



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 05:10 AM GMT

PDB ID : 3IKL  
Title : Crystal structure of Pol gB delta-I4.  
Authors : Lee, Y.S.; Kennedy, W.D.; Yin, Y.W.  
Deposited on : 2009-08-06  
Resolution : 3.10 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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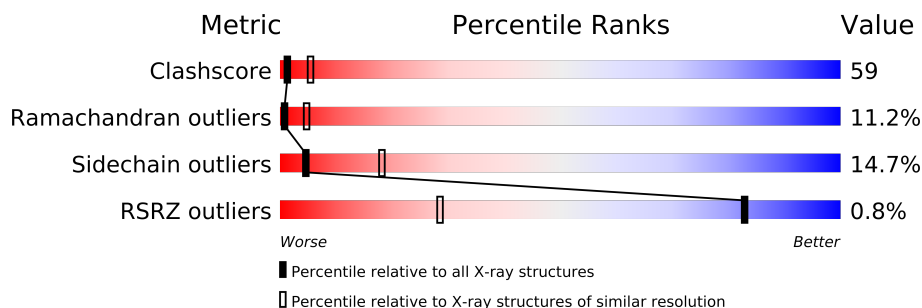
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

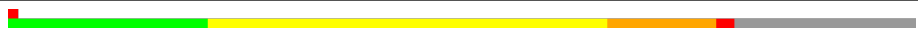
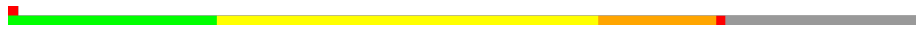
The reported resolution of this entry is 3.10 Å.

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)) |
|-----------------------|-----------------------------|---|
| Clashscore            | 79885                       | 1078 (3.16-3.04)                                      |
| Ramachandran outliers | 78287                       | 1044 (3.16-3.04)                                      |
| Sidechain outliers    | 78261                       | 1044 (3.16-3.04)                                      |
| RSRZ outliers         | 66119                       | 1008 (3.18-3.02)                                      |

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | A     | 459    |  |
| 1   | B     | 459    |  |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5866 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA polymerase subunit gamma-2, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 364      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2931  | 1877 | 515 | 523 | 16 |         |         |       |
| 1   | B     | 364      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2935  | 1880 | 517 | 522 | 16 |         |         |       |

There are 16 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 180     | GLY      | -      | linker         | UNP Q9UHN1 |
| A     | 181     | GLY      | -      | linker         | UNP Q9UHN1 |
| A     | 486     | HIS      | -      | expression tag | UNP Q9UHN1 |
| A     | 487     | HIS      | -      | expression tag | UNP Q9UHN1 |
| A     | 488     | HIS      | -      | expression tag | UNP Q9UHN1 |
| A     | 489     | HIS      | -      | expression tag | UNP Q9UHN1 |
| A     | 490     | HIS      | -      | expression tag | UNP Q9UHN1 |
| A     | 491     | HIS      | -      | expression tag | UNP Q9UHN1 |
| B     | 180     | GLY      | -      | linker         | UNP Q9UHN1 |
| B     | 181     | GLY      | -      | linker         | UNP Q9UHN1 |
| B     | 486     | HIS      | -      | expression tag | UNP Q9UHN1 |
| B     | 487     | HIS      | -      | expression tag | UNP Q9UHN1 |
| B     | 488     | HIS      | -      | expression tag | UNP Q9UHN1 |
| B     | 489     | HIS      | -      | expression tag | UNP Q9UHN1 |
| B     | 490     | HIS      | -      | expression tag | UNP Q9UHN1 |
| B     | 491     | HIS      | -      | expression tag | UNP Q9UHN1 |





## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 41  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 64.43Å 64.43Å 260.70Å<br>90.00° 90.00° 90.00°               | Depositor        |
| Resolution (Å)  | 45.82 – 3.10<br>45.82 – 3.10                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 74.6 (45.82-3.10)<br>74.7 (45.82-3.10)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.80 (at 3.12Å)   | Xtriage          |
| Refinement program  | CNS 1.2   | Depositor        |
| R, $R_{free}$   | 0.257 , 0.294<br>0.260 , (Not available)                    | Depositor<br>DCC |
| $R_{free}$ test set   | No test flags present.                                      | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 61.0  | Xtriage          |
| Anisotropy  | 0.568   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.29 , 12.0   | EDS              |
| Estimated twinning fraction   | 0.448 for h,-k,-l   | Xtriage          |
| L-test for twinning   | $\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$ | Xtriage          |
| Outliers  | 0 of 16475 reflections                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.88  | EDS              |
| Total number of atoms   | 5866  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 76.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |             | Bond angles |               |
|-----|-------|--------------|-------------|-------------|---------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$   |
| 1   | A     | 0.46         | 0/3006      | 0.78        | 1/4067 (0.0%) |
| 1   | B     | 0.46         | 0/3011      | 0.76        | 1/4074 (0.0%) |
| All | All   | 0.46         | 0/6017      | 0.77        | 2/8141 (0.0%) |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 124 | GLN  | N-CA-C   | -6.04 | 94.69       | 111.00   |
| 1   | B     | 455 | LEU  | CA-CB-CG | 5.72  | 128.46      | 115.30   |

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2931  | 0        | 2915     | 376     | 0            |
| 1   | B     | 2935  | 0        | 2917     | 326     | 0            |
| All | All   | 5866  | 0        | 5832     | 691     | 0            |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 59.

All (691) close contacts within the same asymmetric unit are listed below.

| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:231:ILE:H    | 1:A:231:ILE:HD12 | 1.16        | 1.10     |
| 1:B:392:THR:HG22 | 1:B:393:LEU:H    | 1.24        | 1.03     |
| 1:A:280:ASP:H    | 1:A:284:ARG:HA   | 1.23        | 1.03     |
| 1:A:448:LEU:HD23 | 1:A:448:LEU:H    | 1.23        | 1.02     |
| 1:A:450:ASN:HD21 | 1:A:452:LEU:HB2  | 1.24        | 1.01     |
| 1:B:303:LEU:HG   | 1:B:338:VAL:HG22 | 1.43        | 0.99     |
| 1:B:454:HIS:HE1  | 1:B:465:MET:HG2  | 1.27        | 0.99     |
| 1:A:88:ARG:HA    | 1:A:91:LEU:HD12  | 1.44        | 0.96     |
| 1:A:441:VAL:HG12 | 1:A:455:LEU:HB3  | 1.43        | 0.95     |
| 1:B:395:LEU:O    | 1:B:398:VAL:HG12 | 1.66        | 0.94     |
| 1:A:320:SER:HA   | 1:A:323:HIS:NE2  | 1.81        | 0.94     |
| 1:A:197:LEU:HD11 | 1:A:202:LYS:HG3  | 1.48        | 0.94     |
| 1:B:438:LEU:O    | 1:B:458:ARG:HB2  | 1.68        | 0.93     |
| 1:A:186:LEU:HD11 | 1:A:306:LEU:HD11 | 1.51        | 0.91     |
| 1:A:391:PRO:HD2  | 1:A:395:LEU:HD21 | 1.51        | 0.91     |
| 1:A:303:LEU:HD11 | 1:A:338:VAL:HG13 | 1.52        | 0.89     |
| 1:A:88:ARG:N     | 1:A:88:ARG:HD2   | 1.88        | 0.88     |
| 1:A:201:ASN:HD22 | 1:A:203:ARG:NH2  | 1.69        | 0.88     |
| 1:A:369:ARG:HH21 | 1:A:371:VAL:HG21 | 1.37        | 0.88     |
| 1:A:388:GLY:O    | 1:A:390:GLY:N    | 2.07        | 0.87     |
| 1:B:454:HIS:CE1  | 1:B:465:MET:HG2  | 2.10        | 0.86     |
| 1:A:431:LYS:NZ   | 1:A:431:LYS:HB2  | 1.92        | 0.85     |
| 1:A:389:ARG:HH11 | 1:A:444:THR:HG21 | 1.39        | 0.84     |
| 1:B:121:PHE:O    | 1:B:122:ARG:HG2  | 1.78        | 0.84     |
| 1:B:406:LEU:H    | 1:B:406:LEU:HD12 | 1.39        | 0.84     |
| 1:B:252:LEU:HB2  | 1:B:336:LEU:HD11 | 1.57        | 0.84     |
| 1:B:406:LEU:H    | 1:B:406:LEU:CD1  | 1.90        | 0.83     |
| 1:A:450:ASN:ND2  | 1:A:452:LEU:HB2  | 1.92        | 0.83     |
| 1:A:67:GLU:HG2   | 1:A:69:LEU:H     | 1.42        | 0.83     |
| 1:B:280:ASP:HA   | 1:B:284:ARG:HH21 | 1.43        | 0.83     |
| 1:A:393:LEU:HD23 | 1:A:397:GLN:HG3  | 1.60        | 0.83     |
| 1:A:256:LEU:HD22 | 1:A:287:ASN:ND2  | 1.94        | 0.82     |
| 1:A:421:MET:HG3  | 1:A:422:GLN:H    | 1.43        | 0.82     |
| 1:A:201:ASN:HD22 | 1:A:203:ARG:HH22 | 1.24        | 0.82     |
| 1:B:445:GLU:C    | 1:B:447:THR:H    | 1.82        | 0.82     |
| 1:A:116:THR:HA   | 1:A:120:VAL:CG2  | 2.10        | 0.82     |
| 1:A:243:THR:HG23 | 1:A:334:CYS:HB2  | 1.62        | 0.81     |
| 1:A:394:GLU:O    | 1:A:397:GLN:HB2  | 1.81        | 0.81     |
| 1:B:134:LYS:H    | 1:B:180:GLY:HA2  | 1.46        | 0.81     |
| 1:A:381:ILE:HD11 | 1:A:437:ILE:HD12 | 1.62        | 0.81     |
| 1:A:448:LEU:HD23 | 1:A:448:LEU:N    | 1.96        | 0.80     |
| 1:B:320:SER:HA   | 1:B:323:HIS:CD2  | 2.17        | 0.80     |
| 1:B:122:ARG:NH1  | 1:B:122:ARG:HB3  | 1.97        | 0.80     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:450:ASN:HD22 | 1:A:452:LEU:HD23 | 1.46        | 0.80     |
| 1:B:128:VAL:HG13 | 1:B:210:GLN:HB2  | 1.65        | 0.79     |
| 1:A:385:LEU:HD23 | 1:A:385:LEU:H    | 1.45        | 0.79     |
| 1:A:419:GLU:HG3  | 1:A:420:THR:H    | 1.49        | 0.77     |
| 1:A:231:ILE:CD1  | 1:A:231:ILE:H    | 1.96        | 0.77     |
| 1:B:301:GLU:OE2  | 1:B:340:GLY:HA3  | 1.85        | 0.77     |
| 1:B:122:ARG:HB3  | 1:B:122:ARG:HH11 | 1.48        | 0.77     |
| 1:B:445:GLU:HA   | 1:B:445:GLU:OE1  | 1.83        | 0.77     |
| 1:A:353:SER:HB3  | 1:A:374:LEU:HD23 | 1.67        | 0.77     |
| 1:B:406:LEU:HD12 | 1:B:406:LEU:N    | 1.98        | 0.77     |
| 1:B:122:ARG:O    | 1:B:124:GLN:HG3  | 1.85        | 0.77     |
| 1:A:396:ARG:HA   | 1:A:399:CYS:HB2  | 1.65        | 0.77     |
| 1:A:455:LEU:HD11 | 1:A:474:PHE:HE2  | 1.49        | 0.77     |
| 1:A:231:ILE:HD12 | 1:A:231:ILE:N    | 1.97        | 0.76     |
| 1:B:373:LYS:HE2  | 1:B:459:ASP:HA   | 1.64        | 0.76     |
| 1:A:389:ARG:NH1  | 1:A:444:THR:HG21 | 1.98        | 0.76     |
| 1:A:303:LEU:HG   | 1:A:338:VAL:HG22 | 1.66        | 0.76     |
| 1:A:421:MET:CG   | 1:A:422:GLN:H    | 1.95        | 0.76     |
| 1:B:477:LYS:HA   | 1:B:480:SER:HB3  | 1.68        | 0.75     |
| 1:B:122:ARG:HB2  | 1:B:124:GLN:NE2  | 2.00        | 0.75     |
| 1:A:389:ARG:HD2  | 1:A:444:THR:HB   | 1.69        | 0.75     |
| 1:B:384:ALA:O    | 1:B:385:LEU:HB3  | 1.86        | 0.75     |
| 1:B:392:THR:HG22 | 1:B:393:LEU:N    | 2.02        | 0.74     |
| 1:B:229:LYS:HE2  | 1:B:229:LYS:HA   | 1.70        | 0.74     |
| 1:B:280:ASP:O    | 1:B:281:GLU:HB2  | 1.87        | 0.74     |
| 1:A:131:LEU:HD21 | 1:B:97:PRO:O     | 1.88        | 0.74     |
| 1:A:69:LEU:HD13  | 1:A:354:PHE:CD2  | 2.23        | 0.74     |
| 1:A:116:THR:HG23 | 1:A:120:VAL:HG21 | 1.71        | 0.73     |
| 1:A:280:ASP:N    | 1:A:284:ARG:HA   | 2.00        | 0.73     |
| 1:B:389:ARG:HG2  | 1:B:444:THR:HB   | 1.69        | 0.73     |
| 1:A:370:LYS:O    | 1:A:371:VAL:HG12 | 1.87        | 0.72     |
| 1:B:257:ARG:HB3  | 1:B:257:ARG:NH2  | 2.04        | 0.72     |
| 1:B:128:VAL:HG22 | 1:B:129:ASP:N    | 2.05        | 0.71     |
| 1:A:441:VAL:CG1  | 1:A:455:LEU:HB3  | 2.20        | 0.71     |
| 1:A:444:THR:OG1  | 1:A:446:THR:HG22 | 1.91        | 0.71     |
| 1:B:256:LEU:HD22 | 1:B:287:ASN:ND2  | 2.06        | 0.71     |
| 1:B:134:LYS:H    | 1:B:180:GLY:CA   | 2.03        | 0.71     |
| 1:B:289:LEU:HB2  | 1:B:301:GLU:HB3  | 1.72        | 0.71     |
| 1:B:310:GLU:CD   | 1:B:310:GLU:H    | 1.94        | 0.71     |
| 1:B:257:ARG:HB3  | 1:B:257:ARG:HH21 | 1.54        | 0.71     |
| 1:B:325:ARG:HA   | 1:B:329:LYS:O    | 1.90        | 0.71     |
| 1:B:420:THR:HG23 | 1:B:421:MET:H    | 1.54        | 0.71     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:249:ASN:CG   | 1:B:250:GLN:N    | 2.44        | 0.71     |
| 1:A:303:LEU:CD1  | 1:A:338:VAL:HG13 | 2.20        | 0.71     |
| 1:A:243:THR:HG22 | 1:A:334:CYS:O    | 1.91        | 0.71     |
| 1:A:325:ARG:HG2  | 1:A:325:ARG:HH11 | 1.56        | 0.70     |
| 1:A:432:TYR:O    | 1:A:437:ILE:HG12 | 1.91        | 0.70     |
| 1:A:391:PRO:CD   | 1:A:395:LEU:HD21 | 2.21        | 0.70     |
| 1:A:116:THR:HA   | 1:A:120:VAL:HG23 | 1.73        | 0.69     |
| 1:A:133:HIS:HA   | 1:A:181:GLY:HA2  | 1.74        | 0.69     |
| 1:A:327:GLY:O    | 1:A:328:ARG:HB2  | 1.91        | 0.69     |
| 1:B:197:LEU:HD11 | 1:B:202:LYS:HA   | 1.72        | 0.69     |
| 1:A:393:LEU:O    | 1:A:397:GLN:HG2  | 1.92        | 0.69     |
| 1:A:375:HIS:ND1  | 1:A:376:PRO:HD2  | 2.07        | 0.69     |
| 1:B:291:TYR:OH   | 1:B:352:ASP:HB2  | 1.91        | 0.69     |
| 1:B:294:PRO:HD2  | 1:B:295:TRP:CZ3  | 2.28        | 0.69     |
| 1:B:91:LEU:HD13  | 1:B:96:HIS:HB3   | 1.75        | 0.69     |
| 1:A:318:ASN:ND2  | 1:A:319:VAL:H    | 1.91        | 0.69     |
| 1:B:420:THR:HG23 | 1:B:421:MET:N    | 2.08        | 0.69     |
| 1:A:262:TRP:O    | 1:A:265:LYS:HB3  | 1.93        | 0.69     |
| 1:A:231:ILE:HG22 | 1:A:232:GLY:H    | 1.59        | 0.68     |
| 1:A:421:MET:HG3  | 1:A:422:GLN:N    | 2.07        | 0.68     |
| 1:B:422:GLN:HG3  | 1:B:423:SER:N    | 2.07        | 0.68     |
| 1:A:382:LYS:HD2  | 1:A:382:LYS:N    | 2.08        | 0.68     |
| 1:A:251:TRP:O    | 1:A:254:PHE:HB3  | 1.93        | 0.68     |
| 1:B:260:LEU:HD13 | 1:B:275:SER:HB3  | 1.76        | 0.68     |
| 1:A:431:LYS:HZ2  | 1:A:431:LYS:HB2  | 1.56        | 0.68     |
| 1:A:411:ILE:HD11 | 1:A:476:ILE:CD1  | 2.23        | 0.68     |
| 1:B:416:GLY:O    | 1:B:418:LEU:N    | 2.27        | 0.68     |
| 1:A:468:ILE:HD12 | 1:A:469:SER:N    | 2.09        | 0.68     |
| 1:B:128:VAL:CG1  | 1:B:210:GLN:HB2  | 2.23        | 0.67     |
| 1:B:415:PRO:HB2  | 1:B:418:LEU:HD13 | 1.76        | 0.67     |
| 1:A:217:PRO:HB2  | 1:A:229:LYS:HD3  | 1.76        | 0.67     |
| 1:A:460:THR:O    | 1:A:462:MET:N    | 2.27        | 0.67     |
| 1:B:91:LEU:N     | 1:B:91:LEU:HD22  | 2.09        | 0.67     |
| 1:B:112:ALA:O    | 1:B:116:THR:HG23 | 1.93        | 0.67     |
| 1:B:460:THR:HB   | 1:B:462:MET:HG2  | 1.77        | 0.67     |
| 1:A:393:LEU:HD23 | 1:A:397:GLN:CG   | 2.25        | 0.67     |
| 1:B:131:LEU:O    | 1:B:182:ARG:HD3  | 1.94        | 0.67     |
| 1:A:92:LEU:HD22  | 1:A:344:ARG:CZ   | 2.25        | 0.66     |
| 1:B:405:GLU:O    | 1:B:408:GLU:HB2  | 1.96        | 0.66     |
| 1:A:450:ASN:ND2  | 1:A:452:LEU:HD23 | 2.11        | 0.66     |
| 1:A:146:ARG:HH11 | 1:A:146:ARG:HA   | 1.60        | 0.66     |
| 1:A:263:TRP:CZ3  | 1:A:300:ILE:HD12 | 2.29        | 0.66     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:420:THR:OG1  | 1:A:421:MET:N    | 2.29        | 0.66     |
| 1:B:193:TYR:CZ   | 1:B:333:PRO:HG3  | 2.31        | 0.66     |
| 1:B:402:LEU:O    | 1:B:406:LEU:HD13 | 1.96        | 0.66     |
| 1:A:453:ILE:HD12 | 1:A:454:HIS:N    | 2.09        | 0.65     |
| 1:A:477:LYS:HA   | 1:A:480:SER:HB3  | 1.77        | 0.65     |
| 1:A:383:VAL:HG22 | 1:A:384:ALA:N    | 2.12        | 0.65     |
| 1:B:445:GLU:O    | 1:B:447:THR:N    | 2.30        | 0.65     |
| 1:B:325:ARG:HH11 | 1:B:325:ARG:HG2  | 1.61        | 0.65     |
| 1:A:88:ARG:N     | 1:A:88:ARG:CD    | 2.53        | 0.65     |
| 1:B:91:LEU:H     | 1:B:91:LEU:HD22  | 1.61        | 0.65     |
| 1:B:88:ARG:HD2   | 1:B:89:ASP:N     | 2.12        | 0.64     |
| 1:A:123:GLU:O    | 1:A:124:GLN:HG3  | 1.97        | 0.64     |
| 1:B:303:LEU:HG   | 1:B:338:VAL:CG2  | 2.22        | 0.64     |
| 1:A:325:ARG:NH1  | 1:A:330:ASN:HD21 | 1.94        | 0.64     |
| 1:A:96:HIS:H     | 1:A:96:HIS:CD2   | 2.15        | 0.64     |
| 1:B:115:TRP:CZ2  | 1:B:119:VAL:HG11 | 2.33        | 0.64     |
| 1:B:197:LEU:C    | 1:B:199:LEU:H    | 2.00        | 0.64     |
| 1:B:445:GLU:C    | 1:B:447:THR:N    | 2.52        | 0.64     |
| 1:A:122:ARG:HG3  | 1:A:122:ARG:O    | 1.99        | 0.64     |
| 1:B:392:THR:CG2  | 1:B:393:LEU:H    | 2.05        | 0.63     |
| 1:A:448:LEU:CD2  | 1:A:448:LEU:H    | 1.91        | 0.63     |
| 1:B:128:VAL:HG12 | 1:B:209:ALA:O    | 1.98        | 0.63     |
| 1:A:424:SER:OG   | 1:A:427:GLN:HG3  | 1.98        | 0.63     |
| 1:B:424:SER:HB3  | 1:B:427:GLN:CG   | 2.28        | 0.63     |
| 1:A:76:ARG:HB3   | 1:A:435:MET:HG2  | 1.79        | 0.63     |
| 1:B:145:PHE:CZ   | 1:B:217:PRO:HB3  | 2.34        | 0.63     |
| 1:B:457:SER:HB2  | 1:B:462:MET:HG3  | 1.80        | 0.63     |
| 1:B:94:GLY:O     | 1:B:232:GLY:HA2  | 1.98        | 0.63     |
| 1:B:193:TYR:OH   | 1:B:333:PRO:HG3  | 1.97        | 0.63     |
| 1:A:199:LEU:HD21 | 1:B:101:PRO:HG2  | 1.81        | 0.62     |
| 1:A:303:LEU:CD1  | 1:A:338:VAL:HG22 | 2.29        | 0.62     |
| 1:A:460:THR:C    | 1:A:462:MET:H    | 2.02        | 0.62     |
| 1:A:182:ARG:HD2  | 1:A:213:VAL:O    | 1.99        | 0.62     |
| 1:A:290:TYR:HD1  | 1:A:299:LEU:HA   | 1.63        | 0.62     |
| 1:B:69:LEU:HA    | 1:B:72:ILE:HD12  | 1.81        | 0.62     |
| 1:A:404:ASN:O    | 1:A:408:GLU:HG2  | 1.99        | 0.62     |
| 1:B:256:LEU:HD12 | 1:B:256:LEU:C    | 2.20        | 0.62     |
| 1:B:253:ASP:HB3  | 1:B:257:ARG:HH12 | 1.65        | 0.62     |
| 1:B:258:HIS:ND1  | 1:B:259:ARG:N    | 2.48        | 0.62     |
| 1:B:88:ARG:CD    | 1:B:89:ASP:H     | 2.13        | 0.61     |
| 1:A:323:HIS:HB2  | 1:A:331:VAL:C    | 2.21        | 0.61     |
| 1:A:231:ILE:HB   | 1:B:133:HIS:NE2  | 2.16        | 0.61     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:249:ASN:CG   | 1:B:250:GLN:H    | 2.03        | 0.61     |
| 1:A:69:LEU:HD13  | 1:A:354:PHE:CG   | 2.36        | 0.61     |
| 1:A:325:ARG:NH1  | 1:A:330:ASN:ND2  | 2.49        | 0.61     |
| 1:B:252:LEU:HA   | 1:B:336:LEU:HD21 | 1.83        | 0.61     |
| 1:A:422:GLN:HG3  | 1:A:424:SER:H    | 1.66        | 0.61     |
| 1:A:303:LEU:CG   | 1:A:338:VAL:HG22 | 2.31        | 0.60     |
| 1:A:201:ASN:ND2  | 1:A:203:ARG:HH22 | 1.98        | 0.60     |
| 1:A:405:GLU:O    | 1:A:408:GLU:HB2  | 2.00        | 0.60     |
| 1:B:301:GLU:OE2  | 1:B:340:GLY:CA   | 2.49        | 0.60     |
| 1:A:391:PRO:HG2  | 1:A:395:LEU:HD23 | 1.83        | 0.60     |
| 1:A:327:GLY:O    | 1:A:328:ARG:CB   | 2.49        | 0.60     |
| 1:A:385:LEU:HD23 | 1:A:385:LEU:N    | 2.16        | 0.60     |
| 1:A:404:ASN:O    | 1:A:408:GLU:CG   | 2.49        | 0.60     |
| 1:A:466:MET:HE1  | 1:A:471:LEU:HA   | 1.84        | 0.60     |
| 1:A:455:LEU:HD11 | 1:A:474:PHE:CE2  | 2.33        | 0.60     |
| 1:A:88:ARG:CA    | 1:A:91:LEU:HD12  | 2.26        | 0.60     |
| 1:A:389:ARG:HD2  | 1:A:444:THR:CB   | 2.31        | 0.60     |
| 1:A:453:ILE:C    | 1:A:453:ILE:HD12 | 2.22        | 0.60     |
| 1:B:457:SER:OG   | 1:B:458:ARG:N    | 2.28        | 0.60     |
| 1:A:199:LEU:HD13 | 1:B:77:HIS:CD2   | 2.37        | 0.60     |
| 1:B:107:ARG:HG3  | 1:B:108:LYS:N    | 2.17        | 0.59     |
| 1:A:306:LEU:HD12 | 1:A:335:VAL:HG12 | 1.83        | 0.59     |
| 1:B:322:LEU:HD23 | 1:B:322:LEU:N    | 2.18        | 0.59     |
| 1:A:423:SER:O    | 1:A:427:GLN:HB2  | 2.03        | 0.59     |
| 1:B:311:LEU:O    | 1:B:314:MET:HB2  | 2.03        | 0.59     |
| 1:A:233:GLU:HG3  | 1:B:133:HIS:HE1  | 1.68        | 0.59     |
| 1:A:411:ILE:HD11 | 1:A:476:ILE:HD13 | 1.84        | 0.59     |
| 1:B:441:VAL:HG12 | 1:B:455:LEU:CB   | 2.32        | 0.59     |
| 1:A:445:GLU:HA   | 1:A:448:LEU:HD21 | 1.85        | 0.59     |
| 1:A:262:TRP:O    | 1:A:265:LYS:CB   | 2.51        | 0.58     |
| 1:B:376:PRO:C    | 1:B:378:LEU:H    | 2.06        | 0.58     |
| 1:B:286:GLY:HA3  | 1:B:304:TRP:CE3  | 2.38        | 0.58     |
| 1:A:277:ASP:OD2  | 1:A:277:ASP:N    | 2.36        | 0.58     |
| 1:B:325:ARG:NH1  | 1:B:325:ARG:HG2  | 2.16        | 0.58     |
| 1:B:331:VAL:HG22 | 1:B:332:VAL:N    | 2.18        | 0.58     |
| 1:A:309:HIS:O    | 1:A:311:LEU:N    | 2.36        | 0.58     |
| 1:A:432:TYR:CD2  | 1:A:440:THR:HG23 | 2.39        | 0.58     |
| 1:A:468:ILE:O    | 1:A:469:SER:HB3  | 2.03        | 0.58     |
| 1:B:110:LEU:HD13 | 1:B:378:LEU:HD11 | 1.85        | 0.58     |
| 1:B:290:TYR:CD1  | 1:B:299:LEU:HA   | 2.38        | 0.58     |
| 1:B:447:THR:O    | 1:B:449:GLU:N    | 2.37        | 0.58     |
| 1:A:459:ASP:C    | 1:A:461:THR:H    | 2.07        | 0.58     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:279:GLN:HB3  | 1:A:285:LYS:H    | 1.68        | 0.58     |
| 1:A:455:LEU:HD23 | 1:A:455:LEU:H    | 1.68        | 0.58     |
| 1:B:453:ILE:C    | 1:B:453:ILE:HD12 | 2.23        | 0.58     |
| 1:A:395:LEU:N    | 1:A:395:LEU:HD22 | 2.18        | 0.58     |
| 1:A:381:ILE:HA   | 1:A:412:SER:OG   | 2.03        | 0.58     |
| 1:A:299:LEU:HD23 | 1:A:299:LEU:C    | 2.24        | 0.58     |
| 1:B:371:VAL:HA   | 1:B:433:ASP:HB3  | 1.85        | 0.58     |
| 1:A:87:SER:O     | 1:A:89:ASP:N     | 2.37        | 0.58     |
| 1:A:310:GLU:O    | 1:A:313:HIS:HB3  | 2.04        | 0.58     |
| 1:A:243:THR:OG1  | 1:A:244:PRO:HD2  | 2.03        | 0.58     |
| 1:A:259:ARG:HH21 | 1:A:301:GLU:CD   | 2.07        | 0.58     |
| 1:B:87:SER:HB2   | 1:B:88:ARG:CZ    | 2.34        | 0.58     |
| 1:A:466:MET:CE   | 1:A:471:LEU:HA   | 2.34        | 0.57     |
| 1:A:395:LEU:CD2  | 1:A:395:LEU:H    | 2.16        | 0.57     |
| 1:A:437:ILE:O    | 1:A:438:LEU:C    | 2.42        | 0.57     |
| 1:A:139:LEU:HB2  | 1:A:140:PRO:HD2  | 1.86        | 0.57     |
| 1:B:391:PRO:HG2  | 1:B:395:LEU:HD13 | 1.86        | 0.57     |
| 1:A:197:LEU:O    | 1:A:197:LEU:HD12 | 2.05        | 0.57     |
| 1:A:431:LYS:CG   | 1:A:432:TYR:N    | 2.67        | 0.57     |
| 1:B:438:LEU:HD23 | 1:B:458:ARG:NH1  | 2.19        | 0.57     |
| 1:B:420:THR:CG2  | 1:B:421:MET:H    | 2.14        | 0.57     |
| 1:A:389:ARG:O    | 1:A:389:ARG:HG2  | 2.05        | 0.57     |
| 1:A:402:LEU:O    | 1:A:406:LEU:HD23 | 2.05        | 0.57     |
| 1:A:306:LEU:HD12 | 1:A:335:VAL:CG1  | 2.35        | 0.57     |
| 1:B:180:GLY:O    | 1:B:181:GLY:C    | 2.43        | 0.57     |
| 1:B:424:SER:HB3  | 1:B:427:GLN:CD   | 2.25        | 0.57     |
| 1:A:244:PRO:HG2  | 1:A:247:THR:OG1  | 2.05        | 0.57     |
| 1:B:92:LEU:HD22  | 1:B:298:GLU:HG2  | 1.87        | 0.57     |
| 1:A:260:LEU:HD21 | 1:A:264:ARG:NH2  | 2.20        | 0.57     |
| 1:B:302:THR:C    | 1:B:303:LEU:HD12 | 2.26        | 0.56     |
| 1:B:121:PHE:O    | 1:B:122:ARG:CG   | 2.52        | 0.56     |
| 1:A:130:ALA:HB1  | 1:A:188:GLY:HA3  | 1.86        | 0.56     |
| 1:B:392:THR:O    | 1:B:394:GLU:N    | 2.38        | 0.56     |
| 1:A:122:ARG:HH11 | 1:A:122:ARG:HG2  | 1.70        | 0.56     |
| 1:A:321:LYS:C    | 1:A:322:LEU:HD23 | 2.26        | 0.56     |
| 1:B:128:VAL:CG2  | 1:B:129:ASP:N    | 2.67        | 0.56     |
| 1:A:231:ILE:HG22 | 1:A:232:GLY:N    | 2.20        | 0.56     |
| 1:A:411:ILE:HD11 | 1:A:476:ILE:HD11 | 1.86        | 0.56     |
| 1:B:115:TRP:CE3  | 1:B:119:VAL:HG21 | 2.41        | 0.56     |
| 1:A:456:ARG:HA   | 1:A:462:MET:O    | 2.06        | 0.56     |
| 1:B:241:TRP:CD1  | 1:B:243:THR:CG2  | 2.88        | 0.56     |
| 1:B:251:TRP:O    | 1:B:254:PHE:HB3  | 2.05        | 0.56     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:309:HIS:O    | 1:A:310:GLU:C    | 2.44        | 0.56     |
| 1:A:381:ILE:CD1  | 1:A:437:ILE:HD12 | 2.32        | 0.56     |
| 1:B:116:THR:HA   | 1:B:120:VAL:CG2  | 2.35        | 0.56     |
| 1:A:265:LYS:HD2  | 1:A:266:PHE:CZ   | 2.40        | 0.56     |
| 1:B:280:ASP:HA   | 1:B:284:ARG:NH2  | 2.17        | 0.56     |
| 1:B:384:ALA:HB2  | 1:B:437:ILE:HG21 | 1.87        | 0.56     |
| 1:B:120:VAL:HG12 | 1:B:121:PHE:N    | 2.20        | 0.56     |
| 1:A:432:TYR:HD2  | 1:A:440:THR:HG23 | 1.71        | 0.56     |
| 1:B:122:ARG:HB2  | 1:B:124:GLN:HE21 | 1.71        | 0.56     |
| 1:A:460:THR:OG1  | 1:A:462:MET:HB2  | 2.06        | 0.56     |
| 1:A:123:GLU:C    | 1:A:124:GLN:HG3  | 2.26        | 0.56     |
| 1:B:382:LYS:HE3  | 1:B:479:ILE:HD13 | 1.88        | 0.56     |
| 1:B:252:LEU:C    | 1:B:252:LEU:HD13 | 2.26        | 0.55     |
| 1:A:445:GLU:O    | 1:A:448:LEU:HG   | 2.05        | 0.55     |
| 1:A:450:ASN:CG   | 1:A:451:GLY:H    | 2.09        | 0.55     |
| 1:B:428:LEU:N    | 1:B:428:LEU:HD12 | 2.22        | 0.55     |
| 1:B:189:ALA:CB   | 1:B:240:VAL:HG21 | 2.36        | 0.55     |
| 1:B:128:VAL:HG22 | 1:B:129:ASP:H    | 1.71        | 0.55     |
| 1:B:88:ARG:O     | 1:B:91:LEU:N     | 2.40        | 0.55     |
| 1:B:100:GLY:O    | 1:B:104:VAL:HG23 | 2.07        | 0.55     |
| 1:A:395:LEU:N    | 1:A:395:LEU:CD2  | 2.70        | 0.55     |
| 1:A:325:ARG:HH12 | 1:A:330:ASN:HD21 | 1.53        | 0.55     |
| 1:B:111:ALA:O    | 1:B:114:TRP:HB3  | 2.06        | 0.55     |
| 1:A:87:SER:HB3   | 1:A:88:ARG:NH2   | 2.22        | 0.55     |
| 1:A:424:SER:OG   | 1:A:425:LEU:N    | 2.39        | 0.55     |
| 1:B:472:LYS:HD3  | 1:B:473:ASP:N    | 2.21        | 0.55     |
| 1:A:102:LEU:HD12 | 1:A:102:LEU:N    | 2.22        | 0.55     |
| 1:B:395:LEU:C    | 1:B:397:GLN:H    | 2.10        | 0.55     |
| 1:B:405:GLU:HB3  | 1:B:406:LEU:HD12 | 1.89        | 0.55     |
| 1:A:113:GLU:HG2  | 1:A:266:PHE:CZ   | 2.41        | 0.55     |
| 1:B:86:LEU:N     | 1:B:86:LEU:HD22  | 2.22        | 0.55     |
| 1:A:197:LEU:HD21 | 1:A:202:LYS:HE3  | 1.89        | 0.54     |
| 1:B:113:GLU:OE2  | 1:B:266:PHE:HZ   | 1.90        | 0.54     |
| 1:A:105:GLU:O    | 1:A:109:ASN:HB2  | 2.07        | 0.54     |
| 1:A:391:PRO:HG2  | 1:A:395:LEU:CD2  | 2.37        | 0.54     |
| 1:A:381:ILE:HG13 | 1:A:381:ILE:O    | 2.07        | 0.54     |
| 1:B:122:ARG:HH11 | 1:B:122:ARG:CB   | 2.17        | 0.54     |
| 1:A:419:GLU:HG3  | 1:A:420:THR:N    | 2.19        | 0.54     |
| 1:B:128:VAL:CG2  | 1:B:129:ASP:H    | 2.21        | 0.54     |
| 1:B:87:SER:HB2   | 1:B:88:ARG:NE    | 2.22        | 0.54     |
| 1:A:273:PHE:CE1  | 1:A:291:TYR:HD1  | 2.25        | 0.54     |
| 1:A:197:LEU:HD12 | 1:A:202:LYS:HA   | 1.89        | 0.54     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:435:MET:HB3  | 1:A:437:ILE:HD11 | 1.89        | 0.54     |
| 1:B:69:LEU:HD13  | 1:B:354:PHE:CD2  | 2.43        | 0.54     |
| 1:B:441:VAL:HG12 | 1:B:455:LEU:HB2  | 1.89        | 0.54     |
| 1:A:78:PHE:CE1   | 1:A:102:LEU:HB3  | 2.43        | 0.54     |
| 1:B:88:ARG:HD2   | 1:B:89:ASP:H     | 1.70        | 0.54     |
| 1:A:323:HIS:HB3  | 1:A:332:VAL:HG22 | 1.90        | 0.54     |
| 1:A:67:GLU:HG2   | 1:A:69:LEU:N     | 2.19        | 0.54     |
| 1:A:116:THR:HA   | 1:A:120:VAL:HG21 | 1.89        | 0.54     |
| 1:B:91:LEU:O     | 1:B:92:LEU:C     | 2.47        | 0.54     |
| 1:B:114:TRP:O    | 1:B:117:SER:HB3  | 2.08        | 0.54     |
| 1:A:286:GLY:HA3  | 1:A:304:TRP:CE3  | 2.43        | 0.54     |
| 1:B:303:LEU:HD12 | 1:B:303:LEU:N    | 2.22        | 0.54     |
| 1:A:127:PRO:HB2  | 1:B:104:VAL:HG11 | 1.90        | 0.54     |
| 1:A:145:PHE:HE2  | 1:A:229:LYS:HD2  | 1.73        | 0.53     |
| 1:A:260:LEU:HD13 | 1:A:289:LEU:HD12 | 1.90        | 0.53     |
| 1:A:373:LYS:HA   | 1:A:458:ARG:CZ   | 2.38        | 0.53     |
| 1:A:145:PHE:HE2  | 1:A:229:LYS:HZ3  | 1.56        | 0.53     |
| 1:A:466:MET:CE   | 1:A:471:LEU:HD22 | 2.39        | 0.53     |
| 1:A:320:SER:C    | 1:A:322:LEU:H    | 2.11        | 0.53     |
| 1:B:87:SER:OG    | 1:B:88:ARG:CZ    | 2.56        | 0.53     |
| 1:A:321:LYS:O    | 1:A:322:LEU:HD23 | 2.07        | 0.53     |
| 1:A:431:LYS:HZ3  | 1:A:431:LYS:HB2  | 1.72        | 0.53     |
| 1:B:252:LEU:O    | 1:B:252:LEU:HD13 | 2.08        | 0.53     |
| 1:B:95:CYS:O     | 1:B:96:HIS:C     | 2.47        | 0.53     |
| 1:A:243:THR:CG2  | 1:A:334:CYS:HB2  | 2.37        | 0.53     |
| 1:B:192:HIS:O    | 1:B:194:VAL:N    | 2.42        | 0.53     |
| 1:B:351:TYR:C    | 1:B:353:SER:H    | 2.12        | 0.53     |
| 1:A:455:LEU:O    | 1:A:463:LYS:HA   | 2.09        | 0.53     |
| 1:A:320:SER:O    | 1:A:322:LEU:N    | 2.42        | 0.53     |
| 1:B:193:TYR:O    | 1:B:197:LEU:HB2  | 2.08        | 0.53     |
| 1:A:320:SER:HA   | 1:A:323:HIS:CE1  | 2.43        | 0.52     |
| 1:B:121:PHE:C    | 1:B:122:ARG:HG2  | 2.30        | 0.52     |
| 1:A:199:LEU:CD2  | 1:B:101:PRO:HG2  | 2.39        | 0.52     |
| 1:A:279:GLN:CB   | 1:A:285:LYS:H    | 2.22        | 0.52     |
| 1:B:385:LEU:HD12 | 1:B:385:LEU:C    | 2.30        | 0.52     |
| 1:A:394:GLU:C    | 1:A:397:GLN:HB2  | 2.30        | 0.52     |
| 1:B:289:LEU:HD12 | 1:B:301:GLU:HG2  | 1.90        | 0.52     |
| 1:A:126:PHE:HB3  | 1:A:127:PRO:HD2  | 1.91        | 0.52     |
| 1:B:368:HIS:HB3  | 1:B:370:LYS:HE2  | 1.90        | 0.52     |
| 1:B:115:TRP:CE2  | 1:B:119:VAL:HG11 | 2.44        | 0.52     |
| 1:A:407:LEU:HD23 | 1:A:411:ILE:O    | 2.10        | 0.52     |
| 1:B:116:THR:HA   | 1:B:120:VAL:HG23 | 1.91        | 0.52     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:332:VAL:CG1  | 1:B:333:PRO:HD2  | 2.40        | 0.52     |
| 1:A:468:ILE:O    | 1:A:469:SER:CB   | 2.57        | 0.52     |
| 1:B:438:LEU:HA   | 1:B:458:ARG:HD3  | 1.92        | 0.52     |
| 1:B:252:LEU:CB   | 1:B:336:LEU:HD11 | 2.35        | 0.52     |
| 1:A:120:VAL:O    | 1:A:121:PHE:C    | 2.48        | 0.52     |
| 1:A:146:ARG:NH1  | 1:A:146:ARG:O    | 2.43        | 0.52     |
| 1:A:405:GLU:OE2  | 1:A:472:LYS:HB2  | 2.10        | 0.51     |
| 1:A:460:THR:C    | 1:A:462:MET:N    | 2.61        | 0.51     |
| 1:A:397:GLN:OE1  | 1:A:397:GLN:HA   | 2.09        | 0.51     |
| 1:A:369:ARG:HE   | 1:A:371:VAL:CG1  | 2.23        | 0.51     |
| 1:B:421:MET:O    | 1:B:422:GLN:C    | 2.48        | 0.51     |
| 1:A:218:VAL:C    | 1:A:229:LYS:HG3  | 2.30        | 0.51     |
| 1:A:369:ARG:NH2  | 1:A:458:ARG:O    | 2.40        | 0.51     |
| 1:B:87:SER:H     | 1:B:91:LEU:HD21  | 1.75        | 0.51     |
| 1:A:146:ARG:CA   | 1:A:146:ARG:HH11 | 2.24        | 0.51     |
| 1:B:114:TRP:O    | 1:B:117:SER:N    | 2.40        | 0.51     |
| 1:B:321:LYS:HG2  | 1:B:321:LYS:O    | 2.09        | 0.51     |
| 1:B:369:ARG:HH11 | 1:B:369:ARG:HG3  | 1.74        | 0.51     |
| 1:A:369:ARG:NH2  | 1:A:371:VAL:HG21 | 2.16        | 0.51     |
| 1:B:251:TRP:HA   | 1:B:254:PHE:HB3  | 1.92        | 0.51     |
| 1:B:389:ARG:HG2  | 1:B:389:ARG:O    | 2.10        | 0.51     |
| 1:A:450:ASN:ND2  | 1:A:452:LEU:CB   | 2.71        | 0.51     |
| 1:A:471:LEU:O    | 1:A:474:PHE:HB3  | 2.10        | 0.51     |
| 1:B:287:ASN:HB2  | 1:B:303:LEU:HB2  | 1.91        | 0.51     |
| 1:B:87:SER:CB    | 1:B:88:ARG:CZ    | 2.88        | 0.51     |
| 1:B:424:SER:HB3  | 1:B:427:GLN:HB2  | 1.93        | 0.51     |
| 1:A:470:LYS:HA   | 1:A:470:LYS:HE2  | 1.92        | 0.51     |
| 1:A:410:GLY:O    | 1:A:411:ILE:HD13 | 2.10        | 0.51     |
| 1:A:309:HIS:O    | 1:A:312:LEU:N    | 2.41        | 0.51     |
| 1:B:87:SER:O     | 1:B:88:ARG:C     | 2.50        | 0.51     |
| 1:B:297:LYS:O    | 1:B:298:GLU:OE1  | 2.29        | 0.50     |
| 1:A:116:THR:CG2  | 1:A:120:VAL:HG21 | 2.41        | 0.50     |
| 1:A:484:ASN:O    | 1:A:485:VAL:C    | 2.50        | 0.50     |
| 1:A:76:ARG:HG3   | 1:A:434:GLU:O    | 2.11        | 0.50     |
| 1:A:120:VAL:HG12 | 1:A:121:PHE:N    | 2.24        | 0.50     |
| 1:B:182:ARG:NH2  | 1:B:213:VAL:O    | 2.32        | 0.50     |
| 1:B:253:ASP:C    | 1:B:257:ARG:NH1  | 2.64        | 0.50     |
| 1:A:302:THR:O    | 1:A:303:LEU:HD12 | 2.11        | 0.50     |
| 1:A:456:ARG:HH11 | 1:A:456:ARG:HG2  | 1.77        | 0.50     |
| 1:A:128:VAL:HG12 | 1:A:209:ALA:O    | 2.11        | 0.50     |
| 1:B:306:LEU:HB2  | 1:B:335:VAL:HG23 | 1.92        | 0.50     |
| 1:A:456:ARG:HG2  | 1:A:456:ARG:NH1  | 2.27        | 0.50     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:189:ALA:CB   | 1:A:240:VAL:HG21 | 2.42        | 0.50     |
| 1:B:345:GLY:O    | 1:B:348:ALA:N    | 2.44        | 0.50     |
| 1:A:197:LEU:CD1  | 1:A:202:LYS:HG3  | 2.33        | 0.50     |
| 1:A:326:ASP:OD1  | 1:A:326:ASP:C    | 2.49        | 0.50     |
| 1:A:419:GLU:HG3  | 1:A:420:THR:HG22 | 1.94        | 0.50     |
| 1:B:73:CYS:O     | 1:B:78:PHE:HB2   | 2.11        | 0.50     |
| 1:A:114:TRP:O    | 1:A:118:VAL:HG13 | 2.11        | 0.50     |
| 1:A:325:ARG:NH1  | 1:A:325:ARG:HG2  | 2.25        | 0.50     |
| 1:A:466:MET:HG2  | 1:A:467:HIS:N    | 2.27        | 0.49     |
| 1:A:320:SER:C    | 1:A:322:LEU:N    | 2.65        | 0.49     |
| 1:B:389:ARG:CG   | 1:B:389:ARG:O    | 2.59        | 0.49     |
| 1:A:306:LEU:HB2  | 1:A:335:VAL:HB   | 1.94        | 0.49     |
| 1:A:345:GLY:O    | 1:A:348:ALA:N    | 2.44        | 0.49     |
| 1:B:318:ASN:ND2  | 1:B:318:ASN:N    | 2.59        | 0.49     |
| 1:B:281:GLU:C    | 1:B:283:GLY:H    | 2.15        | 0.49     |
| 1:B:110:LEU:CD1  | 1:B:378:LEU:HD11 | 2.42        | 0.49     |
| 1:B:136:GLY:O    | 1:B:138:LEU:HD22 | 2.12        | 0.49     |
| 1:B:460:THR:O    | 1:B:462:MET:N    | 2.45        | 0.49     |
| 1:A:310:GLU:O    | 1:A:313:HIS:N    | 2.46        | 0.49     |
| 1:B:371:VAL:CA   | 1:B:433:ASP:HB3  | 2.41        | 0.49     |
| 1:B:254:PHE:CD2  | 1:B:255:TRP:N    | 2.81        | 0.49     |
| 1:B:386:ASP:HB3  | 1:B:417:TYR:N    | 2.28        | 0.49     |
| 1:B:134:LYS:N    | 1:B:180:GLY:HA2  | 2.21        | 0.49     |
| 1:B:277:ASP:HA   | 1:B:287:ASN:OD1  | 2.12        | 0.49     |
| 1:A:252:LEU:HD11 | 1:A:287:ASN:HD22 | 1.78        | 0.49     |
| 1:B:421:MET:O    | 1:B:423:SER:N    | 2.45        | 0.49     |
| 1:B:437:ILE:O    | 1:B:438:LEU:C    | 2.51        | 0.49     |
| 1:A:383:VAL:CG2  | 1:A:384:ALA:N    | 2.76        | 0.49     |
| 1:B:255:TRP:O    | 1:B:256:LEU:C    | 2.51        | 0.48     |
| 1:B:314:MET:HE1  | 1:B:315:TYR:OH   | 2.13        | 0.48     |
| 1:B:405:GLU:O    | 1:B:408:GLU:N    | 2.46        | 0.48     |
| 1:B:87:SER:O     | 1:B:88:ARG:HD2   | 2.13        | 0.48     |
| 1:B:78:PHE:C     | 1:B:79:LEU:HD22  | 2.34        | 0.48     |
| 1:B:424:SER:O    | 1:B:428:LEU:CD1  | 2.61        | 0.48     |
| 1:A:106:LEU:HD12 | 1:A:106:LEU:O    | 2.14        | 0.48     |
| 1:A:254:PHE:CD2  | 1:A:255:TRP:N    | 2.81        | 0.48     |
| 1:A:459:ASP:O    | 1:A:461:THR:N    | 2.46        | 0.48     |
| 1:B:416:GLY:HA2  | 1:B:419:GLU:OE1  | 2.13        | 0.48     |
| 1:B:415:PRO:HB2  | 1:B:418:LEU:CD1  | 2.44        | 0.48     |
| 1:B:441:VAL:HG12 | 1:B:455:LEU:HB3  | 1.94        | 0.48     |
| 1:B:256:LEU:HG   | 1:B:257:ARG:N    | 2.29        | 0.48     |
| 1:A:420:THR:HG23 | 1:A:421:MET:N    | 2.28        | 0.48     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:266:PHE:HB2  | 1:A:349:TYR:CE1  | 2.49        | 0.48     |
| 1:B:415:PRO:O    | 1:B:418:LEU:HD13 | 2.14        | 0.48     |
| 1:A:451:GLY:O    | 1:A:467:HIS:HA   | 2.13        | 0.48     |
| 1:B:280:ASP:CA   | 1:B:284:ARG:HH21 | 2.22        | 0.48     |
| 1:B:137:PRO:O    | 1:B:138:LEU:HD13 | 2.14        | 0.48     |
| 1:A:372:LEU:HD12 | 1:A:434:GLU:C    | 2.34        | 0.48     |
| 1:A:314:MET:HG2  | 1:A:315:TYR:CE1  | 2.48        | 0.48     |
| 1:B:373:LYS:HE2  | 1:B:459:ASP:CA   | 2.40        | 0.48     |
| 1:A:186:LEU:HD11 | 1:A:306:LEU:CD1  | 2.35        | 0.48     |
| 1:B:290:TYR:HD1  | 1:B:299:LEU:HA   | 1.77        | 0.48     |
| 1:A:200:VAL:C    | 1:A:202:LYS:N    | 2.67        | 0.47     |
| 1:B:77:HIS:O     | 1:B:102:LEU:HB2  | 2.13        | 0.47     |
| 1:B:286:GLY:HA2  | 1:B:303:LEU:O    | 2.14        | 0.47     |
| 1:A:189:ALA:HB3  | 1:A:240:VAL:HG21 | 1.96        | 0.47     |
| 1:B:452:LEU:CD2  | 1:B:452:LEU:N    | 2.77        | 0.47     |
| 1:B:326:ASP:O    | 1:B:329:LYS:HB2  | 2.14        | 0.47     |
| 1:B:102:LEU:O    | 1:B:103:GLY:C    | 2.52        | 0.47     |
| 1:B:256:LEU:HB2  | 1:B:287:ASN:HD22 | 1.79        | 0.47     |
| 1:A:87:SER:O     | 1:A:88:ARG:C     | 2.53        | 0.47     |
| 1:B:190:LEU:C    | 1:B:192:HIS:H    | 2.16        | 0.47     |
| 1:A:382:LYS:N    | 1:A:412:SER:OG   | 2.46        | 0.47     |
| 1:A:255:TRP:O    | 1:A:256:LEU:C    | 2.52        | 0.47     |
| 1:A:306:LEU:HB2  | 1:A:335:VAL:O    | 2.14        | 0.47     |
| 1:A:394:GLU:HA   | 1:A:394:GLU:OE2  | 2.14        | 0.47     |
| 1:A:477:LYS:O    | 1:A:481:SER:HB3  | 2.14        | 0.47     |
| 1:A:390:GLY:HA2  | 1:A:445:GLU:HB3  | 1.97        | 0.47     |
| 1:A:308:ASP:O    | 1:A:309:HIS:O    | 2.32        | 0.47     |
| 1:A:371:VAL:HG23 | 1:A:433:ASP:HB3  | 1.96        | 0.47     |
| 1:A:437:ILE:O    | 1:A:439:PHE:N    | 2.48        | 0.47     |
| 1:A:121:PHE:CD2  | 1:A:121:PHE:N    | 2.77        | 0.47     |
| 1:B:332:VAL:HG13 | 1:B:333:PRO:HD2  | 1.97        | 0.47     |
| 1:A:288:LYS:HD3  | 1:A:299:LEU:HD12 | 1.97        | 0.47     |
| 1:A:192:HIS:O    | 1:A:194:VAL:N    | 2.48        | 0.47     |
| 1:A:459:ASP:C    | 1:A:461:THR:N    | 2.67        | 0.47     |
| 1:A:130:ALA:HB3  | 1:A:210:GLN:HE22 | 1.79        | 0.47     |
| 1:B:88:ARG:O     | 1:B:89:ASP:C     | 2.53        | 0.47     |
| 1:B:145:PHE:CE1  | 1:B:217:PRO:HB3  | 2.48        | 0.47     |
| 1:A:385:LEU:HB3  | 1:A:441:VAL:HG23 | 1.97        | 0.47     |
| 1:B:234:LYS:HD3  | 1:B:341:ASP:OD2  | 2.15        | 0.47     |
| 1:A:88:ARG:H     | 1:A:88:ARG:CD    | 2.24        | 0.47     |
| 1:B:385:LEU:HD12 | 1:B:385:LEU:O    | 2.14        | 0.47     |
| 1:B:115:TRP:HH2  | 1:B:127:PRO:HB3  | 1.80        | 0.47     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:387:VAL:HG12 | 1:B:443:VAL:HG12 | 1.97        | 0.47     |
| 1:B:458:ARG:HB3  | 1:B:459:ASP:H    | 1.59        | 0.46     |
| 1:B:120:VAL:HG12 | 1:B:121:PHE:CD2  | 2.50        | 0.46     |
| 1:A:463:LYS:HD2  | 1:A:463:LYS:N    | 2.30        | 0.46     |
| 1:A:259:ARG:NH2  | 1:A:301:GLU:OE2  | 2.38        | 0.46     |
| 1:A:429:TYR:CE2  | 1:A:456:ARG:HD3  | 2.51        | 0.46     |
| 1:A:229:LYS:HG2  | 1:A:230:SER:N    | 2.30        | 0.46     |
| 1:B:370:LYS:O    | 1:B:371:VAL:O    | 2.32        | 0.46     |
| 1:A:89:ASP:O     | 1:A:91:LEU:N     | 2.49        | 0.46     |
| 1:A:266:PHE:HB2  | 1:A:349:TYR:HE1  | 1.80        | 0.46     |
| 1:A:291:TYR:CG   | 1:A:348:ALA:HB1  | 2.51        | 0.46     |
| 1:A:381:ILE:HD11 | 1:A:437:ILE:CD1  | 2.42        | 0.46     |
| 1:B:447:THR:O    | 1:B:448:LEU:C    | 2.53        | 0.46     |
| 1:B:258:HIS:ND1  | 1:B:258:HIS:C    | 2.69        | 0.46     |
| 1:B:244:PRO:HG2  | 1:B:247:THR:OG1  | 2.16        | 0.46     |
| 1:B:197:LEU:HD21 | 1:B:202:LYS:HG3  | 1.98        | 0.46     |
| 1:A:141:GLY:O    | 1:A:142:ASP:O    | 2.34        | 0.46     |
| 1:B:422:GLN:CG   | 1:B:423:SER:N    | 2.77        | 0.46     |
| 1:A:95:CYS:SG    | 1:A:218:VAL:HG21 | 2.56        | 0.46     |
| 1:A:303:LEU:HD11 | 1:A:338:VAL:CG1  | 2.36        | 0.46     |
| 1:A:244:PRO:O    | 1:A:245:PRO:C    | 2.53        | 0.46     |
| 1:A:468:ILE:HD12 | 1:A:468:ILE:C    | 2.35        | 0.46     |
| 1:B:125:VAL:HA   | 1:B:207:GLY:O    | 2.15        | 0.46     |
| 1:A:392:THR:O    | 1:A:393:LEU:C    | 2.54        | 0.46     |
| 1:A:112:ALA:O    | 1:A:116:THR:OG1  | 2.33        | 0.46     |
| 1:B:376:PRO:C    | 1:B:378:LEU:N    | 2.69        | 0.46     |
| 1:B:369:ARG:HG3  | 1:B:369:ARG:NH1  | 2.31        | 0.46     |
| 1:B:460:THR:HB   | 1:B:462:MET:CG   | 2.45        | 0.46     |
| 1:A:392:THR:HG22 | 1:A:393:LEU:N    | 2.31        | 0.46     |
| 1:A:481:SER:O    | 1:A:482:ALA:C    | 2.54        | 0.46     |
| 1:B:318:ASN:HD22 | 1:B:318:ASN:N    | 2.13        | 0.46     |
| 1:B:460:THR:HB   | 1:B:462:MET:SD   | 2.56        | 0.45     |
| 1:A:369:ARG:HE   | 1:A:371:VAL:HG11 | 1.81        | 0.45     |
| 1:A:301:GLU:OE2  | 1:A:340:GLY:HA3  | 2.16        | 0.45     |
| 1:A:290:TYR:CD1  | 1:A:299:LEU:HA   | 2.49        | 0.45     |
| 1:B:455:LEU:HD12 | 1:B:455:LEU:O    | 2.16        | 0.45     |
| 1:A:293:PHE:O    | 1:A:295:TRP:N    | 2.50        | 0.45     |
| 1:A:318:ASN:OD1  | 1:A:320:SER:HB2  | 2.16        | 0.45     |
| 1:B:126:PHE:HB3  | 1:B:127:PRO:HD2  | 1.97        | 0.45     |
| 1:B:197:LEU:C    | 1:B:199:LEU:N    | 2.69        | 0.45     |
| 1:A:128:VAL:HG23 | 1:A:192:HIS:CD2  | 2.52        | 0.45     |
| 1:A:115:TRP:CZ2  | 1:A:119:VAL:HG11 | 2.51        | 0.45     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:465:MET:O    | 1:B:466:MET:HB2  | 2.16        | 0.45     |
| 1:B:437:ILE:HG22 | 1:B:439:PHE:O    | 2.16        | 0.45     |
| 1:A:263:TRP:CH2  | 1:A:300:ILE:HD12 | 2.51        | 0.45     |
| 1:A:454:HIS:N    | 1:A:454:HIS:ND1  | 2.63        | 0.45     |
| 1:A:481:SER:OG   | 1:A:482:ALA:N    | 2.46        | 0.45     |
| 1:A:119:VAL:O    | 1:A:123:GLU:HG3  | 2.15        | 0.45     |
| 1:B:424:SER:O    | 1:B:428:LEU:HD13 | 2.17        | 0.45     |
| 1:A:394:GLU:O    | 1:A:398:VAL:HG12 | 2.16        | 0.45     |
| 1:A:255:TRP:O    | 1:A:258:HIS:HB3  | 2.17        | 0.45     |
| 1:B:320:SER:HA   | 1:B:323:HIS:NE2  | 2.31        | 0.45     |
| 1:A:403:PHE:HZ   | 1:B:123:GLU:HB2  | 1.82        | 0.45     |
| 1:A:279:GLN:HB2  | 1:A:284:ARG:HA   | 1.99        | 0.45     |
| 1:B:305:ASN:HB2  | 1:B:336:LEU:HD12 | 1.99        | 0.45     |
| 1:B:420:THR:O    | 1:B:422:GLN:N    | 2.50        | 0.45     |
| 1:A:218:VAL:C    | 1:A:229:LYS:CG   | 2.85        | 0.45     |
| 1:B:426:GLU:OE1  | 1:B:426:GLU:HA   | 2.17        | 0.45     |
| 1:A:89:ASP:O     | 1:A:90:SER:C     | 2.55        | 0.45     |
| 1:A:395:LEU:C    | 1:A:397:GLN:H    | 2.20        | 0.45     |
| 1:B:263:TRP:CZ3  | 1:B:300:ILE:HD12 | 2.51        | 0.45     |
| 1:A:281:GLU:OE2  | 1:A:304:TRP:CD1  | 2.70        | 0.45     |
| 1:A:313:HIS:C    | 1:A:313:HIS:CD2  | 2.90        | 0.45     |
| 1:A:394:GLU:HA   | 1:A:397:GLN:HB2  | 1.99        | 0.45     |
| 1:A:205:PRO:HG3  | 1:A:251:TRP:CZ2  | 2.52        | 0.45     |
| 1:A:326:ASP:HB3  | 1:A:329:LYS:O    | 2.16        | 0.45     |
| 1:B:115:TRP:CH2  | 1:B:127:PRO:HB3  | 2.52        | 0.45     |
| 1:A:126:PHE:N    | 1:A:126:PHE:CD1  | 2.84        | 0.45     |
| 1:A:318:ASN:ND2  | 1:A:319:VAL:N    | 2.60        | 0.44     |
| 1:A:369:ARG:HG3  | 1:A:370:LYS:H    | 1.82        | 0.44     |
| 1:B:191:GLU:N    | 1:B:314:MET:HE2  | 2.32        | 0.44     |
| 1:A:145:PHE:CE2  | 1:A:229:LYS:HD2  | 2.51        | 0.44     |
| 1:A:137:PRO:O    | 1:A:138:LEU:HG   | 2.17        | 0.44     |
| 1:B:264:ARG:HB3  | 1:B:270:PRO:HB3  | 1.99        | 0.44     |
| 1:B:392:THR:HG22 | 1:B:393:LEU:HD22 | 1.98        | 0.44     |
| 1:B:256:LEU:O    | 1:B:256:LEU:HD12 | 2.16        | 0.44     |
| 1:A:254:PHE:O    | 1:A:255:TRP:C    | 2.56        | 0.44     |
| 1:A:299:LEU:O    | 1:A:344:ARG:HD2  | 2.17        | 0.44     |
| 1:A:409:ASN:ND2  | 1:A:472:LYS:HD2  | 2.32        | 0.44     |
| 1:B:73:CYS:CB    | 1:B:79:LEU:HD23  | 2.48        | 0.44     |
| 1:A:241:TRP:HB3  | 1:A:336:LEU:HD22 | 2.00        | 0.44     |
| 1:B:73:CYS:HB3   | 1:B:79:LEU:HD23  | 2.00        | 0.44     |
| 1:B:200:VAL:O    | 1:B:203:ARG:HG3  | 2.17        | 0.44     |
| 1:A:85:GLN:HG2   | 1:A:85:GLN:H     | 1.49        | 0.44     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:402:LEU:O    | 1:B:403:PHE:C    | 2.55        | 0.44     |
| 1:B:93:SER:O     | 1:B:94:GLY:C     | 2.54        | 0.44     |
| 1:B:266:PHE:HB3  | 1:B:378:LEU:HD22 | 2.00        | 0.44     |
| 1:B:290:TYR:HE1  | 1:B:299:LEU:HB2  | 1.83        | 0.44     |
| 1:B:264:ARG:HB3  | 1:B:270:PRO:CB   | 2.47        | 0.44     |
| 1:B:319:VAL:O    | 1:B:319:VAL:HG22 | 2.17        | 0.44     |
| 1:B:396:ARG:HA   | 1:B:399:CYS:HB2  | 2.00        | 0.44     |
| 1:A:259:ARG:O    | 1:A:262:TRP:HB3  | 2.18        | 0.44     |
| 1:A:306:LEU:HB3  | 1:A:310:GLU:OE1  | 2.18        | 0.44     |
| 1:A:369:ARG:CG   | 1:A:370:LYS:N    | 2.80        | 0.44     |
| 1:A:431:LYS:HA   | 1:A:434:GLU:HB2  | 2.00        | 0.44     |
| 1:A:322:LEU:O    | 1:A:323:HIS:HD2  | 2.01        | 0.44     |
| 1:A:76:ARG:HB3   | 1:A:435:MET:CG   | 2.46        | 0.44     |
| 1:B:190:LEU:C    | 1:B:314:MET:HE2  | 2.39        | 0.44     |
| 1:B:259:ARG:O    | 1:B:263:TRP:HD1  | 2.00        | 0.44     |
| 1:A:130:ALA:CB   | 1:A:210:GLN:HE22 | 2.30        | 0.44     |
| 1:B:82:SER:OG    | 1:B:83:LYS:N     | 2.51        | 0.44     |
| 1:A:195:ASN:C    | 1:A:197:LEU:H    | 2.21        | 0.44     |
| 1:A:393:LEU:HD21 | 1:A:397:GLN:HE21 | 1.83        | 0.44     |
| 1:B:252:LEU:CD1  | 1:B:252:LEU:C    | 2.86        | 0.44     |
| 1:B:197:LEU:CD1  | 1:B:202:LYS:HA   | 2.45        | 0.44     |
| 1:B:424:SER:HB3  | 1:B:427:GLN:CB   | 2.48        | 0.44     |
| 1:B:395:LEU:C    | 1:B:397:GLN:N    | 2.71        | 0.43     |
| 1:B:122:ARG:O    | 1:B:124:GLN:N    | 2.51        | 0.43     |
| 1:A:252:LEU:O    | 1:A:253:ASP:C    | 2.56        | 0.43     |
| 1:A:403:PHE:CZ   | 1:B:123:GLU:HB2  | 2.53        | 0.43     |
| 1:A:467:HIS:O    | 1:A:470:LYS:HB2  | 2.18        | 0.43     |
| 1:B:130:ALA:CB   | 1:B:210:GLN:HE22 | 2.31        | 0.43     |
| 1:A:443:VAL:HG22 | 1:A:453:ILE:HG22 | 2.01        | 0.43     |
| 1:B:259:ARG:HA   | 1:B:259:ARG:HD2  | 1.72        | 0.43     |
| 1:B:472:LYS:C    | 1:B:472:LYS:HD3  | 2.39        | 0.43     |
| 1:A:106:LEU:HG   | 1:A:346:MET:HG2  | 1.99        | 0.43     |
| 1:B:347:LEU:HA   | 1:B:347:LEU:HD23 | 1.62        | 0.43     |
| 1:A:231:ILE:HD13 | 1:B:133:HIS:CD2  | 2.53        | 0.43     |
| 1:B:130:ALA:HB3  | 1:B:210:GLN:HE22 | 1.83        | 0.43     |
| 1:A:350:LEU:HA   | 1:A:350:LEU:HD23 | 1.72        | 0.43     |
| 1:A:200:VAL:O    | 1:A:202:LYS:N    | 2.52        | 0.43     |
| 1:B:439:PHE:HD1  | 1:B:456:ARG:O    | 2.01        | 0.43     |
| 1:A:432:TYR:HD2  | 1:A:440:THR:CG2  | 2.31        | 0.43     |
| 1:B:92:LEU:CD2   | 1:B:298:GLU:HG2  | 2.47        | 0.43     |
| 1:B:87:SER:H     | 1:B:91:LEU:CD2   | 2.31        | 0.43     |
| 1:B:95:CYS:O     | 1:B:96:HIS:O     | 2.35        | 0.43     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:441:VAL:HG11 | 1:A:471:LEU:HD21 | 2.00        | 0.43     |
| 1:B:286:GLY:CA   | 1:B:303:LEU:O    | 2.66        | 0.43     |
| 1:B:373:LYS:HA   | 1:B:458:ARG:NH2  | 2.33        | 0.43     |
| 1:B:215:PHE:CD1  | 1:B:215:PHE:N    | 2.86        | 0.43     |
| 1:A:103:GLY:O    | 1:A:104:VAL:C    | 2.57        | 0.43     |
| 1:A:96:HIS:H     | 1:A:96:HIS:HD2   | 1.61        | 0.43     |
| 1:A:436:SER:C    | 1:A:437:ILE:HD13 | 2.38        | 0.43     |
| 1:A:235:THR:N    | 1:A:343:ASP:OD2  | 2.38        | 0.43     |
| 1:A:450:ASN:N    | 1:A:450:ASN:OD1  | 2.51        | 0.43     |
| 1:A:466:MET:CG   | 1:A:467:HIS:N    | 2.82        | 0.43     |
| 1:A:393:LEU:C    | 1:A:397:GLN:HG2  | 2.38        | 0.43     |
| 1:B:118:VAL:HG13 | 1:B:119:VAL:H    | 1.84        | 0.43     |
| 1:B:87:SER:C     | 1:B:88:ARG:HD2   | 2.38        | 0.43     |
| 1:B:108:LYS:O    | 1:B:111:ALA:HB3  | 2.19        | 0.43     |
| 1:A:102:LEU:CD1  | 1:A:102:LEU:N    | 2.80        | 0.43     |
| 1:A:381:ILE:CG1  | 1:A:437:ILE:HD12 | 2.49        | 0.43     |
| 1:B:299:LEU:HD13 | 1:B:299:LEU:C    | 2.39        | 0.43     |
| 1:B:82:SER:N     | 1:B:85:GLN:OE1   | 2.42        | 0.43     |
| 1:A:466:MET:HE1  | 1:A:471:LEU:HD13 | 2.00        | 0.42     |
| 1:B:406:LEU:HB3  | 1:B:411:ILE:HB   | 2.00        | 0.42     |
| 1:B:252:LEU:HD23 | 1:B:336:LEU:HD11 | 2.01        | 0.42     |
| 1:B:331:VAL:CG2  | 1:B:332:VAL:N    | 2.80        | 0.42     |
| 1:A:87:SER:C     | 1:A:88:ARG:HD2   | 2.38        | 0.42     |
| 1:A:122:ARG:CG   | 1:A:122:ARG:O    | 2.67        | 0.42     |
| 1:B:287:ASN:N    | 1:B:303:LEU:O    | 2.51        | 0.42     |
| 1:B:278:CYS:SG   | 1:B:304:TRP:CZ2  | 3.12        | 0.42     |
| 1:B:265:LYS:HB2  | 1:B:265:LYS:HE3  | 1.90        | 0.42     |
| 1:B:372:LEU:O    | 1:B:374:LEU:N    | 2.52        | 0.42     |
| 1:B:289:LEU:CB   | 1:B:301:GLU:HB3  | 2.45        | 0.42     |
| 1:B:397:GLN:HG2  | 1:B:397:GLN:O    | 2.13        | 0.42     |
| 1:B:281:GLU:OE1  | 1:B:304:TRP:CE2  | 2.72        | 0.42     |
| 1:A:354:PHE:CG   | 1:A:355:GLN:N    | 2.87        | 0.42     |
| 1:B:87:SER:N     | 1:B:91:LEU:HD21  | 2.35        | 0.42     |
| 1:A:322:LEU:O    | 1:A:323:HIS:C    | 2.58        | 0.42     |
| 1:A:431:LYS:HG2  | 1:A:432:TYR:N    | 2.34        | 0.42     |
| 1:B:119:VAL:HG22 | 1:B:209:ALA:HB3  | 2.01        | 0.42     |
| 1:A:372:LEU:CB   | 1:A:436:SER:HB2  | 2.49        | 0.42     |
| 1:A:407:LEU:O    | 1:A:408:GLU:C    | 2.58        | 0.42     |
| 1:A:407:LEU:HD13 | 1:B:120:VAL:HG12 | 2.01        | 0.42     |
| 1:B:258:HIS:O    | 1:B:261:GLN:N    | 2.53        | 0.42     |
| 1:A:188:GLY:HA2  | 1:A:191:GLU:OE2  | 2.20        | 0.42     |
| 1:B:193:TYR:O    | 1:B:193:TYR:CD1  | 2.73        | 0.42     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:107:ARG:HG2  | 1:B:107:ARG:HH11 | 1.85        | 0.42     |
| 1:B:269:SER:HB2  | 1:B:272:ASN:HD22 | 1.84        | 0.42     |
| 1:A:385:LEU:CB   | 1:A:441:VAL:HG23 | 2.49        | 0.42     |
| 1:A:481:SER:O    | 1:A:483:LYS:N    | 2.53        | 0.42     |
| 1:A:139:LEU:CD1  | 1:A:142:ASP:HB2  | 2.50        | 0.42     |
| 1:B:186:LEU:HD21 | 1:B:306:LEU:HD11 | 2.01        | 0.42     |
| 1:B:481:SER:O    | 1:B:484:ASN:HB2  | 2.20        | 0.42     |
| 1:A:202:LYS:HG2  | 1:A:202:LYS:O    | 2.20        | 0.41     |
| 1:A:389:ARG:HD2  | 1:A:444:THR:CG2  | 2.50        | 0.41     |
| 1:B:244:PRO:HA   | 1:B:245:PRO:HD3  | 1.91        | 0.41     |
| 1:B:82:SER:HB3   | 1:B:85:GLN:OE1   | 2.20        | 0.41     |
| 1:A:375:HIS:HA   | 1:A:376:PRO:HD3  | 1.92        | 0.41     |
| 1:B:76:ARG:HD3   | 1:B:76:ARG:HA    | 1.64        | 0.41     |
| 1:A:121:PHE:HB2  | 1:A:122:ARG:H    | 1.72        | 0.41     |
| 1:A:442:LEU:HA   | 1:A:442:LEU:HD23 | 1.73        | 0.41     |
| 1:B:385:LEU:HD23 | 1:B:413:VAL:CG1  | 2.51        | 0.41     |
| 1:B:391:PRO:HG2  | 1:B:392:THR:H    | 1.84        | 0.41     |
| 1:B:460:THR:CB   | 1:B:462:MET:HG2  | 2.48        | 0.41     |
| 1:B:115:TRP:CZ3  | 1:B:119:VAL:HG21 | 2.55        | 0.41     |
| 1:A:385:LEU:N    | 1:A:385:LEU:CD2  | 2.83        | 0.41     |
| 1:A:435:MET:HE2  | 1:A:435:MET:HB3  | 1.93        | 0.41     |
| 1:A:127:PRO:HA   | 1:A:209:ALA:O    | 2.21        | 0.41     |
| 1:A:448:LEU:CD2  | 1:A:448:LEU:N    | 2.65        | 0.41     |
| 1:B:192:HIS:O    | 1:B:193:TYR:C    | 2.58        | 0.41     |
| 1:B:267:ALA:HB2  | 1:B:273:PHE:HE2  | 1.86        | 0.41     |
| 1:A:96:HIS:HB2   | 1:A:97:PRO:HD2   | 2.03        | 0.41     |
| 1:B:69:LEU:O     | 1:B:72:ILE:HB    | 2.21        | 0.41     |
| 1:A:185:LEU:HD23 | 1:A:185:LEU:HA   | 1.82        | 0.41     |
| 1:B:392:THR:HG22 | 1:B:393:LEU:CD2  | 2.51        | 0.41     |
| 1:A:308:ASP:OD2  | 1:A:308:ASP:N    | 2.26        | 0.41     |
| 1:A:353:SER:HB2  | 1:A:373:LYS:C    | 2.40        | 0.41     |
| 1:B:122:ARG:O    | 1:B:122:ARG:HG3  | 2.20        | 0.41     |
| 1:A:355:GLN:NE2  | 1:A:355:GLN:HA   | 2.35        | 0.41     |
| 1:A:420:THR:CG2  | 1:A:421:MET:N    | 2.84        | 0.41     |
| 1:A:423:SER:HB3  | 1:A:427:GLN:NE2  | 2.35        | 0.41     |
| 1:A:243:THR:OG1  | 1:A:244:PRO:CD   | 2.68        | 0.41     |
| 1:B:260:LEU:CD1  | 1:B:275:SER:HB3  | 2.48        | 0.41     |
| 1:B:69:LEU:O     | 1:B:70:LEU:C     | 2.59        | 0.41     |
| 1:B:104:VAL:O    | 1:B:107:ARG:N    | 2.52        | 0.41     |
| 1:B:368:HIS:ND1  | 1:B:368:HIS:O    | 2.54        | 0.41     |
| 1:A:139:LEU:CB   | 1:A:140:PRO:HD2  | 2.50        | 0.41     |
| 1:A:260:LEU:HD21 | 1:A:264:ARG:CZ   | 2.51        | 0.41     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:387:VAL:HG12 | 1:B:443:VAL:O    | 2.20        | 0.41     |
| 1:B:395:LEU:O    | 1:B:397:GLN:N    | 2.54        | 0.40     |
| 1:A:372:LEU:HB3  | 1:A:436:SER:HB2  | 2.01        | 0.40     |
| 1:A:266:PHE:HB3  | 1:A:378:LEU:HD22 | 2.02        | 0.40     |
| 1:B:294:PRO:HD2  | 1:B:295:TRP:CE3  | 2.56        | 0.40     |
| 1:B:202:LYS:HB3  | 1:B:324:GLY:HA2  | 2.04        | 0.40     |
| 1:A:375:HIS:O    | 1:A:378:LEU:HB2  | 2.22        | 0.40     |
| 1:A:193:TYR:O    | 1:A:197:LEU:HB2  | 2.21        | 0.40     |
| 1:A:200:VAL:C    | 1:A:202:LYS:H    | 2.24        | 0.40     |
| 1:B:122:ARG:CB   | 1:B:124:GLN:HE21 | 2.34        | 0.40     |
| 1:B:193:TYR:HB2  | 1:B:242:PHE:CZ   | 2.56        | 0.40     |
| 1:A:263:TRP:CE3  | 1:A:300:ILE:HD12 | 2.56        | 0.40     |
| 1:A:87:SER:C     | 1:A:89:ASP:N     | 2.74        | 0.40     |
| 1:A:425:LEU:HA   | 1:A:425:LEU:HD23 | 1.86        | 0.40     |
| 1:A:280:ASP:HA   | 1:A:283:GLY:C    | 2.42        | 0.40     |
| 1:A:323:HIS:CB   | 1:A:331:VAL:C    | 2.89        | 0.40     |
| 1:B:273:PHE:CE1  | 1:B:291:TYR:HD1  | 2.40        | 0.40     |
| 1:B:299:LEU:O    | 1:B:344:ARG:HD2  | 2.22        | 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     | 358/459 (78%) | 246 (69%) | 75 (21%)  | 37 (10%) | 1           | 6 |
| 1   | B     | 358/459 (78%) | 242 (68%) | 73 (20%)  | 43 (12%) | 1           | 4 |
| All | All   | 716/918 (78%) | 488 (68%) | 148 (21%) | 80 (11%) | 1           | 5 |

All (80) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 88  | ARG  |
| 1   | A     | 120 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 124 | GLN  |
| 1   | A     | 131 | LEU  |
| 1   | A     | 142 | ASP  |
| 1   | A     | 193 | TYR  |
| 1   | A     | 309 | HIS  |
| 1   | A     | 310 | GLU  |
| 1   | A     | 323 | HIS  |
| 1   | A     | 389 | ARG  |
| 1   | A     | 420 | THR  |
| 1   | A     | 421 | MET  |
| 1   | A     | 461 | THR  |
| 1   | B     | 68  | ALA  |
| 1   | B     | 88  | ARG  |
| 1   | B     | 104 | VAL  |
| 1   | B     | 120 | VAL  |
| 1   | B     | 181 | GLY  |
| 1   | B     | 281 | GLU  |
| 1   | B     | 371 | VAL  |
| 1   | B     | 391 | PRO  |
| 1   | B     | 393 | LEU  |
| 1   | B     | 417 | TYR  |
| 1   | B     | 423 | SER  |
| 1   | B     | 424 | SER  |
| 1   | B     | 448 | LEU  |
| 1   | B     | 461 | THR  |
| 1   | A     | 90  | SER  |
| 1   | A     | 121 | PHE  |
| 1   | A     | 328 | ARG  |
| 1   | A     | 371 | VAL  |
| 1   | A     | 391 | PRO  |
| 1   | A     | 438 | LEU  |
| 1   | A     | 450 | ASN  |
| 1   | A     | 469 | SER  |
| 1   | B     | 121 | PHE  |
| 1   | B     | 130 | ALA  |
| 1   | B     | 146 | ARG  |
| 1   | B     | 191 | GLU  |
| 1   | B     | 193 | TYR  |
| 1   | B     | 309 | HIS  |
| 1   | B     | 421 | MET  |
| 1   | B     | 438 | LEU  |
| 1   | B     | 446 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 89  | ASP  |
| 1   | A     | 254 | PHE  |
| 1   | A     | 271 | SER  |
| 1   | A     | 321 | LYS  |
| 1   | A     | 393 | LEU  |
| 1   | A     | 460 | THR  |
| 1   | B     | 123 | GLU  |
| 1   | B     | 124 | GLN  |
| 1   | B     | 258 | HIS  |
| 1   | B     | 259 | ARG  |
| 1   | B     | 285 | LYS  |
| 1   | B     | 373 | LYS  |
| 1   | B     | 385 | LEU  |
| 1   | B     | 396 | ARG  |
| 1   | B     | 422 | GLN  |
| 1   | B     | 466 | MET  |
| 1   | A     | 146 | ARG  |
| 1   | A     | 294 | PRO  |
| 1   | A     | 392 | THR  |
| 1   | A     | 464 | GLU  |
| 1   | B     | 87  | SER  |
| 1   | B     | 105 | GLU  |
| 1   | B     | 321 | LYS  |
| 1   | B     | 352 | ASP  |
| 1   | B     | 419 | GLU  |
| 1   | A     | 280 | ASP  |
| 1   | B     | 190 | LEU  |
| 1   | B     | 354 | PHE  |
| 1   | A     | 140 | PRO  |
| 1   | A     | 425 | LEU  |
| 1   | B     | 118 | VAL  |
| 1   | A     | 376 | PRO  |
| 1   | A     | 451 | GLY  |
| 1   | B     | 376 | PRO  |
| 1   | A     | 104 | VAL  |
| 1   | B     | 96  | HIS  |

### 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     | 323/401 (80%) | 271 (84%) | 52 (16%) | 3           | 13 |
| 1   | B     | 323/401 (80%) | 280 (87%) | 43 (13%) | 6           | 22 |
| All | All   | 646/802 (80%) | 551 (85%) | 95 (15%) | 4           | 18 |

All (95) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 67  | GLU  |
| 1   | A     | 70  | LEU  |
| 1   | A     | 79  | LEU  |
| 1   | A     | 85  | GLN  |
| 1   | A     | 88  | ARG  |
| 1   | A     | 89  | ASP  |
| 1   | A     | 92  | LEU  |
| 1   | A     | 95  | CYS  |
| 1   | A     | 96  | HIS  |
| 1   | A     | 109 | ASN  |
| 1   | A     | 116 | THR  |
| 1   | A     | 118 | VAL  |
| 1   | A     | 121 | PHE  |
| 1   | A     | 122 | ARG  |
| 1   | A     | 124 | GLN  |
| 1   | A     | 125 | VAL  |
| 1   | A     | 126 | PHE  |
| 1   | A     | 128 | VAL  |
| 1   | A     | 142 | ASP  |
| 1   | A     | 195 | ASN  |
| 1   | A     | 200 | VAL  |
| 1   | A     | 206 | TYR  |
| 1   | A     | 229 | LYS  |
| 1   | A     | 231 | ILE  |
| 1   | A     | 250 | GLN  |
| 1   | A     | 252 | LEU  |
| 1   | A     | 276 | SER  |
| 1   | A     | 277 | ASP  |
| 1   | A     | 278 | CYS  |
| 1   | A     | 280 | ASP  |
| 1   | A     | 298 | GLU  |
| 1   | A     | 308 | ASP  |
| 1   | A     | 323 | HIS  |
| 1   | A     | 328 | ARG  |
| 1   | A     | 330 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 347 | LEU  |
| 1   | A     | 378 | LEU  |
| 1   | A     | 386 | ASP  |
| 1   | A     | 387 | VAL  |
| 1   | A     | 389 | ARG  |
| 1   | A     | 423 | SER  |
| 1   | A     | 426 | GLU  |
| 1   | A     | 431 | LYS  |
| 1   | A     | 443 | VAL  |
| 1   | A     | 445 | GLU  |
| 1   | A     | 448 | LEU  |
| 1   | A     | 449 | GLU  |
| 1   | A     | 454 | HIS  |
| 1   | A     | 460 | THR  |
| 1   | A     | 468 | ILE  |
| 1   | A     | 471 | LEU  |
| 1   | A     | 481 | SER  |
| 1   | B     | 67  | GLU  |
| 1   | B     | 70  | LEU  |
| 1   | B     | 85  | GLN  |
| 1   | B     | 88  | ARG  |
| 1   | B     | 89  | ASP  |
| 1   | B     | 95  | CYS  |
| 1   | B     | 107 | ARG  |
| 1   | B     | 122 | ARG  |
| 1   | B     | 124 | GLN  |
| 1   | B     | 139 | LEU  |
| 1   | B     | 184 | ASN  |
| 1   | B     | 200 | VAL  |
| 1   | B     | 206 | TYR  |
| 1   | B     | 216 | HIS  |
| 1   | B     | 230 | SER  |
| 1   | B     | 234 | LYS  |
| 1   | B     | 248 | SER  |
| 1   | B     | 256 | LEU  |
| 1   | B     | 257 | ARG  |
| 1   | B     | 271 | SER  |
| 1   | B     | 284 | ARG  |
| 1   | B     | 298 | GLU  |
| 1   | B     | 311 | LEU  |
| 1   | B     | 312 | LEU  |
| 1   | B     | 322 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 328 | ARG  |
| 1   | B     | 335 | VAL  |
| 1   | B     | 374 | LEU  |
| 1   | B     | 377 | CYS  |
| 1   | B     | 389 | ARG  |
| 1   | B     | 397 | GLN  |
| 1   | B     | 426 | GLU  |
| 1   | B     | 431 | LYS  |
| 1   | B     | 445 | GLU  |
| 1   | B     | 448 | LEU  |
| 1   | B     | 455 | LEU  |
| 1   | B     | 456 | ARG  |
| 1   | B     | 459 | ASP  |
| 1   | B     | 460 | THR  |
| 1   | B     | 462 | MET  |
| 1   | B     | 472 | LYS  |
| 1   | B     | 473 | ASP  |
| 1   | B     | 481 | SER  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 84  | GLN  |
| 1   | A     | 96  | HIS  |
| 1   | A     | 192 | HIS  |
| 1   | A     | 201 | ASN  |
| 1   | A     | 210 | GLN  |
| 1   | A     | 216 | HIS  |
| 1   | A     | 287 | ASN  |
| 1   | A     | 313 | HIS  |
| 1   | A     | 323 | HIS  |
| 1   | A     | 355 | GLN  |
| 1   | A     | 400 | GLN  |
| 1   | A     | 422 | GLN  |
| 1   | A     | 427 | GLN  |
| 1   | A     | 450 | ASN  |
| 1   | A     | 454 | HIS  |
| 1   | B     | 77  | HIS  |
| 1   | B     | 124 | GLN  |
| 1   | B     | 192 | HIS  |
| 1   | B     | 201 | ASN  |
| 1   | B     | 210 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 272 | ASN  |
| 1   | B     | 287 | ASN  |
| 1   | B     | 305 | ASN  |
| 1   | B     | 313 | HIS  |
| 1   | B     | 318 | ASN  |
| 1   | B     | 323 | HIS  |
| 1   | B     | 375 | HIS  |
| 1   | B     | 400 | GLN  |
| 1   | B     | 454 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2 |       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|---------|-------|-----------------------|-------|
| 1   | A     | 364/459 (79%) | -0.10  | 3 (0%)  | 83 28 | 41, 74, 102, 136      | 0     |
| 1   | B     | 364/459 (79%) | -0.09  | 3 (0%)  | 83 28 | 48, 73, 108, 127      | 0     |
| All | All   | 728/918 (79%) | -0.09  | 6 (0%)  | 83 28 | 41, 73, 107, 136      | 0     |

All (6) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 138 | LEU  | 6.1  |
| 1   | A     | 139 | LEU  | 5.8  |
| 1   | B     | 140 | PRO  | 4.4  |
| 1   | A     | 140 | PRO  | 3.8  |
| 1   | B     | 139 | LEU  | 2.7  |
| 1   | B     | 144 | ALA  | 2.0  |

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.