



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:51 AM GMT

PDB ID : 2BYB
Title : HUMAN MONOAMINE OXIDASE B IN COMPLEX WITH DEPRENYL
Authors : Binda, C.; De Colibus, L.; Edmondson, D.E.; Mattevi, A.
Deposited on : 2005-07-29
Resolution : 2.20 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

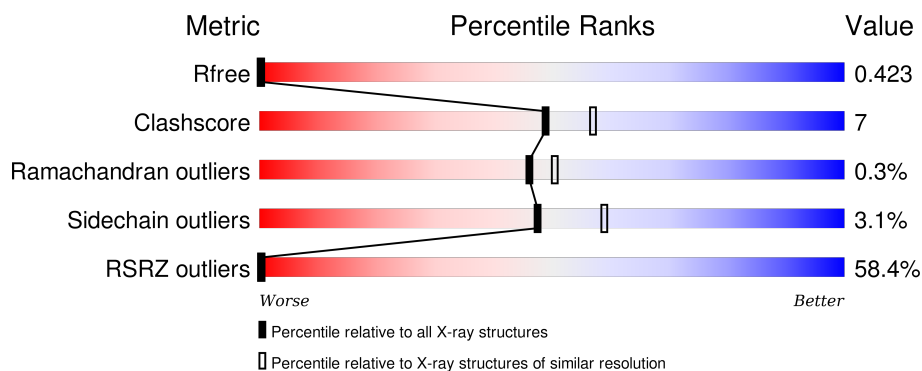
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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)) |
|-----------------------|-----------------------------|---|
| R_{free} | 91344 | 3774 (2.20-2.20) |
| Clashscore | 102246 | 4477 (2.20-2.20) |
| Ramachandran outliers | 100387 | 4404 (2.20-2.20) |
| Sidechain outliers | 100360 | 4405 (2.20-2.20) |
| RSRZ outliers | 91569 | 3781 (2.20-2.20) |

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.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 520 | |
| 1 | B | 520 | |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2 | FAD | A | 600 | - | - | X | - |
| 3 | DPK | A | 601 | - | - | - | X |
| 3 | DPK | B | 601 | - | - | - | X |

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8534 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 AMINE OXIDASE [FLAVIN-CONTAINING] B.

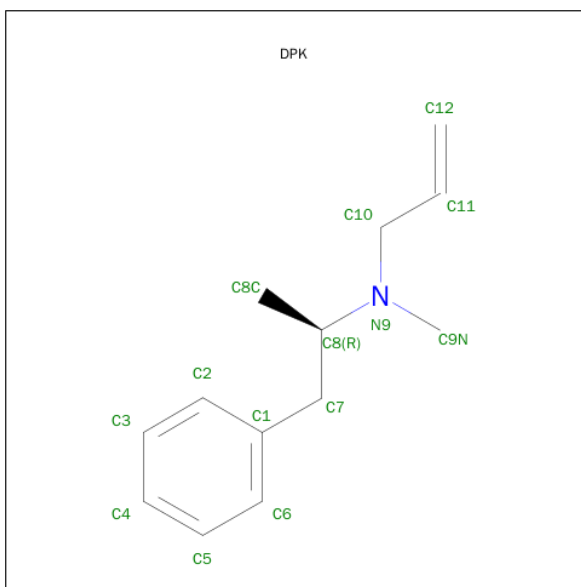
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 499 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3971 | 2538 | 681 | 728 | 24 | | | |
| 1 | B | 494 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3940 | 2519 | 676 | 721 | 24 | | | |

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 2 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 27 | 9 | 15 | 2 | | |
| 2 | B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 27 | 9 | 15 | 2 | | |

- Molecule 3 is DEPRENYL (three-letter code: DPK) (formula: $C_{13}H_{19}N$).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 3 | A | 1 | Total | C | N | 0 | 0 |
| | | | 14 | 13 | 1 | | |
| 3 | B | 1 | Total | C | N | 0 | 0 |
| | | | 14 | 13 | 1 | | |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 4 | A | 233 | Total | O | 0 | 0 |
| | | | 233 | 233 | | |
| 4 | B | 256 | Total | O | 0 | 0 |
| | | | 256 | 256 | | |

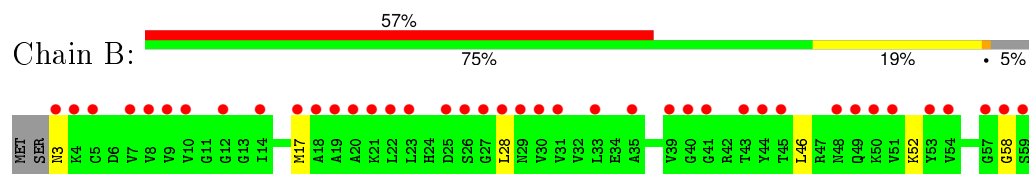
3 Residue-property plots

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

• Molecule 1: AMINE OXIDASE [FLAVIN-CONTAINING] B



• Molecule 1: AMINE OXIDASE [FLAVIN-CONTAINING] B



| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| A474 | Q475 | P476 | I477 | T478 | T479 | T480 | F481 | L482 | E483 | R484 | H485 | V489 | P490 | G491 | L492 | L493 | R494 | L495 | I496 | GLY | LEU | THR | THR | THR | ILE | PHE | SER | ALA | ALA | THR | ALA | LEU | GLY | PHE | LEU | ALA | HIS | LYS | ARG | GLY | LEU | LEU | VAL | ARG | VAL | | | | | | | | | | | | | |
| G411 | R412 | V413 | I414 | R415 | Q416 | P417 | V418 | D419 | R420 | I421 | Y422 | F423 | A424 | G425 | T426 | E427 | T428 | A429 | T430 | H431 | W432 | S433 | G434 | Y435 | V440 | E441 | A442 | G443 | E444 | R445 | A446 | A447 | R448 | E449 | I450 | L451 | R452 | A453 | M454 | G455 | K456 | I457 | P458 | E459 | D460 | E461 | I462 | W463 | Q464 | S465 | E466 | P467 | E468 | S469 | V470 | D471 | V472 | P473 |
| I340 | R341 | F342 | F343 | I344 | I345 | A346 | H347 | K351 | L352 | A353 | R354 | L355 | E358 | L361 | K362 | K363 | L364 | L367 | V368 | A369 | L372 | E376 | A377 | L378 | E379 | P380 | V381 | H382 | V383 | E384 | E385 | K386 | N387 | W388 | Q392 | Y393 | S394 | G395 | G396 | C397 | Y398 | T399 | T400 | V401 | F402 | P403 | I406 | L407 | T408 | Q409 | Y410 | | | | | | | |
| G269 | M270 | K271 | I272 | H273 | F274 | N275 | M280 | M281 | R282 | N283 | I286 | L291 | V294 | I295 | K296 | C297 | I298 | V299 | Y300 | Y301 | K302 | E303 | P304 | F305 | W306 | R307 | K308 | K309 | D310 | Y311 | C312 | G313 | I317 | G319 | E320 | E321 | A322 | P323 | V324 | A325 | H252 | Y326 | T327 | L328 | D329 | D330 | T331 | K332 | P333 | E334 | G335 | N336 | Y337 | | | | | |
| L139 | A140 | W143 | D144 | N145 | M146 | T147 | M148 | K149 | E150 | L151 | L152 | D153 | K154 | L155 | C156 | T158 | E159 | K162 | Q163 | L164 | A165 | T166 | L167 | F168 | V169 | M170 | L171 | G172 | V173 | T174 | A175 | E176 | T177 | H178 | E179 | V180 | S181 | A182 | L183 | W184 | F185 | L186 | W187 | Y188 | V189 | K190 | Q191 | C192 | E193 | G194 | T195 | I198 | I199 | S200 | T201 | | | |
| M66 | R67 | L68 | R70 | L71 | A72 | K73 | L77 | Y80 | K81 | V82 | M83 | E84 | V85 | L88 | V92 | K93 | G94 | K95 | S96 | Y97 | P98 | F99 | R100 | G101 | P102 | F103 | P104 | P105 | V106 | W107 | N108 | P109 | I110 | T111 | Y112 | N116 | N117 | F118 | W119 | R120 | T121 | M122 | G126 | R127 | E128 | I129 | A133 | K136 | A137 | P138 | | | | | | | | |
| G204 | R208 | K209 | F210 | V211 | G212 | G213 | S214 | G215 | Q216 | V217 | R220 | M221 | D222 | L224 | L225 | G226 | D227 | R228 | V229 | K230 | L231 | E232 | R233 | P234 | V235 | I236 | Y237 | L238 | D239 | Q240 | T241 | R242 | E243 | N244 | V245 | L246 | V247 | E248 | T249 | L250 | N251 | H252 | Y255 | K258 | Y259 | V260 | I261 | S262 | A263 | I264 | P265 | L268 | | | | | | |

4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | C 2 2 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 132.84Å 225.84Å 85.68Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 15.00 – 2.20 29.86 – 2.00 | Depositor EDS |
| % Data completeness (in resolution range) | 95.0 (15.00-2.20) 95.7 (29.86-2.00) | Depositor EDS |
| R_{merge} | 0.09 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.72 (at 2.00Å) | Xtriage |
| Refinement program | REFMAC 5.2.0005 | Depositor |
| R, R_{free} | 0.237 , 0.299 0.399 , 0.423 | Depositor DCC |
| R_{free} test set | 1606 reflections (2.65%) | DCC |
| Wilson B-factor (Å ²) | 25.8 | Xtriage |
| Anisotropy | 0.758 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.35 , 46.9 | EDS |
| Estimated twinning fraction | 0.006 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.021 for 1/2*h+1/2*k,3/2*h-1/2*k,-l | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$ | Xtriage |
| Outliers | 23 of 83353 reflections (0.028%) | Xtriage |
| F_o, F_c correlation | 0.74 | EDS |
| Total number of atoms | 8534 | wwPDB-VP |
| Average B, all atoms (Å ²) | 32.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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 | 0.79 | 1/4068 (0.0%) | 0.80 | 2/5522 (0.0%) |
| 1 | B | 0.88 | 3/4037 (0.1%) | 0.86 | 5/5479 (0.1%) |
| All | All | 0.84 | 4/8105 (0.0%) | 0.83 | 7/11001 (0.1%) |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | B | 156 | CYS | CB-SG | -6.55 | 1.71 | 1.82 |
| 1 | B | 176 | GLU | CB-CG | 5.24 | 1.62 | 1.52 |
| 1 | B | 393 | TYR | CD1-CE1 | 5.11 | 1.47 | 1.39 |
| 1 | A | 300 | TYR | CD2-CE2 | 5.03 | 1.46 | 1.39 |

All (7) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | B | 144 | ASP | CB-CG-OD2 | -6.15 | 112.77 | 118.30 |
| 1 | B | 144 | ASP | CB-CG-OD1 | 5.88 | 123.60 | 118.30 |
| 1 | A | 445 | ARG | NE-CZ-NH2 | -5.81 | 117.40 | 120.30 |
| 1 | B | 310 | ASP | CB-CG-OD1 | 5.71 | 123.44 | 118.30 |
| 1 | B | 448 | ARG | NE-CZ-NH2 | -5.24 | 117.68 | 120.30 |
| 1 | B | 146 | MET | CB-CA-C | -5.10 | 100.19 | 110.40 |
| 1 | A | 155 | LEU | CA-CB-CG | 5.10 | 127.03 | 115.30 |

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 | 3971 | 0 | 3967 | 59 | 1344 |
| 1 | B | 3940 | 0 | 3937 | 60 | 22 |
| 2 | A | 53 | 0 | 29 | 2 | 60 |
| 2 | B | 53 | 0 | 29 | 2 | 0 |
| 3 | A | 14 | 0 | 17 | 0 | 0 |
| 3 | B | 14 | 0 | 17 | 1 | 0 |
| 4 | A | 233 | 0 | 0 | 7 | 132 |
| 4 | B | 256 | 0 | 0 | 16 | 3 |
| All | All | 8534 | 0 | 7996 | 116 | 1369 |

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 7.

All (116) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:464:GLN:NE2 | 4:B:2244:HOH:O | 1.79 | 1.14 |
| 1:B:117:ASN:HD22 | 1:B:120:ARG:HH21 | 1.12 | 0.96 |
| 1:A:92:VAL:HG22 | 1:A:318:ASP:OD2 | 1.75 | 0.84 |
| 1:B:414:LEU:HD12 | 4:B:2217:HOH:O | 1.78 | 0.83 |
| 1:A:117:ASN:HD22 | 1:A:120:ARG:HH21 | 1.29 | 0.80 |
| 1:B:195:THR:O | 1:B:199:ILE:HG23 | 1.83 | 0.79 |
| 1:B:28:LEU:HD11 | 1:B:454:MET:HE1 | 1.65 | 0.77 |
| 1:B:159:GLU:O | 1:B:163:GLN:HG3 | 1.86 | 0.74 |
| 1:A:126:GLY:HA2 | 1:A:129:ILE:HD12 | 1.72 | 0.72 |
| 1:A:28:LEU:HD11 | 1:A:454:MET:HE1 | 1.72 | 0.70 |
| 1:A:195:THR:O | 1:A:199:ILE:HG23 | 1.91 | 0.70 |
| 1:A:270:MET:HB3 | 1:B:270:MET:HB3 | 1.75 | 0.68 |
| 1:B:251:ASN:H | 1:B:251:ASN:HD22 | 1.43 | 0.65 |
| 1:A:265:PRO:HD2 | 1:A:268:LEU:HD12 | 1.79 | 0.65 |
| 1:A:296:LYS:NZ | 4:A:2139:HOH:O | 2.21 | 0.65 |
| 1:B:412:ARG:HD2 | 4:B:2219:HOH:O | 1.99 | 0.62 |
| 1:B:92:VAL:HG22 | 1:B:318:ASP:OD2 | 1.99 | 0.62 |
| 1:B:323:PRO:HD2 | 1:B:367:LEU:HD22 | 1.82 | 0.61 |
| 1:A:480:THR:O | 1:A:484:ARG:HG3 | 2.00 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:323:PRO:HD2 | 1:A:367:LEU:HD22 | 1.83 | 0.60 |
| 1:A:321:GLU:CD | 1:A:321:GLU:H | 2.04 | 0.60 |
| 1:B:84:GLU:HG2 | 1:B:84:GLU:O | 2.01 | 0.60 |
| 1:A:149:LYS:HD3 | 4:B:2089:HOH:O | 2.02 | 0.59 |
| 1:A:251:ASN:H | 1:A:251:ASN:HD22 | 1.48 | 0.59 |
| 1:B:363:LYS:HD3 | 4:B:2187:HOH:O | 2.03 | 0.57 |
| 1:B:392:GLN:O | 4:B:2209:HOH:O | 2.17 | 0.57 |
| 1:A:454:MET:HE3 | 1:A:456:LYS:HE3 | 1.88 | 0.56 |
| 1:B:445:ARG:HD2 | 1:B:463:TRP:CZ2 | 2.41 | 0.56 |
| 1:B:398:TYR:N | 4:B:2102:HOH:O | 2.39 | 0.55 |
| 1:A:270:MET:CB | 1:B:270:MET:HB3 | 2.37 | 0.55 |
| 1:A:84:GLU:O | 1:A:84:GLU:HG2 | 2.07 | 0.55 |
| 1:A:445:ARG:HD2 | 1:A:463:TRP:CH2 | 2.42 | 0.55 |
| 1:B:100:ARG:HH11 | 1:B:100:ARG:HG2 | 1.71 | 0.54 |
| 1:B:191:GLN:O | 1:B:431:HIS:HD2 | 1.89 | 0.54 |
| 1:B:116:ASN:HB3 | 4:B:2064:HOH:O | 2.07 | 0.54 |
| 1:A:171:LEU:HD21 | 1:A:326:TYR:CG | 2.43 | 0.54 |
| 1:A:252:HIS:NE2 | 1:B:248:GLU:OE2 | 2.33 | 0.54 |
| 1:B:427:GLU:O | 4:B:2231:HOH:O | 2.18 | 0.53 |
| 1:A:370:LYS:CE | 4:A:2168:HOH:O | 2.56 | 0.53 |
| 1:A:309:LYS:HE3 | 4:A:2144:HOH:O | 2.08 | 0.52 |
| 1:A:270:MET:HB3 | 1:B:270:MET:CB | 2.38 | 0.52 |
| 1:B:321:GLU:CD | 1:B:321:GLU:H | 2.11 | 0.52 |
| 1:B:400:THR:HB | 1:B:427:GLU:HG2 | 1.93 | 0.51 |
| 1:B:265:PRO:HD2 | 1:B:268:LEU:HD12 | 1.93 | 0.51 |
| 1:A:251:ASN:ND2 | 1:A:251:ASN:H | 2.08 | 0.51 |
| 1:A:445:ARG:HD2 | 1:A:463:TRP:CZ2 | 2.46 | 0.51 |
| 1:B:480:THR:O | 1:B:484:ARG:HG3 | 2.11 | 0.50 |
| 1:A:207:GLU:HG2 | 1:A:208:ARG:HG3 | 1.94 | 0.50 |
| 1:B:251:ASN:H | 1:B:251:ASN:ND2 | 2.08 | 0.50 |
| 1:A:88:LEU:HD12 | 1:A:88:LEU:N | 2.27 | 0.49 |
| 1:A:117:ASN:HD22 | 1:A:120:ARG:NH2 | 2.02 | 0.49 |
| 1:B:133:ALA:O | 1:B:136:LYS:HB2 | 2.13 | 0.49 |
| 1:B:445:ARG:HD2 | 1:B:463:TRP:CH2 | 2.47 | 0.49 |
| 1:A:281:MET:HB3 | 1:A:413:VAL:HG21 | 1.95 | 0.49 |
| 1:B:450:ILE:O | 1:B:454:MET:HG3 | 2.13 | 0.49 |
| 2:A:600:FAD:N1 | 2:A:600:FAD:H2' | 2.28 | 0.48 |
| 1:A:350:ARG:HD2 | 1:B:410:TYR:OH | 2.12 | 0.48 |
| 2:B:600:FAD:H2' | 2:B:600:FAD:N1 | 2.28 | 0.48 |
| 1:A:389:CYS:HB3 | 1:B:280:MET:HG3 | 1.95 | 0.48 |
| 1:A:201:THR:O | 1:A:207:GLU:HB2 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:331:THR:HG22 | 1:B:332:LYS:N | 2.29 | 0.48 |
| 1:B:174:THR:OG1 | 4:B:2102:HOH:O | 2.20 | 0.48 |
| 1:A:315:MET:HB2 | 1:A:327:THR:OG1 | 2.14 | 0.47 |
| 1:B:331:THR:HG22 | 1:B:332:LYS:H | 1.80 | 0.47 |
| 1:B:461:GLU:O | 4:B:2244:HOH:O | 2.21 | 0.47 |
| 1:A:217:VAL:O | 1:A:221:ILE:HG13 | 2.14 | 0.46 |
| 1:A:191:GLN:O | 1:A:431:HIS:HD2 | 1.99 | 0.45 |
| 1:B:296:LYS:NZ | 4:B:2155:HOH:O | 2.47 | 0.45 |
| 1:A:149:LYS:CD | 4:B:2089:HOH:O | 2.60 | 0.45 |
| 1:A:400:THR:HB | 1:A:427:GLU:HG2 | 1.97 | 0.45 |
| 1:B:233:ARG:HG3 | 1:B:251:ASN:HD21 | 1.80 | 0.45 |
| 1:A:271:LYS:HG2 | 1:B:270:MET:O | 2.16 | 0.45 |
| 1:A:149:LYS:CE | 4:A:2086:HOH:O | 2.55 | 0.45 |
| 1:A:134:PRO:HD2 | 1:A:135:TRP:CZ3 | 2.52 | 0.45 |
| 1:B:165:ALA:O | 1:B:168:PHE:HB3 | 2.17 | 0.45 |
| 1:A:159:GLU:O | 1:A:163:GLN:HG3 | 2.17 | 0.45 |
| 1:A:188:TYR:O | 1:A:191:GLN:HG3 | 2.16 | 0.44 |
| 1:B:312:CYS:O | 1:B:329:ASP:HB2 | 2.16 | 0.44 |
| 1:B:171:LEU:HD21 | 1:B:326:TYR:CG | 2.52 | 0.44 |
| 1:B:117:ASN:ND2 | 1:B:120:ARG:HH21 | 1.95 | 0.44 |
| 1:A:117:ASN:ND2 | 1:A:120:ARG:HH21 | 2.05 | 0.44 |
| 1:A:406:ILE:HD11 | 4:B:2214:HOH:O | 2.18 | 0.44 |
| 1:B:185:PHE:O | 1:B:189:VAL:HG23 | 2.17 | 0.44 |
| 1:B:281:MET:HB3 | 1:B:413:VAL:HG21 | 1.99 | 0.44 |
| 1:A:370:LYS:HE3 | 4:A:2168:HOH:O | 2.16 | 0.44 |
| 4:A:2186:HOH:O | 1:B:406:ILE:HD11 | 2.17 | 0.44 |
| 1:B:282:ARG:HD2 | 4:B:2220:HOH:O | 2.16 | 0.43 |
| 1:B:176:GLU:OE2 | 1:B:346:ALA:HB1 | 2.18 | 0.43 |
| 1:A:233:ARG:HG3 | 1:A:251:ASN:HD21 | 1.84 | 0.43 |
| 1:B:126:GLY:HA2 | 1:B:129:ILE:HD12 | 2.00 | 0.43 |
| 1:A:134:PRO:HG3 | 1:A:187:TRP:CD1 | 2.53 | 0.43 |
| 1:A:42:ARG:NH2 | 1:A:265:PRO:HG3 | 2.34 | 0.43 |
| 1:A:89:ILE:HG21 | 1:A:371:VAL:CG1 | 2.49 | 0.43 |
| 1:B:237:TYR:HB3 | 1:B:248:GLU:HB3 | 2.01 | 0.43 |
| 1:A:133:ALA:O | 1:A:136:LYS:HB2 | 2.19 | 0.43 |
| 1:A:331:THR:HG22 | 1:A:332:LYS:N | 2.33 | 0.43 |
| 3:B:601:DPK:H9N1 | 3:B:601:DPK:H7C2 | 1.85 | 0.42 |
| 1:A:305:PHE:HA | 1:A:308:LYS:HD3 | 2.00 | 0.42 |
| 1:B:400:THR:HB | 1:B:427:GLU:CG | 2.49 | 0.42 |
| 1:A:278:LEU:HD13 | 1:A:282:ARG:HG2 | 2.02 | 0.42 |
| 1:A:278:LEU:HD23 | 1:A:278:LEU:HA | 1.90 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:143:TRP:O | 1:B:182:ALA:HB3 | 2.20 | 0.42 |
| 1:A:278:LEU:N | 4:A:2129:HOH:O | 2.35 | 0.42 |
| 1:B:327:THR:HG21 | 1:B:368:TYR:CE2 | 2.55 | 0.42 |
| 1:A:109:PRO:O | 1:A:113:LEU:HG | 2.20 | 0.42 |
| 1:B:88:LEU:N | 1:B:88:LEU:HD12 | 2.35 | 0.42 |
| 1:B:343:PHE:HB2 | 4:B:2174:HOH:O | 2.19 | 0.41 |
| 1:A:106:VAL:HG13 | 1:A:112:TYR:CD2 | 2.55 | 0.41 |
| 1:B:295:ILE:HA | 1:B:386:LYS:O | 2.21 | 0.41 |
| 1:B:451:LEU:HD23 | 1:B:454:MET:HE1 | 2.02 | 0.41 |
| 1:B:17:MET:HE3 | 1:B:221:ILE:HG22 | 2.02 | 0.41 |
| 1:A:60:TYR:HB3 | 1:A:206:GLN:HA | 2.02 | 0.41 |
| 2:A:600:FAD:H1'1 | 2:A:600:FAD:H9 | 1.77 | 0.41 |
| 1:B:58:GLY:HA2 | 2:B:600:FAD:C4X | 2.51 | 0.41 |
| 1:A:184:TRP:HB2 | 1:A:407:LEU:HD22 | 2.04 | 0.40 |
| 1:A:296:LYS:O | 1:A:385:GLU:HA | 2.22 | 0.40 |

All (1369) 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:A:67:ARG:NE | 1:A:222:MET:CB[3_655] | 0.21 | 1.99 |
| 1:A:76:GLY:C | 2:A:600:FAD:N1[3_655] | 0.29 | 1.91 |
| 1:A:223:ASP:O | 1:A:441:GLU:OE2[3_655] | 0.32 | 1.88 |
| 1:A:228:ARG:CB | 1:A:462:ILE:O[3_655] | 0.37 | 1.83 |
| 1:A:223:ASP:CA | 1:A:441:GLU:OE1[3_655] | 0.37 | 1.83 |
| 1:A:257:ALA:CB | 1:A:456:LYS:CB[3_655] | 0.38 | 1.82 |
| 1:A:223:ASP:C | 1:A:441:GLU:CD[3_655] | 0.40 | 1.80 |
| 1:A:53:TYR:CZ | 1:A:207:GLU:C[3_655] | 0.40 | 1.80 |
| 1:A:307:ARG:NH1 | 1:A:307:ARG:NH1[3_655] | 0.40 | 1.80 |
| 1:A:53:TYR:CA | 1:A:207:GLU:OE2[3_655] | 0.40 | 1.80 |
| 1:A:23:LEU:CG | 1:A:23:LEU:CG[3_655] | 0.41 | 1.79 |
| 1:A:53:TYR:CD2 | 1:A:207:GLU:CB[3_655] | 0.44 | 1.76 |
| 1:A:61:VAL:O | 1:A:212:GLY:CA[3_655] | 0.45 | 1.75 |
| 1:A:19:ALA:CB | 1:A:22:LEU:N[3_655] | 0.46 | 1.74 |
| 1:A:221:ILE:O | 1:A:441:GLU:CA[3_655] | 0.47 | 1.73 |
| 1:A:75:LEU:O | 1:A:435:TYR:C[3_655] | 0.48 | 1.72 |
| 1:A:29:ASN:CA | 1:A:449:GLU:C[3_655] | 0.48 | 1.72 |
| 1:A:210:PHE:CD1 | 1:A:210:PHE:CD1[3_655] | 0.51 | 1.69 |
| 1:A:83:ASN:CG | 1:A:335:GLY:CA[3_655] | 0.52 | 1.68 |
| 1:A:82:VAL:O | 1:A:332:LYS:CB[3_655] | 0.54 | 1.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:29:ASN:CB | 1:A:449:GLU:O[3_655] | 0.56 | 1.64 |
| 1:A:40:GLY:CA | 1:A:70:ARG:CB[3_655] | 0.57 | 1.63 |
| 1:A:30:VAL:CG2 | 1:A:448:ARG:N[3_655] | 0.59 | 1.61 |
| 1:A:19:ALA:O | 1:A:19:ALA:O[3_655] | 0.59 | 1.61 |
| 1:A:67:ARG:CB | 1:A:218:SER:O[3_655] | 0.61 | 1.59 |
| 1:A:55:ASP:OD2 | 1:A:79:THR:CB[3_655] | 0.61 | 1.59 |
| 1:A:74:GLU:N | 2:A:600:FAD:O4'[3_655] | 0.62 | 1.58 |
| 1:A:74:GLU:CG | 2:A:600:FAD:P[3_655] | 0.63 | 1.57 |
| 1:B:475:GLN:OE1 | 4:B:2058:HOH:O[3_555] | 0.64 | 1.56 |
| 1:A:258:LYS:O | 1:A:456:LYS:NZ[3_655] | 0.64 | 1.56 |
| 1:A:221:ILE:CA | 1:A:441:GLU:N[3_655] | 0.65 | 1.55 |
| 1:A:53:TYR:CE2 | 1:A:207:GLU:CA[3_655] | 0.65 | 1.55 |
| 1:B:478:THR:O | 1:B:478:THR:CB[3_555] | 0.65 | 1.55 |
| 1:A:39:VAL:CA | 1:A:466:GLU:OE2[3_655] | 0.65 | 1.55 |
| 1:A:25:ASP:OD1 | 1:A:424:ALA:CB[3_655] | 0.67 | 1.53 |
| 1:A:28:LEU:CA | 1:A:450:ILE:CG1[3_655] | 0.67 | 1.53 |
| 1:A:258:LYS:C | 1:A:456:LYS:NZ[3_655] | 0.68 | 1.52 |
| 1:A:501:ILE:C | 4:A:2054:HOH:O[6_565] | 0.68 | 1.52 |
| 1:A:84:GLU:C | 1:A:336:ASN:CB[3_655] | 0.69 | 1.51 |
| 1:A:229:VAL:CA | 1:A:464:GLN:CB[3_655] | 0.69 | 1.51 |
| 1:A:3:ASN:N | 1:A:458:PRO:CB[3_655] | 0.70 | 1.50 |
| 1:A:43:THR:OG1 | 1:A:69:LEU:O[3_655] | 0.70 | 1.50 |
| 1:A:47:ARG:NE | 1:A:63:PRO:CA[3_655] | 0.70 | 1.50 |
| 1:A:54:VAL:CA | 1:A:208:ARG:NH2[3_655] | 0.70 | 1.50 |
| 1:A:66:ASN:N | 1:A:219:GLU:CG[3_655] | 0.71 | 1.49 |
| 1:A:74:GLU:CD | 2:A:600:FAD:O1P[3_655] | 0.71 | 1.49 |
| 1:A:210:PHE:N | 1:A:210:PHE:N[3_655] | 0.72 | 1.48 |
| 1:A:26:SER:CA | 1:A:261:ILE:N[3_655] | 0.73 | 1.47 |
| 1:A:42:ARG:O | 1:A:73:LYS:CG[3_655] | 0.73 | 1.47 |
| 1:A:228:ARG:N | 1:A:463:TRP:CA[3_655] | 0.73 | 1.47 |
| 1:A:26:SER:N | 1:A:261:ILE:CB[3_655] | 0.74 | 1.46 |
| 1:A:69:LEU:CB | 1:A:215:GLY:CA[3_655] | 0.74 | 1.46 |
| 1:A:32:VAL:CB | 4:A:2209:HOH:O[3_655] | 0.75 | 1.45 |
| 1:A:14:ILE:CG1 | 1:A:71:LEU:C[3_655] | 0.76 | 1.44 |
| 1:A:221:ILE:CG2 | 1:A:440:VAL:O[3_655] | 0.76 | 1.44 |
| 1:A:68:ILE:CB | 1:A:217:VAL:N[3_655] | 0.76 | 1.44 |
| 1:A:7:VAL:CA | 1:A:451:LEU:CD2[3_655] | 0.76 | 1.44 |
| 1:A:39:VAL:CB | 1:A:466:GLU:CD[3_655] | 0.76 | 1.44 |
| 1:A:52:LYS:CE | 1:A:202:THR:N[3_655] | 0.77 | 1.43 |
| 1:A:46:LEU:N | 1:A:472:VAL:CA[3_655] | 0.77 | 1.43 |
| 1:A:15:SER:CB | 1:A:21:LYS:CE[3_655] | 0.77 | 1.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:46:LEU:CB | 1:A:473:PRO:CD[3_655] | 0.78 | 1.42 |
| 1:A:61:VAL:N | 1:A:211:VAL:O[3_655] | 0.79 | 1.41 |
| 1:A:14:ILE:CD1 | 1:A:72:ALA:N[3_655] | 0.79 | 1.41 |
| 1:A:44:TYR:CA | 4:A:2216:HOH:O[3_655] | 0.79 | 1.41 |
| 1:A:39:VAL:CG1 | 1:A:466:GLU:OE1[3_655] | 0.79 | 1.41 |
| 1:A:16:GLY:N | 4:A:2003:HOH:O[3_655] | 0.80 | 1.40 |
| 1:A:83:ASN:N | 1:A:332:LYS:C[3_655] | 0.80 | 1.40 |
| 1:A:44:TYR:N | 4:A:2216:HOH:O[3_655] | 0.81 | 1.39 |
| 1:A:258:LYS:C | 1:A:456:LYS:CE[3_655] | 0.81 | 1.39 |
| 1:A:83:ASN:ND2 | 1:A:335:GLY:CA[3_655] | 0.81 | 1.39 |
| 1:A:44:TYR:CE1 | 1:A:469:SER:C[3_655] | 0.82 | 1.38 |
| 1:A:68:ILE:CB | 1:A:217:VAL:CA[3_655] | 0.82 | 1.38 |
| 1:A:80:TYR:CA | 1:A:209:LYS:CE[3_655] | 0.82 | 1.38 |
| 1:A:221:ILE:CG1 | 1:A:440:VAL:CA[3_655] | 0.82 | 1.38 |
| 1:A:30:VAL:CG1 | 1:A:447:ALA:O[3_655] | 0.84 | 1.36 |
| 1:A:44:TYR:CE2 | 1:A:470:VAL:CA[3_655] | 0.85 | 1.35 |
| 1:A:54:VAL:CA | 1:A:208:ARG:CZ[3_655] | 0.85 | 1.35 |
| 1:A:53:TYR:N | 1:A:207:GLU:OE1[3_655] | 0.85 | 1.35 |
| 1:A:230:LYS:NZ | 1:A:460:ASP:O[3_655] | 0.85 | 1.35 |
| 1:A:67:ARG:CB | 1:A:218:SER:C[3_655] | 0.86 | 1.34 |
| 1:A:59:SER:OG | 1:A:79:THR:N[3_655] | 0.87 | 1.33 |
| 1:A:52:LYS:CD | 1:A:202:THR:N[3_655] | 0.87 | 1.33 |
| 1:A:228:ARG:CA | 1:A:462:ILE:C[3_655] | 0.87 | 1.33 |
| 1:A:84:GLU:CA | 1:A:336:ASN:OD1[3_655] | 0.87 | 1.33 |
| 1:A:24:HIS:CG | 1:A:446:ALA:CB[3_655] | 0.87 | 1.33 |
| 1:A:52:LYS:C | 1:A:207:GLU:OE1[3_655] | 0.88 | 1.32 |
| 1:A:38:ARG:CB | 1:A:467:PRO:C[3_655] | 0.88 | 1.32 |
| 1:A:221:ILE:C | 1:A:441:GLU:CA[3_655] | 0.88 | 1.32 |
| 1:A:229:VAL:C | 1:A:464:GLN:CB[3_655] | 0.88 | 1.32 |
| 1:A:59:SER:C | 1:A:78:GLU:O[3_655] | 0.88 | 1.32 |
| 1:A:17:MET:CB | 1:A:444:GLU:OE2[3_655] | 0.89 | 1.31 |
| 1:A:28:LEU:CB | 1:A:450:ILE:CB[3_655] | 0.89 | 1.31 |
| 1:A:227:ASP:CA | 1:A:463:TRP:CB[3_655] | 0.90 | 1.30 |
| 1:A:7:VAL:CB | 1:A:451:LEU:CD2[3_655] | 0.90 | 1.30 |
| 1:A:46:LEU:CA | 1:A:473:PRO:N[3_655] | 0.90 | 1.30 |
| 1:B:475:GLN:CD | 4:B:2058:HOH:O[3_555] | 0.90 | 1.30 |
| 1:A:220:ARG:CB | 1:A:437:GLU:C[3_655] | 0.91 | 1.29 |
| 1:A:29:ASN:N | 1:A:450:ILE:N[3_655] | 0.91 | 1.29 |
| 1:A:330:ASP:CG | 4:A:2046:HOH:O[3_655] | 0.91 | 1.29 |
| 1:A:74:GLU:C | 2:A:600:FAD:C4'[3_655] | 0.91 | 1.29 |
| 1:A:25:ASP:CA | 1:A:261:ILE:CG2[3_655] | 0.92 | 1.28 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:80:TYR:N | 1:A:209:LYS:CE[3_655] | 0.92 | 1.28 |
| 1:A:73:LYS:NZ | 1:A:388:TRP:CH2[3_655] | 0.92 | 1.28 |
| 1:A:227:ASP:C | 1:A:463:TRP:CA[3_655] | 0.92 | 1.28 |
| 1:A:333:PRO:CA | 4:A:2154:HOH:O[3_655] | 0.92 | 1.28 |
| 1:A:229:VAL:O | 1:A:464:GLN:CA[3_655] | 0.93 | 1.27 |
| 1:A:501:ILE:CA | 4:A:2054:HOH:O[6_565] | 0.93 | 1.27 |
| 1:A:74:GLU:CB | 2:A:600:FAD:O5'[3_655] | 0.93 | 1.27 |
| 1:A:27:GLY:O | 1:A:422:TYR:CD1[3_655] | 0.94 | 1.26 |
| 1:A:38:ARG:CA | 1:A:467:PRO:N[3_655] | 0.94 | 1.26 |
| 1:A:18:ALA:C | 1:A:18:ALA:C[3_655] | 0.95 | 1.25 |
| 1:A:30:VAL:N | 1:A:448:ARG:C[3_655] | 0.96 | 1.24 |
| 1:A:67:ARG:O | 1:A:218:SER:CB[3_655] | 0.96 | 1.24 |
| 1:A:221:ILE:CG1 | 1:A:440:VAL:CB[3_655] | 0.96 | 1.24 |
| 1:A:30:VAL:CG1 | 1:A:447:ALA:C[3_655] | 0.97 | 1.23 |
| 1:A:29:ASN:N | 1:A:450:ILE:CA[3_655] | 0.97 | 1.23 |
| 1:A:38:ARG:CA | 1:A:467:PRO:CA[3_655] | 0.98 | 1.22 |
| 1:A:43:THR:O | 4:A:2009:HOH:O[3_655] | 0.98 | 1.22 |
| 1:A:77:LEU:CB | 1:A:436:MET:CE[3_655] | 0.99 | 1.21 |
| 1:A:84:GLU:CA | 1:A:336:ASN:CG[3_655] | 0.99 | 1.21 |
| 1:A:30:VAL:CB | 1:A:448:ARG:N[3_655] | 0.99 | 1.21 |
| 1:A:44:TYR:CE2 | 1:A:470:VAL:C[3_655] | 0.99 | 1.21 |
| 1:A:26:SER:C | 1:A:260:VAL:O[3_655] | 0.99 | 1.21 |
| 1:A:219:GLU:C | 1:A:437:GLU:OE1[3_655] | 0.99 | 1.21 |
| 1:A:80:TYR:CE1 | 1:A:80:TYR:CE1[3_655] | 0.99 | 1.21 |
| 1:A:47:ARG:CA | 1:A:473:PRO:O[3_655] | 1.00 | 1.20 |
| 1:A:225:LEU:CD2 | 1:A:445:ARG:N[3_655] | 1.00 | 1.20 |
| 1:A:67:ARG:NH2 | 1:A:222:MET:CG[3_655] | 1.00 | 1.20 |
| 1:A:228:ARG:N | 1:A:463:TRP:N[3_655] | 1.00 | 1.20 |
| 1:A:59:SER:CA | 1:A:78:GLU:C[3_655] | 1.00 | 1.20 |
| 1:A:66:ASN:N | 1:A:219:GLU:CD[3_655] | 1.00 | 1.20 |
| 1:A:84:GLU:C | 1:A:336:ASN:CG[3_655] | 1.00 | 1.20 |
| 1:A:15:SER:CB | 1:A:21:LYS:NZ[3_655] | 1.01 | 1.19 |
| 1:A:330:ASP:OD2 | 4:A:2046:HOH:O[3_655] | 1.01 | 1.19 |
| 1:A:85:VAL:N | 1:A:336:ASN:CA[3_655] | 1.01 | 1.19 |
| 1:A:224:LEU:O | 4:A:2204:HOH:O[3_655] | 1.01 | 1.19 |
| 1:A:42:ARG:C | 1:A:73:LYS:CG[3_655] | 1.01 | 1.19 |
| 1:A:73:LYS:O | 2:A:600:FAD:O2'[3_655] | 1.02 | 1.18 |
| 1:A:68:ILE:CG2 | 1:A:216:GLN:C[3_655] | 1.02 | 1.18 |
| 1:A:43:THR:CG2 | 1:A:73:LYS:N[3_655] | 1.03 | 1.17 |
| 1:A:12:GLY:O | 1:A:70:ARG:NE[3_655] | 1.03 | 1.17 |
| 1:A:260:VAL:CA | 4:A:2006:HOH:O[3_655] | 1.03 | 1.17 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------------|--------------------------|-------------------|
| 1:A:59:SER:CA | 1:A:78:GLU:CA[3_655] | 1.03 | 1.17 |
| 1:A:53:TYR:N | 1:A:207:GLU:CD[3_655] | 1.04 | 1.16 |
| 1:A:329:ASP:CB | 1:A:333:PRO:O[3_655] | 1.04 | 1.16 |
| 1:A:67:ARG:C | 1:A:218:SER:CA[3_655] | 1.04 | 1.16 |
| 1:A:6:ASP:CB | 1:A:450:ILE:O[3_655] | 1.04 | 1.16 |
| 1:A:45:THR:CG2 | 1:A:472:VAL:CG1[3_655] | 1.05 | 1.15 |
| 1:A:30:VAL:CA | 1:A:448:ARG:CA[3_655] | 1.05 | 1.15 |
| 1:A:47:ARG:N | 1:A:473:PRO:O[3_655] | 1.05 | 1.15 |
| 1:A:68:ILE:CG2 | 1:A:217:VAL:N[3_655] | 1.05 | 1.15 |
| 1:A:73:LYS:NZ | 1:A:388:TRP:CZ2[3_655] | 1.06 | 1.14 |
| 1:A:38:ARG:C | 1:A:467:PRO:CD[3_655] | 1.06 | 1.14 |
| 1:A:65:GLN:C | 1:A:219:GLU:OE1[3_655] | 1.06 | 1.14 |
| 1:A:220:ARG:C | 1:A:437:GLU:O[3_655] | 1.07 | 1.13 |
| 1:A:18:ALA:C | 1:A:18:ALA:O[3_655] | 1.07 | 1.13 |
| 1:A:46:LEU:CD1 | 1:A:473:PRO:CG[3_655] | 1.07 | 1.13 |
| 1:A:5:CYS:C | 1:A:451:LEU:O[3_655] | 1.07 | 1.13 |
| 1:A:26:SER:N | 1:A:261:ILE:CA[3_655] | 1.07 | 1.13 |
| 1:A:67:ARG:CA | 1:A:218:SER:C[3_655] | 1.07 | 1.13 |
| 1:A:78:GLU:CG | 4:A:2139:HOH:O[3_655] | 1.07 | 1.13 |
| 1:A:27:GLY:O | 1:A:422:TYR:CE1[3_655] | 1.08 | 1.12 |
| 1:A:46:LEU:N | 1:A:472:VAL:N[3_655] | 1.08 | 1.12 |
| 1:A:44:TYR:CD1 | 1:A:470:VAL:N[3_655] | 1.08 | 1.12 |
| 1:A:61:VAL:CA | 1:A:216:GLN:NE2[3_655] | 1.08 | 1.12 |
| 1:A:438:GLY:CA | 4:A:2121:HOH:O[3_655] | 1.08 | 1.12 |
| 1:A:84:GLU:CB | 1:A:336:ASN:OD1[3_655] | 1.09 | 1.11 |
| 1:A:38:ARG:N | 1:A:467:PRO:CB[3_655] | 1.09 | 1.11 |
| 1:A:18:ALA:CA | 1:A:18:ALA:CA[3_655] | 1.09 | 1.11 |
| 1:A:17:MET:CA | 1:A:444:GLU:OE2[3_655] | 1.09 | 1.11 |
| 1:A:29:ASN:O | 1:A:451:LEU:N[3_655] | 1.09 | 1.11 |
| 1:A:44:TYR:CD2 | 1:A:471:ASP:N[3_655] | 1.09 | 1.11 |
| 1:A:6:ASP:N | 1:A:451:LEU:O[3_655] | 1.10 | 1.10 |
| 1:A:66:ASN:CB | 4:A:2119:HOH:O[3_655] | 1.10 | 1.10 |
| 1:A:74:GLU:CD | 2:A:600:FAD:P[3_655] | 1.11 | 1.09 |
| 1:A:76:GLY:C | 2:A:600:FAD:C2[3_655] | 1.11 | 1.09 |
| 1:A:223:ASP:C | 1:A:441:GLU:OE2[3_655] | 1.11 | 1.09 |
| 1:B:479:THR:N | 1:B:479:THR:N[3_555] | 1.11 | 1.09 |
| 1:A:39:VAL:CB | 1:A:466:GLU:OE1[3_655] | 1.11 | 1.09 |
| 1:A:225:LEU:CG | 1:A:445:ARG:N[3_655] | 1.12 | 1.08 |
| 1:A:68:ILE:CG1 | 1:A:217:VAL:CG2[3_655] | 1.12 | 1.08 |
| 1:A:224:LEU:CG | 1:A:438:GLY:O[3_655] | 1.12 | 1.08 |
| 1:A:23:LEU:CG | 1:A:23:LEU:CD1[3_655] | 1.12 | 1.08 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:15:SER:OG | 1:A:21:LYS:CE[3_655] | 1.13 | 1.07 |
| 1:A:60:TYR:CD2 | 1:A:211:VAL:CG2[3_655] | 1.13 | 1.07 |
| 1:A:53:TYR:CZ | 1:A:207:GLU:O[3_655] | 1.14 | 1.06 |
| 1:A:336:ASN:O | 4:A:2049:HOH:O[3_655] | 1.14 | 1.06 |
| 1:A:257:ALA:CA | 1:A:456:LYS:CA[3_655] | 1.14 | 1.06 |
| 1:A:85:VAL:N | 1:A:336:ASN:CB[3_655] | 1.14 | 1.06 |
| 1:A:307:ARG:CZ | 1:A:307:ARG:NH1[3_655] | 1.14 | 1.06 |
| 1:A:220:ARG:CB | 1:A:437:GLU:CA[3_655] | 1.14 | 1.06 |
| 1:A:68:ILE:N | 1:A:218:SER:N[3_655] | 1.14 | 1.06 |
| 1:A:24:HIS:CG | 1:A:446:ALA:CA[3_655] | 1.14 | 1.06 |
| 1:A:53:TYR:CE2 | 1:A:207:GLU:C[3_655] | 1.14 | 1.06 |
| 1:A:17:MET:SD | 1:A:444:GLU:OE1[3_655] | 1.14 | 1.06 |
| 1:A:74:GLU:CG | 2:A:600:FAD:O5'[3_655] | 1.15 | 1.05 |
| 1:A:39:VAL:CB | 1:A:466:GLU:OE2[3_655] | 1.16 | 1.04 |
| 1:A:221:ILE:CB | 1:A:440:VAL:C[3_655] | 1.16 | 1.04 |
| 1:A:258:LYS:CA | 1:A:456:LYS:CE[3_655] | 1.16 | 1.04 |
| 1:A:210:PHE:CD1 | 1:A:210:PHE:CE1[3_655] | 1.16 | 1.04 |
| 1:A:72:ALA:O | 1:A:436:MET:CG[3_655] | 1.16 | 1.04 |
| 1:A:220:ARG:NH1 | 1:A:435:TYR:CB[3_655] | 1.16 | 1.04 |
| 1:A:26:SER:O | 1:A:260:VAL:O[3_655] | 1.17 | 1.03 |
| 1:A:25:ASP:O | 1:A:262:SER:N[3_655] | 1.17 | 1.03 |
| 1:A:220:ARG:CG | 1:A:437:GLU:CB[3_655] | 1.17 | 1.03 |
| 1:A:17:MET:CE | 1:A:444:GLU:OE1[3_655] | 1.17 | 1.03 |
| 1:A:44:TYR:CE1 | 1:A:470:VAL:N[3_655] | 1.17 | 1.03 |
| 1:A:42:ARG:C | 1:A:73:LYS:CD[3_655] | 1.17 | 1.03 |
| 1:A:4:LYS:O | 1:A:452:HIS:ND1[3_655] | 1.17 | 1.03 |
| 1:A:19:ALA:CB | 1:A:21:LYS:C[3_655] | 1.17 | 1.03 |
| 1:A:14:ILE:CG1 | 1:A:71:LEU:CA[3_655] | 1.18 | 1.02 |
| 1:A:46:LEU:CG | 1:A:473:PRO:CG[3_655] | 1.18 | 1.02 |
| 1:A:209:LYS:N | 1:A:210:PHE:O[3_655] | 1.18 | 1.02 |
| 1:A:23:LEU:C | 1:A:261:ILE:CD1[3_655] | 1.18 | 1.02 |
| 1:A:60:TYR:CD2 | 1:A:211:VAL:CB[3_655] | 1.18 | 1.02 |
| 1:A:74:GLU:C | 2:A:600:FAD:C5'[3_655] | 1.18 | 1.02 |
| 1:A:73:LYS:C | 2:A:600:FAD:O4'[3_655] | 1.19 | 1.01 |
| 1:A:18:ALA:O | 1:A:19:ALA:N[3_655] | 1.19 | 1.01 |
| 1:A:255:TYR:CE1 | 1:A:461:GLU:OE2[3_655] | 1.19 | 1.01 |
| 1:A:52:LYS:CD | 1:A:202:THR:CA[3_655] | 1.19 | 1.01 |
| 1:A:59:SER:O | 1:A:78:GLU:O[3_655] | 1.19 | 1.01 |
| 1:A:82:VAL:C | 1:A:332:LYS:CB[3_655] | 1.19 | 1.01 |
| 1:A:53:TYR:CA | 1:A:207:GLU:CD[3_655] | 1.19 | 1.01 |
| 1:A:32:VAL:O | 1:A:464:GLN:NE2[3_655] | 1.19 | 1.01 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------------|--------------------------|-------------------|
| 1:A:14:ILE:CD1 | 1:A:71:LEU:C[3_655] | 1.20 | 1.00 |
| 1:A:28:LEU:CB | 1:A:450:ILE:CG2[3_655] | 1.20 | 1.00 |
| 1:A:209:LYS:C | 1:A:209:LYS:C[3_655] | 1.20 | 1.00 |
| 1:A:26:SER:O | 1:A:260:VAL:C[3_655] | 1.20 | 1.00 |
| 1:A:46:LEU:CA | 1:A:473:PRO:CD[3_655] | 1.20 | 1.00 |
| 1:A:47:ARG:CG | 1:A:63:PRO:CB[3_655] | 1.20 | 1.00 |
| 1:A:69:LEU:CG | 1:A:215:GLY:CA[3_655] | 1.20 | 1.00 |
| 1:A:66:ASN:CG | 4:A:2119:HOH:O[3_655] | 1.20 | 1.00 |
| 1:A:79:THR:C | 1:A:209:LYS:NZ[3_655] | 1.20 | 1.00 |
| 1:A:209:LYS:C | 1:A:210:PHE:N[3_655] | 1.20 | 1.00 |
| 1:A:45:THR:C | 1:A:472:VAL:CA[3_655] | 1.20 | 1.00 |
| 1:A:28:LEU:N | 1:A:450:ILE:CG1[3_655] | 1.20 | 1.00 |
| 1:A:80:TYR:N | 1:A:209:LYS:NZ[3_655] | 1.21 | 0.99 |
| 1:A:65:GLN:OE1 | 1:A:216:GLN:CD[3_655] | 1.21 | 0.99 |
| 1:A:74:GLU:OE2 | 2:A:600:FAD:O1P[3_655] | 1.21 | 0.99 |
| 1:A:53:TYR:CD2 | 1:A:207:GLU:CG[3_655] | 1.21 | 0.99 |
| 1:A:66:ASN:CA | 1:A:219:GLU:CG[3_655] | 1.22 | 0.98 |
| 1:A:39:VAL:CG2 | 1:A:466:GLU:CD[3_655] | 1.22 | 0.98 |
| 1:A:55:ASP:OD2 | 1:A:79:THR:OG1[3_655] | 1.22 | 0.98 |
| 1:A:67:ARG:N | 1:A:219:GLU:N[3_655] | 1.22 | 0.98 |
| 1:A:76:GLY:O | 2:A:600:FAD:N1[3_655] | 1.22 | 0.98 |
| 1:A:75:LEU:O | 1:A:435:TYR:CA[3_655] | 1.23 | 0.97 |
| 1:A:221:ILE:O | 1:A:441:GLU:C[3_655] | 1.23 | 0.97 |
| 1:A:26:SER:C | 1:A:260:VAL:C[3_655] | 1.23 | 0.97 |
| 1:A:69:LEU:CG | 1:A:215:GLY:N[3_655] | 1.23 | 0.97 |
| 1:A:29:ASN:CA | 1:A:450:ILE:N[3_655] | 1.23 | 0.97 |
| 1:A:9:VAL:CG2 | 1:A:22:LEU:CD2[3_655] | 1.23 | 0.97 |
| 1:A:31:VAL:CG2 | 1:A:457:ILE:CD1[3_655] | 1.23 | 0.97 |
| 1:A:44:TYR:CD2 | 1:A:470:VAL:C[3_655] | 1.23 | 0.97 |
| 1:A:74:GLU:O | 2:A:600:FAD:C5'[3_655] | 1.23 | 0.97 |
| 1:A:68:ILE:CD1 | 1:A:217:VAL:CG2[3_655] | 1.24 | 0.96 |
| 1:A:227:ASP:N | 1:A:463:TRP:CB[3_655] | 1.24 | 0.96 |
| 1:A:223:ASP:O | 1:A:441:GLU:CD[3_655] | 1.24 | 0.96 |
| 1:A:39:VAL:O | 4:A:2215:HOH:O[3_655] | 1.25 | 0.95 |
| 1:A:67:ARG:CZ | 1:A:222:MET:CG[3_655] | 1.25 | 0.95 |
| 1:A:38:ARG:N | 1:A:467:PRO:CG[3_655] | 1.25 | 0.95 |
| 1:A:67:ARG:CA | 1:A:219:GLU:N[3_655] | 1.25 | 0.95 |
| 1:A:26:SER:CA | 1:A:261:ILE:CA[3_655] | 1.25 | 0.95 |
| 1:A:61:VAL:CB | 1:A:213:GLY:O[3_655] | 1.25 | 0.95 |
| 1:A:54:VAL:CB | 1:A:208:ARG:NH2[3_655] | 1.25 | 0.95 |
| 1:A:16:GLY:CA | 4:A:2003:HOH:O[3_655] | 1.26 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:29:ASN:CA | 1:A:449:GLU:O[3_655] | 1.26 | 0.94 |
| 1:A:208:ARG:O | 1:A:211:VAL:CA[3_655] | 1.26 | 0.94 |
| 1:A:81:LYS:CG | 1:A:332:LYS:NZ[3_655] | 1.26 | 0.94 |
| 1:A:228:ARG:CA | 1:A:462:ILE:O[3_655] | 1.26 | 0.94 |
| 1:A:84:GLU:O | 1:A:336:ASN:CB[3_655] | 1.26 | 0.94 |
| 1:A:75:LEU:C | 1:A:435:TYR:C[3_655] | 1.26 | 0.94 |
| 1:A:25:ASP:O | 1:A:261:ILE:C[3_655] | 1.26 | 0.94 |
| 1:A:6:ASP:N | 1:A:451:LEU:C[3_655] | 1.26 | 0.94 |
| 1:A:74:GLU:CA | 2:A:600:FAD:O4'[3_655] | 1.26 | 0.94 |
| 1:A:47:ARG:NH2 | 1:A:62:GLY:O[3_655] | 1.27 | 0.93 |
| 1:A:61:VAL:O | 1:A:212:GLY:C[3_655] | 1.27 | 0.93 |
| 1:A:221:ILE:C | 1:A:441:GLU:N[3_655] | 1.28 | 0.92 |
| 1:A:65:GLN:CA | 1:A:219:GLU:OE1[3_655] | 1.28 | 0.92 |
| 1:A:24:HIS:ND1 | 1:A:446:ALA:CA[3_655] | 1.28 | 0.92 |
| 1:A:44:TYR:CD1 | 1:A:469:SER:C[3_655] | 1.28 | 0.92 |
| 1:A:208:ARG:C | 1:A:210:PHE:O[3_655] | 1.29 | 0.91 |
| 1:A:59:SER:CB | 1:A:78:GLU:C[3_655] | 1.29 | 0.91 |
| 1:A:32:VAL:CA | 4:A:2209:HOH:O[3_655] | 1.29 | 0.91 |
| 1:A:19:ALA:C | 1:A:19:ALA:O[3_655] | 1.29 | 0.91 |
| 1:A:69:LEU:CD2 | 1:A:215:GLY:N[3_655] | 1.29 | 0.91 |
| 1:A:500:THR:O | 4:A:2014:HOH:O[6_565] | 1.29 | 0.91 |
| 1:A:30:VAL:C | 1:A:448:ARG:CA[3_655] | 1.29 | 0.91 |
| 1:A:220:ARG:N | 1:A:437:GLU:CD[3_655] | 1.29 | 0.91 |
| 1:A:32:VAL:CG1 | 4:A:2209:HOH:O[3_655] | 1.29 | 0.91 |
| 1:A:55:ASP:OD2 | 1:A:79:THR:CG2[3_655] | 1.30 | 0.90 |
| 1:A:223:ASP:CA | 1:A:441:GLU:CD[3_655] | 1.30 | 0.90 |
| 1:A:53:TYR:CZ | 1:A:208:ARG:N[3_655] | 1.30 | 0.90 |
| 1:A:27:GLY:C | 1:A:422:TYR:CD1[3_655] | 1.30 | 0.90 |
| 1:A:67:ARG:O | 1:A:218:SER:CA[3_655] | 1.31 | 0.89 |
| 1:A:5:CYS:CB | 1:A:452:HIS:CA[3_655] | 1.31 | 0.89 |
| 1:A:3:ASN:O | 1:A:458:PRO:N[3_655] | 1.32 | 0.88 |
| 1:A:75:LEU:O | 1:A:436:MET:N[3_655] | 1.32 | 0.88 |
| 1:A:52:LYS:CD | 1:A:201:THR:C[3_655] | 1.32 | 0.88 |
| 1:A:500:THR:C | 4:A:2014:HOH:O[6_565] | 1.32 | 0.88 |
| 1:A:45:THR:N | 1:A:469:SER:OG[3_655] | 1.32 | 0.88 |
| 1:A:15:SER:CA | 1:A:21:LYS:CE[3_655] | 1.32 | 0.88 |
| 1:B:478:THR:C | 1:B:478:THR:C[3_555] | 1.33 | 0.87 |
| 1:A:76:GLY:O | 2:A:600:FAD:C2[3_655] | 1.33 | 0.87 |
| 1:A:224:LEU:CD1 | 1:A:438:GLY:O[3_655] | 1.33 | 0.87 |
| 1:A:65:GLN:OE1 | 1:A:216:GLN:OE1[3_655] | 1.33 | 0.87 |
| 1:A:54:VAL:N | 1:A:208:ARG:NH2[3_655] | 1.33 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:6:ASP:CG | 1:A:450:ILE:O[3_655] | 1.33 | 0.87 |
| 1:A:53:TYR:CB | 1:A:207:GLU:OE2[3_655] | 1.33 | 0.87 |
| 1:A:221:ILE:CA | 1:A:440:VAL:C[3_655] | 1.33 | 0.87 |
| 1:A:53:TYR:OH | 1:A:207:GLU:O[3_655] | 1.33 | 0.87 |
| 1:A:40:GLY:N | 1:A:70:ARG:CB[3_655] | 1.34 | 0.86 |
| 1:A:59:SER:CB | 1:A:79:THR:N[3_655] | 1.34 | 0.86 |
| 1:A:75:LEU:CD2 | 1:A:439:ALA:N[3_655] | 1.34 | 0.86 |
| 1:A:220:ARG:NH1 | 1:A:435:TYR:CG[3_655] | 1.34 | 0.86 |
| 1:A:84:GLU:CG | 1:A:336:ASN:ND2[3_655] | 1.34 | 0.86 |
| 1:A:55:ASP:CG | 1:A:79:THR:OG1[3_655] | 1.34 | 0.86 |
| 1:A:28:LEU:C | 1:A:450:ILE:N[3_655] | 1.35 | 0.85 |
| 1:A:256:GLU:O | 1:A:455:GLY:C[3_655] | 1.35 | 0.85 |
| 1:A:30:VAL:CB | 1:A:447:ALA:C[3_655] | 1.35 | 0.85 |
| 1:A:59:SER:N | 1:A:78:GLU:CA[3_655] | 1.35 | 0.85 |
| 1:A:60:TYR:C | 1:A:211:VAL:O[3_655] | 1.35 | 0.85 |
| 1:A:24:HIS:CE1 | 1:A:445:ARG:NH2[3_655] | 1.35 | 0.85 |
| 1:A:30:VAL:C | 1:A:448:ARG:CB[3_655] | 1.35 | 0.85 |
| 1:A:38:ARG:CB | 1:A:467:PRO:O[3_655] | 1.35 | 0.85 |
| 1:A:79:THR:O | 1:A:209:LYS:NZ[3_655] | 1.35 | 0.85 |
| 1:A:74:GLU:CA | 2:A:600:FAD:C4'[3_655] | 1.35 | 0.85 |
| 1:A:334:GLU:CA | 4:A:2048:HOH:O[3_655] | 1.36 | 0.84 |
| 1:A:77:LEU:N | 2:A:600:FAD:C2[3_655] | 1.36 | 0.84 |
| 1:A:14:ILE:CD1 | 1:A:72:ALA:CA[3_655] | 1.36 | 0.84 |
| 1:A:76:GLY:CA | 2:A:600:FAD:N1[3_655] | 1.36 | 0.84 |
| 1:A:77:LEU:CD2 | 4:A:2036:HOH:O[3_655] | 1.36 | 0.84 |
| 1:A:59:SER:C | 1:A:78:GLU:C[3_655] | 1.36 | 0.84 |
| 1:A:259:TYR:N | 1:A:456:LYS:CE[3_655] | 1.36 | 0.84 |
| 1:A:229:VAL:C | 1:A:464:GLN:CA[3_655] | 1.36 | 0.84 |
| 1:A:67:ARG:O | 1:A:218:SER:OG[3_655] | 1.36 | 0.84 |
| 1:A:82:VAL:CA | 1:A:333:PRO:CD[3_655] | 1.36 | 0.84 |
| 1:A:58:GLY:C | 1:A:77:LEU:O[3_655] | 1.36 | 0.84 |
| 1:A:25:ASP:C | 1:A:261:ILE:CA[3_655] | 1.37 | 0.83 |
| 1:A:256:GLU:C | 1:A:455:GLY:O[3_655] | 1.37 | 0.83 |
| 1:A:210:PHE:CG | 1:A:210:PHE:CD1[3_655] | 1.37 | 0.83 |
| 1:A:38:ARG:O | 1:A:467:PRO:CD[3_655] | 1.37 | 0.83 |
| 1:A:39:VAL:CG2 | 1:A:466:GLU:CG[3_655] | 1.37 | 0.83 |
| 1:A:7:VAL:O | 1:A:451:LEU:CD1[3_655] | 1.37 | 0.83 |
| 1:A:40:GLY:N | 1:A:70:ARG:CG[3_655] | 1.37 | 0.83 |
| 1:A:67:ARG:C | 1:A:218:SER:N[3_655] | 1.37 | 0.83 |
| 1:A:53:TYR:OH | 1:A:207:GLU:C[3_655] | 1.37 | 0.83 |
| 1:A:228:ARG:CB | 1:A:462:ILE:C[3_655] | 1.37 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:209:LYS:O | 1:A:209:LYS:CB[3_655] | 1.38 | 0.82 |
| 1:A:5:CYS:CA | 1:A:452:HIS:CA[3_655] | 1.38 | 0.82 |
| 1:A:14:ILE:O | 1:A:71:LEU:CD1[3_655] | 1.38 | 0.82 |
| 1:A:255:TYR:CZ | 1:A:461:GLU:OE2[3_655] | 1.38 | 0.82 |
| 1:A:44:TYR:CZ | 1:A:470:VAL:CA[3_655] | 1.38 | 0.82 |
| 1:A:29:ASN:CG | 1:A:449:GLU:O[3_655] | 1.38 | 0.82 |
| 1:A:75:LEU:CB | 1:A:436:MET:CA[3_655] | 1.38 | 0.82 |
| 1:A:260:VAL:N | 4:A:2006:HOH:O[3_655] | 1.38 | 0.82 |
| 1:A:74:GLU:CA | 2:A:600:FAD:C5'[3_655] | 1.39 | 0.81 |
| 1:A:44:TYR:O | 1:A:471:ASP:CB[3_655] | 1.39 | 0.81 |
| 1:A:42:ARG:N | 4:A:2044:HOH:O[3_655] | 1.39 | 0.81 |
| 1:A:45:THR:CB | 1:A:472:VAL:CB[3_655] | 1.39 | 0.81 |
| 1:A:53:TYR:CG | 1:A:207:GLU:CG[3_655] | 1.39 | 0.81 |
| 1:A:83:ASN:CB | 1:A:335:GLY:N[3_655] | 1.39 | 0.81 |
| 1:A:82:VAL:C | 1:A:332:LYS:CA[3_655] | 1.39 | 0.81 |
| 1:A:422:TYR:C | 4:A:2008:HOH:O[3_655] | 1.39 | 0.81 |
| 1:A:231:LEU:CD2 | 1:A:465:SER:O[3_655] | 1.40 | 0.80 |
| 1:A:68:ILE:CG1 | 1:A:217:VAL:CB[3_655] | 1.40 | 0.80 |
| 1:A:8:VAL:CG2 | 1:A:457:ILE:CG2[3_655] | 1.40 | 0.80 |
| 1:A:43:THR:N | 1:A:73:LYS:CB[3_655] | 1.40 | 0.80 |
| 1:B:81:LYS:NZ | 1:B:100:ARG:NH1[3_555] | 1.40 | 0.80 |
| 1:A:25:ASP:CB | 1:A:261:ILE:CG2[3_655] | 1.40 | 0.80 |
| 1:A:68:ILE:CA | 1:A:217:VAL:CA[3_655] | 1.40 | 0.80 |
| 1:A:7:VAL:N | 1:A:451:LEU:CA[3_655] | 1.40 | 0.80 |
| 1:A:30:VAL:CB | 1:A:448:ARG:CA[3_655] | 1.40 | 0.80 |
| 1:A:18:ALA:N | 4:A:2001:HOH:O[3_655] | 1.40 | 0.80 |
| 1:A:58:GLY:CA | 1:A:77:LEU:O[3_655] | 1.41 | 0.79 |
| 1:A:53:TYR:C | 1:A:207:GLU:OE2[3_655] | 1.41 | 0.79 |
| 1:A:47:ARG:CG | 1:A:63:PRO:CG[3_655] | 1.41 | 0.79 |
| 1:A:257:ALA:N | 1:A:456:LYS:CA[3_655] | 1.41 | 0.79 |
| 1:A:25:ASP:C | 1:A:261:ILE:CB[3_655] | 1.42 | 0.78 |
| 1:A:332:LYS:CD | 4:A:2047:HOH:O[3_655] | 1.42 | 0.78 |
| 1:A:228:ARG:CA | 1:A:463:TRP:N[3_655] | 1.42 | 0.78 |
| 1:A:24:HIS:CB | 1:A:446:ALA:CA[3_655] | 1.42 | 0.78 |
| 1:A:42:ARG:O | 1:A:73:LYS:CD[3_655] | 1.42 | 0.78 |
| 1:A:38:ARG:CB | 1:A:467:PRO:CA[3_655] | 1.42 | 0.78 |
| 1:A:224:LEU:N | 1:A:441:GLU:CG[3_655] | 1.42 | 0.78 |
| 1:A:25:ASP:C | 1:A:261:ILE:CG2[3_655] | 1.42 | 0.78 |
| 1:A:227:ASP:C | 1:A:463:TRP:N[3_655] | 1.42 | 0.78 |
| 1:A:68:ILE:CD1 | 1:A:217:VAL:CB[3_655] | 1.42 | 0.78 |
| 1:A:219:GLU:O | 1:A:437:GLU:OE1[3_655] | 1.43 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:210:PHE:CE2 | 1:A:214:SER:CB[3_655] | 1.43 | 0.77 |
| 1:B:478:THR:O | 1:B:478:THR:OG1[3_555] | 1.43 | 0.77 |
| 1:A:46:LEU:CA | 1:A:472:VAL:C[3_655] | 1.43 | 0.77 |
| 1:A:43:THR:CB | 1:A:69:LEU:O[3_655] | 1.43 | 0.77 |
| 1:A:42:ARG:CB | 4:A:2010:HOH:O[3_655] | 1.43 | 0.77 |
| 1:A:68:ILE:CA | 1:A:218:SER:N[3_655] | 1.43 | 0.77 |
| 1:A:14:ILE:C | 1:A:71:LEU:CD1[3_655] | 1.43 | 0.77 |
| 1:A:28:LEU:CB | 1:A:450:ILE:CG1[3_655] | 1.44 | 0.76 |
| 1:A:47:ARG:CD | 1:A:63:PRO:CB[3_655] | 1.44 | 0.76 |
| 1:A:83:ASN:N | 1:A:332:LYS:O[3_655] | 1.44 | 0.76 |
| 1:A:45:THR:CA | 1:A:472:VAL:CB[3_655] | 1.44 | 0.76 |
| 1:A:61:VAL:C | 1:A:212:GLY:C[3_655] | 1.44 | 0.76 |
| 1:A:259:TYR:N | 1:A:456:LYS:CD[3_655] | 1.44 | 0.76 |
| 1:A:45:THR:CG2 | 1:A:472:VAL:CB[3_655] | 1.44 | 0.76 |
| 1:A:59:SER:CB | 1:A:78:GLU:CA[3_655] | 1.44 | 0.76 |
| 1:A:44:TYR:CG | 1:A:470:VAL:N[3_655] | 1.44 | 0.76 |
| 1:A:23:LEU:CD1 | 1:A:23:LEU:CD2[3_655] | 1.44 | 0.76 |
| 1:A:83:ASN:OD1 | 1:A:335:GLY:C[3_655] | 1.45 | 0.75 |
| 1:A:80:TYR:CA | 1:A:209:LYS:NZ[3_655] | 1.45 | 0.75 |
| 1:A:52:LYS:CG | 1:A:202:THR:CA[3_655] | 1.45 | 0.75 |
| 1:A:39:VAL:CA | 1:A:466:GLU:CD[3_655] | 1.45 | 0.75 |
| 1:A:47:ARG:CD | 1:A:63:PRO:CA[3_655] | 1.45 | 0.75 |
| 1:A:28:LEU:CG | 1:A:450:ILE:CG2[3_655] | 1.46 | 0.74 |
| 1:A:43:THR:OG1 | 1:A:69:LEU:C[3_655] | 1.46 | 0.74 |
| 1:A:59:SER:OG | 1:A:79:THR:CA[3_655] | 1.46 | 0.74 |
| 1:A:60:TYR:CD2 | 1:A:211:VAL:CG1[3_655] | 1.46 | 0.74 |
| 1:A:227:ASP:C | 1:A:463:TRP:C[3_655] | 1.46 | 0.74 |
| 1:A:46:LEU:CG | 1:A:473:PRO:CD[3_655] | 1.46 | 0.74 |
| 1:A:255:TYR:CD2 | 1:A:458:PRO:CD[3_655] | 1.46 | 0.74 |
| 1:A:39:VAL:C | 1:A:466:GLU:OE2[3_655] | 1.47 | 0.73 |
| 1:A:84:GLU:O | 1:A:336:ASN:CG[3_655] | 1.47 | 0.73 |
| 1:A:30:VAL:O | 1:A:448:ARG:CB[3_655] | 1.47 | 0.73 |
| 1:A:60:TYR:CG | 1:A:211:VAL:CB[3_655] | 1.47 | 0.73 |
| 1:A:65:GLN:C | 1:A:219:GLU:CD[3_655] | 1.47 | 0.73 |
| 1:A:74:GLU:OE1 | 2:A:600:FAD:O1P[3_655] | 1.47 | 0.73 |
| 1:A:75:LEU:CD1 | 1:A:436:MET:O[3_655] | 1.47 | 0.73 |
| 1:A:38:ARG:N | 1:A:467:PRO:CA[3_655] | 1.47 | 0.73 |
| 1:A:84:GLU:N | 1:A:336:ASN:OD1[3_655] | 1.48 | 0.72 |
| 1:A:81:LYS:CD | 1:A:332:LYS:NZ[3_655] | 1.48 | 0.72 |
| 1:A:230:LYS:CE | 1:A:461:GLU:CA[3_655] | 1.48 | 0.72 |
| 1:A:30:VAL:CA | 1:A:448:ARG:C[3_655] | 1.48 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:68:ILE:CA | 1:A:217:VAL:C[3_655] | 1.48 | 0.72 |
| 1:A:224:LEU:CB | 1:A:442:ALA:N[3_655] | 1.48 | 0.72 |
| 1:A:83:ASN:O | 1:A:334:GLU:CB[3_655] | 1.48 | 0.72 |
| 1:A:67:ARG:CZ | 1:A:222:MET:CB[3_655] | 1.48 | 0.72 |
| 1:A:7:VAL:C | 1:A:451:LEU:CG[3_655] | 1.48 | 0.72 |
| 1:A:221:ILE:CB | 1:A:440:VAL:CA[3_655] | 1.49 | 0.71 |
| 1:A:83:ASN:CB | 1:A:332:LYS:O[3_655] | 1.49 | 0.71 |
| 1:A:40:GLY:CA | 1:A:70:ARG:CA[3_655] | 1.49 | 0.71 |
| 1:A:5:CYS:O | 1:A:455:GLY:N[3_655] | 1.49 | 0.71 |
| 1:A:59:SER:N | 1:A:78:GLU:N[3_655] | 1.49 | 0.71 |
| 1:A:42:ARG:N | 4:A:2010:HOH:O[3_655] | 1.49 | 0.71 |
| 1:A:221:ILE:N | 1:A:437:GLU:O[3_655] | 1.49 | 0.71 |
| 1:A:61:VAL:O | 1:A:212:GLY:N[3_655] | 1.49 | 0.71 |
| 1:A:336:ASN:C | 4:A:2049:HOH:O[3_655] | 1.49 | 0.71 |
| 1:A:65:GLN:N | 1:A:219:GLU:OE1[3_655] | 1.49 | 0.71 |
| 1:A:223:ASP:C | 1:A:441:GLU:OE1[3_655] | 1.50 | 0.70 |
| 1:A:31:VAL:CB | 1:A:457:ILE:CD1[3_655] | 1.50 | 0.70 |
| 1:A:228:ARG:CG | 1:A:462:ILE:CG2[3_655] | 1.50 | 0.70 |
| 1:A:30:VAL:N | 1:A:449:GLU:N[3_655] | 1.50 | 0.70 |
| 1:A:75:LEU:CD2 | 1:A:439:ALA:CA[3_655] | 1.50 | 0.70 |
| 1:A:60:TYR:CE2 | 1:A:211:VAL:CG2[3_655] | 1.50 | 0.70 |
| 1:A:28:LEU:CA | 1:A:450:ILE:CB[3_655] | 1.50 | 0.70 |
| 1:A:74:GLU:CG | 2:A:600:FAD:O3P[3_655] | 1.50 | 0.70 |
| 1:A:68:ILE:O | 4:A:2018:HOH:O[3_655] | 1.50 | 0.70 |
| 1:A:83:ASN:CA | 1:A:332:LYS:O[3_655] | 1.50 | 0.70 |
| 1:A:76:GLY:O | 2:A:600:FAD:C10[3_655] | 1.50 | 0.70 |
| 1:A:26:SER:N | 1:A:261:ILE:CG1[3_655] | 1.50 | 0.70 |
| 1:A:19:ALA:CA | 1:A:22:LEU:N[3_655] | 1.50 | 0.70 |
| 1:A:226:GLY:CA | 1:A:463:TRP:CE3[3_655] | 1.50 | 0.70 |
| 1:A:223:ASP:C | 1:A:441:GLU:CG[3_655] | 1.50 | 0.70 |
| 1:A:321:GLU:OE2 | 1:A:499:THR:O[6_564] | 1.51 | 0.69 |
| 1:A:221:ILE:CG2 | 1:A:440:VAL:C[3_655] | 1.51 | 0.69 |
| 1:A:60:TYR:O | 4:A:2045:HOH:O[3_655] | 1.51 | 0.69 |
| 1:A:59:SER:N | 1:A:77:LEU:O[3_655] | 1.51 | 0.69 |
| 1:A:230:LYS:CE | 1:A:460:ASP:O[3_655] | 1.51 | 0.69 |
| 1:A:21:LYS:CA | 1:A:443:GLY:C[3_655] | 1.51 | 0.69 |
| 1:A:67:ARG:CD | 1:A:222:MET:CB[3_655] | 1.51 | 0.69 |
| 1:A:225:LEU:CA | 1:A:445:ARG:CB[3_655] | 1.52 | 0.68 |
| 1:A:230:LYS:N | 1:A:464:GLN:CG[3_655] | 1.52 | 0.68 |
| 1:A:70:ARG:O | 4:A:2230:HOH:O[3_655] | 1.52 | 0.68 |
| 1:A:7:VAL:O | 1:A:451:LEU:CG[3_655] | 1.52 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:80:TYR:CD1 | 1:A:80:TYR:OH[3_655] | 1.52 | 0.68 |
| 1:A:7:VAL:CA | 1:A:451:LEU:CG[3_655] | 1.52 | 0.68 |
| 1:A:227:ASP:O | 1:A:463:TRP:O[3_655] | 1.52 | 0.68 |
| 1:A:67:ARG:CG | 1:A:218:SER:O[3_655] | 1.52 | 0.68 |
| 1:A:61:VAL:C | 1:A:212:GLY:CA[3_655] | 1.53 | 0.67 |
| 1:A:28:LEU:N | 1:A:450:ILE:CD1[3_655] | 1.53 | 0.67 |
| 1:A:24:HIS:CB | 1:A:446:ALA:CB[3_655] | 1.53 | 0.67 |
| 1:A:75:LEU:C | 1:A:436:MET:N[3_655] | 1.53 | 0.67 |
| 1:A:40:GLY:CA | 1:A:70:ARG:CG[3_655] | 1.53 | 0.67 |
| 1:A:7:VAL:O | 1:A:451:LEU:CB[3_655] | 1.53 | 0.67 |
| 1:A:12:GLY:O | 1:A:70:ARG:CD[3_655] | 1.53 | 0.67 |
| 1:A:3:ASN:O | 1:A:457:ILE:C[3_655] | 1.53 | 0.67 |
| 1:A:75:LEU:CD2 | 1:A:439:ALA:CB[3_655] | 1.53 | 0.67 |
| 1:A:45:THR:C | 1:A:472:VAL:N[3_655] | 1.53 | 0.67 |
| 1:A:83:ASN:OD1 | 1:A:335:GLY:CA[3_655] | 1.54 | 0.66 |
| 1:A:227:ASP:C | 1:A:463:TRP:CB[3_655] | 1.54 | 0.66 |
| 1:A:44:TYR:CE1 | 1:A:469:SER:O[3_655] | 1.54 | 0.66 |
| 1:A:42:ARG:CA | 4:A:2010:HOH:O[3_655] | 1.54 | 0.66 |
| 1:A:257:ALA:CB | 1:A:456:LYS:CA[3_655] | 1.54 | 0.66 |
| 1:A:17:MET:CG | 1:A:444:GLU:OE2[3_655] | 1.54 | 0.66 |
| 1:A:44:TYR:CZ | 1:A:469:SER:O[3_655] | 1.54 | 0.66 |
| 1:A:21:LYS:CA | 1:A:443:GLY:O[3_655] | 1.54 | 0.66 |
| 1:A:220:ARG:CA | 1:A:437:GLU:O[3_655] | 1.54 | 0.66 |
| 1:A:219:GLU:C | 1:A:437:GLU:CD[3_655] | 1.54 | 0.66 |
| 1:A:321:GLU:CG | 1:A:499:THR:O[6_564] | 1.54 | 0.66 |
| 1:A:67:ARG:NE | 1:A:222:MET:CG[3_655] | 1.54 | 0.66 |
| 1:A:43:THR:CG2 | 1:A:73:LYS:CA[3_655] | 1.54 | 0.66 |
| 1:A:225:LEU:CD1 | 1:A:444:GLU:C[3_655] | 1.54 | 0.66 |
| 1:A:46:LEU:N | 1:A:472:VAL:C[3_655] | 1.54 | 0.66 |
| 1:A:84:GLU:CB | 1:A:336:ASN:CG[3_655] | 1.55 | 0.65 |
| 1:A:55:ASP:N | 1:A:208:ARG:NH1[3_655] | 1.55 | 0.65 |
| 1:A:17:MET:CG | 1:A:70:ARG:NH2[3_655] | 1.55 | 0.65 |
| 1:A:68:ILE:CA | 1:A:217:VAL:N[3_655] | 1.55 | 0.65 |
| 1:A:208:ARG:O | 1:A:211:VAL:C[3_655] | 1.55 | 0.65 |
| 1:A:231:LEU:CG | 1:A:465:SER:O[3_655] | 1.55 | 0.65 |
| 1:A:256:GLU:O | 1:A:455:GLY:O[3_655] | 1.55 | 0.65 |
| 1:A:223:ASP:CB | 1:A:441:GLU:OE1[3_655] | 1.55 | 0.65 |
| 1:A:53:TYR:CD2 | 1:A:207:GLU:CA[3_655] | 1.55 | 0.65 |
| 1:A:321:GLU:CD | 1:A:499:THR:O[6_564] | 1.56 | 0.64 |
| 1:A:67:ARG:NE | 1:A:222:MET:CA[3_655] | 1.56 | 0.64 |
| 1:A:255:TYR:CZ | 1:A:461:GLU:CD[3_655] | 1.56 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:77:LEU:N | 2:A:600:FAD:N1[3_655] | 1.56 | 0.64 |
| 1:A:32:VAL:O | 1:A:464:GLN:CD[3_655] | 1.56 | 0.64 |
| 1:A:74:GLU:CA | 2:A:600:FAD:O5'[3_655] | 1.56 | 0.64 |
| 1:A:44:TYR:CZ | 1:A:470:VAL:N[3_655] | 1.56 | 0.64 |
| 1:A:330:ASP:OD2 | 4:A:2116:HOH:O[3_655] | 1.56 | 0.64 |
| 1:A:209:LYS:CA | 1:A:210:PHE:C[3_655] | 1.56 | 0.64 |
| 1:A:24:HIS:NE2 | 1:A:445:ARG:NH2[3_655] | 1.56 | 0.64 |
| 1:A:422:TYR:O | 4:A:2008:HOH:O[3_655] | 1.56 | 0.64 |
| 1:A:28:LEU:C | 1:A:450:ILE:CA[3_655] | 1.56 | 0.64 |
| 1:A:59:SER:N | 1:A:77:LEU:C[3_655] | 1.57 | 0.63 |
| 1:A:47:ARG:NH1 | 4:A:2037:HOH:O[3_655] | 1.57 | 0.63 |
| 1:A:500:THR:O | 4:A:2149:HOH:O[6_565] | 1.57 | 0.63 |
| 1:A:83:ASN:CG | 1:A:335:GLY:N[3_655] | 1.57 | 0.63 |
| 1:A:80:TYR:CB | 1:A:209:LYS:CD[3_655] | 1.57 | 0.63 |
| 1:A:53:TYR:CE2 | 1:A:207:GLU:CB[3_655] | 1.57 | 0.63 |
| 1:A:44:TYR:CD2 | 1:A:470:VAL:CA[3_655] | 1.58 | 0.62 |
| 1:A:53:TYR:CD1 | 1:A:208:ARG:CG[3_655] | 1.58 | 0.62 |
| 1:A:30:VAL:N | 1:A:448:ARG:O[3_655] | 1.58 | 0.62 |
| 1:A:422:TYR:N | 4:A:2008:HOH:O[3_655] | 1.58 | 0.62 |
| 1:A:14:ILE:CG1 | 1:A:72:ALA:N[3_655] | 1.58 | 0.62 |
| 1:A:65:GLN:CD | 1:A:216:GLN:OE1[3_655] | 1.58 | 0.62 |
| 1:A:225:LEU:CD1 | 1:A:445:ARG:N[3_655] | 1.58 | 0.62 |
| 1:A:60:TYR:CE1 | 1:A:78:GLU:OE1[3_655] | 1.58 | 0.62 |
| 1:A:20:ALA:O | 1:A:447:ALA:CB[3_655] | 1.58 | 0.62 |
| 1:A:38:ARG:CA | 1:A:467:PRO:CB[3_655] | 1.58 | 0.62 |
| 1:A:69:LEU:CA | 1:A:215:GLY:CA[3_655] | 1.58 | 0.62 |
| 1:A:76:GLY:C | 2:A:600:FAD:C10[3_655] | 1.58 | 0.62 |
| 1:A:19:ALA:CB | 1:A:22:LEU:CA[3_655] | 1.59 | 0.61 |
| 1:A:24:HIS:CD2 | 1:A:446:ALA:CB[3_655] | 1.59 | 0.61 |
| 1:A:44:TYR:C | 4:A:2216:HOH:O[3_655] | 1.59 | 0.61 |
| 1:A:44:TYR:CD1 | 1:A:469:SER:CA[3_655] | 1.59 | 0.61 |
| 1:A:80:TYR:CB | 1:A:209:LYS:CE[3_655] | 1.59 | 0.61 |
| 1:A:225:LEU:CD2 | 1:A:445:ARG:CA[3_655] | 1.59 | 0.61 |
| 1:A:46:LEU:C | 1:A:473:PRO:N[3_655] | 1.59 | 0.61 |
| 1:A:83:ASN:O | 1:A:334:GLU:CA[3_655] | 1.59 | 0.61 |
| 1:A:47:ARG:N | 1:A:473:PRO:C[3_655] | 1.59 | 0.61 |
| 1:A:38:ARG:CA | 1:A:467:PRO:CD[3_655] | 1.59 | 0.61 |
| 1:A:26:SER:CA | 1:A:260:VAL:C[3_655] | 1.59 | 0.61 |
| 1:A:73:LYS:O | 2:A:600:FAD:C2'[3_655] | 1.59 | 0.61 |
| 1:A:52:LYS:CE | 1:A:201:THR:C[3_655] | 1.59 | 0.61 |
| 1:A:66:ASN:N | 1:A:219:GLU:CB[3_655] | 1.60 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:5:CYS:CB | 1:A:452:HIS:N[3_655] | 1.60 | 0.60 |
| 1:A:53:TYR:CB | 1:A:207:GLU:CD[3_655] | 1.60 | 0.60 |
| 1:A:54:VAL:N | 1:A:208:ARG:CZ[3_655] | 1.60 | 0.60 |
| 1:A:223:ASP:OD2 | 1:A:431:HIS:O[3_655] | 1.60 | 0.60 |
| 1:A:83:ASN:CG | 1:A:335:GLY:C[3_655] | 1.60 | 0.60 |
| 1:A:229:VAL:C | 1:A:464:GLN:CG[3_655] | 1.60 | 0.60 |
| 1:A:14:ILE:CG2 | 1:A:71:LEU:CG[3_655] | 1.60 | 0.60 |
| 1:A:29:ASN:CB | 1:A:449:GLU:C[3_655] | 1.60 | 0.60 |
| 1:A:43:THR:CA | 1:A:73:LYS:CB[3_655] | 1.60 | 0.60 |
| 1:A:24:HIS:CB | 1:A:446:ALA:C[3_655] | 1.60 | 0.60 |
| 1:A:29:ASN:N | 1:A:449:GLU:C[3_655] | 1.60 | 0.60 |
| 1:A:257:ALA:CA | 1:A:456:LYS:CB[3_655] | 1.61 | 0.59 |
| 1:A:45:THR:O | 1:A:472:VAL:O[3_655] | 1.61 | 0.59 |
| 1:A:5:CYS:SG | 1:A:457:ILE:CG1[3_655] | 1.61 | 0.59 |
| 1:A:61:VAL:CG2 | 1:A:213:GLY:O[3_655] | 1.61 | 0.59 |
| 1:A:32:VAL:N | 1:A:448:ARG:CD[3_655] | 1.61 | 0.59 |
| 1:A:25:ASP:O | 1:A:261:ILE:CA[3_655] | 1.61 | 0.59 |
| 1:A:228:ARG:O | 1:A:461:GLU:O[3_655] | 1.61 | 0.59 |
| 1:A:44:TYR:C | 1:A:469:SER:OG[3_655] | 1.62 | 0.58 |
| 1:A:56:LEU:C | 1:A:471:ASP:OD2[3_655] | 1.62 | 0.58 |
| 1:A:257:ALA:CA | 1:A:456:LYS:N[3_655] | 1.62 | 0.58 |
| 1:A:83:ASN:ND2 | 1:A:335:GLY:N[3_655] | 1.62 | 0.58 |
| 1:A:256:GLU:O | 1:A:456:LYS:N[3_655] | 1.62 | 0.58 |
| 1:A:67:ARG:C | 1:A:218:SER:CB[3_655] | 1.63 | 0.57 |
| 1:A:20:ALA:N | 1:A:22:LEU:CB[3_655] | 1.63 | 0.57 |
| 1:A:61:VAL:CG2 | 1:A:213:GLY:C[3_655] | 1.63 | 0.57 |
| 1:A:257:ALA:CB | 1:A:456:LYS:CG[3_655] | 1.63 | 0.57 |
| 1:A:84:GLU:O | 1:A:336:ASN:ND2[3_655] | 1.63 | 0.57 |
| 1:A:65:GLN:CA | 4:A:2120:HOH:O[3_655] | 1.63 | 0.57 |
| 1:A:15:SER:CA | 1:A:21:LYS:NZ[3_655] | 1.64 | 0.56 |
| 1:A:66:ASN:OD1 | 1:A:219:GLU:OE2[3_655] | 1.64 | 0.56 |
| 1:A:61:VAL:CB | 1:A:216:GLN:NE2[3_655] | 1.64 | 0.56 |
| 1:A:224:LEU:N | 1:A:441:GLU:CD[3_655] | 1.64 | 0.56 |
| 1:A:69:LEU:C | 4:A:2018:HOH:O[3_655] | 1.64 | 0.56 |
| 1:A:6:ASP:O | 1:A:454:MET:CE[3_655] | 1.65 | 0.55 |
| 1:A:59:SER:OG | 1:A:78:GLU:C[3_655] | 1.65 | 0.55 |
| 1:A:47:ARG:NE | 1:A:63:PRO:N[3_655] | 1.65 | 0.55 |
| 1:A:67:ARG:O | 1:A:218:SER:N[3_655] | 1.65 | 0.55 |
| 1:A:206:GLN:O | 4:A:2030:HOH:O[3_655] | 1.65 | 0.55 |
| 1:A:24:HIS:N | 1:A:261:ILE:CD1[3_655] | 1.65 | 0.55 |
| 1:A:54:VAL:O | 1:A:471:ASP:O[3_655] | 1.65 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:83:ASN:N | 1:A:333:PRO:N[3_655] | 1.65 | 0.55 |
| 1:A:84:GLU:N | 1:A:336:ASN:N[3_655] | 1.65 | 0.55 |
| 1:A:501:ILE:N | 4:A:2014:HOH:O[6_565] | 1.65 | 0.55 |
| 1:A:53:TYR:CE1 | 1:A:208:ARG:N[3_655] | 1.65 | 0.55 |
| 1:A:27:GLY:N | 1:A:260:VAL:O[3_655] | 1.65 | 0.55 |
| 1:A:24:HIS:CE1 | 1:A:445:ARG:CZ[3_655] | 1.66 | 0.54 |
| 1:A:45:THR:C | 1:A:472:VAL:C[3_655] | 1.66 | 0.54 |
| 1:A:13:GLY:O | 1:A:70:ARG:NH1[3_655] | 1.66 | 0.54 |
| 1:A:62:GLY:N | 1:A:212:GLY:O[3_655] | 1.66 | 0.54 |
| 1:A:40:GLY:C | 1:A:70:ARG:CG[3_655] | 1.66 | 0.54 |
| 1:A:68:ILE:CG1 | 1:A:217:VAL:CA[3_655] | 1.66 | 0.54 |
| 1:A:259:TYR:N | 1:A:456:LYS:NZ[3_655] | 1.66 | 0.54 |
| 1:A:25:ASP:OD1 | 1:A:424:ALA:CA[3_655] | 1.66 | 0.54 |
| 1:A:25:ASP:CG | 1:A:424:ALA:CB[3_655] | 1.66 | 0.54 |
| 1:A:81:LYS:CG | 4:A:2158:HOH:O[3_655] | 1.67 | 0.53 |
| 1:A:53:TYR:CG | 1:A:207:GLU:CB[3_655] | 1.67 | 0.53 |
| 1:A:68:ILE:N | 1:A:217:VAL:C[3_655] | 1.67 | 0.53 |
| 1:A:307:ARG:NH2 | 4:A:2157:HOH:O[3_655] | 1.67 | 0.53 |
| 1:A:23:LEU:CB | 1:A:23:LEU:CD1[3_655] | 1.67 | 0.53 |
| 1:A:23:LEU:CG | 1:A:23:LEU:CD2[3_655] | 1.67 | 0.53 |
| 1:A:53:TYR:CE1 | 1:A:208:ARG:CG[3_655] | 1.67 | 0.53 |
| 1:A:44:TYR:CZ | 1:A:469:SER:C[3_655] | 1.67 | 0.53 |
| 1:B:475:GLN:NE2 | 4:B:2058:HOH:O[3_555] | 1.67 | 0.53 |
| 1:A:220:ARG:CA | 1:A:437:GLU:C[3_655] | 1.67 | 0.53 |
| 1:A:75:LEU:N | 2:A:600:FAD:C4'[3_655] | 1.67 | 0.53 |
| 1:A:6:ASP:OD2 | 1:A:450:ILE:O[3_655] | 1.67 | 0.53 |
| 1:A:7:VAL:C | 1:A:451:LEU:CD1[3_655] | 1.68 | 0.52 |
| 1:A:26:SER:CB | 1:A:261:ILE:N[3_655] | 1.68 | 0.52 |
| 1:A:7:VAL:CB | 1:A:451:LEU:CG[3_655] | 1.68 | 0.52 |
| 1:A:82:VAL:CB | 1:A:333:PRO:CD[3_655] | 1.68 | 0.52 |
| 1:A:221:ILE:CB | 1:A:440:VAL:CB[3_655] | 1.68 | 0.52 |
| 1:A:202:THR:OG1 | 1:A:337:TYR:CE1[3_655] | 1.68 | 0.52 |
| 1:A:67:ARG:C | 1:A:218:SER:C[3_655] | 1.68 | 0.52 |
| 1:A:75:LEU:O | 1:A:435:TYR:O[3_655] | 1.68 | 0.52 |
| 1:A:75:LEU:CG | 1:A:439:ALA:CB[3_655] | 1.68 | 0.52 |
| 1:A:228:ARG:CG | 1:A:462:ILE:O[3_655] | 1.68 | 0.52 |
| 1:A:67:ARG:CB | 1:A:219:GLU:N[3_655] | 1.68 | 0.52 |
| 1:A:75:LEU:CA | 1:A:435:TYR:O[3_655] | 1.68 | 0.52 |
| 1:A:52:LYS:O | 1:A:207:GLU:OE1[3_655] | 1.68 | 0.52 |
| 1:A:67:ARG:CD | 1:A:222:MET:N[3_655] | 1.68 | 0.52 |
| 1:A:65:GLN:OE1 | 1:A:216:GLN:CG[3_655] | 1.68 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:220:ARG:CB | 1:A:438:GLY:N[3_655] | 1.68 | 0.52 |
| 1:A:45:THR:CA | 1:A:472:VAL:CG2[3_655] | 1.69 | 0.51 |
| 1:A:220:ARG:CB | 1:A:437:GLU:CB[3_655] | 1.69 | 0.51 |
| 1:A:24:HIS:CG | 1:A:446:ALA:N[3_655] | 1.69 | 0.51 |
| 1:A:56:LEU:CB | 1:A:471:ASP:OD2[3_655] | 1.69 | 0.51 |
| 1:B:478:THR:C | 1:B:479:THR:N[3_555] | 1.69 | 0.51 |
| 1:A:210:PHE:CE1 | 1:A:210:PHE:CE1[3_655] | 1.69 | 0.51 |
| 1:B:81:LYS:CE | 1:B:100:ARG:NH1[3_555] | 1.69 | 0.51 |
| 1:A:82:VAL:CG1 | 1:A:333:PRO:CG[3_655] | 1.69 | 0.51 |
| 1:A:230:LYS:NZ | 1:A:460:ASP:C[3_655] | 1.69 | 0.51 |
| 1:A:54:VAL:N | 1:A:208:ARG:NE[3_655] | 1.69 | 0.51 |
| 1:A:221:ILE:O | 1:A:441:GLU:CB[3_655] | 1.69 | 0.51 |
| 1:A:83:ASN:N | 1:A:332:LYS:CA[3_655] | 1.69 | 0.51 |
| 1:A:82:VAL:C | 1:A:332:LYS:C[3_655] | 1.69 | 0.51 |
| 1:A:52:LYS:NZ | 1:A:202:THR:N[3_655] | 1.69 | 0.51 |
| 1:A:45:THR:O | 1:A:472:VAL:C[3_655] | 1.70 | 0.50 |
| 1:A:52:LYS:CB | 1:A:202:THR:CA[3_655] | 1.70 | 0.50 |
| 1:A:226:GLY:O | 4:A:2214:HOH:O[3_655] | 1.70 | 0.50 |
| 1:A:54:VAL:CA | 1:A:208:ARG:NH1[3_655] | 1.70 | 0.50 |
| 1:A:82:VAL:O | 1:A:332:LYS:CG[3_655] | 1.70 | 0.50 |
| 1:A:66:ASN:N | 1:A:219:GLU:OE1[3_655] | 1.70 | 0.50 |
| 1:A:208:ARG:O | 1:A:211:VAL:N[3_655] | 1.70 | 0.50 |
| 1:A:220:ARG:NH1 | 1:A:435:TYR:CD2[3_655] | 1.70 | 0.50 |
| 1:A:68:ILE:CG2 | 1:A:216:GLN:CA[3_655] | 1.71 | 0.49 |
| 1:A:255:TYR:CE2 | 1:A:461:GLU:CD[3_655] | 1.71 | 0.49 |
| 1:A:21:LYS:CB | 1:A:443:GLY:CA[3_655] | 1.71 | 0.49 |
| 1:A:15:SER:CA | 1:A:21:LYS:CD[3_655] | 1.71 | 0.49 |
| 1:A:258:LYS:N | 1:A:456:LYS:CG[3_655] | 1.71 | 0.49 |
| 1:A:26:SER:O | 1:A:260:VAL:CA[3_655] | 1.71 | 0.49 |
| 1:A:38:ARG:O | 1:A:467:PRO:CG[3_655] | 1.71 | 0.49 |
| 1:A:43:THR:N | 1:A:73:LYS:CG[3_655] | 1.71 | 0.49 |
| 1:A:17:MET:CA | 1:A:444:GLU:CD[3_655] | 1.71 | 0.49 |
| 1:A:62:GLY:CA | 1:A:212:GLY:O[3_655] | 1.71 | 0.49 |
| 1:A:55:ASP:CB | 1:A:79:THR:OG1[3_655] | 1.71 | 0.49 |
| 1:A:25:ASP:N | 1:A:261:ILE:CG2[3_655] | 1.71 | 0.49 |
| 1:B:478:THR:CA | 1:B:478:THR:O[3_555] | 1.72 | 0.48 |
| 1:A:76:GLY:O | 2:A:600:FAD:N3[3_655] | 1.72 | 0.48 |
| 1:A:30:VAL:CG2 | 1:A:447:ALA:C[3_655] | 1.72 | 0.48 |
| 1:A:24:HIS:CA | 1:A:446:ALA:C[3_655] | 1.72 | 0.48 |
| 1:A:75:LEU:CB | 1:A:436:MET:C[3_655] | 1.72 | 0.48 |
| 1:A:208:ARG:O | 1:A:210:PHE:O[3_655] | 1.72 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:40:GLY:O | 1:A:70:ARG:O[3_655] | 1.72 | 0.48 |
| 1:A:5:CYS:CA | 1:A:452:HIS:C[3_655] | 1.72 | 0.48 |
| 1:A:80:TYR:CE1 | 1:A:80:TYR:CZ[3_655] | 1.72 | 0.48 |
| 1:A:42:ARG:CG | 4:A:2010:HOH:O[3_655] | 1.72 | 0.48 |
| 1:A:227:ASP:OD2 | 4:A:2212:HOH:O[3_655] | 1.72 | 0.48 |
| 1:A:43:THR:N | 1:A:73:LYS:CD[3_655] | 1.73 | 0.47 |
| 1:A:422:TYR:CA | 4:A:2008:HOH:O[3_655] | 1.73 | 0.47 |
| 1:A:39:VAL:CG2 | 1:A:466:GLU:OE1[3_655] | 1.73 | 0.47 |
| 1:A:28:LEU:C | 1:A:450:ILE:CG1[3_655] | 1.73 | 0.47 |
| 1:A:230:LYS:N | 1:A:464:GLN:NE2[3_655] | 1.73 | 0.47 |
| 1:A:38:ARG:C | 1:A:467:PRO:N[3_655] | 1.73 | 0.47 |
| 1:A:66:ASN:CA | 1:A:219:GLU:CD[3_655] | 1.73 | 0.47 |
| 1:A:67:ARG:N | 1:A:219:GLU:CA[3_655] | 1.73 | 0.47 |
| 1:A:48:ASN:CA | 1:A:475:GLN:CG[3_655] | 1.73 | 0.47 |
| 1:B:478:THR:CA | 1:B:478:THR:C[3_555] | 1.73 | 0.47 |
| 1:A:7:VAL:N | 1:A:451:LEU:CB[3_655] | 1.73 | 0.47 |
| 1:A:224:LEU:C | 4:A:2204:HOH:O[3_655] | 1.73 | 0.47 |
| 1:A:47:ARG:C | 1:A:473:PRO:O[3_655] | 1.74 | 0.46 |
| 1:A:258:LYS:N | 1:A:456:LYS:CE[3_655] | 1.74 | 0.46 |
| 1:A:53:TYR:CE1 | 1:A:208:ARG:CA[3_655] | 1.74 | 0.46 |
| 1:B:478:THR:C | 1:B:478:THR:CB[3_555] | 1.74 | 0.46 |
| 1:A:53:TYR:CE1 | 1:A:207:GLU:C[3_655] | 1.74 | 0.46 |
| 1:A:61:VAL:N | 1:A:211:VAL:C[3_655] | 1.74 | 0.46 |
| 1:A:44:TYR:CD2 | 1:A:470:VAL:N[3_655] | 1.74 | 0.46 |
| 1:A:81:LYS:NZ | 1:A:300:TYR:CE2[3_655] | 1.74 | 0.46 |
| 1:A:53:TYR:N | 1:A:207:GLU:OE2[3_655] | 1.74 | 0.46 |
| 1:A:56:LEU:CA | 1:A:471:ASP:OD2[3_655] | 1.74 | 0.46 |
| 1:A:231:LEU:CD1 | 1:A:465:SER:OG[3_655] | 1.75 | 0.45 |
| 1:A:227:ASP:CA | 1:A:463:TRP:CA[3_655] | 1.75 | 0.45 |
| 1:A:77:LEU:CA | 2:A:600:FAD:N3[3_655] | 1.75 | 0.45 |
| 1:A:15:SER:O | 1:A:21:LYS:CG[3_655] | 1.75 | 0.45 |
| 1:A:228:ARG:N | 1:A:462:ILE:C[3_655] | 1.75 | 0.45 |
| 1:A:14:ILE:CG2 | 1:A:71:LEU:CD1[3_655] | 1.75 | 0.45 |
| 1:A:53:TYR:OH | 1:A:208:ARG:N[3_655] | 1.75 | 0.45 |
| 1:A:259:TYR:C | 4:A:2006:HOH:O[3_655] | 1.75 | 0.45 |
| 1:A:221:ILE:CB | 1:A:440:VAL:CG1[3_655] | 1.75 | 0.45 |
| 1:A:45:THR:C | 1:A:472:VAL:CB[3_655] | 1.75 | 0.45 |
| 1:A:17:MET:CB | 1:A:444:GLU:CD[3_655] | 1.75 | 0.45 |
| 1:A:32:VAL:O | 1:A:464:GLN:OE1[3_655] | 1.76 | 0.44 |
| 1:A:5:CYS:O | 1:A:451:LEU:O[3_655] | 1.76 | 0.44 |
| 1:A:329:ASP:O | 1:A:333:PRO:CB[3_655] | 1.76 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------------|--------------------------|-------------------|
| 1:A:80:TYR:CD2 | 1:A:209:LYS:CD[3_655] | 1.76 | 0.44 |
| 1:A:81:LYS:O | 1:A:331:THR:O[3_655] | 1.76 | 0.44 |
| 1:A:73:LYS:C | 2:A:600:FAD:O2'[3_655] | 1.76 | 0.44 |
| 1:A:83:ASN:OD1 | 1:A:335:GLY:O[3_655] | 1.76 | 0.44 |
| 1:A:14:ILE:CD1 | 1:A:71:LEU:O[3_655] | 1.76 | 0.44 |
| 1:A:24:HIS:NE2 | 1:A:445:ARG:CZ[3_655] | 1.76 | 0.44 |
| 1:A:75:LEU:C | 1:A:435:TYR:O[3_655] | 1.76 | 0.44 |
| 1:A:18:ALA:CA | 1:A:18:ALA:C[3_655] | 1.76 | 0.44 |
| 1:A:14:ILE:CA | 1:A:71:LEU:CD1[3_655] | 1.77 | 0.43 |
| 1:A:65:GLN:NE2 | 1:A:220:ARG:NH2[3_655] | 1.77 | 0.43 |
| 1:A:81:LYS:CA | 4:A:2158:HOH:O[3_655] | 1.77 | 0.43 |
| 1:A:60:TYR:CG | 1:A:211:VAL:CG1[3_655] | 1.77 | 0.43 |
| 1:A:220:ARG:CG | 1:A:437:GLU:CG[3_655] | 1.77 | 0.43 |
| 1:A:330:ASP:CB | 4:A:2046:HOH:O[3_655] | 1.77 | 0.43 |
| 1:A:14:ILE:CB | 1:A:71:LEU:C[3_655] | 1.77 | 0.43 |
| 1:A:85:VAL:N | 1:A:336:ASN:N[3_655] | 1.77 | 0.43 |
| 1:A:52:LYS:CD | 1:A:201:THR:O[3_655] | 1.77 | 0.43 |
| 1:A:14:ILE:CB | 1:A:71:LEU:O[3_655] | 1.77 | 0.43 |
| 1:A:28:LEU:CD2 | 1:A:259:TYR:CG[3_655] | 1.78 | 0.42 |
| 1:A:38:ARG:CD | 1:A:468:GLU:O[3_655] | 1.78 | 0.42 |
| 1:A:45:THR:CB | 1:A:472:VAL:CG2[3_655] | 1.78 | 0.42 |
| 1:A:46:LEU:C | 1:A:472:VAL:C[3_655] | 1.78 | 0.42 |
| 1:A:80:TYR:CG | 1:A:209:LYS:CD[3_655] | 1.78 | 0.42 |
| 1:A:224:LEU:CB | 1:A:442:ALA:CA[3_655] | 1.78 | 0.42 |
| 1:A:69:LEU:CB | 1:A:215:GLY:N[3_655] | 1.78 | 0.42 |
| 1:A:74:GLU:OE1 | 2:A:600:FAD:P[3_655] | 1.78 | 0.42 |
| 1:A:30:VAL:C | 1:A:448:ARG:C[3_655] | 1.78 | 0.42 |
| 1:A:30:VAL:CB | 1:A:447:ALA:O[3_655] | 1.78 | 0.42 |
| 1:A:68:ILE:C | 4:A:2018:HOH:O[3_655] | 1.79 | 0.41 |
| 1:A:28:LEU:O | 1:A:450:ILE:N[3_655] | 1.79 | 0.41 |
| 1:A:60:TYR:CB | 1:A:211:VAL:CB[3_655] | 1.79 | 0.41 |
| 1:A:259:TYR:O | 4:A:2006:HOH:O[3_655] | 1.79 | 0.41 |
| 1:A:65:GLN:O | 1:A:215:GLY:C[3_655] | 1.79 | 0.41 |
| 1:A:21:LYS:CG | 1:A:443:GLY:CA[3_655] | 1.79 | 0.41 |
| 1:A:220:ARG:N | 1:A:437:GLU:OE1[3_655] | 1.79 | 0.41 |
| 1:A:26:SER:O | 1:A:260:VAL:N[3_655] | 1.79 | 0.41 |
| 1:A:229:VAL:CB | 1:A:464:GLN:CB[3_655] | 1.79 | 0.41 |
| 1:A:223:ASP:N | 1:A:441:GLU:OE1[3_655] | 1.79 | 0.41 |
| 1:A:30:VAL:O | 1:A:448:ARG:C[3_655] | 1.79 | 0.41 |
| 1:A:73:LYS:O | 2:A:600:FAD:C3'[3_655] | 1.79 | 0.41 |
| 1:A:74:GLU:O | 2:A:600:FAD:C4'[3_655] | 1.80 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------------|--------------------------|-------------------|
| 1:A:214:SER:OG | 4:A:2043:HOH:O[3_655] | 1.80 | 0.40 |
| 1:A:54:VAL:C | 1:A:208:ARG:CZ[3_655] | 1.80 | 0.40 |
| 1:A:72:ALA:CB | 1:A:436:MET:SD[3_655] | 1.80 | 0.40 |
| 1:A:54:VAL:C | 1:A:208:ARG:NH1[3_655] | 1.80 | 0.40 |
| 1:A:14:ILE:CG1 | 1:A:71:LEU:CB[3_655] | 1.80 | 0.40 |
| 1:A:45:THR:CG2 | 1:A:472:VAL:CG2[3_655] | 1.80 | 0.40 |
| 1:A:217:VAL:O | 1:A:440:VAL:CG2[3_655] | 1.80 | 0.40 |
| 1:A:44:TYR:CE2 | 1:A:470:VAL:N[3_655] | 1.80 | 0.40 |
| 1:A:229:VAL:N | 1:A:464:GLN:N[3_655] | 1.80 | 0.40 |
| 1:A:68:ILE:CB | 1:A:216:GLN:C[3_655] | 1.80 | 0.40 |
| 1:A:334:GLU:CB | 4:A:2048:HOH:O[3_655] | 1.81 | 0.39 |
| 1:A:23:LEU:CB | 1:A:23:LEU:CG[3_655] | 1.81 | 0.39 |
| 1:A:14:ILE:CG1 | 1:A:71:LEU:O[3_655] | 1.81 | 0.39 |
| 1:A:230:LYS:CE | 1:A:460:ASP:C[3_655] | 1.81 | 0.39 |
| 1:A:312:CYS:CB | 1:A:334:GLU:O[3_655] | 1.81 | 0.39 |
| 1:A:28:LEU:CD2 | 1:A:259:TYR:CD1[3_655] | 1.81 | 0.39 |
| 1:A:501:ILE:O | 4:A:2054:HOH:O[6_565] | 1.81 | 0.39 |
| 1:A:21:LYS:N | 1:A:443:GLY:O[3_655] | 1.81 | 0.39 |
| 1:A:230:LYS:N | 1:A:464:GLN:CD[3_655] | 1.81 | 0.39 |
| 1:A:60:TYR:N | 1:A:78:GLU:N[3_655] | 1.81 | 0.39 |
| 1:A:230:LYS:CE | 1:A:461:GLU:N[3_655] | 1.81 | 0.39 |
| 1:A:29:ASN:O | 1:A:451:LEU:CA[3_655] | 1.81 | 0.39 |
| 1:A:13:GLY:CA | 1:A:70:ARG:CD[3_655] | 1.81 | 0.39 |
| 1:A:47:ARG:NE | 1:A:63:PRO:C[3_655] | 1.81 | 0.39 |
| 1:A:74:GLU:OE1 | 2:A:600:FAD:O2P[3_655] | 1.81 | 0.39 |
| 1:A:3:ASN:CA | 1:A:458:PRO:CB[3_655] | 1.81 | 0.39 |
| 1:A:85:VAL:CA | 1:A:336:ASN:CA[3_655] | 1.81 | 0.39 |
| 1:A:7:VAL:CG1 | 1:A:451:LEU:CD2[3_655] | 1.81 | 0.39 |
| 1:A:60:TYR:N | 1:A:78:GLU:O[3_655] | 1.81 | 0.39 |
| 1:A:227:ASP:CB | 1:A:463:TRP:CB[3_655] | 1.81 | 0.39 |
| 1:A:227:ASP:O | 1:A:463:TRP:N[3_655] | 1.81 | 0.39 |
| 1:A:59:SER:CA | 1:A:78:GLU:N[3_655] | 1.82 | 0.38 |
| 1:A:67:ARG:CD | 1:A:222:MET:CA[3_655] | 1.82 | 0.38 |
| 1:A:81:LYS:CB | 4:A:2158:HOH:O[3_655] | 1.82 | 0.38 |
| 1:A:227:ASP:C | 1:A:463:TRP:O[3_655] | 1.82 | 0.38 |
| 1:A:24:HIS:CB | 1:A:447:ALA:N[3_655] | 1.82 | 0.38 |
| 1:A:55:ASP:CG | 1:A:79:THR:CG2[3_655] | 1.82 | 0.38 |
| 1:A:39:VAL:CG1 | 1:A:466:GLU:CD[3_655] | 1.82 | 0.38 |
| 1:A:71:LEU:N | 1:A:218:SER:OG[3_655] | 1.82 | 0.38 |
| 1:A:76:GLY:N | 2:A:600:FAD:C2'[3_655] | 1.82 | 0.38 |
| 1:A:20:ALA:CB | 1:A:22:LEU:CD1[3_655] | 1.82 | 0.38 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------------|--------------------------|-------------------|
| 1:A:463:TRP:O | 4:A:2122:HOH:O[3_655] | 1.82 | 0.38 |
| 1:A:47:ARG:CB | 1:A:473:PRO:O[3_655] | 1.82 | 0.38 |
| 1:A:32:VAL:CG2 | 4:A:2209:HOH:O[3_655] | 1.82 | 0.38 |
| 1:A:7:VAL:C | 1:A:451:LEU:CD2[3_655] | 1.82 | 0.38 |
| 1:A:53:TYR:CE1 | 1:A:208:ARG:CB[3_655] | 1.82 | 0.38 |
| 1:A:227:ASP:N | 1:A:463:TRP:CG[3_655] | 1.82 | 0.38 |
| 1:A:225:LEU:CG | 1:A:441:GLU:O[3_655] | 1.82 | 0.38 |
| 1:A:83:ASN:O | 1:A:334:GLU:C[3_655] | 1.82 | 0.38 |
| 1:A:73:LYS:O | 2:A:600:FAD:O4'[3_655] | 1.82 | 0.38 |
| 1:A:59:SER:CB | 1:A:78:GLU:CB[3_655] | 1.83 | 0.37 |
| 1:A:77:LEU:CA | 2:A:600:FAD:C2[3_655] | 1.83 | 0.37 |
| 1:A:24:HIS:ND1 | 1:A:446:ALA:N[3_655] | 1.83 | 0.37 |
| 1:A:66:ASN:CG | 1:A:219:GLU:OE2[3_655] | 1.83 | 0.37 |
| 1:A:85:VAL:CG1 | 4:A:2142:HOH:O[3_655] | 1.83 | 0.37 |
| 1:A:55:ASP:CG | 1:A:79:THR:CB[3_655] | 1.83 | 0.37 |
| 1:A:41:GLY:C | 4:A:2044:HOH:O[3_655] | 1.83 | 0.37 |
| 1:A:225:LEU:CB | 1:A:445:ARG:CB[3_655] | 1.83 | 0.37 |
| 1:A:67:ARG:CA | 1:A:218:SER:CA[3_655] | 1.83 | 0.37 |
| 1:A:220:ARG:N | 1:A:437:GLU:OE2[3_655] | 1.83 | 0.37 |
| 1:A:26:SER:C | 1:A:261:ILE:N[3_655] | 1.83 | 0.37 |
| 1:A:333:PRO:N | 4:A:2154:HOH:O[3_655] | 1.83 | 0.37 |
| 1:A:30:VAL:CG2 | 1:A:448:ARG:CA[3_655] | 1.83 | 0.37 |
| 1:A:77:LEU:N | 2:A:600:FAD:O2[3_655] | 1.83 | 0.37 |
| 1:A:23:LEU:CA | 1:A:261:ILE:CD1[3_655] | 1.83 | 0.37 |
| 1:A:27:GLY:CA | 1:A:422:TYR:CD1[3_655] | 1.83 | 0.37 |
| 1:A:29:ASN:CA | 1:A:449:GLU:CA[3_655] | 1.83 | 0.37 |
| 1:A:59:SER:C | 1:A:78:GLU:N[3_655] | 1.84 | 0.36 |
| 1:A:67:ARG:NH2 | 1:A:222:MET:SD[3_655] | 1.84 | 0.36 |
| 1:A:224:LEU:CB | 1:A:442:ALA:CB[3_655] | 1.84 | 0.36 |
| 1:A:52:LYS:CD | 1:A:202:THR:C[3_655] | 1.84 | 0.36 |
| 1:A:38:ARG:N | 1:A:467:PRO:N[3_655] | 1.84 | 0.36 |
| 1:A:220:ARG:CD | 1:A:437:GLU:CB[3_655] | 1.84 | 0.36 |
| 1:A:23:LEU:O | 1:A:261:ILE:CG1[3_655] | 1.84 | 0.36 |
| 1:A:14:ILE:CB | 1:A:71:LEU:CA[3_655] | 1.84 | 0.36 |
| 1:A:221:ILE:CB | 1:A:440:VAL:O[3_655] | 1.84 | 0.36 |
| 1:A:29:ASN:C | 1:A:448:ARG:O[3_655] | 1.84 | 0.36 |
| 1:A:84:GLU:C | 1:A:336:ASN:CA[3_655] | 1.84 | 0.36 |
| 1:A:210:PHE:CG | 1:A:210:PHE:CE1[3_655] | 1.85 | 0.35 |
| 1:A:28:LEU:C | 1:A:450:ILE:CB[3_655] | 1.85 | 0.35 |
| 1:A:4:LYS:C | 1:A:457:ILE:O[3_655] | 1.85 | 0.35 |
| 1:A:221:ILE:O | 1:A:441:GLU:N[3_655] | 1.85 | 0.35 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:219:GLU:CA | 1:A:437:GLU:OE1[3_655] | 1.85 | 0.35 |
| 1:A:65:GLN:O | 1:A:216:GLN:N[3_655] | 1.85 | 0.35 |
| 1:A:74:GLU:CG | 2:A:600:FAD:O1P[3_655] | 1.85 | 0.35 |
| 1:A:56:LEU:N | 1:A:471:ASP:CB[3_655] | 1.85 | 0.35 |
| 1:A:229:VAL:CA | 1:A:464:GLN:CA[3_655] | 1.85 | 0.35 |
| 1:A:257:ALA:CA | 1:A:456:LYS:CG[3_655] | 1.85 | 0.35 |
| 1:A:43:THR:CG2 | 1:A:73:LYS:CB[3_655] | 1.85 | 0.35 |
| 1:A:500:THR:OG1 | 4:A:2168:HOH:O[6_565] | 1.86 | 0.34 |
| 1:A:230:LYS:N | 1:A:464:GLN:CB[3_655] | 1.86 | 0.34 |
| 1:A:69:LEU:N | 1:A:215:GLY:C[3_655] | 1.86 | 0.34 |
| 1:A:208:ARG:CB | 4:A:2118:HOH:O[3_655] | 1.86 | 0.34 |
| 1:A:59:SER:CA | 1:A:79:THR:N[3_655] | 1.86 | 0.34 |
| 1:A:76:GLY:O | 2:A:600:FAD:C4X[3_655] | 1.87 | 0.33 |
| 1:A:7:VAL:C | 1:A:451:LEU:CB[3_655] | 1.87 | 0.33 |
| 1:A:65:GLN:O | 1:A:215:GLY:O[3_655] | 1.87 | 0.33 |
| 1:A:17:MET:CG | 1:A:70:ARG:NH1[3_655] | 1.87 | 0.33 |
| 1:A:229:VAL:CG2 | 1:A:448:ARG:NH2[3_655] | 1.87 | 0.33 |
| 1:A:221:ILE:CG1 | 1:A:440:VAL:CG2[3_655] | 1.87 | 0.33 |
| 1:A:25:ASP:C | 1:A:261:ILE:C[3_655] | 1.87 | 0.33 |
| 1:A:84:GLU:CB | 1:A:336:ASN:ND2[3_655] | 1.87 | 0.33 |
| 1:A:228:ARG:NH1 | 1:A:445:ARG:CD[3_655] | 1.87 | 0.33 |
| 1:A:53:TYR:CZ | 1:A:207:GLU:CA[3_655] | 1.87 | 0.33 |
| 1:A:78:GLU:CD | 4:A:2139:HOH:O[3_655] | 1.87 | 0.33 |
| 1:A:312:CYS:O | 1:A:334:GLU:O[3_655] | 1.87 | 0.33 |
| 1:A:229:VAL:O | 1:A:464:GLN:CB[3_655] | 1.87 | 0.33 |
| 1:A:386:LYS:NZ | 1:A:470:VAL:CG2[3_655] | 1.87 | 0.33 |
| 1:A:31:VAL:N | 1:A:448:ARG:CB[3_655] | 1.87 | 0.33 |
| 1:A:83:ASN:CB | 1:A:335:GLY:CA[3_655] | 1.88 | 0.32 |
| 1:A:52:LYS:CG | 1:A:202:THR:C[3_655] | 1.88 | 0.32 |
| 1:A:29:ASN:C | 1:A:449:GLU:C[3_655] | 1.88 | 0.32 |
| 1:A:3:ASN:C | 1:A:458:PRO:CA[3_655] | 1.88 | 0.32 |
| 1:A:256:GLU:C | 1:A:455:GLY:C[3_655] | 1.88 | 0.32 |
| 1:A:3:ASN:N | 1:A:458:PRO:CA[3_655] | 1.88 | 0.32 |
| 1:A:47:ARG:CZ | 1:A:63:PRO:CA[3_655] | 1.88 | 0.32 |
| 1:A:68:ILE:CD1 | 1:A:217:VAL:CG1[3_655] | 1.88 | 0.32 |
| 1:A:39:VAL:C | 4:A:2215:HOH:O[3_655] | 1.88 | 0.32 |
| 1:A:221:ILE:CG1 | 1:A:440:VAL:CG1[3_655] | 1.89 | 0.31 |
| 1:A:75:LEU:CG | 1:A:436:MET:O[3_655] | 1.89 | 0.31 |
| 1:A:22:LEU:O | 1:A:261:ILE:CD1[3_655] | 1.89 | 0.31 |
| 1:A:23:LEU:O | 1:A:261:ILE:CD1[3_655] | 1.89 | 0.31 |
| 1:A:228:ARG:CG | 1:A:462:ILE:C[3_655] | 1.89 | 0.31 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------------|--------------------------|-------------------|
| 1:A:21:LYS:CA | 1:A:443:GLY:CA[3_655] | 1.89 | 0.31 |
| 1:A:25:ASP:OD2 | 1:A:263:ALA:CB[3_655] | 1.89 | 0.31 |
| 1:A:221:ILE:C | 1:A:441:GLU:CB[3_655] | 1.89 | 0.31 |
| 1:A:83:ASN:ND2 | 1:A:335:GLY:C[3_655] | 1.89 | 0.31 |
| 1:A:59:SER:CA | 1:A:78:GLU:O[3_655] | 1.89 | 0.31 |
| 1:A:258:LYS:CG | 1:A:454:MET:CB[3_655] | 1.89 | 0.31 |
| 1:A:59:SER:OG | 1:A:79:THR:C[3_655] | 1.89 | 0.31 |
| 1:A:38:ARG:CB | 1:A:467:PRO:CB[3_655] | 1.89 | 0.31 |
| 1:A:59:SER:C | 1:A:78:GLU:CA[3_655] | 1.89 | 0.31 |
| 1:A:220:ARG:CB | 1:A:437:GLU:O[3_655] | 1.90 | 0.30 |
| 1:A:208:ARG:O | 1:A:210:PHE:C[3_655] | 1.90 | 0.30 |
| 1:A:228:ARG:N | 1:A:463:TRP:C[3_655] | 1.90 | 0.30 |
| 1:A:30:VAL:O | 1:A:448:ARG:CA[3_655] | 1.90 | 0.30 |
| 1:A:81:LYS:CG | 4:A:2156:HOH:O[3_655] | 1.90 | 0.30 |
| 1:A:28:LEU:CD1 | 1:A:450:ILE:CG2[3_655] | 1.90 | 0.30 |
| 1:A:18:ALA:O | 1:A:18:ALA:O[3_655] | 1.90 | 0.30 |
| 1:A:257:ALA:C | 1:A:456:LYS:CG[3_655] | 1.90 | 0.30 |
| 1:A:208:ARG:N | 1:A:212:GLY:N[3_655] | 1.90 | 0.30 |
| 1:A:80:TYR:C | 1:A:209:LYS:CE[3_655] | 1.90 | 0.30 |
| 1:B:102:PRO:N | 1:B:475:GLN:NE2[3_555] | 1.90 | 0.30 |
| 1:A:44:TYR:CE2 | 1:A:470:VAL:O[3_655] | 1.91 | 0.29 |
| 1:A:224:LEU:N | 1:A:441:GLU:CB[3_655] | 1.91 | 0.29 |
| 1:A:29:ASN:O | 1:A:450:ILE:C[3_655] | 1.91 | 0.29 |
| 1:A:49:GLN:N | 1:A:475:GLN:NE2[3_655] | 1.91 | 0.29 |
| 1:A:332:LYS:CG | 4:A:2047:HOH:O[3_655] | 1.91 | 0.29 |
| 1:A:81:LYS:N | 4:A:2158:HOH:O[3_655] | 1.91 | 0.29 |
| 1:A:17:MET:SD | 1:A:70:ARG:NH2[3_655] | 1.91 | 0.29 |
| 1:A:74:GLU:CD | 2:A:600:FAD:O3P[3_655] | 1.91 | 0.29 |
| 1:A:42:ARG:C | 1:A:73:LYS:CB[3_655] | 1.91 | 0.29 |
| 1:A:17:MET:CG | 1:A:70:ARG:CZ[3_655] | 1.92 | 0.28 |
| 1:A:27:GLY:CA | 1:A:422:TYR:CB[3_655] | 1.92 | 0.28 |
| 1:A:4:LYS:O | 1:A:452:HIS:CE1[3_655] | 1.92 | 0.28 |
| 1:A:44:TYR:CE2 | 1:A:471:ASP:N[3_655] | 1.92 | 0.28 |
| 1:A:6:ASP:CA | 1:A:451:LEU:O[3_655] | 1.92 | 0.28 |
| 1:B:477:ILE:O | 1:B:480:THR:N[3_555] | 1.92 | 0.28 |
| 1:A:38:ARG:N | 1:A:467:PRO:CD[3_655] | 1.92 | 0.28 |
| 1:A:28:LEU:O | 1:A:446:ALA:O[3_655] | 1.92 | 0.28 |
| 1:A:24:HIS:ND1 | 1:A:446:ALA:CB[3_655] | 1.92 | 0.28 |
| 1:A:19:ALA:C | 1:A:19:ALA:C[3_655] | 1.92 | 0.28 |
| 1:A:46:LEU:CA | 1:A:472:VAL:CA[3_655] | 1.92 | 0.28 |
| 1:A:6:ASP:OD1 | 1:A:454:MET:N[3_655] | 1.92 | 0.28 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:85:VAL:CA | 1:A:336:ASN:CB[3_655] | 1.92 | 0.28 |
| 1:A:16:GLY:CA | 4:A:2005:HOH:O[3_655] | 1.93 | 0.27 |
| 1:A:225:LEU:CD1 | 1:A:444:GLU:CB[3_655] | 1.93 | 0.27 |
| 1:A:52:LYS:CE | 1:A:202:THR:CA[3_655] | 1.93 | 0.27 |
| 1:A:30:VAL:N | 1:A:448:ARG:CA[3_655] | 1.93 | 0.27 |
| 1:A:219:GLU:CB | 1:A:437:GLU:OE2[3_655] | 1.93 | 0.27 |
| 1:A:69:LEU:N | 1:A:215:GLY:O[3_655] | 1.93 | 0.27 |
| 1:A:84:GLU:C | 1:A:336:ASN:ND2[3_655] | 1.93 | 0.27 |
| 1:B:102:PRO:CD | 1:B:475:GLN:NE2[3_555] | 1.93 | 0.27 |
| 1:A:229:VAL:N | 1:A:464:GLN:CB[3_655] | 1.93 | 0.27 |
| 1:A:47:ARG:N | 1:A:473:PRO:N[3_655] | 1.93 | 0.27 |
| 1:A:40:GLY:O | 4:A:2044:HOH:O[3_655] | 1.93 | 0.27 |
| 1:A:231:LEU:CD1 | 1:A:465:SER:C[3_655] | 1.93 | 0.27 |
| 1:A:209:LYS:CA | 1:A:209:LYS:C[3_655] | 1.94 | 0.26 |
| 1:A:60:TYR:CG | 1:A:211:VAL:CG2[3_655] | 1.94 | 0.26 |
| 1:A:69:LEU:N | 4:A:2018:HOH:O[3_655] | 1.94 | 0.26 |
| 1:A:5:CYS:CA | 1:A:452:HIS:O[3_655] | 1.94 | 0.26 |
| 1:A:255:TYR:CD2 | 1:A:461:GLU:OE1[3_655] | 1.94 | 0.26 |
| 1:A:29:ASN:C | 1:A:451:LEU:N[3_655] | 1.94 | 0.26 |
| 1:A:53:TYR:CA | 1:A:207:GLU:OE1[3_655] | 1.94 | 0.26 |
| 1:A:38:ARG:CZ | 4:A:2217:HOH:O[3_655] | 1.94 | 0.26 |
| 1:A:17:MET:N | 4:A:2001:HOH:O[3_655] | 1.94 | 0.26 |
| 1:A:29:ASN:C | 1:A:450:ILE:N[3_655] | 1.94 | 0.26 |
| 1:A:221:ILE:N | 1:A:441:GLU:N[3_655] | 1.94 | 0.26 |
| 1:A:225:LEU:CB | 4:A:2207:HOH:O[3_655] | 1.94 | 0.26 |
| 1:A:256:GLU:C | 1:A:456:LYS:CA[3_655] | 1.94 | 0.26 |
| 1:A:72:ALA:C | 1:A:436:MET:CG[3_655] | 1.94 | 0.26 |
| 1:A:332:LYS:CE | 4:A:2047:HOH:O[3_655] | 1.95 | 0.25 |
| 1:A:17:MET:N | 1:A:444:GLU:OE2[3_655] | 1.95 | 0.25 |
| 1:A:53:TYR:CE2 | 1:A:207:GLU:O[3_655] | 1.95 | 0.25 |
| 1:A:333:PRO:CB | 4:A:2154:HOH:O[3_655] | 1.95 | 0.25 |
| 1:A:220:ARG:CG | 1:A:437:GLU:CA[3_655] | 1.95 | 0.25 |
| 1:A:65:GLN:NE2 | 1:A:216:GLN:OE1[3_655] | 1.95 | 0.25 |
| 1:A:68:ILE:N | 1:A:218:SER:CA[3_655] | 1.95 | 0.25 |
| 1:B:477:ILE:O | 1:B:480:THR:CG2[3_555] | 1.95 | 0.25 |
| 1:A:225:LEU:CD1 | 1:A:444:GLU:CA[3_655] | 1.95 | 0.25 |
| 1:A:40:GLY:C | 1:A:70:ARG:CB[3_655] | 1.95 | 0.25 |
| 1:A:41:GLY:N | 1:A:70:ARG:CG[3_655] | 1.95 | 0.25 |
| 1:A:38:ARG:CA | 1:A:467:PRO:C[3_655] | 1.95 | 0.25 |
| 1:A:38:ARG:CA | 1:A:467:PRO:CG[3_655] | 1.95 | 0.25 |
| 1:A:82:VAL:CB | 4:A:2030:HOH:O[3_655] | 1.95 | 0.25 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:52:LYS:CG | 1:A:203:ASN:N[3_655] | 1.95 | 0.25 |
| 1:A:81:LYS:CB | 1:A:332:LYS:NZ[3_655] | 1.95 | 0.25 |
| 1:A:42:ARG:O | 1:A:73:LYS:CE[3_655] | 1.95 | 0.25 |
| 1:A:220:ARG:N | 1:A:437:GLU:CG[3_655] | 1.95 | 0.25 |
| 1:A:15:SER:OG | 1:A:21:LYS:CD[3_655] | 1.96 | 0.24 |
| 1:A:74:GLU:C | 2:A:600:FAD:O5'[3_655] | 1.96 | 0.24 |
| 1:A:39:VAL:N | 1:A:466:GLU:OE2[3_655] | 1.96 | 0.24 |
| 1:A:304:PRO:CG | 4:A:2052:HOH:O[3_655] | 1.96 | 0.24 |
| 1:A:39:VAL:N | 1:A:466:GLU:CD[3_655] | 1.96 | 0.24 |
| 1:A:330:ASP:OD1 | 4:A:2046:HOH:O[3_655] | 1.96 | 0.24 |
| 1:A:5:CYS:C | 1:A:451:LEU:C[3_655] | 1.96 | 0.24 |
| 1:A:30:VAL:CA | 1:A:448:ARG:O[3_655] | 1.96 | 0.24 |
| 1:A:231:LEU:CG | 1:A:465:SER:C[3_655] | 1.96 | 0.24 |
| 1:A:76:GLY:C | 2:A:600:FAD:O2[3_655] | 1.96 | 0.24 |
| 1:A:221:ILE:O | 1:A:441:GLU:O[3_655] | 1.96 | 0.24 |
| 1:A:15:SER:C | 1:A:21:LYS:NZ[3_655] | 1.96 | 0.24 |
| 1:A:60:TYR:C | 4:A:2045:HOH:O[3_655] | 1.96 | 0.24 |
| 1:A:220:ARG:CA | 1:A:437:GLU:CG[3_655] | 1.96 | 0.24 |
| 1:A:31:VAL:CG1 | 1:A:461:GLU:CB[3_655] | 1.96 | 0.24 |
| 1:A:84:GLU:C | 1:A:336:ASN:OD1[3_655] | 1.96 | 0.24 |
| 1:A:74:GLU:N | 2:A:600:FAD:C4'[3_655] | 1.97 | 0.23 |
| 1:A:61:VAL:C | 1:A:212:GLY:O[3_655] | 1.97 | 0.23 |
| 1:A:225:LEU:N | 1:A:441:GLU:O[3_655] | 1.97 | 0.23 |
| 1:A:231:LEU:CG | 1:A:465:SER:OG[3_655] | 1.97 | 0.23 |
| 1:A:221:ILE:CA | 1:A:441:GLU:CA[3_655] | 1.97 | 0.23 |
| 1:A:45:THR:OG1 | 1:A:69:LEU:CD2[3_655] | 1.97 | 0.23 |
| 1:A:225:LEU:O | 1:A:445:ARG:CG[3_655] | 1.97 | 0.23 |
| 1:A:46:LEU:CB | 1:A:473:PRO:CG[3_655] | 1.97 | 0.23 |
| 1:A:84:GLU:CA | 1:A:336:ASN:ND2[3_655] | 1.97 | 0.23 |
| 1:A:82:VAL:O | 1:A:332:LYS:CA[3_655] | 1.97 | 0.23 |
| 1:A:221:ILE:CB | 1:A:441:GLU:N[3_655] | 1.97 | 0.23 |
| 1:A:65:GLN:CB | 1:A:216:GLN:CG[3_655] | 1.97 | 0.23 |
| 1:A:67:ARG:C | 1:A:219:GLU:N[3_655] | 1.97 | 0.23 |
| 1:A:69:LEU:CA | 4:A:2018:HOH:O[3_655] | 1.97 | 0.23 |
| 1:A:24:HIS:CE1 | 1:A:445:ARG:NE[3_655] | 1.97 | 0.23 |
| 1:A:20:ALA:O | 1:A:443:GLY:O[3_655] | 1.97 | 0.23 |
| 1:A:83:ASN:CA | 1:A:332:LYS:C[3_655] | 1.98 | 0.22 |
| 1:A:15:SER:OG | 1:A:21:LYS:NZ[3_655] | 1.98 | 0.22 |
| 1:A:12:GLY:O | 1:A:70:ARG:CZ[3_655] | 1.98 | 0.22 |
| 1:A:44:TYR:CE1 | 1:A:469:SER:CA[3_655] | 1.98 | 0.22 |
| 1:A:208:ARG:O | 1:A:212:GLY:N[3_655] | 1.98 | 0.22 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:18:ALA:CA | 1:A:18:ALA:CB[3_655] | 1.98 | 0.22 |
| 1:A:28:LEU:CD2 | 1:A:259:TYR:CB[3_655] | 1.98 | 0.22 |
| 1:A:17:MET:O | 1:A:444:GLU:CG[3_655] | 1.98 | 0.22 |
| 1:A:24:HIS:CB | 1:A:446:ALA:N[3_655] | 1.98 | 0.22 |
| 1:A:68:ILE:CB | 1:A:217:VAL:CB[3_655] | 1.98 | 0.22 |
| 1:A:30:VAL:C | 1:A:448:ARG:O[3_655] | 1.98 | 0.22 |
| 1:A:209:LYS:CA | 1:A:209:LYS:O[3_655] | 1.98 | 0.22 |
| 1:A:14:ILE:CA | 1:A:71:LEU:CA[3_655] | 1.98 | 0.22 |
| 1:A:229:VAL:CB | 1:A:464:GLN:O[3_655] | 1.98 | 0.22 |
| 1:A:30:VAL:CG1 | 1:A:447:ALA:CA[3_655] | 1.99 | 0.21 |
| 1:A:38:ARG:CG | 1:A:467:PRO:CB[3_655] | 1.99 | 0.21 |
| 1:A:15:SER:C | 4:A:2003:HOH:O[3_655] | 1.99 | 0.21 |
| 1:A:202:THR:OG1 | 1:A:337:TYR:CZ[3_655] | 1.99 | 0.21 |
| 1:A:223:ASP:N | 1:A:441:GLU:CB[3_655] | 1.99 | 0.21 |
| 1:A:23:LEU:CB | 1:A:23:LEU:CD2[3_655] | 1.99 | 0.21 |
| 1:A:329:ASP:CA | 1:A:333:PRO:O[3_655] | 1.99 | 0.21 |
| 1:A:337:TYR:N | 4:A:2049:HOH:O[3_655] | 1.99 | 0.21 |
| 1:A:74:GLU:CG | 2:A:600:FAD:O2P[3_655] | 1.99 | 0.21 |
| 1:A:229:VAL:O | 1:A:464:GLN:C[3_655] | 1.99 | 0.21 |
| 1:A:223:ASP:OD2 | 1:A:431:HIS:C[3_655] | 1.99 | 0.21 |
| 1:A:38:ARG:CB | 1:A:468:GLU:N[3_655] | 2.00 | 0.20 |
| 1:A:74:GLU:O | 2:A:600:FAD:O3'[3_655] | 2.00 | 0.20 |
| 1:B:476:PRO:CB | 1:B:483:GLU:OE2[3_555] | 2.00 | 0.20 |
| 1:A:66:ASN:CA | 1:A:219:GLU:OE2[3_655] | 2.00 | 0.20 |
| 1:A:26:SER:N | 1:A:261:ILE:CG2[3_655] | 2.00 | 0.20 |
| 1:A:61:VAL:CA | 1:A:211:VAL:O[3_655] | 2.00 | 0.20 |
| 1:A:82:VAL:CG1 | 1:A:334:GLU:OE1[3_655] | 2.00 | 0.20 |
| 1:A:45:THR:OG1 | 1:A:69:LEU:CD1[3_655] | 2.00 | 0.20 |
| 1:A:229:VAL:CA | 1:A:464:GLN:CG[3_655] | 2.00 | 0.20 |
| 1:A:260:VAL:CB | 4:A:2006:HOH:O[3_655] | 2.00 | 0.20 |
| 1:A:80:TYR:CD1 | 1:A:80:TYR:CZ[3_655] | 2.00 | 0.20 |
| 1:A:37:ASP:C | 1:A:467:PRO:CA[3_655] | 2.00 | 0.20 |
| 1:A:219:GLU:CA | 1:A:437:GLU:OE2[3_655] | 2.00 | 0.20 |
| 1:A:227:ASP:O | 1:A:463:TRP:C[3_655] | 2.00 | 0.20 |
| 1:A:222:MET:C | 1:A:441:GLU:CG[3_655] | 2.00 | 0.20 |
| 1:A:76:GLY:O | 2:A:600:FAD:C4[3_655] | 2.00 | 0.20 |
| 1:A:32:VAL:CG2 | 1:A:448:ARG:NE[3_655] | 2.00 | 0.20 |
| 1:A:65:GLN:C | 1:A:219:GLU:CG[3_655] | 2.00 | 0.20 |
| 1:A:27:GLY:C | 1:A:422:TYR:CG[3_655] | 2.01 | 0.19 |
| 1:A:23:LEU:O | 1:A:450:ILE:CD1[3_655] | 2.01 | 0.19 |
| 1:A:228:ARG:NH1 | 1:A:445:ARG:CG[3_655] | 2.01 | 0.19 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:43:THR:C | 4:A:2216:HOH:O[3_655] | 2.01 | 0.19 |
| 1:A:210:PHE:CD1 | 1:A:210:PHE:CZ[3_655] | 2.01 | 0.19 |
| 1:A:258:LYS:N | 1:A:456:LYS:CD[3_655] | 2.01 | 0.19 |
| 1:A:255:TYR:CE2 | 1:A:461:GLU:CG[3_655] | 2.01 | 0.19 |
| 1:A:65:GLN:O | 1:A:219:GLU:OE1[3_655] | 2.01 | 0.19 |
| 1:A:67:ARG:CA | 1:A:218:SER:O[3_655] | 2.01 | 0.19 |
| 1:A:46:LEU:CD1 | 1:A:473:PRO:CB[3_655] | 2.01 | 0.19 |
| 1:A:79:THR:O | 4:A:2138:HOH:O[3_655] | 2.01 | 0.19 |
| 1:A:75:LEU:CB | 1:A:436:MET:O[3_655] | 2.01 | 0.19 |
| 1:A:329:ASP:CG | 1:A:333:PRO:O[3_655] | 2.02 | 0.18 |
| 1:A:12:GLY:C | 1:A:70:ARG:NE[3_655] | 2.02 | 0.18 |
| 1:A:74:GLU:CB | 2:A:600:FAD:P[3_655] | 2.02 | 0.18 |
| 2:A:600:FAD:O2A | 4:A:2044:HOH:O[3_655] | 2.02 | 0.18 |
| 1:A:7:VAL:CA | 1:A:451:LEU:CB[3_655] | 2.02 | 0.18 |
| 1:A:66:ASN:CB | 1:A:219:GLU:CG[3_655] | 2.02 | 0.18 |
| 1:A:258:LYS:O | 1:A:456:LYS:CE[3_655] | 2.02 | 0.18 |
| 1:A:53:TYR:CE1 | 1:A:207:GLU:O[3_655] | 2.02 | 0.18 |
| 1:A:40:GLY:C | 1:A:70:ARG:CA[3_655] | 2.02 | 0.18 |
| 1:A:20:ALA:C | 1:A:443:GLY:O[3_655] | 2.02 | 0.18 |
| 1:A:55:ASP:OD2 | 1:A:79:THR:CA[3_655] | 2.02 | 0.18 |
| 1:A:26:SER:CA | 1:A:261:ILE:CB[3_655] | 2.02 | 0.18 |
| 1:A:225:LEU:CD2 | 1:A:444:GLU:C[3_655] | 2.02 | 0.18 |
| 1:A:220:ARG:O | 1:A:437:GLU:O[3_655] | 2.02 | 0.18 |
| 1:A:6:ASP:CB | 1:A:450:ILE:C[3_655] | 2.02 | 0.18 |
| 1:A:80:TYR:N | 1:A:209:LYS:CD[3_655] | 2.02 | 0.18 |
| 1:A:29:ASN:O | 1:A:452:HIS:N[3_655] | 2.02 | 0.18 |
| 1:A:52:LYS:NZ | 1:A:201:THR:CB[3_655] | 2.02 | 0.18 |
| 1:A:17:MET:SD | 1:A:444:GLU:CD[3_655] | 2.03 | 0.17 |
| 1:A:45:THR:CA | 1:A:472:VAL:N[3_655] | 2.03 | 0.17 |
| 1:A:54:VAL:CA | 1:A:208:ARG:NE[3_655] | 2.03 | 0.17 |
| 1:A:26:SER:N | 1:A:261:ILE:N[3_655] | 2.03 | 0.17 |
| 1:A:47:ARG:CZ | 1:A:63:PRO:C[3_655] | 2.03 | 0.17 |
| 1:A:18:ALA:CA | 1:A:18:ALA:O[3_655] | 2.03 | 0.17 |
| 1:A:30:VAL:CG1 | 1:A:448:ARG:N[3_655] | 2.03 | 0.17 |
| 1:A:475:GLN:CD | 4:A:2026:HOH:O[3_655] | 2.03 | 0.17 |
| 1:A:17:MET:C | 4:A:2001:HOH:O[3_655] | 2.03 | 0.17 |
| 1:A:62:GLY:N | 1:A:212:GLY:C[3_655] | 2.03 | 0.17 |
| 1:A:43:THR:C | 4:A:2009:HOH:O[3_655] | 2.03 | 0.17 |
| 1:A:222:MET:O | 1:A:441:GLU:CG[3_655] | 2.03 | 0.17 |
| 1:A:74:GLU:CB | 4:A:2230:HOH:O[3_655] | 2.03 | 0.17 |
| 1:A:14:ILE:CB | 1:A:71:LEU:CG[3_655] | 2.03 | 0.17 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:29:ASN:N | 1:A:449:GLU:O[3_655] | 2.03 | 0.17 |
| 1:A:229:VAL:CG1 | 1:A:464:GLN:CG[3_655] | 2.03 | 0.17 |
| 1:A:82:VAL:CA | 1:A:333:PRO:N[3_655] | 2.03 | 0.17 |
| 1:A:45:THR:CA | 1:A:472:VAL:CA[3_655] | 2.03 | 0.17 |
| 1:A:40:GLY:O | 1:A:70:ARG:CA[3_655] | 2.03 | 0.17 |
| 1:A:221:ILE:CG1 | 1:A:440:VAL:N[3_655] | 2.03 | 0.17 |
| 1:A:66:ASN:ND2 | 4:A:2119:HOH:O[3_655] | 2.03 | 0.17 |
| 1:A:53:TYR:CD1 | 1:A:208:ARG:CD[3_655] | 2.03 | 0.17 |
| 1:A:258:LYS:C | 1:A:456:LYS:CD[3_655] | 2.03 | 0.17 |
| 1:A:221:ILE:CD1 | 1:A:440:VAL:CB[3_655] | 2.03 | 0.17 |
| 1:A:321:GLU:CG | 1:A:499:THR:C[6_564] | 2.03 | 0.17 |
| 1:A:38:ARG:C | 1:A:467:PRO:CG[3_655] | 2.04 | 0.16 |
| 1:A:66:ASN:OD1 | 4:A:2119:HOH:O[3_655] | 2.04 | 0.16 |
| 1:A:38:ARG:NH2 | 4:A:2217:HOH:O[3_655] | 2.04 | 0.16 |
| 1:A:501:ILE:CA | 4:A:2014:HOH:O[6_565] | 2.04 | 0.16 |
| 1:A:6:ASP:OD1 | 1:A:453:ALA:C[3_655] | 2.04 | 0.16 |
| 1:A:83:ASN:C | 1:A:335:GLY:N[3_655] | 2.04 | 0.16 |
| 1:A:29:ASN:C | 1:A:448:ARG:C[3_655] | 2.04 | 0.16 |
| 1:A:43:THR:CB | 1:A:73:LYS:CB[3_655] | 2.04 | 0.16 |
| 1:A:68:ILE:CG1 | 1:A:217:VAL:N[3_655] | 2.04 | 0.16 |
| 1:A:73:LYS:CE | 1:A:388:TRP:CZ2[3_655] | 2.04 | 0.16 |
| 1:A:46:LEU:C | 1:A:473:PRO:CD[3_655] | 2.04 | 0.16 |
| 1:A:65:GLN:CG | 4:A:2120:HOH:O[3_655] | 2.04 | 0.16 |
| 1:A:220:ARG:C | 1:A:437:GLU:C[3_655] | 2.04 | 0.16 |
| 1:A:73:LYS:CE | 1:A:388:TRP:CH2[3_655] | 2.04 | 0.16 |
| 1:A:3:ASN:O | 1:A:458:PRO:CA[3_655] | 2.04 | 0.16 |
| 1:A:28:LEU:CD2 | 1:A:450:ILE:CG2[3_655] | 2.04 | 0.16 |
| 1:A:7:VAL:CG2 | 1:A:451:LEU:CD2[3_655] | 2.05 | 0.15 |
| 1:A:501:ILE:N | 4:A:2054:HOH:O[6_565] | 2.05 | 0.15 |
| 1:A:226:GLY:N | 4:A:2214:HOH:O[3_655] | 2.05 | 0.15 |
| 1:A:59:SER:OG | 1:A:79:THR:O[3_655] | 2.05 | 0.15 |
| 1:A:222:MET:N | 1:A:441:GLU:CA[3_655] | 2.05 | 0.15 |
| 1:A:68:ILE:O | 1:A:214:SER:O[3_655] | 2.05 | 0.15 |
| 1:A:307:ARG:NE | 1:A:307:ARG:NH1[3_655] | 2.05 | 0.15 |
| 1:A:47:ARG:O | 1:A:473:PRO:O[3_655] | 2.05 | 0.15 |
| 1:A:53:TYR:C | 1:A:208:ARG:NE[3_655] | 2.05 | 0.15 |
| 1:A:28:LEU:CB | 1:A:450:ILE:CD1[3_655] | 2.05 | 0.15 |
| 1:A:44:TYR:CA | 1:A:469:SER:OG[3_655] | 2.06 | 0.14 |
| 1:A:80:TYR:CG | 1:A:80:TYR:OH[3_655] | 2.06 | 0.14 |
| 1:A:82:VAL:CG1 | 1:A:333:PRO:CD[3_655] | 2.06 | 0.14 |
| 1:A:76:GLY:CA | 2:A:600:FAD:C2'[3_655] | 2.06 | 0.14 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:61:VAL:CG1 | 1:A:213:GLY:O[3_655] | 2.06 | 0.14 |
| 1:A:6:ASP:N | 1:A:452:HIS:N[3_655] | 2.06 | 0.14 |
| 4:A:2116:HOH:O | 4:A:2155:HOH:O[3_655] | 2.06 | 0.14 |
| 1:A:255:TYR:CZ | 1:A:461:GLU:CG[3_655] | 2.06 | 0.14 |
| 1:A:224:LEU:N | 1:A:441:GLU:OE2[3_655] | 2.06 | 0.14 |
| 1:A:61:VAL:C | 1:A:216:GLN:NE2[3_655] | 2.06 | 0.14 |
| 1:A:24:HIS:CA | 1:A:446:ALA:CB[3_655] | 2.06 | 0.14 |
| 1:A:53:TYR:CE2 | 1:A:207:GLU:N[3_655] | 2.06 | 0.14 |
| 1:A:68:ILE:CA | 1:A:217:VAL:CB[3_655] | 2.06 | 0.14 |
| 1:A:47:ARG:N | 1:A:473:PRO:CA[3_655] | 2.06 | 0.14 |
| 1:A:47:ARG:NE | 1:A:63:PRO:CB[3_655] | 2.06 | 0.14 |
| 1:A:386:LYS:CD | 1:A:470:VAL:CG2[3_655] | 2.06 | 0.14 |
| 1:A:52:LYS:CG | 1:A:201:THR:O[3_655] | 2.06 | 0.14 |
| 1:A:255:TYR:OH | 1:A:461:GLU:CG[3_655] | 2.06 | 0.14 |
| 1:A:30:VAL:CA | 1:A:448:ARG:N[3_655] | 2.07 | 0.13 |
| 1:A:81:LYS:O | 1:A:332:LYS:CA[3_655] | 2.07 | 0.13 |
| 1:A:334:GLU:CG | 4:A:2048:HOH:O[3_655] | 2.07 | 0.13 |
| 1:A:74:GLU:C | 2:A:600:FAD:O4'[3_655] | 2.07 | 0.13 |
| 1:A:19:ALA:CB | 1:A:21:LYS:O[3_655] | 2.07 | 0.13 |
| 1:A:83:ASN:CA | 1:A:335:GLY:N[3_655] | 2.07 | 0.13 |
| 1:A:70:ARG:N | 4:A:2018:HOH:O[3_655] | 2.07 | 0.13 |
| 1:A:84:GLU:CA | 1:A:336:ASN:CB[3_655] | 2.07 | 0.13 |
| 1:A:85:VAL:CG2 | 4:A:2142:HOH:O[3_655] | 2.07 | 0.13 |
| 1:A:39:VAL:O | 4:A:2038:HOH:O[3_655] | 2.07 | 0.13 |
| 1:A:228:ARG:CD | 1:A:462:ILE:CG2[3_655] | 2.08 | 0.12 |
| 1:A:44:TYR:OH | 1:A:469:SER:O[3_655] | 2.08 | 0.12 |
| 1:A:74:GLU:CB | 2:A:600:FAD:C5'[3_655] | 2.08 | 0.12 |
| 1:A:7:VAL:N | 1:A:451:LEU:CD2[3_655] | 2.08 | 0.12 |
| 1:A:74:GLU:N | 4:A:2230:HOH:O[3_655] | 2.08 | 0.12 |
| 1:A:19:ALA:CA | 1:A:19:ALA:O[3_655] | 2.08 | 0.12 |
| 1:A:20:ALA:C | 1:A:447:ALA:CB[3_655] | 2.08 | 0.12 |
| 1:A:55:ASP:OD1 | 1:A:79:THR:CG2[3_655] | 2.08 | 0.12 |
| 1:A:52:LYS:C | 1:A:207:GLU:CD[3_655] | 2.08 | 0.12 |
| 1:A:44:TYR:CB | 1:A:471:ASP:OD1[3_655] | 2.08 | 0.12 |
| 1:A:53:TYR:CG | 1:A:207:GLU:CD[3_655] | 2.08 | 0.12 |
| 1:A:82:VAL:C | 1:A:333:PRO:N[3_655] | 2.08 | 0.12 |
| 1:A:221:ILE:CD1 | 1:A:440:VAL:CG1[3_655] | 2.08 | 0.12 |
| 1:A:41:GLY:CA | 4:A:2044:HOH:O[3_655] | 2.09 | 0.11 |
| 1:A:60:TYR:CA | 1:A:211:VAL:CB[3_655] | 2.09 | 0.11 |
| 1:A:228:ARG:NE | 1:A:462:ILE:CG2[3_655] | 2.09 | 0.11 |
| 1:A:228:ARG:CD | 1:A:445:ARG:O[3_655] | 2.09 | 0.11 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:52:LYS:NZ | 1:A:84:GLU:OE1[3_655] | 2.09 | 0.11 |
| 1:A:257:ALA:N | 1:A:455:GLY:O[3_655] | 2.09 | 0.11 |
| 1:A:80:TYR:CD2 | 1:A:209:LYS:CG[3_655] | 2.09 | 0.11 |
| 1:A:69:LEU:CA | 1:A:214:SER:O[3_655] | 2.09 | 0.11 |
| 1:A:65:GLN:OE1 | 1:A:216:GLN:CB[3_655] | 2.09 | 0.11 |
| 1:A:81:LYS:O | 1:A:331:THR:C[3_655] | 2.09 | 0.11 |
| 1:A:256:GLU:C | 1:A:456:LYS:C[3_655] | 2.09 | 0.11 |
| 1:A:46:LEU:N | 1:A:471:ASP:C[3_655] | 2.09 | 0.11 |
| 1:A:227:ASP:O | 1:A:463:TRP:CA[3_655] | 2.09 | 0.11 |
| 1:A:52:LYS:CB | 1:A:202:THR:CG2[3_655] | 2.09 | 0.11 |
| 1:A:21:LYS:N | 1:A:443:GLY:C[3_655] | 2.09 | 0.11 |
| 1:A:3:ASN:C | 1:A:458:PRO:N[3_655] | 2.09 | 0.11 |
| 1:A:61:VAL:O | 1:A:213:GLY:N[3_655] | 2.09 | 0.11 |
| 1:A:43:THR:OG1 | 1:A:70:ARG:N[3_655] | 2.09 | 0.11 |
| 1:A:40:GLY:O | 1:A:70:ARG:C[3_655] | 2.09 | 0.11 |
| 1:A:220:ARG:CZ | 1:A:435:TYR:CB[3_655] | 2.09 | 0.11 |
| 1:A:32:VAL:CB | 1:A:448:ARG:NE[3_655] | 2.09 | 0.11 |
| 1:A:15:SER:O | 1:A:21:LYS:CD[3_655] | 2.09 | 0.11 |
| 1:A:14:ILE:CB | 1:A:71:LEU:CD1[3_655] | 2.09 | 0.11 |
| 1:A:17:MET:CA | 1:A:444:GLU:CG[3_655] | 2.09 | 0.11 |
| 1:A:255:TYR:CE2 | 1:A:461:GLU:OE1[3_655] | 2.09 | 0.11 |
| 1:A:68:ILE:C | 1:A:214:SER:O[3_655] | 2.09 | 0.11 |
| 1:A:68:ILE:CG2 | 1:A:216:GLN:O[3_655] | 2.09 | 0.11 |
| 1:A:30:VAL:O | 1:A:448:ARG:O[3_655] | 2.10 | 0.10 |
| 1:A:3:ASN:O | 1:A:457:ILE:O[3_655] | 2.10 | 0.10 |
| 1:A:229:VAL:O | 1:A:464:GLN:N[3_655] | 2.10 | 0.10 |
| 1:A:3:ASN:N | 1:A:458:PRO:CG[3_655] | 2.10 | 0.10 |
| 1:A:60:TYR:CA | 1:A:211:VAL:O[3_655] | 2.10 | 0.10 |
| 1:A:256:GLU:C | 1:A:456:LYS:N[3_655] | 2.10 | 0.10 |
| 1:A:12:GLY:C | 1:A:70:ARG:CD[3_655] | 2.10 | 0.10 |
| 1:A:221:ILE:CG1 | 1:A:440:VAL:C[3_655] | 2.10 | 0.10 |
| 1:A:27:GLY:CA | 1:A:422:TYR:CG[3_655] | 2.10 | 0.10 |
| 1:A:46:LEU:CB | 1:A:473:PRO:N[3_655] | 2.10 | 0.10 |
| 1:A:61:VAL:CG2 | 1:A:213:GLY:CA[3_655] | 2.10 | 0.10 |
| 1:A:225:LEU:CG | 1:A:445:ARG:CA[3_655] | 2.10 | 0.10 |
| 1:A:257:ALA:N | 1:A:456:LYS:N[3_655] | 2.10 | 0.10 |
| 1:A:222:MET:CE | 1:A:466:GLU:CB[3_655] | 2.10 | 0.10 |
| 1:A:79:THR:C | 1:A:209:LYS:CE[3_655] | 2.10 | 0.10 |
| 1:A:223:ASP:N | 1:A:441:GLU:CG[3_655] | 2.10 | 0.10 |
| 1:A:208:ARG:C | 1:A:210:PHE:C[3_655] | 2.10 | 0.10 |
| 1:A:65:GLN:C | 1:A:219:GLU:CB[3_655] | 2.10 | 0.10 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:17:MET:CG | 1:A:444:GLU:CD[3_655] | 2.10 | 0.10 |
| 1:A:312:CYS:C | 1:A:334:GLU:O[3_655] | 2.10 | 0.10 |
| 1:A:37:ASP:C | 1:A:467:PRO:CB[3_655] | 2.10 | 0.10 |
| 1:A:46:LEU:N | 1:A:473:PRO:N[3_655] | 2.11 | 0.09 |
| 1:A:227:ASP:CA | 1:A:463:TRP:C[3_655] | 2.11 | 0.09 |
| 1:A:7:VAL:CG2 | 1:A:28:LEU:CD1[3_655] | 2.11 | 0.09 |
| 1:A:210:PHE:CD1 | 1:A:210:PHE:CD2[3_655] | 2.11 | 0.09 |
| 1:A:68:ILE:CB | 1:A:217:VAL:C[3_655] | 2.11 | 0.09 |
| 1:A:67:ARG:CA | 1:A:218:SER:CB[3_655] | 2.11 | 0.09 |
| 1:A:60:TYR:CB | 1:A:211:VAL:CG1[3_655] | 2.11 | 0.09 |
| 1:A:255:TYR:CG | 1:A:458:PRO:CD[3_655] | 2.11 | 0.09 |
| 1:A:228:ARG:N | 1:A:463:TRP:CB[3_655] | 2.11 | 0.09 |
| 1:A:76:GLY:CA | 2:A:600:FAD:C1'[3_655] | 2.11 | 0.09 |
| 1:A:39:VAL:N | 1:A:467:PRO:CD[3_655] | 2.11 | 0.09 |
| 1:A:66:ASN:N | 1:A:219:GLU:OE2[3_655] | 2.11 | 0.09 |
| 1:A:53:TYR:C | 1:A:208:ARG:NH2[3_655] | 2.11 | 0.09 |
| 1:A:37:ASP:O | 1:A:467:PRO:CA[3_655] | 2.11 | 0.09 |
| 1:A:28:LEU:CA | 1:A:450:ILE:CD1[3_655] | 2.11 | 0.09 |
| 1:A:65:GLN:O | 1:A:216:GLN:CA[3_655] | 2.11 | 0.09 |
| 1:A:44:TYR:CG | 1:A:471:ASP:N[3_655] | 2.11 | 0.09 |
| 1:A:61:VAL:CG2 | 1:A:213:GLY:N[3_655] | 2.11 | 0.09 |
| 1:A:228:ARG:N | 1:A:462:ILE:O[3_655] | 2.11 | 0.09 |
| 1:A:337:TYR:CD1 | 4:A:2113:HOH:O[3_655] | 2.11 | 0.09 |
| 1:A:255:TYR:CD1 | 1:A:461:GLU:OE2[3_655] | 2.11 | 0.09 |
| 1:A:8:VAL:O | 1:A:26:SER:OG[3_655] | 2.11 | 0.09 |
| 1:A:60:TYR:CD1 | 1:A:78:GLU:OE1[3_655] | 2.12 | 0.08 |
| 1:A:6:ASP:CA | 1:A:450:ILE:O[3_655] | 2.12 | 0.08 |
| 1:A:220:ARG:CB | 1:A:437:GLU:CG[3_655] | 2.12 | 0.08 |
| 1:A:255:TYR:CE1 | 1:A:461:GLU:CD[3_655] | 2.12 | 0.08 |
| 1:A:258:LYS:CA | 1:A:456:LYS:NZ[3_655] | 2.12 | 0.08 |
| 1:A:3:ASN:CB | 4:A:2211:HOH:O[3_655] | 2.12 | 0.08 |
| 1:A:220:ARG:CZ | 1:A:435:TYR:CG[3_655] | 2.12 | 0.08 |
| 1:A:221:ILE:CA | 1:A:440:VAL:CA[3_655] | 2.12 | 0.08 |
| 1:A:209:LYS:C | 1:A:209:LYS:O[3_655] | 2.12 | 0.08 |
| 1:B:101:GLY:C | 1:B:475:GLN:NE2[3_555] | 2.12 | 0.08 |
| 1:A:32:VAL:CG1 | 4:A:2208:HOH:O[3_655] | 2.12 | 0.08 |
| 1:A:221:ILE:CD1 | 1:A:440:VAL:CG2[3_655] | 2.12 | 0.08 |
| 1:A:27:GLY:O | 1:A:422:TYR:CG[3_655] | 2.12 | 0.08 |
| 1:A:66:ASN:C | 1:A:219:GLU:CG[3_655] | 2.13 | 0.07 |
| 1:A:80:TYR:CD1 | 1:A:80:TYR:CE1[3_655] | 2.13 | 0.07 |
| 1:A:24:HIS:CA | 1:A:446:ALA:O[3_655] | 2.13 | 0.07 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:83:ASN:O | 1:A:334:GLU:N[3_655] | 2.13 | 0.07 |
| 1:A:74:GLU:OE2 | 4:A:2126:HOH:O[3_655] | 2.13 | 0.07 |
| 1:A:39:VAL:N | 1:A:466:GLU:CG[3_655] | 2.13 | 0.07 |
| 1:A:59:SER:O | 1:A:78:GLU:C[3_655] | 2.13 | 0.07 |
| 1:A:312:CYS:CA | 1:A:334:GLU:O[3_655] | 2.13 | 0.07 |
| 1:A:75:LEU:CA | 1:A:435:TYR:C[3_655] | 2.13 | 0.07 |
| 1:A:16:GLY:C | 4:A:2003:HOH:O[3_655] | 2.13 | 0.07 |
| 1:A:23:LEU:C | 1:A:261:ILE:CG1[3_655] | 2.13 | 0.07 |
| 1:A:39:VAL:CG2 | 1:A:466:GLU:OE2[3_655] | 2.13 | 0.07 |
| 1:A:14:ILE:CA | 1:A:71:LEU:CB[3_655] | 2.13 | 0.07 |
| 1:A:255:TYR:OH | 1:A:461:GLU:OE2[3_655] | 2.13 | 0.07 |
| 1:A:65:GLN:CB | 4:A:2120:HOH:O[3_655] | 2.13 | 0.07 |
| 1:A:65:GLN:CD | 1:A:216:GLN:CD[3_655] | 2.13 | 0.07 |
| 4:A:2050:HOH:O | 4:A:2159:HOH:O[3_655] | 2.14 | 0.06 |
| 1:A:81:LYS:CD | 4:A:2156:HOH:O[3_655] | 2.14 | 0.06 |
| 1:A:226:GLY:O | 1:A:464:GLN:N[3_655] | 2.14 | 0.06 |
| 1:A:44:TYR:CB | 4:A:2216:HOH:O[3_655] | 2.14 | 0.06 |
| 1:A:23:LEU:CA | 1:A:23:LEU:CD1[3_655] | 2.14 | 0.06 |
| 1:A:14:ILE:N | 1:A:71:LEU:CA[3_655] | 2.14 | 0.06 |
| 1:B:478:THR:O | 1:B:478:THR:CG2[3_555] | 2.14 | 0.06 |
| 1:A:9:VAL:CG2 | 1:A:22:LEU:CG[3_655] | 2.14 | 0.06 |
| 1:A:69:LEU:N | 1:A:215:GLY:CA[3_655] | 2.14 | 0.06 |
| 1:A:20:ALA:CA | 1:A:447:ALA:CB[3_655] | 2.14 | 0.06 |
| 1:A:74:GLU:CG | 2:A:600:FAD:C5'[3_655] | 2.14 | 0.06 |
| 1:A:231:LEU:CD1 | 1:A:466:GLU:N[3_655] | 2.14 | 0.06 |
| 1:A:221:ILE:CD1 | 1:A:440:VAL:CA[3_655] | 2.14 | 0.06 |
| 1:A:47:ARG:CZ | 1:A:62:GLY:O[3_655] | 2.14 | 0.06 |
| 1:A:466:GLU:CB | 4:A:2017:HOH:O[3_655] | 2.14 | 0.06 |
| 1:A:29:ASN:OD1 | 1:A:449:GLU:O[3_655] | 2.15 | 0.05 |
| 1:A:28:LEU:CA | 1:A:450:ILE:CA[3_655] | 2.15 | 0.05 |
| 1:A:68:ILE:N | 1:A:219:GLU:N[3_655] | 2.15 | 0.05 |
| 1:A:69:LEU:CA | 1:A:215:GLY:N[3_655] | 2.15 | 0.05 |
| 1:A:24:HIS:C | 1:A:446:ALA:CB[3_655] | 2.15 | 0.05 |
| 1:A:31:VAL:C | 1:A:448:ARG:CD[3_655] | 2.15 | 0.05 |
| 1:A:227:ASP:N | 1:A:463:TRP:CA[3_655] | 2.15 | 0.05 |
| 1:A:6:ASP:OD2 | 1:A:453:ALA:CB[3_655] | 2.15 | 0.05 |
| 1:A:52:LYS:CB | 1:A:202:THR:CB[3_655] | 2.15 | 0.05 |
| 1:A:65:GLN:N | 4:A:2120:HOH:O[3_655] | 2.15 | 0.05 |
| 1:A:219:GLU:C | 1:A:437:GLU:OE2[3_655] | 2.15 | 0.05 |
| 1:A:256:GLU:O | 1:A:456:LYS:CA[3_655] | 2.15 | 0.05 |
| 1:A:82:VAL:CA | 1:A:332:LYS:CA[3_655] | 2.15 | 0.05 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:228:ARG:CA | 1:A:463:TRP:CA[3_655] | 2.15 | 0.05 |
| 1:A:224:LEU:CD2 | 1:A:438:GLY:O[3_655] | 2.15 | 0.05 |
| 1:A:73:LYS:O | 2:A:600:FAD:C4'[3_655] | 2.15 | 0.05 |
| 1:A:501:ILE:CB | 4:A:2054:HOH:O[6_565] | 2.15 | 0.05 |
| 1:A:85:VAL:CB | 4:A:2142:HOH:O[3_655] | 2.16 | 0.04 |
| 1:A:210:PHE:CD2 | 4:A:2034:HOH:O[3_655] | 2.16 | 0.04 |
| 1:A:5:CYS:O | 1:A:454:MET:C[3_655] | 2.16 | 0.04 |
| 1:A:6:ASP:C | 1:A:451:LEU:CA[3_655] | 2.16 | 0.04 |
| 1:A:54:VAL:C | 1:A:208:ARG:NH2[3_655] | 2.16 | 0.04 |
| 1:A:52:LYS:CA | 1:A:207:GLU:OE1[3_655] | 2.16 | 0.04 |
| 1:A:77:LEU:CG | 1:A:436:MET:CE[3_655] | 2.16 | 0.04 |
| 1:A:225:LEU:CG | 1:A:444:GLU:C[3_655] | 2.16 | 0.04 |
| 1:A:45:THR:CB | 1:A:472:VAL:CG1[3_655] | 2.16 | 0.04 |
| 1:A:83:ASN:N | 1:A:332:LYS:CB[3_655] | 2.16 | 0.04 |
| 1:A:29:ASN:N | 1:A:450:ILE:C[3_655] | 2.16 | 0.04 |
| 1:A:210:PHE:N | 1:A:210:PHE:CA[3_655] | 2.16 | 0.04 |
| 1:A:80:TYR:CD2 | 1:A:209:LYS:CB[3_655] | 2.16 | 0.04 |
| 1:A:321:GLU:CG | 1:A:499:THR:OG1[6_564] | 2.16 | 0.04 |
| 1:A:45:THR:C | 1:A:472:VAL:O[3_655] | 2.16 | 0.04 |
| 1:A:227:ASP:OD2 | 1:A:463:TRP:CD1[3_655] | 2.16 | 0.04 |
| 1:A:83:ASN:ND2 | 1:A:334:GLU:C[3_655] | 2.16 | 0.04 |
| 1:A:84:GLU:CG | 1:A:336:ASN:CG[3_655] | 2.16 | 0.04 |
| 1:A:69:LEU:N | 1:A:214:SER:O[3_655] | 2.17 | 0.03 |
| 1:A:69:LEU:CB | 1:A:215:GLY:C[3_655] | 2.17 | 0.03 |
| 1:A:80:TYR:CA | 1:A:209:LYS:CD[3_655] | 2.17 | 0.03 |
| 1:A:23:LEU:N | 1:A:261:ILE:CD1[3_655] | 2.17 | 0.03 |
| 1:A:220:ARG:CD | 1:A:437:GLU:N[3_655] | 2.17 | 0.03 |
| 1:A:25:ASP:CA | 1:A:261:ILE:CB[3_655] | 2.17 | 0.03 |
| 1:A:74:GLU:C | 2:A:600:FAD:C3'[3_655] | 2.17 | 0.03 |
| 1:A:68:ILE:CD1 | 1:A:217:VAL:CA[3_655] | 2.17 | 0.03 |
| 1:A:256:GLU:CA | 1:A:455:GLY:O[3_655] | 2.17 | 0.03 |
| 1:A:60:TYR:CA | 4:A:2045:HOH:O[3_655] | 2.17 | 0.03 |
| 1:A:258:LYS:NZ | 1:A:454:MET:CA[3_655] | 2.17 | 0.03 |
| 1:A:32:VAL:N | 1:A:448:ARG:NE[3_655] | 2.17 | 0.03 |
| 1:A:219:GLU:CA | 1:A:437:GLU:CD[3_655] | 2.17 | 0.03 |
| 1:A:69:LEU:CG | 1:A:215:GLY:C[3_655] | 2.17 | 0.03 |
| 1:A:210:PHE:CE2 | 1:A:214:SER:CA[3_655] | 2.17 | 0.03 |
| 1:A:15:SER:C | 1:A:21:LYS:CD[3_655] | 2.17 | 0.03 |
| 1:A:17:MET:CE | 1:A:444:GLU:CD[3_655] | 2.17 | 0.03 |
| 1:A:22:LEU:C | 1:A:261:ILE:CD1[3_655] | 2.17 | 0.03 |
| 1:A:76:GLY:N | 2:A:600:FAD:O3'[3_655] | 2.17 | 0.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------------|--------------------------|-------------------|
| 1:A:466:GLU:CG | 4:A:2017:HOH:O[3_655] | 2.17 | 0.03 |
| 1:A:223:ASP:CG | 1:A:431:HIS:CB[3_655] | 2.18 | 0.02 |
| 1:A:228:ARG:NE | 1:A:449:GLU:CG[3_655] | 2.18 | 0.02 |
| 1:A:21:LYS:CB | 1:A:443:GLY:C[3_655] | 2.18 | 0.02 |
| 1:A:386:LYS:NZ | 1:A:470:VAL:CG1[3_655] | 2.18 | 0.02 |
| 1:A:228:ARG:CA | 1:A:462:ILE:CA[3_655] | 2.18 | 0.02 |
| 1:B:100:ARG:NE | 1:B:208:ARG:NH2[3_555] | 2.18 | 0.02 |
| 1:A:466:GLU:O | 4:A:2017:HOH:O[3_655] | 2.18 | 0.02 |
| 1:A:74:GLU:CD | 2:A:600:FAD:O2P[3_655] | 2.18 | 0.02 |
| 1:A:29:ASN:CA | 1:A:450:ILE:CA[3_655] | 2.18 | 0.02 |
| 1:A:53:TYR:CZ | 1:A:208:ARG:CA[3_655] | 2.18 | 0.02 |
| 1:A:40:GLY:N | 1:A:466:GLU:OE2[3_655] | 2.18 | 0.02 |
| 1:A:83:ASN:O | 1:A:335:GLY:N[3_655] | 2.18 | 0.02 |
| 1:A:56:LEU:CD1 | 1:A:470:VAL:O[3_655] | 2.18 | 0.02 |
| 1:A:227:ASP:CG | 1:A:463:TRP:CD1[3_655] | 2.18 | 0.02 |
| 1:A:81:LYS:NZ | 1:A:300:TYR:CZ[3_655] | 2.19 | 0.01 |
| 1:A:14:ILE:CB | 1:A:71:LEU:CB[3_655] | 2.19 | 0.01 |
| 1:A:24:HIS:CA | 1:A:447:ALA:N[3_655] | 2.19 | 0.01 |
| 1:A:44:TYR:CG | 1:A:469:SER:C[3_655] | 2.19 | 0.01 |
| 1:A:6:ASP:O | 1:A:456:LYS:CG[3_655] | 2.19 | 0.01 |
| 1:A:21:LYS:CD | 1:A:439:ALA:O[3_655] | 2.19 | 0.01 |
| 1:A:438:GLY:C | 4:A:2121:HOH:O[3_655] | 2.19 | 0.01 |
| 1:A:62:GLY:N | 1:A:216:GLN:CD[3_655] | 2.19 | 0.01 |
| 1:A:223:ASP:CA | 1:A:441:GLU:CG[3_655] | 2.19 | 0.01 |
| 1:A:333:PRO:CB | 4:A:2153:HOH:O[3_655] | 2.19 | 0.01 |
| 1:A:5:CYS:C | 1:A:452:HIS:C[3_655] | 2.19 | 0.01 |
| 1:A:19:ALA:CA | 1:A:21:LYS:N[3_655] | 2.19 | 0.01 |
| 1:A:44:TYR:CE1 | 1:A:470:VAL:CA[3_655] | 2.19 | 0.01 |
| 1:A:370:LYS:NZ | 1:A:497:GLY:O[6_564] | 2.19 | 0.01 |
| 1:A:223:ASP:O | 1:A:441:GLU:OE1[3_655] | 2.19 | 0.01 |
| 1:A:16:GLY:C | 4:A:2001:HOH:O[3_655] | 2.19 | 0.01 |
| 1:A:60:TYR:N | 1:A:78:GLU:CA[3_655] | 2.19 | 0.01 |
| 1:A:38:ARG:CA | 1:A:466:GLU:C[3_655] | 2.19 | 0.01 |
| 1:A:47:ARG:CZ | 1:A:64:THR:N[3_655] | 2.19 | 0.01 |
| 1:A:56:LEU:O | 1:A:471:ASP:OD2[3_655] | 2.19 | 0.01 |
| 1:A:47:ARG:CB | 1:A:63:PRO:CB[3_655] | 2.19 | 0.01 |
| 1:B:478:THR:C | 1:B:478:THR:O[3_555] | 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 | 497/520 (96%) | 476 (96%) | 20 (4%) | 1 (0%) | 52 | 59 |
| 1 | B | 492/520 (95%) | 470 (96%) | 20 (4%) | 2 (0%) | 39 | 42 |
| All | All | 989/1040 (95%) | 946 (96%) | 40 (4%) | 3 (0%) | 46 | 50 |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 52 | LYS |
| 1 | A | 52 | LYS |
| 1 | B | 460 | ASP |

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 | 427/444 (96%) | 413 (97%) | 14 (3%) | 45 | 56 |
| 1 | B | 424/444 (96%) | 412 (97%) | 12 (3%) | 51 | 63 |
| All | All | 851/888 (96%) | 825 (97%) | 26 (3%) | 47 | 59 |

All (26) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 3 | ASN |
| 1 | A | 106 | VAL |
| 1 | A | 155 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 242 | ARG |
| 1 | A | 251 | ASN |
| 1 | A | 350 | ARG |
| 1 | A | 364 | LEU |
| 1 | A | 379 | GLU |
| 1 | A | 397 | CYS |
| 1 | A | 398 | TYR |
| 1 | A | 412 | ARG |
| 1 | A | 460 | ASP |
| 1 | A | 494 | ARG |
| 1 | A | 495 | LEU |
| 1 | B | 3 | ASN |
| 1 | B | 46 | LEU |
| 1 | B | 155 | LEU |
| 1 | B | 167 | LEU |
| 1 | B | 198 | ILE |
| 1 | B | 242 | ARG |
| 1 | B | 251 | ASN |
| 1 | B | 364 | LEU |
| 1 | B | 379 | GLU |
| 1 | B | 412 | ARG |
| 1 | B | 460 | ASP |
| 1 | B | 494 | ARG |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 117 | ASN |
| 1 | A | 251 | ASN |
| 1 | A | 431 | HIS |
| 1 | B | 117 | ASN |
| 1 | B | 251 | ASN |
| 1 | B | 431 | HIS |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | # $ Z > 2$ | Counts | RMSZ | # $ Z > 2$ |
| 2 | FAD | A | 600 | 1,3 | 48,58,58 | 1.61 | 7 (14%) | 54,89,89 | 2.39 | 11 (20%) |
| 3 | DPK | A | 601 | 2 | 14,14,14 | 0.54 | 0 | 15,17,17 | 2.26 | 4 (26%) |
| 2 | FAD | B | 600 | 1,3 | 48,58,58 | 1.42 | 9 (18%) | 54,89,89 | 2.45 | 12 (22%) |
| 3 | DPK | B | 601 | 2 | 14,14,14 | 0.61 | 0 | 15,17,17 | 2.35 | 4 (26%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 2 | FAD | A | 600 | 1,3 | - | 0/30/50/50 | 0/6/6/6 |
| 3 | DPK | A | 601 | 2 | - | 1/11/11/11 | 0/1/1/1 |
| 2 | FAD | B | 600 | 1,3 | - | 0/30/50/50 | 0/6/6/6 |
| 3 | DPK | B | 601 | 2 | - | 1/11/11/11 | 0/1/1/1 |

All (16) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | B | 600 | FAD | O4B-C4B | -2.34 | 1.39 | 1.45 |
| 2 | A | 600 | FAD | C10-N10 | -2.28 | 1.36 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | B | 600 | FAD | C9A-N10 | 2.03 | 1.41 | 1.38 |
| 2 | B | 600 | FAD | C5'-C4' | 2.13 | 1.54 | 1.51 |
| 2 | B | 600 | FAD | C10-N1 | 2.13 | 1.39 | 1.35 |
| 2 | A | 600 | FAD | C4-N3 | 2.19 | 1.37 | 1.33 |
| 2 | A | 600 | FAD | C5X-N5 | 2.21 | 1.38 | 1.35 |
| 2 | A | 600 | FAD | C2A-N1A | 2.82 | 1.39 | 1.33 |
| 2 | B | 600 | FAD | C4-N3 | 2.97 | 1.38 | 1.33 |
| 2 | B | 600 | FAD | C1'-N10 | 3.10 | 1.51 | 1.48 |
| 2 | B | 600 | FAD | C2A-N1A | 3.13 | 1.39 | 1.33 |
| 2 | B | 600 | FAD | C2A-N3A | 3.42 | 1.38 | 1.32 |
| 2 | A | 600 | FAD | C2A-N3A | 3.60 | 1.38 | 1.32 |
| 2 | B | 600 | FAD | C4X-N5 | 3.99 | 1.39 | 1.33 |
| 2 | A | 600 | FAD | C4X-N5 | 4.16 | 1.39 | 1.33 |
| 2 | A | 600 | FAD | C1'-N10 | 6.28 | 1.55 | 1.48 |

All (31) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 2 | B | 600 | FAD | N3A-C2A-N1A | -12.64 | 119.22 | 128.89 |
| 2 | A | 600 | FAD | N3A-C2A-N1A | -10.17 | 121.11 | 128.89 |
| 2 | A | 600 | FAD | C4X-C4-N3 | -4.85 | 116.96 | 123.59 |
| 2 | A | 600 | FAD | C4A-C5A-N7A | -3.84 | 105.94 | 109.48 |
| 2 | B | 600 | FAD | C9A-C5X-N5 | -3.79 | 116.75 | 122.36 |
| 2 | B | 600 | FAD | C1'-N10-C9A | -3.70 | 114.71 | 118.86 |
| 2 | A | 600 | FAD | C1B-N9A-C4A | -3.69 | 121.37 | 126.94 |
| 2 | A | 600 | FAD | O3'-C3'-C4' | -3.28 | 100.48 | 108.75 |
| 2 | B | 600 | FAD | C4X-C4-N3 | -3.28 | 119.11 | 123.59 |
| 2 | B | 600 | FAD | C1B-N9A-C4A | -2.81 | 122.71 | 126.94 |
| 2 | B | 600 | FAD | C4A-C5A-N7A | -2.63 | 107.06 | 109.48 |
| 2 | B | 600 | FAD | P-O3P-PA | -2.55 | 125.57 | 132.73 |
| 2 | A | 600 | FAD | C9A-C5X-N5 | -2.27 | 119.00 | 122.36 |
| 2 | A | 600 | FAD | P-O3P-PA | -2.09 | 126.85 | 132.73 |
| 2 | A | 600 | FAD | O2A-PA-O3P | 2.02 | 114.26 | 105.09 |
| 3 | B | 601 | DPK | C9N-N9-C8 | 2.07 | 117.19 | 113.78 |
| 3 | A | 601 | DPK | C9N-N9-C8 | 2.12 | 117.27 | 113.78 |
| 2 | A | 600 | FAD | C4-C4X-N5 | 2.12 | 121.29 | 118.72 |
| 2 | B | 600 | FAD | C4-C4X-N5 | 2.47 | 121.71 | 118.72 |
| 2 | B | 600 | FAD | O2A-PA-O3P | 2.83 | 117.91 | 105.09 |
| 3 | B | 601 | DPK | C10-N9-C8 | 3.49 | 123.65 | 113.71 |
| 2 | B | 600 | FAD | C2B-C1B-N9A | 3.62 | 119.82 | 114.29 |
| 3 | A | 601 | DPK | C10-N9-C8 | 3.63 | 124.07 | 113.71 |
| 2 | A | 600 | FAD | C2B-C1B-N9A | 3.68 | 119.92 | 114.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 3 | A | 601 | DPK | C11-C10-N9 | 3.93 | 121.51 | 112.62 |
| 3 | B | 601 | DPK | C11-C10-N9 | 4.00 | 121.66 | 112.62 |
| 2 | B | 600 | FAD | C4-N3-C2 | 4.46 | 119.10 | 115.25 |
| 2 | B | 600 | FAD | C4X-N5-C5X | 4.93 | 122.43 | 116.76 |
| 3 | A | 601 | DPK | C9N-N9-C10 | 6.42 | 118.67 | 110.04 |
| 3 | B | 601 | DPK | C9N-N9-C10 | 6.78 | 119.16 | 110.04 |
| 2 | A | 600 | FAD | C4-N3-C2 | 8.57 | 122.66 | 115.25 |

There are no chirality outliers.

All (2) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|----------------|
| 3 | A | 601 | DPK | C11-C10-N9-C9N |
| 3 | B | 601 | DPK | C11-C10-N9-C9N |

There are no ring outliers.

3 monomers are involved in 65 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2 | A | 600 | FAD | 2 | 60 |
| 2 | B | 600 | FAD | 2 | 0 |
| 3 | B | 601 | DPK | 1 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 1 | A | 499/520 (95%) | 2.56 | 284 (56%) 0 0 | 24, 31, 46, 64 | 0 |
| 1 | B | 494/520 (95%) | 2.63 | 296 (59%) 0 0 | 23, 31, 42, 60 | 0 |
| All | All | 993/1040 (95%) | 2.59 | 580 (58%) 0 0 | 23, 31, 44, 64 | 0 |

All (580) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | B | 495 | LEU | 14.6 |
| 1 | B | 212 | GLY | 12.7 |
| 1 | B | 496 | ILE | 12.1 |
| 1 | B | 244 | ASN | 11.8 |
| 1 | A | 13 | GLY | 10.5 |
| 1 | A | 226 | GLY | 8.9 |
| 1 | A | 94 | GLY | 8.8 |
| 1 | A | 481 | PHE | 8.8 |
| 1 | A | 302 | LYS | 8.2 |
| 1 | A | 246 | LEU | 8.1 |
| 1 | B | 453 | ALA | 7.7 |
| 1 | B | 494 | ARG | 7.4 |
| 1 | B | 491 | GLY | 7.3 |
| 1 | B | 110 | ILE | 7.2 |
| 1 | A | 245 | VAL | 7.0 |
| 1 | B | 243 | GLU | 7.0 |
| 1 | B | 252 | HIS | 7.0 |
| 1 | A | 459 | GLU | 7.0 |
| 1 | A | 138 | PRO | 6.9 |
| 1 | B | 395 | GLY | 6.9 |
| 1 | A | 263 | ALA | 6.9 |
| 1 | A | 477 | ILE | 6.9 |
| 1 | B | 446 | ALA | 6.7 |
| 1 | A | 107 | TRP | 6.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 224 | LEU | 6.3 |
| 1 | B | 92 | VAL | 6.3 |
| 1 | A | 241 | THR | 6.3 |
| 1 | A | 264 | ILE | 6.2 |
| 1 | A | 9 | VAL | 6.2 |
| 1 | A | 92 | VAL | 6.1 |
| 1 | A | 486 | LEU | 6.1 |
| 1 | A | 105 | PRO | 6.0 |
| 1 | B | 460 | ASP | 6.0 |
| 1 | A | 352 | LEU | 6.0 |
| 1 | B | 85 | VAL | 5.9 |
| 1 | A | 33 | LEU | 5.8 |
| 1 | A | 374 | SER | 5.8 |
| 1 | A | 465 | SER | 5.8 |
| 1 | A | 242 | ARG | 5.7 |
| 1 | A | 259 | TYR | 5.7 |
| 1 | A | 425 | GLY | 5.7 |
| 1 | A | 429 | ALA | 5.6 |
| 1 | B | 230 | LYS | 5.6 |
| 1 | A | 22 | LEU | 5.6 |
| 1 | B | 241 | THR | 5.6 |
| 1 | A | 8 | VAL | 5.6 |
| 1 | B | 250 | LEU | 5.5 |
| 1 | B | 462 | ILE | 5.5 |
| 1 | A | 328 | LEU | 5.5 |
| 1 | A | 110 | ILE | 5.5 |
| 1 | B | 81 | LYS | 5.5 |
| 1 | A | 231 | LEU | 5.5 |
| 1 | A | 355 | LEU | 5.5 |
| 1 | A | 452 | HIS | 5.4 |
| 1 | A | 189 | VAL | 5.4 |
| 1 | A | 354 | ARG | 5.4 |
| 1 | B | 458 | PRO | 5.4 |
| 1 | B | 242 | ARG | 5.4 |
| 1 | A | 214 | SER | 5.3 |
| 1 | A | 499 | THR | 5.2 |
| 1 | A | 98 | PRO | 5.2 |
| 1 | B | 450 | ILE | 5.2 |
| 1 | B | 35 | ALA | 5.1 |
| 1 | A | 433 | SER | 5.1 |
| 1 | B | 105 | PRO | 5.0 |
| 1 | A | 341 | MET | 5.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | B | 54 | VAL | 5.0 |
| 1 | B | 246 | LEU | 5.0 |
| 1 | B | 236 | ILE | 5.0 |
| 1 | B | 493 | LEU | 5.0 |
| 1 | A | 298 | ILE | 5.0 |
| 1 | B | 263 | ALA | 5.0 |
| 1 | B | 465 | SER | 4.9 |
| 1 | B | 457 | ILE | 4.9 |
| 1 | A | 3 | ASN | 4.9 |
| 1 | A | 236 | ILE | 4.9 |
| 1 | A | 12 | GLY | 4.9 |
| 1 | B | 424 | ALA | 4.9 |
| 1 | A | 10 | VAL | 4.9 |
| 1 | A | 342 | GLY | 4.9 |
| 1 | A | 470 | VAL | 4.8 |
| 1 | A | 106 | VAL | 4.8 |
| 1 | B | 235 | VAL | 4.8 |
| 1 | A | 119 | TRP | 4.8 |
| 1 | A | 498 | LEU | 4.7 |
| 1 | A | 247 | VAL | 4.7 |
| 1 | A | 97 | TYR | 4.7 |
| 1 | A | 304 | PRO | 4.7 |
| 1 | B | 43 | THR | 4.7 |
| 1 | B | 156 | CYS | 4.7 |
| 1 | A | 343 | PHE | 4.6 |
| 1 | B | 485 | HIS | 4.6 |
| 1 | B | 23 | LEU | 4.6 |
| 1 | B | 29 | ASN | 4.6 |
| 1 | A | 20 | ALA | 4.6 |
| 1 | A | 327 | THR | 4.6 |
| 1 | A | 279 | PRO | 4.6 |
| 1 | A | 383 | TYR | 4.6 |
| 1 | B | 82 | VAL | 4.6 |
| 1 | B | 27 | GLY | 4.6 |
| 1 | B | 455 | GLY | 4.6 |
| 1 | B | 335 | GLY | 4.6 |
| 1 | A | 318 | ASP | 4.6 |
| 1 | A | 495 | LEU | 4.6 |
| 1 | A | 222 | MET | 4.5 |
| 1 | A | 372 | LEU | 4.5 |
| 1 | A | 457 | ILE | 4.5 |
| 1 | A | 478 | THR | 4.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 337 | TYR | 4.5 |
| 1 | B | 467 | PRO | 4.5 |
| 1 | B | 238 | ILE | 4.5 |
| 1 | B | 103 | PHE | 4.5 |
| 1 | B | 58 | GLY | 4.5 |
| 1 | B | 264 | ILE | 4.5 |
| 1 | B | 463 | TRP | 4.5 |
| 1 | A | 104 | PRO | 4.4 |
| 1 | A | 243 | GLU | 4.4 |
| 1 | B | 227 | ASP | 4.4 |
| 1 | A | 71 | LEU | 4.4 |
| 1 | B | 31 | VAL | 4.4 |
| 1 | B | 429 | ALA | 4.4 |
| 1 | B | 226 | GLY | 4.4 |
| 1 | B | 482 | LEU | 4.3 |
| 1 | B | 217 | VAL | 4.3 |
| 1 | B | 93 | LYS | 4.3 |
| 1 | B | 394 | SER | 4.3 |
| 1 | A | 93 | LYS | 4.3 |
| 1 | B | 261 | ILE | 4.3 |
| 1 | B | 336 | ASN | 4.3 |
| 1 | B | 340 | ILE | 4.3 |
| 1 | A | 484 | ARG | 4.3 |
| 1 | B | 136 | LYS | 4.3 |
| 1 | A | 133 | ALA | 4.2 |
| 1 | B | 143 | TRP | 4.2 |
| 1 | A | 442 | ALA | 4.2 |
| 1 | A | 265 | PRO | 4.2 |
| 1 | B | 456 | LYS | 4.2 |
| 1 | A | 475 | GLN | 4.2 |
| 1 | B | 22 | LEU | 4.2 |
| 1 | B | 259 | TYR | 4.2 |
| 1 | B | 492 | LEU | 4.2 |
| 1 | B | 107 | TRP | 4.1 |
| 1 | B | 9 | VAL | 4.1 |
| 1 | B | 221 | ILE | 4.1 |
| 1 | B | 119 | TRP | 4.1 |
| 1 | A | 458 | PRO | 4.1 |
| 1 | A | 418 | VAL | 4.0 |
| 1 | B | 443 | GLY | 4.0 |
| 1 | A | 305 | PHE | 4.0 |
| 1 | A | 300 | TYR | 4.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | B | 311 | TYR | 4.0 |
| 1 | A | 454 | MET | 4.0 |
| 1 | B | 398 | TYR | 4.0 |
| 1 | A | 252 | HIS | 4.0 |
| 1 | B | 237 | TYR | 4.0 |
| 1 | A | 345 | LEU | 4.0 |
| 1 | A | 331 | THR | 3.9 |
| 1 | B | 163 | GLN | 3.9 |
| 1 | A | 432 | TRP | 3.9 |
| 1 | A | 317 | ILE | 3.9 |
| 1 | B | 476 | PRO | 3.9 |
| 1 | A | 423 | PHE | 3.9 |
| 1 | A | 421 | ILE | 3.9 |
| 1 | B | 260 | VAL | 3.9 |
| 1 | B | 303 | GLU | 3.9 |
| 1 | A | 389 | CYS | 3.9 |
| 1 | B | 4 | LYS | 3.9 |
| 1 | B | 220 | ARG | 3.9 |
| 1 | B | 229 | VAL | 3.9 |
| 1 | B | 247 | VAL | 3.9 |
| 1 | B | 53 | TYR | 3.9 |
| 1 | B | 139 | LEU | 3.9 |
| 1 | A | 37 | ASP | 3.8 |
| 1 | A | 453 | ALA | 3.8 |
| 1 | A | 255 | TYR | 3.8 |
| 1 | A | 294 | VAL | 3.8 |
| 1 | B | 274 | PHE | 3.8 |
| 1 | A | 426 | THR | 3.8 |
| 1 | A | 313 | GLY | 3.8 |
| 1 | B | 193 | GLY | 3.8 |
| 1 | B | 251 | ASN | 3.8 |
| 1 | A | 72 | ALA | 3.8 |
| 1 | A | 491 | GLY | 3.8 |
| 1 | B | 305 | PHE | 3.7 |
| 1 | B | 189 | VAL | 3.7 |
| 1 | B | 461 | GLU | 3.7 |
| 1 | B | 204 | GLY | 3.7 |
| 1 | B | 77 | LEU | 3.7 |
| 1 | B | 431 | HIS | 3.7 |
| 1 | A | 225 | LEU | 3.7 |
| 1 | A | 316 | ILE | 3.7 |
| 1 | A | 439 | ALA | 3.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 77 | LEU | 3.6 |
| 1 | B | 14 | ILE | 3.6 |
| 1 | B | 255 | TYR | 3.6 |
| 1 | B | 352 | LEU | 3.6 |
| 1 | A | 297 | CYS | 3.6 |
| 1 | A | 434 | GLY | 3.6 |
| 1 | B | 121 | THR | 3.6 |
| 1 | A | 229 | VAL | 3.6 |
| 1 | A | 235 | VAL | 3.6 |
| 1 | A | 476 | PRO | 3.6 |
| 1 | A | 301 | TYR | 3.6 |
| 1 | B | 343 | PHE | 3.6 |
| 1 | A | 23 | LEU | 3.6 |
| 1 | A | 375 | LEU | 3.6 |
| 1 | B | 228 | ARG | 3.6 |
| 1 | B | 420 | ARG | 3.6 |
| 1 | A | 363 | LYS | 3.6 |
| 1 | A | 312 | CYS | 3.5 |
| 1 | A | 268 | LEU | 3.5 |
| 1 | B | 270 | MET | 3.5 |
| 1 | B | 328 | LEU | 3.5 |
| 1 | B | 422 | TYR | 3.5 |
| 1 | B | 66 | ASN | 3.5 |
| 1 | A | 326 | TYR | 3.5 |
| 1 | B | 425 | GLY | 3.5 |
| 1 | B | 39 | VAL | 3.5 |
| 1 | B | 21 | LYS | 3.5 |
| 1 | A | 319 | GLY | 3.5 |
| 1 | A | 244 | ASN | 3.5 |
| 1 | A | 496 | ILE | 3.5 |
| 1 | A | 6 | ASP | 3.5 |
| 1 | B | 231 | LEU | 3.5 |
| 1 | A | 198 | ILE | 3.5 |
| 1 | A | 463 | TRP | 3.5 |
| 1 | B | 449 | GLU | 3.5 |
| 1 | B | 50 | LYS | 3.4 |
| 1 | B | 418 | VAL | 3.4 |
| 1 | A | 387 | ASN | 3.4 |
| 1 | B | 185 | PHE | 3.4 |
| 1 | B | 472 | VAL | 3.4 |
| 1 | A | 364 | LEU | 3.4 |
| 1 | B | 258 | LYS | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | B | 97 | TYR | 3.4 |
| 1 | A | 50 | LYS | 3.4 |
| 1 | B | 245 | VAL | 3.4 |
| 1 | B | 215 | GLY | 3.4 |
| 1 | B | 401 | TYR | 3.4 |
| 1 | B | 410 | TYR | 3.4 |
| 1 | B | 490 | PRO | 3.4 |
| 1 | B | 440 | VAL | 3.4 |
| 1 | B | 489 | VAL | 3.4 |
| 1 | B | 222 | MET | 3.4 |
| 1 | B | 140 | ALA | 3.4 |
| 1 | A | 340 | ILE | 3.4 |
| 1 | A | 31 | VAL | 3.3 |
| 1 | B | 451 | LEU | 3.3 |
| 1 | B | 187 | TRP | 3.3 |
| 1 | B | 376 | GLU | 3.3 |
| 1 | B | 448 | ARG | 3.3 |
| 1 | B | 20 | ALA | 3.3 |
| 1 | A | 266 | PRO | 3.3 |
| 1 | A | 173 | VAL | 3.3 |
| 1 | A | 424 | ALA | 3.3 |
| 1 | B | 171 | LEU | 3.3 |
| 1 | B | 355 | LEU | 3.3 |
| 1 | B | 116 | ASN | 3.3 |
| 1 | A | 479 | THR | 3.3 |
| 1 | A | 472 | VAL | 3.3 |
| 1 | B | 347 | HIS | 3.3 |
| 1 | B | 272 | ILE | 3.3 |
| 1 | A | 171 | LEU | 3.3 |
| 1 | A | 393 | TYR | 3.2 |
| 1 | B | 88 | LEU | 3.2 |
| 1 | B | 138 | PRO | 3.2 |
| 1 | A | 184 | TRP | 3.2 |
| 1 | A | 258 | LYS | 3.2 |
| 1 | A | 188 | TYR | 3.2 |
| 1 | B | 137 | ALA | 3.2 |
| 1 | B | 322 | ALA | 3.2 |
| 1 | B | 341 | MET | 3.2 |
| 1 | A | 296 | LYS | 3.2 |
| 1 | A | 388 | TRP | 3.2 |
| 1 | B | 367 | LEU | 3.2 |
| 1 | B | 108 | ASN | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 160 | SER | 3.2 |
| 1 | B | 309 | LYS | 3.2 |
| 1 | A | 249 | THR | 3.2 |
| 1 | B | 337 | TYR | 3.1 |
| 1 | A | 101 | GLY | 3.1 |
| 1 | A | 175 | ALA | 3.1 |
| 1 | B | 306 | TRP | 3.1 |
| 1 | B | 265 | PRO | 3.1 |
| 1 | B | 473 | PRO | 3.1 |
| 1 | A | 469 | SER | 3.1 |
| 1 | B | 59 | SER | 3.1 |
| 1 | A | 49 | GLN | 3.1 |
| 1 | B | 155 | LEU | 3.1 |
| 1 | B | 224 | LEU | 3.1 |
| 1 | A | 51 | VAL | 3.1 |
| 1 | B | 225 | LEU | 3.1 |
| 1 | B | 249 | THR | 3.1 |
| 1 | A | 462 | ILE | 3.1 |
| 1 | B | 325 | ALA | 3.1 |
| 1 | A | 399 | THR | 3.1 |
| 1 | A | 54 | VAL | 3.1 |
| 1 | B | 49 | GLN | 3.1 |
| 1 | A | 41 | GLY | 3.0 |
| 1 | B | 95 | LYS | 3.0 |
| 1 | B | 362 | LYS | 3.0 |
| 1 | B | 111 | THR | 3.0 |
| 1 | B | 408 | THR | 3.0 |
| 1 | A | 413 | VAL | 3.0 |
| 1 | A | 182 | ALA | 3.0 |
| 1 | A | 412 | ARG | 3.0 |
| 1 | B | 435 | TYR | 3.0 |
| 1 | A | 485 | HIS | 3.0 |
| 1 | B | 129 | ILE | 3.0 |
| 1 | A | 367 | LEU | 3.0 |
| 1 | A | 381 | VAL | 3.0 |
| 1 | B | 409 | GLN | 3.0 |
| 1 | B | 198 | ILE | 3.0 |
| 1 | A | 187 | TRP | 3.0 |
| 1 | A | 404 | PRO | 2.9 |
| 1 | A | 497 | GLY | 2.9 |
| 1 | B | 173 | VAL | 2.9 |
| 1 | A | 398 | TYR | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | B | 307 | ARG | 2.9 |
| 1 | B | 211 | VAL | 2.9 |
| 1 | B | 175 | ALA | 2.9 |
| 1 | B | 426 | THR | 2.9 |
| 1 | A | 414 | LEU | 2.9 |
| 1 | B | 28 | LEU | 2.9 |
| 1 | A | 169 | VAL | 2.9 |
| 1 | A | 325 | ALA | 2.9 |
| 1 | B | 432 | TRP | 2.9 |
| 1 | B | 470 | VAL | 2.9 |
| 1 | B | 275 | ASN | 2.9 |
| 1 | B | 64 | THR | 2.9 |
| 1 | A | 205 | GLY | 2.9 |
| 1 | A | 250 | LEU | 2.9 |
| 1 | B | 169 | VAL | 2.9 |
| 1 | A | 400 | THR | 2.9 |
| 1 | B | 188 | TYR | 2.9 |
| 1 | A | 494 | ARG | 2.9 |
| 1 | B | 477 | ILE | 2.9 |
| 1 | B | 69 | LEU | 2.9 |
| 1 | B | 299 | VAL | 2.9 |
| 1 | B | 298 | ILE | 2.9 |
| 1 | A | 7 | VAL | 2.8 |
| 1 | B | 104 | PRO | 2.8 |
| 1 | A | 254 | MET | 2.8 |
| 1 | B | 454 | MET | 2.8 |
| 1 | A | 251 | ASN | 2.8 |
| 1 | B | 94 | GLY | 2.8 |
| 1 | B | 61 | VAL | 2.8 |
| 1 | B | 112 | TYR | 2.8 |
| 1 | B | 333 | PRO | 2.8 |
| 1 | B | 379 | GLU | 2.8 |
| 1 | A | 64 | THR | 2.8 |
| 1 | A | 428 | THR | 2.8 |
| 1 | B | 8 | VAL | 2.8 |
| 1 | B | 469 | SER | 2.8 |
| 1 | A | 203 | ASN | 2.8 |
| 1 | A | 5 | CYS | 2.8 |
| 1 | B | 428 | THR | 2.8 |
| 1 | A | 468 | GLU | 2.8 |
| 1 | A | 11 | GLY | 2.8 |
| 1 | B | 423 | PHE | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | B | 102 | PRO | 2.8 |
| 1 | A | 262 | SER | 2.7 |
| 1 | A | 420 | ARG | 2.7 |
| 1 | A | 379 | GLU | 2.7 |
| 1 | A | 293 | SER | 2.7 |
| 1 | B | 283 | ASN | 2.7 |
| 1 | B | 301 | TYR | 2.7 |
| 1 | A | 309 | LYS | 2.7 |
| 1 | A | 43 | THR | 2.7 |
| 1 | B | 396 | GLY | 2.7 |
| 1 | B | 459 | GLU | 2.7 |
| 1 | B | 73 | LYS | 2.7 |
| 1 | A | 339 | ALA | 2.7 |
| 1 | B | 72 | ALA | 2.7 |
| 1 | B | 214 | SER | 2.7 |
| 1 | B | 393 | TYR | 2.7 |
| 1 | A | 70 | ARG | 2.7 |
| 1 | B | 167 | LEU | 2.7 |
| 1 | B | 416 | GLN | 2.7 |
| 1 | A | 276 | PRO | 2.7 |
| 1 | A | 155 | LEU | 2.7 |
| 1 | B | 421 | ILE | 2.7 |
| 1 | B | 442 | ALA | 2.7 |
| 1 | B | 400 | THR | 2.7 |
| 1 | A | 368 | TYR | 2.7 |
| 1 | A | 167 | LEU | 2.6 |
| 1 | B | 152 | LEU | 2.6 |
| 1 | A | 35 | ALA | 2.6 |
| 1 | B | 26 | SER | 2.6 |
| 1 | B | 118 | PHE | 2.6 |
| 1 | A | 480 | THR | 2.6 |
| 1 | A | 500 | THR | 2.6 |
| 1 | B | 150 | GLU | 2.6 |
| 1 | B | 80 | TYR | 2.6 |
| 1 | A | 351 | LYS | 2.6 |
| 1 | B | 302 | LYS | 2.6 |
| 1 | B | 403 | PRO | 2.6 |
| 1 | B | 51 | VAL | 2.6 |
| 1 | A | 57 | GLY | 2.6 |
| 1 | A | 267 | THR | 2.6 |
| 1 | A | 460 | ASP | 2.6 |
| 1 | B | 180 | VAL | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | B | 324 | VAL | 2.6 |
| 1 | A | 291 | LEU | 2.6 |
| 1 | B | 346 | ALA | 2.6 |
| 1 | B | 464 | GLN | 2.6 |
| 1 | A | 292 | GLY | 2.6 |
| 1 | B | 213 | GLY | 2.6 |
| 1 | B | 411 | GLY | 2.6 |
| 1 | B | 33 | LEU | 2.6 |
| 1 | B | 120 | ARG | 2.6 |
| 1 | A | 53 | TYR | 2.6 |
| 1 | A | 211 | VAL | 2.6 |
| 1 | B | 48 | ASN | 2.6 |
| 1 | A | 334 | GLU | 2.6 |
| 1 | A | 438 | GLY | 2.6 |
| 1 | A | 275 | ASN | 2.6 |
| 1 | A | 278 | LEU | 2.6 |
| 1 | B | 7 | VAL | 2.6 |
| 1 | A | 58 | GLY | 2.5 |
| 1 | B | 12 | GLY | 2.5 |
| 1 | B | 157 | TRP | 2.5 |
| 1 | A | 81 | LYS | 2.5 |
| 1 | B | 209 | LYS | 2.5 |
| 1 | A | 482 | LEU | 2.5 |
| 1 | B | 5 | CYS | 2.5 |
| 1 | A | 396 | GLY | 2.5 |
| 1 | A | 135 | TRP | 2.5 |
| 1 | B | 153 | ASP | 2.5 |
| 1 | B | 291 | LEU | 2.5 |
| 1 | A | 180 | VAL | 2.5 |
| 1 | A | 102 | PRO | 2.5 |
| 1 | B | 330 | ASP | 2.5 |
| 1 | A | 174 | THR | 2.5 |
| 1 | A | 25 | ASP | 2.5 |
| 1 | A | 366 | GLU | 2.5 |
| 1 | B | 60 | TYR | 2.5 |
| 1 | B | 148 | MET | 2.5 |
| 1 | B | 268 | LEU | 2.5 |
| 1 | B | 342 | GLY | 2.5 |
| 1 | A | 487 | PRO | 2.5 |
| 1 | B | 417 | PRO | 2.5 |
| 1 | A | 199 | ILE | 2.5 |
| 1 | A | 308 | LYS | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | B | 3 | ASN | 2.5 |
| 1 | B | 466 | GLU | 2.5 |
| 1 | B | 369 | ALA | 2.5 |
| 1 | B | 45 | THR | 2.5 |
| 1 | A | 143 | TRP | 2.5 |
| 1 | A | 178 | HIS | 2.5 |
| 1 | A | 435 | TYR | 2.5 |
| 1 | A | 473 | PRO | 2.5 |
| 1 | B | 98 | PRO | 2.5 |
| 1 | A | 217 | VAL | 2.5 |
| 1 | B | 30 | VAL | 2.5 |
| 1 | A | 501 | ILE | 2.5 |
| 1 | B | 321 | GLU | 2.5 |
| 1 | A | 402 | PHE | 2.5 |
| 1 | A | 66 | ASN | 2.4 |
| 1 | A | 403 | PRO | 2.4 |
| 1 | A | 82 | VAL | 2.4 |
| 1 | B | 40 | GLY | 2.4 |
| 1 | A | 46 | LEU | 2.4 |
| 1 | B | 388 | TRP | 2.4 |
| 1 | A | 27 | GLY | 2.4 |
| 1 | A | 233 | ARG | 2.4 |
| 1 | A | 75 | LEU | 2.4 |
| 1 | A | 401 | TYR | 2.4 |
| 1 | B | 317 | ILE | 2.4 |
| 1 | B | 481 | PHE | 2.4 |
| 1 | B | 327 | THR | 2.4 |
| 1 | A | 163 | GLN | 2.4 |
| 1 | B | 381 | VAL | 2.4 |
| 1 | B | 178 | HIS | 2.4 |
| 1 | A | 430 | THR | 2.4 |
| 1 | B | 358 | GLU | 2.4 |
| 1 | B | 354 | ARG | 2.4 |
| 1 | B | 122 | MET | 2.4 |
| 1 | A | 124 | ASP | 2.4 |
| 1 | B | 25 | ASP | 2.4 |
| 1 | B | 68 | ILE | 2.4 |
| 1 | A | 99 | PHE | 2.4 |
| 1 | A | 103 | PHE | 2.4 |
| 1 | A | 127 | ARG | 2.4 |
| 1 | B | 190 | LYS | 2.4 |
| 1 | A | 384 | GLU | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | B | 17 | MET | 2.3 |
| 1 | B | 44 | TYR | 2.3 |
| 1 | B | 19 | ALA | 2.3 |
| 1 | A | 48 | ASN | 2.3 |
| 1 | B | 345 | LEU | 2.3 |
| 1 | B | 10 | VAL | 2.3 |
| 1 | A | 257 | ALA | 2.3 |
| 1 | A | 269 | GLY | 2.3 |
| 1 | B | 240 | GLN | 2.3 |
| 1 | A | 40 | GLY | 2.3 |
| 1 | B | 216 | GLN | 2.3 |
| 1 | B | 452 | HIS | 2.3 |
| 1 | B | 471 | ASP | 2.3 |
| 1 | B | 286 | ILE | 2.3 |
| 1 | A | 60 | TYR | 2.3 |
| 1 | A | 443 | GLY | 2.3 |
| 1 | A | 100 | ARG | 2.3 |
| 1 | A | 467 | PRO | 2.3 |
| 1 | A | 80 | TYR | 2.3 |
| 1 | A | 338 | ALA | 2.3 |
| 1 | A | 489 | VAL | 2.3 |
| 1 | A | 216 | GLN | 2.2 |
| 1 | A | 213 | GLY | 2.2 |
| 1 | B | 363 | LYS | 2.2 |
| 1 | A | 237 | TYR | 2.2 |
| 1 | A | 390 | GLU | 2.2 |
| 1 | B | 281 | MET | 2.2 |
| 1 | A | 227 | ASP | 2.2 |
| 1 | B | 447 | ALA | 2.2 |
| 1 | A | 299 | VAL | 2.2 |
| 1 | A | 336 | ASN | 2.2 |
| 1 | A | 392 | GLN | 2.2 |
| 1 | A | 220 | ARG | 2.2 |
| 1 | B | 100 | ARG | 2.2 |
| 1 | A | 159 | GLU | 2.2 |
| 1 | B | 223 | ASP | 2.2 |
| 1 | A | 415 | ARG | 2.2 |
| 1 | B | 127 | ARG | 2.2 |
| 1 | B | 378 | LEU | 2.2 |
| 1 | A | 347 | HIS | 2.2 |
| 1 | B | 331 | THR | 2.2 |
| 1 | A | 272 | ILE | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 330 | ASP | 2.2 |
| 1 | A | 24 | HIS | 2.2 |
| 1 | A | 321 | GLU | 2.2 |
| 1 | B | 71 | LEU | 2.2 |
| 1 | B | 83 | ASN | 2.2 |
| 1 | B | 361 | LEU | 2.2 |
| 1 | A | 289 | VAL | 2.1 |
| 1 | A | 490 | PRO | 2.1 |
| 1 | A | 152 | LEU | 2.1 |
| 1 | A | 397 | CYS | 2.1 |
| 1 | A | 447 | ALA | 2.1 |
| 1 | B | 57 | GLY | 2.1 |
| 1 | B | 319 | GLY | 2.1 |
| 1 | B | 294 | VAL | 2.1 |
| 1 | A | 140 | ALA | 2.1 |
| 1 | A | 204 | GLY | 2.1 |
| 1 | B | 41 | GLY | 2.1 |
| 1 | B | 126 | GLY | 2.1 |
| 1 | A | 277 | PRO | 2.1 |
| 1 | A | 324 | VAL | 2.1 |
| 1 | B | 385 | GLU | 2.1 |
| 1 | B | 372 | LEU | 2.1 |
| 1 | B | 430 | THR | 2.1 |
| 1 | B | 351 | LYS | 2.1 |
| 1 | A | 112 | TYR | 2.1 |
| 1 | A | 422 | TYR | 2.1 |
| 1 | B | 184 | TRP | 2.1 |
| 1 | B | 18 | ALA | 2.1 |
| 1 | A | 394 | SER | 2.1 |
| 1 | B | 162 | LYS | 2.1 |
| 1 | A | 32 | VAL | 2.1 |
| 1 | B | 384 | GLU | 2.0 |
| 1 | A | 196 | THR | 2.0 |
| 1 | A | 307 | ARG | 2.0 |
| 1 | A | 314 | THR | 2.0 |
| 1 | B | 145 | ASN | 2.0 |
| 1 | B | 383 | TYR | 2.0 |
| 1 | B | 474 | ALA | 2.0 |
| 1 | B | 382 | HIS | 2.0 |
| 1 | A | 461 | GLU | 2.0 |
| 1 | B | 344 | ILE | 2.0 |
| 1 | A | 373 | GLY | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | B | 313 | GLY | 2.0 |
| 1 | B | 434 | GLY | 2.0 |
| 1 | B | 201 | THR | 2.0 |
| 1 | A | 270 | MET | 2.0 |
| 1 | A | 115 | HIS | 2.0 |
| 1 | B | 233 | ARG | 2.0 |
| 1 | A | 29 | ASN | 2.0 |
| 1 | B | 177 | THR | 2.0 |
| 1 | A | 197 | ARG | 2.0 |
| 1 | A | 290 | PRO | 2.0 |

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|----------------------------|-------|
| 3 | DPK | A | 601 | 14/14 | 0.59 | 0.56 | 5.28 | 49,57,64,64 | 0 |
| 3 | DPK | B | 601 | 14/14 | 0.54 | 0.57 | 4.79 | 49,57,64,64 | 0 |
| 2 | FAD | A | 600 | 53/53 | 0.83 | 0.22 | -0.82 | 23,29,32,33 | 0 |
| 2 | FAD | B | 600 | 53/53 | 0.79 | 0.20 | -1.33 | 22,29,32,33 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.