:D:146:LEU:CB   | 1:D:542:LEU:HD12 | 2.46                     | 0.42              |
| 1:A:123:SER:O    | 1:A:126:TYR:HB3  | 2.19                     | 0.42              |
| 1:B:267:GLN:O    | 1:B:268:ASP:C    | 2.62                     | 0.42              |
| 1:C:231:ILE:HD13 | 1:C:232:GLY:O    | 2.18                     | 0.42              |
| 1:D:191:PHE:C    | 1:D:193:THR:H    | 2.27                     | 0.42              |
| 1:A:194:ARG:HH11 | 1:A:194:ARG:CB   | 2.33                     | 0.42              |
| 1:A:349:VAL:O    | 1:A:350:PHE:C    | 2.63                     | 0.42              |
| 1:A:403:MET:HG2  | 1:A:404:LEU:H    | 1.84                     | 0.42              |
| 1:B:259:VAL:HG12 | 1:B:261:LEU:CB   | 2.50                     | 0.42              |
| 1:C:206:ASN:O    | 1:C:210:VAL:HG23 | 2.19                     | 0.42              |
| 1:C:303:PRO:C    | 1:C:305:GLY:H    | 2.28                     | 0.42              |
| 1:C:569:ARG:HG2  | 1:D:567:ILE:HG12 | 2.01                     | 0.42              |
| 1:A:200:VAL:HG12 | 1:A:246:LEU:HD21 | 2.00                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:385:ARG:NE   | 1:D:341:GLY:HA3  | 2.35                     | 0.42              |
| 1:C:420:MET:HE2  | 1:C:424:ILE:CG1  | 2.50                     | 0.42              |
| 1:D:419:LYS:O    | 1:D:422:HIS:HB3  | 2.19                     | 0.42              |
| 1:B:70:LEU:CD2   | 1:D:362:LEU:HD12 | 2.50                     | 0.42              |
| 1:B:348:LYS:O    | 1:B:349:VAL:C    | 2.62                     | 0.42              |
| 1:B:446:PRO:O    | 1:B:447:LEU:C    | 2.63                     | 0.42              |
| 1:D:267:GLN:O    | 1:D:268:ASP:C    | 2.61                     | 0.42              |
| 1:B:135:ARG:O    | 1:B:139:GLU:HG2  | 2.19                     | 0.42              |
| 1:A:232:GLY:HA2  | 1:A:233:PRO:HD3  | 1.84                     | 0.42              |
| 1:A:286:SER:CA   | 1:A:313:LYS:HE2  | 2.50                     | 0.42              |
| 1:A:377:MET:C    | 1:A:379:THR:N    | 2.77                     | 0.42              |
| 1:D:478:GLY:O    | 1:D:479:ARG:C    | 2.61                     | 0.42              |
| 1:B:559:ARG:HD3  | 1:B:560:PRO:O    | 2.20                     | 0.41              |
| 1:D:290:LYS:O    | 1:D:291:ALA:C    | 2.63                     | 0.41              |
| 1:A:347:GLU:CG   | 1:C:423:ALA:HB1  | 2.49                     | 0.41              |
| 1:B:534:GLN:O    | 1:B:535:PHE:C    | 2.61                     | 0.41              |
| 1:C:506:VAL:HG13 | 1:C:512:VAL:CG1  | 2.51                     | 0.41              |
| 1:B:264:LEU:HD12 | 1:B:268:ASP:CB   | 2.50                     | 0.41              |
| 1:A:76:LEU:HD23  | 1:A:76:LEU:HA    | 1.74                     | 0.41              |
| 1:A:100:SER:O    | 1:A:101:VAL:C    | 2.64                     | 0.41              |
| 1:A:175:VAL:HG11 | 1:A:197:ALA:N    | 2.35                     | 0.41              |
| 1:B:206:ASN:O    | 1:B:210:VAL:HG23 | 2.20                     | 0.41              |
| 1:B:385:ARG:HG2  | 1:D:372:GLN:OE1  | 2.19                     | 0.41              |
| 1:C:61:LEU:HD12  | 1:C:61:LEU:HA    | 1.95                     | 0.41              |
| 1:C:87:SER:H     | 1:C:429:GLU:CD   | 2.29                     | 0.41              |
| 1:C:559:ARG:HD2  | 1:C:564:TYR:CE1  | 2.55                     | 0.41              |
| 1:B:370:ALA:HB1  | 1:B:403:MET:HE2  | 2.01                     | 0.41              |
| 1:C:230:LYS:CB   | 1:C:237:VAL:HB   | 2.51                     | 0.41              |
| 1:D:98:SER:HB2   | 1:D:107:MET:SD   | 2.60                     | 0.41              |
| 1:D:157:THR:HG22 | 1:D:286:SER:CB   | 2.51                     | 0.41              |
| 1:B:357:ILE:O    | 1:B:358:GLY:C    | 2.63                     | 0.41              |
| 1:C:87:SER:HB3   | 1:C:511:GLY:HA2  | 2.02                     | 0.41              |
| 1:C:296:ALA:O    | 1:C:299:ALA:HB3  | 2.20                     | 0.41              |
| 1:D:175:VAL:HG12 | 1:D:177:LEU:HD22 | 2.03                     | 0.41              |
| 1:A:86:ARG:NH2   | 1:A:113:ASN:OD1  | 2.54                     | 0.41              |
| 1:A:188:ASP:HA   | 1:A:189:PRO:HD3  | 1.89                     | 0.41              |
| 1:A:351:LEU:O    | 1:A:352:ALA:C    | 2.59                     | 0.41              |
| 1:A:437:LEU:HD21 | 1:A:488:ARG:HG3  | 2.03                     | 0.41              |
| 1:D:68:THR:OG1   | 1:D:71:GLU:HB2   | 2.20                     | 0.41              |
| 1:A:59:GLN:O     | 1:A:60:GLN:C     | 2.64                     | 0.41              |
| 1:A:86:ARG:HA    | 1:A:429:GLU:OE1  | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:95:GLY:O     | 1:A:96:PRO:C     | 2.64                     | 0.41              |
| 1:A:499:SER:O    | 1:A:500:ALA:C    | 2.63                     | 0.41              |
| 1:C:372:GLN:HA   | 1:C:375:GLU:HG2  | 2.02                     | 0.41              |
| 1:A:99:ARG:HH11  | 1:A:99:ARG:HD3   | 1.72                     | 0.41              |
| 1:A:559:ARG:HD2  | 1:A:564:TYR:CE1  | 2.56                     | 0.41              |
| 1:C:210:VAL:O    | 1:C:212:PRO:HD2  | 2.21                     | 0.41              |
| 1:A:194:ARG:HB3  | 1:A:194:ARG:NH1  | 2.36                     | 0.41              |
| 1:A:483:LEU:O    | 1:A:486:ARG:HB2  | 2.21                     | 0.41              |
| 1:B:521:PRO:HA   | 1:B:528:ASP:OD1  | 2.21                     | 0.41              |
| 1:C:182:GLN:O    | 1:C:198:ASN:OD1  | 2.39                     | 0.41              |
| 1:C:187:VAL:O    | 1:C:189:PRO:HD3  | 2.20                     | 0.41              |
| 1:C:553:ILE:HG23 | 1:C:568:MET:HE3  | 2.03                     | 0.41              |
| 1:A:98:SER:HB2   | 1:A:107:MET:SD   | 2.61                     | 0.40              |
| 1:A:276:VAL:HG21 | 1:A:301:LEU:O    | 2.21                     | 0.40              |
| 1:A:336:ALA:HB1  | 3:A:581:PGA:C1   | 2.52                     | 0.40              |
| 1:A:339:ASP:O    | 1:A:340:LEU:C    | 2.64                     | 0.40              |
| 1:A:525:TRP:CE2  | 1:A:560:PRO:HG3  | 2.56                     | 0.40              |
| 1:D:334:MET:HA   | 1:D:368:VAL:HB   | 2.03                     | 0.40              |
| 1:A:229:GLN:O    | 1:A:230:LYS:HD3  | 2.21                     | 0.40              |
| 1:A:301:LEU:HD12 | 1:A:301:LEU:HA   | 1.78                     | 0.40              |
| 1:D:95:GLY:O     | 1:D:96:PRO:C     | 2.65                     | 0.40              |
| 1:B:98:SER:HA    | 1:B:103:ARG:HG2  | 2.04                     | 0.40              |
| 1:C:433:TYR:O    | 1:C:434:HIS:C    | 2.62                     | 0.40              |
| 1:D:274:PHE:CD2  | 1:D:274:PHE:C    | 2.99                     | 0.40              |
| 1:B:325:GLU:HG3  | 1:B:326:ILE:N    | 2.36                     | 0.40              |
| 1:B:517:TYR:CE2  | 1:B:519:GLU:HB2  | 2.57                     | 0.40              |
| 1:C:76:LEU:HA    | 1:C:76:LEU:HD23  | 1.78                     | 0.40              |
| 1:A:87:SER:HB3   | 1:A:511:GLY:CA   | 2.47                     | 0.40              |
| 1:A:506:VAL:CG1  | 1:A:512:VAL:HG12 | 2.51                     | 0.40              |
| 1:B:287:PHE:O    | 1:B:288:VAL:C    | 2.65                     | 0.40              |
| 1:C:70:LEU:O     | 1:C:73:LEU:HB2   | 2.22                     | 0.40              |
| 1:D:91:ILE:HB    | 1:D:403:MET:HG3  | 2.04                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

of similar resolution.

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1   | A     | 515/528 (98%)   | 454 (88%)  | 44 (8%)  | 17 (3%)  | 3           | 5  |
| 1   | B     | 483/528 (92%)   | 436 (90%)  | 38 (8%)  | 9 (2%)   | 6           | 12 |
| 1   | C     | 515/528 (98%)   | 465 (90%)  | 37 (7%)  | 13 (2%)  | 4           | 8  |
| 1   | D     | 508/528 (96%)   | 452 (89%)  | 43 (8%)  | 13 (3%)  | 4           | 7  |
| All | All   | 2021/2112 (96%) | 1807 (89%) | 162 (8%) | 52 (3%)  | 4           | 7  |

All (52) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 192 | ARG  |
| 1   | B     | 447 | LEU  |
| 1   | C     | 171 | PRO  |
| 1   | C     | 433 | TYR  |
| 1   | D     | 172 | GLU  |
| 1   | D     | 197 | ALA  |
| 1   | D     | 447 | LEU  |
| 1   | A     | 83  | VAL  |
| 1   | A     | 447 | LEU  |
| 1   | B     | 59  | GLN  |
| 1   | B     | 287 | PHE  |
| 1   | C     | 83  | VAL  |
| 1   | C     | 168 | GLN  |
| 1   | C     | 169 | GLY  |
| 1   | C     | 447 | LEU  |
| 1   | D     | 83  | VAL  |
| 1   | D     | 259 | VAL  |
| 1   | D     | 433 | TYR  |
| 1   | A     | 197 | ALA  |
| 1   | A     | 328 | GLU  |
| 1   | A     | 433 | TYR  |
| 1   | B     | 83  | VAL  |
| 1   | B     | 220 | ASP  |
| 1   | C     | 164 | THR  |
| 1   | D     | 206 | ASN  |
| 1   | A     | 84  | ALA  |
| 1   | A     | 160 | PRO  |
| 1   | A     | 299 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 304 | GLU  |
| 1   | B     | 160 | PRO  |
| 1   | D     | 193 | THR  |
| 1   | D     | 287 | PHE  |
| 1   | A     | 193 | THR  |
| 1   | A     | 220 | ASP  |
| 1   | A     | 371 | THR  |
| 1   | A     | 486 | ARG  |
| 1   | B     | 249 | ARG  |
| 1   | C     | 160 | PRO  |
| 1   | C     | 206 | ASN  |
| 1   | C     | 220 | ASP  |
| 1   | C     | 566 | ASN  |
| 1   | D     | 160 | PRO  |
| 1   | D     | 299 | ALA  |
| 1   | B     | 371 | THR  |
| 1   | A     | 213 | VAL  |
| 1   | A     | 338 | GLY  |
| 1   | B     | 338 | GLY  |
| 1   | C     | 205 | PRO  |
| 1   | D     | 178 | VAL  |
| 1   | D     | 338 | GLY  |
| 1   | C     | 338 | GLY  |
| 1   | A     | 398 | 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.

| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |   |
|-----|-------|-----------------|------------|-----------|-------------|---|
| 1   | A     | 414/423 (98%)   | 365 (88%)  | 49 (12%)  | 5           | 9 |
| 1   | B     | 394/423 (93%)   | 343 (87%)  | 51 (13%)  | 4           | 7 |
| 1   | C     | 414/423 (98%)   | 355 (86%)  | 59 (14%)  | 3           | 5 |
| 1   | D     | 411/423 (97%)   | 362 (88%)  | 49 (12%)  | 5           | 8 |
| All | All   | 1633/1692 (96%) | 1425 (87%) | 208 (13%) | 4           | 8 |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 59  | GLN  |
| 1   | A     | 61  | LEU  |
| 1   | A     | 83  | VAL  |
| 1   | A     | 87  | SER  |
| 1   | A     | 99  | ARG  |
| 1   | A     | 100 | SER  |
| 1   | A     | 103 | ARG  |
| 1   | A     | 104 | LEU  |
| 1   | A     | 120 | SER  |
| 1   | A     | 124 | HIS  |
| 1   | A     | 157 | THR  |
| 1   | A     | 174 | GLU  |
| 1   | A     | 182 | GLN  |
| 1   | A     | 186 | THR  |
| 1   | A     | 187 | VAL  |
| 1   | A     | 202 | VAL  |
| 1   | A     | 210 | VAL  |
| 1   | A     | 224 | ILE  |
| 1   | A     | 231 | ILE  |
| 1   | A     | 258 | GLN  |
| 1   | A     | 294 | VAL  |
| 1   | A     | 301 | LEU  |
| 1   | A     | 304 | GLU  |
| 1   | A     | 327 | LEU  |
| 1   | A     | 329 | VAL  |
| 1   | A     | 337 | ARG  |
| 1   | A     | 359 | ARG  |
| 1   | A     | 362 | LEU  |
| 1   | A     | 374 | LEU  |
| 1   | A     | 379 | THR  |
| 1   | A     | 384 | MET  |
| 1   | A     | 388 | THR  |
| 1   | A     | 396 | LEU  |
| 1   | A     | 410 | LYS  |
| 1   | A     | 457 | ILE  |
| 1   | A     | 473 | VAL  |
| 1   | A     | 485 | SER  |
| 1   | A     | 486 | ARG  |
| 1   | A     | 506 | VAL  |
| 1   | A     | 508 | LEU  |
| 1   | A     | 539 | SER  |
| 1   | A     | 542 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 543 | ARG  |
| 1   | A     | 546 | LEU  |
| 1   | A     | 547 | ARG  |
| 1   | A     | 552 | VAL  |
| 1   | A     | 559 | ARG  |
| 1   | A     | 562 | SER  |
| 1   | A     | 568 | MET  |
| 1   | B     | 59  | GLN  |
| 1   | B     | 61  | LEU  |
| 1   | B     | 83  | VAL  |
| 1   | B     | 86  | ARG  |
| 1   | B     | 99  | ARG  |
| 1   | B     | 100 | SER  |
| 1   | B     | 103 | ARG  |
| 1   | B     | 104 | LEU  |
| 1   | B     | 120 | SER  |
| 1   | B     | 124 | HIS  |
| 1   | B     | 141 | PHE  |
| 1   | B     | 144 | SER  |
| 1   | B     | 157 | THR  |
| 1   | B     | 175 | VAL  |
| 1   | B     | 177 | LEU  |
| 1   | B     | 182 | GLN  |
| 1   | B     | 185 | VAL  |
| 1   | B     | 202 | VAL  |
| 1   | B     | 210 | VAL  |
| 1   | B     | 219 | ILE  |
| 1   | B     | 254 | LEU  |
| 1   | B     | 294 | VAL  |
| 1   | B     | 301 | LEU  |
| 1   | B     | 304 | GLU  |
| 1   | B     | 327 | LEU  |
| 1   | B     | 329 | VAL  |
| 1   | B     | 337 | ARG  |
| 1   | B     | 347 | GLU  |
| 1   | B     | 359 | ARG  |
| 1   | B     | 362 | LEU  |
| 1   | B     | 374 | LEU  |
| 1   | B     | 379 | THR  |
| 1   | B     | 384 | MET  |
| 1   | B     | 388 | THR  |
| 1   | B     | 396 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 410 | LYS  |
| 1   | B     | 457 | ILE  |
| 1   | B     | 473 | VAL  |
| 1   | B     | 485 | SER  |
| 1   | B     | 486 | ARG  |
| 1   | B     | 506 | VAL  |
| 1   | B     | 508 | LEU  |
| 1   | B     | 534 | GLN  |
| 1   | B     | 539 | SER  |
| 1   | B     | 542 | LEU  |
| 1   | B     | 546 | LEU  |
| 1   | B     | 547 | ARG  |
| 1   | B     | 552 | VAL  |
| 1   | B     | 559 | ARG  |
| 1   | B     | 562 | SER  |
| 1   | B     | 568 | MET  |
| 1   | C     | 61  | LEU  |
| 1   | C     | 65  | MET  |
| 1   | C     | 83  | VAL  |
| 1   | C     | 86  | ARG  |
| 1   | C     | 99  | ARG  |
| 1   | C     | 100 | SER  |
| 1   | C     | 103 | ARG  |
| 1   | C     | 104 | LEU  |
| 1   | C     | 120 | SER  |
| 1   | C     | 124 | HIS  |
| 1   | C     | 147 | SER  |
| 1   | C     | 157 | THR  |
| 1   | C     | 164 | THR  |
| 1   | C     | 166 | ILE  |
| 1   | C     | 167 | LEU  |
| 1   | C     | 173 | SER  |
| 1   | C     | 175 | VAL  |
| 1   | C     | 193 | THR  |
| 1   | C     | 200 | VAL  |
| 1   | C     | 202 | VAL  |
| 1   | C     | 210 | VAL  |
| 1   | C     | 225 | SER  |
| 1   | C     | 228 | VAL  |
| 1   | C     | 231 | ILE  |
| 1   | C     | 234 | GLU  |
| 1   | C     | 248 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 250 | LYS  |
| 1   | C     | 258 | GLN  |
| 1   | C     | 294 | VAL  |
| 1   | C     | 301 | LEU  |
| 1   | C     | 304 | GLU  |
| 1   | C     | 327 | LEU  |
| 1   | C     | 329 | VAL  |
| 1   | C     | 337 | ARG  |
| 1   | C     | 359 | ARG  |
| 1   | C     | 362 | LEU  |
| 1   | C     | 374 | LEU  |
| 1   | C     | 379 | THR  |
| 1   | C     | 384 | MET  |
| 1   | C     | 388 | THR  |
| 1   | C     | 396 | LEU  |
| 1   | C     | 410 | LYS  |
| 1   | C     | 453 | GLU  |
| 1   | C     | 457 | ILE  |
| 1   | C     | 473 | VAL  |
| 1   | C     | 485 | SER  |
| 1   | C     | 486 | ARG  |
| 1   | C     | 506 | VAL  |
| 1   | C     | 508 | LEU  |
| 1   | C     | 534 | GLN  |
| 1   | C     | 539 | SER  |
| 1   | C     | 542 | LEU  |
| 1   | C     | 546 | LEU  |
| 1   | C     | 547 | ARG  |
| 1   | C     | 552 | VAL  |
| 1   | C     | 559 | ARG  |
| 1   | C     | 562 | SER  |
| 1   | C     | 568 | MET  |
| 1   | C     | 572 | SER  |
| 1   | D     | 59  | GLN  |
| 1   | D     | 61  | LEU  |
| 1   | D     | 83  | VAL  |
| 1   | D     | 86  | ARG  |
| 1   | D     | 99  | ARG  |
| 1   | D     | 100 | SER  |
| 1   | D     | 103 | ARG  |
| 1   | D     | 104 | LEU  |
| 1   | D     | 120 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 124 | HIS  |
| 1   | D     | 157 | THR  |
| 1   | D     | 176 | GLU  |
| 1   | D     | 177 | LEU  |
| 1   | D     | 182 | GLN  |
| 1   | D     | 186 | THR  |
| 1   | D     | 193 | THR  |
| 1   | D     | 202 | VAL  |
| 1   | D     | 210 | VAL  |
| 1   | D     | 216 | ARG  |
| 1   | D     | 231 | ILE  |
| 1   | D     | 248 | SER  |
| 1   | D     | 250 | LYS  |
| 1   | D     | 254 | LEU  |
| 1   | D     | 261 | LEU  |
| 1   | D     | 294 | VAL  |
| 1   | D     | 301 | LEU  |
| 1   | D     | 304 | GLU  |
| 1   | D     | 308 | ILE  |
| 1   | D     | 327 | LEU  |
| 1   | D     | 329 | VAL  |
| 1   | D     | 337 | ARG  |
| 1   | D     | 359 | ARG  |
| 1   | D     | 362 | LEU  |
| 1   | D     | 374 | LEU  |
| 1   | D     | 379 | THR  |
| 1   | D     | 388 | THR  |
| 1   | D     | 396 | LEU  |
| 1   | D     | 410 | LYS  |
| 1   | D     | 457 | ILE  |
| 1   | D     | 473 | VAL  |
| 1   | D     | 486 | ARG  |
| 1   | D     | 508 | LEU  |
| 1   | D     | 539 | SER  |
| 1   | D     | 542 | LEU  |
| 1   | D     | 547 | ARG  |
| 1   | D     | 552 | VAL  |
| 1   | D     | 559 | ARG  |
| 1   | D     | 562 | SER  |
| 1   | D     | 568 | MET  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 121 | HIS  |
| 1   | A     | 124 | HIS  |
| 1   | A     | 133 | ASN  |
| 1   | A     | 198 | ASN  |
| 1   | A     | 253 | ASN  |
| 1   | A     | 421 | GLN  |
| 1   | A     | 434 | HIS  |
| 1   | B     | 72  | HIS  |
| 1   | B     | 121 | HIS  |
| 1   | B     | 124 | HIS  |
| 1   | B     | 133 | ASN  |
| 1   | B     | 421 | GLN  |
| 1   | C     | 57  | GLN  |
| 1   | C     | 124 | HIS  |
| 1   | C     | 133 | ASN  |
| 1   | C     | 198 | ASN  |
| 1   | C     | 421 | GLN  |
| 1   | C     | 534 | GLN  |
| 1   | D     | 124 | HIS  |
| 1   | D     | 133 | ASN  |
| 1   | D     | 229 | GLN  |
| 1   | D     | 242 | ASN  |
| 1   | D     | 421 | GLN  |
| 1   | D     | 434 | HIS  |
| 1   | D     | 534 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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 | $\# Z  > 2$ |
| 2   | FBP  | D     | 580 | -    | 18,20,20     | 1.08 | 1 (5%)      | 21,32,32    | 0.86 | 0           |
| 2   | FBP  | A     | 580 | -    | 18,20,20     | 0.91 | 1 (5%)      | 21,32,32    | 0.77 | 0           |
| 3   | PGA  | C     | 581 | 5,4  | 8,8,8        | 1.48 | 1 (12%)     | 10,11,11    | 1.05 | 0           |
| 3   | PGA  | B     | 581 | 5,4  | 8,8,8        | 1.24 | 1 (12%)     | 10,11,11    | 1.18 | 2 (20%)     |
| 2   | FBP  | B     | 580 | -    | 18,20,20     | 1.08 | 0           | 21,32,32    | 0.85 | 1 (4%)      |
| 3   | PGA  | A     | 581 | 5,4  | 8,8,8        | 1.30 | 1 (12%)     | 10,11,11    | 1.14 | 0           |
| 2   | FBP  | C     | 580 | -    | 18,20,20     | 1.09 | 1 (5%)      | 21,32,32    | 0.90 | 1 (4%)      |
| 3   | PGA  | D     | 581 | 5,4  | 8,8,8        | 1.18 | 1 (12%)     | 10,11,11    | 1.09 | 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   | FBP  | D     | 580 | -    | -       | 5/13/32/32 | 0/1/1/1 |
| 2   | FBP  | A     | 580 | -    | -       | 5/13/32/32 | 0/1/1/1 |
| 3   | PGA  | C     | 581 | 5,4  | -       | 3/6/6/6    | -       |
| 3   | PGA  | B     | 581 | 5,4  | -       | 4/6/6/6    | -       |
| 2   | FBP  | B     | 580 | -    | -       | 5/13/32/32 | 0/1/1/1 |
| 3   | PGA  | A     | 581 | 5,4  | -       | 3/6/6/6    | -       |
| 2   | FBP  | C     | 580 | -    | -       | 5/13/32/32 | 0/1/1/1 |
| 3   | PGA  | D     | 581 | 5,4  | -       | 3/6/6/6    | -       |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | C     | 581 | PGA  | O1P-C2 | -3.10 | 1.40        | 1.43     |
| 3   | A     | 581 | PGA  | O1P-C2 | -2.88 | 1.40        | 1.43     |
| 3   | D     | 581 | PGA  | O1P-C2 | -2.47 | 1.40        | 1.43     |
| 3   | B     | 581 | PGA  | O1P-C2 | -2.37 | 1.41        | 1.43     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2   | C     | 580 | FBP  | O2-C2 | 2.25 | 1.44        | 1.40     |
| 2   | A     | 580 | FBP  | O2-C2 | 2.04 | 1.44        | 1.40     |
| 2   | D     | 580 | FBP  | O2-C2 | 2.02 | 1.44        | 1.40     |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | B     | 580 | FBP  | O2P-P1-O1 | 2.36  | 112.81      | 106.67   |
| 2   | C     | 580 | FBP  | O2P-P1-O1 | 2.35  | 112.80      | 106.67   |
| 3   | B     | 581 | PGA  | O3P-P-O1P | 2.27  | 112.60      | 106.67   |
| 3   | B     | 581 | PGA  | O2-C1-O1  | -2.18 | 117.72      | 123.33   |

There are no chirality outliers.

All (33) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 2   | A     | 580 | FBP  | C6-O6-P2-O5P |
| 2   | A     | 580 | FBP  | C6-O6-P2-O6P |
| 2   | B     | 580 | FBP  | C6-O6-P2-O4P |
| 2   | B     | 580 | FBP  | C6-O6-P2-O5P |
| 2   | C     | 580 | FBP  | C6-O6-P2-O4P |
| 2   | C     | 580 | FBP  | C6-O6-P2-O5P |
| 2   | D     | 580 | FBP  | C6-O6-P2-O5P |
| 2   | D     | 580 | FBP  | C6-O6-P2-O6P |
| 3   | A     | 581 | PGA  | C2-O1P-P-O3P |
| 3   | A     | 581 | PGA  | C2-O1P-P-O4P |
| 3   | B     | 581 | PGA  | C2-O1P-P-O3P |
| 3   | B     | 581 | PGA  | C2-O1P-P-O4P |
| 3   | C     | 581 | PGA  | C2-O1P-P-O3P |
| 3   | C     | 581 | PGA  | C2-O1P-P-O4P |
| 3   | D     | 581 | PGA  | C2-O1P-P-O3P |
| 3   | D     | 581 | PGA  | C2-O1P-P-O4P |
| 2   | A     | 580 | FBP  | O5-C5-C6-O6  |
| 2   | B     | 580 | FBP  | C4-C5-C6-O6  |
| 2   | C     | 580 | FBP  | C4-C5-C6-O6  |
| 2   | D     | 580 | FBP  | O5-C5-C6-O6  |
| 2   | A     | 580 | FBP  | C4-C5-C6-O6  |
| 2   | B     | 580 | FBP  | O5-C5-C6-O6  |
| 2   | D     | 580 | FBP  | C4-C5-C6-O6  |
| 2   | C     | 580 | FBP  | O5-C5-C6-O6  |
| 2   | A     | 580 | FBP  | C6-O6-P2-O4P |
| 2   | D     | 580 | FBP  | C6-O6-P2-O4P |

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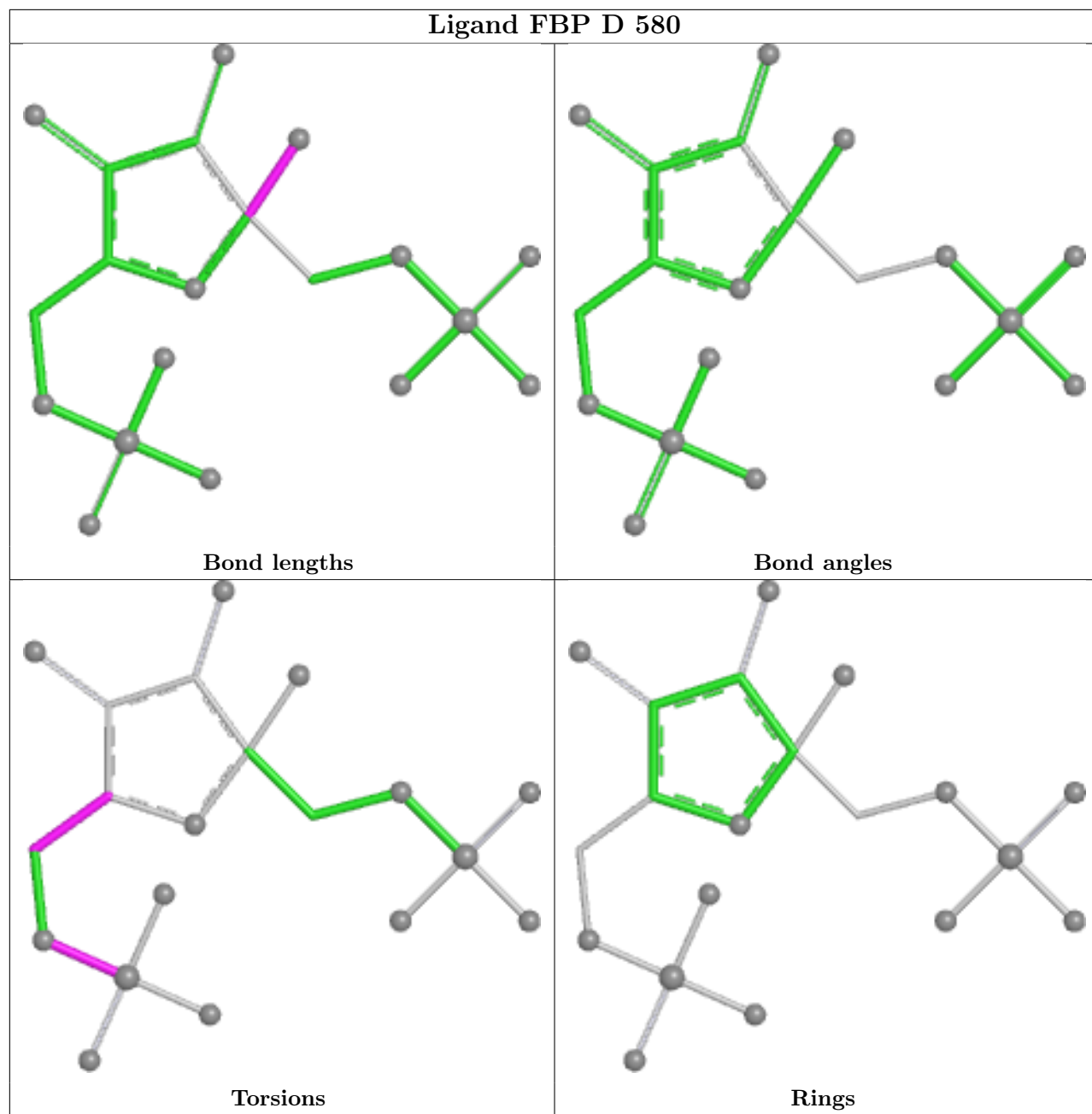
| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 3   | A     | 581 | PGA  | C2-O1P-P-O2P |
| 3   | B     | 581 | PGA  | C2-O1P-P-O2P |
| 3   | C     | 581 | PGA  | C2-O1P-P-O2P |
| 3   | D     | 581 | PGA  | C2-O1P-P-O2P |
| 2   | B     | 580 | FBP  | C6-O6-P2-O6P |
| 2   | C     | 580 | FBP  | C6-O6-P2-O6P |
| 3   | B     | 581 | PGA  | C1-C2-O1P-P  |

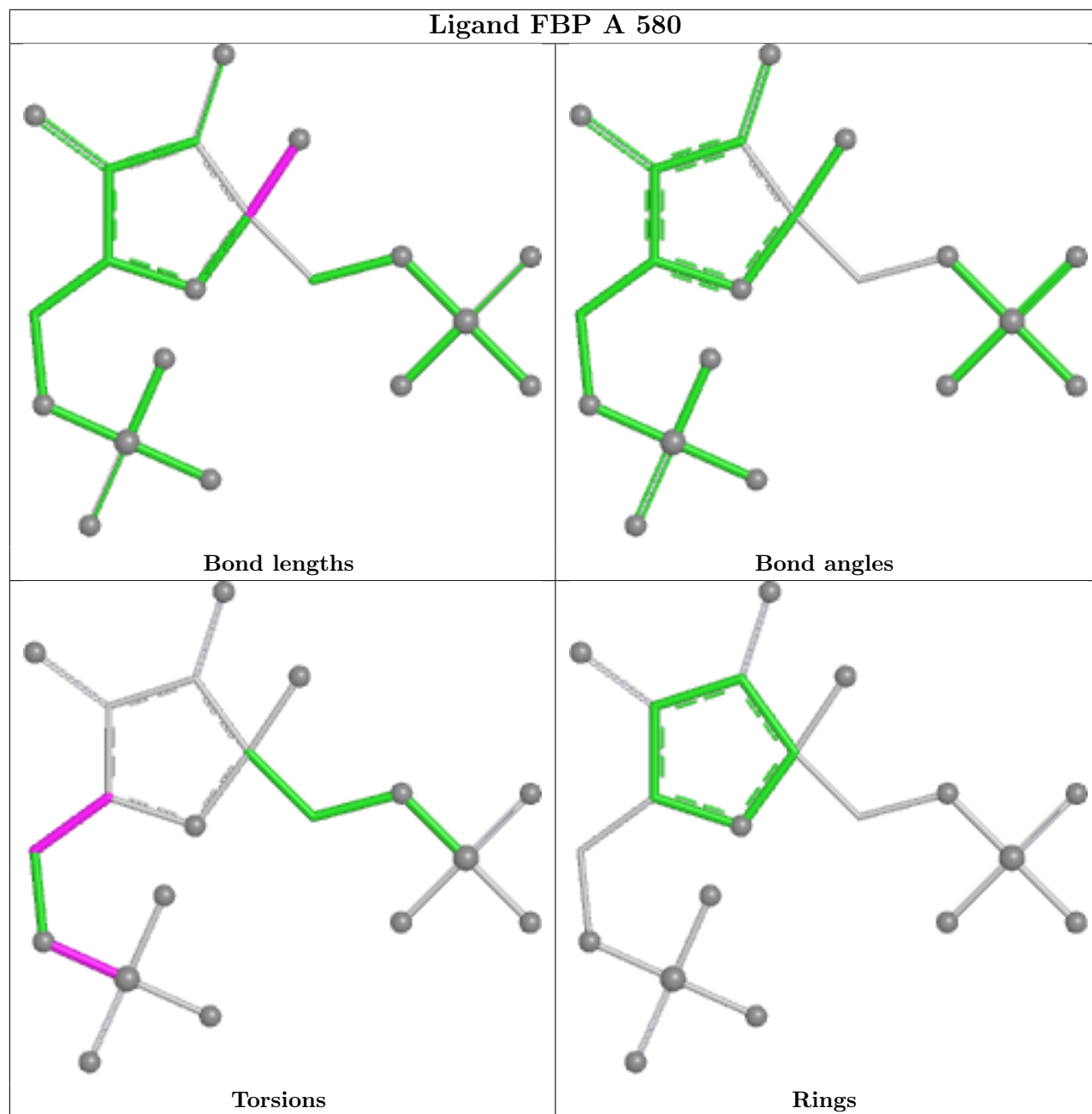
There are no ring outliers.

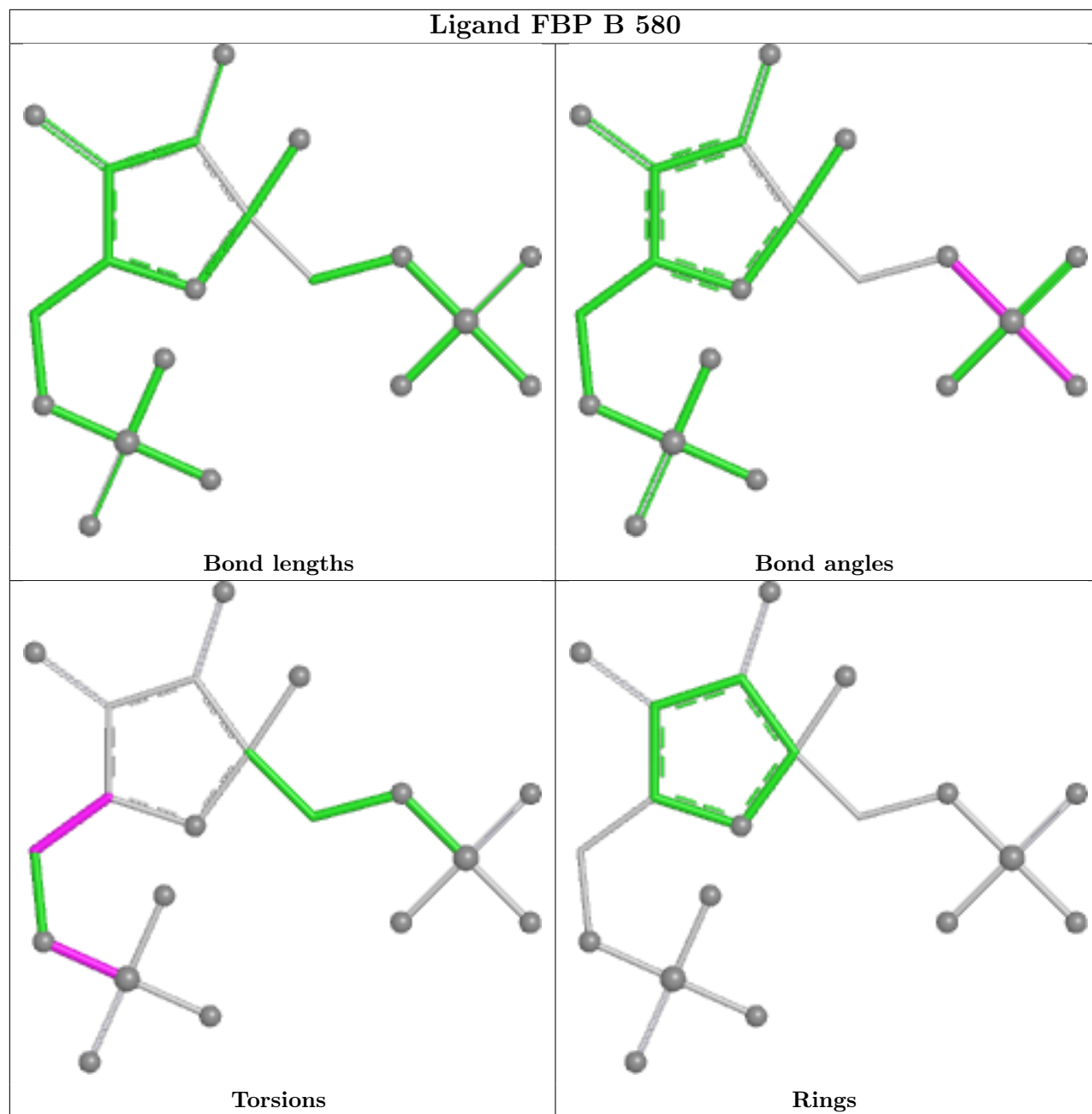
5 monomers are involved in 6 short contacts:

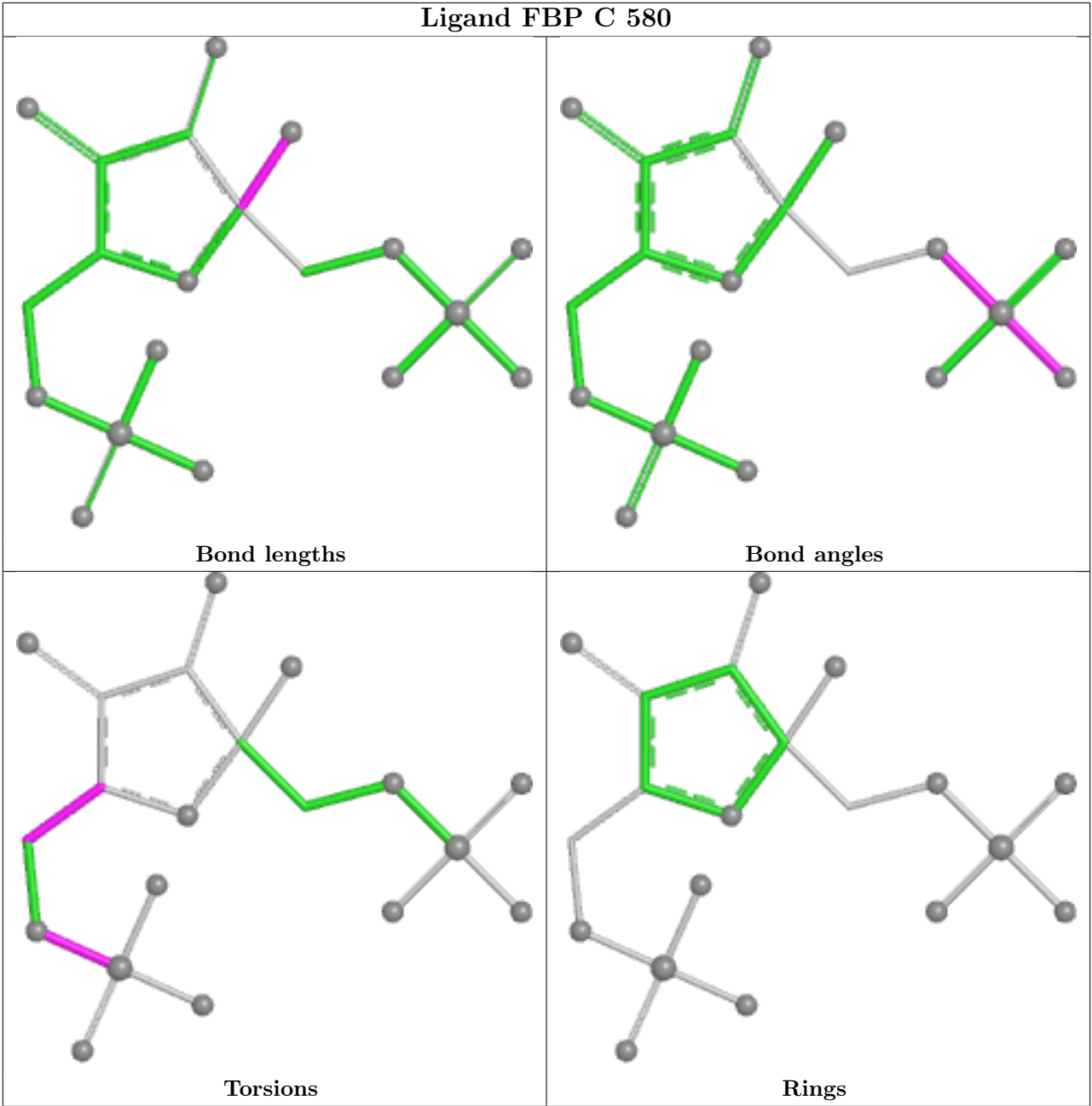
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | D     | 580 | FBP  | 2       | 0            |
| 2   | A     | 580 | FBP  | 1       | 0            |
| 2   | B     | 580 | FBP  | 1       | 0            |
| 3   | A     | 581 | PGA  | 1       | 0            |
| 3   | D     | 581 | PGA  | 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.









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1   | D     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | D     | 171:PRO   | C      | 172:GLU   | N      | 1.95         |

## 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     | 517/528 (97%)   | 0.94   | 62 (11%) 9 7  | 9, 12, 23, 32         | 0     |
| 1   | B     | 491/528 (92%)   | 1.01   | 71 (14%) 6 5  | 10, 12, 22, 32        | 0     |
| 1   | C     | 517/528 (97%)   | 0.75   | 38 (7%) 20 20 | 10, 12, 23, 32        | 0     |
| 1   | D     | 511/528 (96%)   | 1.06   | 63 (12%) 8 6  | 10, 12, 22, 32        | 0     |
| All | All   | 2036/2112 (96%) | 0.94   | 234 (11%) 9 8 | 9, 12, 22, 32         | 0     |

All (234) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 129 | GLU  | 7.3  |
| 1   | D     | 232 | GLY  | 7.1  |
| 1   | D     | 231 | ILE  | 6.8  |
| 1   | B     | 208 | VAL  | 6.3  |
| 1   | B     | 165 | GLY  | 6.0  |
| 1   | B     | 180 | GLY  | 5.9  |
| 1   | A     | 119 | PHE  | 5.7  |
| 1   | D     | 98  | SER  | 5.6  |
| 1   | A     | 122 | GLY  | 5.5  |
| 1   | D     | 173 | SER  | 5.3  |
| 1   | D     | 122 | GLY  | 5.3  |
| 1   | D     | 123 | SER  | 5.1  |
| 1   | B     | 142 | ALA  | 4.8  |
| 1   | C     | 247 | GLY  | 4.8  |
| 1   | D     | 126 | TYR  | 4.6  |
| 1   | B     | 143 | GLY  | 4.5  |
| 1   | C     | 227 | VAL  | 4.5  |
| 1   | B     | 200 | VAL  | 4.5  |
| 1   | A     | 103 | ARG  | 4.4  |
| 1   | A     | 123 | SER  | 4.4  |
| 1   | D     | 182 | GLN  | 4.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 95  | GLY  | 4.3  |
| 1   | A     | 279 | GLY  | 4.2  |
| 1   | B     | 238 | THR  | 4.1  |
| 1   | B     | 213 | VAL  | 4.1  |
| 1   | B     | 214 | GLY  | 4.0  |
| 1   | B     | 181 | SER  | 4.0  |
| 1   | D     | 94  | ILE  | 4.0  |
| 1   | A     | 126 | TYR  | 4.0  |
| 1   | D     | 259 | VAL  | 4.0  |
| 1   | B     | 305 | GLY  | 3.9  |
| 1   | B     | 527 | ASP  | 3.9  |
| 1   | A     | 256 | GLY  | 3.8  |
| 1   | C     | 167 | LEU  | 3.8  |
| 1   | D     | 130 | SER  | 3.8  |
| 1   | D     | 185 | VAL  | 3.8  |
| 1   | B     | 258 | GLN  | 3.7  |
| 1   | B     | 209 | ARG  | 3.7  |
| 1   | B     | 161 | GLU  | 3.6  |
| 1   | B     | 249 | ARG  | 3.6  |
| 1   | B     | 201 | TRP  | 3.6  |
| 1   | B     | 215 | GLY  | 3.6  |
| 1   | D     | 238 | THR  | 3.5  |
| 1   | C     | 182 | GLN  | 3.5  |
| 1   | A     | 280 | VAL  | 3.5  |
| 1   | B     | 226 | LEU  | 3.5  |
| 1   | B     | 227 | VAL  | 3.5  |
| 1   | B     | 198 | ASN  | 3.5  |
| 1   | C     | 399 | ALA  | 3.4  |
| 1   | D     | 184 | LEU  | 3.4  |
| 1   | B     | 260 | ASP  | 3.4  |
| 1   | B     | 217 | ILE  | 3.4  |
| 1   | C     | 199 | THR  | 3.4  |
| 1   | A     | 125 | GLU  | 3.4  |
| 1   | D     | 304 | GLU  | 3.4  |
| 1   | B     | 219 | ILE  | 3.3  |
| 1   | D     | 271 | ASP  | 3.3  |
| 1   | D     | 119 | PHE  | 3.3  |
| 1   | A     | 421 | GLN  | 3.2  |
| 1   | D     | 120 | SER  | 3.2  |
| 1   | D     | 248 | SER  | 3.2  |
| 1   | A     | 141 | PHE  | 3.2  |
| 1   | B     | 239 | GLN  | 3.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 263 | GLY  | 3.2  |
| 1   | A     | 523 | ALA  | 3.2  |
| 1   | A     | 120 | SER  | 3.2  |
| 1   | D     | 107 | MET  | 3.2  |
| 1   | A     | 409 | ALA  | 3.1  |
| 1   | C     | 263 | GLY  | 3.1  |
| 1   | D     | 301 | LEU  | 3.1  |
| 1   | A     | 414 | PRO  | 3.1  |
| 1   | C     | 169 | GLY  | 3.1  |
| 1   | D     | 209 | ARG  | 3.0  |
| 1   | C     | 208 | VAL  | 3.0  |
| 1   | A     | 133 | ASN  | 3.0  |
| 1   | C     | 231 | ILE  | 3.0  |
| 1   | B     | 262 | PRO  | 3.0  |
| 1   | B     | 182 | GLN  | 3.0  |
| 1   | C     | 168 | GLN  | 3.0  |
| 1   | A     | 108 | ILE  | 3.0  |
| 1   | A     | 497 | THR  | 3.0  |
| 1   | B     | 177 | LEU  | 3.0  |
| 1   | B     | 185 | VAL  | 3.0  |
| 1   | D     | 183 | VAL  | 3.0  |
| 1   | D     | 134 | VAL  | 2.9  |
| 1   | A     | 503 | ALA  | 2.9  |
| 1   | C     | 491 | ALA  | 2.9  |
| 1   | D     | 165 | GLY  | 2.9  |
| 1   | B     | 228 | VAL  | 2.9  |
| 1   | A     | 557 | GLY  | 2.9  |
| 1   | C     | 367 | VAL  | 2.9  |
| 1   | B     | 164 | THR  | 2.8  |
| 1   | B     | 243 | GLY  | 2.8  |
| 1   | B     | 244 | GLY  | 2.8  |
| 1   | D     | 95  | GLY  | 2.8  |
| 1   | B     | 65  | MET  | 2.8  |
| 1   | B     | 564 | TYR  | 2.8  |
| 1   | D     | 176 | GLU  | 2.8  |
| 1   | C     | 195 | GLY  | 2.8  |
| 1   | D     | 278 | HIS  | 2.8  |
| 1   | A     | 215 | GLY  | 2.7  |
| 1   | A     | 275 | GLY  | 2.7  |
| 1   | B     | 221 | ASP  | 2.7  |
| 1   | C     | 260 | ASP  | 2.7  |
| 1   | C     | 336 | ALA  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 547 | ARG  | 2.7  |
| 1   | D     | 112 | MET  | 2.7  |
| 1   | B     | 146 | LEU  | 2.7  |
| 1   | D     | 104 | LEU  | 2.7  |
| 1   | C     | 122 | GLY  | 2.7  |
| 1   | B     | 322 | ARG  | 2.7  |
| 1   | A     | 152 | ALA  | 2.7  |
| 1   | D     | 410 | LYS  | 2.7  |
| 1   | A     | 311 | ILE  | 2.7  |
| 1   | D     | 193 | THR  | 2.7  |
| 1   | A     | 130 | SER  | 2.6  |
| 1   | B     | 259 | VAL  | 2.6  |
| 1   | D     | 187 | VAL  | 2.6  |
| 1   | A     | 129 | GLU  | 2.6  |
| 1   | B     | 205 | PRO  | 2.6  |
| 1   | A     | 92  | ALA  | 2.6  |
| 1   | D     | 239 | GLN  | 2.6  |
| 1   | B     | 266 | GLU  | 2.6  |
| 1   | C     | 256 | GLY  | 2.6  |
| 1   | B     | 382 | ARG  | 2.5  |
| 1   | B     | 242 | ASN  | 2.5  |
| 1   | D     | 233 | PRO  | 2.5  |
| 1   | A     | 101 | VAL  | 2.5  |
| 1   | A     | 413 | PHE  | 2.5  |
| 1   | D     | 256 | GLY  | 2.5  |
| 1   | B     | 210 | VAL  | 2.5  |
| 1   | D     | 101 | VAL  | 2.5  |
| 1   | C     | 238 | THR  | 2.4  |
| 1   | A     | 160 | PRO  | 2.4  |
| 1   | A     | 209 | ARG  | 2.4  |
| 1   | C     | 186 | THR  | 2.4  |
| 1   | B     | 144 | SER  | 2.4  |
| 1   | C     | 129 | GLU  | 2.4  |
| 1   | B     | 175 | VAL  | 2.4  |
| 1   | D     | 245 | VAL  | 2.4  |
| 1   | C     | 229 | GLN  | 2.4  |
| 1   | C     | 184 | LEU  | 2.3  |
| 1   | D     | 306 | HIS  | 2.3  |
| 1   | A     | 266 | GLU  | 2.3  |
| 1   | A     | 230 | LYS  | 2.3  |
| 1   | B     | 212 | PRO  | 2.3  |
| 1   | A     | 175 | VAL  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 237 | VAL  | 2.3  |
| 1   | B     | 245 | VAL  | 2.3  |
| 1   | D     | 178 | VAL  | 2.3  |
| 1   | B     | 125 | GLU  | 2.3  |
| 1   | D     | 158 | LYS  | 2.3  |
| 1   | C     | 237 | VAL  | 2.3  |
| 1   | A     | 392 | ALA  | 2.3  |
| 1   | B     | 261 | LEU  | 2.3  |
| 1   | D     | 542 | LEU  | 2.3  |
| 1   | A     | 283 | VAL  | 2.3  |
| 1   | A     | 506 | VAL  | 2.3  |
| 1   | D     | 272 | LEU  | 2.3  |
| 1   | A     | 154 | ALA  | 2.3  |
| 1   | A     | 357 | ILE  | 2.3  |
| 1   | A     | 379 | THR  | 2.3  |
| 1   | B     | 241 | GLU  | 2.3  |
| 1   | A     | 98  | SER  | 2.3  |
| 1   | C     | 214 | GLY  | 2.3  |
| 1   | C     | 259 | VAL  | 2.3  |
| 1   | B     | 63  | ALA  | 2.2  |
| 1   | C     | 126 | TYR  | 2.2  |
| 1   | D     | 482 | GLN  | 2.2  |
| 1   | A     | 254 | LEU  | 2.2  |
| 1   | A     | 231 | ILE  | 2.2  |
| 1   | B     | 207 | ILE  | 2.2  |
| 1   | B     | 524 | ILE  | 2.2  |
| 1   | C     | 274 | PHE  | 2.2  |
| 1   | C     | 218 | TYR  | 2.2  |
| 1   | C     | 490 | ARG  | 2.2  |
| 1   | A     | 542 | LEU  | 2.2  |
| 1   | D     | 61  | LEU  | 2.2  |
| 1   | A     | 208 | VAL  | 2.2  |
| 1   | C     | 242 | ASN  | 2.2  |
| 1   | D     | 549 | GLY  | 2.2  |
| 1   | B     | 248 | SER  | 2.2  |
| 1   | D     | 138 | VAL  | 2.2  |
| 1   | A     | 121 | HIS  | 2.2  |
| 1   | A     | 84  | ALA  | 2.2  |
| 1   | D     | 263 | GLY  | 2.2  |
| 1   | A     | 271 | ASP  | 2.2  |
| 1   | D     | 220 | ASP  | 2.2  |
| 1   | D     | 227 | VAL  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 535 | PHE  | 2.2  |
| 1   | B     | 88  | THR  | 2.1  |
| 1   | B     | 253 | ASN  | 2.1  |
| 1   | C     | 258 | GLN  | 2.1  |
| 1   | D     | 133 | ASN  | 2.1  |
| 1   | B     | 539 | SER  | 2.1  |
| 1   | C     | 333 | ILE  | 2.1  |
| 1   | D     | 240 | VAL  | 2.1  |
| 1   | A     | 257 | ALA  | 2.1  |
| 1   | B     | 64  | ALA  | 2.1  |
| 1   | D     | 197 | ALA  | 2.1  |
| 1   | A     | 371 | THR  | 2.1  |
| 1   | D     | 180 | GLY  | 2.1  |
| 1   | A     | 142 | ALA  | 2.1  |
| 1   | B     | 386 | ALA  | 2.1  |
| 1   | A     | 416 | GLU  | 2.1  |
| 1   | B     | 518 | ARG  | 2.1  |
| 1   | D     | 273 | ARG  | 2.1  |
| 1   | A     | 88  | THR  | 2.1  |
| 1   | B     | 303 | PRO  | 2.1  |
| 1   | C     | 267 | GLN  | 2.1  |
| 1   | B     | 223 | LEU  | 2.1  |
| 1   | D     | 236 | LEU  | 2.1  |
| 1   | A     | 259 | VAL  | 2.1  |
| 1   | B     | 89  | SER  | 2.1  |
| 1   | B     | 463 | ALA  | 2.1  |
| 1   | A     | 211 | VAL  | 2.1  |
| 1   | A     | 260 | ASP  | 2.0  |
| 1   | D     | 194 | ARG  | 2.0  |
| 1   | A     | 137 | ALA  | 2.0  |
| 1   | D     | 394 | ALA  | 2.0  |
| 1   | D     | 199 | THR  | 2.0  |
| 1   | D     | 264 | LEU  | 2.0  |
| 1   | C     | 306 | HIS  | 2.0  |
| 1   | B     | 91  | ILE  | 2.0  |
| 1   | C     | 458 | GLY  | 2.0  |
| 1   | A     | 289 | ARG  | 2.0  |
| 1   | C     | 216 | ARG  | 2.0  |
| 1   | D     | 106 | GLU  | 2.0  |
| 1   | B     | 132 | ALA  | 2.0  |
| 1   | C     | 558 | TRP  | 2.0  |
| 1   | A     | 358 | GLY  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 275 | GLY  | 2.0  |
| 1   | B     | 342 | ILE  | 2.0  |
| 1   | D     | 322 | ARG  | 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](#)

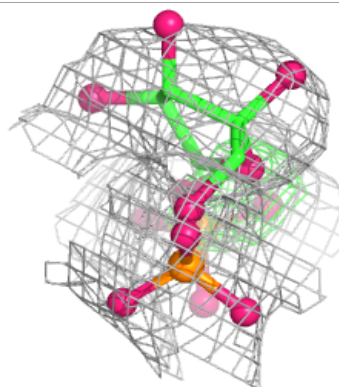
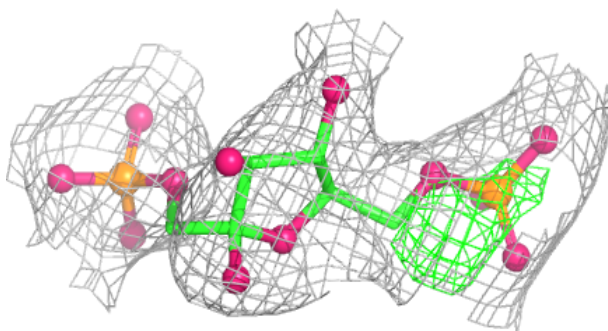
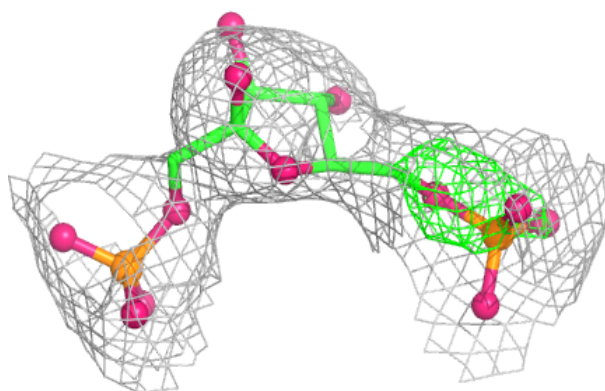
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 4   | K    | A     | 582 | 1/1   | 0.54 | 0.20 | 52,52,52,52                | 0     |
| 3   | PGA  | A     | 581 | 9/9   | 0.75 | 0.20 | 85,86,86,86                | 0     |
| 2   | FBP  | A     | 580 | 20/20 | 0.78 | 0.19 | 56,61,63,63                | 0     |
| 3   | PGA  | D     | 581 | 9/9   | 0.79 | 0.14 | 85,86,86,86                | 0     |
| 3   | PGA  | C     | 581 | 9/9   | 0.79 | 0.20 | 85,86,86,86                | 0     |
| 3   | PGA  | B     | 581 | 9/9   | 0.80 | 0.20 | 85,86,86,86                | 0     |
| 4   | K    | C     | 590 | 1/1   | 0.80 | 0.12 | 41,41,41,41                | 0     |
| 4   | K    | D     | 594 | 1/1   | 0.80 | 0.08 | 77,77,77,77                | 0     |
| 2   | FBP  | C     | 580 | 20/20 | 0.81 | 0.18 | 56,61,63,63                | 0     |
| 2   | FBP  | B     | 580 | 20/20 | 0.83 | 0.22 | 56,61,63,63                | 0     |
| 2   | FBP  | D     | 580 | 20/20 | 0.86 | 0.21 | 56,61,63,63                | 0     |
| 4   | K    | B     | 586 | 1/1   | 0.91 | 0.10 | 33,33,33,33                | 0     |
| 5   | MN   | A     | 583 | 1/1   | 0.96 | 0.05 | 64,64,64,64                | 0     |
| 5   | MN   | D     | 595 | 1/1   | 0.98 | 0.03 | 38,38,38,38                | 0     |
| 5   | MN   | B     | 587 | 1/1   | 0.99 | 0.08 | 35,35,35,35                | 0     |
| 5   | MN   | C     | 591 | 1/1   | 1.00 | 0.05 | 37,37,37,37                | 0     |

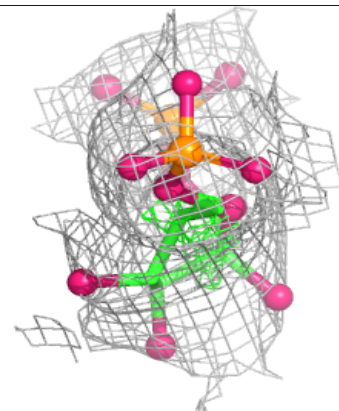
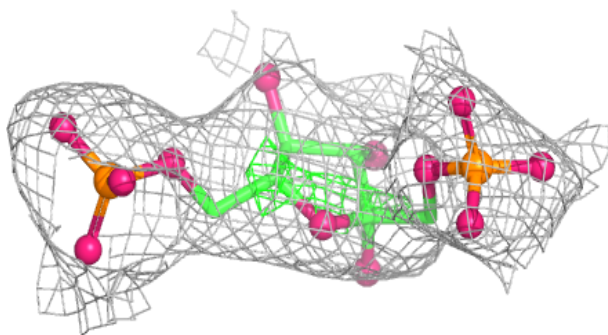
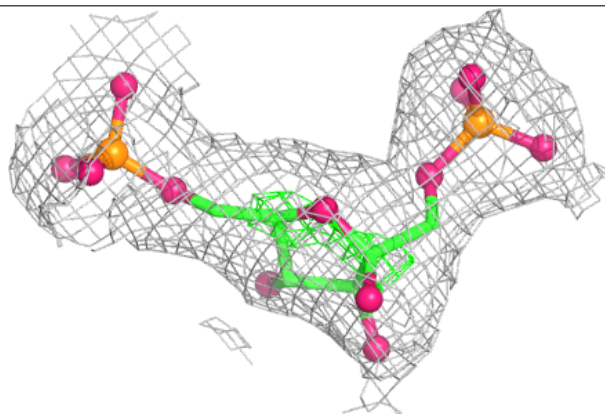
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around FBP A 580:**

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

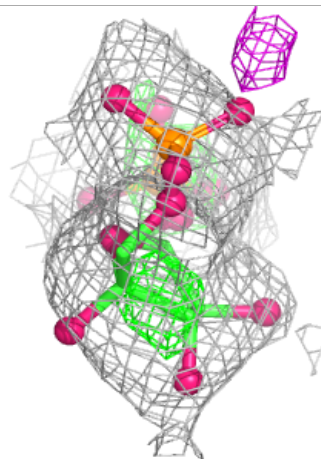
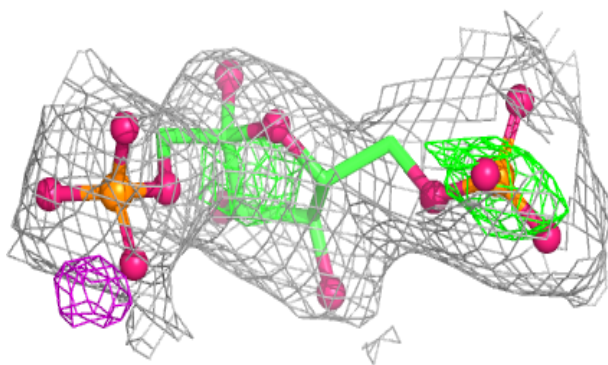
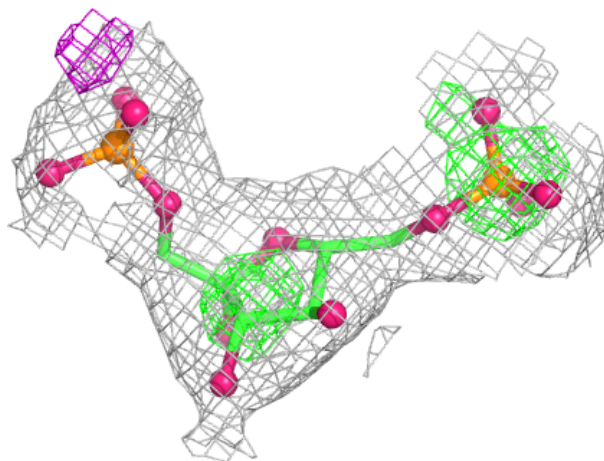
**Electron density around FBP C 580:**

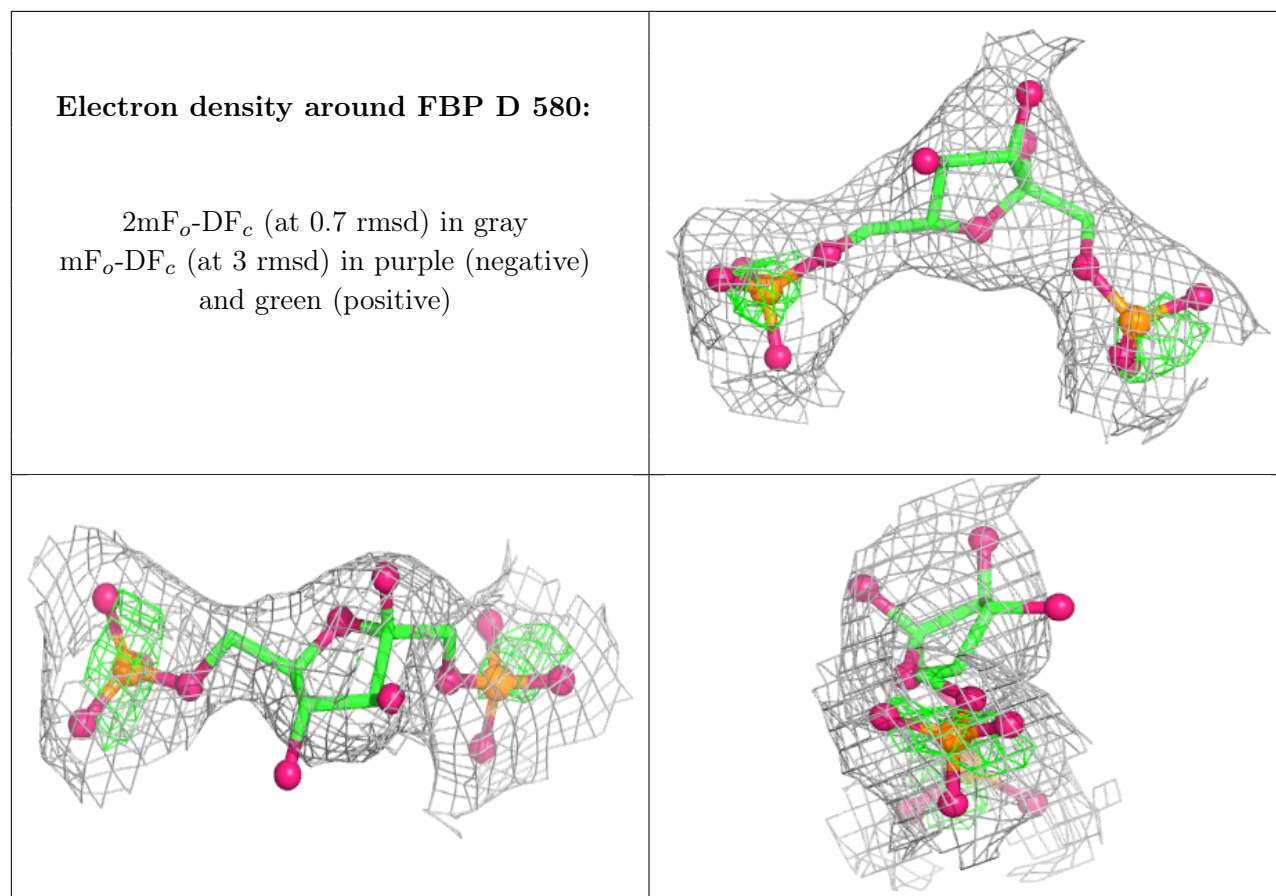
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FBP B 580:**

$2mF_o-DF_c$  (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.