



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:52 am GMT

PDB ID : 1O7X
Title : CITRATE SYNTHASE FROM SULFOLOBUS SOLFATARICUS
Authors : Bell, G.S.; Russell, R.J.M.; Connaris, H.; Hough, D.W.; Danson, M.J.; Taylor, G.L.
Deposited on : 2002-11-19
Resolution : 2.70 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

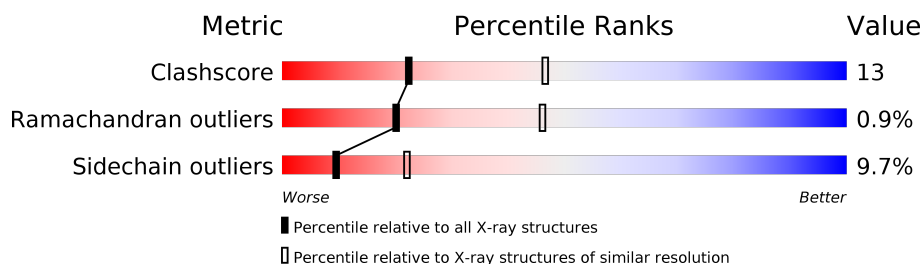
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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 (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore | 112137 | 2590 (2.70-2.70) |
| Ramachandran outliers | 110173 | 2550 (2.70-2.70) |
| Sidechain outliers | 110143 | 2550 (2.70-2.70) |

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 377 | |
| 1 | B | 377 | |
| 1 | C | 377 | |
| 1 | D | 377 | |

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11738 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 CITRATE SYNTHASE.

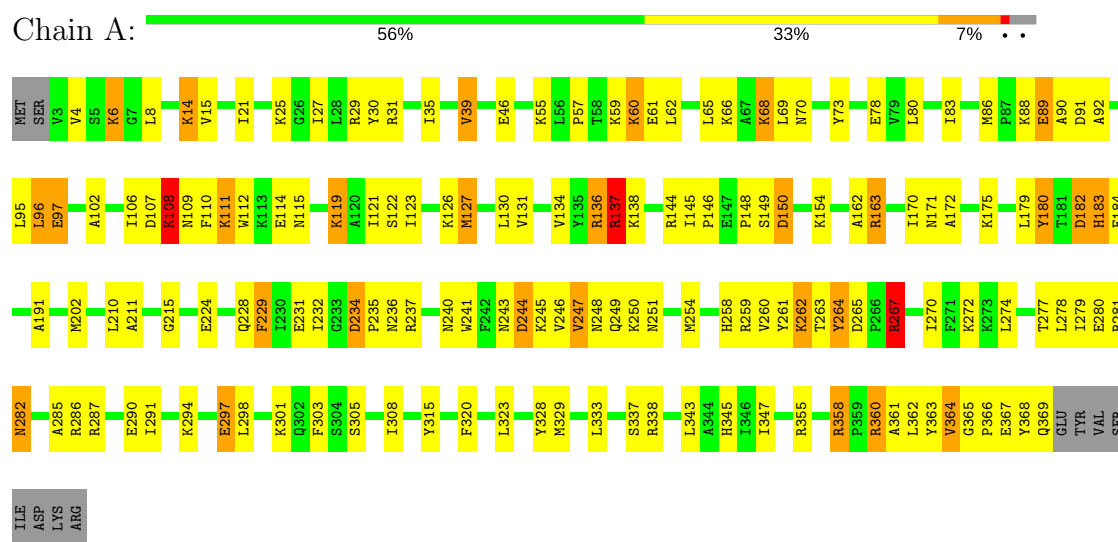
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1 | A | 367 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2935 | 1897 | 487 | 544 | 7 | | | |
| 1 | B | 366 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2926 | 1892 | 485 | 542 | 7 | | | |
| 1 | C | 370 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2963 | 1916 | 490 | 550 | 7 | | | |
| 1 | D | 365 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2914 | 1883 | 484 | 540 | 7 | | | |

3 Residue-property plots

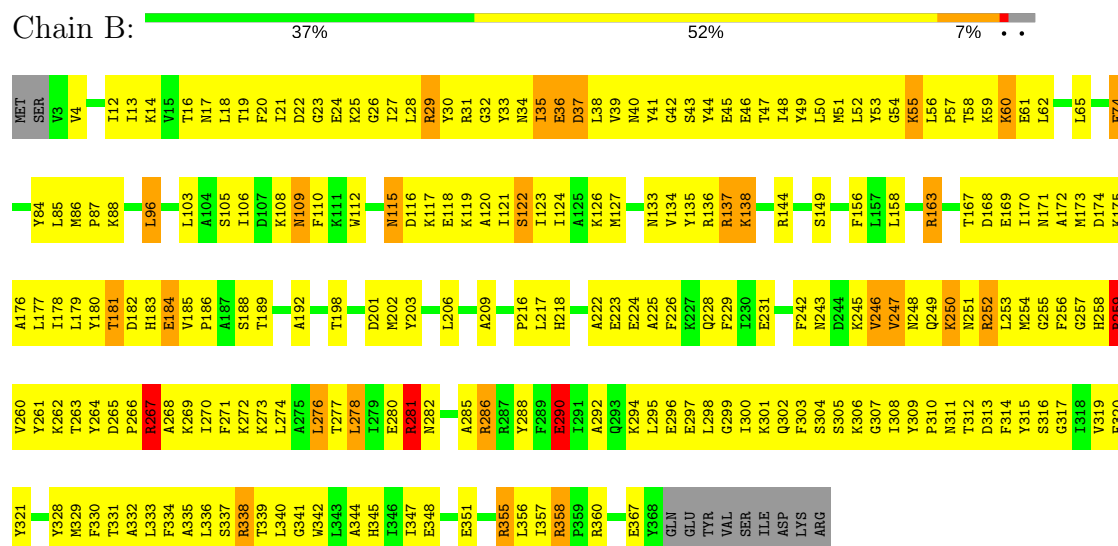
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

• Molecule 1: CITRATE SYNTHASE

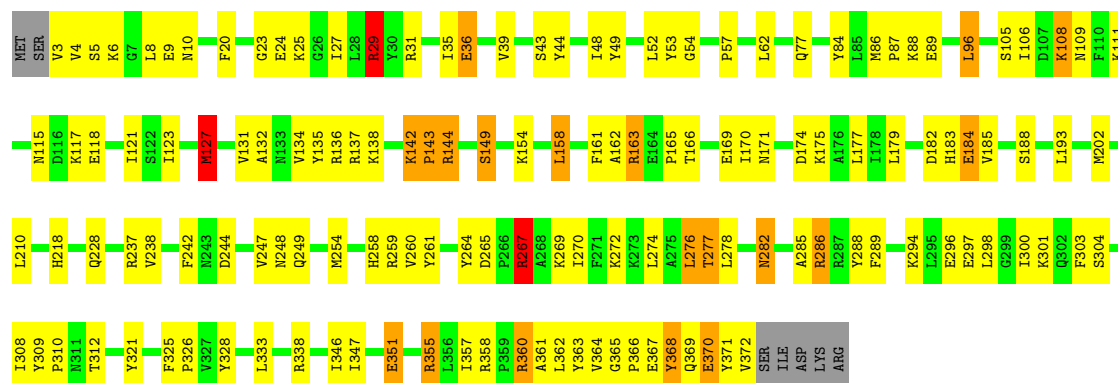


• Molecule 1: CITRATE SYNTHASE



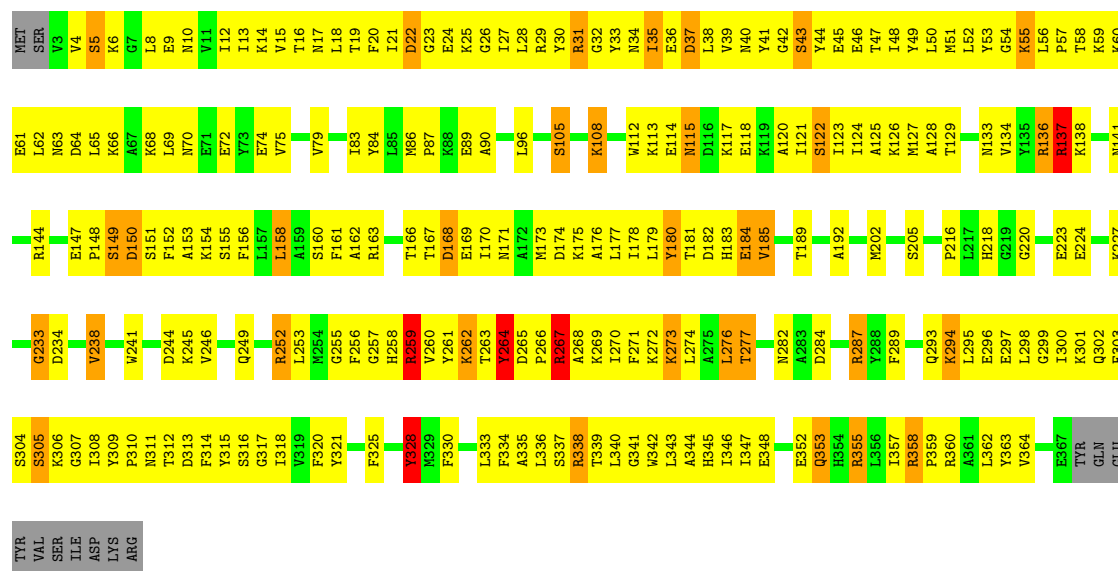
• Molecule 1: CITRATE SYNTHASE

Chain C: 



• Molecule 1: CITRATE SYNTHASE

Chain D: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property | Value | Source |
|--|--|-----------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 77.34Å 97.86Å 119.33Å 90.00° 107.60° 90.00° | Depositor |
| Resolution (Å) | 20.00 – 2.70 | Depositor |
| % Data completeness (in resolution range) | 88.6 (20.00-2.70) | Depositor |
| R_{merge} | 0.07 | Depositor |
| R_{sym} | (Not available) | Depositor |
| Refinement program | REFMAC | Depositor |
| R, R_{free} | 0.208 , 0.285 | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 11738 | wwPDB-VP |
| Average B, all atoms (Å ²) | 37.0 | wwPDB-VP |

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 | 0.47 | 0/2998 | 1.31 | 19/4055 (0.5%) |
| 1 | B | 0.53 | 0/2989 | 1.45 | 29/4043 (0.7%) |
| 1 | C | 0.48 | 0/3027 | 1.36 | 22/4095 (0.5%) |
| 1 | D | 0.52 | 0/2976 | 1.44 | 32/4025 (0.8%) |
| All | All | 0.50 | 0/11990 | 1.39 | 102/16218 (0.6%) |

There are no bond length outliers.

All (102) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | C | 355 | ARG | NE-CZ-NH2 | -12.70 | 113.95 | 120.30 |
| 1 | D | 252 | ARG | NE-CZ-NH1 | 12.03 | 126.32 | 120.30 |
| 1 | B | 281 | ARG | CD-NE-CZ | 11.05 | 139.08 | 123.60 |
| 1 | A | 267 | ARG | CD-NE-CZ | 10.93 | 138.90 | 123.60 |
| 1 | B | 338 | ARG | NE-CZ-NH1 | 10.67 | 125.64 | 120.30 |
| 1 | B | 281 | ARG | NE-CZ-NH1 | 10.46 | 125.53 | 120.30 |
| 1 | D | 259 | ARG | CD-NE-CZ | 9.88 | 137.44 | 123.60 |
| 1 | B | 355 | ARG | NE-CZ-NH1 | 9.63 | 125.11 | 120.30 |
| 1 | C | 136 | ARG | NE-CZ-NH1 | 9.13 | 124.86 | 120.30 |
| 1 | C | 136 | ARG | NE-CZ-NH2 | -9.01 | 115.80 | 120.30 |
| 1 | B | 267 | ARG | NE-CZ-NH2 | -8.89 | 115.85 | 120.30 |
| 1 | C | 29 | ARG | NE-CZ-NH2 | -8.81 | 115.89 | 120.30 |
| 1 | C | 358 | ARG | CD-NE-CZ | 8.72 | 135.81 | 123.60 |
| 1 | A | 360 | ARG | NE-CZ-NH2 | -8.71 | 115.94 | 120.30 |
| 1 | D | 137 | ARG | NE-CZ-NH2 | 8.69 | 124.64 | 120.30 |
| 1 | B | 136 | ARG | CD-NE-CZ | 8.63 | 135.68 | 123.60 |
| 1 | C | 358 | ARG | NE-CZ-NH1 | 8.59 | 124.59 | 120.30 |
| 1 | A | 182 | ASP | CB-CG-OD2 | 8.57 | 126.01 | 118.30 |
| 1 | B | 355 | ARG | NE-CZ-NH2 | -8.55 | 116.03 | 120.30 |
| 1 | D | 252 | ARG | CD-NE-CZ | 8.43 | 135.41 | 123.60 |
| 1 | B | 163 | ARG | NE-CZ-NH1 | 8.41 | 124.51 | 120.30 |
| 1 | C | 163 | ARG | NE-CZ-NH1 | 8.20 | 124.40 | 120.30 |
| 1 | A | 264 | TYR | CA-CB-CG | 8.16 | 128.91 | 113.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | B | 286 | ARG | CD-NE-CZ | 8.14 | 134.99 | 123.60 |
| 1 | C | 184 | GLU | OE1-CD-OE2 | -8.04 | 113.65 | 123.30 |
| 1 | B | 252 | ARG | NE-CZ-NH1 | 8.00 | 124.30 | 120.30 |
| 1 | B | 281 | ARG | NE-CZ-NH2 | -7.62 | 116.49 | 120.30 |
| 1 | D | 259 | ARG | NE-CZ-NH1 | 7.59 | 124.10 | 120.30 |
| 1 | D | 338 | ARG | NE-CZ-NH1 | 7.57 | 124.09 | 120.30 |
| 1 | D | 360 | ARG | CD-NE-CZ | 7.54 | 134.15 | 123.60 |
| 1 | A | 338 | ARG | NE-CZ-NH1 | -7.45 | 116.57 | 120.30 |
| 1 | D | 136 | ARG | NE-CZ-NH2 | -7.40 | 116.60 | 120.30 |
| 1 | D | 37 | ASP | CB-CG-OD2 | 7.25 | 124.83 | 118.30 |
| 1 | A | 137 | ARG | NE-CZ-NH2 | 7.21 | 123.90 | 120.30 |
| 1 | B | 355 | ARG | CD-NE-CZ | 7.12 | 133.57 | 123.60 |
| 1 | A | 364 | VAL | CA-C-N | 7.11 | 130.42 | 116.20 |
| 1 | A | 163 | ARG | NE-CZ-NH1 | 7.07 | 123.84 | 120.30 |
| 1 | B | 338 | ARG | NE-CZ-NH2 | -7.07 | 116.76 | 120.30 |
| 1 | B | 105 | SER | N-CA-CB | -6.98 | 100.02 | 110.50 |
| 1 | D | 358 | ARG | CD-NE-CZ | 6.94 | 133.32 | 123.60 |
| 1 | C | 265 | ASP | CB-CG-OD1 | 6.94 | 124.55 | 118.30 |
| 1 | A | 191 | ALA | N-CA-CB | 6.90 | 119.76 | 110.10 |
| 1 | B | 29 | ARG | NE-CZ-NH1 | -6.88 | 116.86 | 120.30 |
| 1 | D | 137 | ARG | CD-NE-CZ | -6.86 | 114.00 | 123.60 |
| 1 | C | 144 | ARG | NE-CZ-NH1 | -6.77 | 116.91 | 120.30 |
| 1 | B | 163 | ARG | NE-CZ-NH2 | -6.77 | 116.92 | 120.30 |
| 1 | D | 184 | GLU | OE1-CD-OE2 | -6.63 | 115.34 | 123.30 |
| 1 | D | 144 | ARG | NE-CZ-NH1 | -6.61 | 116.99 | 120.30 |
| 1 | B | 252 | ARG | NE-CZ-NH2 | -6.56 | 117.02 | 120.30 |
| 1 | C | 127 | MET | CA-CB-CG | 6.53 | 124.41 | 113.30 |
| 1 | C | 368 | TYR | CB-CG-CD1 | -6.51 | 117.09 | 121.00 |
| 1 | C | 163 | ARG | CD-NE-CZ | 6.45 | 132.62 | 123.60 |
| 1 | B | 358 | ARG | CD-NE-CZ | 6.42 | 132.58 | 123.60 |
| 1 | C | 286 | ARG | NE-CZ-NH2 | -6.41 | 117.10 | 120.30 |
| 1 | D | 358 | ARG | NE-CZ-NH1 | 6.36 | 123.48 | 120.30 |
| 1 | D | 338 | ARG | NE-CZ-NH2 | -6.35 | 117.12 | 120.30 |
| 1 | B | 74 | GLU | OE1-CD-OE2 | 6.24 | 130.79 | 123.30 |
| 1 | D | 328 | TYR | CA-CB-CG | 6.12 | 125.03 | 113.40 |
| 1 | D | 31 | ARG | NE-CZ-NH1 | -6.10 | 117.25 | 120.30 |
| 1 | A | 267 | ARG | CB-CA-C | 6.09 | 122.58 | 110.40 |
| 1 | B | 259 | ARG | NE-CZ-NH2 | 6.05 | 123.33 | 120.30 |
| 1 | D | 287 | ARG | NE-CZ-NH2 | 6.04 | 123.32 | 120.30 |
| 1 | D | 364 | VAL | CA-C-N | 5.99 | 128.18 | 116.20 |
| 1 | C | 370 | GLU | OE1-CD-OE2 | -5.96 | 116.14 | 123.30 |
| 1 | A | 355 | ARG | NE-CZ-NH1 | 5.92 | 123.26 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 265 | ASP | CB-CG-OD1 | 5.88 | 123.59 | 118.30 |
| 1 | D | 259 | ARG | CG-CD-NE | 5.85 | 124.08 | 111.80 |
| 1 | B | 37 | ASP | CB-CG-OD2 | 5.79 | 123.51 | 118.30 |
| 1 | D | 31 | ARG | NE-CZ-NH2 | 5.71 | 123.15 | 120.30 |
| 1 | B | 184 | GLU | OE1-CD-OE2 | -5.70 | 116.46 | 123.30 |
| 1 | D | 168 | ASP | CB-CG-OD2 | -5.67 | 113.19 | 118.30 |
| 1 | A | 97 | GLU | CA-CB-CG | 5.60 | 125.73 | 113.40 |
| 1 | A | 91 | ASP | CB-CG-OD1 | 5.58 | 123.33 | 118.30 |
| 1 | D | 328 | TYR | CB-CG-CD2 | 5.58 | 124.35 | 121.00 |
| 1 | C | 267 | ARG | CA-CB-CG | 5.57 | 125.66 | 113.40 |
| 1 | C | 360 | ARG | CA-CB-CG | 5.57 | 125.65 | 113.40 |
| 1 | C | 267 | ARG | CB-CA-C | 5.56 | 121.53 | 110.40 |
| 1 | D | 355 | ARG | NE-CZ-NH1 | -5.49 | 117.56 | 120.30 |
| 1 | D | 264 | TYR | CB-CG-CD2 | -5.45 | 117.73 | 121.00 |
| 1 | D | 267 | ARG | NE-CZ-NH1 | -5.45 | 117.58 | 120.30 |
| 1 | A | 30 | TYR | CB-CG-CD2 | 5.41 | 124.25 | 121.00 |
| 1 | A | 102 | ALA | CB-CA-C | 5.40 | 118.20 | 110.10 |
| 1 | C | 136 | ARG | CD-NE-CZ | 5.40 | 131.16 | 123.60 |
| 1 | D | 137 | ARG | CG-CD-NE | 5.37 | 123.09 | 111.80 |
| 1 | D | 22 | ASP | CB-CG-OD1 | 5.35 | 123.11 | 118.30 |
| 1 | B | 267 | ARG | CA-CB-CG | 5.30 | 125.05 | 113.40 |
| 1 | B | 360 | ARG | NE-CZ-NH2 | -5.28 | 117.66 | 120.30 |
| 1 | B | 338 | ARG | CD-NE-CZ | 5.27 | 130.98 | 123.60 |
| 1 | B | 290 | GLU | OE1-CD-OE2 | 5.26 | 129.62 | 123.30 |
| 1 | A | 31 | ARG | NE-CZ-NH1 | -5.24 | 117.68 | 120.30 |
| 1 | C | 265 | ASP | CA-CB-CG | 5.23 | 124.91 | 113.40 |
| 1 | D | 234 | ASP | CB-CG-OD1 | 5.22 | 123.00 | 118.30 |
| 1 | A | 136 | ARG | CD-NE-CZ | 5.21 | 130.89 | 123.60 |
| 1 | D | 168 | ASP | CB-CG-OD1 | 5.20 | 122.97 | 118.30 |
| 1 | D | 267 | ARG | CA-CB-CG | 5.19 | 124.82 | 113.40 |
| 1 | B | 267 | ARG | CB-CA-C | 5.18 | 120.75 | 110.40 |
| 1 | C | 288 | TYR | CB-CG-CD2 | -5.13 | 117.92 | 121.00 |
| 1 | D | 136 | ARG | NE-CZ-NH1 | 5.13 | 122.86 | 120.30 |
| 1 | B | 223 | GLU | OE1-CD-OE2 | -5.07 | 117.22 | 123.30 |
| 1 | C | 321 | TYR | CB-CG-CD2 | -5.06 | 117.96 | 121.00 |
| 1 | B | 136 | ARG | NE-CZ-NH2 | -5.04 | 117.78 | 120.30 |
| 1 | A | 163 | ARG | CD-NE-CZ | 5.02 | 130.62 | 123.60 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 2935 | 0 | 2966 | 97 | 328 |
| 1 | B | 2926 | 0 | 2958 | 70 | 2668 |
| 1 | C | 2963 | 0 | 2990 | 91 | 240 |
| 1 | D | 2914 | 0 | 2949 | 84 | 2525 |
| All | All | 11738 | 0 | 11863 | 309 | 2931 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (309) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:358:ARG:HD2 | 1:B:259:ARG:NH1 | 1.81 | 0.96 |
| 1:D:35:ILE:HD11 | 1:D:266:PRO:HB2 | 1.55 | 0.88 |
| 1:A:358:ARG:NH1 | 1:B:259:ARG:HD2 | 1.89 | 0.87 |
| 1:A:358:ARG:HD2 | 1:B:259:ARG:HH11 | 1.40 | 0.87 |
| 1:C:258:HIS:HD2 | 1:C:260:VAL:H | 1.20 | 0.86 |
| 1:C:179:LEU:HD22 | 1:C:267:ARG:HB2 | 1.58 | 0.86 |
| 1:A:179:LEU:HD22 | 1:A:267:ARG:HB2 | 1.61 | 0.82 |
| 1:A:358:ARG:HH11 | 1:B:259:ARG:HD2 | 1.42 | 0.81 |
| 1:B:134:VAL:HG12 | 1:B:329:MET:HE1 | 1.63 | 0.79 |
| 1:B:88:LYS:N | 1:B:137:ARG:HH21 | 1.82 | 0.78 |
| 1:C:277:THR:HG22 | 1:C:278:LEU:HG | 1.66 | 0.77 |
| 1:D:258:HIS:HD2 | 1:D:261:TYR:H | 1.31 | 0.77 |
| 1:A:228:GLN:HE22 | 1:A:254:MET:H | 1.32 | 0.76 |
| 1:D:179:LEU:HD22 | 1:D:267:ARG:HB2 | 1.67 | 0.76 |
| 1:D:15:VAL:HG22 | 1:D:353:GLN:HE22 | 1.52 | 0.75 |
| 1:A:62:LEU:HD21 | 1:A:66:LYS:HE3 | 1.69 | 0.75 |
| 1:A:258:HIS:HD2 | 1:A:260:VAL:H | 1.35 | 0.74 |
| 1:A:25:LYS:HD2 | 1:A:27:ILE:HD11 | 1.70 | 0.74 |
| 1:B:123:ILE:HD12 | 1:B:202:MET:HE3 | 1.69 | 0.74 |
| 1:A:366:PRO:HG3 | 1:A:369:GLN:NE2 | 2.04 | 0.72 |
| 1:C:228:GLN:HE22 | 1:C:254:MET:H | 1.39 | 0.71 |
| 1:A:366:PRO:HG3 | 1:A:369:GLN:HE21 | 1.56 | 0.71 |
| 1:A:119:LYS:HB3 | 1:A:202:MET:HE1 | 1.71 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:309:TYR:HB3 | 1:D:310:PRO:CD | 2.22 | 0.70 |
| 1:C:258:HIS:CD2 | 1:C:260:VAL:H | 2.08 | 0.70 |
| 1:A:232:ILE:HD12 | 1:A:291:ILE:HG23 | 1.74 | 0.69 |
| 1:D:15:VAL:CG2 | 1:D:353:GLN:HE22 | 2.06 | 0.68 |
| 1:D:258:HIS:CD2 | 1:D:261:TYR:H | 2.12 | 0.67 |
| 1:C:106:ILE:HG13 | 1:D:86:MET:HE1 | 1.76 | 0.67 |
| 1:D:147:GLU:HB3 | 1:D:148:PRO:HD2 | 1.76 | 0.67 |
| 1:B:35:ILE:HD11 | 1:B:266:PRO:HB2 | 1.78 | 0.66 |
| 1:B:173:MET:HE2 | 1:B:173:MET:O | 1.95 | 0.66 |
| 1:A:245:LYS:HB3 | 1:A:251:ASN:HD22 | 1.61 | 0.65 |
| 1:A:303:PHE:HB3 | 1:A:308:ILE:HB | 1.78 | 0.65 |
| 1:A:88:LYS:N | 1:A:137:ARG:HH21 | 1.94 | 0.65 |
| 1:C:25:LYS:HE2 | 1:C:27:ILE:HD11 | 1.79 | 0.65 |
| 1:C:193:LEU:HD23 | 1:C:346:ILE:HG22 | 1.78 | 0.64 |
| 1:A:111:LYS:HB3 | 1:A:114:GLU:HG3 | 1.78 | 0.64 |
| 1:A:215:GLY:HA3 | 1:B:198:THR:O | 1.98 | 0.64 |
| 1:C:303:PHE:HB3 | 1:C:308:ILE:HB | 1.81 | 0.62 |
| 1:B:243:ASN:O | 1:B:247:VAL:HB | 2.00 | 0.61 |
| 1:C:88:LYS:N | 1:C:137:ARG:HH21 | 1.98 | 0.61 |
| 1:A:138:LYS:HD3 | 1:A:328:TYR:CE1 | 2.36 | 0.61 |
| 1:A:14:LYS:HE2 | 1:A:345:HIS:ND1 | 2.16 | 0.61 |
| 1:A:90:ALA:O | 1:A:138:LYS:HE3 | 2.01 | 0.61 |
| 1:A:272:LYS:HE2 | 1:A:315:TYR:CZ | 2.36 | 0.59 |
| 1:D:39:VAL:HG21 | 1:D:270:ILE:HD13 | 1.82 | 0.59 |
| 1:A:343:LEU:O | 1:A:347:ILE:HG13 | 2.03 | 0.59 |
| 1:B:84:TYR:HA | 1:B:137:ARG:HD3 | 1.83 | 0.59 |
| 1:B:86:MET:HB3 | 1:B:87:PRO:HD2 | 1.84 | 0.59 |
| 1:C:86:MET:HE2 | 1:D:105:SER:OG | 2.03 | 0.59 |
| 1:D:233:GLY:O | 1:D:287:ARG:NH1 | 2.35 | 0.59 |
| 1:C:242:PHE:CG | 1:C:298:LEU:HD12 | 2.38 | 0.58 |
| 1:D:303:PHE:HB3 | 1:D:308:ILE:HB | 1.83 | 0.58 |
| 1:D:90:ALA:O | 1:D:138:LYS:HE3 | 2.04 | 0.58 |
| 1:D:220:GLY:O | 1:D:224:GLU:HG2 | 2.03 | 0.58 |
| 1:D:238:VAL:HG11 | 1:D:294:LYS:HB2 | 1.86 | 0.58 |
| 1:C:355:ARG:HD3 | 1:D:6:LYS:HB2 | 1.86 | 0.57 |
| 1:D:255:GLY:HA3 | 1:D:314:PHE:HD1 | 1.70 | 0.57 |
| 1:D:53:TYR:CE2 | 1:D:117:LYS:HD2 | 2.40 | 0.57 |
| 1:D:153:ALA:HB1 | 1:D:173:MET:HB3 | 1.87 | 0.57 |
| 1:D:75:VAL:HG12 | 1:D:126:LYS:HG3 | 1.86 | 0.57 |
| 1:A:228:GLN:NE2 | 1:A:254:MET:H | 2.00 | 0.57 |
| 1:C:106:ILE:HG13 | 1:D:86:MET:CE | 2.35 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:258:HIS:CD2 | 1:C:261:TYR:H | 2.23 | 0.57 |
| 1:A:259:ARG:HD3 | 1:B:358:ARG:NH1 | 2.20 | 0.56 |
| 1:C:272:LYS:NZ | 1:C:296:GLU:OE1 | 2.38 | 0.56 |
| 1:B:356:LEU:HD23 | 1:B:358:ARG:HH21 | 1.70 | 0.56 |
| 1:A:240:ASN:O | 1:A:244:ASP:HB2 | 2.05 | 0.56 |
| 1:C:144:ARG:NH1 | 1:C:162:ALA:HA | 2.21 | 0.56 |
| 1:C:8:LEU:O | 1:D:359:PRO:HA | 2.05 | 0.56 |
| 1:B:258:HIS:CD2 | 1:B:261:TYR:H | 2.23 | 0.56 |
| 1:B:49:TYR:OH | 1:B:55:LYS:HE3 | 2.04 | 0.56 |
| 1:D:15:VAL:HG22 | 1:D:353:GLN:NE2 | 2.21 | 0.55 |
| 1:B:258:HIS:HD2 | 1:B:260:VAL:H | 1.54 | 0.55 |
| 1:C:367:GLU:O | 1:D:29:ARG:HD2 | 2.07 | 0.55 |
| 1:C:158:LEU:CD1 | 1:C:165:PRO:HD3 | 2.38 | 0.54 |
| 1:D:112:TRP:HH2 | 1:D:346:ILE:HG13 | 1.72 | 0.54 |
| 1:D:138:LYS:HD3 | 1:D:328:TYR:CE1 | 2.42 | 0.54 |
| 1:B:21:ILE:HG12 | 1:B:183:HIS:CE1 | 2.43 | 0.54 |
| 1:C:132:ALA:O | 1:C:135:TYR:HB3 | 2.08 | 0.54 |
| 1:D:75:VAL:HG12 | 1:D:126:LYS:CG | 2.37 | 0.54 |
| 1:C:171:ASN:O | 1:C:175:LYS:HG2 | 2.08 | 0.54 |
| 1:C:44:TYR:O | 1:C:48:ILE:HG13 | 2.08 | 0.53 |
| 1:A:171:ASN:O | 1:A:175:LYS:HG2 | 2.08 | 0.53 |
| 1:C:123:ILE:HD12 | 1:C:202:MET:CE | 2.39 | 0.53 |
| 1:A:8:LEU:HD12 | 1:B:357:ILE:HG23 | 1.90 | 0.53 |
| 1:A:224:GLU:HB3 | 1:A:254:MET:HE2 | 1.91 | 0.53 |
| 1:A:172:ALA:HA | 1:A:274:LEU:HD22 | 1.91 | 0.53 |
| 1:C:88:LYS:O | 1:C:138:LYS:HD2 | 2.09 | 0.53 |
| 1:C:144:ARG:HH12 | 1:C:162:ALA:HA | 1.73 | 0.53 |
| 1:C:108:LYS:O | 1:C:109:ASN:HB2 | 2.09 | 0.53 |
| 1:D:70:ASN:OD1 | 1:D:148:PRO:HA | 2.08 | 0.53 |
| 1:A:287:ARG:O | 1:A:291:ILE:HD12 | 2.09 | 0.52 |
| 1:B:74:GLU:O | 1:B:126:LYS:HE3 | 2.09 | 0.52 |
| 1:A:127:MET:HE3 | 1:A:130:LEU:HB2 | 1.92 | 0.52 |
| 1:B:347:ILE:HG23 | 1:B:351:GLU:OE1 | 2.10 | 0.52 |
| 1:A:119:LYS:HG3 | 1:A:202:MET:HE1 | 1.91 | 0.52 |
| 1:D:133:ASN:O | 1:D:137:ARG:HB2 | 2.08 | 0.52 |
| 1:D:137:ARG:HD2 | 1:D:137:ARG:O | 2.10 | 0.52 |
| 1:D:123:ILE:HD12 | 1:D:202:MET:CE | 2.40 | 0.52 |
| 1:A:119:LYS:HG3 | 1:A:202:MET:CE | 2.39 | 0.52 |
| 1:D:309:TYR:HB3 | 1:D:310:PRO:HD2 | 1.91 | 0.51 |
| 1:D:72:GLU:HG3 | 1:D:122:SER:HB3 | 1.92 | 0.51 |
| 1:C:118:GLU:HA | 1:C:121:ILE:HD12 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:123:ILE:HD12 | 1:B:202:MET:CE | 2.37 | 0.51 |
| 1:A:274:LEU:O | 1:A:278:LEU:HD12 | 2.11 | 0.51 |
| 1:D:171:ASN:O | 1:D:175:LYS:HG2 | 2.11 | 0.51 |
| 1:D:171:ASN:OD1 | 1:D:175:LYS:HE3 | 2.11 | 0.51 |
| 1:B:328:TYR:CD1 | 1:B:329:MET:HG2 | 2.46 | 0.51 |
| 1:B:103:LEU:HD13 | 1:B:203:TYR:CE2 | 2.46 | 0.51 |
| 1:D:72:GLU:CG | 1:D:122:SER:HB3 | 2.41 | 0.51 |
| 1:D:258:HIS:CD2 | 1:D:260:VAL:H | 2.28 | 0.51 |
| 1:A:122:SER:O | 1:A:126:LYS:HD2 | 2.10 | 0.51 |
| 1:A:183:HIS:HE1 | 1:A:261:TYR:OH | 1.94 | 0.51 |
| 1:C:228:GLN:NE2 | 1:C:254:MET:H | 2.06 | 0.51 |
| 1:C:267:ARG:NH1 | 1:C:312:THR:HG21 | 2.26 | 0.50 |
| 1:B:258:HIS:CD2 | 1:B:260:VAL:H | 2.30 | 0.50 |
| 1:B:258:HIS:HD2 | 1:B:261:TYR:H | 1.60 | 0.50 |
| 1:B:122:SER:O | 1:B:126:LYS:HG3 | 2.11 | 0.50 |
| 1:C:309:TYR:HB3 | 1:C:310:PRO:HD2 | 1.93 | 0.50 |
| 1:C:238:VAL:HG21 | 1:C:294:LYS:HD2 | 1.93 | 0.50 |
| 1:A:97:GLU:OE2 | 1:A:211:ALA:HA | 2.11 | 0.50 |
| 1:C:300:ILE:HG23 | 1:C:304:SER:HB3 | 1.94 | 0.50 |
| 1:D:14:LYS:HB2 | 1:D:353:GLN:OE1 | 2.12 | 0.50 |
| 1:B:280:GLU:H | 1:B:280:GLU:CD | 2.15 | 0.49 |
| 1:C:84:TYR:HA | 1:C:137:ARG:HD3 | 1.94 | 0.49 |
| 1:C:154:LYS:HG3 | 1:C:170:ILE:HD13 | 1.95 | 0.49 |
| 1:C:183:HIS:O | 1:C:184:GLU:HB2 | 2.12 | 0.49 |
| 1:D:31:ARG:NE | 1:D:54:GLY:HA2 | 2.27 | 0.49 |
| 1:A:83:ILE:O | 1:A:137:ARG:HD3 | 2.12 | 0.49 |
| 1:A:106:ILE:HG13 | 1:B:86:MET:HE1 | 1.95 | 0.49 |
| 1:A:95:LEU:HD12 | 1:A:134:VAL:HG13 | 1.95 | 0.49 |
| 1:A:80:LEU:HD11 | 1:A:145:ILE:HD11 | 1.94 | 0.49 |
| 1:A:241:TRP:CE2 | 1:A:245:LYS:HG3 | 2.47 | 0.49 |
| 1:A:286:ARG:O | 1:A:290:GLU:HG3 | 2.13 | 0.49 |
| 1:B:171:ASN:OD1 | 1:B:175:LYS:HE3 | 2.13 | 0.49 |
| 1:A:119:LYS:CB | 1:A:202:MET:HE1 | 2.41 | 0.48 |
| 1:B:115:ASN:ND2 | 1:B:118:GLU:HG2 | 2.26 | 0.48 |
| 1:C:166:THR:O | 1:C:169:GLU:HB2 | 2.13 | 0.48 |
| 1:A:89:GLU:O | 1:B:108:LYS:HE3 | 2.14 | 0.48 |
| 1:C:347:ILE:O | 1:C:351:GLU:HB2 | 2.13 | 0.48 |
| 1:C:297:GLU:HG2 | 1:C:301:LYS:NZ | 2.28 | 0.48 |
| 1:A:70:ASN:OD1 | 1:A:148:PRO:HA | 2.12 | 0.48 |
| 1:B:88:LYS:CA | 1:B:137:ARG:HH21 | 2.26 | 0.48 |
| 1:C:57:PRO:HG3 | 1:C:62:LEU:HD13 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:280:GLU:H | 1:A:280:GLU:CD | 2.17 | 0.48 |
| 1:D:296:GLU:O | 1:D:300:ILE:HG13 | 2.13 | 0.48 |
| 1:A:232:ILE:HD12 | 1:A:291:ILE:CG2 | 2.41 | 0.48 |
| 1:A:106:ILE:HG13 | 1:B:86:MET:CE | 2.44 | 0.48 |
| 1:B:290:GLU:O | 1:B:294:LYS:HG3 | 2.14 | 0.48 |
| 1:D:86:MET:HB3 | 1:D:87:PRO:HD2 | 1.96 | 0.48 |
| 1:A:154:LYS:HD2 | 1:A:170:ILE:CD1 | 2.44 | 0.48 |
| 1:C:185:VAL:O | 1:D:359:PRO:HD2 | 2.14 | 0.48 |
| 1:C:35:ILE:HD13 | 1:C:179:LEU:HD23 | 1.96 | 0.48 |
| 1:D:161:PHE:O | 1:D:162:ALA:HB3 | 2.14 | 0.47 |
| 1:B:88:LYS:HB2 | 1:B:137:ARG:NH2 | 2.29 | 0.47 |
| 1:D:262:LYS:HA | 1:D:262:LYS:HD3 | 1.73 | 0.47 |
| 1:D:154:LYS:HG2 | 1:D:158:LEU:HD22 | 1.95 | 0.47 |
| 1:A:282:ASN:HB3 | 1:A:285:ALA:CB | 2.44 | 0.47 |
| 1:A:46:GLU:HG3 | 1:A:57:PRO:CG | 2.44 | 0.47 |
| 1:B:179:LEU:HD22 | 1:B:267:ARG:HB2 | 1.96 | 0.47 |
| 1:B:116:ASP:HB3 | 1:B:347:ILE:HG12 | 1.97 | 0.47 |
| 1:C:27:ILE:HG21 | 1:C:29:ARG:NH2 | 2.30 | 0.46 |
| 1:D:134:VAL:O | 1:D:138:LYS:HG3 | 2.14 | 0.46 |
| 1:A:96:LEU:HB3 | 1:A:210:LEU:HD13 | 1.96 | 0.46 |
| 1:B:281:ARG:HD2 | 1:B:281:ARG:N | 2.31 | 0.46 |
| 1:C:35:ILE:CD1 | 1:C:179:LEU:HD23 | 2.46 | 0.46 |
| 1:D:84:TYR:CE1 | 1:D:137:ARG:HG2 | 2.50 | 0.46 |
| 1:A:119:LYS:O | 1:A:123:ILE:HG13 | 2.15 | 0.46 |
| 1:A:29:ARG:HD2 | 1:B:367:GLU:O | 2.15 | 0.46 |
| 1:A:229:PHE:HA | 1:A:291:ILE:HG21 | 1.96 | 0.46 |
| 1:A:57:PRO:HB2 | 1:A:62:LEU:HB2 | 1.97 | 0.46 |
| 1:B:228:GLN:HE22 | 1:B:254:MET:H | 1.62 | 0.46 |
| 1:A:89:GLU:CD | 1:A:89:GLU:H | 2.17 | 0.46 |
| 1:D:84:TYR:CD1 | 1:D:137:ARG:HG2 | 2.49 | 0.46 |
| 1:D:223:GLU:O | 1:D:227:LYS:HG3 | 2.16 | 0.46 |
| 1:C:282:ASN:ND2 | 1:C:285:ALA:H | 2.13 | 0.46 |
| 1:B:13:ILE:HG23 | 1:B:14:LYS:HG2 | 1.97 | 0.46 |
| 1:C:96:LEU:CD1 | 1:C:134:VAL:HG21 | 2.46 | 0.46 |
| 1:A:282:ASN:HD22 | 1:A:282:ASN:HA | 1.56 | 0.46 |
| 1:A:297:GLU:HG3 | 1:A:301:LYS:HZ2 | 1.80 | 0.46 |
| 1:A:14:LYS:HE2 | 1:A:345:HIS:CE1 | 2.51 | 0.46 |
| 1:D:136:ARG:NH1 | 1:D:141:ASN:HB3 | 2.31 | 0.46 |
| 1:C:123:ILE:HD12 | 1:C:202:MET:HE2 | 1.98 | 0.45 |
| 1:C:138:LYS:HE3 | 1:C:328:TYR:CE1 | 2.50 | 0.45 |
| 1:C:87:PRO:HB2 | 1:D:108:LYS:HZ1 | 1.80 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:108:LYS:CE | 1:D:89:GLU:HB2 | 2.45 | 0.45 |
| 1:A:96:LEU:HD13 | 1:A:134:VAL:HG21 | 1.98 | 0.45 |
| 1:D:245:LYS:HA | 1:D:249:GLN:OE1 | 2.16 | 0.45 |
| 1:A:73:TYR:CG | 1:A:146:PRO:HB2 | 2.51 | 0.45 |
| 1:B:328:TYR:CE1 | 1:B:329:MET:HG2 | 2.51 | 0.45 |
| 1:C:4:VAL:CG2 | 1:D:15:VAL:HG13 | 2.47 | 0.45 |
| 1:C:309:TYR:HB3 | 1:C:310:PRO:CD | 2.47 | 0.45 |
| 1:D:83:ILE:HG22 | 1:D:137:ARG:HG3 | 1.98 | 0.45 |
| 1:A:78:GLU:CD | 1:A:78:GLU:H | 2.20 | 0.45 |
| 1:B:119:LYS:HB3 | 1:B:202:MET:HE1 | 1.98 | 0.45 |
| 1:B:179:LEU:HD22 | 1:B:267:ARG:CB | 2.47 | 0.45 |
| 1:A:262:LYS:HB3 | 1:A:262:LYS:NZ | 2.32 | 0.45 |
| 1:C:23:GLY:HA3 | 1:C:260:VAL:O | 2.17 | 0.45 |
| 1:D:74:GLU:O | 1:D:126:LYS:HE3 | 2.17 | 0.45 |
| 1:C:127:MET:O | 1:C:131:VAL:HG23 | 2.16 | 0.45 |
| 1:B:119:LYS:HG3 | 1:B:202:MET:CE | 2.47 | 0.44 |
| 1:C:188:SER:HB3 | 1:C:218:HIS:CD2 | 2.52 | 0.44 |
| 1:B:192:ALA:HB2 | 1:B:209:ALA:HB2 | 2.00 | 0.44 |
| 1:C:142:LYS:HB2 | 1:C:143:PRO:HD2 | 1.98 | 0.44 |
| 1:B:88:LYS:O | 1:B:138:LYS:HD2 | 2.17 | 0.44 |
| 1:B:172:ALA:CB | 1:B:278:LEU:HD11 | 2.47 | 0.44 |
| 1:B:108:LYS:O | 1:B:109:ASN:HB2 | 2.18 | 0.44 |
| 1:C:242:PHE:CB | 1:C:298:LEU:HD12 | 2.48 | 0.44 |
| 1:C:36:GLU:H | 1:C:36:GLU:HG2 | 1.20 | 0.44 |
| 1:B:272:LYS:HE3 | 1:B:315:TYR:OH | 2.18 | 0.44 |
| 1:B:135:TYR:HA | 1:B:329:MET:HE3 | 1.99 | 0.44 |
| 1:B:127:MET:HG3 | 1:B:339:THR:HG21 | 1.99 | 0.44 |
| 1:C:149:SER:OG | 1:C:154:LYS:HD2 | 2.17 | 0.44 |
| 1:C:158:LEU:HD12 | 1:C:165:PRO:HD3 | 2.00 | 0.44 |
| 1:D:325:PHE:CG | 1:D:333:LEU:HD11 | 2.53 | 0.44 |
| 1:C:276:LEU:HD13 | 1:C:289:PHE:CZ | 2.53 | 0.44 |
| 1:C:363:TYR:HA | 1:D:16:THR:O | 2.18 | 0.44 |
| 1:D:276:LEU:HD13 | 1:D:289:PHE:CZ | 2.53 | 0.44 |
| 1:A:86:MET:CE | 1:B:106:ILE:HG13 | 2.48 | 0.43 |
| 1:C:106:ILE:CG1 | 1:D:86:MET:HE1 | 2.47 | 0.43 |
| 1:C:44:TYR:CD1 | 1:C:177:LEU:HB3 | 2.53 | 0.43 |
| 1:C:244:ASP:HA | 1:C:248:ASN:OD1 | 2.18 | 0.43 |
| 1:D:68:LYS:HA | 1:D:68:LYS:HD2 | 1.79 | 0.43 |
| 1:A:134:VAL:O | 1:A:138:LYS:HG3 | 2.18 | 0.43 |
| 1:A:320:PHE:CD2 | 1:A:333:LEU:HD13 | 2.52 | 0.43 |
| 1:B:281:ARG:HH11 | 1:B:281:ARG:HB3 | 1.82 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:129:THR:O | 1:D:133:ASN:ND2 | 2.51 | 0.43 |
| 1:A:65:LEU:CD1 | 1:A:121:ILE:HG12 | 2.48 | 0.43 |
| 1:D:96:LEU:HD13 | 1:D:134:VAL:HG21 | 2.01 | 0.43 |
| 1:C:360:ARG:O | 1:D:13:ILE:HG22 | 2.19 | 0.43 |
| 1:A:180:TYR:HB2 | 1:A:337:SER:OG | 2.19 | 0.43 |
| 1:A:183:HIS:HD2 | 1:A:184:GLU:OE2 | 2.00 | 0.43 |
| 1:A:6:LYS:HB3 | 1:B:355:ARG:HE | 1.83 | 0.43 |
| 1:C:188:SER:HB3 | 1:C:218:HIS:NE2 | 2.32 | 0.43 |
| 1:B:119:LYS:HG3 | 1:B:202:MET:HE2 | 2.01 | 0.43 |
| 1:C:4:VAL:HG21 | 1:D:15:VAL:HG13 | 2.01 | 0.43 |
| 1:D:149:SER:HB3 | 1:D:155:SER:OG | 2.18 | 0.43 |
| 1:D:241:TRP:CZ2 | 1:D:245:LYS:HD2 | 2.53 | 0.43 |
| 1:B:118:GLU:HA | 1:B:121:ILE:HD12 | 2.00 | 0.43 |
| 1:D:16:THR:HA | 1:D:348:GLU:OE2 | 2.18 | 0.43 |
| 1:A:172:ALA:HB2 | 1:A:278:LEU:HD11 | 2.00 | 0.43 |
| 1:A:21:ILE:HG21 | 1:A:260:VAL:HG11 | 2.00 | 0.43 |
| 1:B:110:PHE:CE1 | 1:B:119:LYS:HG2 | 2.54 | 0.43 |
| 1:B:183:HIS:CD2 | 1:B:184:GLU:HG3 | 2.54 | 0.43 |
| 1:C:20:PHE:HB2 | 1:D:363:TYR:CD2 | 2.54 | 0.42 |
| 1:A:144:ARG:NH1 | 1:A:162:ALA:HA | 2.34 | 0.42 |
| 1:A:297:GLU:HG2 | 1:A:298:LEU:HD23 | 2.00 | 0.42 |
| 1:A:172:ALA:HB3 | 1:A:323:LEU:HD21 | 2.02 | 0.42 |
| 1:A:263:THR:OG1 | 1:A:264:TYR:N | 2.52 | 0.42 |
| 1:B:133:ASN:O | 1:B:137:ARG:HB3 | 2.20 | 0.42 |
| 1:D:179:LEU:HD22 | 1:D:267:ARG:CB | 2.45 | 0.42 |
| 1:D:45:GLU:HG2 | 1:D:66:LYS:HG2 | 2.01 | 0.42 |
| 1:D:5:SER:OG | 1:D:8:LEU:HD23 | 2.18 | 0.42 |
| 1:A:183:HIS:O | 1:A:184:GLU:HB2 | 2.20 | 0.42 |
| 1:A:243:ASN:HA | 1:A:247:VAL:CG2 | 2.49 | 0.42 |
| 1:B:96:LEU:HA | 1:B:96:LEU:HD12 | 1.93 | 0.42 |
| 1:C:31:ARG:NE | 1:C:54:GLY:HA2 | 2.34 | 0.42 |
| 1:A:127:MET:O | 1:A:131:VAL:HG23 | 2.19 | 0.42 |
| 1:A:245:LYS:O | 1:A:249:GLN:HB3 | 2.19 | 0.42 |
| 1:A:60:LYS:HD3 | 1:A:61:GLU:N | 2.35 | 0.42 |
| 1:C:274:LEU:O | 1:C:277:THR:HB | 2.20 | 0.42 |
| 1:C:325:PHE:CG | 1:C:333:LEU:HD11 | 2.55 | 0.42 |
| 1:A:282:ASN:HB3 | 1:A:285:ALA:HB3 | 2.01 | 0.42 |
| 1:B:84:TYR:CZ | 1:B:137:ARG:HB2 | 2.55 | 0.42 |
| 1:C:9:GLU:HG2 | 1:C:259:ARG:HH21 | 1.84 | 0.42 |
| 1:C:286:ARG:HH11 | 1:C:286:ARG:HD3 | 1.63 | 0.42 |
| 1:C:4:VAL:HG22 | 1:D:12:ILE:CG2 | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:15:VAL:HG13 | 1:B:4:VAL:CG2 | 2.49 | 0.42 |
| 1:B:272:LYS:HG3 | 1:B:315:TYR:CZ | 2.55 | 0.42 |
| 1:C:264:TYR:CD2 | 1:C:269:LYS:HG3 | 2.55 | 0.42 |
| 1:C:87:PRO:HB2 | 1:D:108:LYS:NZ | 2.35 | 0.42 |
| 1:C:297:GLU:HG2 | 1:C:301:LYS:HE3 | 2.02 | 0.41 |
| 1:C:43:SER:HA | 1:C:174:ASP:OD1 | 2.19 | 0.41 |
| 1:C:89:GLU:CD | 1:C:89:GLU:H | 2.22 | 0.41 |
| 1:A:68:LYS:O | 1:A:69:LEU:C | 2.57 | 0.41 |
| 1:B:36:GLU:HG2 | 1:B:36:GLU:H | 1.28 | 0.41 |
| 1:C:244:ASP:O | 1:C:249:GLN:HB2 | 2.19 | 0.41 |
| 1:D:22:ASP:OD2 | 1:D:25:LYS:HD2 | 2.20 | 0.41 |
| 1:A:39:VAL:HG21 | 1:A:270:ILE:HG21 | 2.01 | 0.41 |
| 1:A:92:ALA:HB1 | 1:A:329:MET:HE1 | 2.02 | 0.41 |
| 1:C:52:LEU:O | 1:C:117:LYS:HD3 | 2.20 | 0.41 |
| 1:A:150:ASP:OD1 | 1:A:154:LYS:NZ | 2.46 | 0.41 |
| 1:B:282:ASN:HB3 | 1:B:285:ALA:HB3 | 2.01 | 0.41 |
| 1:C:49:TYR:O | 1:C:53:TYR:HB2 | 2.21 | 0.41 |
| 1:C:357:ILE:N | 1:C:357:ILE:HD12 | 2.36 | 0.41 |
| 1:D:79:VAL:O | 1:D:83:ILE:HD12 | 2.20 | 0.41 |
| 1:A:182:ASP:O | 1:A:183:HIS:HB2 | 2.21 | 0.41 |
| 1:C:161:PHE:O | 1:C:162:ALA:HB3 | 2.21 | 0.41 |
| 1:C:39:VAL:HG21 | 1:C:270:ILE:HD13 | 2.01 | 0.41 |
| 1:A:234:ASP:HA | 1:A:235:PRO:HD3 | 1.80 | 0.41 |
| 1:A:279:ILE:HG22 | 1:A:285:ALA:HB1 | 2.03 | 0.41 |
| 1:A:138:LYS:HD3 | 1:A:328:TYR:CD1 | 2.56 | 0.40 |
| 1:D:263:THR:HG23 | 1:D:264:TYR:O | 2.21 | 0.40 |
| 1:D:289:PHE:HA | 1:D:318:ILE:HD13 | 2.03 | 0.40 |
| 1:A:88:LYS:HB3 | 1:A:137:ARG:NH2 | 2.36 | 0.40 |
| 1:A:25:LYS:HB2 | 1:A:27:ILE:HG13 | 2.02 | 0.40 |
| 1:B:303:PHE:HB3 | 1:B:308:ILE:HB | 2.03 | 0.40 |
| 1:C:96:LEU:HB3 | 1:C:210:LEU:HD13 | 2.03 | 0.40 |
| 1:D:297:GLU:O | 1:D:297:GLU:HG2 | 2.20 | 0.40 |
| 1:D:309:TYR:CB | 1:D:310:PRO:CD | 2.92 | 0.40 |
| 1:B:22:ASP:HB3 | 1:B:27:ILE:HB | 2.03 | 0.40 |
| 1:C:325:PHE:HA | 1:C:326:PRO:HD3 | 1.89 | 0.40 |
| 1:C:360:ARG:NH2 | 1:D:10:ASN:OD1 | 2.54 | 0.40 |
| 1:A:259:ARG:HA | 1:A:259:ARG:HD2 | 1.80 | 0.40 |
| 1:C:108:LYS:NZ | 1:D:89:GLU:HB2 | 2.37 | 0.40 |
| 1:C:182:ASP:HA | 1:C:338:ARG:NE | 2.36 | 0.40 |
| 1:D:175:LYS:HB2 | 1:D:274:LEU:HD11 | 2.03 | 0.40 |

All (2931) symmetry-related close contacts are listed below. The label for Atom-2 includes the

symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:312:THR:OG1 | 1:D:28:LEU:CB[2_546] | 0.15 | 2.05 |
| 1:B:44:TYR:N | 1:D:31:ARG:NH2[2_546] | 0.18 | 2.02 |
| 1:A:365:GLY:C | 1:D:152:PHE:O[2_546] | 0.21 | 1.99 |
| 1:B:48:ILE:N | 1:D:49:TYR:O[2_546] | 0.22 | 1.98 |
| 1:B:49:TYR:CB | 1:D:53:TYR:CE1[2_546] | 0.24 | 1.96 |
| 1:B:265:ASP:C | 1:D:267:ARG:CZ[2_546] | 0.25 | 1.95 |
| 1:B:336:LEU:O | 1:D:33:TYR:CZ[2_546] | 0.25 | 1.95 |
| 1:B:333:LEU:CB | 1:C:368:TYR:CA[2_546] | 0.28 | 1.92 |
| 1:B:175:LYS:O | 1:D:18:LEU:O[2_546] | 0.31 | 1.89 |
| 1:B:53:TYR:C | 1:D:65:LEU:CA[2_546] | 0.31 | 1.89 |
| 1:A:367:GLU:CG | 1:D:156:PHE:CZ[2_546] | 0.33 | 1.87 |
| 1:B:184:GLU:O | 1:D:39:VAL:O[2_546] | 0.35 | 1.85 |
| 1:B:58:THR:O | 1:D:115:ASN:ND2[2_546] | 0.35 | 1.85 |
| 1:B:271:PHE:CD2 | 1:D:20:PHE:C[2_546] | 0.35 | 1.85 |
| 1:A:369:GLN:CB | 1:D:124:ILE:O[2_546] | 0.35 | 1.85 |
| 1:B:120:ALA:N | 1:D:58:THR:CG2[2_546] | 0.36 | 1.84 |
| 1:B:299:GLY:CA | 1:D:308:ILE:N[2_546] | 0.36 | 1.84 |
| 1:B:175:LYS:N | 1:D:18:LEU:N[2_546] | 0.37 | 1.83 |
| 1:B:48:ILE:O | 1:D:49:TYR:CG[2_546] | 0.38 | 1.82 |
| 1:B:20:PHE:O | 1:D:177:LEU:N[2_546] | 0.39 | 1.81 |
| 1:B:242:PHE:CG | 1:D:305:SER:O[2_546] | 0.39 | 1.81 |
| 1:A:360:ARG:CZ | 1:D:277:THR:OG1[2_546] | 0.40 | 1.80 |
| 1:B:46:GLU:N | 1:D:52:LEU:O[2_546] | 0.41 | 1.79 |
| 1:B:117:LYS:CB | 1:D:61:GLU:N[2_546] | 0.42 | 1.78 |
| 1:B:263:THR:CB | 1:D:313:ASP:CA[2_546] | 0.43 | 1.77 |
| 1:B:302:GLN:CA | 1:D:303:PHE:CB[2_546] | 0.43 | 1.77 |
| 1:B:59:LYS:N | 1:D:115:ASN:CA[2_546] | 0.43 | 1.77 |
| 1:B:266:PRO:N | 1:D:267:ARG:NH1[2_546] | 0.43 | 1.77 |
| 1:B:308:ILE:C | 1:D:310:PRO:CA[2_546] | 0.44 | 1.76 |
| 1:A:109:ASN:OD1 | 1:A:250:LYS:CA[2_556] | 0.44 | 1.76 |
| 1:B:21:ILE:CA | 1:D:176:ALA:CA[2_546] | 0.45 | 1.75 |
| 1:B:17:ASN:CG | 1:D:151:SER:CA[2_546] | 0.46 | 1.74 |
| 1:B:342:TRP:CG | 1:C:371:TYR:CE2[2_546] | 0.46 | 1.74 |
| 1:B:264:TYR:O | 1:D:312:THR:CG2[2_546] | 0.47 | 1.73 |
| 1:B:264:TYR:OH | 1:D:258:HIS:CD2[2_546] | 0.47 | 1.73 |
| 1:B:186:PRO:CB | 1:D:40:ASN:ND2[2_546] | 0.48 | 1.72 |
| 1:B:332:ALA:CA | 1:C:368:TYR:CE2[2_546] | 0.48 | 1.72 |
| 1:B:56:LEU:N | 1:D:121:ILE:CB[2_546] | 0.49 | 1.71 |
| 1:B:269:LYS:N | 1:D:183:HIS:NE2[2_546] | 0.49 | 1.71 |
| 1:B:342:TRP:CD2 | 1:C:371:TYR:CD2[2_546] | 0.49 | 1.71 |
| 1:B:336:LEU:CG | 1:C:369:GLN:CD[2_546] | 0.49 | 1.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:308:ILE:CB | 1:D:310:PRO:CG[2_546] | 0.49 | 1.71 |
| 1:B:311:ASN:CB | 1:D:266:PRO:N[2_546] | 0.51 | 1.69 |
| 1:B:341:GLY:CA | 1:D:46:GLU:OE2[2_546] | 0.51 | 1.69 |
| 1:B:309:TYR:N | 1:D:310:PRO:C[2_546] | 0.51 | 1.69 |
| 1:B:169:GLU:C | 1:C:364:VAL:CB[2_546] | 0.51 | 1.69 |
| 1:B:30:TYR:N | 1:D:44:TYR:CE1[2_546] | 0.52 | 1.68 |
| 1:B:28:LEU:CD1 | 1:D:178:ILE:C[2_546] | 0.52 | 1.68 |
| 1:A:107:ASP:O | 1:A:248:ASN:OD1[2_556] | 0.52 | 1.68 |
| 1:B:299:GLY:C | 1:D:308:ILE:CA[2_546] | 0.53 | 1.67 |
| 1:B:303:PHE:C | 1:D:256:PHE:CD2[2_546] | 0.53 | 1.67 |
| 1:A:360:ARG:NH1 | 1:D:277:THR:CB[2_546] | 0.53 | 1.67 |
| 1:A:111:LYS:CA | 1:A:245:LYS:CD[2_556] | 0.54 | 1.66 |
| 1:B:309:TYR:CE1 | 1:D:255:GLY:O[2_546] | 0.54 | 1.66 |
| 1:B:188:SER:CA | 1:D:41:TYR:OH[2_546] | 0.54 | 1.66 |
| 1:B:18:LEU:CD1 | 1:D:43:SER:OG[2_546] | 0.54 | 1.66 |
| 1:B:172:ALA:CB | 1:C:363:TYR:CA[2_546] | 0.55 | 1.65 |
| 1:B:256:PHE:CA | 1:D:264:TYR:CA[2_546] | 0.56 | 1.64 |
| 1:A:108:LYS:N | 1:A:248:ASN:CB[2_556] | 0.56 | 1.64 |
| 1:A:361:ALA:O | 1:D:171:ASN:CB[2_546] | 0.56 | 1.64 |
| 1:B:40:ASN:OD1 | 1:D:189:THR:CG2[2_546] | 0.57 | 1.63 |
| 1:B:258:HIS:CB | 1:D:269:LYS:N[2_546] | 0.57 | 1.63 |
| 1:B:179:LEU:CA | 1:D:30:TYR:CD2[2_546] | 0.59 | 1.61 |
| 1:B:260:VAL:CG2 | 1:D:270:ILE:O[2_546] | 0.59 | 1.61 |
| 1:B:262:LYS:CB | 1:D:315:TYR:N[2_546] | 0.59 | 1.61 |
| 1:B:56:LEU:CB | 1:D:121:ILE:N[2_546] | 0.59 | 1.61 |
| 1:B:342:TRP:N | 1:C:371:TYR:OH[2_546] | 0.59 | 1.61 |
| 1:B:172:ALA:O | 1:C:363:TYR:CD1[2_546] | 0.60 | 1.60 |
| 1:B:265:ASP:OD1 | 1:D:267:ARG:CD[2_546] | 0.60 | 1.60 |
| 1:A:280:GLU:CA | 1:B:248:ASN:O[2_546] | 0.60 | 1.60 |
| 1:B:112:TRP:CH2 | 1:D:59:LYS:CE[2_546] | 0.61 | 1.59 |
| 1:B:206:LEU:CD1 | 1:C:372:VAL:CG1[2_546] | 0.61 | 1.59 |
| 1:B:183:HIS:C | 1:D:39:VAL:CB[2_546] | 0.61 | 1.59 |
| 1:A:363:TYR:N | 1:D:170:ILE:C[2_546] | 0.62 | 1.58 |
| 1:B:171:ASN:O | 1:D:16:THR:C[2_546] | 0.62 | 1.58 |
| 1:B:35:ILE:CB | 1:D:181:THR:C[2_546] | 0.62 | 1.58 |
| 1:B:177:LEU:CA | 1:D:31:ARG:CA[2_546] | 0.62 | 1.58 |
| 1:B:61:GLU:CD | 1:D:118:GLU:CD[2_546] | 0.63 | 1.57 |
| 1:B:256:PHE:C | 1:D:264:TYR:CB[2_546] | 0.64 | 1.56 |
| 1:B:175:LYS:C | 1:D:18:LEU:C[2_546] | 0.64 | 1.56 |
| 1:B:179:LEU:CD1 | 1:D:19:THR:CG2[2_546] | 0.64 | 1.56 |
| 1:B:334:PHE:CD1 | 1:D:34:ASN:CB[2_546] | 0.64 | 1.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:308:ILE:CA | 1:D:310:PRO:CB[2_546] | 0.65 | 1.55 |
| 1:B:24:GLU:CD | 1:D:317:GLY:O[2_546] | 0.65 | 1.55 |
| 1:B:304:SER:CA | 1:D:256:PHE:CB[2_546] | 0.65 | 1.55 |
| 1:B:256:PHE:O | 1:D:264:TYR:CB[2_546] | 0.66 | 1.54 |
| 1:B:273:LYS:NZ | 1:D:185:VAL:CB[2_546] | 0.66 | 1.54 |
| 1:B:171:ASN:CB | 1:D:15:VAL:C[2_546] | 0.66 | 1.54 |
| 1:B:308:ILE:CG2 | 1:D:310:PRO:CD[2_546] | 0.66 | 1.54 |
| 1:B:264:TYR:CE2 | 1:D:258:HIS:CE1[2_546] | 0.66 | 1.54 |
| 1:B:24:GLU:CA | 1:D:317:GLY:N[2_546] | 0.66 | 1.54 |
| 1:B:56:LEU:CD1 | 1:D:120:ALA:O[2_546] | 0.66 | 1.54 |
| 1:B:188:SER:C | 1:D:41:TYR:CE2[2_546] | 0.67 | 1.53 |
| 1:B:259:ARG:O | 1:D:273:LYS:N[2_546] | 0.67 | 1.53 |
| 1:B:315:TYR:C | 1:D:22:ASP:N[2_546] | 0.67 | 1.53 |
| 1:B:17:ASN:OD1 | 1:D:151:SER:C[2_546] | 0.67 | 1.53 |
| 1:B:351:GLU:OE1 | 1:D:63:ASN:ND2[2_546] | 0.67 | 1.53 |
| 1:B:171:ASN:CB | 1:D:16:THR:N[2_546] | 0.68 | 1.52 |
| 1:B:242:PHE:CE2 | 1:D:306:LYS:N[2_546] | 0.68 | 1.52 |
| 1:A:364:VAL:C | 1:D:154:LYS:N[2_546] | 0.68 | 1.52 |
| 1:B:23:GLY:C | 1:D:316:SER:CA[2_546] | 0.68 | 1.52 |
| 1:B:26:GLY:C | 1:D:180:TYR:CZ[2_546] | 0.69 | 1.51 |
| 1:A:367:GLU:CB | 1:D:156:PHE:CD1[2_546] | 0.69 | 1.51 |
| 1:B:262:LYS:CD | 1:D:315:TYR:CG[2_546] | 0.69 | 1.51 |
| 1:B:27:ILE:CA | 1:D:180:TYR:CD1[2_546] | 0.70 | 1.50 |
| 1:B:50:LEU:CG | 1:D:48:ILE:CG2[2_546] | 0.70 | 1.50 |
| 1:B:34:ASN:ND2 | 1:D:335:ALA:O[2_546] | 0.70 | 1.50 |
| 1:B:229:PHE:CE1 | 1:D:24:GLU:CB[2_546] | 0.71 | 1.49 |
| 1:B:320:PHE:C | 1:C:367:GLU:OE1[2_546] | 0.71 | 1.49 |
| 1:B:345:HIS:NE2 | 1:D:42:GLY:C[2_546] | 0.72 | 1.48 |
| 1:B:55:LYS:CA | 1:D:121:ILE:CG2[2_546] | 0.72 | 1.48 |
| 1:B:41:TYR:O | 1:D:347:ILE:N[2_546] | 0.72 | 1.48 |
| 1:B:169:GLU:CA | 1:C:364:VAL:CG1[2_546] | 0.73 | 1.47 |
| 1:B:269:LYS:O | 1:D:184:GLU:CG[2_546] | 0.73 | 1.47 |
| 1:B:121:ILE:CG1 | 1:D:61:GLU:OE2[2_546] | 0.74 | 1.46 |
| 1:B:124:ILE:CD1 | 1:D:56:LEU:O[2_546] | 0.74 | 1.46 |
| 1:B:312:THR:N | 1:D:266:PRO:CG[2_546] | 0.75 | 1.45 |
| 1:B:226:PHE:CB | 1:D:25:LYS:CD[2_546] | 0.75 | 1.45 |
| 1:B:57:PRO:C | 1:D:118:GLU:N[2_546] | 0.76 | 1.44 |
| 1:B:331:THR:O | 1:C:368:TYR:CE1[2_546] | 0.76 | 1.44 |
| 1:B:276:LEU:O | 1:C:360:ARG:NH1[2_546] | 0.77 | 1.43 |
| 1:B:24:GLU:N | 1:D:316:SER:CA[2_546] | 0.77 | 1.43 |
| 1:B:169:GLU:O | 1:C:364:VAL:CA[2_546] | 0.77 | 1.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:336:LEU:CB | 1:C:369:GLN:CG[2_546] | 0.78 | 1.42 |
| 1:A:111:LYS:NZ | 1:A:241:TRP:CH2[2_556] | 0.78 | 1.42 |
| 1:B:27:ILE:N | 1:D:180:TYR:CE1[2_546] | 0.79 | 1.41 |
| 1:B:255:GLY:O | 1:D:264:TYR:O[2_546] | 0.79 | 1.41 |
| 1:B:28:LEU:CB | 1:D:180:TYR:N[2_546] | 0.79 | 1.41 |
| 1:B:309:TYR:CB | 1:D:311:ASN:CA[2_546] | 0.79 | 1.41 |
| 1:B:345:HIS:CE1 | 1:D:42:GLY:O[2_546] | 0.79 | 1.41 |
| 1:B:188:SER:C | 1:D:41:TYR:CZ[2_546] | 0.79 | 1.41 |
| 1:B:311:ASN:C | 1:D:266:PRO:CD[2_546] | 0.80 | 1.40 |
| 1:B:27:ILE:N | 1:D:180:TYR:CD1[2_546] | 0.80 | 1.40 |
| 1:B:262:LYS:CE | 1:D:315:TYR:CG[2_546] | 0.80 | 1.40 |
| 1:B:180:TYR:CB | 1:D:33:TYR:O[2_546] | 0.80 | 1.40 |
| 1:B:340:LEU:N | 1:D:56:LEU:CD2[2_546] | 0.81 | 1.39 |
| 1:B:181:THR:OG1 | 1:D:50:LEU:CD2[2_546] | 0.81 | 1.39 |
| 1:B:24:GLU:CG | 1:D:317:GLY:C[2_546] | 0.81 | 1.39 |
| 1:B:300:ILE:CD1 | 1:D:258:HIS:N[2_546] | 0.81 | 1.39 |
| 1:B:264:TYR:CZ | 1:D:258:HIS:CG[2_546] | 0.81 | 1.39 |
| 1:B:61:GLU:CG | 1:D:118:GLU:OE2[2_546] | 0.82 | 1.38 |
| 1:B:33:TYR:CE1 | 1:D:124:ILE:CB[2_546] | 0.82 | 1.38 |
| 1:B:304:SER:CB | 1:D:256:PHE:CB[2_546] | 0.82 | 1.38 |
| 1:B:266:PRO:O | 1:D:183:HIS:CB[2_546] | 0.82 | 1.38 |
| 1:B:24:GLU:CB | 1:D:317:GLY:CA[2_546] | 0.82 | 1.38 |
| 1:B:61:GLU:OE1 | 1:D:118:GLU:CG[2_546] | 0.82 | 1.38 |
| 1:B:62:LEU:CD1 | 1:D:117:LYS:CE[2_546] | 0.82 | 1.38 |
| 1:B:336:LEU:CB | 1:C:369:GLN:CB[2_546] | 0.83 | 1.37 |
| 1:B:257:GLY:CA | 1:D:264:TYR:CD2[2_546] | 0.83 | 1.37 |
| 1:B:22:ASP:CB | 1:D:320:PHE:CZ[2_546] | 0.83 | 1.37 |
| 1:B:313:ASP:C | 1:D:26:GLY:C[2_546] | 0.84 | 1.36 |
| 1:B:177:LEU:CB | 1:D:31:ARG:CB[2_546] | 0.84 | 1.36 |
| 1:B:242:PHE:CD2 | 1:D:305:SER:C[2_546] | 0.84 | 1.36 |
| 1:B:304:SER:CA | 1:D:256:PHE:CG[2_546] | 0.84 | 1.36 |
| 1:B:345:HIS:CD2 | 1:D:42:GLY:CA[2_546] | 0.84 | 1.36 |
| 1:B:340:LEU:CA | 1:D:56:LEU:CD2[2_546] | 0.84 | 1.36 |
| 1:B:302:GLN:OE1 | 1:D:302:GLN:O[2_546] | 0.85 | 1.35 |
| 1:B:30:TYR:CA | 1:D:44:TYR:CD1[2_546] | 0.85 | 1.35 |
| 1:B:337:SER:CA | 1:D:33:TYR:CG[2_546] | 0.85 | 1.35 |
| 1:B:34:ASN:CB | 1:D:338:ARG:N[2_546] | 0.85 | 1.35 |
| 1:B:305:SER:CA | 1:D:253:LEU:CG[2_546] | 0.85 | 1.35 |
| 1:B:23:GLY:O | 1:D:316:SER:N[2_546] | 0.85 | 1.35 |
| 1:B:175:LYS:CA | 1:D:18:LEU:CA[2_546] | 0.86 | 1.34 |
| 1:B:171:ASN:C | 1:D:16:THR:O[2_546] | 0.86 | 1.34 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:303:PHE:O | 1:D:256:PHE:CZ[2_546] | 0.86 | 1.34 |
| 1:B:316:SER:N | 1:D:22:ASP:N[2_546] | 0.87 | 1.33 |
| 1:B:177:LEU:CD2 | 1:D:31:ARG:O[2_546] | 0.87 | 1.33 |
| 1:B:263:THR:O | 1:D:312:THR:CA[2_546] | 0.87 | 1.33 |
| 1:B:188:SER:CA | 1:D:41:TYR:CZ[2_546] | 0.87 | 1.33 |
| 1:B:171:ASN:C | 1:D:16:THR:C[2_546] | 0.87 | 1.33 |
| 1:B:46:GLU:OE1 | 1:D:347:ILE:CD1[2_546] | 0.87 | 1.33 |
| 1:B:120:ALA:CB | 1:D:58:THR:CA[2_546] | 0.87 | 1.33 |
| 1:B:337:SER:CA | 1:D:33:TYR:CD1[2_546] | 0.87 | 1.33 |
| 1:B:169:GLU:O | 1:C:364:VAL:CB[2_546] | 0.87 | 1.33 |
| 1:B:174:ASP:N | 1:D:17:ASN:CA[2_546] | 0.87 | 1.33 |
| 1:B:269:LYS:N | 1:D:183:HIS:CD2[2_546] | 0.88 | 1.32 |
| 1:B:316:SER:O | 1:D:20:PHE:CE2[2_546] | 0.88 | 1.32 |
| 1:B:35:ILE:C | 1:D:181:THR:O[2_546] | 0.88 | 1.32 |
| 1:B:36:GLU:CG | 1:D:338:ARG:CG[2_546] | 0.88 | 1.32 |
| 1:A:110:PHE:O | 1:A:245:LYS:N[2_556] | 0.88 | 1.32 |
| 1:B:21:ILE:N | 1:D:176:ALA:N[2_546] | 0.88 | 1.32 |
| 1:B:47:THR:CB | 1:D:51:MET:N[2_546] | 0.89 | 1.31 |
| 1:B:19:THR:C | 1:D:174:ASP:O[2_546] | 0.89 | 1.31 |
| 1:B:263:THR:O | 1:D:312:THR:N[2_546] | 0.89 | 1.31 |
| 1:B:226:PHE:CG | 1:D:25:LYS:CE[2_546] | 0.89 | 1.31 |
| 1:B:169:GLU:C | 1:C:364:VAL:CG1[2_546] | 0.89 | 1.31 |
| 1:B:304:SER:N | 1:D:256:PHE:CD2[2_546] | 0.89 | 1.31 |
| 1:B:62:LEU:CG | 1:D:117:LYS:CE[2_546] | 0.89 | 1.31 |
| 1:B:186:PRO:CD | 1:D:40:ASN:CB[2_546] | 0.90 | 1.30 |
| 1:B:20:PHE:CE2 | 1:D:173:MET:CE[2_546] | 0.90 | 1.30 |
| 1:B:341:GLY:C | 1:D:46:GLU:OE2[2_546] | 0.90 | 1.30 |
| 1:A:363:TYR:CA | 1:D:170:ILE:O[2_546] | 0.90 | 1.30 |
| 1:B:337:SER:C | 1:D:33:TYR:CG[2_546] | 0.90 | 1.30 |
| 1:B:46:GLU:N | 1:D:52:LEU:C[2_546] | 0.90 | 1.30 |
| 1:B:263:THR:OG1 | 1:D:313:ASP:CB[2_546] | 0.90 | 1.30 |
| 1:B:47:THR:O | 1:D:49:TYR:CA[2_546] | 0.91 | 1.29 |
| 1:B:61:GLU:CD | 1:D:118:GLU:OE2[2_546] | 0.91 | 1.29 |
| 1:B:26:GLY:O | 1:D:180:TYR:CE2[2_546] | 0.91 | 1.29 |
| 1:A:237:ARG:NH1 | 1:B:217:LEU:C[2_546] | 0.91 | 1.29 |
| 1:B:296:GLU:N | 1:D:262:LYS:CD[2_546] | 0.91 | 1.29 |
| 1:B:47:THR:N | 1:D:52:LEU:N[2_546] | 0.91 | 1.29 |
| 1:A:364:VAL:CG1 | 1:D:170:ILE:CD1[2_546] | 0.91 | 1.29 |
| 1:B:302:GLN:NE2 | 1:D:302:GLN:C[2_546] | 0.91 | 1.29 |
| 1:B:26:GLY:CA | 1:D:180:TYR:OH[2_546] | 0.92 | 1.28 |
| 1:B:181:THR:O | 1:D:38:LEU:CD2[2_546] | 0.92 | 1.28 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:315:TYR:C | 1:D:22:ASP:CA[2_546] | 0.92 | 1.28 |
| 1:B:52:LEU:CG | 1:D:57:PRO:CB[2_546] | 0.92 | 1.28 |
| 1:A:368:TYR:OH | 1:D:127:MET:CE[2_546] | 0.92 | 1.28 |
| 1:B:303:PHE:C | 1:D:256:PHE:CE2[2_546] | 0.92 | 1.28 |
| 1:B:27:ILE:CD1 | 1:D:334:PHE:CA[2_546] | 0.92 | 1.28 |
| 1:B:256:PHE:CD2 | 1:D:309:TYR:CB[2_546] | 0.93 | 1.27 |
| 1:B:305:SER:CB | 1:D:253:LEU:CD2[2_546] | 0.93 | 1.27 |
| 1:B:300:ILE:C | 1:D:308:ILE:CG2[2_546] | 0.93 | 1.27 |
| 1:B:18:LEU:O | 1:D:44:TYR:CA[2_546] | 0.93 | 1.27 |
| 1:B:156:PHE:CD2 | 1:C:366:PRO:CG[2_546] | 0.93 | 1.27 |
| 1:B:61:GLU:OE1 | 1:D:118:GLU:CD[2_546] | 0.93 | 1.27 |
| 1:B:18:LEU:CB | 1:D:43:SER:CB[2_546] | 0.93 | 1.27 |
| 1:B:338:ARG:CZ | 1:D:38:LEU:N[2_546] | 0.93 | 1.27 |
| 1:B:178:ILE:CG2 | 1:D:51:MET:SD[2_546] | 0.93 | 1.27 |
| 1:B:314:PHE:C | 1:D:22:ASP:O[2_546] | 0.93 | 1.27 |
| 1:B:302:GLN:CB | 1:D:303:PHE:CA[2_546] | 0.94 | 1.26 |
| 1:B:24:GLU:N | 1:D:316:SER:C[2_546] | 0.94 | 1.26 |
| 1:B:226:PHE:N | 1:D:25:LYS:CG[2_546] | 0.94 | 1.26 |
| 1:B:20:PHE:C | 1:D:177:LEU:N[2_546] | 0.94 | 1.26 |
| 1:B:229:PHE:CZ | 1:D:24:GLU:CA[2_546] | 0.94 | 1.26 |
| 1:B:268:ALA:C | 1:D:183:HIS:NE2[2_546] | 0.95 | 1.25 |
| 1:B:45:GLU:C | 1:D:53:TYR:CA[2_546] | 0.95 | 1.25 |
| 1:B:186:PRO:CB | 1:D:40:ASN:CG[2_546] | 0.95 | 1.25 |
| 1:B:229:PHE:CZ | 1:D:24:GLU:CB[2_546] | 0.95 | 1.25 |
| 1:B:18:LEU:O | 1:D:44:TYR:CB[2_546] | 0.96 | 1.24 |
| 1:B:17:ASN:ND2 | 1:D:150:ASP:C[2_546] | 0.96 | 1.24 |
| 1:B:333:LEU:CA | 1:C:368:TYR:C[2_546] | 0.96 | 1.24 |
| 1:B:305:SER:CA | 1:D:253:LEU:CD2[2_546] | 0.96 | 1.24 |
| 1:B:47:THR:C | 1:D:49:TYR:C[2_546] | 0.96 | 1.24 |
| 1:B:345:HIS:NE2 | 1:D:42:GLY:O[2_546] | 0.96 | 1.24 |
| 1:B:273:LYS:CE | 1:D:185:VAL:CG2[2_546] | 0.97 | 1.23 |
| 1:B:302:GLN:CG | 1:D:303:PHE:CA[2_546] | 0.97 | 1.23 |
| 1:B:315:TYR:CA | 1:D:22:ASP:C[2_546] | 0.97 | 1.23 |
| 1:B:271:PHE:CB | 1:D:21:ILE:CG1[2_546] | 0.97 | 1.23 |
| 1:B:117:LYS:O | 1:D:58:THR:OG1[2_546] | 0.97 | 1.23 |
| 1:B:174:ASP:C | 1:D:17:ASN:C[2_546] | 0.97 | 1.23 |
| 1:B:24:GLU:CA | 1:D:316:SER:C[2_546] | 0.97 | 1.23 |
| 1:B:262:LYS:CG | 1:D:315:TYR:CA[2_546] | 0.98 | 1.22 |
| 1:B:184:GLU:OE2 | 1:D:270:ILE:CG2[2_546] | 0.98 | 1.22 |
| 1:B:47:THR:OG1 | 1:D:51:MET:CA[2_546] | 0.98 | 1.22 |
| 1:B:267:ARG:CG | 1:D:28:LEU:CD2[2_546] | 0.98 | 1.22 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:21:ILE:N | 1:D:176:ALA:CA[2_546] | 0.98 | 1.22 |
| 1:A:367:GLU:O | 1:D:336:LEU:CD2[2_546] | 0.98 | 1.22 |
| 1:B:299:GLY:O | 1:D:308:ILE:O[2_546] | 0.98 | 1.22 |
| 1:B:44:TYR:CE1 | 1:D:50:LEU:CD1[2_546] | 0.98 | 1.22 |
| 1:B:178:ILE:CB | 1:D:51:MET:SD[2_546] | 0.99 | 1.21 |
| 1:B:336:LEU:CG | 1:C:369:GLN:CG[2_546] | 0.99 | 1.21 |
| 1:B:28:LEU:N | 1:D:180:TYR:CB[2_546] | 0.99 | 1.21 |
| 1:B:26:GLY:CA | 1:D:180:TYR:CZ[2_546] | 0.99 | 1.21 |
| 1:B:46:GLU:C | 1:D:52:LEU:CB[2_546] | 0.99 | 1.21 |
| 1:B:270:ILE:CA | 1:D:184:GLU:N[2_546] | 1.00 | 1.20 |
| 1:B:59:LYS:CB | 1:D:114:GLU:C[2_546] | 1.00 | 1.20 |
| 1:B:34:ASN:CA | 1:D:337:SER:O[2_546] | 1.00 | 1.20 |
| 1:B:320:PHE:CA | 1:C:367:GLU:OE1[2_546] | 1.00 | 1.20 |
| 1:B:296:GLU:CB | 1:D:262:LYS:NZ[2_546] | 1.00 | 1.20 |
| 1:B:50:LEU:O | 1:D:65:LEU:CD2[2_546] | 1.01 | 1.19 |
| 1:B:315:TYR:O | 1:D:21:ILE:O[2_546] | 1.01 | 1.19 |
| 1:B:315:TYR:N | 1:D:22:ASP:O[2_546] | 1.01 | 1.19 |
| 1:B:175:LYS:O | 1:D:18:LEU:C[2_546] | 1.01 | 1.19 |
| 1:B:333:LEU:N | 1:C:368:TYR:CG[2_546] | 1.01 | 1.19 |
| 1:B:180:TYR:CE2 | 1:D:28:LEU:O[2_546] | 1.01 | 1.19 |
| 1:B:36:GLU:CB | 1:D:338:ARG:CD[2_546] | 1.01 | 1.19 |
| 1:B:33:TYR:CZ | 1:D:124:ILE:CB[2_546] | 1.01 | 1.19 |
| 1:B:268:ALA:N | 1:D:183:HIS:CE1[2_546] | 1.01 | 1.19 |
| 1:B:183:HIS:CE1 | 1:D:179:LEU:CD2[2_546] | 1.01 | 1.19 |
| 1:B:21:ILE:CG1 | 1:D:175:LYS:O[2_546] | 1.01 | 1.19 |
| 1:B:43:SER:O | 1:D:51:MET:O[2_546] | 1.01 | 1.19 |
| 1:B:55:LYS:C | 1:D:121:ILE:CB[2_546] | 1.01 | 1.19 |
| 1:B:57:PRO:O | 1:D:118:GLU:N[2_546] | 1.01 | 1.19 |
| 1:B:45:GLU:O | 1:D:53:TYR:CA[2_546] | 1.01 | 1.19 |
| 1:A:111:LYS:CA | 1:A:245:LYS:CG[2_556] | 1.01 | 1.19 |
| 1:B:313:ASP:C | 1:D:27:ILE:N[2_546] | 1.01 | 1.19 |
| 1:B:271:PHE:CB | 1:D:21:ILE:CB[2_546] | 1.02 | 1.18 |
| 1:B:186:PRO:CD | 1:D:40:ASN:CA[2_546] | 1.02 | 1.18 |
| 1:B:226:PHE:CB | 1:D:25:LYS:CE[2_546] | 1.02 | 1.18 |
| 1:B:57:PRO:CA | 1:D:118:GLU:N[2_546] | 1.02 | 1.18 |
| 1:B:262:LYS:O | 1:D:314:PHE:CA[2_546] | 1.02 | 1.18 |
| 1:B:59:LYS:CD | 1:D:113:LYS:O[2_546] | 1.02 | 1.18 |
| 1:B:55:LYS:O | 1:D:121:ILE:CG1[2_546] | 1.03 | 1.17 |
| 1:B:189:THR:CA | 1:D:41:TYR:CD2[2_546] | 1.03 | 1.17 |
| 1:B:338:ARG:O | 1:C:371:TYR:CE1[2_546] | 1.03 | 1.17 |
| 1:B:242:PHE:CD1 | 1:D:305:SER:O[2_546] | 1.03 | 1.17 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:308:ILE:CA | 1:D:310:PRO:CG[2_546] | 1.03 | 1.17 |
| 1:B:300:ILE:CG1 | 1:D:257:GLY:CA[2_546] | 1.03 | 1.17 |
| 1:B:19:THR:O | 1:D:174:ASP:C[2_546] | 1.03 | 1.17 |
| 1:B:268:ALA:CA | 1:D:183:HIS:CE1[2_546] | 1.04 | 1.16 |
| 1:B:30:TYR:N | 1:D:44:TYR:CD1[2_546] | 1.04 | 1.16 |
| 1:B:309:TYR:CA | 1:D:310:PRO:O[2_546] | 1.04 | 1.16 |
| 1:B:274:LEU:CD1 | 1:D:19:THR:O[2_546] | 1.04 | 1.16 |
| 1:B:261:TYR:OH | 1:D:179:LEU:CB[2_546] | 1.04 | 1.16 |
| 1:B:47:THR:N | 1:D:52:LEU:CA[2_546] | 1.05 | 1.15 |
| 1:B:262:LYS:CB | 1:D:314:PHE:C[2_546] | 1.05 | 1.15 |
| 1:B:333:LEU:CB | 1:C:368:TYR:N[2_546] | 1.05 | 1.15 |
| 1:B:308:ILE:O | 1:D:310:PRO:N[2_546] | 1.05 | 1.15 |
| 1:B:256:PHE:CA | 1:D:264:TYR:N[2_546] | 1.05 | 1.15 |
| 1:B:22:ASP:CG | 1:D:320:PHE:CE1[2_546] | 1.05 | 1.15 |
| 1:B:58:THR:C | 1:D:115:ASN:ND2[2_546] | 1.05 | 1.15 |
| 1:B:264:TYR:CZ | 1:D:258:HIS:ND1[2_546] | 1.05 | 1.15 |
| 1:B:20:PHE:N | 1:D:174:ASP:O[2_546] | 1.05 | 1.15 |
| 1:B:53:TYR:CA | 1:D:65:LEU:N[2_546] | 1.05 | 1.15 |
| 1:B:268:ALA:CB | 1:D:261:TYR:CE1[2_546] | 1.06 | 1.14 |
| 1:B:262:LYS:C | 1:D:314:PHE:N[2_546] | 1.06 | 1.14 |
| 1:B:189:THR:CG2 | 1:D:41:TYR:CA[2_546] | 1.06 | 1.14 |
| 1:B:156:PHE:CE2 | 1:C:366:PRO:CG[2_546] | 1.06 | 1.14 |
| 1:B:173:MET:CB | 1:C:364:VAL:O[2_546] | 1.06 | 1.14 |
| 1:B:265:ASP:O | 1:D:267:ARG:CZ[2_546] | 1.06 | 1.14 |
| 1:B:315:TYR:N | 1:D:22:ASP:C[2_546] | 1.06 | 1.14 |
| 1:B:37:ASP:O | 1:D:342:TRP:C[2_546] | 1.07 | 1.13 |
| 1:B:21:ILE:C | 1:D:176:ALA:CB[2_546] | 1.07 | 1.13 |
| 1:A:110:PHE:CB | 1:A:249:GLN:OE1[2_556] | 1.07 | 1.13 |
| 1:B:48:ILE:CG2 | 1:D:49:TYR:CE2[2_546] | 1.07 | 1.13 |
| 1:B:260:VAL:CA | 1:D:271:PHE:CA[2_546] | 1.07 | 1.13 |
| 1:B:45:GLU:CA | 1:D:53:TYR:C[2_546] | 1.07 | 1.13 |
| 1:A:363:TYR:N | 1:D:170:ILE:O[2_546] | 1.07 | 1.13 |
| 1:B:270:ILE:CD1 | 1:D:183:HIS:N[2_546] | 1.08 | 1.12 |
| 1:B:271:PHE:CD2 | 1:D:20:PHE:O[2_546] | 1.08 | 1.12 |
| 1:B:24:GLU:CG | 1:D:318:ILE:N[2_546] | 1.08 | 1.12 |
| 1:B:314:PHE:CZ | 1:D:262:LYS:CB[2_546] | 1.08 | 1.12 |
| 1:B:311:ASN:CB | 1:D:265:ASP:C[2_546] | 1.08 | 1.12 |
| 1:B:57:PRO:CG | 1:D:117:LYS:CB[2_546] | 1.08 | 1.12 |
| 1:A:363:TYR:CB | 1:D:170:ILE:O[2_546] | 1.08 | 1.12 |
| 1:A:367:GLU:CB | 1:D:156:PHE:CE1[2_546] | 1.09 | 1.11 |
| 1:B:30:TYR:CE1 | 1:D:47:THR:CG2[2_546] | 1.09 | 1.11 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:313:ASP:CA | 1:D:26:GLY:C[2_546] | 1.09 | 1.11 |
| 1:B:264:TYR:CE1 | 1:D:258:HIS:ND1[2_546] | 1.09 | 1.11 |
| 1:B:56:LEU:CG | 1:D:120:ALA:C[2_546] | 1.09 | 1.11 |
| 1:B:256:PHE:N | 1:D:264:TYR:N[2_546] | 1.09 | 1.11 |
| 1:B:35:ILE:CA | 1:D:181:THR:O[2_546] | 1.09 | 1.11 |
| 1:B:334:PHE:CD1 | 1:D:34:ASN:CA[2_546] | 1.09 | 1.11 |
| 1:B:298:LEU:CB | 1:D:306:LYS:O[2_546] | 1.09 | 1.11 |
| 1:B:271:PHE:CE2 | 1:D:20:PHE:C[2_546] | 1.09 | 1.11 |
| 1:B:28:LEU:CD2 | 1:D:178:ILE:O[2_546] | 1.09 | 1.11 |
| 1:A:107:ASP:O | 1:A:248:ASN:CG[2_556] | 1.09 | 1.11 |
| 1:B:263:THR:CA | 1:D:313:ASP:N[2_546] | 1.09 | 1.11 |
| 1:A:367:GLU:CG | 1:D:156:PHE:CE1[2_546] | 1.10 | 1.10 |
| 1:B:266:PRO:CA | 1:D:267:ARG:NH1[2_546] | 1.10 | 1.10 |
| 1:B:46:GLU:O | 1:D:52:LEU:CB[2_546] | 1.10 | 1.10 |
| 1:B:48:ILE:O | 1:D:49:TYR:CD1[2_546] | 1.10 | 1.10 |
| 1:B:320:PHE:CE1 | 1:D:29:ARG:NH1[2_546] | 1.10 | 1.10 |
| 1:B:186:PRO:CA | 1:D:40:ASN:CG[2_546] | 1.10 | 1.10 |
| 1:B:298:LEU:CA | 1:D:306:LYS:O[2_546] | 1.10 | 1.10 |
| 1:A:279:ILE:CD1 | 1:B:249:GLN:NE2[2_546] | 1.10 | 1.10 |
| 1:B:55:LYS:O | 1:D:121:ILE:CD1[2_546] | 1.10 | 1.10 |
| 1:B:269:LYS:CA | 1:D:183:HIS:CD2[2_546] | 1.10 | 1.10 |
| 1:B:302:GLN:CD | 1:D:303:PHE:N[2_546] | 1.10 | 1.10 |
| 1:B:34:ASN:CA | 1:D:337:SER:C[2_546] | 1.10 | 1.10 |
| 1:B:299:GLY:O | 1:D:308:ILE:C[2_546] | 1.10 | 1.10 |
| 1:B:177:LEU:CA | 1:D:31:ARG:N[2_546] | 1.10 | 1.10 |
| 1:B:308:ILE:C | 1:D:310:PRO:N[2_546] | 1.10 | 1.10 |
| 1:A:108:LYS:CA | 1:A:248:ASN:CB[2_556] | 1.10 | 1.10 |
| 1:B:304:SER:N | 1:D:256:PHE:CG[2_546] | 1.11 | 1.09 |
| 1:A:236:ASN:ND2 | 1:B:254:MET:CE[2_546] | 1.11 | 1.09 |
| 1:B:260:VAL:CA | 1:D:271:PHE:C[2_546] | 1.11 | 1.09 |
| 1:B:55:LYS:C | 1:D:121:ILE:CG1[2_546] | 1.11 | 1.09 |
| 1:B:41:TYR:CA | 1:D:346:ILE:N[2_546] | 1.11 | 1.09 |
| 1:B:58:THR:C | 1:D:115:ASN:CG[2_546] | 1.11 | 1.09 |
| 1:A:362:LEU:CB | 1:D:167:THR:O[2_546] | 1.12 | 1.08 |
| 1:A:111:LYS:C | 1:A:245:LYS:CD[2_556] | 1.12 | 1.08 |
| 1:B:260:VAL:CB | 1:D:271:PHE:CA[2_546] | 1.12 | 1.08 |
| 1:B:36:GLU:CG | 1:D:338:ARG:CD[2_546] | 1.12 | 1.08 |
| 1:B:172:ALA:O | 1:C:363:TYR:CE1[2_546] | 1.12 | 1.08 |
| 1:B:183:HIS:CA | 1:D:39:VAL:CG1[2_546] | 1.12 | 1.08 |
| 1:B:257:GLY:CA | 1:D:264:TYR:CE2[2_546] | 1.12 | 1.08 |
| 1:B:267:ARG:NH1 | 1:D:35:ILE:CB[2_546] | 1.12 | 1.08 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:42:GLY:N | 1:D:344:ALA:C[2_546] | 1.12 | 1.08 |
| 1:B:24:GLU:CB | 1:D:317:GLY:N[2_546] | 1.12 | 1.08 |
| 1:B:299:GLY:N | 1:D:308:ILE:N[2_546] | 1.12 | 1.08 |
| 1:B:222:ALA:CA | 1:D:27:ILE:CD1[2_546] | 1.12 | 1.08 |
| 1:A:367:GLU:CB | 1:D:156:PHE:CG[2_546] | 1.12 | 1.08 |
| 1:B:117:LYS:CB | 1:D:60:LYS:C[2_546] | 1.12 | 1.08 |
| 1:B:226:PHE:CA | 1:D:25:LYS:CG[2_546] | 1.13 | 1.07 |
| 1:A:109:ASN:CB | 1:A:250:LYS:N[2_556] | 1.13 | 1.07 |
| 1:B:267:ARG:C | 1:D:183:HIS:ND1[2_546] | 1.13 | 1.07 |
| 1:B:44:TYR:CB | 1:D:31:ARG:NE[2_546] | 1.13 | 1.07 |
| 1:B:267:ARG:NH1 | 1:D:35:ILE:CG2[2_546] | 1.13 | 1.07 |
| 1:B:183:HIS:C | 1:D:39:VAL:CG1[2_546] | 1.13 | 1.07 |
| 1:B:337:SER:OG | 1:D:30:TYR:O[2_546] | 1.13 | 1.07 |
| 1:A:368:TYR:O | 1:D:127:MET:C[2_546] | 1.13 | 1.07 |
| 1:B:37:ASP:OD2 | 1:D:339:THR:CA[2_546] | 1.14 | 1.06 |
| 1:B:175:LYS:N | 1:D:17:ASN:C[2_546] | 1.14 | 1.06 |
| 1:B:257:GLY:C | 1:D:264:TYR:CD2[2_546] | 1.14 | 1.06 |
| 1:B:184:GLU:O | 1:D:39:VAL:C[2_546] | 1.14 | 1.06 |
| 1:B:336:LEU:C | 1:D:33:TYR:CE2[2_546] | 1.14 | 1.06 |
| 1:B:37:ASP:CA | 1:D:342:TRP:N[2_546] | 1.14 | 1.06 |
| 1:B:35:ILE:CG2 | 1:D:181:THR:CB[2_546] | 1.14 | 1.06 |
| 1:B:120:ALA:CB | 1:D:58:THR:N[2_546] | 1.14 | 1.06 |
| 1:A:360:ARG:NH1 | 1:D:277:THR:OG1[2_546] | 1.14 | 1.06 |
| 1:B:40:ASN:ND2 | 1:D:189:THR:OG1[2_546] | 1.14 | 1.06 |
| 1:B:18:LEU:C | 1:D:44:TYR:N[2_546] | 1.14 | 1.06 |
| 1:B:299:GLY:C | 1:D:308:ILE:CB[2_546] | 1.14 | 1.06 |
| 1:B:48:ILE:CA | 1:D:49:TYR:O[2_546] | 1.15 | 1.05 |
| 1:B:172:ALA:N | 1:D:16:THR:O[2_546] | 1.15 | 1.05 |
| 1:B:184:GLU:C | 1:D:39:VAL:O[2_546] | 1.15 | 1.05 |
| 1:B:331:THR:O | 1:C:368:TYR:CZ[2_546] | 1.15 | 1.05 |
| 1:A:279:ILE:CD1 | 1:B:249:GLN:CD[2_546] | 1.15 | 1.05 |
| 1:A:109:ASN:N | 1:A:249:GLN:N[2_556] | 1.15 | 1.05 |
| 1:B:22:ASP:CB | 1:D:320:PHE:CE2[2_546] | 1.16 | 1.04 |
| 1:B:39:VAL:O | 1:D:345:HIS:CG[2_546] | 1.16 | 1.04 |
| 1:B:168:ASP:N | 1:D:15:VAL:CG1[2_546] | 1.16 | 1.04 |
| 1:B:44:TYR:CA | 1:D:31:ARG:NH2[2_546] | 1.16 | 1.04 |
| 1:B:59:LYS:CD | 1:D:113:LYS:C[2_546] | 1.16 | 1.04 |
| 1:A:368:TYR:O | 1:D:128:ALA:N[2_546] | 1.16 | 1.04 |
| 1:B:260:VAL:C | 1:D:271:PHE:CB[2_546] | 1.16 | 1.04 |
| 1:B:302:GLN:CD | 1:D:302:GLN:C[2_546] | 1.16 | 1.04 |
| 1:B:261:TYR:CD1 | 1:D:267:ARG:O[2_546] | 1.16 | 1.04 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:121:ILE:CD1 | 1:D:61:GLU:OE2[2_546] | 1.16 | 1.04 |
| 1:B:263:THR:OG1 | 1:D:313:ASP:CG[2_546] | 1.16 | 1.04 |
| 1:B:186:PRO:CG | 1:D:40:ASN:CB[2_546] | 1.17 | 1.03 |
| 1:B:336:LEU:CD1 | 1:C:369:GLN:NE2[2_546] | 1.17 | 1.03 |
| 1:B:336:LEU:O | 1:D:33:TYR:CE2[2_546] | 1.17 | 1.03 |
| 1:B:320:PHE:CD1 | 1:D:29:ARG:NH1[2_546] | 1.17 | 1.03 |
| 1:B:257:GLY:N | 1:D:264:TYR:CG[2_546] | 1.17 | 1.03 |
| 1:B:38:LEU:CA | 1:D:340:LEU:O[2_546] | 1.17 | 1.03 |
| 1:B:265:ASP:O | 1:D:267:ARG:NH2[2_546] | 1.17 | 1.03 |
| 1:B:183:HIS:C | 1:D:39:VAL:CA[2_546] | 1.18 | 1.02 |
| 1:B:38:LEU:O | 1:D:344:ALA:CB[2_546] | 1.18 | 1.02 |
| 1:A:366:PRO:N | 1:D:152:PHE:O[2_546] | 1.18 | 1.02 |
| 1:B:17:ASN:OD1 | 1:D:151:SER:CA[2_546] | 1.18 | 1.02 |
| 1:B:268:ALA:N | 1:D:183:HIS:ND1[2_546] | 1.18 | 1.02 |
| 1:B:332:ALA:N | 1:C:368:TYR:CE2[2_546] | 1.18 | 1.02 |
| 1:B:37:ASP:C | 1:D:342:TRP:N[2_546] | 1.18 | 1.02 |
| 1:B:258:HIS:CA | 1:D:269:LYS:N[2_546] | 1.18 | 1.02 |
| 1:B:268:ALA:C | 1:D:183:HIS:CE1[2_546] | 1.18 | 1.02 |
| 1:B:336:LEU:CG | 1:C:369:GLN:OE1[2_546] | 1.18 | 1.02 |
| 1:B:183:HIS:CE1 | 1:D:179:LEU:CG[2_546] | 1.19 | 1.01 |
| 1:B:340:LEU:N | 1:D:56:LEU:CG[2_546] | 1.19 | 1.01 |
| 1:B:316:SER:OG | 1:D:27:ILE:CG2[2_546] | 1.19 | 1.01 |
| 1:B:242:PHE:CE1 | 1:D:304:SER:O[2_546] | 1.19 | 1.01 |
| 1:B:316:SER:O | 1:D:20:PHE:CZ[2_546] | 1.19 | 1.01 |
| 1:B:179:LEU:C | 1:D:30:TYR:CG[2_546] | 1.19 | 1.01 |
| 1:A:364:VAL:CA | 1:D:154:LYS:N[2_546] | 1.19 | 1.01 |
| 1:B:265:ASP:C | 1:D:267:ARG:NE[2_546] | 1.19 | 1.01 |
| 1:B:26:GLY:C | 1:D:180:TYR:CE1[2_546] | 1.19 | 1.01 |
| 1:B:333:LEU:CA | 1:C:368:TYR:CA[2_546] | 1.19 | 1.01 |
| 1:B:262:LYS:O | 1:D:314:PHE:CB[2_546] | 1.19 | 1.01 |
| 1:B:31:ARG:N | 1:D:44:TYR:CD2[2_546] | 1.19 | 1.01 |
| 1:B:179:LEU:C | 1:D:30:TYR:CD2[2_546] | 1.19 | 1.01 |
| 1:B:309:TYR:CG | 1:D:311:ASN:N[2_546] | 1.19 | 1.01 |
| 1:B:262:LYS:O | 1:D:314:PHE:N[2_546] | 1.19 | 1.01 |
| 1:B:112:TRP:CH2 | 1:D:59:LYS:NZ[2_546] | 1.20 | 1.00 |
| 1:B:30:TYR:CA | 1:D:44:TYR:CE1[2_546] | 1.20 | 1.00 |
| 1:A:361:ALA:C | 1:D:171:ASN:CB[2_546] | 1.20 | 1.00 |
| 1:B:265:ASP:CG | 1:D:267:ARG:CD[2_546] | 1.20 | 1.00 |
| 1:B:342:TRP:CA | 1:C:371:TYR:OH[2_546] | 1.20 | 1.00 |
| 1:B:178:ILE:CG2 | 1:D:51:MET:CE[2_546] | 1.20 | 1.00 |
| 1:B:189:THR:N | 1:D:41:TYR:CE2[2_546] | 1.21 | 0.99 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:367:GLU:CA | 1:D:156:PHE:CG[2_546] | 1.21 | 0.99 |
| 1:A:110:PHE:CG | 1:A:249:GLN:OE1[2_556] | 1.21 | 0.99 |
| 1:A:109:ASN:CG | 1:A:250:LYS:N[2_556] | 1.21 | 0.99 |
| 1:B:52:LEU:O | 1:D:62:LEU:C[2_546] | 1.21 | 0.99 |
| 1:B:256:PHE:C | 1:D:264:TYR:CA[2_546] | 1.21 | 0.99 |
| 1:B:314:PHE:N | 1:D:26:GLY:CA[2_546] | 1.21 | 0.99 |
| 1:B:17:ASN:ND2 | 1:D:151:SER:N[2_546] | 1.21 | 0.99 |
| 1:B:38:LEU:CG | 1:D:340:LEU:CG[2_546] | 1.21 | 0.99 |
| 1:B:188:SER:O | 1:D:41:TYR:CE2[2_546] | 1.21 | 0.99 |
| 1:B:258:HIS:CD2 | 1:D:270:ILE:N[2_546] | 1.21 | 0.99 |
| 1:B:309:TYR:CD2 | 1:D:311:ASN:ND2[2_546] | 1.21 | 0.99 |
| 1:A:110:PHE:N | 1:A:244:ASP:O[2_556] | 1.21 | 0.99 |
| 1:B:299:GLY:CA | 1:D:308:ILE:CA[2_546] | 1.21 | 0.99 |
| 1:B:46:GLU:C | 1:D:52:LEU:CA[2_546] | 1.22 | 0.98 |
| 1:A:365:GLY:CA | 1:D:152:PHE:C[2_546] | 1.22 | 0.98 |
| 1:B:172:ALA:CB | 1:C:363:TYR:C[2_546] | 1.22 | 0.98 |
| 1:B:313:ASP:CA | 1:D:27:ILE:N[2_546] | 1.22 | 0.98 |
| 1:B:117:LYS:N | 1:D:60:LYS:N[2_546] | 1.22 | 0.98 |
| 1:B:309:TYR:CE2 | 1:D:311:ASN:ND2[2_546] | 1.22 | 0.98 |
| 1:B:175:LYS:C | 1:D:18:LEU:O[2_546] | 1.22 | 0.98 |
| 1:B:337:SER:CB | 1:D:33:TYR:N[2_546] | 1.22 | 0.98 |
| 1:B:206:LEU:CG | 1:C:372:VAL:CG1[2_546] | 1.22 | 0.98 |
| 1:B:265:ASP:C | 1:D:267:ARG:NH2[2_546] | 1.22 | 0.98 |
| 1:B:247:VAL:CG2 | 1:D:305:SER:OG[2_546] | 1.22 | 0.98 |
| 1:B:225:ALA:CB | 1:D:25:LYS:C[2_546] | 1.22 | 0.98 |
| 1:B:259:ARG:O | 1:D:272:LYS:C[2_546] | 1.22 | 0.98 |
| 1:B:309:TYR:CE1 | 1:D:255:GLY:C[2_546] | 1.23 | 0.97 |
| 1:B:180:TYR:CD1 | 1:D:29:ARG:CB[2_546] | 1.23 | 0.97 |
| 1:B:117:LYS:CD | 1:D:60:LYS:O[2_546] | 1.23 | 0.97 |
| 1:B:333:LEU:N | 1:C:368:TYR:CD2[2_546] | 1.23 | 0.97 |
| 1:B:117:LYS:CG | 1:D:60:LYS:C[2_546] | 1.23 | 0.97 |
| 1:B:338:ARG:NE | 1:D:38:LEU:N[2_546] | 1.23 | 0.97 |
| 1:B:263:THR:CB | 1:D:313:ASP:N[2_546] | 1.23 | 0.97 |
| 1:B:302:GLN:CB | 1:D:303:PHE:C[2_546] | 1.23 | 0.97 |
| 1:B:331:THR:C | 1:C:368:TYR:CZ[2_546] | 1.23 | 0.97 |
| 1:B:120:ALA:CA | 1:D:58:THR:CG2[2_546] | 1.23 | 0.97 |
| 1:B:49:TYR:CG | 1:D:53:TYR:OH[2_546] | 1.23 | 0.97 |
| 1:B:260:VAL:CB | 1:D:271:PHE:N[2_546] | 1.23 | 0.97 |
| 1:B:20:PHE:CD1 | 1:D:173:MET:CA[2_546] | 1.23 | 0.97 |
| 1:A:369:GLN:O | 1:D:127:MET:CB[2_546] | 1.24 | 0.96 |
| 1:B:28:LEU:CG | 1:D:178:ILE:O[2_546] | 1.24 | 0.96 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:20:PHE:O | 1:D:176:ALA:C[2_546] | 1.24 | 0.96 |
| 1:B:28:LEU:CG | 1:D:178:ILE:C[2_546] | 1.24 | 0.96 |
| 1:B:34:ASN:CB | 1:D:338:ARG:CA[2_546] | 1.24 | 0.96 |
| 1:B:41:TYR:CD2 | 1:D:346:ILE:CG2[2_546] | 1.24 | 0.96 |
| 1:B:342:TRP:CZ3 | 1:C:371:TYR:C[2_546] | 1.24 | 0.96 |
| 1:B:30:TYR:CZ | 1:D:47:THR:CG2[2_546] | 1.24 | 0.96 |
| 1:A:109:ASN:OD1 | 1:A:250:LYS:C[2_556] | 1.25 | 0.95 |
| 1:B:314:PHE:CD2 | 1:D:23:GLY:O[2_546] | 1.25 | 0.95 |
| 1:B:35:ILE:CG1 | 1:D:181:THR:C[2_546] | 1.25 | 0.95 |
| 1:B:19:THR:O | 1:D:174:ASP:CA[2_546] | 1.25 | 0.95 |
| 1:B:315:TYR:OH | 1:D:260:VAL:O[2_546] | 1.25 | 0.95 |
| 1:B:22:ASP:OD2 | 1:D:320:PHE:CD1[2_546] | 1.25 | 0.95 |
| 1:B:271:PHE:CD2 | 1:D:21:ILE:N[2_546] | 1.25 | 0.95 |
| 1:B:183:HIS:O | 1:D:39:VAL:CA[2_546] | 1.25 | 0.95 |
| 1:B:306:LYS:NZ | 1:D:297:GLU:O[2_546] | 1.25 | 0.95 |
| 1:B:258:HIS:CA | 1:D:269:LYS:CA[2_546] | 1.25 | 0.95 |
| 1:B:302:GLN:CG | 1:D:303:PHE:C[2_546] | 1.25 | 0.95 |
| 1:B:271:PHE:CA | 1:D:21:ILE:CG1[2_546] | 1.25 | 0.95 |
| 1:B:258:HIS:CB | 1:D:268:ALA:C[2_546] | 1.26 | 0.94 |
| 1:B:24:GLU:OE1 | 1:D:317:GLY:O[2_546] | 1.26 | 0.94 |
| 1:B:179:LEU:CA | 1:D:30:TYR:CG[2_546] | 1.26 | 0.94 |
| 1:B:51:MET:CG | 1:D:46:GLU:C[2_546] | 1.26 | 0.94 |
| 1:A:360:ARG:NE | 1:D:277:THR:OG1[2_546] | 1.26 | 0.94 |
| 1:A:364:VAL:O | 1:D:153:ALA:CA[2_546] | 1.26 | 0.94 |
| 1:B:302:GLN:CA | 1:D:303:PHE:CG[2_546] | 1.26 | 0.94 |
| 1:B:47:THR:CB | 1:D:51:MET:CA[2_546] | 1.26 | 0.94 |
| 1:A:363:TYR:CD2 | 1:D:153:ALA:CB[2_546] | 1.26 | 0.94 |
| 1:B:45:GLU:C | 1:D:53:TYR:N[2_546] | 1.26 | 0.94 |
| 1:B:333:LEU:CA | 1:C:369:GLN:N[2_546] | 1.26 | 0.94 |
| 1:B:33:TYR:OH | 1:D:124:ILE:N[2_546] | 1.26 | 0.94 |
| 1:B:309:TYR:CZ | 1:D:255:GLY:C[2_546] | 1.26 | 0.94 |
| 1:B:45:GLU:O | 1:D:53:TYR:N[2_546] | 1.26 | 0.94 |
| 1:B:270:ILE:CG1 | 1:D:183:HIS:C[2_546] | 1.27 | 0.93 |
| 1:B:35:ILE:CG2 | 1:D:181:THR:CG2[2_546] | 1.27 | 0.93 |
| 1:B:47:THR:OG1 | 1:D:51:MET:CB[2_546] | 1.27 | 0.93 |
| 1:B:27:ILE:CD1 | 1:D:334:PHE:CB[2_546] | 1.27 | 0.93 |
| 1:B:310:PRO:O | 1:D:265:ASP:CB[2_546] | 1.27 | 0.93 |
| 1:B:263:THR:CB | 1:D:313:ASP:CB[2_546] | 1.27 | 0.93 |
| 1:B:39:VAL:CG1 | 1:D:182:ASP:OD2[2_546] | 1.27 | 0.93 |
| 1:A:108:LYS:C | 1:A:248:ASN:N[2_556] | 1.27 | 0.93 |
| 1:B:175:LYS:CA | 1:D:18:LEU:C[2_546] | 1.27 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:111:LYS:CE | 1:A:241:TRP:CZ3[2_556] | 1.27 | 0.93 |
| 1:B:178:ILE:CD1 | 1:D:18:LEU:CD2[2_546] | 1.27 | 0.93 |
| 1:B:189:THR:CB | 1:D:41:TYR:CA[2_546] | 1.28 | 0.92 |
| 1:B:299:GLY:C | 1:D:308:ILE:C[2_546] | 1.28 | 0.92 |
| 1:B:48:ILE:C | 1:D:49:TYR:CG[2_546] | 1.28 | 0.92 |
| 1:B:59:LYS:N | 1:D:115:ASN:CB[2_546] | 1.28 | 0.92 |
| 1:B:262:LYS:CB | 1:D:315:TYR:CA[2_546] | 1.28 | 0.92 |
| 1:B:57:PRO:N | 1:D:117:LYS:C[2_546] | 1.28 | 0.92 |
| 1:B:47:THR:O | 1:D:49:TYR:C[2_546] | 1.28 | 0.92 |
| 1:B:259:ARG:N | 1:D:269:LYS:O[2_546] | 1.28 | 0.92 |
| 1:B:242:PHE:CG | 1:D:305:SER:C[2_546] | 1.28 | 0.92 |
| 1:B:20:PHE:CZ | 1:D:173:MET:CE[2_546] | 1.29 | 0.91 |
| 1:B:262:LYS:CD | 1:D:315:TYR:CD2[2_546] | 1.29 | 0.91 |
| 1:A:365:GLY:CA | 1:D:152:PHE:O[2_546] | 1.29 | 0.91 |
| 1:B:256:PHE:CD1 | 1:D:263:THR:C[2_546] | 1.29 | 0.91 |
| 1:A:367:GLU:N | 1:D:156:PHE:CB[2_546] | 1.29 | 0.91 |
| 1:B:55:LYS:CG | 1:D:68:LYS:CG[2_546] | 1.29 | 0.91 |
| 1:B:271:PHE:N | 1:D:21:ILE:CD1[2_546] | 1.29 | 0.91 |
| 1:B:336:LEU:N | 1:C:369:GLN:C[2_546] | 1.29 | 0.91 |
| 1:B:309:TYR:CB | 1:D:311:ASN:N[2_546] | 1.29 | 0.91 |
| 1:B:189:THR:N | 1:D:41:TYR:CD2[2_546] | 1.29 | 0.91 |
| 1:B:242:PHE:CD2 | 1:D:306:LYS:N[2_546] | 1.29 | 0.91 |
| 1:B:38:LEU:CD1 | 1:D:340:LEU:CG[2_546] | 1.29 | 0.91 |
| 1:B:309:TYR:N | 1:D:310:PRO:O[2_546] | 1.30 | 0.90 |
| 1:B:309:TYR:OH | 1:D:255:GLY:C[2_546] | 1.30 | 0.90 |
| 1:B:30:TYR:CD1 | 1:D:47:THR:CG2[2_546] | 1.30 | 0.90 |
| 1:B:56:LEU:N | 1:D:121:ILE:CA[2_546] | 1.30 | 0.90 |
| 1:B:298:LEU:CB | 1:D:306:LYS:C[2_546] | 1.30 | 0.90 |
| 1:B:303:PHE:O | 1:D:256:PHE:CE2[2_546] | 1.30 | 0.90 |
| 1:B:56:LEU:CB | 1:D:120:ALA:C[2_546] | 1.30 | 0.90 |
| 1:B:183:HIS:O | 1:D:39:VAL:CB[2_546] | 1.30 | 0.90 |
| 1:B:33:TYR:O | 1:D:44:TYR:OH[2_546] | 1.30 | 0.90 |
| 1:B:311:ASN:N | 1:D:265:ASP:CA[2_546] | 1.30 | 0.90 |
| 1:B:17:ASN:OD1 | 1:D:151:SER:O[2_546] | 1.30 | 0.90 |
| 1:B:320:PHE:CE2 | 1:C:367:GLU:O[2_546] | 1.30 | 0.90 |
| 1:B:177:LEU:CB | 1:D:31:ARG:CA[2_546] | 1.30 | 0.90 |
| 1:B:311:ASN:CA | 1:D:266:PRO:N[2_546] | 1.30 | 0.90 |
| 1:B:184:GLU:N | 1:D:39:VAL:CB[2_546] | 1.30 | 0.90 |
| 1:B:177:LEU:N | 1:D:31:ARG:N[2_546] | 1.30 | 0.90 |
| 1:A:368:TYR:CZ | 1:D:127:MET:CE[2_546] | 1.30 | 0.90 |
| 1:B:302:GLN:N | 1:D:303:PHE:CB[2_546] | 1.31 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:271:PHE:CE2 | 1:D:20:PHE:O[2_546] | 1.31 | 0.89 |
| 1:B:264:TYR:CE1 | 1:D:258:HIS:CG[2_546] | 1.31 | 0.89 |
| 1:B:49:TYR:CB | 1:D:53:TYR:CZ[2_546] | 1.31 | 0.89 |
| 1:B:57:PRO:N | 1:D:117:LYS:O[2_546] | 1.31 | 0.89 |
| 1:B:174:ASP:C | 1:D:18:LEU:N[2_546] | 1.31 | 0.89 |
| 1:B:303:PHE:CA | 1:D:256:PHE:CE2[2_546] | 1.31 | 0.89 |
| 1:B:44:TYR:CB | 1:D:31:ARG:CZ[2_546] | 1.31 | 0.89 |
| 1:B:117:LYS:CE | 1:D:60:LYS:O[2_546] | 1.31 | 0.89 |
| 1:B:170:ILE:C | 1:C:364:VAL:CG2[2_546] | 1.31 | 0.89 |
| 1:B:51:MET:CG | 1:D:46:GLU:O[2_546] | 1.31 | 0.89 |
| 1:B:340:LEU:CD2 | 1:D:50:LEU:CB[2_546] | 1.31 | 0.89 |
| 1:B:49:TYR:CD1 | 1:D:53:TYR:OH[2_546] | 1.31 | 0.89 |
| 1:B:332:ALA:CA | 1:C:368:TYR:CD2[2_546] | 1.31 | 0.89 |
| 1:B:331:THR:O | 1:C:368:TYR:OH[2_546] | 1.32 | 0.88 |
| 1:B:171:ASN:O | 1:D:16:THR:O[2_546] | 1.32 | 0.88 |
| 1:B:50:LEU:CB | 1:D:48:ILE:CG2[2_546] | 1.32 | 0.88 |
| 1:B:49:TYR:N | 1:D:53:TYR:CD1[2_546] | 1.32 | 0.88 |
| 1:B:309:TYR:N | 1:D:310:PRO:CA[2_546] | 1.32 | 0.88 |
| 1:B:51:MET:CE | 1:D:47:THR:N[2_546] | 1.32 | 0.88 |
| 1:B:309:TYR:CA | 1:D:310:PRO:C[2_546] | 1.32 | 0.88 |
| 1:B:296:GLU:OE2 | 1:D:258:HIS:C[2_546] | 1.32 | 0.88 |
| 1:B:262:LYS:NZ | 1:D:315:TYR:CD1[2_546] | 1.32 | 0.88 |
| 1:B:339:THR:CA | 1:D:56:LEU:CD1[2_546] | 1.32 | 0.88 |
| 1:B:309:TYR:CZ | 1:D:255:GLY:O[2_546] | 1.32 | 0.88 |
| 1:B:24:GLU:CD | 1:D:317:GLY:C[2_546] | 1.32 | 0.88 |
| 1:B:44:TYR:N | 1:D:31:ARG:CZ[2_546] | 1.32 | 0.88 |
| 1:B:28:LEU:CD1 | 1:D:179:LEU:N[2_546] | 1.32 | 0.88 |
| 1:B:320:PHE:CA | 1:C:367:GLU:CD[2_546] | 1.32 | 0.88 |
| 1:B:29:ARG:N | 1:D:177:LEU:O[2_546] | 1.32 | 0.88 |
| 1:B:29:ARG:N | 1:D:177:LEU:C[2_546] | 1.33 | 0.87 |
| 1:B:302:GLN:CB | 1:D:303:PHE:CB[2_546] | 1.33 | 0.87 |
| 1:B:174:ASP:C | 1:D:17:ASN:O[2_546] | 1.33 | 0.87 |
| 1:B:39:VAL:C | 1:D:345:HIS:CG[2_546] | 1.33 | 0.87 |
| 1:B:53:TYR:O | 1:D:65:LEU:CA[2_546] | 1.33 | 0.87 |
| 1:B:43:SER:C | 1:D:31:ARG:NH2[2_546] | 1.33 | 0.87 |
| 1:B:336:LEU:CD1 | 1:C:369:GLN:CD[2_546] | 1.33 | 0.87 |
| 1:B:56:LEU:CD1 | 1:D:120:ALA:C[2_546] | 1.33 | 0.87 |
| 1:B:188:SER:OG | 1:D:41:TYR:CE1[2_546] | 1.33 | 0.87 |
| 1:B:272:LYS:NZ | 1:D:259:ARG:O[2_546] | 1.33 | 0.87 |
| 1:B:53:TYR:O | 1:D:65:LEU:C[2_546] | 1.33 | 0.87 |
| 1:A:369:GLN:C | 1:D:127:MET:CB[2_546] | 1.33 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:308:ILE:CG1 | 1:D:310:PRO:CG[2_546] | 1.33 | 0.87 |
| 1:B:177:LEU:N | 1:D:31:ARG:CA[2_546] | 1.33 | 0.87 |
| 1:B:35:ILE:O | 1:D:341:GLY:CA[2_546] | 1.33 | 0.87 |
| 1:B:332:ALA:C | 1:C:368:TYR:CD2[2_546] | 1.33 | 0.87 |
| 1:B:271:PHE:CZ | 1:D:20:PHE:O[2_546] | 1.33 | 0.87 |
| 1:B:303:PHE:O | 1:D:256:PHE:CE1[2_546] | 1.33 | 0.87 |
| 1:B:167:THR:O | 1:D:15:VAL:CG2[2_546] | 1.33 | 0.87 |
| 1:B:261:TYR:CD1 | 1:D:267:ARG:C[2_546] | 1.33 | 0.87 |
| 1:A:280:GLU:CB | 1:B:248:ASN:O[2_546] | 1.34 | 0.86 |
| 1:B:50:LEU:CD2 | 1:D:48:ILE:CB[2_546] | 1.34 | 0.86 |
| 1:B:28:LEU:CD1 | 1:D:178:ILE:CA[2_546] | 1.34 | 0.86 |
| 1:B:331:THR:C | 1:C:368:TYR:CE1[2_546] | 1.34 | 0.86 |
| 1:B:342:TRP:CE2 | 1:C:371:TYR:CD2[2_546] | 1.34 | 0.86 |
| 1:A:237:ARG:NH1 | 1:B:217:LEU:CA[2_546] | 1.34 | 0.86 |
| 1:B:37:ASP:CB | 1:D:339:THR:O[2_546] | 1.34 | 0.86 |
| 1:B:175:LYS:C | 1:D:19:THR:N[2_546] | 1.34 | 0.86 |
| 1:B:273:LYS:CE | 1:D:185:VAL:CB[2_546] | 1.34 | 0.86 |
| 1:B:35:ILE:CD1 | 1:D:182:ASP:N[2_546] | 1.34 | 0.86 |
| 1:B:300:ILE:N | 1:D:308:ILE:CA[2_546] | 1.34 | 0.86 |
| 1:B:180:TYR:CD1 | 1:D:29:ARG:CA[2_546] | 1.34 | 0.86 |
| 1:B:182:ASP:OD1 | 1:D:38:LEU:O[2_546] | 1.34 | 0.86 |
| 1:B:264:TYR:O | 1:D:312:THR:CB[2_546] | 1.34 | 0.86 |
| 1:B:332:ALA:C | 1:C:368:TYR:CE2[2_546] | 1.34 | 0.86 |
| 1:B:256:PHE:C | 1:D:264:TYR:CG[2_546] | 1.34 | 0.86 |
| 1:B:320:PHE:C | 1:C:367:GLU:CD[2_546] | 1.34 | 0.86 |
| 1:B:169:GLU:N | 1:C:364:VAL:CG1[2_546] | 1.34 | 0.86 |
| 1:B:46:GLU:CA | 1:D:52:LEU:C[2_546] | 1.34 | 0.86 |
| 1:B:342:TRP:CZ3 | 1:C:371:TYR:O[2_546] | 1.34 | 0.86 |
| 1:B:38:LEU:CB | 1:D:340:LEU:O[2_546] | 1.34 | 0.86 |
| 1:B:168:ASP:CA | 1:D:15:VAL:CG1[2_546] | 1.34 | 0.86 |
| 1:A:237:ARG:CZ | 1:B:217:LEU:CA[2_546] | 1.34 | 0.86 |
| 1:A:237:ARG:CD | 1:B:216:PRO:O[2_546] | 1.35 | 0.85 |
| 1:B:42:GLY:C | 1:D:344:ALA:O[2_546] | 1.35 | 0.85 |
| 1:B:180:TYR:CE1 | 1:D:29:ARG:CG[2_546] | 1.35 | 0.85 |
| 1:B:22:ASP:CG | 1:D:320:PHE:CZ[2_546] | 1.35 | 0.85 |
| 1:B:308:ILE:CA | 1:D:310:PRO:CA[2_546] | 1.35 | 0.85 |
| 1:B:59:LYS:CB | 1:D:115:ASN:N[2_546] | 1.35 | 0.85 |
| 1:B:271:PHE:CG | 1:D:20:PHE:O[2_546] | 1.35 | 0.85 |
| 1:A:109:ASN:O | 1:A:249:GLN:CB[2_556] | 1.35 | 0.85 |
| 1:B:302:GLN:O | 1:D:299:GLY:O[2_546] | 1.35 | 0.85 |
| 1:A:279:ILE:CG1 | 1:B:249:GLN:CG[2_546] | 1.35 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:313:ASP:CA | 1:D:26:GLY:O[2_546] | 1.35 | 0.85 |
| 1:B:265:ASP:C | 1:D:267:ARG:NH1[2_546] | 1.35 | 0.85 |
| 1:B:17:ASN:ND2 | 1:D:150:ASP:O[2_546] | 1.35 | 0.85 |
| 1:B:246:VAL:CG1 | 1:D:305:SER:N[2_546] | 1.35 | 0.85 |
| 1:B:336:LEU:CD2 | 1:C:369:GLN:CD[2_546] | 1.35 | 0.85 |
| 1:B:46:GLU:OE2 | 1:D:52:LEU:CD2[2_546] | 1.35 | 0.85 |
| 1:A:369:GLN:CA | 1:D:124:ILE:O[2_546] | 1.35 | 0.85 |
| 1:B:12:ILE:CG2 | 1:D:167:THR:CG2[2_546] | 1.35 | 0.85 |
| 1:B:304:SER:CB | 1:D:256:PHE:CA[2_546] | 1.35 | 0.85 |
| 1:B:47:THR:CA | 1:D:52:LEU:N[2_546] | 1.35 | 0.85 |
| 1:B:56:LEU:O | 1:D:118:GLU:O[2_546] | 1.36 | 0.84 |
| 1:B:33:TYR:CE2 | 1:D:124:ILE:CA[2_546] | 1.36 | 0.84 |
| 1:A:360:ARG:NH1 | 1:D:277:THR:CG2[2_546] | 1.36 | 0.84 |
| 1:B:261:TYR:CD2 | 1:D:271:PHE:CD1[2_546] | 1.36 | 0.84 |
| 1:B:260:VAL:C | 1:D:271:PHE:CA[2_546] | 1.36 | 0.84 |
| 1:B:312:THR:O | 1:D:27:ILE:C[2_546] | 1.36 | 0.84 |
| 1:B:334:PHE:CE2 | 1:D:37:ASP:CG[2_546] | 1.36 | 0.84 |
| 1:B:36:GLU:N | 1:D:181:THR:O[2_546] | 1.36 | 0.84 |
| 1:B:338:ARG:N | 1:D:33:TYR:CB[2_546] | 1.36 | 0.84 |
| 1:B:40:ASN:CG | 1:D:189:THR:CG2[2_546] | 1.36 | 0.84 |
| 1:A:110:PHE:CD1 | 1:A:249:GLN:OE1[2_556] | 1.36 | 0.84 |
| 1:B:333:LEU:O | 1:D:32:GLY:O[2_546] | 1.36 | 0.84 |
| 1:B:183:HIS:NE2 | 1:D:179:LEU:CD2[2_546] | 1.36 | 0.84 |
| 1:B:33:TYR:CZ | 1:D:124:ILE:N[2_546] | 1.36 | 0.84 |
| 1:A:367:GLU:CG | 1:D:156:PHE:CE2[2_546] | 1.36 | 0.84 |
| 1:B:23:GLY:C | 1:D:316:SER:N[2_546] | 1.37 | 0.83 |
| 1:B:20:PHE:O | 1:D:177:LEU:CA[2_546] | 1.37 | 0.83 |
| 1:B:312:THR:CB | 1:D:28:LEU:CB[2_546] | 1.37 | 0.83 |
| 1:B:35:ILE:CB | 1:D:181:THR:O[2_546] | 1.37 | 0.83 |
| 1:A:369:GLN:CB | 1:D:124:ILE:C[2_546] | 1.37 | 0.83 |
| 1:B:257:GLY:N | 1:D:264:TYR:CD2[2_546] | 1.37 | 0.83 |
| 1:B:45:GLU:O | 1:D:53:TYR:CB[2_546] | 1.37 | 0.83 |
| 1:B:174:ASP:CA | 1:D:17:ASN:CB[2_546] | 1.37 | 0.83 |
| 1:B:26:GLY:O | 1:D:180:TYR:CD2[2_546] | 1.37 | 0.83 |
| 1:B:189:THR:OG1 | 1:D:41:TYR:N[2_546] | 1.37 | 0.83 |
| 1:B:117:LYS:NZ | 1:D:64:ASP:OD1[2_546] | 1.37 | 0.83 |
| 1:B:302:GLN:C | 1:D:303:PHE:CG[2_546] | 1.37 | 0.83 |
| 1:A:364:VAL:C | 1:D:153:ALA:C[2_546] | 1.37 | 0.83 |
| 1:B:174:ASP:CA | 1:D:17:ASN:CA[2_546] | 1.37 | 0.83 |
| 1:B:258:HIS:CG | 1:D:269:LYS:N[2_546] | 1.38 | 0.82 |
| 1:A:363:TYR:N | 1:D:171:ASN:N[2_546] | 1.38 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:50:LEU:CD2 | 1:D:48:ILE:CG2[2_546] | 1.38 | 0.82 |
| 1:B:171:ASN:O | 1:D:17:ASN:N[2_546] | 1.38 | 0.82 |
| 1:B:47:THR:CG2 | 1:D:51:MET:N[2_546] | 1.38 | 0.82 |
| 1:B:315:TYR:CA | 1:D:22:ASP:CA[2_546] | 1.38 | 0.82 |
| 1:B:312:THR:OG1 | 1:D:28:LEU:CG[2_546] | 1.38 | 0.82 |
| 1:B:55:LYS:CG | 1:D:68:LYS:CB[2_546] | 1.38 | 0.82 |
| 1:A:365:GLY:N | 1:D:154:LYS:N[2_546] | 1.38 | 0.82 |
| 1:A:109:ASN:CG | 1:A:250:LYS:CA[2_556] | 1.38 | 0.82 |
| 1:B:17:ASN:ND2 | 1:D:151:SER:CA[2_546] | 1.38 | 0.82 |
| 1:B:257:GLY:C | 1:D:264:TYR:CE2[2_546] | 1.38 | 0.82 |
| 1:B:347:ILE:CG1 | 1:D:59:LYS:CG[2_546] | 1.38 | 0.82 |
| 1:B:44:TYR:CA | 1:D:31:ARG:CZ[2_546] | 1.38 | 0.82 |
| 1:B:96:LEU:CG | 1:C:370:GLU:OE1[2_546] | 1.38 | 0.82 |
| 1:B:53:TYR:CA | 1:D:65:LEU:CA[2_546] | 1.39 | 0.81 |
| 1:B:309:TYR:CD1 | 1:D:255:GLY:O[2_546] | 1.39 | 0.81 |
| 1:B:313:ASP:N | 1:D:26:GLY:O[2_546] | 1.39 | 0.81 |
| 1:B:262:LYS:CA | 1:D:315:TYR:N[2_546] | 1.39 | 0.81 |
| 1:B:260:VAL:O | 1:D:271:PHE:CB[2_546] | 1.39 | 0.81 |
| 1:B:112:TRP:CZ3 | 1:D:59:LYS:CD[2_546] | 1.39 | 0.81 |
| 1:B:225:ALA:CB | 1:D:25:LYS:CA[2_546] | 1.39 | 0.81 |
| 1:B:338:ARG:C | 1:C:371:TYR:CD1[2_546] | 1.39 | 0.81 |
| 1:B:50:LEU:CG | 1:D:48:ILE:CB[2_546] | 1.39 | 0.81 |
| 1:B:338:ARG:NH1 | 1:D:37:ASP:C[2_546] | 1.39 | 0.81 |
| 1:A:366:PRO:CG | 1:D:152:PHE:CD1[2_546] | 1.39 | 0.81 |
| 1:B:35:ILE:CG1 | 1:D:181:THR:CA[2_546] | 1.39 | 0.81 |
| 1:B:308:ILE:O | 1:D:309:TYR:C[2_546] | 1.39 | 0.81 |
| 1:B:229:PHE:CE1 | 1:D:24:GLU:CG[2_546] | 1.39 | 0.81 |
| 1:B:117:LYS:CA | 1:D:61:GLU:N[2_546] | 1.39 | 0.81 |
| 1:B:58:THR:OG1 | 1:D:115:ASN:OD1[2_546] | 1.39 | 0.81 |
| 1:B:36:GLU:OE1 | 1:D:338:ARG:NH1[2_546] | 1.40 | 0.80 |
| 1:A:109:ASN:OD1 | 1:A:250:LYS:N[2_556] | 1.40 | 0.80 |
| 1:B:339:THR:C | 1:D:56:LEU:CD1[2_546] | 1.40 | 0.80 |
| 1:B:264:TYR:CZ | 1:D:258:HIS:CE1[2_546] | 1.40 | 0.80 |
| 1:B:56:LEU:N | 1:D:121:ILE:CG1[2_546] | 1.40 | 0.80 |
| 1:A:368:TYR:O | 1:D:127:MET:O[2_546] | 1.40 | 0.80 |
| 1:B:266:PRO:N | 1:D:267:ARG:CZ[2_546] | 1.40 | 0.80 |
| 1:A:107:ASP:C | 1:A:248:ASN:CG[2_556] | 1.40 | 0.80 |
| 1:B:23:GLY:C | 1:D:316:SER:CB[2_546] | 1.40 | 0.80 |
| 1:A:286:ARG:CG | 1:B:251:ASN:ND2[2_546] | 1.40 | 0.80 |
| 1:B:112:TRP:CZ3 | 1:D:59:LYS:CE[2_546] | 1.40 | 0.80 |
| 1:B:314:PHE:CG | 1:D:23:GLY:O[2_546] | 1.40 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:33:TYR:CZ | 1:D:124:ILE:CA[2_546] | 1.40 | 0.80 |
| 1:B:170:ILE:N | 1:C:364:VAL:CB[2_546] | 1.40 | 0.80 |
| 1:B:264:TYR:CZ | 1:D:258:HIS:CD2[2_546] | 1.40 | 0.80 |
| 1:B:48:ILE:CD1 | 1:D:55:LYS:N[2_546] | 1.40 | 0.80 |
| 1:B:302:GLN:O | 1:D:303:PHE:CD1[2_546] | 1.40 | 0.80 |
| 1:B:306:LYS:NZ | 1:D:298:LEU:O[2_546] | 1.41 | 0.79 |
| 1:B:61:GLU:OE2 | 1:D:118:GLU:OE1[2_546] | 1.41 | 0.79 |
| 1:B:49:TYR:CA | 1:D:53:TYR:CE1[2_546] | 1.41 | 0.79 |
| 1:B:20:PHE:CB | 1:D:173:MET:O[2_546] | 1.41 | 0.79 |
| 1:B:242:PHE:CZ | 1:D:306:LYS:N[2_546] | 1.41 | 0.79 |
| 1:B:48:ILE:N | 1:D:49:TYR:C[2_546] | 1.41 | 0.79 |
| 1:B:265:ASP:N | 1:D:265:ASP:OD2[2_546] | 1.41 | 0.79 |
| 1:B:253:LEU:CB | 1:D:309:TYR:CE1[2_546] | 1.41 | 0.79 |
| 1:B:336:LEU:C | 1:D:33:TYR:CZ[2_546] | 1.41 | 0.79 |
| 1:B:262:LYS:CG | 1:D:315:TYR:CB[2_546] | 1.41 | 0.79 |
| 1:B:265:ASP:CB | 1:D:265:ASP:OD1[2_546] | 1.41 | 0.79 |
| 1:B:44:TYR:C | 1:D:54:GLY:N[2_546] | 1.41 | 0.79 |
| 1:B:39:VAL:C | 1:D:345:HIS:CD2[2_546] | 1.41 | 0.79 |
| 1:B:45:GLU:N | 1:D:54:GLY:N[2_546] | 1.41 | 0.79 |
| 1:B:309:TYR:CB | 1:D:311:ASN:CB[2_546] | 1.41 | 0.79 |
| 1:B:28:LEU:C | 1:D:177:LEU:O[2_546] | 1.41 | 0.79 |
| 1:B:256:PHE:CD1 | 1:D:263:THR:O[2_546] | 1.41 | 0.79 |
| 1:B:188:SER:N | 1:D:41:TYR:OH[2_546] | 1.41 | 0.79 |
| 1:B:51:MET:O | 1:D:62:LEU:CD1[2_546] | 1.41 | 0.79 |
| 1:B:260:VAL:CA | 1:D:272:LYS:N[2_546] | 1.42 | 0.78 |
| 1:A:108:LYS:CE | 1:A:243:ASN:ND2[2_556] | 1.42 | 0.78 |
| 1:B:177:LEU:C | 1:D:31:ARG:N[2_546] | 1.42 | 0.78 |
| 1:B:52:LEU:CD2 | 1:D:57:PRO:CB[2_546] | 1.42 | 0.78 |
| 1:B:50:LEU:O | 1:D:65:LEU:CG[2_546] | 1.42 | 0.78 |
| 1:B:313:ASP:CB | 1:D:26:GLY:O[2_546] | 1.42 | 0.78 |
| 1:A:110:PHE:C | 1:A:245:LYS:CA[2_556] | 1.42 | 0.78 |
| 1:B:225:ALA:CB | 1:D:25:LYS:O[2_546] | 1.42 | 0.78 |
| 1:B:186:PRO:CD | 1:D:40:ASN:N[2_546] | 1.42 | 0.78 |
| 1:B:28:LEU:C | 1:D:337:SER:OG[2_546] | 1.42 | 0.78 |
| 1:B:171:ASN:CA | 1:D:16:THR:N[2_546] | 1.42 | 0.78 |
| 1:B:314:PHE:N | 1:D:26:GLY:C[2_546] | 1.42 | 0.78 |
| 1:B:18:LEU:CG | 1:D:43:SER:OG[2_546] | 1.42 | 0.78 |
| 1:A:286:ARG:NH1 | 1:B:251:ASN:N[2_546] | 1.42 | 0.78 |
| 1:B:174:ASP:N | 1:D:17:ASN:CB[2_546] | 1.42 | 0.78 |
| 1:B:315:TYR:CZ | 1:D:260:VAL:O[2_546] | 1.42 | 0.78 |
| 1:B:65:LEU:CD1 | 1:D:53:TYR:CD2[2_546] | 1.42 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:174:ASP:CB | 1:D:17:ASN:CB[2_546] | 1.42 | 0.78 |
| 1:B:179:LEU:CD1 | 1:D:19:THR:CB[2_546] | 1.43 | 0.77 |
| 1:B:206:LEU:CD2 | 1:C:372:VAL:C[2_546] | 1.43 | 0.77 |
| 1:B:174:ASP:OD2 | 1:D:31:ARG:NH1[2_546] | 1.43 | 0.77 |
| 1:A:110:PHE:CD1 | 1:A:249:GLN:NE2[2_556] | 1.43 | 0.77 |
| 1:B:265:ASP:CB | 1:D:267:ARG:NE[2_546] | 1.43 | 0.77 |
| 1:B:305:SER:OG | 1:D:253:LEU:CD2[2_546] | 1.43 | 0.77 |
| 1:B:302:GLN:OE1 | 1:D:302:GLN:C[2_546] | 1.43 | 0.77 |
| 1:B:50:LEU:C | 1:D:65:LEU:CD1[2_546] | 1.43 | 0.77 |
| 1:A:294:LYS:NZ | 1:B:231:GLU:OE2[2_546] | 1.43 | 0.77 |
| 1:A:365:GLY:O | 1:D:152:PHE:O[2_546] | 1.43 | 0.77 |
| 1:B:264:TYR:CE2 | 1:D:258:HIS:ND1[2_546] | 1.43 | 0.77 |
| 1:B:299:GLY:N | 1:D:307:GLY:C[2_546] | 1.43 | 0.77 |
| 1:B:119:LYS:C | 1:D:58:THR:CG2[2_546] | 1.43 | 0.77 |
| 1:B:33:TYR:CD1 | 1:D:124:ILE:CG1[2_546] | 1.43 | 0.77 |
| 1:B:173:MET:CE | 1:C:363:TYR:OH[2_546] | 1.43 | 0.77 |
| 1:B:34:ASN:ND2 | 1:D:335:ALA:C[2_546] | 1.43 | 0.77 |
| 1:B:319:VAL:CB | 1:D:20:PHE:CD1[2_546] | 1.43 | 0.77 |
| 1:B:42:GLY:O | 1:D:344:ALA:O[2_546] | 1.43 | 0.77 |
| 1:A:368:TYR:CA | 1:D:336:LEU:CD1[2_546] | 1.43 | 0.77 |
| 1:B:302:GLN:CD | 1:D:302:GLN:O[2_546] | 1.43 | 0.77 |
| 1:B:38:LEU:N | 1:D:340:LEU:C[2_546] | 1.43 | 0.77 |
| 1:B:24:GLU:OE2 | 1:D:318:ILE:O[2_546] | 1.43 | 0.77 |
| 1:B:189:THR:CA | 1:D:41:TYR:CG[2_546] | 1.43 | 0.77 |
| 1:B:22:ASP:CG | 1:D:320:PHE:CE2[2_546] | 1.43 | 0.77 |
| 1:A:111:LYS:NZ | 1:A:241:TRP:CZ3[2_556] | 1.43 | 0.77 |
| 1:B:37:ASP:O | 1:D:343:LEU:N[2_546] | 1.44 | 0.76 |
| 1:A:364:VAL:CB | 1:D:154:LYS:CB[2_546] | 1.44 | 0.76 |
| 1:B:173:MET:SD | 1:C:366:PRO:O[2_546] | 1.44 | 0.76 |
| 1:B:22:ASP:OD2 | 1:D:320:PHE:CG[2_546] | 1.44 | 0.76 |
| 1:B:351:GLU:CD | 1:D:63:ASN:ND2[2_546] | 1.44 | 0.76 |
| 1:B:47:THR:C | 1:D:49:TYR:O[2_546] | 1.44 | 0.76 |
| 1:B:260:VAL:CB | 1:D:270:ILE:O[2_546] | 1.44 | 0.76 |
| 1:B:272:LYS:NZ | 1:D:259:ARG:C[2_546] | 1.44 | 0.76 |
| 1:B:26:GLY:C | 1:D:180:TYR:CE2[2_546] | 1.44 | 0.76 |
| 1:B:171:ASN:CG | 1:D:16:THR:CA[2_546] | 1.44 | 0.76 |
| 1:B:17:ASN:CG | 1:D:151:SER:N[2_546] | 1.45 | 0.75 |
| 1:B:330:PHE:O | 1:C:368:TYR:CD1[2_546] | 1.45 | 0.75 |
| 1:A:111:LYS:O | 1:A:245:LYS:NZ[2_556] | 1.45 | 0.75 |
| 1:B:172:ALA:CA | 1:C:363:TYR:CA[2_546] | 1.45 | 0.75 |
| 1:B:18:LEU:N | 1:D:45:GLU:OE1[2_546] | 1.45 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:120:ALA:N | 1:D:58:THR:CB[2_546] | 1.45 | 0.75 |
| 1:B:22:ASP:OD2 | 1:D:320:PHE:CD2[2_546] | 1.45 | 0.75 |
| 1:B:37:ASP:CA | 1:D:342:TRP:CA[2_546] | 1.45 | 0.75 |
| 1:B:181:THR:C | 1:D:38:LEU:CD2[2_546] | 1.45 | 0.75 |
| 1:B:20:PHE:CA | 1:D:173:MET:O[2_546] | 1.45 | 0.75 |
| 1:A:368:TYR:O | 1:D:128:ALA:CA[2_546] | 1.45 | 0.75 |
| 1:B:259:ARG:CA | 1:D:269:LYS:O[2_546] | 1.45 | 0.75 |
| 1:B:263:THR:CG2 | 1:D:313:ASP:CA[2_546] | 1.45 | 0.75 |
| 1:B:315:TYR:CA | 1:D:23:GLY:N[2_546] | 1.45 | 0.75 |
| 1:B:315:TYR:C | 1:D:21:ILE:C[2_546] | 1.45 | 0.75 |
| 1:B:256:PHE:CA | 1:D:264:TYR:CB[2_546] | 1.45 | 0.75 |
| 1:B:112:TRP:CZ2 | 1:D:59:LYS:NZ[2_546] | 1.45 | 0.75 |
| 1:A:363:TYR:CG | 1:D:153:ALA:CB[2_546] | 1.45 | 0.75 |
| 1:B:53:TYR:C | 1:D:65:LEU:C[2_546] | 1.46 | 0.74 |
| 1:B:319:VAL:CG1 | 1:D:20:PHE:CD1[2_546] | 1.46 | 0.74 |
| 1:B:260:VAL:N | 1:D:272:LYS:N[2_546] | 1.46 | 0.74 |
| 1:B:182:ASP:O | 1:D:178:ILE:CG2[2_546] | 1.46 | 0.74 |
| 1:B:338:ARG:NH1 | 1:D:38:LEU:N[2_546] | 1.46 | 0.74 |
| 1:B:273:LYS:NZ | 1:D:185:VAL:CA[2_546] | 1.46 | 0.74 |
| 1:B:269:LYS:N | 1:D:183:HIS:CE1[2_546] | 1.46 | 0.74 |
| 1:B:17:ASN:CG | 1:D:151:SER:C[2_546] | 1.46 | 0.74 |
| 1:B:35:ILE:CB | 1:D:181:THR:CA[2_546] | 1.46 | 0.74 |
| 1:B:336:LEU:O | 1:D:33:TYR:CE1[2_546] | 1.46 | 0.74 |
| 1:B:156:PHE:CE2 | 1:C:366:PRO:CB[2_546] | 1.46 | 0.74 |
| 1:B:261:TYR:CE2 | 1:D:271:PHE:CE1[2_546] | 1.46 | 0.74 |
| 1:B:121:ILE:CG1 | 1:D:61:GLU:CD[2_546] | 1.46 | 0.74 |
| 1:B:36:GLU:CD | 1:D:338:ARG:CZ[2_546] | 1.47 | 0.73 |
| 1:B:59:LYS:CG | 1:D:114:GLU:O[2_546] | 1.47 | 0.73 |
| 1:B:33:TYR:CD1 | 1:D:124:ILE:CB[2_546] | 1.47 | 0.73 |
| 1:B:19:THR:C | 1:D:174:ASP:C[2_546] | 1.47 | 0.73 |
| 1:B:336:LEU:N | 1:C:369:GLN:O[2_546] | 1.47 | 0.73 |
| 1:B:334:PHE:CE2 | 1:D:37:ASP:OD2[2_546] | 1.47 | 0.73 |
| 1:B:181:THR:N | 1:D:38:LEU:CD1[2_546] | 1.47 | 0.73 |
| 1:A:111:LYS:O | 1:A:245:LYS:CE[2_556] | 1.47 | 0.73 |
| 1:B:336:LEU:O | 1:D:33:TYR:OH[2_546] | 1.47 | 0.73 |
| 1:B:312:THR:N | 1:D:266:PRO:CD[2_546] | 1.47 | 0.73 |
| 1:A:108:LYS:NZ | 1:A:243:ASN:ND2[2_556] | 1.47 | 0.73 |
| 1:B:264:TYR:CE2 | 1:D:258:HIS:NE2[2_546] | 1.47 | 0.73 |
| 1:B:338:ARG:O | 1:C:371:TYR:CD1[2_546] | 1.47 | 0.73 |
| 1:B:308:ILE:O | 1:D:309:TYR:O[2_546] | 1.47 | 0.73 |
| 1:B:183:HIS:O | 1:D:39:VAL:CG2[2_546] | 1.47 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:267:ARG:NH2 | 1:D:35:ILE:CD1[2_546] | 1.47 | 0.73 |
| 1:B:58:THR:N | 1:D:118:GLU:CB[2_546] | 1.47 | 0.73 |
| 1:B:258:HIS:N | 1:D:264:TYR:CE2[2_546] | 1.47 | 0.73 |
| 1:B:40:ASN:C | 1:D:345:HIS:CB[2_546] | 1.47 | 0.73 |
| 1:B:34:ASN:C | 1:D:337:SER:O[2_546] | 1.47 | 0.73 |
| 1:B:29:ARG:CG | 1:D:337:SER:CA[2_546] | 1.48 | 0.72 |
| 1:B:334:PHE:CB | 1:D:34:ASN:ND2[2_546] | 1.48 | 0.72 |
| 1:B:342:TRP:CD2 | 1:C:371:TYR:CE2[2_546] | 1.48 | 0.72 |
| 1:B:33:TYR:CE1 | 1:D:124:ILE:CG1[2_546] | 1.48 | 0.72 |
| 1:B:319:VAL:CB | 1:D:20:PHE:CE1[2_546] | 1.48 | 0.72 |
| 1:B:308:ILE:O | 1:D:310:PRO:CA[2_546] | 1.48 | 0.72 |
| 1:B:270:ILE:CG1 | 1:D:183:HIS:CA[2_546] | 1.48 | 0.72 |
| 1:B:333:LEU:CB | 1:C:368:TYR:C[2_546] | 1.48 | 0.72 |
| 1:B:28:LEU:O | 1:D:337:SER:OG[2_546] | 1.48 | 0.72 |
| 1:B:117:LYS:CB | 1:D:61:GLU:CA[2_546] | 1.48 | 0.72 |
| 1:B:28:LEU:CB | 1:D:179:LEU:C[2_546] | 1.48 | 0.72 |
| 1:B:271:PHE:CE2 | 1:D:20:PHE:CA[2_546] | 1.48 | 0.72 |
| 1:B:38:LEU:N | 1:D:341:GLY:C[2_546] | 1.48 | 0.72 |
| 1:B:308:ILE:CB | 1:D:310:PRO:CD[2_546] | 1.48 | 0.72 |
| 1:B:35:ILE:CB | 1:D:182:ASP:N[2_546] | 1.48 | 0.72 |
| 1:B:24:GLU:OE2 | 1:D:317:GLY:O[2_546] | 1.48 | 0.72 |
| 1:A:360:ARG:CZ | 1:D:277:THR:CB[2_546] | 1.49 | 0.71 |
| 1:B:38:LEU:CD2 | 1:D:340:LEU:CD1[2_546] | 1.49 | 0.71 |
| 1:B:33:TYR:CE2 | 1:D:124:ILE:N[2_546] | 1.49 | 0.71 |
| 1:B:34:ASN:OD1 | 1:D:337:SER:N[2_546] | 1.49 | 0.71 |
| 1:B:189:THR:CB | 1:D:41:TYR:N[2_546] | 1.49 | 0.71 |
| 1:B:58:THR:C | 1:D:115:ASN:CB[2_546] | 1.49 | 0.71 |
| 1:B:21:ILE:CA | 1:D:176:ALA:N[2_546] | 1.49 | 0.71 |
| 1:B:305:SER:CB | 1:D:253:LEU:CG[2_546] | 1.49 | 0.71 |
| 1:B:300:ILE:CA | 1:D:308:ILE:CG2[2_546] | 1.49 | 0.71 |
| 1:B:25:LYS:NZ | 1:D:330:PHE:CB[2_546] | 1.49 | 0.71 |
| 1:B:300:ILE:CG1 | 1:D:257:GLY:C[2_546] | 1.49 | 0.71 |
| 1:B:46:GLU:N | 1:D:53:TYR:N[2_546] | 1.49 | 0.71 |
| 1:B:29:ARG:NH2 | 1:D:336:LEU:N[2_546] | 1.49 | 0.71 |
| 1:B:37:ASP:C | 1:D:341:GLY:C[2_546] | 1.49 | 0.71 |
| 1:A:111:LYS:CB | 1:A:245:LYS:CG[2_556] | 1.50 | 0.70 |
| 1:B:56:LEU:C | 1:D:117:LYS:O[2_546] | 1.50 | 0.70 |
| 1:B:246:VAL:CG1 | 1:D:304:SER:C[2_546] | 1.50 | 0.70 |
| 1:B:253:LEU:CB | 1:D:309:TYR:CZ[2_546] | 1.50 | 0.70 |
| 1:B:300:ILE:N | 1:D:308:ILE:CB[2_546] | 1.50 | 0.70 |
| 1:B:311:ASN:CA | 1:D:266:PRO:CD[2_546] | 1.50 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:108:LYS:CA | 1:A:248:ASN:CG[2_556] | 1.50 | 0.70 |
| 1:B:175:LYS:CA | 1:D:18:LEU:N[2_546] | 1.50 | 0.70 |
| 1:B:254:MET:O | 1:D:263:THR:OG1[2_546] | 1.50 | 0.70 |
| 1:B:320:PHE:CZ | 1:C:367:GLU:O[2_546] | 1.50 | 0.70 |
| 1:A:365:GLY:C | 1:D:152:PHE:C[2_546] | 1.50 | 0.70 |
| 1:A:112:TRP:O | 1:A:231:GLU:OE1[2_556] | 1.50 | 0.70 |
| 1:B:179:LEU:CG | 1:D:19:THR:OG1[2_546] | 1.50 | 0.70 |
| 1:A:290:GLU:OE2 | 1:B:251:ASN:OD1[2_546] | 1.50 | 0.70 |
| 1:B:309:TYR:OH | 1:D:256:PHE:N[2_546] | 1.50 | 0.70 |
| 1:B:38:LEU:N | 1:D:341:GLY:N[2_546] | 1.51 | 0.69 |
| 1:B:56:LEU:CA | 1:D:121:ILE:CG1[2_546] | 1.51 | 0.69 |
| 1:B:127:MET:CE | 1:C:370:GLU:CG[2_546] | 1.51 | 0.69 |
| 1:B:59:LYS:CE | 1:D:113:LYS:O[2_546] | 1.51 | 0.69 |
| 1:B:206:LEU:CD2 | 1:C:372:VAL:O[2_546] | 1.51 | 0.69 |
| 1:B:44:TYR:CA | 1:D:31:ARG:NE[2_546] | 1.51 | 0.69 |
| 1:A:109:ASN:CA | 1:A:249:GLN:N[2_556] | 1.51 | 0.69 |
| 1:B:340:LEU:CD2 | 1:D:50:LEU:CA[2_546] | 1.51 | 0.69 |
| 1:B:182:ASP:CA | 1:D:38:LEU:CB[2_546] | 1.51 | 0.69 |
| 1:B:256:PHE:O | 1:D:264:TYR:CG[2_546] | 1.51 | 0.69 |
| 1:B:173:MET:C | 1:D:17:ASN:ND2[2_546] | 1.51 | 0.69 |
| 1:B:315:TYR:O | 1:D:21:ILE:C[2_546] | 1.51 | 0.69 |
| 1:B:180:TYR:CG | 1:D:33:TYR:O[2_546] | 1.51 | 0.69 |
| 1:B:303:PHE:C | 1:D:256:PHE:CG[2_546] | 1.51 | 0.69 |
| 1:B:45:GLU:C | 1:D:52:LEU:O[2_546] | 1.51 | 0.69 |
| 1:B:22:ASP:CG | 1:D:320:PHE:CD1[2_546] | 1.51 | 0.69 |
| 1:B:337:SER:N | 1:D:33:TYR:CD2[2_546] | 1.51 | 0.69 |
| 1:B:265:ASP:O | 1:D:267:ARG:NE[2_546] | 1.51 | 0.69 |
| 1:A:368:TYR:CD1 | 1:D:336:LEU:CA[2_546] | 1.51 | 0.69 |
| 1:B:270:ILE:CD1 | 1:D:182:ASP:C[2_546] | 1.51 | 0.69 |
| 1:B:340:LEU:CD1 | 1:D:57:PRO:CD[2_546] | 1.51 | 0.69 |
| 1:B:242:PHE:CE2 | 1:D:305:SER:C[2_546] | 1.51 | 0.69 |
| 1:B:17:ASN:OD1 | 1:D:151:SER:N[2_546] | 1.51 | 0.69 |
| 1:B:22:ASP:OD2 | 1:D:320:PHE:CE1[2_546] | 1.51 | 0.69 |
| 1:B:313:ASP:O | 1:D:27:ILE:N[2_546] | 1.52 | 0.68 |
| 1:B:33:TYR:CE2 | 1:D:124:ILE:CB[2_546] | 1.52 | 0.68 |
| 1:B:309:TYR:CD2 | 1:D:311:ASN:CG[2_546] | 1.52 | 0.68 |
| 1:A:280:GLU:CA | 1:B:248:ASN:C[2_546] | 1.52 | 0.68 |
| 1:B:315:TYR:CE1 | 1:D:260:VAL:C[2_546] | 1.52 | 0.68 |
| 1:B:36:GLU:OE2 | 1:D:338:ARG:CZ[2_546] | 1.52 | 0.68 |
| 1:B:272:LYS:CD | 1:D:260:VAL:CG2[2_546] | 1.52 | 0.68 |
| 1:B:262:LYS:NZ | 1:D:315:TYR:CE1[2_546] | 1.52 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:109:ASN:ND2 | 1:A:246:VAL:O[2_556] | 1.52 | 0.68 |
| 1:B:179:LEU:N | 1:D:30:TYR:CB[2_546] | 1.52 | 0.68 |
| 1:B:303:PHE:CZ | 1:D:304:SER:CB[2_546] | 1.52 | 0.68 |
| 1:B:36:GLU:CG | 1:D:338:ARG:NE[2_546] | 1.52 | 0.68 |
| 1:B:333:LEU:CG | 1:C:368:TYR:N[2_546] | 1.52 | 0.68 |
| 1:B:22:ASP:OD1 | 1:D:320:PHE:CD1[2_546] | 1.52 | 0.68 |
| 1:B:268:ALA:CB | 1:D:261:TYR:CZ[2_546] | 1.52 | 0.68 |
| 1:B:20:PHE:C | 1:D:176:ALA:C[2_546] | 1.52 | 0.68 |
| 1:B:50:LEU:CA | 1:D:65:LEU:CD1[2_546] | 1.52 | 0.68 |
| 1:B:38:LEU:O | 1:D:344:ALA:CA[2_546] | 1.52 | 0.68 |
| 1:B:184:GLU:CD | 1:D:270:ILE:CG2[2_546] | 1.52 | 0.68 |
| 1:B:171:ASN:O | 1:D:16:THR:CA[2_546] | 1.52 | 0.68 |
| 1:B:21:ILE:CG1 | 1:D:175:LYS:C[2_546] | 1.52 | 0.68 |
| 1:B:333:LEU:CB | 1:C:368:TYR:CB[2_546] | 1.53 | 0.67 |
| 1:B:57:PRO:CD | 1:D:117:LYS:C[2_546] | 1.53 | 0.67 |
| 1:B:117:LYS:NZ | 1:D:64:ASP:CG[2_546] | 1.53 | 0.67 |
| 1:B:49:TYR:CG | 1:D:53:TYR:CZ[2_546] | 1.53 | 0.67 |
| 1:B:254:MET:C | 1:D:263:THR:OG1[2_546] | 1.53 | 0.67 |
| 1:B:21:ILE:O | 1:D:176:ALA:CB[2_546] | 1.53 | 0.67 |
| 1:B:301:LYS:O | 1:D:303:PHE:CD2[2_546] | 1.53 | 0.67 |
| 1:B:260:VAL:CG2 | 1:D:270:ILE:C[2_546] | 1.53 | 0.67 |
| 1:A:286:ARG:CG | 1:B:251:ASN:CG[2_546] | 1.53 | 0.67 |
| 1:B:269:LYS:C | 1:D:184:GLU:CG[2_546] | 1.53 | 0.67 |
| 1:A:4:VAL:CG2 | 1:D:167:THR:OG1[2_546] | 1.53 | 0.67 |
| 1:B:33:TYR:CD1 | 1:D:124:ILE:CG2[2_546] | 1.53 | 0.67 |
| 1:B:175:LYS:CG | 1:D:16:THR:OG1[2_546] | 1.53 | 0.67 |
| 1:B:186:PRO:CG | 1:D:40:ASN:CG[2_546] | 1.53 | 0.67 |
| 1:B:40:ASN:ND2 | 1:D:189:THR:CA[2_546] | 1.53 | 0.67 |
| 1:A:110:PHE:O | 1:A:245:LYS:CA[2_556] | 1.53 | 0.67 |
| 1:B:27:ILE:CG1 | 1:D:334:PHE:CB[2_546] | 1.53 | 0.67 |
| 1:B:35:ILE:CG1 | 1:D:181:THR:N[2_546] | 1.53 | 0.67 |
| 1:B:18:LEU:C | 1:D:44:TYR:CA[2_546] | 1.53 | 0.67 |
| 1:B:310:PRO:C | 1:D:265:ASP:CA[2_546] | 1.53 | 0.67 |
| 1:B:263:THR:OG1 | 1:D:313:ASP:CA[2_546] | 1.53 | 0.67 |
| 1:B:263:THR:CG2 | 1:D:312:THR:O[2_546] | 1.53 | 0.67 |
| 1:B:258:HIS:ND1 | 1:D:266:PRO:O[2_546] | 1.53 | 0.67 |
| 1:B:315:TYR:N | 1:D:23:GLY:N[2_546] | 1.54 | 0.66 |
| 1:B:259:ARG:NE | 1:D:273:LYS:CB[2_546] | 1.54 | 0.66 |
| 1:B:341:GLY:C | 1:D:46:GLU:CD[2_546] | 1.54 | 0.66 |
| 1:A:236:ASN:CG | 1:B:254:MET:CE[2_546] | 1.54 | 0.66 |
| 1:B:334:PHE:CE1 | 1:D:34:ASN:CB[2_546] | 1.54 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:177:LEU:CA | 1:D:31:ARG:CB[2_546] | 1.54 | 0.66 |
| 1:B:300:ILE:CB | 1:D:257:GLY:CA[2_546] | 1.54 | 0.66 |
| 1:B:51:MET:CA | 1:D:45:GLU:O[2_546] | 1.54 | 0.66 |
| 1:B:57:PRO:CG | 1:D:117:LYS:CA[2_546] | 1.54 | 0.66 |
| 1:B:337:SER:C | 1:D:33:TYR:CD1[2_546] | 1.54 | 0.66 |
| 1:B:335:ALA:C | 1:C:370:GLU:C[2_546] | 1.54 | 0.66 |
| 1:B:277:THR:OG1 | 1:C:362:LEU:CA[2_546] | 1.55 | 0.65 |
| 1:B:49:TYR:CB | 1:D:53:TYR:CD1[2_546] | 1.55 | 0.65 |
| 1:B:309:TYR:CG | 1:D:311:ASN:CG[2_546] | 1.55 | 0.65 |
| 1:B:270:ILE:CB | 1:D:184:GLU:N[2_546] | 1.55 | 0.65 |
| 1:B:186:PRO:CA | 1:D:40:ASN:OD1[2_546] | 1.55 | 0.65 |
| 1:B:301:LYS:N | 1:D:308:ILE:CD1[2_546] | 1.55 | 0.65 |
| 1:A:364:VAL:O | 1:D:153:ALA:N[2_546] | 1.55 | 0.65 |
| 1:B:56:LEU:CA | 1:D:121:ILE:N[2_546] | 1.55 | 0.65 |
| 1:B:299:GLY:O | 1:D:308:ILE:CB[2_546] | 1.55 | 0.65 |
| 1:A:110:PHE:C | 1:A:245:LYS:N[2_556] | 1.55 | 0.65 |
| 1:B:175:LYS:CE | 1:D:16:THR:OG1[2_546] | 1.55 | 0.65 |
| 1:B:172:ALA:C | 1:C:363:TYR:CD1[2_546] | 1.55 | 0.65 |
| 1:B:302:GLN:CG | 1:D:304:SER:N[2_546] | 1.55 | 0.65 |
| 1:B:18:LEU:O | 1:D:44:TYR:N[2_546] | 1.55 | 0.65 |
| 1:B:38:LEU:CG | 1:D:340:LEU:O[2_546] | 1.55 | 0.65 |
| 1:B:40:ASN:ND2 | 1:D:189:THR:CB[2_546] | 1.55 | 0.65 |
| 1:B:24:GLU:CG | 1:D:317:GLY:CA[2_546] | 1.55 | 0.65 |
| 1:A:109:ASN:C | 1:A:249:GLN:CB[2_556] | 1.56 | 0.64 |
| 1:B:58:THR:C | 1:D:115:ASN:CA[2_546] | 1.56 | 0.64 |
| 1:B:26:GLY:O | 1:D:180:TYR:CZ[2_546] | 1.56 | 0.64 |
| 1:B:26:GLY:N | 1:D:180:TYR:OH[2_546] | 1.56 | 0.64 |
| 1:B:112:TRP:CZ3 | 1:D:59:LYS:NZ[2_546] | 1.56 | 0.64 |
| 1:B:342:TRP:CG | 1:C:371:TYR:CZ[2_546] | 1.56 | 0.64 |
| 1:B:62:LEU:CD1 | 1:D:117:LYS:CD[2_546] | 1.56 | 0.64 |
| 1:B:27:ILE:CA | 1:D:180:TYR:CG[2_546] | 1.56 | 0.64 |
| 1:B:35:ILE:CA | 1:D:181:THR:C[2_546] | 1.56 | 0.64 |
| 1:B:338:ARG:N | 1:D:33:TYR:CG[2_546] | 1.56 | 0.64 |
| 1:B:304:SER:N | 1:D:256:PHE:CB[2_546] | 1.56 | 0.64 |
| 1:B:314:PHE:O | 1:D:24:GLU:N[2_546] | 1.56 | 0.64 |
| 1:B:178:ILE:CG2 | 1:D:51:MET:CG[2_546] | 1.56 | 0.64 |
| 1:B:304:SER:C | 1:D:256:PHE:CD1[2_546] | 1.56 | 0.64 |
| 1:B:117:LYS:NZ | 1:D:64:ASP:CB[2_546] | 1.56 | 0.64 |
| 1:A:367:GLU:C | 1:D:336:LEU:CD2[2_546] | 1.56 | 0.64 |
| 1:B:20:PHE:CG | 1:D:173:MET:O[2_546] | 1.56 | 0.64 |
| 1:B:52:LEU:CD1 | 1:D:57:PRO:CA[2_546] | 1.56 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:117:LYS:C | 1:D:58:THR:OG1[2_546] | 1.56 | 0.64 |
| 1:B:42:GLY:N | 1:D:344:ALA:CA[2_546] | 1.56 | 0.64 |
| 1:B:310:PRO:CB | 1:D:261:TYR:CB[2_546] | 1.56 | 0.64 |
| 1:B:58:THR:N | 1:D:118:GLU:CG[2_546] | 1.56 | 0.64 |
| 1:B:54:GLY:N | 1:D:65:LEU:C[2_546] | 1.56 | 0.64 |
| 1:B:42:GLY:CA | 1:D:344:ALA:O[2_546] | 1.56 | 0.64 |
| 1:B:345:HIS:CD2 | 1:D:42:GLY:C[2_546] | 1.56 | 0.64 |
| 1:B:253:LEU:CD2 | 1:D:309:TYR:CE1[2_546] | 1.56 | 0.64 |
| 1:B:47:THR:OG1 | 1:D:51:MET:C[2_546] | 1.56 | 0.64 |
| 1:B:338:ARG:CZ | 1:D:37:ASP:C[2_546] | 1.56 | 0.64 |
| 1:B:19:THR:N | 1:D:44:TYR:N[2_546] | 1.56 | 0.64 |
| 1:B:302:GLN:NE2 | 1:D:303:PHE:N[2_546] | 1.56 | 0.64 |
| 1:B:56:LEU:CG | 1:D:121:ILE:N[2_546] | 1.56 | 0.64 |
| 1:B:34:ASN:CB | 1:D:337:SER:C[2_546] | 1.57 | 0.63 |
| 1:B:173:MET:CE | 1:C:366:PRO:O[2_546] | 1.57 | 0.63 |
| 1:B:246:VAL:CG1 | 1:D:304:SER:OG[2_546] | 1.57 | 0.63 |
| 1:B:18:LEU:CG | 1:D:43:SER:CB[2_546] | 1.57 | 0.63 |
| 1:B:18:LEU:C | 1:D:44:TYR:CB[2_546] | 1.57 | 0.63 |
| 1:A:111:LYS:CB | 1:A:245:LYS:CD[2_556] | 1.57 | 0.63 |
| 1:B:253:LEU:N | 1:D:309:TYR:OH[2_546] | 1.57 | 0.63 |
| 1:B:31:ARG:N | 1:D:44:TYR:CG[2_546] | 1.57 | 0.63 |
| 1:B:52:LEU:O | 1:D:62:LEU:O[2_546] | 1.57 | 0.63 |
| 1:B:40:ASN:CA | 1:D:345:HIS:CB[2_546] | 1.57 | 0.63 |
| 1:A:286:ARG:NE | 1:B:245:LYS:O[2_546] | 1.57 | 0.63 |
| 1:B:255:GLY:C | 1:D:264:TYR:O[2_546] | 1.57 | 0.63 |
| 1:B:38:LEU:N | 1:D:340:LEU:O[2_546] | 1.57 | 0.63 |
| 1:B:269:LYS:CA | 1:D:183:HIS:NE2[2_546] | 1.57 | 0.63 |
| 1:B:264:TYR:OH | 1:D:258:HIS:NE2[2_546] | 1.57 | 0.63 |
| 1:B:314:PHE:C | 1:D:22:ASP:C[2_546] | 1.57 | 0.63 |
| 1:B:58:THR:O | 1:D:115:ASN:CG[2_546] | 1.57 | 0.63 |
| 1:A:109:ASN:N | 1:A:248:ASN:N[2_556] | 1.57 | 0.63 |
| 1:A:280:GLU:C | 1:B:248:ASN:O[2_546] | 1.57 | 0.63 |
| 1:B:258:HIS:NE2 | 1:D:270:ILE:N[2_546] | 1.58 | 0.62 |
| 1:B:54:GLY:O | 1:D:69:LEU:CG[2_546] | 1.58 | 0.62 |
| 1:B:34:ASN:CG | 1:D:338:ARG:N[2_546] | 1.58 | 0.62 |
| 1:A:362:LEU:C | 1:D:170:ILE:C[2_546] | 1.58 | 0.62 |
| 1:A:362:LEU:CA | 1:D:171:ASN:N[2_546] | 1.58 | 0.62 |
| 1:B:19:THR:O | 1:D:174:ASP:O[2_546] | 1.58 | 0.62 |
| 1:B:52:LEU:O | 1:D:62:LEU:CA[2_546] | 1.58 | 0.62 |
| 1:B:315:TYR:CD1 | 1:D:260:VAL:CG1[2_546] | 1.58 | 0.62 |
| 1:B:49:TYR:CA | 1:D:53:TYR:CD1[2_546] | 1.58 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:262:LYS:CE | 1:D:315:TYR:CD2[2_546] | 1.58 | 0.62 |
| 1:B:334:PHE:CE1 | 1:D:34:ASN:C[2_546] | 1.58 | 0.62 |
| 1:B:167:THR:O | 1:D:15:VAL:CB[2_546] | 1.58 | 0.62 |
| 1:B:186:PRO:N | 1:D:40:ASN:CA[2_546] | 1.58 | 0.62 |
| 1:B:55:LYS:CD | 1:D:68:LYS:CG[2_546] | 1.58 | 0.62 |
| 1:B:303:PHE:O | 1:D:256:PHE:CD2[2_546] | 1.58 | 0.62 |
| 1:B:57:PRO:C | 1:D:118:GLU:CA[2_546] | 1.58 | 0.62 |
| 1:A:107:ASP:C | 1:A:248:ASN:CB[2_556] | 1.58 | 0.62 |
| 1:A:364:VAL:N | 1:D:170:ILE:CG2[2_546] | 1.58 | 0.62 |
| 1:B:53:TYR:C | 1:D:65:LEU:CB[2_546] | 1.58 | 0.62 |
| 1:B:175:LYS:NZ | 1:D:348:GLU:OE1[2_546] | 1.58 | 0.62 |
| 1:B:302:GLN:C | 1:D:303:PHE:CB[2_546] | 1.58 | 0.62 |
| 1:B:61:GLU:CD | 1:D:118:GLU:OE1[2_546] | 1.59 | 0.61 |
| 1:B:183:HIS:N | 1:D:39:VAL:N[2_546] | 1.59 | 0.61 |
| 1:B:59:LYS:CA | 1:D:115:ASN:CA[2_546] | 1.59 | 0.61 |
| 1:B:263:THR:C | 1:D:312:THR:N[2_546] | 1.59 | 0.61 |
| 1:B:19:THR:O | 1:D:174:ASP:CB[2_546] | 1.59 | 0.61 |
| 1:B:171:ASN:CG | 1:D:16:THR:N[2_546] | 1.59 | 0.61 |
| 1:B:41:TYR:OH | 1:D:192:ALA:CB[2_546] | 1.59 | 0.61 |
| 1:B:313:ASP:CB | 1:D:26:GLY:C[2_546] | 1.59 | 0.61 |
| 1:B:170:ILE:CA | 1:C:364:VAL:CG2[2_546] | 1.59 | 0.61 |
| 1:B:186:PRO:N | 1:D:40:ASN:OD1[2_546] | 1.59 | 0.61 |
| 1:B:260:VAL:CG1 | 1:D:271:PHE:CA[2_546] | 1.59 | 0.61 |
| 1:B:53:TYR:N | 1:D:65:LEU:CB[2_546] | 1.59 | 0.61 |
| 1:B:178:ILE:C | 1:D:30:TYR:CB[2_546] | 1.59 | 0.61 |
| 1:A:362:LEU:CD2 | 1:D:167:THR:CA[2_546] | 1.59 | 0.61 |
| 1:B:333:LEU:C | 1:C:369:GLN:N[2_546] | 1.59 | 0.61 |
| 1:B:188:SER:CA | 1:D:41:TYR:CE1[2_546] | 1.59 | 0.61 |
| 1:B:177:LEU:C | 1:D:30:TYR:C[2_546] | 1.59 | 0.61 |
| 1:B:54:GLY:N | 1:D:65:LEU:CA[2_546] | 1.59 | 0.61 |
| 1:B:314:PHE:CE2 | 1:D:262:LYS:N[2_546] | 1.59 | 0.61 |
| 1:A:237:ARG:NH1 | 1:B:218:HIS:N[2_546] | 1.59 | 0.61 |
| 1:B:54:GLY:N | 1:D:65:LEU:CB[2_546] | 1.59 | 0.61 |
| 1:B:47:THR:O | 1:D:49:TYR:N[2_546] | 1.59 | 0.61 |
| 1:A:367:GLU:CD | 1:D:156:PHE:CZ[2_546] | 1.59 | 0.61 |
| 1:B:39:VAL:CG1 | 1:D:182:ASP:CG[2_546] | 1.59 | 0.61 |
| 1:A:286:ARG:CD | 1:B:251:ASN:N[2_546] | 1.59 | 0.61 |
| 1:B:189:THR:N | 1:D:41:TYR:CG[2_546] | 1.59 | 0.61 |
| 1:B:19:THR:CG2 | 1:D:178:ILE:CG1[2_546] | 1.60 | 0.60 |
| 1:A:362:LEU:CA | 1:D:167:THR:O[2_546] | 1.60 | 0.60 |
| 1:B:48:ILE:C | 1:D:49:TYR:CD2[2_546] | 1.60 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:226:PHE:CA | 1:D:25:LYS:CD[2_546] | 1.60 | 0.60 |
| 1:B:186:PRO:N | 1:D:40:ASN:CG[2_546] | 1.60 | 0.60 |
| 1:B:29:ARG:NE | 1:D:337:SER:N[2_546] | 1.60 | 0.60 |
| 1:B:303:PHE:O | 1:D:256:PHE:CG[2_546] | 1.60 | 0.60 |
| 1:B:41:TYR:CD1 | 1:D:342:TRP:C[2_546] | 1.60 | 0.60 |
| 1:B:41:TYR:O | 1:D:346:ILE:C[2_546] | 1.60 | 0.60 |
| 1:B:117:LYS:CG | 1:D:60:LYS:O[2_546] | 1.60 | 0.60 |
| 1:B:296:GLU:CG | 1:D:258:HIS:O[2_546] | 1.60 | 0.60 |
| 1:B:17:ASN:C | 1:D:45:GLU:OE1[2_546] | 1.60 | 0.60 |
| 1:B:341:GLY:CA | 1:D:46:GLU:CD[2_546] | 1.60 | 0.60 |
| 1:B:176:ALA:C | 1:D:31:ARG:N[2_546] | 1.60 | 0.60 |
| 1:B:264:TYR:OH | 1:D:258:HIS:CG[2_546] | 1.60 | 0.60 |
| 1:B:37:ASP:CA | 1:D:342:TRP:CB[2_546] | 1.60 | 0.60 |
| 1:B:44:TYR:CD2 | 1:D:54:GLY:O[2_546] | 1.60 | 0.60 |
| 1:B:295:LEU:O | 1:D:307:GLY:CA[2_546] | 1.60 | 0.60 |
| 1:B:342:TRP:CB | 1:C:371:TYR:CE2[2_546] | 1.60 | 0.60 |
| 1:B:302:GLN:CD | 1:D:303:PHE:CA[2_546] | 1.60 | 0.60 |
| 1:B:44:TYR:CG | 1:D:31:ARG:NE[2_546] | 1.60 | 0.60 |
| 1:B:339:THR:CB | 1:D:56:LEU:CD1[2_546] | 1.60 | 0.60 |
| 1:B:345:HIS:CD2 | 1:D:42:GLY:N[2_546] | 1.61 | 0.59 |
| 1:B:176:ALA:O | 1:D:30:TYR:C[2_546] | 1.61 | 0.59 |
| 1:B:61:GLU:OE2 | 1:D:118:GLU:CD[2_546] | 1.61 | 0.59 |
| 1:B:265:ASP:CA | 1:D:267:ARG:NE[2_546] | 1.61 | 0.59 |
| 1:B:260:VAL:CB | 1:D:270:ILE:C[2_546] | 1.61 | 0.59 |
| 1:B:44:TYR:CG | 1:D:31:ARG:CD[2_546] | 1.61 | 0.59 |
| 1:B:313:ASP:C | 1:D:26:GLY:CA[2_546] | 1.61 | 0.59 |
| 1:B:334:PHE:CG | 1:D:34:ASN:CG[2_546] | 1.61 | 0.59 |
| 1:B:171:ASN:C | 1:D:16:THR:CA[2_546] | 1.61 | 0.59 |
| 1:B:296:GLU:OE2 | 1:D:258:HIS:O[2_546] | 1.61 | 0.59 |
| 1:B:188:SER:C | 1:D:41:TYR:CE1[2_546] | 1.61 | 0.59 |
| 1:B:19:THR:OG1 | 1:D:178:ILE:CD1[2_546] | 1.61 | 0.59 |
| 1:B:302:GLN:C | 1:D:303:PHE:CD1[2_546] | 1.61 | 0.59 |
| 1:B:29:ARG:N | 1:D:177:LEU:CA[2_546] | 1.61 | 0.59 |
| 1:B:51:MET:SD | 1:D:47:THR:N[2_546] | 1.61 | 0.59 |
| 1:A:360:ARG:NH2 | 1:D:277:THR:OG1[2_546] | 1.61 | 0.59 |
| 1:B:332:ALA:N | 1:C:368:TYR:CZ[2_546] | 1.61 | 0.59 |
| 1:B:335:ALA:N | 1:C:369:GLN:O[2_546] | 1.61 | 0.59 |
| 1:B:312:THR:O | 1:D:28:LEU:N[2_546] | 1.61 | 0.59 |
| 1:B:262:LYS:CG | 1:D:315:TYR:CG[2_546] | 1.61 | 0.59 |
| 1:B:121:ILE:CA | 1:D:55:LYS:NZ[2_546] | 1.61 | 0.59 |
| 1:B:54:GLY:CA | 1:D:65:LEU:O[2_546] | 1.61 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:301:LYS:N | 1:D:308:ILE:CG2[2_546] | 1.61 | 0.59 |
| 1:B:259:ARG:CB | 1:D:269:LYS:O[2_546] | 1.61 | 0.59 |
| 1:B:36:GLU:CD | 1:D:338:ARG:NH1[2_546] | 1.61 | 0.59 |
| 1:B:339:THR:C | 1:D:56:LEU:CG[2_546] | 1.61 | 0.59 |
| 1:B:48:ILE:CG1 | 1:D:55:LYS:O[2_546] | 1.62 | 0.58 |
| 1:B:56:LEU:CG | 1:D:120:ALA:O[2_546] | 1.62 | 0.58 |
| 1:B:263:THR:C | 1:D:313:ASP:N[2_546] | 1.62 | 0.58 |
| 1:B:315:TYR:CE1 | 1:D:260:VAL:CB[2_546] | 1.62 | 0.58 |
| 1:B:321:TYR:N | 1:C:367:GLU:OE1[2_546] | 1.62 | 0.58 |
| 1:B:351:GLU:OE1 | 1:D:63:ASN:CG[2_546] | 1.62 | 0.58 |
| 1:B:342:TRP:CH2 | 1:C:371:TYR:CB[2_546] | 1.62 | 0.58 |
| 1:B:341:GLY:N | 1:D:46:GLU:OE2[2_546] | 1.62 | 0.58 |
| 1:B:172:ALA:CB | 1:C:363:TYR:N[2_546] | 1.62 | 0.58 |
| 1:B:115:ASN:ND2 | 1:D:60:LYS:CG[2_546] | 1.62 | 0.58 |
| 1:B:184:GLU:OE2 | 1:D:270:ILE:CB[2_546] | 1.62 | 0.58 |
| 1:B:222:ALA:N | 1:D:27:ILE:CD1[2_546] | 1.62 | 0.58 |
| 1:B:334:PHE:CG | 1:D:34:ASN:ND2[2_546] | 1.62 | 0.58 |
| 1:B:296:GLU:OE1 | 1:D:259:ARG:C[2_546] | 1.62 | 0.58 |
| 1:B:34:ASN:CA | 1:D:338:ARG:N[2_546] | 1.62 | 0.58 |
| 1:B:189:THR:OG1 | 1:D:41:TYR:CA[2_546] | 1.62 | 0.58 |
| 1:B:263:THR:O | 1:D:311:ASN:C[2_546] | 1.62 | 0.58 |
| 1:B:124:ILE:CG2 | 1:D:55:LYS:CB[2_546] | 1.62 | 0.58 |
| 1:A:111:LYS:CB | 1:A:245:LYS:CE[2_556] | 1.63 | 0.57 |
| 1:B:35:ILE:CG1 | 1:D:182:ASP:N[2_546] | 1.63 | 0.57 |
| 1:B:169:GLU:O | 1:C:364:VAL:C[2_546] | 1.63 | 0.57 |
| 1:B:189:THR:CG2 | 1:D:41:TYR:C[2_546] | 1.63 | 0.57 |
| 1:B:259:ARG:N | 1:D:269:LYS:C[2_546] | 1.63 | 0.57 |
| 1:B:271:PHE:N | 1:D:21:ILE:CG1[2_546] | 1.63 | 0.57 |
| 1:B:306:LYS:CB | 1:D:296:GLU:C[2_546] | 1.63 | 0.57 |
| 1:B:260:VAL:C | 1:D:271:PHE:C[2_546] | 1.63 | 0.57 |
| 1:B:37:ASP:N | 1:D:342:TRP:N[2_546] | 1.63 | 0.57 |
| 1:B:53:TYR:C | 1:D:65:LEU:N[2_546] | 1.63 | 0.57 |
| 1:B:303:PHE:O | 1:D:256:PHE:CD1[2_546] | 1.63 | 0.57 |
| 1:A:363:TYR:CE2 | 1:D:153:ALA:CB[2_546] | 1.63 | 0.57 |
| 1:B:264:TYR:CD2 | 1:D:258:HIS:CE1[2_546] | 1.63 | 0.57 |
| 1:B:54:GLY:N | 1:D:65:LEU:CG[2_546] | 1.63 | 0.57 |
| 1:B:171:ASN:CB | 1:D:15:VAL:O[2_546] | 1.63 | 0.57 |
| 1:B:38:LEU:CD1 | 1:D:340:LEU:CD1[2_546] | 1.63 | 0.57 |
| 1:B:258:HIS:NE2 | 1:D:270:ILE:CB[2_546] | 1.63 | 0.57 |
| 1:B:25:LYS:NZ | 1:D:223:GLU:OE2[2_546] | 1.63 | 0.57 |
| 1:B:347:ILE:CD1 | 1:D:59:LYS:CA[2_546] | 1.63 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:18:LEU:CD2 | 1:D:45:GLU:CB[2_546] | 1.64 | 0.56 |
| 1:B:53:TYR:CA | 1:D:65:LEU:CB[2_546] | 1.64 | 0.56 |
| 1:B:171:ASN:CG | 1:D:15:VAL:O[2_546] | 1.64 | 0.56 |
| 1:B:302:GLN:CA | 1:D:303:PHE:CA[2_546] | 1.64 | 0.56 |
| 1:B:20:PHE:N | 1:D:174:ASP:C[2_546] | 1.64 | 0.56 |
| 1:B:21:ILE:N | 1:D:176:ALA:C[2_546] | 1.64 | 0.56 |
| 1:B:38:LEU:CG | 1:D:340:LEU:C[2_546] | 1.64 | 0.56 |
| 1:B:174:ASP:CA | 1:D:17:ASN:C[2_546] | 1.64 | 0.56 |
| 1:B:311:ASN:CB | 1:D:266:PRO:CA[2_546] | 1.64 | 0.56 |
| 1:B:269:LYS:CB | 1:D:183:HIS:CD2[2_546] | 1.64 | 0.56 |
| 1:B:296:GLU:OE2 | 1:D:259:ARG:N[2_546] | 1.64 | 0.56 |
| 1:B:117:LYS:N | 1:D:60:LYS:CA[2_546] | 1.64 | 0.56 |
| 1:B:256:PHE:CB | 1:D:264:TYR:N[2_546] | 1.64 | 0.56 |
| 1:B:296:GLU:OE1 | 1:D:260:VAL:N[2_546] | 1.64 | 0.56 |
| 1:B:271:PHE:CE1 | 1:D:20:PHE:O[2_546] | 1.64 | 0.56 |
| 1:B:263:THR:CG2 | 1:D:313:ASP:N[2_546] | 1.64 | 0.56 |
| 1:B:338:ARG:NH1 | 1:D:37:ASP:N[2_546] | 1.64 | 0.56 |
| 1:B:263:THR:N | 1:D:314:PHE:N[2_546] | 1.64 | 0.56 |
| 1:B:272:LYS:CG | 1:D:260:VAL:CG1[2_546] | 1.64 | 0.56 |
| 1:B:311:ASN:O | 1:D:261:TYR:CE2[2_546] | 1.64 | 0.56 |
| 1:B:117:LYS:CG | 1:D:61:GLU:N[2_546] | 1.64 | 0.56 |
| 1:B:254:MET:O | 1:D:263:THR:CB[2_546] | 1.64 | 0.56 |
| 1:B:260:VAL:CA | 1:D:271:PHE:N[2_546] | 1.64 | 0.56 |
| 1:B:171:ASN:CG | 1:D:15:VAL:C[2_546] | 1.64 | 0.56 |
| 1:B:181:THR:C | 1:D:38:LEU:CG[2_546] | 1.64 | 0.56 |
| 1:B:48:ILE:O | 1:D:49:TYR:CD2[2_546] | 1.65 | 0.55 |
| 1:B:314:PHE:CE2 | 1:D:23:GLY:O[2_546] | 1.65 | 0.55 |
| 1:B:45:GLU:CA | 1:D:53:TYR:CA[2_546] | 1.65 | 0.55 |
| 1:B:262:LYS:CE | 1:D:315:TYR:CD1[2_546] | 1.65 | 0.55 |
| 1:B:39:VAL:O | 1:D:345:HIS:ND1[2_546] | 1.65 | 0.55 |
| 1:B:39:VAL:N | 1:D:341:GLY:O[2_546] | 1.65 | 0.55 |
| 1:B:31:ARG:CZ | 1:D:45:GLU:CG[2_546] | 1.65 | 0.55 |
| 1:B:188:SER:CB | 1:D:41:TYR:OH[2_546] | 1.65 | 0.55 |
| 1:B:257:GLY:CA | 1:D:264:TYR:CG[2_546] | 1.65 | 0.55 |
| 1:B:37:ASP:C | 1:D:342:TRP:CA[2_546] | 1.65 | 0.55 |
| 1:B:298:LEU:N | 1:D:306:LYS:O[2_546] | 1.65 | 0.55 |
| 1:B:50:LEU:CD2 | 1:D:48:ILE:CG1[2_546] | 1.65 | 0.55 |
| 1:B:342:TRP:CD1 | 1:C:371:TYR:CE2[2_546] | 1.65 | 0.55 |
| 1:B:19:THR:OG1 | 1:D:178:ILE:CG1[2_546] | 1.65 | 0.55 |
| 1:B:25:LYS:NZ | 1:D:223:GLU:CD[2_546] | 1.65 | 0.55 |
| 1:B:278:LEU:CD2 | 1:C:362:LEU:CG[2_546] | 1.65 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:173:MET:O | 1:D:17:ASN:ND2[2_546] | 1.65 | 0.55 |
| 1:B:52:LEU:CD1 | 1:D:57:PRO:CB[2_546] | 1.65 | 0.55 |
| 1:B:265:ASP:CG | 1:D:267:ARG:NE[2_546] | 1.65 | 0.55 |
| 1:B:177:LEU:O | 1:D:30:TYR:C[2_546] | 1.65 | 0.55 |
| 1:B:186:PRO:CD | 1:D:40:ASN:CG[2_546] | 1.65 | 0.55 |
| 1:B:308:ILE:C | 1:D:310:PRO:CB[2_546] | 1.66 | 0.54 |
| 1:B:337:SER:CA | 1:D:33:TYR:CD2[2_546] | 1.66 | 0.54 |
| 1:B:270:ILE:N | 1:D:184:GLU:N[2_546] | 1.66 | 0.54 |
| 1:B:270:ILE:CG1 | 1:D:183:HIS:N[2_546] | 1.66 | 0.54 |
| 1:B:180:TYR:C | 1:D:38:LEU:CD1[2_546] | 1.66 | 0.54 |
| 1:B:24:GLU:OE2 | 1:D:318:ILE:C[2_546] | 1.66 | 0.54 |
| 1:B:310:PRO:O | 1:D:265:ASP:CG[2_546] | 1.66 | 0.54 |
| 1:B:17:ASN:CB | 1:D:45:GLU:OE2[2_546] | 1.66 | 0.54 |
| 1:B:303:PHE:CA | 1:D:256:PHE:CD2[2_546] | 1.66 | 0.54 |
| 1:B:255:GLY:CA | 1:D:263:THR:CG2[2_546] | 1.66 | 0.54 |
| 1:B:259:ARG:O | 1:D:272:LYS:CA[2_546] | 1.66 | 0.54 |
| 1:B:37:ASP:OD1 | 1:D:342:TRP:CD2[2_546] | 1.66 | 0.54 |
| 1:B:340:LEU:CB | 1:D:56:LEU:CD2[2_546] | 1.66 | 0.54 |
| 1:A:361:ALA:CB | 1:D:171:ASN:OD1[2_546] | 1.66 | 0.54 |
| 1:B:53:TYR:CD2 | 1:D:64:ASP:CB[2_546] | 1.66 | 0.54 |
| 1:B:261:TYR:CG | 1:D:267:ARG:O[2_546] | 1.66 | 0.54 |
| 1:B:271:PHE:CE1 | 1:D:29:ARG:N[2_546] | 1.66 | 0.54 |
| 1:B:180:TYR:N | 1:D:30:TYR:CB[2_546] | 1.66 | 0.54 |
| 1:B:338:ARG:NH1 | 1:D:37:ASP:CA[2_546] | 1.66 | 0.54 |
| 1:B:312:THR:CA | 1:D:266:PRO:CG[2_546] | 1.66 | 0.54 |
| 1:B:24:GLU:C | 1:D:317:GLY:N[2_546] | 1.66 | 0.54 |
| 1:B:19:THR:N | 1:D:174:ASP:OD2[2_546] | 1.66 | 0.54 |
| 1:A:362:LEU:CD1 | 1:D:166:THR:O[2_546] | 1.66 | 0.54 |
| 1:B:262:LYS:C | 1:D:314:PHE:CA[2_546] | 1.66 | 0.54 |
| 1:B:265:ASP:CA | 1:D:267:ARG:CZ[2_546] | 1.66 | 0.54 |
| 1:A:109:ASN:N | 1:A:248:ASN:C[2_556] | 1.66 | 0.54 |
| 1:B:127:MET:SD | 1:C:370:GLU:OE2[2_546] | 1.66 | 0.54 |
| 1:B:259:ARG:C | 1:D:272:LYS:N[2_546] | 1.66 | 0.54 |
| 1:B:46:GLU:CA | 1:D:52:LEU:O[2_546] | 1.67 | 0.53 |
| 1:B:278:LEU:CG | 1:C:362:LEU:CD1[2_546] | 1.67 | 0.53 |
| 1:B:337:SER:OG | 1:D:33:TYR:CB[2_546] | 1.67 | 0.53 |
| 1:B:302:GLN:CG | 1:D:303:PHE:N[2_546] | 1.67 | 0.53 |
| 1:B:33:TYR:C | 1:D:44:TYR:OH[2_546] | 1.67 | 0.53 |
| 1:B:309:TYR:C | 1:D:310:PRO:O[2_546] | 1.67 | 0.53 |
| 1:B:175:LYS:CB | 1:D:19:THR:N[2_546] | 1.67 | 0.53 |
| 1:B:304:SER:CA | 1:D:256:PHE:CD1[2_546] | 1.67 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:39:VAL:O | 1:D:345:HIS:CB[2_546] | 1.67 | 0.53 |
| 1:B:229:PHE:CD1 | 1:D:24:GLU:CD[2_546] | 1.67 | 0.53 |
| 1:B:62:LEU:CB | 1:D:117:LYS:CE[2_546] | 1.67 | 0.53 |
| 1:B:59:LYS:N | 1:D:115:ASN:N[2_546] | 1.67 | 0.53 |
| 1:B:44:TYR:CD2 | 1:D:54:GLY:C[2_546] | 1.67 | 0.53 |
| 1:B:313:ASP:CA | 1:D:27:ILE:CA[2_546] | 1.67 | 0.53 |
| 1:B:47:THR:CB | 1:D:51:MET:C[2_546] | 1.67 | 0.53 |
| 1:A:362:LEU:CB | 1:D:167:THR:C[2_546] | 1.67 | 0.53 |
| 1:B:23:GLY:O | 1:D:316:SER:CA[2_546] | 1.67 | 0.53 |
| 1:B:258:HIS:CB | 1:D:268:ALA:CA[2_546] | 1.67 | 0.53 |
| 1:B:38:LEU:N | 1:D:341:GLY:CA[2_546] | 1.67 | 0.53 |
| 1:B:296:GLU:CA | 1:D:262:LYS:NZ[2_546] | 1.67 | 0.53 |
| 1:B:156:PHE:CD2 | 1:C:366:PRO:CD[2_546] | 1.67 | 0.53 |
| 1:B:22:ASP:CG | 1:D:320:PHE:CD2[2_546] | 1.67 | 0.53 |
| 1:A:108:LYS:N | 1:A:248:ASN:CG[2_556] | 1.67 | 0.53 |
| 1:A:111:LYS:O | 1:A:245:LYS:CD[2_556] | 1.67 | 0.53 |
| 1:A:363:TYR:CA | 1:D:170:ILE:C[2_546] | 1.67 | 0.53 |
| 1:B:180:TYR:CD2 | 1:D:35:ILE:N[2_546] | 1.67 | 0.53 |
| 1:B:342:TRP:CG | 1:C:371:TYR:CD2[2_546] | 1.67 | 0.53 |
| 1:B:342:TRP:CD2 | 1:C:371:TYR:CG[2_546] | 1.68 | 0.52 |
| 1:B:338:ARG:NH2 | 1:D:35:ILE:O[2_546] | 1.68 | 0.52 |
| 1:B:338:ARG:NH2 | 1:D:35:ILE:C[2_546] | 1.68 | 0.52 |
| 1:B:306:LYS:CD | 1:D:299:GLY:N[2_546] | 1.68 | 0.52 |
| 1:B:48:ILE:CA | 1:D:49:TYR:CD2[2_546] | 1.68 | 0.52 |
| 1:B:30:TYR:N | 1:D:44:TYR:CZ[2_546] | 1.68 | 0.52 |
| 1:B:264:TYR:CZ | 1:D:258:HIS:NE2[2_546] | 1.68 | 0.52 |
| 1:B:28:LEU:CA | 1:D:180:TYR:N[2_546] | 1.68 | 0.52 |
| 1:B:35:ILE:CB | 1:D:181:THR:CB[2_546] | 1.68 | 0.52 |
| 1:B:314:PHE:CA | 1:D:26:GLY:CA[2_546] | 1.68 | 0.52 |
| 1:A:362:LEU:CD1 | 1:D:170:ILE:N[2_546] | 1.68 | 0.52 |
| 1:B:306:LYS:CE | 1:D:299:GLY:CA[2_546] | 1.68 | 0.52 |
| 1:B:42:GLY:N | 1:D:344:ALA:O[2_546] | 1.68 | 0.52 |
| 1:B:229:PHE:CZ | 1:D:24:GLU:C[2_546] | 1.68 | 0.52 |
| 1:B:29:ARG:CZ | 1:D:336:LEU:CB[2_546] | 1.68 | 0.52 |
| 1:B:311:ASN:CA | 1:D:265:ASP:CA[2_546] | 1.68 | 0.52 |
| 1:B:59:LYS:N | 1:D:115:ASN:C[2_546] | 1.68 | 0.52 |
| 1:B:112:TRP:CE2 | 1:D:59:LYS:NZ[2_546] | 1.68 | 0.52 |
| 1:B:305:SER:C | 1:D:253:LEU:CD2[2_546] | 1.68 | 0.52 |
| 1:B:59:LYS:CB | 1:D:114:GLU:O[2_546] | 1.68 | 0.52 |
| 1:B:335:ALA:CB | 1:C:370:GLU:CA[2_546] | 1.68 | 0.52 |
| 1:B:22:ASP:OD1 | 1:D:320:PHE:CE1[2_546] | 1.68 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:369:GLN:CG | 1:D:124:ILE:O[2_546] | 1.68 | 0.52 |
| 1:B:36:GLU:OE2 | 1:D:338:ARG:NH2[2_546] | 1.68 | 0.52 |
| 1:B:276:LEU:CB | 1:C:360:ARG:NE[2_546] | 1.68 | 0.52 |
| 1:B:28:LEU:CD1 | 1:D:178:ILE:O[2_546] | 1.68 | 0.52 |
| 1:B:242:PHE:CZ | 1:D:304:SER:C[2_546] | 1.68 | 0.52 |
| 1:B:347:ILE:CG1 | 1:D:59:LYS:CB[2_546] | 1.68 | 0.52 |
| 1:B:169:GLU:O | 1:C:364:VAL:CG2[2_546] | 1.68 | 0.52 |
| 1:B:180:TYR:CG | 1:D:29:ARG:CA[2_546] | 1.68 | 0.52 |
| 1:B:337:SER:C | 1:D:33:TYR:CB[2_546] | 1.69 | 0.51 |
| 1:B:37:ASP:N | 1:D:338:ARG:O[2_546] | 1.69 | 0.51 |
| 1:B:30:TYR:C | 1:D:44:TYR:CG[2_546] | 1.69 | 0.51 |
| 1:B:311:ASN:CA | 1:D:265:ASP:C[2_546] | 1.69 | 0.51 |
| 1:B:242:PHE:CE1 | 1:D:307:GLY:N[2_546] | 1.69 | 0.51 |
| 1:B:45:GLU:C | 1:D:52:LEU:C[2_546] | 1.69 | 0.51 |
| 1:B:335:ALA:CA | 1:C:369:GLN:O[2_546] | 1.69 | 0.51 |
| 1:B:59:LYS:CG | 1:D:114:GLU:C[2_546] | 1.69 | 0.51 |
| 1:B:171:ASN:C | 1:D:16:THR:N[2_546] | 1.69 | 0.51 |
| 1:B:186:PRO:N | 1:D:40:ASN:CB[2_546] | 1.69 | 0.51 |
| 1:B:242:PHE:CD2 | 1:D:305:SER:CA[2_546] | 1.69 | 0.51 |
| 1:B:300:ILE:CD1 | 1:D:257:GLY:C[2_546] | 1.69 | 0.51 |
| 1:B:342:TRP:CZ3 | 1:C:371:TYR:CA[2_546] | 1.69 | 0.51 |
| 1:A:111:LYS:C | 1:A:245:LYS:CE[2_556] | 1.69 | 0.51 |
| 1:B:36:GLU:N | 1:D:338:ARG:CD[2_546] | 1.69 | 0.51 |
| 1:B:315:TYR:CE1 | 1:D:260:VAL:CA[2_546] | 1.69 | 0.51 |
| 1:B:37:ASP:CB | 1:D:339:THR:C[2_546] | 1.69 | 0.51 |
| 1:B:36:GLU:CA | 1:D:338:ARG:CD[2_546] | 1.69 | 0.51 |
| 1:B:334:PHE:CE1 | 1:D:34:ASN:CA[2_546] | 1.69 | 0.51 |
| 1:B:306:LYS:CD | 1:D:296:GLU:O[2_546] | 1.69 | 0.51 |
| 1:A:109:ASN:CG | 1:A:246:VAL:O[2_556] | 1.69 | 0.51 |
| 1:B:267:ARG:NH1 | 1:D:35:ILE:CG1[2_546] | 1.69 | 0.51 |
| 1:B:41:TYR:CD1 | 1:D:342:TRP:O[2_546] | 1.69 | 0.51 |
| 1:B:33:TYR:CG | 1:D:124:ILE:CG1[2_546] | 1.70 | 0.50 |
| 1:B:21:ILE:CD1 | 1:D:175:LYS:CB[2_546] | 1.70 | 0.50 |
| 1:A:361:ALA:N | 1:D:171:ASN:CG[2_546] | 1.70 | 0.50 |
| 1:B:311:ASN:C | 1:D:266:PRO:CG[2_546] | 1.70 | 0.50 |
| 1:B:20:PHE:CD1 | 1:D:173:MET:C[2_546] | 1.70 | 0.50 |
| 1:B:264:TYR:CE1 | 1:D:258:HIS:CB[2_546] | 1.70 | 0.50 |
| 1:B:309:TYR:CG | 1:D:311:ASN:CA[2_546] | 1.70 | 0.50 |
| 1:B:182:ASP:N | 1:D:38:LEU:CB[2_546] | 1.70 | 0.50 |
| 1:B:183:HIS:CB | 1:D:39:VAL:CG1[2_546] | 1.70 | 0.50 |
| 1:B:314:PHE:CA | 1:D:26:GLY:N[2_546] | 1.70 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:170:ILE:N | 1:C:364:VAL:CG2[2_546] | 1.70 | 0.50 |
| 1:A:362:LEU:CD2 | 1:D:167:THR:N[2_546] | 1.70 | 0.50 |
| 1:B:226:PHE:N | 1:D:25:LYS:CB[2_546] | 1.70 | 0.50 |
| 1:B:262:LYS:CG | 1:D:315:TYR:N[2_546] | 1.70 | 0.50 |
| 1:B:172:ALA:CA | 1:D:16:THR:O[2_546] | 1.70 | 0.50 |
| 1:B:177:LEU:O | 1:D:30:TYR:O[2_546] | 1.70 | 0.50 |
| 1:B:23:GLY:CA | 1:D:271:PHE:CD2[2_546] | 1.70 | 0.50 |
| 1:B:52:LEU:CD2 | 1:D:57:PRO:CG[2_546] | 1.70 | 0.50 |
| 1:B:34:ASN:O | 1:D:338:ARG:O[2_546] | 1.70 | 0.50 |
| 1:B:315:TYR:O | 1:D:22:ASP:CA[2_546] | 1.70 | 0.50 |
| 1:B:172:ALA:CB | 1:C:363:TYR:CB[2_546] | 1.71 | 0.49 |
| 1:B:306:LYS:CB | 1:D:296:GLU:CA[2_546] | 1.71 | 0.49 |
| 1:B:30:TYR:CE2 | 1:D:47:THR:CG2[2_546] | 1.71 | 0.49 |
| 1:B:297:GLU:O | 1:D:308:ILE:CG1[2_546] | 1.71 | 0.49 |
| 1:B:46:GLU:CD | 1:D:347:ILE:CD1[2_546] | 1.71 | 0.49 |
| 1:B:345:HIS:CE1 | 1:D:42:GLY:C[2_546] | 1.71 | 0.49 |
| 1:B:314:PHE:O | 1:D:22:ASP:O[2_546] | 1.71 | 0.49 |
| 1:B:37:ASP:O | 1:D:342:TRP:O[2_546] | 1.71 | 0.49 |
| 1:B:34:ASN:CB | 1:D:338:ARG:C[2_546] | 1.71 | 0.49 |
| 1:A:237:ARG:CZ | 1:B:217:LEU:C[2_546] | 1.71 | 0.49 |
| 1:A:363:TYR:OH | 1:D:152:PHE:CD2[2_546] | 1.71 | 0.49 |
| 1:B:306:LYS:O | 1:D:296:GLU:CB[2_546] | 1.71 | 0.49 |
| 1:B:124:ILE:CD1 | 1:D:56:LEU:C[2_546] | 1.71 | 0.49 |
| 1:B:49:TYR:CG | 1:D:53:TYR:CE1[2_546] | 1.71 | 0.49 |
| 1:B:173:MET:CB | 1:C:364:VAL:C[2_546] | 1.71 | 0.49 |
| 1:B:27:ILE:CG1 | 1:D:334:PHE:CA[2_546] | 1.71 | 0.49 |
| 1:B:264:TYR:CD2 | 1:D:258:HIS:ND1[2_546] | 1.71 | 0.49 |
| 1:B:55:LYS:CB | 1:D:121:ILE:CG2[2_546] | 1.71 | 0.49 |
| 1:B:39:VAL:CG2 | 1:D:345:HIS:NE2[2_546] | 1.71 | 0.49 |
| 1:B:335:ALA:C | 1:C:369:GLN:O[2_546] | 1.71 | 0.49 |
| 1:B:337:SER:N | 1:D:33:TYR:CE2[2_546] | 1.71 | 0.49 |
| 1:B:263:THR:OG1 | 1:D:313:ASP:N[2_546] | 1.71 | 0.49 |
| 1:B:316:SER:OG | 1:D:27:ILE:CB[2_546] | 1.72 | 0.48 |
| 1:A:110:PHE:CA | 1:A:244:ASP:O[2_556] | 1.72 | 0.48 |
| 1:B:180:TYR:CZ | 1:D:28:LEU:O[2_546] | 1.72 | 0.48 |
| 1:B:59:LYS:N | 1:D:115:ASN:CG[2_546] | 1.72 | 0.48 |
| 1:B:306:LYS:CE | 1:D:299:GLY:C[2_546] | 1.72 | 0.48 |
| 1:B:302:GLN:NE2 | 1:D:302:GLN:CA[2_546] | 1.72 | 0.48 |
| 1:B:174:ASP:CG | 1:D:31:ARG:NH1[2_546] | 1.72 | 0.48 |
| 1:B:341:GLY:O | 1:D:46:GLU:CD[2_546] | 1.72 | 0.48 |
| 1:B:304:SER:OG | 1:D:256:PHE:CB[2_546] | 1.72 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:31:ARG:NE | 1:D:45:GLU:CG[2_546] | 1.72 | 0.48 |
| 1:A:109:ASN:ND2 | 1:A:251:ASN:N[2_556] | 1.72 | 0.48 |
| 1:B:173:MET:SD | 1:C:366:PRO:C[2_546] | 1.72 | 0.48 |
| 1:B:332:ALA:N | 1:C:368:TYR:CD2[2_546] | 1.72 | 0.48 |
| 1:B:57:PRO:O | 1:D:117:LYS:C[2_546] | 1.72 | 0.48 |
| 1:B:263:THR:C | 1:D:312:THR:CA[2_546] | 1.72 | 0.48 |
| 1:B:308:ILE:C | 1:D:310:PRO:C[2_546] | 1.72 | 0.48 |
| 1:B:301:LYS:O | 1:D:303:PHE:CG[2_546] | 1.72 | 0.48 |
| 1:B:57:PRO:CA | 1:D:118:GLU:CA[2_546] | 1.72 | 0.48 |
| 1:B:170:ILE:N | 1:C:364:VAL:CG1[2_546] | 1.72 | 0.48 |
| 1:B:320:PHE:CE1 | 1:D:29:ARG:CZ[2_546] | 1.72 | 0.48 |
| 1:A:367:GLU:CB | 1:D:156:PHE:CD2[2_546] | 1.72 | 0.48 |
| 1:A:290:GLU:CD | 1:B:245:LYS:NZ[2_546] | 1.72 | 0.48 |
| 1:B:222:ALA:CB | 1:D:27:ILE:CD1[2_546] | 1.72 | 0.48 |
| 1:B:320:PHE:CD2 | 1:C:367:GLU:CB[2_546] | 1.72 | 0.48 |
| 1:B:306:LYS:CE | 1:D:299:GLY:N[2_546] | 1.72 | 0.48 |
| 1:B:39:VAL:CB | 1:D:182:ASP:OD2[2_546] | 1.72 | 0.48 |
| 1:B:268:ALA:CA | 1:D:183:HIS:NE2[2_546] | 1.72 | 0.48 |
| 1:B:261:TYR:CD2 | 1:D:271:PHE:CE1[2_546] | 1.72 | 0.48 |
| 1:B:314:PHE:CZ | 1:D:262:LYS:CA[2_546] | 1.72 | 0.48 |
| 1:B:186:PRO:CG | 1:D:40:ASN:ND2[2_546] | 1.73 | 0.47 |
| 1:B:259:ARG:C | 1:D:273:LYS:N[2_546] | 1.73 | 0.47 |
| 1:B:36:GLU:CD | 1:D:338:ARG:NE[2_546] | 1.73 | 0.47 |
| 1:B:24:GLU:CB | 1:D:317:GLY:C[2_546] | 1.73 | 0.47 |
| 1:B:262:LYS:CD | 1:D:315:TYR:CD1[2_546] | 1.73 | 0.47 |
| 1:B:47:THR:CG2 | 1:D:47:THR:O[2_546] | 1.73 | 0.47 |
| 1:B:314:PHE:C | 1:D:23:GLY:N[2_546] | 1.73 | 0.47 |
| 1:A:286:ARG:CZ | 1:B:251:ASN:N[2_546] | 1.73 | 0.47 |
| 1:B:189:THR:N | 1:D:41:TYR:CZ[2_546] | 1.73 | 0.47 |
| 1:B:38:LEU:C | 1:D:341:GLY:O[2_546] | 1.73 | 0.47 |
| 1:B:312:THR:O | 1:D:27:ILE:O[2_546] | 1.73 | 0.47 |
| 1:B:27:ILE:CD1 | 1:D:334:PHE:C[2_546] | 1.73 | 0.47 |
| 1:B:62:LEU:CA | 1:D:117:LYS:NZ[2_546] | 1.73 | 0.47 |
| 1:B:117:LYS:N | 1:D:60:LYS:CB[2_546] | 1.73 | 0.47 |
| 1:B:311:ASN:CG | 1:D:266:PRO:N[2_546] | 1.73 | 0.47 |
| 1:B:29:ARG:CG | 1:D:337:SER:CB[2_546] | 1.73 | 0.47 |
| 1:B:335:ALA:O | 1:C:370:GLU:O[2_546] | 1.73 | 0.47 |
| 1:B:242:PHE:CB | 1:D:305:SER:O[2_546] | 1.73 | 0.47 |
| 1:B:38:LEU:CD1 | 1:D:340:LEU:CD2[2_546] | 1.73 | 0.47 |
| 1:B:188:SER:C | 1:D:41:TYR:CD2[2_546] | 1.73 | 0.47 |
| 1:A:110:PHE:CD1 | 1:A:249:GLN:CD[2_556] | 1.73 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:341:GLY:C | 1:C:371:TYR:OH[2_546] | 1.74 | 0.46 |
| 1:B:339:THR:C | 1:D:56:LEU:CD2[2_546] | 1.74 | 0.46 |
| 1:B:296:GLU:CD | 1:D:258:HIS:O[2_546] | 1.74 | 0.46 |
| 1:B:271:PHE:CB | 1:D:21:ILE:CA[2_546] | 1.74 | 0.46 |
| 1:B:47:THR:OG1 | 1:D:51:MET:N[2_546] | 1.74 | 0.46 |
| 1:B:316:SER:N | 1:D:21:ILE:C[2_546] | 1.74 | 0.46 |
| 1:B:189:THR:OG1 | 1:D:41:TYR:CB[2_546] | 1.74 | 0.46 |
| 1:A:108:LYS:O | 1:A:248:ASN:N[2_556] | 1.74 | 0.46 |
| 1:B:33:TYR:OH | 1:D:121:ILE:O[2_546] | 1.74 | 0.46 |
| 1:B:31:ARG:CG | 1:D:48:ILE:CD1[2_546] | 1.74 | 0.46 |
| 1:B:171:ASN:CB | 1:D:16:THR:CA[2_546] | 1.74 | 0.46 |
| 1:B:40:ASN:N | 1:D:345:HIS:CD2[2_546] | 1.74 | 0.46 |
| 1:B:314:PHE:C | 1:D:23:GLY:CA[2_546] | 1.74 | 0.46 |
| 1:B:59:LYS:CG | 1:D:113:LYS:O[2_546] | 1.74 | 0.46 |
| 1:B:46:GLU:CA | 1:D:52:LEU:CA[2_546] | 1.74 | 0.46 |
| 1:B:306:LYS:CE | 1:D:298:LEU:O[2_546] | 1.74 | 0.46 |
| 1:B:256:PHE:CE2 | 1:D:309:TYR:N[2_546] | 1.74 | 0.46 |
| 1:B:173:MET:CA | 1:C:364:VAL:O[2_546] | 1.74 | 0.46 |
| 1:A:364:VAL:CG1 | 1:D:170:ILE:CG1[2_546] | 1.74 | 0.46 |
| 1:A:286:ARG:NH2 | 1:B:246:VAL:CA[2_546] | 1.74 | 0.46 |
| 1:B:56:LEU:O | 1:D:118:GLU:C[2_546] | 1.74 | 0.46 |
| 1:B:175:LYS:C | 1:D:18:LEU:CA[2_546] | 1.74 | 0.46 |
| 1:B:59:LYS:C | 1:D:114:GLU:O[2_546] | 1.74 | 0.46 |
| 1:B:316:SER:N | 1:D:22:ASP:CA[2_546] | 1.74 | 0.46 |
| 1:B:188:SER:CB | 1:D:41:TYR:CE1[2_546] | 1.74 | 0.46 |
| 1:B:39:VAL:CB | 1:D:345:HIS:NE2[2_546] | 1.74 | 0.46 |
| 1:B:315:TYR:O | 1:D:22:ASP:N[2_546] | 1.75 | 0.45 |
| 1:B:309:TYR:OH | 1:D:255:GLY:CA[2_546] | 1.75 | 0.45 |
| 1:B:26:GLY:C | 1:D:180:TYR:CD1[2_546] | 1.75 | 0.45 |
| 1:B:347:ILE:CG1 | 1:D:59:LYS:CA[2_546] | 1.75 | 0.45 |
| 1:B:306:LYS:CB | 1:D:296:GLU:O[2_546] | 1.75 | 0.45 |
| 1:B:44:TYR:CB | 1:D:31:ARG:CD[2_546] | 1.75 | 0.45 |
| 1:B:299:GLY:O | 1:D:308:ILE:CA[2_546] | 1.75 | 0.45 |
| 1:B:315:TYR:CA | 1:D:22:ASP:N[2_546] | 1.75 | 0.45 |
| 1:B:169:GLU:C | 1:C:364:VAL:CA[2_546] | 1.75 | 0.45 |
| 1:B:261:TYR:OH | 1:D:179:LEU:CG[2_546] | 1.75 | 0.45 |
| 1:B:55:LYS:C | 1:D:121:ILE:CG2[2_546] | 1.75 | 0.45 |
| 1:A:111:LYS:CE | 1:A:241:TRP:CH2[2_556] | 1.75 | 0.45 |
| 1:B:180:TYR:N | 1:D:30:TYR:N[2_546] | 1.75 | 0.45 |
| 1:B:302:GLN:NE2 | 1:D:302:GLN:O[2_546] | 1.75 | 0.45 |
| 1:B:312:THR:OG1 | 1:D:28:LEU:CA[2_546] | 1.75 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:39:VAL:CG2 | 1:D:345:HIS:CD2[2_546] | 1.75 | 0.45 |
| 1:B:268:ALA:CA | 1:D:261:TYR:OH[2_546] | 1.75 | 0.45 |
| 1:B:23:GLY:N | 1:D:271:PHE:CD2[2_546] | 1.75 | 0.45 |
| 1:B:167:THR:C | 1:D:15:VAL:CG1[2_546] | 1.75 | 0.45 |
| 1:B:333:LEU:N | 1:C:368:TYR:CB[2_546] | 1.75 | 0.45 |
| 1:B:309:TYR:N | 1:D:311:ASN:N[2_546] | 1.75 | 0.45 |
| 1:B:338:ARG:NE | 1:D:37:ASP:C[2_546] | 1.75 | 0.45 |
| 1:B:181:THR:C | 1:D:38:LEU:CD1[2_546] | 1.75 | 0.45 |
| 1:A:362:LEU:C | 1:D:171:ASN:N[2_546] | 1.75 | 0.45 |
| 1:A:368:TYR:C | 1:D:128:ALA:N[2_546] | 1.75 | 0.45 |
| 1:B:337:SER:CB | 1:D:33:TYR:CG[2_546] | 1.75 | 0.45 |
| 1:B:36:GLU:CB | 1:D:338:ARG:CG[2_546] | 1.75 | 0.45 |
| 1:A:111:LYS:CB | 1:A:245:LYS:CB[2_556] | 1.75 | 0.45 |
| 1:B:301:LYS:O | 1:D:303:PHE:CE2[2_546] | 1.75 | 0.45 |
| 1:B:58:THR:C | 1:D:115:ASN:C[2_546] | 1.75 | 0.45 |
| 1:B:264:TYR:C | 1:D:312:THR:CG2[2_546] | 1.76 | 0.44 |
| 1:A:237:ARG:NH2 | 1:B:217:LEU:O[2_546] | 1.76 | 0.44 |
| 1:B:62:LEU:CG | 1:D:117:LYS:NZ[2_546] | 1.76 | 0.44 |
| 1:B:342:TRP:CE3 | 1:C:371:TYR:CD2[2_546] | 1.76 | 0.44 |
| 1:B:178:ILE:CA | 1:D:51:MET:SD[2_546] | 1.76 | 0.44 |
| 1:B:179:LEU:CB | 1:D:30:TYR:CD2[2_546] | 1.76 | 0.44 |
| 1:A:363:TYR:CE2 | 1:D:153:ALA:CA[2_546] | 1.76 | 0.44 |
| 1:B:37:ASP:CG | 1:D:339:THR:CA[2_546] | 1.76 | 0.44 |
| 1:B:336:LEU:CA | 1:C:369:GLN:CB[2_546] | 1.76 | 0.44 |
| 1:B:299:GLY:O | 1:D:308:ILE:CG2[2_546] | 1.76 | 0.44 |
| 1:B:309:TYR:O | 1:D:265:ASP:N[2_546] | 1.76 | 0.44 |
| 1:B:50:LEU:O | 1:D:65:LEU:CD1[2_546] | 1.76 | 0.44 |
| 1:B:309:TYR:CG | 1:D:311:ASN:CB[2_546] | 1.76 | 0.44 |
| 1:B:334:PHE:O | 1:D:33:TYR:CA[2_546] | 1.76 | 0.44 |
| 1:B:309:TYR:CZ | 1:D:256:PHE:N[2_546] | 1.76 | 0.44 |
| 1:B:259:ARG:O | 1:D:272:LYS:N[2_546] | 1.76 | 0.44 |
| 1:B:258:HIS:CB | 1:D:269:LYS:CA[2_546] | 1.76 | 0.44 |
| 1:B:270:ILE:CA | 1:D:184:GLU:CA[2_546] | 1.76 | 0.44 |
| 1:B:171:ASN:CA | 1:D:16:THR:CA[2_546] | 1.76 | 0.44 |
| 1:B:184:GLU:C | 1:D:39:VAL:C[2_546] | 1.76 | 0.44 |
| 1:B:12:ILE:CD1 | 1:D:168:ASP:N[2_546] | 1.76 | 0.44 |
| 1:A:367:GLU:CA | 1:D:156:PHE:CD2[2_546] | 1.76 | 0.44 |
| 1:B:337:SER:CB | 1:D:33:TYR:CA[2_546] | 1.76 | 0.44 |
| 1:B:345:HIS:NE2 | 1:D:42:GLY:CA[2_546] | 1.76 | 0.44 |
| 1:B:57:PRO:N | 1:D:118:GLU:N[2_546] | 1.77 | 0.43 |
| 1:B:121:ILE:CB | 1:D:55:LYS:NZ[2_546] | 1.77 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:44:TYR:CZ | 1:D:50:LEU:CD1[2_546] | 1.77 | 0.43 |
| 1:B:175:LYS:O | 1:D:19:THR:N[2_546] | 1.77 | 0.43 |
| 1:B:28:LEU:CB | 1:D:180:TYR:CA[2_546] | 1.77 | 0.43 |
| 1:B:21:ILE:CA | 1:D:176:ALA:C[2_546] | 1.77 | 0.43 |
| 1:B:37:ASP:C | 1:D:342:TRP:C[2_546] | 1.77 | 0.43 |
| 1:B:57:PRO:CA | 1:D:117:LYS:C[2_546] | 1.77 | 0.43 |
| 1:B:222:ALA:CB | 1:D:27:ILE:CG1[2_546] | 1.77 | 0.43 |
| 1:B:226:PHE:CG | 1:D:25:LYS:NZ[2_546] | 1.77 | 0.43 |
| 1:A:362:LEU:CD2 | 1:D:166:THR:O[2_546] | 1.77 | 0.43 |
| 1:B:267:ARG:CZ | 1:D:35:ILE:CD1[2_546] | 1.77 | 0.43 |
| 1:B:174:ASP:N | 1:D:17:ASN:CG[2_546] | 1.77 | 0.43 |
| 1:B:33:TYR:CD2 | 1:D:124:ILE:CG1[2_546] | 1.77 | 0.43 |
| 1:B:23:GLY:N | 1:D:271:PHE:CE2[2_546] | 1.77 | 0.43 |
| 1:B:264:TYR:CD1 | 1:D:258:HIS:ND1[2_546] | 1.77 | 0.43 |
| 1:B:177:LEU:CG | 1:D:31:ARG:O[2_546] | 1.77 | 0.43 |
| 1:B:59:LYS:CG | 1:D:113:LYS:C[2_546] | 1.77 | 0.43 |
| 1:B:40:ASN:CG | 1:D:189:THR:CB[2_546] | 1.77 | 0.43 |
| 1:B:60:LYS:N | 1:D:114:GLU:O[2_546] | 1.78 | 0.42 |
| 1:B:54:GLY:CA | 1:D:65:LEU:C[2_546] | 1.78 | 0.42 |
| 1:B:20:PHE:CE1 | 1:D:173:MET:CE[2_546] | 1.78 | 0.42 |
| 1:B:32:GLY:CA | 1:D:152:PHE:CE2[2_546] | 1.78 | 0.42 |
| 1:B:253:LEU:CB | 1:D:309:TYR:OH[2_546] | 1.78 | 0.42 |
| 1:B:332:ALA:O | 1:C:369:GLN:CA[2_546] | 1.78 | 0.42 |
| 1:A:367:GLU:CB | 1:D:156:PHE:CZ[2_546] | 1.78 | 0.42 |
| 1:A:111:LYS:CD | 1:A:245:LYS:CB[2_556] | 1.78 | 0.42 |
| 1:A:361:ALA:O | 1:D:171:ASN:CG[2_546] | 1.78 | 0.42 |
| 1:B:55:LYS:CA | 1:D:121:ILE:CB[2_546] | 1.78 | 0.42 |
| 1:B:242:PHE:CD1 | 1:D:305:SER:C[2_546] | 1.78 | 0.42 |
| 1:B:175:LYS:N | 1:D:17:ASN:O[2_546] | 1.78 | 0.42 |
| 1:B:347:ILE:CD1 | 1:D:59:LYS:N[2_546] | 1.78 | 0.42 |
| 1:B:22:ASP:C | 1:D:271:PHE:CE2[2_546] | 1.78 | 0.42 |
| 1:B:189:THR:OG1 | 1:D:41:TYR:CG[2_546] | 1.78 | 0.42 |
| 1:B:29:ARG:NE | 1:D:336:LEU:C[2_546] | 1.78 | 0.42 |
| 1:B:306:LYS:CE | 1:D:298:LEU:C[2_546] | 1.78 | 0.42 |
| 1:B:299:GLY:CA | 1:D:307:GLY:C[2_546] | 1.78 | 0.42 |
| 1:B:30:TYR:CA | 1:D:44:TYR:CG[2_546] | 1.79 | 0.41 |
| 1:B:263:THR:C | 1:D:312:THR:C[2_546] | 1.79 | 0.41 |
| 1:B:226:PHE:CB | 1:D:25:LYS:NZ[2_546] | 1.79 | 0.41 |
| 1:B:49:TYR:CD1 | 1:D:53:TYR:CZ[2_546] | 1.79 | 0.41 |
| 1:B:320:PHE:O | 1:C:367:GLU:OE2[2_546] | 1.79 | 0.41 |
| 1:B:40:ASN:OD1 | 1:D:189:THR:CB[2_546] | 1.79 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:44:TYR:O | 1:D:54:GLY:N[2_546] | 1.79 | 0.41 |
| 1:B:171:ASN:CA | 1:D:16:THR:C[2_546] | 1.79 | 0.41 |
| 1:B:319:VAL:CA | 1:D:20:PHE:CE1[2_546] | 1.79 | 0.41 |
| 1:B:298:LEU:CA | 1:D:306:LYS:C[2_546] | 1.79 | 0.41 |
| 1:B:31:ARG:NE | 1:D:45:GLU:CB[2_546] | 1.79 | 0.41 |
| 1:B:263:THR:C | 1:D:311:ASN:C[2_546] | 1.79 | 0.41 |
| 1:B:183:HIS:CG | 1:D:39:VAL:CG1[2_546] | 1.79 | 0.41 |
| 1:B:242:PHE:CZ | 1:D:304:SER:O[2_546] | 1.79 | 0.41 |
| 1:B:259:ARG:N | 1:D:269:LYS:CA[2_546] | 1.79 | 0.41 |
| 1:B:320:PHE:C | 1:C:367:GLU:OE2[2_546] | 1.79 | 0.41 |
| 1:B:336:LEU:CD2 | 1:C:369:GLN:NE2[2_546] | 1.79 | 0.41 |
| 1:B:41:TYR:CG | 1:D:342:TRP:O[2_546] | 1.79 | 0.41 |
| 1:B:45:GLU:N | 1:D:53:TYR:C[2_546] | 1.79 | 0.41 |
| 1:B:175:LYS:CE | 1:D:348:GLU:OE1[2_546] | 1.79 | 0.41 |
| 1:B:27:ILE:C | 1:D:180:TYR:CB[2_546] | 1.79 | 0.41 |
| 1:B:257:GLY:O | 1:D:264:TYR:CD2[2_546] | 1.79 | 0.41 |
| 1:B:29:ARG:CZ | 1:D:333:LEU:O[2_546] | 1.79 | 0.41 |
| 1:B:303:PHE:CZ | 1:D:304:SER:CA[2_546] | 1.79 | 0.41 |
| 1:B:27:ILE:N | 1:D:180:TYR:CZ[2_546] | 1.79 | 0.41 |
| 1:B:314:PHE:CD1 | 1:D:23:GLY:O[2_546] | 1.79 | 0.41 |
| 1:A:110:PHE:CA | 1:A:249:GLN:OE1[2_556] | 1.79 | 0.41 |
| 1:B:41:TYR:C | 1:D:346:ILE:N[2_546] | 1.80 | 0.40 |
| 1:A:362:LEU:CG | 1:D:167:THR:CA[2_546] | 1.80 | 0.40 |
| 1:B:169:GLU:C | 1:C:364:VAL:CG2[2_546] | 1.80 | 0.40 |
| 1:B:171:ASN:N | 1:C:364:VAL:CG2[2_546] | 1.80 | 0.40 |
| 1:B:37:ASP:OD1 | 1:D:342:TRP:CE3[2_546] | 1.80 | 0.40 |
| 1:B:260:VAL:O | 1:D:271:PHE:C[2_546] | 1.80 | 0.40 |
| 1:B:31:ARG:CD | 1:D:45:GLU:CG[2_546] | 1.80 | 0.40 |
| 1:B:171:ASN:CG | 1:D:16:THR:CB[2_546] | 1.80 | 0.40 |
| 1:B:337:SER:CB | 1:D:33:TYR:CB[2_546] | 1.80 | 0.40 |
| 1:A:364:VAL:CA | 1:D:154:LYS:CA[2_546] | 1.80 | 0.40 |
| 1:B:342:TRP:N | 1:D:46:GLU:OE2[2_546] | 1.80 | 0.40 |
| 1:B:35:ILE:CA | 1:D:181:THR:CA[2_546] | 1.80 | 0.40 |
| 1:B:334:PHE:CD1 | 1:D:34:ASN:CG[2_546] | 1.80 | 0.40 |
| 1:B:38:LEU:O | 1:D:345:HIS:N[2_546] | 1.80 | 0.40 |
| 1:B:242:PHE:CD2 | 1:D:305:SER:O[2_546] | 1.80 | 0.40 |
| 1:B:175:LYS:N | 1:D:18:LEU:CA[2_546] | 1.80 | 0.40 |
| 1:B:121:ILE:CB | 1:D:61:GLU:OE2[2_546] | 1.80 | 0.40 |
| 1:A:362:LEU:O | 1:D:170:ILE:CG2[2_546] | 1.80 | 0.40 |
| 1:B:23:GLY:CA | 1:D:316:SER:CB[2_546] | 1.80 | 0.40 |
| 1:B:320:PHE:O | 1:C:367:GLU:CD[2_546] | 1.80 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:29:ARG:CD | 1:D:177:LEU:CD2[2_546] | 1.80 | 0.40 |
| 1:B:206:LEU:CD1 | 1:C:372:VAL:CB[2_546] | 1.80 | 0.40 |
| 1:A:369:GLN:O | 1:D:127:MET:CG[2_546] | 1.80 | 0.40 |
| 1:B:337:SER:C | 1:D:33:TYR:CD2[2_546] | 1.80 | 0.40 |
| 1:B:315:TYR:OH | 1:D:260:VAL:C[2_546] | 1.80 | 0.40 |
| 1:B:34:ASN:CB | 1:D:339:THR:N[2_546] | 1.81 | 0.39 |
| 1:B:20:PHE:CB | 1:D:177:LEU:CG[2_546] | 1.81 | 0.39 |
| 1:B:171:ASN:ND2 | 1:D:16:THR:CB[2_546] | 1.81 | 0.39 |
| 1:B:303:PHE:CD1 | 1:D:308:ILE:O[2_546] | 1.81 | 0.39 |
| 1:B:314:PHE:O | 1:D:23:GLY:N[2_546] | 1.81 | 0.39 |
| 1:B:341:GLY:O | 1:D:46:GLU:OE1[2_546] | 1.81 | 0.39 |
| 1:B:263:THR:CG2 | 1:D:312:THR:C[2_546] | 1.81 | 0.39 |
| 1:B:20:PHE:CE1 | 1:D:173:MET:CA[2_546] | 1.81 | 0.39 |
| 1:B:306:LYS:CG | 1:D:299:GLY:N[2_546] | 1.81 | 0.39 |
| 1:B:340:LEU:N | 1:D:56:LEU:CD1[2_546] | 1.81 | 0.39 |
| 1:B:17:ASN:CB | 1:D:151:SER:CA[2_546] | 1.81 | 0.39 |
| 1:B:309:TYR:CB | 1:D:310:PRO:C[2_546] | 1.81 | 0.39 |
| 1:B:306:LYS:NZ | 1:D:298:LEU:C[2_546] | 1.81 | 0.39 |
| 1:B:189:THR:N | 1:D:41:TYR:CD1[2_546] | 1.81 | 0.39 |
| 1:B:58:THR:CA | 1:D:115:ASN:O[2_546] | 1.81 | 0.39 |
| 1:B:33:TYR:CZ | 1:D:124:ILE:CG1[2_546] | 1.81 | 0.39 |
| 1:B:34:ASN:O | 1:D:340:LEU:N[2_546] | 1.81 | 0.39 |
| 1:A:367:GLU:OE1 | 1:D:160:SER:OG[2_546] | 1.81 | 0.39 |
| 1:B:21:ILE:CD1 | 1:D:175:LYS:O[2_546] | 1.81 | 0.39 |
| 1:B:292:ALA:O | 1:D:262:LYS:CG[2_546] | 1.81 | 0.39 |
| 1:B:276:LEU:C | 1:C:360:ARG:NH1[2_546] | 1.81 | 0.39 |
| 1:B:179:LEU:N | 1:D:30:TYR:CG[2_546] | 1.81 | 0.39 |
| 1:B:46:GLU:CD | 1:D:52:LEU:CD2[2_546] | 1.82 | 0.38 |
| 1:A:109:ASN:CB | 1:A:249:GLN:C[2_556] | 1.82 | 0.38 |
| 1:A:361:ALA:CA | 1:D:171:ASN:OD1[2_546] | 1.82 | 0.38 |
| 1:B:112:TRP:CZ2 | 1:D:59:LYS:CE[2_546] | 1.82 | 0.38 |
| 1:B:22:ASP:OD2 | 1:D:320:PHE:CE2[2_546] | 1.82 | 0.38 |
| 1:B:24:GLU:CD | 1:D:318:ILE:C[2_546] | 1.82 | 0.38 |
| 1:B:38:LEU:O | 1:D:344:ALA:C[2_546] | 1.82 | 0.38 |
| 1:B:188:SER:O | 1:D:41:TYR:CD2[2_546] | 1.82 | 0.38 |
| 1:B:226:PHE:CD2 | 1:D:25:LYS:CE[2_546] | 1.82 | 0.38 |
| 1:A:107:ASP:C | 1:A:248:ASN:OD1[2_556] | 1.82 | 0.38 |
| 1:A:368:TYR:CE2 | 1:D:127:MET:CE[2_546] | 1.82 | 0.38 |
| 1:B:311:ASN:O | 1:D:266:PRO:CD[2_546] | 1.82 | 0.38 |
| 1:B:38:LEU:N | 1:D:342:TRP:N[2_546] | 1.82 | 0.38 |
| 1:B:242:PHE:CE2 | 1:D:305:SER:CA[2_546] | 1.82 | 0.38 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:174:ASP:CA | 1:D:17:ASN:CG[2_546] | 1.82 | 0.38 |
| 1:B:300:ILE:N | 1:D:308:ILE:CG1[2_546] | 1.82 | 0.38 |
| 1:A:235:PRO:O | 1:B:224:GLU:OE1[2_546] | 1.82 | 0.38 |
| 1:B:256:PHE:N | 1:D:263:THR:C[2_546] | 1.82 | 0.38 |
| 1:B:307:GLY:CA | 1:D:314:PHE:CG[2_546] | 1.82 | 0.38 |
| 1:B:265:ASP:OD2 | 1:D:267:ARG:N[2_546] | 1.82 | 0.38 |
| 1:B:336:LEU:CG | 1:C:369:GLN:NE2[2_546] | 1.82 | 0.38 |
| 1:B:34:ASN:OD1 | 1:D:334:PHE:O[2_546] | 1.82 | 0.38 |
| 1:B:267:ARG:C | 1:D:183:HIS:CE1[2_546] | 1.82 | 0.38 |
| 1:B:175:LYS:CD | 1:D:16:THR:OG1[2_546] | 1.82 | 0.38 |
| 1:B:51:MET:SD | 1:D:46:GLU:N[2_546] | 1.82 | 0.38 |
| 1:B:34:ASN:OD1 | 1:D:337:SER:CA[2_546] | 1.82 | 0.38 |
| 1:B:265:ASP:OD1 | 1:D:267:ARG:NE[2_546] | 1.82 | 0.38 |
| 1:A:365:GLY:O | 1:D:153:ALA:C[2_546] | 1.82 | 0.38 |
| 1:B:180:TYR:CE1 | 1:D:29:ARG:CB[2_546] | 1.82 | 0.38 |
| 1:B:27:ILE:CD1 | 1:D:334:PHE:CG[2_546] | 1.82 | 0.38 |
| 1:A:361:ALA:O | 1:D:171:ASN:CA[2_546] | 1.82 | 0.38 |
| 1:B:27:ILE:C | 1:D:180:TYR:CG[2_546] | 1.82 | 0.38 |
| 1:B:33:TYR:CA | 1:D:44:TYR:OH[2_546] | 1.82 | 0.38 |
| 1:B:258:HIS:CE1 | 1:D:266:PRO:O[2_546] | 1.82 | 0.38 |
| 1:B:61:GLU:OE1 | 1:D:118:GLU:OE1[2_546] | 1.82 | 0.38 |
| 1:B:59:LYS:CG | 1:D:114:GLU:CA[2_546] | 1.83 | 0.37 |
| 1:B:57:PRO:CD | 1:D:117:LYS:O[2_546] | 1.83 | 0.37 |
| 1:B:33:TYR:CE2 | 1:D:124:ILE:CG1[2_546] | 1.83 | 0.37 |
| 1:B:303:PHE:C | 1:D:256:PHE:CZ[2_546] | 1.83 | 0.37 |
| 1:B:51:MET:CE | 1:D:46:GLU:N[2_546] | 1.83 | 0.37 |
| 1:B:302:GLN:NE2 | 1:D:301:LYS:O[2_546] | 1.83 | 0.37 |
| 1:B:39:VAL:C | 1:D:345:HIS:CB[2_546] | 1.83 | 0.37 |
| 1:B:20:PHE:C | 1:D:176:ALA:N[2_546] | 1.83 | 0.37 |
| 1:B:30:TYR:C | 1:D:44:TYR:CD2[2_546] | 1.83 | 0.37 |
| 1:B:25:LYS:CD | 1:D:330:PHE:CB[2_546] | 1.83 | 0.37 |
| 1:B:308:ILE:N | 1:D:310:PRO:CB[2_546] | 1.83 | 0.37 |
| 1:B:344:ALA:N | 1:D:46:GLU:OE1[2_546] | 1.83 | 0.37 |
| 1:B:56:LEU:N | 1:D:121:ILE:N[2_546] | 1.83 | 0.37 |
| 1:A:363:TYR:C | 1:D:170:ILE:CG2[2_546] | 1.83 | 0.37 |
| 1:B:271:PHE:CD1 | 1:D:20:PHE:O[2_546] | 1.83 | 0.37 |
| 1:B:38:LEU:CD2 | 1:D:340:LEU:O[2_546] | 1.83 | 0.37 |
| 1:B:29:ARG:CG | 1:D:337:SER:N[2_546] | 1.83 | 0.37 |
| 1:B:335:ALA:O | 1:C:370:GLU:C[2_546] | 1.83 | 0.37 |
| 1:B:31:ARG:NH1 | 1:D:45:GLU:CG[2_546] | 1.83 | 0.37 |
| 1:B:334:PHE:CE1 | 1:D:34:ASN:O[2_546] | 1.83 | 0.37 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:181:THR:OG1 | 1:D:50:LEU:CG[2_546] | 1.83 | 0.37 |
| 1:B:266:PRO:O | 1:D:183:HIS:CG[2_546] | 1.83 | 0.37 |
| 1:B:320:PHE:CB | 1:C:367:GLU:OE1[2_546] | 1.83 | 0.37 |
| 1:B:263:THR:CA | 1:D:313:ASP:CA[2_546] | 1.83 | 0.37 |
| 1:B:183:HIS:O | 1:D:39:VAL:C[2_546] | 1.83 | 0.37 |
| 1:B:47:THR:C | 1:D:50:LEU:N[2_546] | 1.83 | 0.37 |
| 1:B:335:ALA:CA | 1:C:371:TYR:N[2_546] | 1.83 | 0.37 |
| 1:B:44:TYR:CE2 | 1:D:54:GLY:O[2_546] | 1.83 | 0.37 |
| 1:A:369:GLN:CG | 1:D:125:ALA:CA[2_546] | 1.84 | 0.36 |
| 1:B:32:GLY:N | 1:D:44:TYR:CE2[2_546] | 1.84 | 0.36 |
| 1:B:29:ARG:NE | 1:D:336:LEU:CA[2_546] | 1.84 | 0.36 |
| 1:B:259:ARG:CD | 1:D:273:LYS:CB[2_546] | 1.84 | 0.36 |
| 1:B:206:LEU:CB | 1:C:372:VAL:CG1[2_546] | 1.84 | 0.36 |
| 1:A:366:PRO:CD | 1:D:152:PHE:CA[2_546] | 1.84 | 0.36 |
| 1:B:298:LEU:CB | 1:D:306:LYS:CA[2_546] | 1.84 | 0.36 |
| 1:B:17:ASN:O | 1:D:45:GLU:OE1[2_546] | 1.84 | 0.36 |
| 1:A:286:ARG:NE | 1:B:251:ASN:CB[2_546] | 1.84 | 0.36 |
| 1:B:313:ASP:O | 1:D:26:GLY:N[2_546] | 1.84 | 0.36 |
| 1:B:258:HIS:CG | 1:D:268:ALA:N[2_546] | 1.84 | 0.36 |
| 1:B:20:PHE:CD2 | 1:D:173:MET:CE[2_546] | 1.84 | 0.36 |
| 1:B:301:LYS:C | 1:D:303:PHE:CG[2_546] | 1.84 | 0.36 |
| 1:B:52:LEU:C | 1:D:62:LEU:CA[2_546] | 1.84 | 0.36 |
| 1:B:180:TYR:CD2 | 1:D:34:ASN:C[2_546] | 1.84 | 0.36 |
| 1:B:21:ILE:CB | 1:D:176:ALA:CA[2_546] | 1.84 | 0.36 |
| 1:B:30:TYR:C | 1:D:44:TYR:CZ[2_546] | 1.84 | 0.36 |
| 1:B:24:GLU:CB | 1:D:316:SER:C[2_546] | 1.84 | 0.36 |
| 1:B:314:PHE:O | 1:D:22:ASP:C[2_546] | 1.84 | 0.36 |
| 1:B:314:PHE:O | 1:D:23:GLY:C[2_546] | 1.84 | 0.36 |
| 1:B:302:GLN:OE1 | 1:D:303:PHE:N[2_546] | 1.84 | 0.36 |
| 1:B:45:GLU:CA | 1:D:53:TYR:O[2_546] | 1.84 | 0.36 |
| 1:B:45:GLU:O | 1:D:53:TYR:CG[2_546] | 1.84 | 0.36 |
| 1:B:33:TYR:CD1 | 1:D:124:ILE:CD1[2_546] | 1.84 | 0.36 |
| 1:B:256:PHE:CD1 | 1:D:263:THR:CA[2_546] | 1.84 | 0.36 |
| 1:B:338:ARG:CA | 1:C:371:TYR:CD1[2_546] | 1.84 | 0.36 |
| 1:B:32:GLY:O | 1:D:336:LEU:O[2_546] | 1.84 | 0.36 |
| 1:B:176:ALA:CB | 1:C:363:TYR:CE1[2_546] | 1.84 | 0.36 |
| 1:B:334:PHE:N | 1:C:368:TYR:CD1[2_546] | 1.84 | 0.36 |
| 1:B:24:GLU:N | 1:D:316:SER:O[2_546] | 1.84 | 0.36 |
| 1:B:184:GLU:N | 1:D:39:VAL:CG1[2_546] | 1.84 | 0.36 |
| 1:B:311:ASN:CB | 1:D:266:PRO:CD[2_546] | 1.84 | 0.36 |
| 1:B:185:VAL:N | 1:D:39:VAL:O[2_546] | 1.84 | 0.36 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:42:GLY:CA | 1:D:344:ALA:C[2_546] | 1.85 | 0.35 |
| 1:B:342:TRP:CB | 1:C:371:TYR:CZ[2_546] | 1.85 | 0.35 |
| 1:B:38:LEU:CD2 | 1:D:340:LEU:CG[2_546] | 1.85 | 0.35 |
| 1:B:334:PHE:CD1 | 1:D:34:ASN:N[2_546] | 1.85 | 0.35 |
| 1:B:260:VAL:C | 1:D:272:LYS:N[2_546] | 1.85 | 0.35 |
| 1:B:61:GLU:OE1 | 1:D:118:GLU:CB[2_546] | 1.85 | 0.35 |
| 1:B:315:TYR:CE1 | 1:D:260:VAL:CG1[2_546] | 1.85 | 0.35 |
| 1:B:302:GLN:O | 1:D:303:PHE:CG[2_546] | 1.85 | 0.35 |
| 1:A:110:PHE:O | 1:A:244:ASP:C[2_556] | 1.85 | 0.35 |
| 1:B:22:ASP:N | 1:D:176:ALA:CB[2_546] | 1.85 | 0.35 |
| 1:B:29:ARG:NH1 | 1:D:333:LEU:O[2_546] | 1.85 | 0.35 |
| 1:A:363:TYR:O | 1:D:170:ILE:CA[2_546] | 1.85 | 0.35 |
| 1:B:342:TRP:N | 1:C:371:TYR:CZ[2_546] | 1.85 | 0.35 |
| 1:A:366:PRO:N | 1:D:152:PHE:C[2_546] | 1.85 | 0.35 |
| 1:B:21:ILE:CA | 1:D:176:ALA:CB[2_546] | 1.85 | 0.35 |
| 1:A:369:GLN:C | 1:D:124:ILE:O[2_546] | 1.85 | 0.35 |
| 1:B:338:ARG:NH1 | 1:D:36:GLU:C[2_546] | 1.85 | 0.35 |
| 1:B:273:LYS:NZ | 1:D:185:VAL:CG1[2_546] | 1.85 | 0.35 |
| 1:B:271:PHE:CZ | 1:D:29:ARG:N[2_546] | 1.85 | 0.35 |
| 1:B:305:SER:N | 1:D:253:LEU:CB[2_546] | 1.85 | 0.35 |
| 1:B:188:SER:N | 1:D:41:TYR:CZ[2_546] | 1.85 | 0.35 |
| 1:B:176:ALA:O | 1:D:31:ARG:N[2_546] | 1.85 | 0.35 |
| 1:B:296:GLU:CB | 1:D:262:LYS:CE[2_546] | 1.85 | 0.35 |
| 1:A:367:GLU:CA | 1:D:156:PHE:CD1[2_546] | 1.85 | 0.35 |
| 1:A:279:ILE:CG1 | 1:B:249:GLN:CD[2_546] | 1.85 | 0.35 |
| 1:B:117:LYS:CG | 1:D:61:GLU:C[2_546] | 1.85 | 0.35 |
| 1:B:302:GLN:N | 1:D:303:PHE:CG[2_546] | 1.85 | 0.35 |
| 1:B:169:GLU:O | 1:C:364:VAL:N[2_546] | 1.85 | 0.35 |
| 1:B:21:ILE:C | 1:D:176:ALA:CA[2_546] | 1.85 | 0.35 |
| 1:B:46:GLU:CG | 1:D:52:LEU:CB[2_546] | 1.85 | 0.35 |
| 1:B:306:LYS:CE | 1:D:300:ILE:N[2_546] | 1.86 | 0.34 |
| 1:B:345:HIS:NE2 | 1:D:43:SER:N[2_546] | 1.86 | 0.34 |
| 1:B:116:ASP:C | 1:D:60:LYS:N[2_546] | 1.86 | 0.34 |
| 1:B:334:PHE:CG | 1:D:34:ASN:CB[2_546] | 1.86 | 0.34 |
| 1:B:264:TYR:N | 1:D:312:THR:N[2_546] | 1.86 | 0.34 |
| 1:B:317:GLY:N | 1:D:22:ASP:CB[2_546] | 1.86 | 0.34 |
| 1:A:367:GLU:N | 1:D:156:PHE:CG[2_546] | 1.86 | 0.34 |
| 1:B:183:HIS:CA | 1:D:39:VAL:CB[2_546] | 1.86 | 0.34 |
| 1:B:171:ASN:CB | 1:D:15:VAL:CA[2_546] | 1.86 | 0.34 |
| 1:A:361:ALA:N | 1:D:171:ASN:OD1[2_546] | 1.86 | 0.34 |
| 1:B:273:LYS:CD | 1:D:185:VAL:N[2_546] | 1.86 | 0.34 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:237:ARG:NE | 1:B:217:LEU:CA[2_546] | 1.86 | 0.34 |
| 1:B:172:ALA:C | 1:C:363:TYR:CG[2_546] | 1.86 | 0.34 |
| 1:B:171:ASN:OD1 | 1:D:16:THR:CB[2_546] | 1.86 | 0.34 |
| 1:B:180:TYR:CB | 1:D:30:TYR:N[2_546] | 1.86 | 0.34 |
| 1:B:258:HIS:C | 1:D:269:LYS:CA[2_546] | 1.86 | 0.34 |
| 1:B:44:TYR:OH | 1:D:50:LEU:CD1[2_546] | 1.86 | 0.34 |
| 1:B:30:TYR:O | 1:D:44:TYR:CZ[2_546] | 1.86 | 0.34 |
| 1:B:180:TYR:CZ | 1:D:28:LEU:C[2_546] | 1.86 | 0.34 |
| 1:B:41:TYR:N | 1:D:345:HIS:N[2_546] | 1.86 | 0.34 |
| 1:B:62:LEU:CD1 | 1:D:117:LYS:NZ[2_546] | 1.86 | 0.34 |
| 1:B:41:TYR:N | 1:D:346:ILE:N[2_546] | 1.86 | 0.34 |
| 1:B:172:ALA:C | 1:D:16:THR:O[2_546] | 1.86 | 0.34 |
| 1:B:48:ILE:CA | 1:D:49:TYR:C[2_546] | 1.86 | 0.34 |
| 1:B:59:LYS:CA | 1:D:115:ASN:N[2_546] | 1.86 | 0.34 |
| 1:B:34:ASN:CG | 1:D:335:ALA:O[2_546] | 1.86 | 0.34 |
| 1:B:263:THR:CB | 1:D:313:ASP:C[2_546] | 1.86 | 0.34 |
| 1:B:314:PHE:CD2 | 1:D:262:LYS:N[2_546] | 1.86 | 0.34 |
| 1:B:179:LEU:O | 1:D:30:TYR:CD2[2_546] | 1.86 | 0.34 |
| 1:B:263:THR:OG1 | 1:D:313:ASP:OD2[2_546] | 1.87 | 0.33 |
| 1:B:259:ARG:CG | 1:D:269:LYS:O[2_546] | 1.87 | 0.33 |
| 1:B:177:LEU:CD2 | 1:D:31:ARG:C[2_546] | 1.87 | 0.33 |
| 1:B:265:ASP:CG | 1:D:267:ARG:CG[2_546] | 1.87 | 0.33 |
| 1:B:344:ALA:CB | 1:D:46:GLU:CB[2_546] | 1.87 | 0.33 |
| 1:B:331:THR:C | 1:C:368:TYR:OH[2_546] | 1.87 | 0.33 |
| 1:B:258:HIS:NE2 | 1:D:270:ILE:CA[2_546] | 1.87 | 0.33 |
| 1:B:263:THR:O | 1:D:312:THR:C[2_546] | 1.87 | 0.33 |
| 1:B:309:TYR:CD1 | 1:D:311:ASN:N[2_546] | 1.87 | 0.33 |
| 1:B:24:GLU:CG | 1:D:317:GLY:O[2_546] | 1.87 | 0.33 |
| 1:B:40:ASN:O | 1:D:345:HIS:CB[2_546] | 1.87 | 0.33 |
| 1:B:188:SER:O | 1:D:41:TYR:CZ[2_546] | 1.87 | 0.33 |
| 1:B:184:GLU:O | 1:D:39:VAL:CA[2_546] | 1.87 | 0.33 |
| 1:B:37:ASP:OD1 | 1:D:342:TRP:CG[2_546] | 1.87 | 0.33 |
| 1:A:109:ASN:O | 1:A:249:GLN:CA[2_556] | 1.87 | 0.33 |
| 1:B:47:THR:CB | 1:D:52:LEU:N[2_546] | 1.87 | 0.33 |
| 1:B:175:LYS:NZ | 1:D:348:GLU:CD[2_546] | 1.87 | 0.33 |
| 1:B:19:THR:O | 1:D:174:ASP:CG[2_546] | 1.87 | 0.33 |
| 1:B:25:LYS:O | 1:D:180:TYR:OH[2_546] | 1.87 | 0.33 |
| 1:B:39:VAL:CG2 | 1:D:182:ASP:OD1[2_546] | 1.87 | 0.33 |
| 1:B:256:PHE:CA | 1:D:264:TYR:C[2_546] | 1.87 | 0.33 |
| 1:B:305:SER:CA | 1:D:253:LEU:CB[2_546] | 1.88 | 0.32 |
| 1:B:177:LEU:CB | 1:D:31:ARG:CG[2_546] | 1.88 | 0.32 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:48:ILE:O | 1:D:49:TYR:CB[2_546] | 1.88 | 0.32 |
| 1:B:175:LYS:CD | 1:D:18:LEU:CB[2_546] | 1.88 | 0.32 |
| 1:B:47:THR:O | 1:D:48:ILE:O[2_546] | 1.88 | 0.32 |
| 1:A:365:GLY:O | 1:D:153:ALA:O[2_546] | 1.88 | 0.32 |
| 1:A:367:GLU:CD | 1:D:156:PHE:CE1[2_546] | 1.88 | 0.32 |
| 1:B:262:LYS:CE | 1:D:315:TYR:CB[2_546] | 1.88 | 0.32 |
| 1:B:56:LEU:CB | 1:D:120:ALA:CA[2_546] | 1.88 | 0.32 |
| 1:B:276:LEU:O | 1:C:360:ARG:CZ[2_546] | 1.88 | 0.32 |
| 1:A:364:VAL:O | 1:D:153:ALA:C[2_546] | 1.88 | 0.32 |
| 1:A:109:ASN:ND2 | 1:A:246:VAL:C[2_556] | 1.88 | 0.32 |
| 1:A:367:GLU:CA | 1:D:156:PHE:CB[2_546] | 1.88 | 0.32 |
| 1:A:364:VAL:O | 1:D:153:ALA:CB[2_546] | 1.88 | 0.32 |
| 1:B:261:TYR:CE1 | 1:D:267:ARG:CB[2_546] | 1.88 | 0.32 |
| 1:B:57:PRO:CD | 1:D:117:LYS:CA[2_546] | 1.88 | 0.32 |
| 1:B:256:PHE:CB | 1:D:264:TYR:CA[2_546] | 1.88 | 0.32 |
| 1:B:229:PHE:CD1 | 1:D:24:GLU:CB[2_546] | 1.88 | 0.32 |
| 1:B:29:ARG:C | 1:D:44:TYR:CD1[2_546] | 1.88 | 0.32 |
| 1:B:277:THR:O | 1:C:362:LEU:CD1[2_546] | 1.88 | 0.32 |
| 1:B:61:GLU:CD | 1:D:118:GLU:CG[2_546] | 1.88 | 0.32 |
| 1:B:28:LEU:O | 1:D:177:LEU:O[2_546] | 1.88 | 0.32 |
| 1:A:364:VAL:CB | 1:D:154:LYS:CA[2_546] | 1.88 | 0.32 |
| 1:B:27:ILE:C | 1:D:180:TYR:CD1[2_546] | 1.88 | 0.32 |
| 1:B:308:ILE:CG2 | 1:D:310:PRO:N[2_546] | 1.88 | 0.32 |
| 1:B:179:LEU:CG | 1:D:19:THR:CB[2_546] | 1.88 | 0.32 |
| 1:B:335:ALA:O | 1:C:371:TYR:N[2_546] | 1.88 | 0.32 |
| 1:B:28:LEU:CG | 1:D:179:LEU:N[2_546] | 1.88 | 0.32 |
| 1:B:37:ASP:OD2 | 1:D:339:THR:CB[2_546] | 1.88 | 0.32 |
| 1:B:59:LYS:CD | 1:D:113:LYS:CA[2_546] | 1.88 | 0.32 |
| 1:B:53:TYR:O | 1:D:64:ASP:O[2_546] | 1.88 | 0.32 |
| 1:B:49:TYR:O | 1:D:65:LEU:CD1[2_546] | 1.88 | 0.32 |
| 1:B:172:ALA:O | 1:C:363:TYR:CG[2_546] | 1.88 | 0.32 |
| 1:B:17:ASN:CG | 1:D:151:SER:CB[2_546] | 1.88 | 0.32 |
| 1:B:183:HIS:ND1 | 1:D:179:LEU:CD2[2_546] | 1.89 | 0.31 |
| 1:B:29:ARG:C | 1:D:44:TYR:CE1[2_546] | 1.89 | 0.31 |
| 1:B:46:GLU:CG | 1:D:52:LEU:CD2[2_546] | 1.89 | 0.31 |
| 1:B:120:ALA:CB | 1:D:58:THR:CB[2_546] | 1.89 | 0.31 |
| 1:B:179:LEU:O | 1:D:30:TYR:CE2[2_546] | 1.89 | 0.31 |
| 1:A:111:LYS:CG | 1:A:245:LYS:CG[2_556] | 1.89 | 0.31 |
| 1:B:171:ASN:OD1 | 1:D:15:VAL:O[2_546] | 1.89 | 0.31 |
| 1:B:41:TYR:CB | 1:D:346:ILE:CG1[2_546] | 1.89 | 0.31 |
| 1:B:26:GLY:O | 1:D:180:TYR:CG[2_546] | 1.89 | 0.31 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:59:LYS:CG | 1:D:114:GLU:N[2_546] | 1.89 | 0.31 |
| 1:B:345:HIS:ND1 | 1:D:42:GLY:O[2_546] | 1.89 | 0.31 |
| 1:B:334:PHE:CD2 | 1:D:37:ASP:OD2[2_546] | 1.89 | 0.31 |
| 1:B:48:ILE:CD1 | 1:D:55:LYS:CG[2_546] | 1.89 | 0.31 |
| 1:B:310:PRO:C | 1:D:265:ASP:CB[2_546] | 1.89 | 0.31 |
| 1:B:178:ILE:O | 1:D:30:TYR:CG[2_546] | 1.89 | 0.31 |
| 1:B:29:ARG:NH2 | 1:D:333:LEU:O[2_546] | 1.89 | 0.31 |
| 1:B:175:LYS:CA | 1:D:19:THR:N[2_546] | 1.89 | 0.31 |
| 1:B:180:TYR:CD1 | 1:D:29:ARG:CG[2_546] | 1.89 | 0.31 |
| 1:B:333:LEU:C | 1:D:32:GLY:O[2_546] | 1.89 | 0.31 |
| 1:B:29:ARG:CB | 1:D:177:LEU:CD2[2_546] | 1.89 | 0.31 |
| 1:B:31:ARG:N | 1:D:44:TYR:CE2[2_546] | 1.89 | 0.31 |
| 1:B:337:SER:N | 1:D:33:TYR:CG[2_546] | 1.89 | 0.31 |
| 1:B:45:GLU:CA | 1:D:54:GLY:N[2_546] | 1.89 | 0.31 |
| 1:B:307:GLY:CA | 1:D:314:PHE:CD2[2_546] | 1.89 | 0.31 |
| 1:B:309:TYR:OH | 1:D:255:GLY:N[2_546] | 1.89 | 0.31 |
| 1:B:271:PHE:CA | 1:D:21:ILE:CB[2_546] | 1.89 | 0.31 |
| 1:B:40:ASN:N | 1:D:341:GLY:O[2_546] | 1.89 | 0.31 |
| 1:B:271:PHE:CE2 | 1:D:20:PHE:N[2_546] | 1.89 | 0.31 |
| 1:B:47:THR:C | 1:D:49:TYR:CA[2_546] | 1.89 | 0.31 |
| 1:B:96:LEU:CD1 | 1:C:370:GLU:OE1[2_546] | 1.89 | 0.31 |
| 1:B:182:ASP:N | 1:D:38:LEU:CD1[2_546] | 1.89 | 0.31 |
| 1:B:29:ARG:N | 1:D:337:SER:OG[2_546] | 1.89 | 0.31 |
| 1:B:271:PHE:CD2 | 1:D:20:PHE:CA[2_546] | 1.89 | 0.31 |
| 1:B:331:THR:C | 1:C:368:TYR:CD1[2_546] | 1.89 | 0.31 |
| 1:B:179:LEU:CG | 1:D:19:THR:CG2[2_546] | 1.89 | 0.31 |
| 1:B:306:LYS:CG | 1:D:299:GLY:CA[2_546] | 1.89 | 0.31 |
| 1:B:319:VAL:O | 1:C:367:GLU:OE2[2_546] | 1.90 | 0.30 |
| 1:B:341:GLY:O | 1:D:46:GLU:OE2[2_546] | 1.90 | 0.30 |
| 1:B:242:PHE:CE2 | 1:D:306:LYS:CA[2_546] | 1.90 | 0.30 |
| 1:B:333:LEU:CD2 | 1:C:368:TYR:O[2_546] | 1.90 | 0.30 |
| 1:A:108:LYS:CB | 1:A:248:ASN:CB[2_556] | 1.90 | 0.30 |
| 1:B:333:LEU:N | 1:C:368:TYR:C[2_546] | 1.90 | 0.30 |
| 1:B:24:GLU:C | 1:D:316:SER:C[2_546] | 1.90 | 0.30 |
| 1:B:61:GLU:OE2 | 1:D:118:GLU:OE2[2_546] | 1.90 | 0.30 |
| 1:B:183:HIS:O | 1:D:39:VAL:N[2_546] | 1.90 | 0.30 |
| 1:B:335:ALA:O | 1:D:33:TYR:CE2[2_546] | 1.90 | 0.30 |
| 1:B:175:LYS:CA | 1:D:18:LEU:CB[2_546] | 1.90 | 0.30 |
| 1:B:54:GLY:O | 1:D:69:LEU:CD2[2_546] | 1.90 | 0.30 |
| 1:B:38:LEU:CG | 1:D:340:LEU:CD1[2_546] | 1.90 | 0.30 |
| 1:B:19:THR:CB | 1:D:178:ILE:CG1[2_546] | 1.90 | 0.30 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:269:LYS:N | 1:D:183:HIS:CG[2_546] | 1.90 | 0.30 |
| 1:B:310:PRO:CG | 1:D:258:HIS:CB[2_546] | 1.90 | 0.30 |
| 1:A:368:TYR:CB | 1:D:336:LEU:CD2[2_546] | 1.90 | 0.30 |
| 1:B:29:ARG:O | 1:D:177:LEU:C[2_546] | 1.90 | 0.30 |
| 1:B:271:PHE:C | 1:D:21:ILE:CB[2_546] | 1.90 | 0.30 |
| 1:B:117:LYS:O | 1:D:61:GLU:CD[2_546] | 1.90 | 0.30 |
| 1:B:300:ILE:O | 1:D:308:ILE:CG2[2_546] | 1.90 | 0.30 |
| 1:B:277:THR:CG2 | 1:C:361:ALA:O[2_546] | 1.90 | 0.30 |
| 1:B:48:ILE:C | 1:D:49:TYR:CD1[2_546] | 1.90 | 0.30 |
| 1:B:332:ALA:O | 1:C:369:GLN:C[2_546] | 1.90 | 0.30 |
| 1:B:264:TYR:C | 1:D:312:THR:CB[2_546] | 1.90 | 0.30 |
| 1:B:229:PHE:CD1 | 1:D:24:GLU:CG[2_546] | 1.90 | 0.30 |
| 1:B:120:ALA:CB | 1:D:57:PRO:C[2_546] | 1.90 | 0.30 |
| 1:A:109:ASN:N | 1:A:248:ASN:CA[2_556] | 1.90 | 0.30 |
| 1:A:108:LYS:CA | 1:A:248:ASN:CA[2_556] | 1.90 | 0.30 |
| 1:B:180:TYR:N | 1:D:30:TYR:CG[2_546] | 1.90 | 0.30 |
| 1:B:271:PHE:CG | 1:D:20:PHE:C[2_546] | 1.90 | 0.30 |
| 1:B:39:VAL:O | 1:D:345:HIS:CA[2_546] | 1.91 | 0.29 |
| 1:B:17:ASN:OD1 | 1:D:152:PHE:N[2_546] | 1.91 | 0.29 |
| 1:B:55:LYS:N | 1:D:121:ILE:CG2[2_546] | 1.91 | 0.29 |
| 1:B:333:LEU:N | 1:C:368:TYR:CE2[2_546] | 1.91 | 0.29 |
| 1:B:18:LEU:CB | 1:D:43:SER:CA[2_546] | 1.91 | 0.29 |
| 1:A:366:PRO:CG | 1:D:152:PHE:CE1[2_546] | 1.91 | 0.29 |
| 1:B:295:LEU:C | 1:D:262:LYS:CD[2_546] | 1.91 | 0.29 |
| 1:B:263:THR:N | 1:D:313:ASP:N[2_546] | 1.91 | 0.29 |
| 1:B:177:LEU:CA | 1:D:31:ARG:C[2_546] | 1.91 | 0.29 |
| 1:B:32:GLY:CA | 1:D:152:PHE:CZ[2_546] | 1.91 | 0.29 |
| 1:B:261:TYR:CG | 1:D:312:THR:OG1[2_546] | 1.91 | 0.29 |
| 1:A:368:TYR:CD1 | 1:D:336:LEU:CB[2_546] | 1.91 | 0.29 |
| 1:B:342:TRP:CE2 | 1:C:371:TYR:CG[2_546] | 1.91 | 0.29 |
| 1:B:222:ALA:CA | 1:D:27:ILE:CG1[2_546] | 1.91 | 0.29 |
| 1:B:262:LYS:CD | 1:D:315:TYR:CB[2_546] | 1.91 | 0.29 |
| 1:B:340:LEU:O | 1:D:46:GLU:CD[2_546] | 1.91 | 0.29 |
| 1:B:117:LYS:CB | 1:D:60:LYS:CA[2_546] | 1.91 | 0.29 |
| 1:B:31:ARG:CB | 1:D:48:ILE:CD1[2_546] | 1.91 | 0.29 |
| 1:B:333:LEU:O | 1:C:369:GLN:N[2_546] | 1.91 | 0.29 |
| 1:B:44:TYR:CD1 | 1:D:31:ARG:NE[2_546] | 1.91 | 0.29 |
| 1:B:53:TYR:O | 1:D:65:LEU:O[2_546] | 1.91 | 0.29 |
| 1:B:16:THR:CG2 | 1:D:174:ASP:CG[2_546] | 1.91 | 0.29 |
| 1:B:314:PHE:CE2 | 1:D:262:LYS:CB[2_546] | 1.91 | 0.29 |
| 1:B:20:PHE:O | 1:D:176:ALA:O[2_546] | 1.91 | 0.29 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:320:PHE:N | 1:D:20:PHE:CE1[2_546] | 1.91 | 0.29 |
| 1:B:169:GLU:O | 1:C:364:VAL:CG1[2_546] | 1.91 | 0.29 |
| 1:B:180:TYR:O | 1:D:38:LEU:CD1[2_546] | 1.91 | 0.29 |
| 1:B:62:LEU:CD2 | 1:D:117:LYS:CE[2_546] | 1.91 | 0.29 |
| 1:B:263:THR:CA | 1:D:312:THR:C[2_546] | 1.91 | 0.29 |
| 1:B:269:LYS:O | 1:D:184:GLU:CB[2_546] | 1.91 | 0.29 |
| 1:B:39:VAL:CB | 1:D:345:HIS:CD2[2_546] | 1.91 | 0.29 |
| 1:B:30:TYR:C | 1:D:44:TYR:CE2[2_546] | 1.92 | 0.28 |
| 1:B:342:TRP:NE1 | 1:D:41:TYR:CD1[2_546] | 1.92 | 0.28 |
| 1:A:109:ASN:CG | 1:A:250:LYS:C[2_556] | 1.92 | 0.28 |
| 1:B:315:TYR:CG | 1:D:23:GLY:N[2_546] | 1.92 | 0.28 |
| 1:B:315:TYR:CE1 | 1:D:260:VAL:O[2_546] | 1.92 | 0.28 |
| 1:B:259:ARG:O | 1:D:273:LYS:CA[2_546] | 1.92 | 0.28 |
| 1:B:48:ILE:CD1 | 1:D:55:LYS:CA[2_546] | 1.92 | 0.28 |
| 1:B:340:LEU:O | 1:D:46:GLU:OE1[2_546] | 1.92 | 0.28 |
| 1:B:183:HIS:C | 1:D:39:VAL:CG2[2_546] | 1.92 | 0.28 |
| 1:B:345:HIS:CD2 | 1:D:41:TYR:O[2_546] | 1.92 | 0.28 |
| 1:B:176:ALA:O | 1:D:30:TYR:CA[2_546] | 1.92 | 0.28 |
| 1:B:61:GLU:OE1 | 1:D:118:GLU:OE2[2_546] | 1.92 | 0.28 |
| 1:B:62:LEU:CB | 1:D:117:LYS:NZ[2_546] | 1.92 | 0.28 |
| 1:B:261:TYR:CD2 | 1:D:312:THR:OG1[2_546] | 1.92 | 0.28 |
| 1:B:37:ASP:C | 1:D:343:LEU:N[2_546] | 1.92 | 0.28 |
| 1:B:229:PHE:CE2 | 1:D:24:GLU:CB[2_546] | 1.92 | 0.28 |
| 1:B:180:TYR:CD2 | 1:D:28:LEU:O[2_546] | 1.92 | 0.28 |
| 1:B:51:MET:SD | 1:D:48:ILE:N[2_546] | 1.92 | 0.28 |
| 1:B:351:GLU:CD | 1:D:63:ASN:CG[2_546] | 1.92 | 0.28 |
| 1:B:338:ARG:CG | 1:D:37:ASP:CB[2_546] | 1.92 | 0.28 |
| 1:B:20:PHE:CA | 1:D:174:ASP:C[2_546] | 1.92 | 0.28 |
| 1:B:333:LEU:O | 1:D:32:GLY:C[2_546] | 1.92 | 0.28 |
| 1:B:256:PHE:CE2 | 1:D:309:TYR:CB[2_546] | 1.92 | 0.28 |
| 1:B:20:PHE:CG | 1:D:173:MET:C[2_546] | 1.92 | 0.28 |
| 1:B:300:ILE:CG1 | 1:D:258:HIS:N[2_546] | 1.92 | 0.28 |
| 1:B:24:GLU:OE2 | 1:D:318:ILE:CA[2_546] | 1.92 | 0.28 |
| 1:B:33:TYR:CG | 1:D:124:ILE:CG2[2_546] | 1.92 | 0.28 |
| 1:B:258:HIS:CG | 1:D:270:ILE:N[2_546] | 1.92 | 0.28 |
| 1:B:268:ALA:CB | 1:D:261:TYR:OH[2_546] | 1.92 | 0.28 |
| 1:B:19:THR:CB | 1:D:178:ILE:CD1[2_546] | 1.92 | 0.28 |
| 1:B:271:PHE:CG | 1:D:21:ILE:CA[2_546] | 1.92 | 0.28 |
| 1:B:18:LEU:O | 1:D:44:TYR:CG[2_546] | 1.93 | 0.27 |
| 1:B:56:LEU:C | 1:D:121:ILE:CD1[2_546] | 1.93 | 0.27 |
| 1:B:256:PHE:CD2 | 1:D:309:TYR:CG[2_546] | 1.93 | 0.27 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:56:LEU:N | 1:D:121:ILE:CG2[2_546] | 1.93 | 0.27 |
| 1:B:44:TYR:CB | 1:D:31:ARG:NH1[2_546] | 1.93 | 0.27 |
| 1:B:18:LEU:CB | 1:D:43:SER:C[2_546] | 1.93 | 0.27 |
| 1:B:173:MET:N | 1:C:364:VAL:O[2_546] | 1.93 | 0.27 |
| 1:B:189:THR:CB | 1:D:40:ASN:O[2_546] | 1.93 | 0.27 |
| 1:B:18:LEU:O | 1:D:44:TYR:C[2_546] | 1.93 | 0.27 |
| 1:B:336:LEU:CD1 | 1:C:369:GLN:CG[2_546] | 1.93 | 0.27 |
| 1:B:266:PRO:CD | 1:D:267:ARG:NH1[2_546] | 1.93 | 0.27 |
| 1:B:320:PHE:CG | 1:C:367:GLU:CB[2_546] | 1.93 | 0.27 |
| 1:A:108:LYS:C | 1:A:248:ASN:CA[2_556] | 1.93 | 0.27 |
| 1:B:30:TYR:CG | 1:D:47:THR:CG2[2_546] | 1.93 | 0.27 |
| 1:B:112:TRP:CH2 | 1:D:59:LYS:CD[2_546] | 1.93 | 0.27 |
| 1:B:308:ILE:CB | 1:D:310:PRO:CB[2_546] | 1.93 | 0.27 |
| 1:B:306:LYS:CG | 1:D:296:GLU:O[2_546] | 1.93 | 0.27 |
| 1:B:336:LEU:CD2 | 1:C:369:GLN:OE1[2_546] | 1.93 | 0.27 |
| 1:B:258:HIS:CG | 1:D:268:ALA:C[2_546] | 1.93 | 0.27 |
| 1:B:47:THR:N | 1:D:52:LEU:CB[2_546] | 1.93 | 0.27 |
| 1:B:40:ASN:O | 1:D:346:ILE:N[2_546] | 1.93 | 0.27 |
| 1:B:26:GLY:CA | 1:D:180:TYR:CE1[2_546] | 1.93 | 0.27 |
| 1:B:336:LEU:CB | 1:C:369:GLN:CD[2_546] | 1.93 | 0.27 |
| 1:B:169:GLU:CA | 1:C:364:VAL:CB[2_546] | 1.93 | 0.27 |
| 1:B:33:TYR:CE1 | 1:D:124:ILE:CG2[2_546] | 1.93 | 0.27 |
| 1:B:315:TYR:C | 1:D:21:ILE:O[2_546] | 1.93 | 0.27 |
| 1:A:286:ARG:C | 1:B:251:ASN:ND2[2_546] | 1.93 | 0.27 |
| 1:B:303:PHE:CE2 | 1:D:300:ILE:O[2_546] | 1.93 | 0.27 |
| 1:B:56:LEU:CB | 1:D:121:ILE:CA[2_546] | 1.93 | 0.27 |
| 1:B:48:ILE:CG1 | 1:D:55:LYS:N[2_546] | 1.93 | 0.27 |
| 1:B:309:TYR:O | 1:D:310:PRO:O[2_546] | 1.93 | 0.27 |
| 1:B:117:LYS:NZ | 1:D:64:ASP:CA[2_546] | 1.93 | 0.27 |
| 1:B:186:PRO:CA | 1:D:40:ASN:ND2[2_546] | 1.93 | 0.27 |
| 1:B:181:THR:O | 1:D:38:LEU:CG[2_546] | 1.93 | 0.27 |
| 1:A:279:ILE:CD1 | 1:B:249:GLN:CG[2_546] | 1.93 | 0.27 |
| 1:B:277:THR:CG2 | 1:C:361:ALA:C[2_546] | 1.94 | 0.26 |
| 1:B:267:ARG:CA | 1:D:183:HIS:ND1[2_546] | 1.94 | 0.26 |
| 1:B:310:PRO:O | 1:D:265:ASP:CA[2_546] | 1.94 | 0.26 |
| 1:B:229:PHE:CE2 | 1:D:24:GLU:CA[2_546] | 1.94 | 0.26 |
| 1:A:364:VAL:O | 1:D:154:LYS:N[2_546] | 1.94 | 0.26 |
| 1:A:286:ARG:CB | 1:B:251:ASN:ND2[2_546] | 1.94 | 0.26 |
| 1:B:39:VAL:CG2 | 1:D:182:ASP:CG[2_546] | 1.94 | 0.26 |
| 1:B:256:PHE:CG | 1:D:309:TYR:CB[2_546] | 1.94 | 0.26 |
| 1:B:180:TYR:CE2 | 1:D:28:LEU:C[2_546] | 1.94 | 0.26 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:335:ALA:C | 1:C:370:GLU:O[2_546] | 1.94 | 0.26 |
| 1:A:107:ASP:O | 1:A:248:ASN:ND2[2_556] | 1.94 | 0.26 |
| 1:A:111:LYS:CE | 1:A:241:TRP:CE3[2_556] | 1.94 | 0.26 |
| 1:B:174:ASP:O | 1:D:18:LEU:N[2_546] | 1.94 | 0.26 |
| 1:B:312:THR:CA | 1:D:261:TYR:OH[2_546] | 1.94 | 0.26 |
| 1:B:41:TYR:C | 1:D:347:ILE:N[2_546] | 1.94 | 0.26 |
| 1:B:262:LYS:C | 1:D:314:PHE:CB[2_546] | 1.94 | 0.26 |
| 1:B:332:ALA:O | 1:C:370:GLU:N[2_546] | 1.94 | 0.26 |
| 1:B:312:THR:N | 1:D:266:PRO:CB[2_546] | 1.94 | 0.26 |
| 1:B:178:ILE:CG1 | 1:D:18:LEU:CD2[2_546] | 1.94 | 0.26 |
| 1:B:315:TYR:CD2 | 1:D:23:GLY:N[2_546] | 1.94 | 0.26 |
| 1:B:53:TYR:CB | 1:D:65:LEU:N[2_546] | 1.94 | 0.26 |
| 1:B:266:PRO:C | 1:D:183:HIS:CB[2_546] | 1.94 | 0.26 |
| 1:B:39:VAL:CA | 1:D:345:HIS:CD2[2_546] | 1.94 | 0.26 |
| 1:B:333:LEU:N | 1:C:368:TYR:CA[2_546] | 1.94 | 0.26 |
| 1:B:56:LEU:CA | 1:D:121:ILE:CB[2_546] | 1.94 | 0.26 |
| 1:B:304:SER:CA | 1:D:256:PHE:CA[2_546] | 1.95 | 0.25 |
| 1:B:31:ARG:CA | 1:D:44:TYR:CD2[2_546] | 1.95 | 0.25 |
| 1:B:265:ASP:CA | 1:D:267:ARG:NH2[2_546] | 1.95 | 0.25 |
| 1:B:22:ASP:CG | 1:D:320:PHE:CG[2_546] | 1.95 | 0.25 |
| 1:A:286:ARG:CD | 1:B:251:ASN:ND2[2_546] | 1.95 | 0.25 |
| 1:B:296:GLU:N | 1:D:262:LYS:CE[2_546] | 1.95 | 0.25 |
| 1:B:42:GLY:CA | 1:D:344:ALA:CA[2_546] | 1.95 | 0.25 |
| 1:B:315:TYR:OH | 1:D:260:VAL:CA[2_546] | 1.95 | 0.25 |
| 1:B:23:GLY:O | 1:D:315:TYR:C[2_546] | 1.95 | 0.25 |
| 1:B:315:TYR:CZ | 1:D:260:VAL:C[2_546] | 1.95 | 0.25 |
| 1:B:30:TYR:C | 1:D:44:TYR:CD1[2_546] | 1.95 | 0.25 |
| 1:B:300:ILE:CG2 | 1:D:257:GLY:CA[2_546] | 1.95 | 0.25 |
| 1:B:58:THR:CB | 1:D:115:ASN:CB[2_546] | 1.95 | 0.25 |
| 1:B:304:SER:O | 1:D:256:PHE:CD1[2_546] | 1.95 | 0.25 |
| 1:B:302:GLN:CB | 1:D:303:PHE:O[2_546] | 1.95 | 0.25 |
| 1:B:47:THR:O | 1:D:50:LEU:N[2_546] | 1.95 | 0.25 |
| 1:B:27:ILE:O | 1:D:176:ALA:O[2_546] | 1.95 | 0.25 |
| 1:B:342:TRP:CZ3 | 1:C:371:TYR:CB[2_546] | 1.95 | 0.25 |
| 1:B:18:LEU:CA | 1:D:44:TYR:N[2_546] | 1.95 | 0.25 |
| 1:B:36:GLU:C | 1:D:342:TRP:N[2_546] | 1.95 | 0.25 |
| 1:B:336:LEU:N | 1:C:370:GLU:N[2_546] | 1.95 | 0.25 |
| 1:B:309:TYR:N | 1:D:310:PRO:N[2_546] | 1.95 | 0.25 |
| 1:B:256:PHE:N | 1:D:264:TYR:CA[2_546] | 1.95 | 0.25 |
| 1:B:172:ALA:C | 1:C:363:TYR:CE1[2_546] | 1.95 | 0.25 |
| 1:B:336:LEU:CD2 | 1:C:369:GLN:CG[2_546] | 1.95 | 0.25 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:256:PHE:O | 1:D:264:TYR:CA[2_546] | 1.95 | 0.25 |
| 1:B:333:LEU:CB | 1:C:367:GLU:C[2_546] | 1.95 | 0.25 |
| 1:B:183:HIS:CA | 1:D:39:VAL:CA[2_546] | 1.95 | 0.25 |
| 1:B:335:ALA:C | 1:C:371:TYR:N[2_546] | 1.95 | 0.25 |
| 1:B:336:LEU:CB | 1:C:369:GLN:CA[2_546] | 1.95 | 0.25 |
| 1:B:171:ASN:OD1 | 1:D:16:THR:CA[2_546] | 1.95 | 0.25 |
| 1:A:237:ARG:NH1 | 1:B:217:LEU:O[2_546] | 1.95 | 0.25 |
| 1:A:110:PHE:N | 1:A:249:GLN:CB[2_556] | 1.95 | 0.25 |
| 1:B:226:PHE:CG | 1:D:25:LYS:CD[2_546] | 1.95 | 0.25 |
| 1:B:267:ARG:CG | 1:D:28:LEU:CG[2_546] | 1.96 | 0.24 |
| 1:B:21:ILE:N | 1:D:176:ALA:CB[2_546] | 1.96 | 0.24 |
| 1:B:20:PHE:CA | 1:D:177:LEU:N[2_546] | 1.96 | 0.24 |
| 1:B:171:ASN:CA | 1:D:15:VAL:C[2_546] | 1.96 | 0.24 |
| 1:B:315:TYR:CA | 1:D:22:ASP:O[2_546] | 1.96 | 0.24 |
| 1:B:320:PHE:CD2 | 1:C:367:GLU:O[2_546] | 1.96 | 0.24 |
| 1:A:290:GLU:OE1 | 1:B:245:LYS:NZ[2_546] | 1.96 | 0.24 |
| 1:B:270:ILE:N | 1:D:183:HIS:C[2_546] | 1.96 | 0.24 |
| 1:B:260:VAL:N | 1:D:271:PHE:N[2_546] | 1.96 | 0.24 |
| 1:B:58:THR:CA | 1:D:115:ASN:CG[2_546] | 1.96 | 0.24 |
| 1:B:189:THR:C | 1:D:41:TYR:CD2[2_546] | 1.96 | 0.24 |
| 1:B:320:PHE:O | 1:C:367:GLU:OE1[2_546] | 1.96 | 0.24 |
| 1:B:309:TYR:CA | 1:D:311:ASN:N[2_546] | 1.96 | 0.24 |
| 1:B:189:THR:CB | 1:D:40:ASN:C[2_546] | 1.96 | 0.24 |
| 1:B:296:GLU:OE1 | 1:D:259:ARG:O[2_546] | 1.96 | 0.24 |
| 1:B:306:LYS:CD | 1:D:299:GLY:CA[2_546] | 1.96 | 0.24 |
| 1:B:180:TYR:CB | 1:D:33:TYR:C[2_546] | 1.96 | 0.24 |
| 1:B:58:THR:CA | 1:D:115:ASN:CB[2_546] | 1.96 | 0.24 |
| 1:B:258:HIS:C | 1:D:268:ALA:O[2_546] | 1.96 | 0.24 |
| 1:B:183:HIS:N | 1:D:38:LEU:C[2_546] | 1.96 | 0.24 |
| 1:A:362:LEU:CD1 | 1:D:169:GLU:N[2_546] | 1.96 | 0.24 |
| 1:B:59:LYS:N | 1:D:115:ASN:ND2[2_546] | 1.96 | 0.24 |
| 1:B:334:PHE:CE2 | 1:D:37:ASP:OD1[2_546] | 1.96 | 0.24 |
| 1:B:337:SER:O | 1:D:33:TYR:CD1[2_546] | 1.96 | 0.24 |
| 1:B:53:TYR:O | 1:D:65:LEU:N[2_546] | 1.96 | 0.24 |
| 1:B:311:ASN:CB | 1:D:265:ASP:CA[2_546] | 1.96 | 0.24 |
| 1:B:51:MET:CE | 1:D:46:GLU:C[2_546] | 1.96 | 0.24 |
| 1:B:120:ALA:C | 1:D:58:THR:CG2[2_546] | 1.96 | 0.24 |
| 1:B:309:TYR:CD2 | 1:D:311:ASN:CB[2_546] | 1.96 | 0.24 |
| 1:B:19:THR:CG2 | 1:D:178:ILE:CD1[2_546] | 1.96 | 0.24 |
| 1:B:174:ASP:N | 1:D:17:ASN:ND2[2_546] | 1.96 | 0.24 |
| 1:A:111:LYS:CA | 1:A:245:LYS:CE[2_556] | 1.96 | 0.24 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:24:GLU:CB | 1:D:316:SER:O[2_546] | 1.97 | 0.23 |
| 1:A:286:ARG:NH1 | 1:B:250:LYS:C[2_546] | 1.97 | 0.23 |
| 1:B:320:PHE:CD2 | 1:C:367:GLU:CA[2_546] | 1.97 | 0.23 |
| 1:B:21:ILE:CB | 1:D:176:ALA:N[2_546] | 1.97 | 0.23 |
| 1:B:277:THR:OG1 | 1:C:362:LEU:N[2_546] | 1.97 | 0.23 |
| 1:B:271:PHE:CG | 1:D:21:ILE:CG1[2_546] | 1.97 | 0.23 |
| 1:B:225:ALA:CA | 1:D:25:LYS:CA[2_546] | 1.97 | 0.23 |
| 1:B:334:PHE:CZ | 1:D:37:ASP:CG[2_546] | 1.97 | 0.23 |
| 1:B:180:TYR:CE1 | 1:D:29:ARG:CA[2_546] | 1.97 | 0.23 |
| 1:B:257:GLY:CA | 1:D:264:TYR:CZ[2_546] | 1.97 | 0.23 |
| 1:B:261:TYR:N | 1:D:271:PHE:CB[2_546] | 1.97 | 0.23 |
| 1:B:174:ASP:CA | 1:D:17:ASN:O[2_546] | 1.97 | 0.23 |
| 1:B:173:MET:SD | 1:C:366:PRO:N[2_546] | 1.97 | 0.23 |
| 1:B:331:THR:O | 1:C:368:TYR:CD1[2_546] | 1.97 | 0.23 |
| 1:A:109:ASN:O | 1:A:245:LYS:O[2_556] | 1.97 | 0.23 |
| 1:B:270:ILE:CG1 | 1:D:184:GLU:N[2_546] | 1.97 | 0.23 |
| 1:B:270:ILE:CG1 | 1:D:183:HIS:O[2_546] | 1.97 | 0.23 |
| 1:B:303:PHE:CB | 1:D:256:PHE:CE2[2_546] | 1.97 | 0.23 |
| 1:B:276:LEU:CB | 1:C:360:ARG:CD[2_546] | 1.97 | 0.23 |
| 1:B:332:ALA:C | 1:C:368:TYR:CG[2_546] | 1.97 | 0.23 |
| 1:B:308:ILE:C | 1:D:310:PRO:CD[2_546] | 1.97 | 0.23 |
| 1:B:335:ALA:CB | 1:C:370:GLU:C[2_546] | 1.97 | 0.23 |
| 1:B:36:GLU:OE1 | 1:D:338:ARG:CZ[2_546] | 1.97 | 0.23 |
| 1:B:124:ILE:CG1 | 1:D:56:LEU:O[2_546] | 1.97 | 0.23 |
| 1:B:25:LYS:CE | 1:D:330:PHE:CB[2_546] | 1.97 | 0.23 |
| 1:B:34:ASN:CA | 1:D:338:ARG:CA[2_546] | 1.97 | 0.23 |
| 1:B:301:LYS:C | 1:D:303:PHE:CD2[2_546] | 1.97 | 0.23 |
| 1:A:362:LEU:CG | 1:D:167:THR:C[2_546] | 1.97 | 0.23 |
| 1:B:305:SER:C | 1:D:253:LEU:CG[2_546] | 1.97 | 0.23 |
| 1:B:18:LEU:CA | 1:D:45:GLU:OE1[2_546] | 1.97 | 0.23 |
| 1:B:28:LEU:N | 1:D:180:TYR:CA[2_546] | 1.97 | 0.23 |
| 1:B:305:SER:N | 1:D:253:LEU:CD2[2_546] | 1.97 | 0.23 |
| 1:B:296:GLU:CG | 1:D:262:LYS:NZ[2_546] | 1.97 | 0.23 |
| 1:A:366:PRO:CG | 1:D:152:PHE:CG[2_546] | 1.97 | 0.23 |
| 1:B:258:HIS:CE1 | 1:D:270:ILE:CG1[2_546] | 1.98 | 0.22 |
| 1:B:120:ALA:CA | 1:D:58:THR:CB[2_546] | 1.98 | 0.22 |
| 1:B:41:TYR:CZ | 1:D:192:ALA:CB[2_546] | 1.98 | 0.22 |
| 1:B:311:ASN:O | 1:D:261:TYR:CZ[2_546] | 1.98 | 0.22 |
| 1:B:262:LYS:CG | 1:D:315:TYR:CD2[2_546] | 1.98 | 0.22 |
| 1:A:365:GLY:N | 1:D:153:ALA:C[2_546] | 1.98 | 0.22 |
| 1:B:127:MET:CE | 1:C:370:GLU:CD[2_546] | 1.98 | 0.22 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:332:ALA:CA | 1:C:368:TYR:CZ[2_546] | 1.98 | 0.22 |
| 1:B:34:ASN:C | 1:D:338:ARG:C[2_546] | 1.98 | 0.22 |
| 1:B:302:GLN:NE2 | 1:D:301:LYS:C[2_546] | 1.98 | 0.22 |
| 1:B:262:LYS:CB | 1:D:314:PHE:O[2_546] | 1.98 | 0.22 |
| 1:A:110:PHE:CB | 1:A:249:GLN:CD[2_556] | 1.98 | 0.22 |
| 1:B:35:ILE:CG2 | 1:D:181:THR:C[2_546] | 1.98 | 0.22 |
| 1:B:168:ASP:OD1 | 1:C:4:VAL:CG2[2_546] | 1.98 | 0.22 |
| 1:B:18:LEU:CB | 1:D:44:TYR:N[2_546] | 1.98 | 0.22 |
| 1:B:189:THR:CG2 | 1:D:41:TYR:O[2_546] | 1.98 | 0.22 |
| 1:A:286:ARG:CZ | 1:B:245:LYS:O[2_546] | 1.98 | 0.22 |
| 1:B:186:PRO:CB | 1:D:40:ASN:CB[2_546] | 1.98 | 0.22 |
| 1:B:315:TYR:CG | 1:D:260:VAL:CG1[2_546] | 1.98 | 0.22 |
| 1:B:188:SER:CB | 1:D:41:TYR:CZ[2_546] | 1.98 | 0.22 |
| 1:B:29:ARG:CD | 1:D:337:SER:N[2_546] | 1.98 | 0.22 |
| 1:B:340:LEU:CD2 | 1:D:50:LEU:N[2_546] | 1.98 | 0.22 |
| 1:B:181:THR:CA | 1:D:38:LEU:CD2[2_546] | 1.98 | 0.22 |
| 1:B:47:THR:CA | 1:D:48:ILE:O[2_546] | 1.98 | 0.22 |
| 1:B:180:TYR:O | 1:D:38:LEU:CG[2_546] | 1.98 | 0.22 |
| 1:B:186:PRO:CA | 1:D:40:ASN:CB[2_546] | 1.98 | 0.22 |
| 1:B:44:TYR:O | 1:D:50:LEU:O[2_546] | 1.98 | 0.22 |
| 1:B:301:LYS:O | 1:D:303:PHE:CD1[2_546] | 1.98 | 0.22 |
| 1:B:121:ILE:CD1 | 1:D:61:GLU:CD[2_546] | 1.98 | 0.22 |
| 1:B:46:GLU:C | 1:D:52:LEU:C[2_546] | 1.98 | 0.22 |
| 1:B:33:TYR:CD2 | 1:D:124:ILE:CB[2_546] | 1.98 | 0.22 |
| 1:A:286:ARG:CG | 1:B:251:ASN:OD1[2_546] | 1.98 | 0.22 |
| 1:B:278:LEU:CD2 | 1:C:362:LEU:CD1[2_546] | 1.98 | 0.22 |
| 1:B:258:HIS:CA | 1:D:268:ALA:C[2_546] | 1.98 | 0.22 |
| 1:B:181:THR:CA | 1:D:38:LEU:CD1[2_546] | 1.98 | 0.22 |
| 1:B:24:GLU:CA | 1:D:316:SER:CA[2_546] | 1.98 | 0.22 |
| 1:B:35:ILE:C | 1:D:181:THR:C[2_546] | 1.98 | 0.22 |
| 1:B:39:VAL:CG2 | 1:D:182:ASP:OD2[2_546] | 1.98 | 0.22 |
| 1:B:333:LEU:CA | 1:C:368:TYR:CG[2_546] | 1.98 | 0.22 |
| 1:B:51:MET:CE | 1:D:46:GLU:CA[2_546] | 1.98 | 0.22 |
| 1:B:49:TYR:CA | 1:D:49:TYR:CD1[2_546] | 1.98 | 0.22 |
| 1:B:333:LEU:CG | 1:C:368:TYR:CA[2_546] | 1.98 | 0.22 |
| 1:B:46:GLU:CA | 1:D:52:LEU:CB[2_546] | 1.98 | 0.22 |
| 1:B:338:ARG:N | 1:D:33:TYR:CD2[2_546] | 1.98 | 0.22 |
| 1:B:226:PHE:CD2 | 1:D:25:LYS:NZ[2_546] | 1.98 | 0.22 |
| 1:B:41:TYR:CA | 1:D:346:ILE:CA[2_546] | 1.99 | 0.21 |
| 1:A:286:ARG:NE | 1:B:251:ASN:N[2_546] | 1.99 | 0.21 |
| 1:B:41:TYR:N | 1:D:342:TRP:O[2_546] | 1.99 | 0.21 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:242:PHE:CE1 | 1:D:305:SER:C[2_546] | 1.99 | 0.21 |
| 1:B:345:HIS:CG | 1:D:41:TYR:O[2_546] | 1.99 | 0.21 |
| 1:B:30:TYR:CD1 | 1:D:47:THR:CB[2_546] | 1.99 | 0.21 |
| 1:B:242:PHE:CE2 | 1:D:305:SER:N[2_546] | 1.99 | 0.21 |
| 1:B:40:ASN:N | 1:D:345:HIS:CB[2_546] | 1.99 | 0.21 |
| 1:B:242:PHE:CZ | 1:D:305:SER:N[2_546] | 1.99 | 0.21 |
| 1:A:364:VAL:CA | 1:D:153:ALA:C[2_546] | 1.99 | 0.21 |
| 1:B:242:PHE:CZ | 1:D:305:SER:C[2_546] | 1.99 | 0.21 |
| 1:B:168:ASP:CB | 1:C:362:LEU:CD2[2_546] | 1.99 | 0.21 |
| 1:B:272:LYS:CB | 1:D:260:VAL:CG2[2_546] | 1.99 | 0.21 |
| 1:B:34:ASN:N | 1:D:339:THR:N[2_546] | 1.99 | 0.21 |
| 1:B:333:LEU:CD1 | 1:C:368:TYR:N[2_546] | 1.99 | 0.21 |
| 1:B:175:LYS:CB | 1:D:18:LEU:C[2_546] | 1.99 | 0.21 |
| 1:B:58:THR:OG1 | 1:D:115:ASN:CG[2_546] | 1.99 | 0.21 |
| 1:B:313:ASP:O | 1:D:25:LYS:C[2_546] | 1.99 | 0.21 |
| 1:B:188:SER:C | 1:D:41:TYR:OH[2_546] | 1.99 | 0.21 |
| 1:B:57:PRO:C | 1:D:118:GLU:CB[2_546] | 1.99 | 0.21 |
| 1:B:51:MET:SD | 1:D:45:GLU:C[2_546] | 1.99 | 0.21 |
| 1:B:183:HIS:NE2 | 1:D:179:LEU:CG[2_546] | 1.99 | 0.21 |
| 1:B:267:ARG:CB | 1:D:28:LEU:CD2[2_546] | 1.99 | 0.21 |
| 1:B:189:THR:CA | 1:D:41:TYR:CB[2_546] | 1.99 | 0.21 |
| 1:B:302:GLN:OE1 | 1:D:303:PHE:CA[2_546] | 1.99 | 0.21 |
| 1:B:61:GLU:CG | 1:D:118:GLU:CD[2_546] | 1.99 | 0.21 |
| 1:B:256:PHE:CD2 | 1:D:309:TYR:CA[2_546] | 1.99 | 0.21 |
| 1:B:18:LEU:CB | 1:D:43:SER:OG[2_546] | 1.99 | 0.21 |
| 1:B:185:VAL:CA | 1:D:39:VAL:O[2_546] | 1.99 | 0.21 |
| 1:A:109:ASN:CB | 1:A:249:GLN:N[2_556] | 1.99 | 0.21 |
| 1:B:265:ASP:OD1 | 1:D:267:ARG:CG[2_546] | 1.99 | 0.21 |
| 1:B:258:HIS:CD2 | 1:D:269:LYS:C[2_546] | 2.00 | 0.20 |
| 1:B:276:LEU:CA | 1:C:360:ARG:NE[2_546] | 2.00 | 0.20 |
| 1:B:59:LYS:CA | 1:D:114:GLU:C[2_546] | 2.00 | 0.20 |
| 1:B:256:PHE:CA | 1:D:263:THR:C[2_546] | 2.00 | 0.20 |
| 1:B:260:VAL:CA | 1:D:271:PHE:CB[2_546] | 2.00 | 0.20 |
| 1:A:290:GLU:OE2 | 1:B:251:ASN:CG[2_546] | 2.00 | 0.20 |
| 1:B:27:ILE:CB | 1:D:180:TYR:CD1[2_546] | 2.00 | 0.20 |
| 1:A:111:LYS:N | 1:A:245:LYS:CD[2_556] | 2.00 | 0.20 |
| 1:B:21:ILE:CG2 | 1:D:179:LEU:CD1[2_546] | 2.00 | 0.20 |
| 1:B:51:MET:SD | 1:D:46:GLU:C[2_546] | 2.00 | 0.20 |
| 1:B:182:ASP:OD2 | 1:D:43:SER:N[2_546] | 2.00 | 0.20 |
| 1:B:338:ARG:NH2 | 1:D:38:LEU:N[2_546] | 2.00 | 0.20 |
| 1:B:298:LEU:C | 1:D:306:LYS:O[2_546] | 2.00 | 0.20 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:362:LEU:CG | 1:D:170:ILE:N[2_546] | 2.00 | 0.20 |
| 1:B:262:LYS:NZ | 1:D:315:TYR:CG[2_546] | 2.00 | 0.20 |
| 1:B:52:LEU:CA | 1:D:62:LEU:CA[2_546] | 2.00 | 0.20 |
| 1:B:33:TYR:N | 1:D:44:TYR:OH[2_546] | 2.00 | 0.20 |
| 1:B:29:ARG:CG | 1:D:177:LEU:CD2[2_546] | 2.00 | 0.20 |
| 1:B:51:MET:CB | 1:D:46:GLU:O[2_546] | 2.00 | 0.20 |
| 1:B:24:GLU:N | 1:D:316:SER:N[2_546] | 2.00 | 0.20 |
| 1:B:306:LYS:CA | 1:D:296:GLU:CA[2_546] | 2.00 | 0.20 |
| 1:B:312:THR:CG2 | 1:D:28:LEU:CB[2_546] | 2.00 | 0.20 |
| 1:B:308:ILE:CG2 | 1:D:310:PRO:CG[2_546] | 2.00 | 0.20 |
| 1:B:112:TRP:CD2 | 1:D:59:LYS:NZ[2_546] | 2.00 | 0.20 |
| 1:B:269:LYS:N | 1:D:183:HIS:ND1[2_546] | 2.00 | 0.20 |
| 1:B:315:TYR:C | 1:D:22:ASP:CB[2_546] | 2.00 | 0.20 |
| 1:B:41:TYR:O | 1:D:347:ILE:CA[2_546] | 2.00 | 0.20 |
| 1:A:369:GLN:OE1 | 1:D:125:ALA:N[2_546] | 2.00 | 0.20 |
| 1:B:186:PRO:CG | 1:D:36:GLU:O[2_546] | 2.00 | 0.20 |
| 1:B:316:SER:C | 1:D:20:PHE:CE2[2_546] | 2.00 | 0.20 |
| 1:B:23:GLY:CA | 1:D:316:SER:CA[2_546] | 2.00 | 0.20 |
| 1:A:368:TYR:CE1 | 1:D:336:LEU:CA[2_546] | 2.00 | 0.20 |
| 1:B:174:ASP:O | 1:D:17:ASN:O[2_546] | 2.00 | 0.20 |
| 1:B:42:GLY:N | 1:D:345:HIS:N[2_546] | 2.00 | 0.20 |
| 1:B:226:PHE:CD1 | 1:D:25:LYS:CE[2_546] | 2.01 | 0.19 |
| 1:B:28:LEU:CB | 1:D:179:LEU:N[2_546] | 2.01 | 0.19 |
| 1:B:59:LYS:CB | 1:D:114:GLU:CA[2_546] | 2.01 | 0.19 |
| 1:A:365:GLY:CA | 1:D:153:ALA:N[2_546] | 2.01 | 0.19 |
| 1:B:29:ARG:CA | 1:D:177:LEU:O[2_546] | 2.01 | 0.19 |
| 1:B:22:ASP:OD2 | 1:D:320:PHE:CZ[2_546] | 2.01 | 0.19 |
| 1:B:117:LYS:CG | 1:D:61:GLU:CA[2_546] | 2.01 | 0.19 |
| 1:B:17:ASN:CG | 1:D:152:PHE:N[2_546] | 2.01 | 0.19 |
| 1:B:272:LYS:CD | 1:D:260:VAL:CB[2_546] | 2.01 | 0.19 |
| 1:B:51:MET:N | 1:D:49:TYR:N[2_546] | 2.01 | 0.19 |
| 1:B:44:TYR:CE2 | 1:D:54:GLY:C[2_546] | 2.01 | 0.19 |
| 1:B:53:TYR:CE2 | 1:D:64:ASP:OD2[2_546] | 2.01 | 0.19 |
| 1:B:173:MET:C | 1:D:17:ASN:CA[2_546] | 2.01 | 0.19 |
| 1:B:332:ALA:O | 1:C:369:GLN:N[2_546] | 2.01 | 0.19 |
| 1:B:54:GLY:C | 1:D:65:LEU:O[2_546] | 2.01 | 0.19 |
| 1:B:247:VAL:CG2 | 1:D:305:SER:CB[2_546] | 2.01 | 0.19 |
| 1:B:17:ASN:CA | 1:D:151:SER:CB[2_546] | 2.01 | 0.19 |
| 1:A:369:GLN:CD | 1:D:125:ALA:N[2_546] | 2.01 | 0.19 |
| 1:B:345:HIS:CD2 | 1:D:41:TYR:C[2_546] | 2.01 | 0.19 |
| 1:B:38:LEU:CD2 | 1:D:340:LEU:CA[2_546] | 2.01 | 0.19 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:24:GLU:OE1 | 1:D:320:PHE:N[2_546] | 2.01 | 0.19 |
| 1:B:180:TYR:N | 1:D:30:TYR:CA[2_546] | 2.01 | 0.19 |
| 1:B:253:LEU:CA | 1:D:309:TYR:OH[2_546] | 2.01 | 0.19 |
| 1:B:314:PHE:CZ | 1:D:262:LYS:N[2_546] | 2.01 | 0.19 |
| 1:B:273:LYS:CD | 1:D:185:VAL:CG2[2_546] | 2.01 | 0.19 |
| 1:B:45:GLU:O | 1:D:52:LEU:C[2_546] | 2.01 | 0.19 |
| 1:B:330:PHE:O | 1:C:368:TYR:CG[2_546] | 2.01 | 0.19 |
| 1:B:18:LEU:CD1 | 1:D:43:SER:CB[2_546] | 2.01 | 0.19 |
| 1:B:271:PHE:CA | 1:D:21:ILE:CD1[2_546] | 2.01 | 0.19 |
| 1:A:363:TYR:N | 1:D:170:ILE:CA[2_546] | 2.01 | 0.19 |
| 1:B:30:TYR:OH | 1:D:30:TYR:CD1[2_546] | 2.01 | 0.19 |
| 1:B:34:ASN:CA | 1:D:338:ARG:C[2_546] | 2.01 | 0.19 |
| 1:A:368:TYR:N | 1:D:336:LEU:CD2[2_546] | 2.01 | 0.19 |
| 1:B:333:LEU:CG | 1:C:368:TYR:CB[2_546] | 2.01 | 0.19 |
| 1:B:320:PHE:CA | 1:C:367:GLU:CG[2_546] | 2.02 | 0.18 |
| 1:B:351:GLU:OE2 | 1:D:63:ASN:ND2[2_546] | 2.02 | 0.18 |
| 1:B:265:ASP:CB | 1:D:267:ARG:CG[2_546] | 2.02 | 0.18 |
| 1:B:189:THR:N | 1:D:41:TYR:CE1[2_546] | 2.02 | 0.18 |
| 1:B:44:TYR:CD1 | 1:D:31:ARG:CG[2_546] | 2.02 | 0.18 |
| 1:B:255:GLY:O | 1:D:264:TYR:C[2_546] | 2.02 | 0.18 |
| 1:B:299:GLY:C | 1:D:308:ILE:N[2_546] | 2.02 | 0.18 |
| 1:B:261:TYR:N | 1:D:268:ALA:O[2_546] | 2.02 | 0.18 |
| 1:B:24:GLU:N | 1:D:316:SER:CB[2_546] | 2.02 | 0.18 |
| 1:B:180:TYR:OH | 1:D:28:LEU:N[2_546] | 2.02 | 0.18 |
| 1:B:304:SER:N | 1:D:256:PHE:CE2[2_546] | 2.02 | 0.18 |
| 1:B:43:SER:C | 1:D:51:MET:O[2_546] | 2.02 | 0.18 |
| 1:A:109:ASN:C | 1:A:249:GLN:CA[2_556] | 2.02 | 0.18 |
| 1:B:40:ASN:CG | 1:D:189:THR:OG1[2_546] | 2.02 | 0.18 |
| 1:B:334:PHE:N | 1:C:368:TYR:CE1[2_546] | 2.02 | 0.18 |
| 1:B:38:LEU:CD2 | 1:D:340:LEU:C[2_546] | 2.02 | 0.18 |
| 1:B:21:ILE:CD1 | 1:D:175:LYS:C[2_546] | 2.02 | 0.18 |
| 1:B:182:ASP:CG | 1:D:38:LEU:O[2_546] | 2.02 | 0.18 |
| 1:B:35:ILE:N | 1:D:337:SER:O[2_546] | 2.02 | 0.18 |
| 1:B:30:TYR:OH | 1:D:30:TYR:CE1[2_546] | 2.02 | 0.18 |
| 1:B:47:THR:CB | 1:D:50:LEU:C[2_546] | 2.02 | 0.18 |
| 1:B:36:GLU:O | 1:D:342:TRP:N[2_546] | 2.02 | 0.18 |
| 1:B:174:ASP:CB | 1:D:17:ASN:CA[2_546] | 2.02 | 0.18 |
| 1:A:237:ARG:CZ | 1:B:217:LEU:O[2_546] | 2.02 | 0.18 |
| 1:B:19:THR:CG2 | 1:D:178:ILE:CB[2_546] | 2.02 | 0.18 |
| 1:B:41:TYR:C | 1:D:343:LEU:O[2_546] | 2.02 | 0.18 |
| 1:B:304:SER:C | 1:D:256:PHE:CG[2_546] | 2.02 | 0.18 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:29:ARG:NH2 | 1:D:336:LEU:CB[2_546] | 2.02 | 0.18 |
| 1:B:41:TYR:CG | 1:D:346:ILE:CG2[2_546] | 2.02 | 0.18 |
| 1:B:345:HIS:CB | 1:D:41:TYR:O[2_546] | 2.02 | 0.18 |
| 1:B:117:LYS:NZ | 1:D:64:ASP:N[2_546] | 2.02 | 0.18 |
| 1:B:22:ASP:CB | 1:D:320:PHE:CE1[2_546] | 2.02 | 0.18 |
| 1:A:108:LYS:CA | 1:A:248:ASN:ND2[2_556] | 2.02 | 0.18 |
| 1:A:368:TYR:C | 1:D:336:LEU:CD1[2_546] | 2.02 | 0.18 |
| 1:B:30:TYR:C | 1:D:44:TYR:CE1[2_546] | 2.02 | 0.18 |
| 1:B:336:LEU:CA | 1:C:369:GLN:CG[2_546] | 2.02 | 0.18 |
| 1:B:127:MET:CE | 1:C:370:GLU:OE2[2_546] | 2.02 | 0.18 |
| 1:B:167:THR:C | 1:D:15:VAL:CG2[2_546] | 2.02 | 0.18 |
| 1:B:25:LYS:N | 1:D:316:SER:OG[2_546] | 2.03 | 0.17 |
| 1:B:117:LYS:CA | 1:D:60:LYS:N[2_546] | 2.03 | 0.17 |
| 1:B:37:ASP:O | 1:D:342:TRP:CA[2_546] | 2.03 | 0.17 |
| 1:B:177:LEU:C | 1:D:30:TYR:O[2_546] | 2.03 | 0.17 |
| 1:B:229:PHE:CD1 | 1:D:24:GLU:OE1[2_546] | 2.03 | 0.17 |
| 1:B:115:ASN:ND2 | 1:D:60:LYS:CD[2_546] | 2.03 | 0.17 |
| 1:B:338:ARG:NE | 1:D:38:LEU:CA[2_546] | 2.03 | 0.17 |
| 1:B:33:TYR:CG | 1:D:124:ILE:CD1[2_546] | 2.03 | 0.17 |
| 1:B:340:LEU:CA | 1:D:56:LEU:CG[2_546] | 2.03 | 0.17 |
| 1:B:308:ILE:CD1 | 1:D:296:GLU:OE2[2_546] | 2.03 | 0.17 |
| 1:B:272:LYS:NZ | 1:D:260:VAL:N[2_546] | 2.03 | 0.17 |
| 1:B:20:PHE:N | 1:D:177:LEU:CB[2_546] | 2.03 | 0.17 |
| 1:B:309:TYR:CG | 1:D:311:ASN:ND2[2_546] | 2.03 | 0.17 |
| 1:B:295:LEU:CB | 1:D:262:LYS:CG[2_546] | 2.03 | 0.17 |
| 1:B:334:PHE:CB | 1:D:34:ASN:CG[2_546] | 2.03 | 0.17 |
| 1:B:112:TRP:CE3 | 1:D:59:LYS:NZ[2_546] | 2.03 | 0.17 |
| 1:B:65:LEU:CD1 | 1:D:53:TYR:CG[2_546] | 2.03 | 0.17 |
| 1:B:37:ASP:OD2 | 1:D:339:THR:N[2_546] | 2.03 | 0.17 |
| 1:B:59:LYS:CB | 1:D:115:ASN:CA[2_546] | 2.03 | 0.17 |
| 1:B:338:ARG:CD | 1:D:37:ASP:C[2_546] | 2.03 | 0.17 |
| 1:B:303:PHE:CD2 | 1:D:300:ILE:CA[2_546] | 2.03 | 0.17 |
| 1:B:305:SER:CB | 1:D:253:LEU:CD1[2_546] | 2.03 | 0.17 |
| 1:B:306:LYS:O | 1:D:296:GLU:CA[2_546] | 2.03 | 0.17 |
| 1:B:38:LEU:C | 1:D:344:ALA:CB[2_546] | 2.03 | 0.17 |
| 1:A:109:ASN:O | 1:A:249:GLN:C[2_556] | 2.03 | 0.17 |
| 1:B:337:SER:CA | 1:D:33:TYR:CE1[2_546] | 2.03 | 0.17 |
| 1:B:338:ARG:CZ | 1:D:37:ASP:CA[2_546] | 2.03 | 0.17 |
| 1:B:35:ILE:O | 1:D:181:THR:O[2_546] | 2.03 | 0.17 |
| 1:B:265:ASP:CB | 1:D:267:ARG:CD[2_546] | 2.03 | 0.17 |
| 1:B:51:MET:CG | 1:D:46:GLU:CA[2_546] | 2.03 | 0.17 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:28:LEU:CD2 | 1:D:30:TYR:OH[2_546] | 2.03 | 0.17 |
| 1:B:36:GLU:O | 1:D:341:GLY:C[2_546] | 2.03 | 0.17 |
| 1:B:40:ASN:N | 1:D:345:HIS:CG[2_546] | 2.03 | 0.17 |
| 1:B:320:PHE:CB | 1:C:367:GLU:CB[2_546] | 2.03 | 0.17 |
| 1:B:288:TYR:O | 1:D:24:GLU:OE2[2_546] | 2.03 | 0.17 |
| 1:A:109:ASN:C | 1:A:245:LYS:O[2_556] | 2.03 | 0.17 |
| 1:B:176:ALA:N | 1:D:18:LEU:C[2_546] | 2.04 | 0.16 |
| 1:B:19:THR:OG1 | 1:D:43:SER:C[2_546] | 2.04 | 0.16 |
| 1:B:51:MET:C | 1:D:62:LEU:CD1[2_546] | 2.04 | 0.16 |
| 1:B:40:ASN:C | 1:D:345:HIS:CA[2_546] | 2.04 | 0.16 |
| 1:B:314:PHE:O | 1:D:23:GLY:CA[2_546] | 2.04 | 0.16 |
| 1:B:33:TYR:OH | 1:D:124:ILE:CA[2_546] | 2.04 | 0.16 |
| 1:B:338:ARG:NE | 1:D:38:LEU:CG[2_546] | 2.04 | 0.16 |
| 1:B:253:LEU:CG | 1:D:309:TYR:CE1[2_546] | 2.04 | 0.16 |
| 1:A:109:ASN:OD1 | 1:A:250:LYS:CB[2_556] | 2.04 | 0.16 |
| 1:B:29:ARG:NE | 1:D:336:LEU:CB[2_546] | 2.04 | 0.16 |
| 1:B:338:ARG:O | 1:C:371:TYR:CZ[2_546] | 2.04 | 0.16 |
| 1:A:368:TYR:CA | 1:D:336:LEU:CG[2_546] | 2.04 | 0.16 |
| 1:B:178:ILE:CB | 1:D:51:MET:CE[2_546] | 2.04 | 0.16 |
| 1:A:237:ARG:CD | 1:B:216:PRO:C[2_546] | 2.04 | 0.16 |
| 1:B:34:ASN:CA | 1:D:339:THR:N[2_546] | 2.04 | 0.16 |
| 1:B:297:GLU:O | 1:D:308:ILE:CD1[2_546] | 2.04 | 0.16 |
| 1:B:334:PHE:CZ | 1:D:34:ASN:O[2_546] | 2.04 | 0.16 |
| 1:B:188:SER:C | 1:D:41:TYR:CD1[2_546] | 2.04 | 0.16 |
| 1:B:28:LEU:CB | 1:D:179:LEU:CA[2_546] | 2.04 | 0.16 |
| 1:B:313:ASP:O | 1:D:26:GLY:C[2_546] | 2.04 | 0.16 |
| 1:B:258:HIS:CD2 | 1:D:267:ARG:O[2_546] | 2.04 | 0.16 |
| 1:B:313:ASP:CB | 1:D:27:ILE:N[2_546] | 2.04 | 0.16 |
| 1:A:280:GLU:CB | 1:B:248:ASN:C[2_546] | 2.04 | 0.16 |
| 1:B:313:ASP:N | 1:D:26:GLY:C[2_546] | 2.04 | 0.16 |
| 1:B:309:TYR:CE2 | 1:D:311:ASN:CG[2_546] | 2.04 | 0.16 |
| 1:B:258:HIS:CD2 | 1:D:270:ILE:CA[2_546] | 2.04 | 0.16 |
| 1:B:334:PHE:CG | 1:D:34:ASN:N[2_546] | 2.04 | 0.16 |
| 1:A:280:GLU:N | 1:B:248:ASN:O[2_546] | 2.04 | 0.16 |
| 1:B:320:PHE:CE1 | 1:C:367:GLU:O[2_546] | 2.04 | 0.16 |
| 1:B:28:LEU:C | 1:D:177:LEU:C[2_546] | 2.04 | 0.16 |
| 1:B:264:TYR:CG | 1:D:258:HIS:ND1[2_546] | 2.04 | 0.16 |
| 1:B:337:SER:CB | 1:D:30:TYR:O[2_546] | 2.04 | 0.16 |
| 1:A:237:ARG:NH1 | 1:B:217:LEU:N[2_546] | 2.04 | 0.16 |
| 1:B:261:TYR:CE2 | 1:D:271:PHE:CD1[2_546] | 2.04 | 0.16 |
| 1:B:257:GLY:N | 1:D:264:TYR:CB[2_546] | 2.04 | 0.16 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:121:ILE:CA | 1:D:55:LYS:CE[2_546] | 2.04 | 0.16 |
| 1:B:46:GLU:CB | 1:D:52:LEU:CA[2_546] | 2.04 | 0.16 |
| 1:B:182:ASP:N | 1:D:38:LEU:CG[2_546] | 2.04 | 0.16 |
| 1:B:36:GLU:OE2 | 1:D:338:ARG:NH1[2_546] | 2.04 | 0.16 |
| 1:B:335:ALA:O | 1:C:371:TYR:CA[2_546] | 2.04 | 0.16 |
| 1:B:179:LEU:N | 1:D:30:TYR:CD2[2_546] | 2.04 | 0.16 |
| 1:A:368:TYR:CA | 1:D:336:LEU:CD2[2_546] | 2.04 | 0.16 |
| 1:A:286:ARG:CD | 1:B:251:ASN:CG[2_546] | 2.04 | 0.16 |
| 1:B:340:LEU:C | 1:D:56:LEU:CD2[2_546] | 2.04 | 0.16 |
| 1:A:368:TYR:CZ | 1:D:127:MET:CG[2_546] | 2.04 | 0.16 |
| 1:B:268:ALA:N | 1:D:183:HIS:NE2[2_546] | 2.04 | 0.16 |
| 1:B:17:ASN:CG | 1:D:150:ASP:C[2_546] | 2.05 | 0.15 |
| 1:B:116:ASP:CB | 1:D:60:LYS:N[2_546] | 2.05 | 0.15 |
| 1:B:263:THR:C | 1:D:311:ASN:O[2_546] | 2.05 | 0.15 |
| 1:B:40:ASN:O | 1:D:345:HIS:C[2_546] | 2.05 | 0.15 |
| 1:A:368:TYR:C | 1:D:127:MET:C[2_546] | 2.05 | 0.15 |
| 1:B:258:HIS:CG | 1:D:269:LYS:CA[2_546] | 2.05 | 0.15 |
| 1:B:272:LYS:NZ | 1:D:259:ARG:CD[2_546] | 2.05 | 0.15 |
| 1:B:258:HIS:O | 1:D:268:ALA:O[2_546] | 2.05 | 0.15 |
| 1:B:311:ASN:O | 1:D:261:TYR:CD2[2_546] | 2.05 | 0.15 |
| 1:B:174:ASP:N | 1:D:17:ASN:N[2_546] | 2.05 | 0.15 |
| 1:B:304:SER:CB | 1:D:256:PHE:N[2_546] | 2.05 | 0.15 |
| 1:B:272:LYS:CB | 1:D:260:VAL:CG1[2_546] | 2.05 | 0.15 |
| 1:B:264:TYR:CE2 | 1:D:258:HIS:CG[2_546] | 2.05 | 0.15 |
| 1:B:299:GLY:C | 1:D:308:ILE:CG1[2_546] | 2.05 | 0.15 |
| 1:B:265:ASP:CA | 1:D:267:ARG:CG[2_546] | 2.05 | 0.15 |
| 1:B:24:GLU:N | 1:D:317:GLY:N[2_546] | 2.05 | 0.15 |
| 1:B:252:ARG:C | 1:D:309:TYR:OH[2_546] | 2.05 | 0.15 |
| 1:A:368:TYR:CE2 | 1:D:127:MET:CG[2_546] | 2.05 | 0.15 |
| 1:A:287:ARG:N | 1:B:251:ASN:ND2[2_546] | 2.05 | 0.15 |
| 1:B:59:LYS:CB | 1:D:114:GLU:N[2_546] | 2.05 | 0.15 |
| 1:B:20:PHE:C | 1:D:176:ALA:CA[2_546] | 2.05 | 0.15 |
| 1:B:226:PHE:CB | 1:D:25:LYS:CG[2_546] | 2.05 | 0.15 |
| 1:B:179:LEU:O | 1:D:30:TYR:CG[2_546] | 2.05 | 0.15 |
| 1:B:121:ILE:CG2 | 1:D:55:LYS:NZ[2_546] | 2.05 | 0.15 |
| 1:B:258:HIS:CB | 1:D:268:ALA:N[2_546] | 2.05 | 0.15 |
| 1:B:342:TRP:CE3 | 1:C:371:TYR:CG[2_546] | 2.05 | 0.15 |
| 1:B:18:LEU:CD2 | 1:D:45:GLU:CA[2_546] | 2.05 | 0.15 |
| 1:A:361:ALA:C | 1:D:171:ASN:CG[2_546] | 2.05 | 0.15 |
| 1:B:24:GLU:CD | 1:D:318:ILE:N[2_546] | 2.05 | 0.15 |
| 1:B:171:ASN:C | 1:D:17:ASN:N[2_546] | 2.05 | 0.15 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:369:GLN:CD | 1:D:125:ALA:CA[2_546] | 2.05 | 0.15 |
| 1:A:367:GLU:CB | 1:D:156:PHE:CE2[2_546] | 2.05 | 0.15 |
| 1:B:341:GLY:C | 1:D:46:GLU:OE1[2_546] | 2.06 | 0.14 |
| 1:B:57:PRO:CB | 1:D:53:TYR:OH[2_546] | 2.06 | 0.14 |
| 1:B:21:ILE:N | 1:D:177:LEU:N[2_546] | 2.06 | 0.14 |
| 1:A:111:LYS:NZ | 1:A:241:TRP:CZ2[2_556] | 2.06 | 0.14 |
| 1:A:362:LEU:CD2 | 1:D:166:THR:C[2_546] | 2.06 | 0.14 |
| 1:B:256:PHE:CE1 | 1:D:263:THR:O[2_546] | 2.06 | 0.14 |
| 1:A:108:LYS:O | 1:A:247:VAL:CB[2_556] | 2.06 | 0.14 |
| 1:A:363:TYR:CB | 1:D:174:ASP:N[2_546] | 2.06 | 0.14 |
| 1:B:29:ARG:CB | 1:D:177:LEU:CB[2_546] | 2.06 | 0.14 |
| 1:B:303:PHE:CE1 | 1:D:304:SER:CA[2_546] | 2.06 | 0.14 |
| 1:B:20:PHE:CD1 | 1:D:173:MET:O[2_546] | 2.06 | 0.14 |
| 1:A:108:LYS:N | 1:A:248:ASN:CA[2_556] | 2.06 | 0.14 |
| 1:B:269:LYS:O | 1:D:184:GLU:CD[2_546] | 2.06 | 0.14 |
| 1:B:345:HIS:CG | 1:D:42:GLY:CA[2_546] | 2.06 | 0.14 |
| 1:A:361:ALA:CA | 1:D:171:ASN:CG[2_546] | 2.06 | 0.14 |
| 1:B:30:TYR:O | 1:D:44:TYR:CE2[2_546] | 2.06 | 0.14 |
| 1:B:46:GLU:CB | 1:D:52:LEU:CB[2_546] | 2.06 | 0.14 |
| 1:B:299:GLY:C | 1:D:308:ILE:O[2_546] | 2.06 | 0.14 |
| 1:B:37:ASP:O | 1:D:341:GLY:O[2_546] | 2.06 | 0.14 |
| 1:B:272:LYS:CE | 1:D:259:ARG:O[2_546] | 2.06 | 0.14 |
| 1:B:17:ASN:CB | 1:D:152:PHE:N[2_546] | 2.06 | 0.14 |
| 1:B:38:LEU:CB | 1:D:340:LEU:C[2_546] | 2.06 | 0.14 |
| 1:B:44:TYR:CD1 | 1:D:31:ARG:CD[2_546] | 2.06 | 0.14 |
| 1:B:338:ARG:CD | 1:D:37:ASP:O[2_546] | 2.06 | 0.14 |
| 1:B:313:ASP:C | 1:D:26:GLY:O[2_546] | 2.06 | 0.14 |
| 1:A:286:ARG:NH1 | 1:B:246:VAL:O[2_546] | 2.06 | 0.14 |
| 1:B:265:ASP:CG | 1:D:267:ARG:CB[2_546] | 2.06 | 0.14 |
| 1:A:286:ARG:NE | 1:B:251:ASN:CG[2_546] | 2.06 | 0.14 |
| 1:B:342:TRP:CD1 | 1:C:371:TYR:CZ[2_546] | 2.06 | 0.14 |
| 1:A:108:LYS:CA | 1:A:248:ASN:N[2_556] | 2.06 | 0.14 |
| 1:B:256:PHE:CG | 1:D:263:THR:C[2_546] | 2.06 | 0.14 |
| 1:B:337:SER:O | 1:D:33:TYR:CG[2_546] | 2.07 | 0.13 |
| 1:B:335:ALA:CB | 1:C:371:TYR:N[2_546] | 2.07 | 0.13 |
| 1:A:108:LYS:C | 1:A:248:ASN:CG[2_556] | 2.07 | 0.13 |
| 1:B:121:ILE:CG1 | 1:D:61:GLU:OE1[2_546] | 2.07 | 0.13 |
| 1:B:308:ILE:C | 1:D:310:PRO:CG[2_546] | 2.07 | 0.13 |
| 1:B:43:SER:O | 1:D:51:MET:C[2_546] | 2.07 | 0.13 |
| 1:A:367:GLU:CG | 1:D:156:PHE:CD1[2_546] | 2.07 | 0.13 |
| 1:B:33:TYR:CG | 1:D:124:ILE:CB[2_546] | 2.07 | 0.13 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:47:THR:O | 1:D:48:ILE:C[2_546] | 2.07 | 0.13 |
| 1:B:174:ASP:N | 1:D:17:ASN:C[2_546] | 2.07 | 0.13 |
| 1:A:360:ARG:NH1 | 1:D:277:THR:CA[2_546] | 2.07 | 0.13 |
| 1:B:260:VAL:O | 1:D:271:PHE:CA[2_546] | 2.07 | 0.13 |
| 1:B:260:VAL:CG2 | 1:D:271:PHE:N[2_546] | 2.07 | 0.13 |
| 1:B:171:ASN:O | 1:D:17:ASN:CA[2_546] | 2.07 | 0.13 |
| 1:B:183:HIS:O | 1:D:39:VAL:CG1[2_546] | 2.07 | 0.13 |
| 1:B:315:TYR:CB | 1:D:23:GLY:N[2_546] | 2.07 | 0.13 |
| 1:B:175:LYS:CD | 1:D:18:LEU:CG[2_546] | 2.07 | 0.13 |
| 1:B:116:ASP:O | 1:D:58:THR:OG1[2_546] | 2.07 | 0.13 |
| 1:B:36:GLU:OE2 | 1:D:338:ARG:NE[2_546] | 2.07 | 0.13 |
| 1:A:286:ARG:CD | 1:B:245:LYS:O[2_546] | 2.07 | 0.13 |
| 1:B:271:PHE:CG | 1:D:21:ILE:N[2_546] | 2.07 | 0.13 |
| 1:B:167:THR:O | 1:D:15:VAL:CG1[2_546] | 2.07 | 0.13 |
| 1:B:116:ASP:O | 1:D:58:THR:CB[2_546] | 2.07 | 0.13 |
| 1:B:337:SER:N | 1:D:33:TYR:CD1[2_546] | 2.08 | 0.12 |
| 1:B:302:GLN:NE2 | 1:D:302:GLN:N[2_546] | 2.08 | 0.12 |
| 1:B:34:ASN:OD1 | 1:D:338:ARG:N[2_546] | 2.08 | 0.12 |
| 1:B:342:TRP:CE3 | 1:C:371:TYR:C[2_546] | 2.08 | 0.12 |
| 1:B:30:TYR:CG | 1:D:47:THR:CB[2_546] | 2.08 | 0.12 |
| 1:B:189:THR:CB | 1:D:41:TYR:CB[2_546] | 2.08 | 0.12 |
| 1:B:304:SER:CB | 1:D:256:PHE:CG[2_546] | 2.08 | 0.12 |
| 1:B:48:ILE:CB | 1:D:49:TYR:CE2[2_546] | 2.08 | 0.12 |
| 1:B:333:LEU:CA | 1:C:368:TYR:CB[2_546] | 2.08 | 0.12 |
| 1:B:334:PHE:CZ | 1:D:37:ASP:OD1[2_546] | 2.08 | 0.12 |
| 1:B:179:LEU:CA | 1:D:30:TYR:CE2[2_546] | 2.08 | 0.12 |
| 1:B:262:LYS:CB | 1:D:315:TYR:CB[2_546] | 2.08 | 0.12 |
| 1:B:267:ARG:CD | 1:D:28:LEU:CD2[2_546] | 2.08 | 0.12 |
| 1:B:44:TYR:CD2 | 1:D:54:GLY:CA[2_546] | 2.08 | 0.12 |
| 1:B:12:ILE:CG1 | 1:D:168:ASP:OD1[2_546] | 2.08 | 0.12 |
| 1:B:338:ARG:NH1 | 1:D:36:GLU:O[2_546] | 2.08 | 0.12 |
| 1:B:316:SER:CA | 1:D:21:ILE:C[2_546] | 2.08 | 0.12 |
| 1:B:29:ARG:CA | 1:D:177:LEU:C[2_546] | 2.08 | 0.12 |
| 1:B:302:GLN:CA | 1:D:303:PHE:CD2[2_546] | 2.08 | 0.12 |
| 1:B:256:PHE:CG | 1:D:263:THR:O[2_546] | 2.08 | 0.12 |
| 1:A:362:LEU:CB | 1:D:167:THR:CA[2_546] | 2.08 | 0.12 |
| 1:B:242:PHE:CD2 | 1:D:306:LYS:CA[2_546] | 2.08 | 0.12 |
| 1:B:320:PHE:CD2 | 1:C:367:GLU:C[2_546] | 2.08 | 0.12 |
| 1:B:184:GLU:CA | 1:D:39:VAL:CB[2_546] | 2.08 | 0.12 |
| 1:B:46:GLU:CG | 1:D:52:LEU:CG[2_546] | 2.08 | 0.12 |
| 1:B:37:ASP:O | 1:D:341:GLY:C[2_546] | 2.08 | 0.12 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:109:ASN:CG | 1:A:249:GLN:C[2_556] | 2.08 | 0.12 |
| 1:B:34:ASN:N | 1:D:337:SER:O[2_546] | 2.08 | 0.12 |
| 1:B:23:GLY:C | 1:D:316:SER:OG[2_546] | 2.08 | 0.12 |
| 1:B:311:ASN:CG | 1:D:266:PRO:CD[2_546] | 2.08 | 0.12 |
| 1:B:41:TYR:C | 1:D:344:ALA:C[2_546] | 2.08 | 0.12 |
| 1:B:338:ARG:CZ | 1:D:37:ASP:N[2_546] | 2.08 | 0.12 |
| 1:A:109:ASN:CA | 1:A:249:GLN:CA[2_556] | 2.09 | 0.11 |
| 1:B:57:PRO:C | 1:D:117:LYS:C[2_546] | 2.09 | 0.11 |
| 1:B:298:LEU:C | 1:D:308:ILE:N[2_546] | 2.09 | 0.11 |
| 1:B:246:VAL:CB | 1:D:305:SER:CA[2_546] | 2.09 | 0.11 |
| 1:B:24:GLU:CA | 1:D:316:SER:O[2_546] | 2.09 | 0.11 |
| 1:A:109:ASN:OD1 | 1:A:250:LYS:O[2_556] | 2.09 | 0.11 |
| 1:B:338:ARG:CB | 1:C:371:TYR:CD1[2_546] | 2.09 | 0.11 |
| 1:B:253:LEU:N | 1:D:309:TYR:CZ[2_546] | 2.09 | 0.11 |
| 1:B:25:LYS:C | 1:D:316:SER:OG[2_546] | 2.09 | 0.11 |
| 1:B:117:LYS:O | 1:D:61:GLU:CG[2_546] | 2.09 | 0.11 |
| 1:B:35:ILE:N | 1:D:181:THR:CA[2_546] | 2.09 | 0.11 |
| 1:B:47:THR:CG2 | 1:D:51:MET:CA[2_546] | 2.09 | 0.11 |
| 1:B:36:GLU:CG | 1:D:338:ARG:CB[2_546] | 2.09 | 0.11 |
| 1:B:178:ILE:O | 1:D:30:TYR:CB[2_546] | 2.09 | 0.11 |
| 1:B:265:ASP:O | 1:D:267:ARG:NH1[2_546] | 2.09 | 0.11 |
| 1:A:110:PHE:CA | 1:A:244:ASP:C[2_556] | 2.09 | 0.11 |
| 1:B:25:LYS:CB | 1:D:320:PHE:CE1[2_546] | 2.09 | 0.11 |
| 1:B:336:LEU:CG | 1:C:369:GLN:CB[2_546] | 2.09 | 0.11 |
| 1:B:173:MET:N | 1:C:364:VAL:N[2_546] | 2.09 | 0.11 |
| 1:B:37:ASP:OD1 | 1:D:342:TRP:CB[2_546] | 2.09 | 0.11 |
| 1:B:175:LYS:CB | 1:D:18:LEU:CA[2_546] | 2.09 | 0.11 |
| 1:B:48:ILE:C | 1:D:49:TYR:O[2_546] | 2.09 | 0.11 |
| 1:B:182:ASP:CB | 1:D:47:THR:OG1[2_546] | 2.09 | 0.11 |
| 1:B:344:ALA:CA | 1:D:62:LEU:CD2[2_546] | 2.09 | 0.11 |
| 1:A:364:VAL:CB | 1:D:154:LYS:N[2_546] | 2.09 | 0.11 |
| 1:A:286:ARG:NE | 1:B:251:ASN:CA[2_546] | 2.09 | 0.11 |
| 1:B:307:GLY:CA | 1:D:314:PHE:CD1[2_546] | 2.09 | 0.11 |
| 1:B:336:LEU:C | 1:D:33:TYR:CD2[2_546] | 2.09 | 0.11 |
| 1:B:178:ILE:O | 1:D:30:TYR:CD1[2_546] | 2.09 | 0.11 |
| 1:A:286:ARG:CZ | 1:B:246:VAL:CA[2_546] | 2.09 | 0.11 |
| 1:B:179:LEU:N | 1:D:30:TYR:CA[2_546] | 2.09 | 0.11 |
| 1:A:280:GLU:CB | 1:B:248:ASN:CB[2_546] | 2.09 | 0.11 |
| 1:B:188:SER:CA | 1:D:41:TYR:CE2[2_546] | 2.09 | 0.11 |
| 1:A:286:ARG:CD | 1:B:251:ASN:CA[2_546] | 2.09 | 0.11 |
| 1:B:180:TYR:CE1 | 1:D:29:ARG:N[2_546] | 2.09 | 0.11 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:309:TYR:CB | 1:D:310:PRO:O[2_546] | 2.09 | 0.11 |
| 1:B:58:THR:N | 1:D:118:GLU:N[2_546] | 2.09 | 0.11 |
| 1:B:334:PHE:N | 1:D:32:GLY:O[2_546] | 2.09 | 0.11 |
| 1:B:27:ILE:N | 1:D:180:TYR:CG[2_546] | 2.09 | 0.11 |
| 1:B:296:GLU:CB | 1:D:261:TYR:O[2_546] | 2.09 | 0.11 |
| 1:B:262:LYS:NZ | 1:D:272:LYS:CG[2_546] | 2.10 | 0.10 |
| 1:A:290:GLU:CG | 1:B:245:LYS:NZ[2_546] | 2.10 | 0.10 |
| 1:B:332:ALA:N | 1:C:368:TYR:CG[2_546] | 2.10 | 0.10 |
| 1:B:314:PHE:CE1 | 1:D:262:LYS:CB[2_546] | 2.10 | 0.10 |
| 1:B:42:GLY:N | 1:D:343:LEU:O[2_546] | 2.10 | 0.10 |
| 1:B:55:LYS:C | 1:D:121:ILE:CD1[2_546] | 2.10 | 0.10 |
| 1:B:61:GLU:CB | 1:D:115:ASN:OD1[2_546] | 2.10 | 0.10 |
| 1:B:37:ASP:CB | 1:D:342:TRP:CB[2_546] | 2.10 | 0.10 |
| 1:B:301:LYS:N | 1:D:308:ILE:CB[2_546] | 2.10 | 0.10 |
| 1:B:56:LEU:CG | 1:D:120:ALA:CA[2_546] | 2.10 | 0.10 |
| 1:B:338:ARG:CD | 1:D:38:LEU:N[2_546] | 2.10 | 0.10 |
| 1:A:367:GLU:CG | 1:D:156:PHE:CD2[2_546] | 2.10 | 0.10 |
| 1:B:316:SER:O | 1:D:20:PHE:CD2[2_546] | 2.10 | 0.10 |
| 1:B:189:THR:CA | 1:D:41:TYR:CE2[2_546] | 2.10 | 0.10 |
| 1:B:22:ASP:OD1 | 1:D:320:PHE:CG[2_546] | 2.10 | 0.10 |
| 1:B:179:LEU:CD2 | 1:D:30:TYR:CE2[2_546] | 2.10 | 0.10 |
| 1:A:362:LEU:C | 1:D:170:ILE:O[2_546] | 2.10 | 0.10 |
| 1:A:364:VAL:C | 1:D:153:ALA:CA[2_546] | 2.10 | 0.10 |
| 1:B:19:THR:CA | 1:D:174:ASP:O[2_546] | 2.10 | 0.10 |
| 1:B:316:SER:CA | 1:D:22:ASP:N[2_546] | 2.10 | 0.10 |
| 1:A:236:ASN:OD1 | 1:B:224:GLU:CB[2_546] | 2.10 | 0.10 |
| 1:B:242:PHE:CZ | 1:D:306:LYS:CA[2_546] | 2.10 | 0.10 |
| 1:B:173:MET:CG | 1:C:365:GLY:CA[2_546] | 2.10 | 0.10 |
| 1:B:56:LEU:CD2 | 1:D:120:ALA:CB[2_546] | 2.10 | 0.10 |
| 1:A:110:PHE:N | 1:A:244:ASP:C[2_556] | 2.10 | 0.10 |
| 1:B:28:LEU:CD1 | 1:D:178:ILE:N[2_546] | 2.10 | 0.10 |
| 1:B:258:HIS:C | 1:D:268:ALA:C[2_546] | 2.10 | 0.10 |
| 1:B:61:GLU:CB | 1:D:118:GLU:OE2[2_546] | 2.10 | 0.10 |
| 1:A:366:PRO:CA | 1:D:152:PHE:O[2_546] | 2.10 | 0.10 |
| 1:B:44:TYR:CD1 | 1:D:50:LEU:CD1[2_546] | 2.10 | 0.10 |
| 1:B:169:GLU:CB | 1:C:364:VAL:CG1[2_546] | 2.10 | 0.10 |
| 1:B:27:ILE:CA | 1:D:180:TYR:CE1[2_546] | 2.10 | 0.10 |
| 1:B:179:LEU:O | 1:D:30:TYR:CD1[2_546] | 2.10 | 0.10 |
| 1:B:25:LYS:NZ | 1:D:223:GLU:OE1[2_546] | 2.10 | 0.10 |
| 1:B:347:ILE:CD1 | 1:D:58:THR:O[2_546] | 2.10 | 0.10 |
| 1:B:174:ASP:O | 1:D:17:ASN:C[2_546] | 2.10 | 0.10 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:46:GLU:C | 1:D:52:LEU:N[2_546] | 2.10 | 0.10 |
| 1:B:315:TYR:CZ | 1:D:260:VAL:CA[2_546] | 2.11 | 0.09 |
| 1:B:26:GLY:C | 1:D:180:TYR:OH[2_546] | 2.11 | 0.09 |
| 1:B:246:VAL:CG1 | 1:D:304:SER:CB[2_546] | 2.11 | 0.09 |
| 1:B:178:ILE:CG1 | 1:D:51:MET:SD[2_546] | 2.11 | 0.09 |
| 1:B:270:ILE:CB | 1:D:183:HIS:C[2_546] | 2.11 | 0.09 |
| 1:B:188:SER:OG | 1:D:41:TYR:CZ[2_546] | 2.11 | 0.09 |
| 1:A:111:LYS:N | 1:A:245:LYS:CA[2_556] | 2.11 | 0.09 |
| 1:B:34:ASN:OD1 | 1:D:337:SER:CB[2_546] | 2.11 | 0.09 |
| 1:B:222:ALA:O | 1:D:25:LYS:CB[2_546] | 2.11 | 0.09 |
| 1:B:59:LYS:CA | 1:D:114:GLU:O[2_546] | 2.11 | 0.09 |
| 1:B:17:ASN:N | 1:D:151:SER:CB[2_546] | 2.11 | 0.09 |
| 1:B:49:TYR:CE1 | 1:D:53:TYR:OH[2_546] | 2.11 | 0.09 |
| 1:B:174:ASP:CA | 1:D:17:ASN:OD1[2_546] | 2.11 | 0.09 |
| 1:B:226:PHE:CA | 1:D:25:LYS:CE[2_546] | 2.11 | 0.09 |
| 1:B:45:GLU:CB | 1:D:53:TYR:O[2_546] | 2.11 | 0.09 |
| 1:B:12:ILE:CD1 | 1:D:168:ASP:CA[2_546] | 2.11 | 0.09 |
| 1:B:333:LEU:N | 1:C:368:TYR:CD1[2_546] | 2.11 | 0.09 |
| 1:A:368:TYR:CE2 | 1:D:127:MET:SD[2_546] | 2.11 | 0.09 |
| 1:B:312:THR:OG1 | 1:D:28:LEU:CD1[2_546] | 2.11 | 0.09 |
| 1:B:268:ALA:O | 1:D:183:HIS:NE2[2_546] | 2.11 | 0.09 |
| 1:B:332:ALA:CB | 1:C:368:TYR:CD2[2_546] | 2.11 | 0.09 |
| 1:B:50:LEU:CD1 | 1:D:48:ILE:CG2[2_546] | 2.11 | 0.09 |
| 1:B:23:GLY:O | 1:D:316:SER:CB[2_546] | 2.11 | 0.09 |
| 1:B:263:THR:N | 1:D:312:THR:C[2_546] | 2.11 | 0.09 |
| 1:B:337:SER:CB | 1:D:33:TYR:CD1[2_546] | 2.11 | 0.09 |
| 1:B:304:SER:CA | 1:D:256:PHE:CD2[2_546] | 2.11 | 0.09 |
| 1:B:173:MET:SD | 1:C:366:PRO:CA[2_546] | 2.11 | 0.09 |
| 1:B:48:ILE:CB | 1:D:53:TYR:CB[2_546] | 2.11 | 0.09 |
| 1:B:176:ALA:N | 1:D:19:THR:N[2_546] | 2.11 | 0.09 |
| 1:B:347:ILE:CD1 | 1:D:58:THR:C[2_546] | 2.11 | 0.09 |
| 1:B:305:SER:N | 1:D:253:LEU:CG[2_546] | 2.11 | 0.09 |
| 1:B:36:GLU:CD | 1:D:338:ARG:CG[2_546] | 2.11 | 0.09 |
| 1:A:112:TRP:C | 1:A:231:GLU:OE1[2_556] | 2.11 | 0.09 |
| 1:B:256:PHE:CD2 | 1:D:309:TYR:N[2_546] | 2.11 | 0.09 |
| 1:B:47:THR:CG2 | 1:D:51:MET:CB[2_546] | 2.11 | 0.09 |
| 1:B:338:ARG:C | 1:C:371:TYR:CE1[2_546] | 2.11 | 0.09 |
| 1:B:34:ASN:CG | 1:D:337:SER:N[2_546] | 2.11 | 0.09 |
| 1:B:257:GLY:CA | 1:D:264:TYR:CD1[2_546] | 2.11 | 0.09 |
| 1:B:35:ILE:CB | 1:D:181:THR:CG2[2_546] | 2.12 | 0.08 |
| 1:B:184:GLU:N | 1:D:39:VAL:CA[2_546] | 2.12 | 0.08 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:265:ASP:C | 1:D:267:ARG:CD[2_546] | 2.12 | 0.08 |
| 1:B:183:HIS:CD2 | 1:D:179:LEU:CD2[2_546] | 2.12 | 0.08 |
| 1:A:279:ILE:CB | 1:B:249:GLN:CG[2_546] | 2.12 | 0.08 |
| 1:B:30:TYR:CD2 | 1:D:47:THR:CG2[2_546] | 2.12 | 0.08 |
| 1:B:48:ILE:CG2 | 1:D:49:TYR:CZ[2_546] | 2.12 | 0.08 |
| 1:B:288:TYR:C | 1:D:24:GLU:OE2[2_546] | 2.12 | 0.08 |
| 1:B:29:ARG:CZ | 1:D:336:LEU:N[2_546] | 2.12 | 0.08 |
| 1:B:117:LYS:CD | 1:D:61:GLU:O[2_546] | 2.12 | 0.08 |
| 1:A:286:ARG:CZ | 1:B:251:ASN:CA[2_546] | 2.12 | 0.08 |
| 1:A:294:LYS:CE | 1:B:231:GLU:OE2[2_546] | 2.12 | 0.08 |
| 1:B:52:LEU:CG | 1:D:57:PRO:CG[2_546] | 2.12 | 0.08 |
| 1:B:264:TYR:CE2 | 1:D:258:HIS:CD2[2_546] | 2.12 | 0.08 |
| 1:B:315:TYR:CD1 | 1:D:260:VAL:CB[2_546] | 2.12 | 0.08 |
| 1:B:301:LYS:CG | 1:D:308:ILE:CD1[2_546] | 2.12 | 0.08 |
| 1:A:280:GLU:CG | 1:B:248:ASN:CG[2_546] | 2.12 | 0.08 |
| 1:B:25:LYS:C | 1:D:180:TYR:OH[2_546] | 2.12 | 0.08 |
| 1:B:51:MET:SD | 1:D:44:TYR:O[2_546] | 2.12 | 0.08 |
| 1:A:109:ASN:O | 1:A:249:GLN:O[2_556] | 2.12 | 0.08 |
| 1:A:361:ALA:C | 1:D:171:ASN:CA[2_546] | 2.12 | 0.08 |
| 1:B:311:ASN:N | 1:D:265:ASP:N[2_546] | 2.12 | 0.08 |
| 1:B:264:TYR:CA | 1:D:312:THR:N[2_546] | 2.12 | 0.08 |
| 1:B:259:ARG:C | 1:D:272:LYS:CA[2_546] | 2.12 | 0.08 |
| 1:B:339:THR:O | 1:D:56:LEU:CD2[2_546] | 2.12 | 0.08 |
| 1:B:51:MET:CG | 1:D:47:THR:N[2_546] | 2.12 | 0.08 |
| 1:B:313:ASP:C | 1:D:26:GLY:N[2_546] | 2.12 | 0.08 |
| 1:B:311:ASN:OD1 | 1:D:266:PRO:CD[2_546] | 2.12 | 0.08 |
| 1:B:261:TYR:CB | 1:D:268:ALA:CA[2_546] | 2.12 | 0.08 |
| 1:B:173:MET:C | 1:D:17:ASN:CG[2_546] | 2.12 | 0.08 |
| 1:A:290:GLU:CG | 1:B:245:LYS:CE[2_546] | 2.12 | 0.08 |
| 1:B:313:ASP:CG | 1:D:26:GLY:O[2_546] | 2.12 | 0.08 |
| 1:B:263:THR:CG2 | 1:D:313:ASP:OD1[2_546] | 2.12 | 0.08 |
| 1:B:156:PHE:CZ | 1:C:366:PRO:CG[2_546] | 2.12 | 0.08 |
| 1:B:308:ILE:C | 1:D:309:TYR:C[2_546] | 2.12 | 0.08 |
| 1:A:111:LYS:N | 1:A:245:LYS:CG[2_556] | 2.12 | 0.08 |
| 1:B:335:ALA:O | 1:D:33:TYR:CD2[2_546] | 2.12 | 0.08 |
| 1:B:177:LEU:CG | 1:D:31:ARG:C[2_546] | 2.12 | 0.08 |
| 1:B:52:LEU:C | 1:D:61:GLU:O[2_546] | 2.12 | 0.08 |
| 1:B:178:ILE:C | 1:D:30:TYR:CG[2_546] | 2.12 | 0.08 |
| 1:B:262:LYS:CD | 1:D:315:TYR:CE2[2_546] | 2.13 | 0.07 |
| 1:B:182:ASP:OD2 | 1:D:178:ILE:CD1[2_546] | 2.13 | 0.07 |
| 1:B:274:LEU:CD1 | 1:D:19:THR:C[2_546] | 2.13 | 0.07 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:256:PHE:CG | 1:D:309:TYR:CG[2_546] | 2.13 | 0.07 |
| 1:B:186:PRO:CB | 1:D:40:ASN:OD1[2_546] | 2.13 | 0.07 |
| 1:B:246:VAL:CB | 1:D:305:SER:N[2_546] | 2.13 | 0.07 |
| 1:A:279:ILE:CD1 | 1:B:249:GLN:OE1[2_546] | 2.13 | 0.07 |
| 1:B:259:ARG:C | 1:D:269:LYS:O[2_546] | 2.13 | 0.07 |
| 1:B:34:ASN:N | 1:D:337:SER:C[2_546] | 2.13 | 0.07 |
| 1:B:172:ALA:N | 1:C:362:LEU:O[2_546] | 2.13 | 0.07 |
| 1:B:337:SER:OG | 1:D:30:TYR:C[2_546] | 2.13 | 0.07 |
| 1:B:296:GLU:OE1 | 1:D:260:VAL:C[2_546] | 2.13 | 0.07 |
| 1:B:32:GLY:N | 1:D:44:TYR:CD2[2_546] | 2.13 | 0.07 |
| 1:B:172:ALA:CB | 1:C:363:TYR:CG[2_546] | 2.13 | 0.07 |
| 1:B:61:GLU:N | 1:D:115:ASN:OD1[2_546] | 2.13 | 0.07 |
| 1:B:56:LEU:CA | 1:D:117:LYS:O[2_546] | 2.13 | 0.07 |
| 1:B:47:THR:N | 1:D:52:LEU:C[2_546] | 2.13 | 0.07 |
| 1:B:263:THR:CB | 1:D:313:ASP:CG[2_546] | 2.13 | 0.07 |
| 1:B:174:ASP:O | 1:D:18:LEU:CA[2_546] | 2.13 | 0.07 |
| 1:B:47:THR:N | 1:D:51:MET:C[2_546] | 2.13 | 0.07 |
| 1:B:28:LEU:CA | 1:D:180:TYR:CA[2_546] | 2.13 | 0.07 |
| 1:B:19:THR:O | 1:D:175:LYS:N[2_546] | 2.13 | 0.07 |
| 1:B:276:LEU:C | 1:C:360:ARG:CZ[2_546] | 2.13 | 0.07 |
| 1:B:22:ASP:O | 1:D:316:SER:CB[2_546] | 2.13 | 0.07 |
| 1:B:29:ARG:O | 1:D:177:LEU:CB[2_546] | 2.13 | 0.07 |
| 1:A:362:LEU:N | 1:D:171:ASN:CB[2_546] | 2.13 | 0.07 |
| 1:B:31:ARG:CZ | 1:D:45:GLU:CB[2_546] | 2.13 | 0.07 |
| 1:B:35:ILE:CG2 | 1:D:181:THR:CA[2_546] | 2.13 | 0.07 |
| 1:B:19:THR:C | 1:D:174:ASP:CA[2_546] | 2.14 | 0.06 |
| 1:B:336:LEU:C | 1:D:33:TYR:CE1[2_546] | 2.14 | 0.06 |
| 1:B:117:LYS:N | 1:D:61:GLU:N[2_546] | 2.14 | 0.06 |
| 1:B:256:PHE:CE1 | 1:D:263:THR:N[2_546] | 2.14 | 0.06 |
| 1:B:308:ILE:CA | 1:D:310:PRO:N[2_546] | 2.14 | 0.06 |
| 1:B:30:TYR:N | 1:D:44:TYR:CG[2_546] | 2.14 | 0.06 |
| 1:B:117:LYS:CD | 1:D:60:LYS:C[2_546] | 2.14 | 0.06 |
| 1:B:263:THR:OG1 | 1:D:313:ASP:OD1[2_546] | 2.14 | 0.06 |
| 1:B:182:ASP:C | 1:D:178:ILE:CG2[2_546] | 2.14 | 0.06 |
| 1:B:47:THR:OG1 | 1:D:52:LEU:N[2_546] | 2.14 | 0.06 |
| 1:B:30:TYR:CA | 1:D:44:TYR:CZ[2_546] | 2.14 | 0.06 |
| 1:B:272:LYS:N | 1:D:21:ILE:CD1[2_546] | 2.14 | 0.06 |
| 1:B:314:PHE:N | 1:D:27:ILE:N[2_546] | 2.14 | 0.06 |
| 1:B:57:PRO:O | 1:D:118:GLU:CA[2_546] | 2.14 | 0.06 |
| 1:B:28:LEU:CG | 1:D:181:THR:N[2_546] | 2.14 | 0.06 |
| 1:A:368:TYR:CB | 1:D:336:LEU:CG[2_546] | 2.14 | 0.06 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:49:TYR:N | 1:D:49:TYR:CD1[2_546] | 2.14 | 0.06 |
| 1:B:22:ASP:OD1 | 1:D:316:SER:O[2_546] | 2.14 | 0.06 |
| 1:B:45:GLU:C | 1:D:53:TYR:C[2_546] | 2.14 | 0.06 |
| 1:B:20:PHE:CB | 1:D:173:MET:C[2_546] | 2.14 | 0.06 |
| 1:B:48:ILE:CG1 | 1:D:55:LYS:C[2_546] | 2.14 | 0.06 |
| 1:A:362:LEU:CD1 | 1:D:169:GLU:C[2_546] | 2.14 | 0.06 |
| 1:B:28:LEU:CD2 | 1:D:178:ILE:C[2_546] | 2.14 | 0.06 |
| 1:B:172:ALA:CB | 1:C:364:VAL:N[2_546] | 2.14 | 0.06 |
| 1:B:300:ILE:N | 1:D:308:ILE:CG2[2_546] | 2.14 | 0.06 |
| 1:B:269:LYS:C | 1:D:183:HIS:CD2[2_546] | 2.14 | 0.06 |
| 1:B:26:GLY:N | 1:D:180:TYR:CE1[2_546] | 2.14 | 0.06 |
| 1:B:278:LEU:CA | 1:C:362:LEU:CD1[2_546] | 2.14 | 0.06 |
| 1:B:270:ILE:CD1 | 1:D:182:ASP:CA[2_546] | 2.14 | 0.06 |
| 1:B:29:ARG:O | 1:D:178:ILE:N[2_546] | 2.14 | 0.06 |
| 1:B:53:TYR:O | 1:D:64:ASP:C[2_546] | 2.14 | 0.06 |
| 1:B:262:LYS:CA | 1:D:314:PHE:CA[2_546] | 2.14 | 0.06 |
| 1:B:310:PRO:O | 1:D:265:ASP:OD2[2_546] | 2.14 | 0.06 |
| 1:B:258:HIS:NE2 | 1:D:270:ILE:CG1[2_546] | 2.14 | 0.06 |
| 1:B:261:TYR:N | 1:D:271:PHE:N[2_546] | 2.14 | 0.06 |
| 1:B:47:THR:O | 1:D:49:TYR:CB[2_546] | 2.14 | 0.06 |
| 1:B:23:GLY:CA | 1:D:271:PHE:CG[2_546] | 2.14 | 0.06 |
| 1:B:24:GLU:CG | 1:D:318:ILE:CA[2_546] | 2.14 | 0.06 |
| 1:B:170:ILE:O | 1:C:364:VAL:CG2[2_546] | 2.14 | 0.06 |
| 1:B:348:GLU:CG | 1:D:66:LYS:NZ[2_546] | 2.14 | 0.06 |
| 1:B:41:TYR:CD1 | 1:D:343:LEU:N[2_546] | 2.14 | 0.06 |
| 1:B:46:GLU:N | 1:D:53:TYR:CA[2_546] | 2.14 | 0.06 |
| 1:B:172:ALA:CA | 1:C:363:TYR:CG[2_546] | 2.14 | 0.06 |
| 1:A:109:ASN:CB | 1:A:246:VAL:O[2_556] | 2.14 | 0.06 |
| 1:B:34:ASN:C | 1:D:338:ARG:O[2_546] | 2.14 | 0.06 |
| 1:B:300:ILE:N | 1:D:308:ILE:C[2_546] | 2.15 | 0.05 |
| 1:B:311:ASN:CB | 1:D:265:ASP:O[2_546] | 2.15 | 0.05 |
| 1:B:41:TYR:CB | 1:D:343:LEU:O[2_546] | 2.15 | 0.05 |
| 1:B:182:ASP:OD1 | 1:D:38:LEU:C[2_546] | 2.15 | 0.05 |
| 1:A:368:TYR:C | 1:D:128:ALA:CA[2_546] | 2.15 | 0.05 |
| 1:B:46:GLU:OE1 | 1:D:347:ILE:CG1[2_546] | 2.15 | 0.05 |
| 1:B:262:LYS:CA | 1:D:314:PHE:C[2_546] | 2.15 | 0.05 |
| 1:B:58:THR:OG1 | 1:D:115:ASN:CB[2_546] | 2.15 | 0.05 |
| 1:B:28:LEU:N | 1:D:180:TYR:N[2_546] | 2.15 | 0.05 |
| 1:B:43:SER:CA | 1:D:31:ARG:NH2[2_546] | 2.15 | 0.05 |
| 1:B:270:ILE:C | 1:D:21:ILE:CD1[2_546] | 2.15 | 0.05 |
| 1:B:183:HIS:O | 1:D:40:ASN:N[2_546] | 2.15 | 0.05 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:320:PHE:CZ | 1:D:29:ARG:CD[2_546] | 2.15 | 0.05 |
| 1:B:16:THR:O | 1:D:151:SER:OG[2_546] | 2.15 | 0.05 |
| 1:B:338:ARG:CG | 1:C:371:TYR:CD1[2_546] | 2.15 | 0.05 |
| 1:B:314:PHE:CA | 1:D:22:ASP:O[2_546] | 2.15 | 0.05 |
| 1:B:272:LYS:CE | 1:D:260:VAL:CA[2_546] | 2.15 | 0.05 |
| 1:B:319:VAL:C | 1:D:20:PHE:CE1[2_546] | 2.15 | 0.05 |
| 1:B:44:TYR:N | 1:D:31:ARG:NE[2_546] | 2.15 | 0.05 |
| 1:B:342:TRP:CA | 1:C:371:TYR:CZ[2_546] | 2.15 | 0.05 |
| 1:B:186:PRO:C | 1:D:40:ASN:CG[2_546] | 2.15 | 0.05 |
| 1:B:309:TYR:CD1 | 1:D:311:ASN:OD1[2_546] | 2.15 | 0.05 |
| 1:B:174:ASP:CB | 1:D:17:ASN:N[2_546] | 2.15 | 0.05 |
| 1:B:342:TRP:CZ2 | 1:C:371:TYR:CB[2_546] | 2.15 | 0.05 |
| 1:B:49:TYR:CA | 1:D:49:TYR:CE1[2_546] | 2.15 | 0.05 |
| 1:A:362:LEU:CD1 | 1:D:167:THR:C[2_546] | 2.15 | 0.05 |
| 1:B:33:TYR:O | 1:D:337:SER:O[2_546] | 2.15 | 0.05 |
| 1:B:46:GLU:O | 1:D:52:LEU:CG[2_546] | 2.15 | 0.05 |
| 1:B:278:LEU:CD2 | 1:C:362:LEU:CD2[2_546] | 2.15 | 0.05 |
| 1:B:176:ALA:O | 1:D:30:TYR:N[2_546] | 2.15 | 0.05 |
| 1:B:306:LYS:NZ | 1:D:297:GLU:C[2_546] | 2.15 | 0.05 |
| 1:B:19:THR:N | 1:D:44:TYR:CB[2_546] | 2.15 | 0.05 |
| 1:A:110:PHE:CB | 1:A:244:ASP:O[2_556] | 2.15 | 0.05 |
| 1:B:172:ALA:N | 1:D:16:THR:C[2_546] | 2.15 | 0.05 |
| 1:B:334:PHE:CA | 1:D:32:GLY:O[2_546] | 2.15 | 0.05 |
| 1:B:179:LEU:CA | 1:D:30:TYR:CB[2_546] | 2.15 | 0.05 |
| 1:B:267:ARG:NE | 1:D:28:LEU:CD2[2_546] | 2.15 | 0.05 |
| 1:B:56:LEU:O | 1:D:118:GLU:CA[2_546] | 2.15 | 0.05 |
| 1:B:117:LYS:CG | 1:D:59:LYS:O[2_546] | 2.15 | 0.05 |
| 1:A:237:ARG:CZ | 1:B:217:LEU:CB[2_546] | 2.15 | 0.05 |
| 1:B:267:ARG:NH1 | 1:D:35:ILE:CD1[2_546] | 2.15 | 0.05 |
| 1:B:314:PHE:CD1 | 1:D:263:THR:CG2[2_546] | 2.15 | 0.05 |
| 1:B:298:LEU:C | 1:D:306:LYS:C[2_546] | 2.15 | 0.05 |
| 1:B:246:VAL:CG1 | 1:D:304:SER:CA[2_546] | 2.15 | 0.05 |
| 1:B:35:ILE:CD1 | 1:D:182:ASP:CA[2_546] | 2.15 | 0.05 |
| 1:B:24:GLU:C | 1:D:316:SER:OG[2_546] | 2.16 | 0.04 |
| 1:B:16:THR:CG2 | 1:D:174:ASP:OD1[2_546] | 2.16 | 0.04 |
| 1:B:37:ASP:CG | 1:D:339:THR:C[2_546] | 2.16 | 0.04 |
| 1:B:332:ALA:CB | 1:C:368:TYR:CE2[2_546] | 2.16 | 0.04 |
| 1:B:242:PHE:CE1 | 1:D:306:LYS:N[2_546] | 2.16 | 0.04 |
| 1:B:182:ASP:OD2 | 1:D:42:GLY:C[2_546] | 2.16 | 0.04 |
| 1:B:31:ARG:N | 1:D:44:TYR:CB[2_546] | 2.16 | 0.04 |
| 1:B:258:HIS:CG | 1:D:267:ARG:C[2_546] | 2.16 | 0.04 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:167:THR:C | 1:D:15:VAL:CB[2_546] | 2.16 | 0.04 |
| 1:B:117:LYS:O | 1:D:58:THR:CB[2_546] | 2.16 | 0.04 |
| 1:B:36:GLU:CB | 1:D:338:ARG:NE[2_546] | 2.16 | 0.04 |
| 1:B:116:ASP:CB | 1:D:59:LYS:CB[2_546] | 2.16 | 0.04 |
| 1:B:257:GLY:O | 1:D:265:ASP:O[2_546] | 2.16 | 0.04 |
| 1:B:40:ASN:CA | 1:D:345:HIS:CG[2_546] | 2.16 | 0.04 |
| 1:B:319:VAL:O | 1:C:367:GLU:CD[2_546] | 2.16 | 0.04 |
| 1:B:263:THR:O | 1:D:311:ASN:O[2_546] | 2.16 | 0.04 |
| 1:B:185:VAL:C | 1:D:40:ASN:CA[2_546] | 2.16 | 0.04 |
| 1:B:268:ALA:C | 1:D:183:HIS:CD2[2_546] | 2.16 | 0.04 |
| 1:B:33:TYR:OH | 1:D:123:ILE:C[2_546] | 2.16 | 0.04 |
| 1:A:363:TYR:CZ | 1:D:153:ALA:N[2_546] | 2.16 | 0.04 |
| 1:B:56:LEU:CG | 1:D:121:ILE:CA[2_546] | 2.16 | 0.04 |
| 1:A:363:TYR:C | 1:D:170:ILE:CA[2_546] | 2.16 | 0.04 |
| 1:B:33:TYR:O | 1:D:44:TYR:CZ[2_546] | 2.16 | 0.04 |
| 1:A:111:LYS:N | 1:A:245:LYS:CB[2_556] | 2.16 | 0.04 |
| 1:B:341:GLY:N | 1:D:46:GLU:CD[2_546] | 2.16 | 0.04 |
| 1:A:363:TYR:C | 1:D:170:ILE:CB[2_546] | 2.16 | 0.04 |
| 1:B:22:ASP:CA | 1:D:320:PHE:CZ[2_546] | 2.16 | 0.04 |
| 1:A:362:LEU:CG | 1:D:166:THR:O[2_546] | 2.16 | 0.04 |
| 1:B:273:LYS:NZ | 1:D:185:VAL:CG2[2_546] | 2.16 | 0.04 |
| 1:B:337:SER:CA | 1:D:33:TYR:CB[2_546] | 2.16 | 0.04 |
| 1:B:58:THR:CG2 | 1:D:118:GLU:OE1[2_546] | 2.16 | 0.04 |
| 1:B:48:ILE:CG2 | 1:D:49:TYR:CD2[2_546] | 2.16 | 0.04 |
| 1:B:263:THR:CA | 1:D:314:PHE:N[2_546] | 2.16 | 0.04 |
| 1:B:255:GLY:C | 1:D:263:THR:CG2[2_546] | 2.16 | 0.04 |
| 1:B:189:THR:CG2 | 1:D:41:TYR:N[2_546] | 2.16 | 0.04 |
| 1:B:300:ILE:CD1 | 1:D:258:HIS:CA[2_546] | 2.16 | 0.04 |
| 1:B:335:ALA:CA | 1:C:370:GLU:C[2_546] | 2.16 | 0.04 |
| 1:B:314:PHE:CE2 | 1:D:262:LYS:CA[2_546] | 2.16 | 0.04 |
| 1:B:121:ILE:N | 1:D:58:THR:CG2[2_546] | 2.16 | 0.04 |
| 1:B:338:ARG:NH2 | 1:D:35:ILE:CA[2_546] | 2.16 | 0.04 |
| 1:B:18:LEU:CA | 1:D:45:GLU:N[2_546] | 2.16 | 0.04 |
| 1:B:260:VAL:CG1 | 1:D:271:PHE:CD2[2_546] | 2.16 | 0.04 |
| 1:B:313:ASP:O | 1:D:25:LYS:O[2_546] | 2.16 | 0.04 |
| 1:B:264:TYR:N | 1:D:311:ASN:OD1[2_546] | 2.16 | 0.04 |
| 1:B:316:SER:O | 1:D:20:PHE:CE1[2_546] | 2.17 | 0.03 |
| 1:B:278:LEU:CB | 1:C:362:LEU:CD1[2_546] | 2.17 | 0.03 |
| 1:B:271:PHE:CZ | 1:D:20:PHE:C[2_546] | 2.17 | 0.03 |
| 1:B:269:LYS:C | 1:D:184:GLU:CB[2_546] | 2.17 | 0.03 |
| 1:B:41:TYR:CB | 1:D:343:LEU:C[2_546] | 2.17 | 0.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:57:PRO:CB | 1:D:118:GLU:N[2_546] | 2.17 | 0.03 |
| 1:B:267:ARG:O | 1:D:183:HIS:ND1[2_546] | 2.17 | 0.03 |
| 1:B:26:GLY:N | 1:D:316:SER:OG[2_546] | 2.17 | 0.03 |
| 1:B:175:LYS:CE | 1:D:348:GLU:CD[2_546] | 2.17 | 0.03 |
| 1:B:225:ALA:C | 1:D:25:LYS:CA[2_546] | 2.17 | 0.03 |
| 1:B:24:GLU:OE1 | 1:D:321:TYR:N[2_546] | 2.17 | 0.03 |
| 1:B:173:MET:CA | 1:C:363:TYR:CZ[2_546] | 2.17 | 0.03 |
| 1:B:308:ILE:O | 1:D:310:PRO:CD[2_546] | 2.17 | 0.03 |
| 1:B:177:LEU:N | 1:D:31:ARG:C[2_546] | 2.17 | 0.03 |
| 1:B:254:MET:C | 1:D:263:THR:CB[2_546] | 2.17 | 0.03 |
| 1:B:254:MET:CA | 1:D:263:THR:OG1[2_546] | 2.17 | 0.03 |
| 1:A:108:LYS:CB | 1:A:247:VAL:CG1[2_556] | 2.17 | 0.03 |
| 1:B:320:PHE:CA | 1:C:367:GLU:CB[2_546] | 2.17 | 0.03 |
| 1:B:180:TYR:CZ | 1:D:29:ARG:N[2_546] | 2.17 | 0.03 |
| 1:A:365:GLY:N | 1:D:154:LYS:CA[2_546] | 2.17 | 0.03 |
| 1:A:366:PRO:C | 1:D:156:PHE:CB[2_546] | 2.17 | 0.03 |
| 1:B:263:THR:CA | 1:D:311:ASN:O[2_546] | 2.17 | 0.03 |
| 1:B:347:ILE:CD1 | 1:D:59:LYS:CG[2_546] | 2.17 | 0.03 |
| 1:B:320:PHE:CE2 | 1:C:367:GLU:C[2_546] | 2.17 | 0.03 |
| 1:A:108:LYS:CB | 1:A:248:ASN:CA[2_556] | 2.17 | 0.03 |
| 1:B:303:PHE:CG | 1:D:308:ILE:O[2_546] | 2.17 | 0.03 |
| 1:B:260:VAL:C | 1:D:271:PHE:N[2_546] | 2.17 | 0.03 |
| 1:B:329:MET:O | 1:C:368:TYR:CB[2_546] | 2.17 | 0.03 |
| 1:B:340:LEU:O | 1:D:46:GLU:CG[2_546] | 2.17 | 0.03 |
| 1:B:51:MET:CB | 1:D:49:TYR:N[2_546] | 2.17 | 0.03 |
| 1:B:57:PRO:CB | 1:D:117:LYS:CB[2_546] | 2.17 | 0.03 |
| 1:B:17:ASN:OD1 | 1:D:151:SER:CB[2_546] | 2.17 | 0.03 |
| 1:B:258:HIS:CB | 1:D:268:ALA:CB[2_546] | 2.17 | 0.03 |
| 1:B:296:GLU:OE1 | 1:D:260:VAL:CA[2_546] | 2.17 | 0.03 |
| 1:B:179:LEU:C | 1:D:30:TYR:CB[2_546] | 2.17 | 0.03 |
| 1:B:259:ARG:CG | 1:D:273:LYS:CB[2_546] | 2.17 | 0.03 |
| 1:A:367:GLU:O | 1:D:336:LEU:CG[2_546] | 2.18 | 0.02 |
| 1:B:39:VAL:O | 1:D:345:HIS:CD2[2_546] | 2.18 | 0.02 |
| 1:B:345:HIS:CG | 1:D:42:GLY:C[2_546] | 2.18 | 0.02 |
| 1:B:342:TRP:CB | 1:C:371:TYR:OH[2_546] | 2.18 | 0.02 |
| 1:B:265:ASP:N | 1:D:267:ARG:NH2[2_546] | 2.18 | 0.02 |
| 1:B:261:TYR:CE1 | 1:D:267:ARG:CG[2_546] | 2.18 | 0.02 |
| 1:B:41:TYR:CD2 | 1:D:346:ILE:CD1[2_546] | 2.18 | 0.02 |
| 1:B:20:PHE:CD1 | 1:D:173:MET:CB[2_546] | 2.18 | 0.02 |
| 1:A:364:VAL:C | 1:D:154:LYS:CA[2_546] | 2.18 | 0.02 |
| 1:B:256:PHE:CG | 1:D:264:TYR:N[2_546] | 2.18 | 0.02 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:46:GLU:CA | 1:D:53:TYR:N[2_546] | 2.18 | 0.02 |
| 1:A:363:TYR:CG | 1:D:174:ASP:N[2_546] | 2.18 | 0.02 |
| 1:B:168:ASP:O | 1:C:362:LEU:O[2_546] | 2.18 | 0.02 |
| 1:B:156:PHE:CE2 | 1:C:366:PRO:CD[2_546] | 2.18 | 0.02 |
| 1:A:240:ASN:ND2 | 1:B:216:PRO:CA[2_546] | 2.18 | 0.02 |
| 1:B:48:ILE:O | 1:D:49:TYR:CE1[2_546] | 2.18 | 0.02 |
| 1:B:256:PHE:CD1 | 1:D:264:TYR:N[2_546] | 2.18 | 0.02 |
| 1:B:261:TYR:CE1 | 1:D:267:ARG:O[2_546] | 2.18 | 0.02 |
| 1:B:35:ILE:CA | 1:D:181:THR:CB[2_546] | 2.18 | 0.02 |
| 1:A:111:LYS:CA | 1:A:245:LYS:CB[2_556] | 2.18 | 0.02 |
| 1:A:119:LYS:CG | 1:A:249:GLN:NE2[2_556] | 2.18 | 0.02 |
| 1:B:310:PRO:C | 1:D:265:ASP:N[2_546] | 2.18 | 0.02 |
| 1:B:270:ILE:CD1 | 1:D:183:HIS:CA[2_546] | 2.18 | 0.02 |
| 1:B:296:GLU:CG | 1:D:261:TYR:O[2_546] | 2.18 | 0.02 |
| 1:B:26:GLY:N | 1:D:180:TYR:CZ[2_546] | 2.18 | 0.02 |
| 1:B:117:LYS:CD | 1:D:61:GLU:C[2_546] | 2.18 | 0.02 |
| 1:B:269:LYS:CA | 1:D:184:GLU:CD[2_546] | 2.18 | 0.02 |
| 1:B:271:PHE:CE1 | 1:D:28:LEU:C[2_546] | 2.18 | 0.02 |
| 1:B:178:ILE:N | 1:D:31:ARG:N[2_546] | 2.18 | 0.02 |
| 1:B:296:GLU:CA | 1:D:262:LYS:CD[2_546] | 2.18 | 0.02 |
| 1:B:262:LYS:CA | 1:D:314:PHE:N[2_546] | 2.18 | 0.02 |
| 1:B:57:PRO:N | 1:D:118:GLU:CA[2_546] | 2.18 | 0.02 |
| 1:B:177:LEU:CA | 1:D:30:TYR:C[2_546] | 2.18 | 0.02 |
| 1:B:31:ARG:C | 1:D:44:TYR:CE2[2_546] | 2.18 | 0.02 |
| 1:B:265:ASP:CB | 1:D:265:ASP:CG[2_546] | 2.18 | 0.02 |
| 1:B:26:GLY:C | 1:D:180:TYR:CD2[2_546] | 2.18 | 0.02 |
| 1:B:62:LEU:C | 1:D:117:LYS:NZ[2_546] | 2.18 | 0.02 |
| 1:B:20:PHE:CD1 | 1:D:173:MET:CE[2_546] | 2.18 | 0.02 |
| 1:A:369:GLN:CB | 1:D:125:ALA:N[2_546] | 2.18 | 0.02 |
| 1:A:368:TYR:CG | 1:D:336:LEU:CD1[2_546] | 2.18 | 0.02 |
| 1:B:28:LEU:CA | 1:D:176:ALA:O[2_546] | 2.18 | 0.02 |
| 1:B:37:ASP:O | 1:D:342:TRP:N[2_546] | 2.19 | 0.01 |
| 1:B:173:MET:O | 1:D:17:ASN:CG[2_546] | 2.19 | 0.01 |
| 1:B:172:ALA:CA | 1:C:363:TYR:CB[2_546] | 2.19 | 0.01 |
| 1:B:320:PHE:N | 1:C:367:GLU:OE1[2_546] | 2.19 | 0.01 |
| 1:B:179:LEU:C | 1:D:30:TYR:CD1[2_546] | 2.19 | 0.01 |
| 1:B:314:PHE:N | 1:D:26:GLY:N[2_546] | 2.19 | 0.01 |
| 1:B:52:LEU:CB | 1:D:62:LEU:N[2_546] | 2.19 | 0.01 |
| 1:B:20:PHE:C | 1:D:173:MET:O[2_546] | 2.19 | 0.01 |
| 1:B:29:ARG:O | 1:D:44:TYR:CD1[2_546] | 2.19 | 0.01 |
| 1:B:242:PHE:CE1 | 1:D:304:SER:C[2_546] | 2.19 | 0.01 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:51:MET:CG | 1:D:49:TYR:N[2_546] | 2.19 | 0.01 |
| 1:A:362:LEU:C | 1:D:170:ILE:CG2[2_546] | 2.19 | 0.01 |
| 1:B:308:ILE:CA | 1:D:310:PRO:CD[2_546] | 2.19 | 0.01 |
| 1:B:262:LYS:C | 1:D:313:ASP:C[2_546] | 2.19 | 0.01 |
| 1:A:362:LEU:CA | 1:D:170:ILE:C[2_546] | 2.19 | 0.01 |
| 1:B:52:LEU:CD1 | 1:D:57:PRO:C[2_546] | 2.19 | 0.01 |
| 1:B:184:GLU:OE2 | 1:D:270:ILE:CA[2_546] | 2.19 | 0.01 |
| 1:B:45:GLU:C | 1:D:53:TYR:CB[2_546] | 2.19 | 0.01 |
| 1:B:49:TYR:CD2 | 1:D:53:TYR:OH[2_546] | 2.19 | 0.01 |
| 1:B:255:GLY:N | 1:D:263:THR:OG1[2_546] | 2.19 | 0.01 |
| 1:B:306:LYS:CD | 1:D:297:GLU:C[2_546] | 2.19 | 0.01 |
| 1:B:314:PHE:C | 1:D:23:GLY:C[2_546] | 2.19 | 0.01 |
| 1:B:183:HIS:C | 1:D:39:VAL:C[2_546] | 2.19 | 0.01 |
| 1:B:333:LEU:N | 1:C:369:GLN:N[2_546] | 2.19 | 0.01 |
| 1:B:303:PHE:CZ | 1:D:304:SER:N[2_546] | 2.19 | 0.01 |
| 1:B:56:LEU:CD1 | 1:D:120:ALA:CA[2_546] | 2.19 | 0.01 |
| 1:B:45:GLU:N | 1:D:54:GLY:CA[2_546] | 2.19 | 0.01 |
| 1:B:44:TYR:CD1 | 1:D:50:LEU:O[2_546] | 2.19 | 0.01 |
| 1:A:369:GLN:CG | 1:D:124:ILE:C[2_546] | 2.19 | 0.01 |
| 1:B:229:PHE:CZ | 1:D:24:GLU:N[2_546] | 2.19 | 0.01 |

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 | 365/377 (97%) | 338 (93%) | 24 (7%) | 3 (1%) | 22 | 49 |
| 1 | B | 364/377 (97%) | 343 (94%) | 18 (5%) | 3 (1%) | 22 | 49 |
| 1 | C | 368/377 (98%) | 344 (94%) | 22 (6%) | 2 (0%) | 32 | 60 |
| 1 | D | 363/377 (96%) | 344 (95%) | 14 (4%) | 5 (1%) | 13 | 33 |
| All | All | 1460/1508 (97%) | 1369 (94%) | 78 (5%) | 13 (1%) | 20 | 46 |

All (13) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 247 | VAL |
| 1 | B | 247 | VAL |
| 1 | D | 233 | GLY |
| 1 | B | 109 | ASN |
| 1 | D | 238 | VAL |
| 1 | B | 246 | VAL |
| 1 | C | 247 | VAL |
| 1 | A | 108 | LYS |
| 1 | A | 183 | HIS |
| 1 | D | 244 | ASP |
| 1 | C | 143 | PRO |
| 1 | D | 246 | VAL |
| 1 | D | 216 | PRO |

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 | 309/319 (97%) | 277 (90%) | 32 (10%) | 8 | 18 |
| 1 | B | 308/319 (97%) | 284 (92%) | 24 (8%) | 15 | 33 |
| 1 | C | 312/319 (98%) | 288 (92%) | 24 (8%) | 15 | 34 |
| 1 | D | 307/319 (96%) | 267 (87%) | 40 (13%) | 5 | 11 |
| All | All | 1236/1276 (97%) | 1116 (90%) | 120 (10%) | 9 | 22 |

All (120) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 6 | LYS |
| 1 | A | 14 | LYS |
| 1 | A | 35 | ILE |
| 1 | A | 39 | VAL |
| 1 | A | 55 | LYS |
| 1 | A | 59 | LYS |
| 1 | A | 60 | LYS |
| 1 | A | 68 | LYS |
| 1 | A | 89 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 96 | LEU |
| 1 | A | 108 | LYS |
| 1 | A | 111 | LYS |
| 1 | A | 115 | ASN |
| 1 | A | 119 | LYS |
| 1 | A | 127 | MET |
| 1 | A | 136 | ARG |
| 1 | A | 137 | ARG |
| 1 | A | 149 | SER |
| 1 | A | 150 | ASP |
| 1 | A | 163 | ARG |
| 1 | A | 180 | TYR |
| 1 | A | 229 | PHE |
| 1 | A | 234 | ASP |
| 1 | A | 244 | ASP |
| 1 | A | 262 | LYS |
| 1 | A | 267 | ARG |
| 1 | A | 277 | THR |
| 1 | A | 281 | ARG |
| 1 | A | 282 | ASN |
| 1 | A | 297 | GLU |
| 1 | A | 305 | SER |
| 1 | A | 358 | ARG |
| 1 | B | 35 | ILE |
| 1 | B | 36 | GLU |
| 1 | B | 55 | LYS |
| 1 | B | 60 | LYS |
| 1 | B | 85 | LEU |
| 1 | B | 96 | LEU |
| 1 | B | 115 | ASN |
| 1 | B | 122 | SER |
| 1 | B | 137 | ARG |
| 1 | B | 138 | LYS |
| 1 | B | 144 | ARG |
| 1 | B | 149 | SER |
| 1 | B | 158 | LEU |
| 1 | B | 163 | ARG |
| 1 | B | 181 | THR |
| 1 | B | 201 | ASP |
| 1 | B | 250 | LYS |
| 1 | B | 259 | ARG |
| 1 | B | 267 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 276 | LEU |
| 1 | B | 278 | LEU |
| 1 | B | 281 | ARG |
| 1 | B | 286 | ARG |
| 1 | B | 290 | GLU |
| 1 | C | 3 | VAL |
| 1 | C | 5 | SER |
| 1 | C | 6 | LYS |
| 1 | C | 10 | ASN |
| 1 | C | 24 | GLU |
| 1 | C | 29 | ARG |
| 1 | C | 36 | GLU |
| 1 | C | 77 | GLN |
| 1 | C | 96 | LEU |
| 1 | C | 105 | SER |
| 1 | C | 108 | LYS |
| 1 | C | 111 | LYS |
| 1 | C | 115 | ASN |
| 1 | C | 127 | MET |
| 1 | C | 142 | LYS |
| 1 | C | 149 | SER |
| 1 | C | 158 | LEU |
| 1 | C | 163 | ARG |
| 1 | C | 237 | ARG |
| 1 | C | 267 | ARG |
| 1 | C | 276 | LEU |
| 1 | C | 277 | THR |
| 1 | C | 282 | ASN |
| 1 | C | 351 | GLU |
| 1 | D | 4 | VAL |
| 1 | D | 5 | SER |
| 1 | D | 9 | GLU |
| 1 | D | 35 | ILE |
| 1 | D | 43 | SER |
| 1 | D | 55 | LYS |
| 1 | D | 105 | SER |
| 1 | D | 108 | LYS |
| 1 | D | 115 | ASN |
| 1 | D | 122 | SER |
| 1 | D | 137 | ARG |
| 1 | D | 149 | SER |
| 1 | D | 150 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 158 | LEU |
| 1 | D | 163 | ARG |
| 1 | D | 180 | TYR |
| 1 | D | 185 | VAL |
| 1 | D | 205 | SER |
| 1 | D | 218 | HIS |
| 1 | D | 252 | ARG |
| 1 | D | 259 | ARG |
| 1 | D | 262 | LYS |
| 1 | D | 264 | TYR |
| 1 | D | 267 | ARG |
| 1 | D | 273 | LYS |
| 1 | D | 276 | LEU |
| 1 | D | 277 | THR |
| 1 | D | 282 | ASN |
| 1 | D | 284 | ASP |
| 1 | D | 293 | GLN |
| 1 | D | 294 | LYS |
| 1 | D | 295 | LEU |
| 1 | D | 305 | SER |
| 1 | D | 328 | TYR |
| 1 | D | 352 | GLU |
| 1 | D | 353 | GLN |
| 1 | D | 355 | ARG |
| 1 | D | 357 | ILE |
| 1 | D | 358 | ARG |
| 1 | D | 362 | LEU |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 115 | ASN |
| 1 | A | 183 | HIS |
| 1 | A | 228 | GLN |
| 1 | A | 251 | ASN |
| 1 | A | 258 | HIS |
| 1 | A | 282 | ASN |
| 1 | A | 369 | GLN |
| 1 | B | 115 | ASN |
| 1 | B | 183 | HIS |
| 1 | B | 228 | GLN |
| 1 | B | 258 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 354 | HIS |
| 1 | C | 77 | GLN |
| 1 | C | 115 | ASN |
| 1 | C | 183 | HIS |
| 1 | C | 228 | GLN |
| 1 | C | 258 | HIS |
| 1 | C | 282 | ASN |
| 1 | D | 115 | ASN |
| 1 | D | 183 | HIS |
| 1 | D | 228 | GLN |
| 1 | D | 258 | HIS |
| 1 | D | 282 | ASN |
| 1 | D | 293 | GLN |
| 1 | D | 353 | 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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.