



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:12 PM GMT

PDB ID : 1EFL
Title : HUMAN MALIC ENZYME IN A QUATERNARY COMPLEX WITH NAD,
MG, AND TARTRONATE
Authors : Yang, Z.; Floyd, D.L.; Loeber, G.; Tong, L.
Deposited on : 2000-02-09
Resolution : 2.60 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

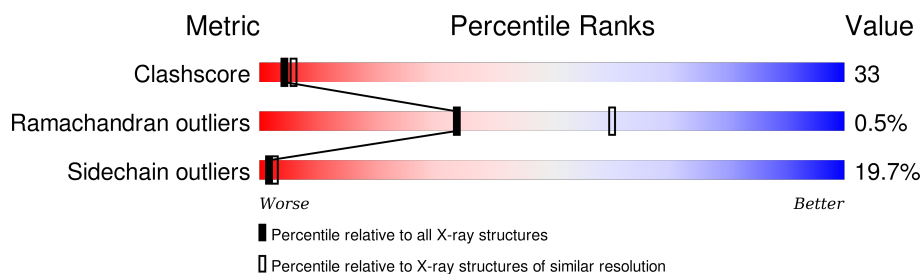
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

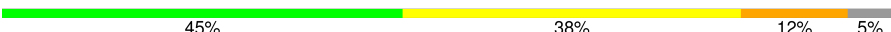

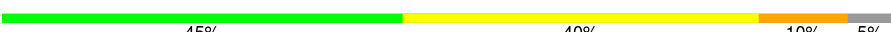
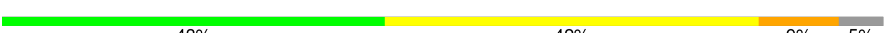
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore | 102246 | 2679 (2.60-2.60) |
| Ramachandran outliers | 100387 | 2635 (2.60-2.60) |
| Sidechain outliers | 100360 | 2635 (2.60-2.60) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 584 |  |
| 1 | B | 584 |  |
| 1 | C | 584 |  |
| 1 | D | 584 |  |

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17947 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 MALIC ENZYME.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|----|---------|---------|-------|
| 1 | A | 553 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 4367 | 2796 | 744 | 804 | 9 | 14 | | | |
| 1 | B | 553 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 4367 | 2796 | 744 | 804 | 9 | 14 | | | |
| 1 | C | 553 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 4367 | 2796 | 744 | 804 | 9 | 14 | | | |
| 1 | D | 553 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 4367 | 2796 | 744 | 804 | 9 | 14 | | | |

There are 56 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------------|------------|
| A | 29 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| A | 38 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| A | 47 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| A | 75 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| A | 86 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| A | 108 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| A | 177 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| A | 219 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| A | 239 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| A | 325 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| A | 327 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| A | 343 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| A | 407 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| A | 539 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| B | 29 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| B | 38 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| B | 47 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| B | 75 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| B | 86 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| B | 108 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| B | 177 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------------|------------|
| B | 219 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| B | 239 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| B | 325 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| B | 327 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| B | 343 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| B | 407 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| B | 539 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| C | 29 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| C | 38 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| C | 47 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| C | 75 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| C | 86 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| C | 108 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| C | 177 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| C | 219 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| C | 239 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| C | 325 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| C | 327 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| C | 343 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| C | 407 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| C | 539 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| D | 29 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| D | 38 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| D | 47 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| D | 75 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| D | 86 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| D | 108 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| D | 177 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| D | 219 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| D | 239 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| D | 325 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| D | 327 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| D | 343 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| D | 407 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |
| D | 539 | MSE | MET | MODIFIED RESIDUE | UNP P23368 |

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

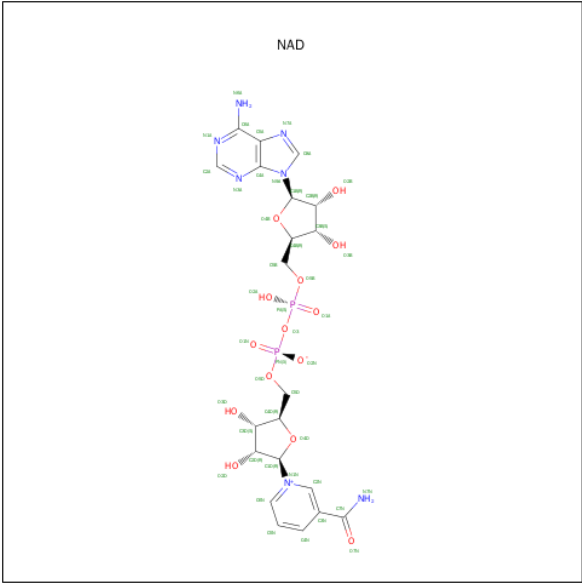
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 2 | B | 1 | Total Mg 1 1 | 0 | 0 |
| 2 | A | 1 | Total Mg 1 1 | 0 | 0 |

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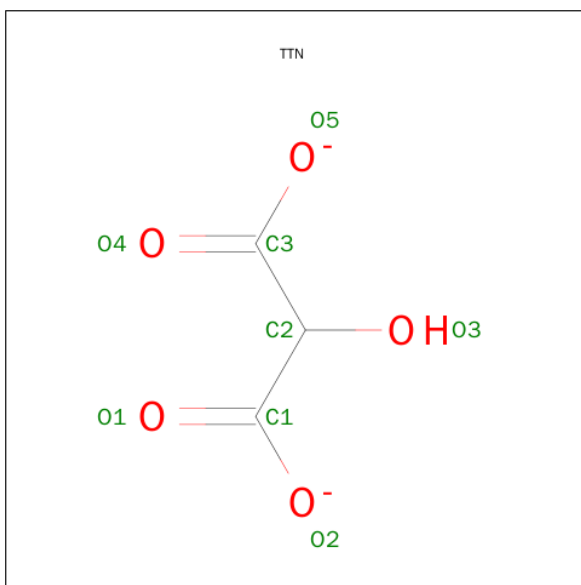
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2 | D | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 2 | C | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 3 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 44 | 21 | 7 | 14 | 2 | | |
| 3 | A | 1 | Total | C | N | O | P | 9 | 0 |
| | | | 44 | 21 | 7 | 14 | 2 | | |
| 3 | B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 44 | 21 | 7 | 14 | 2 | | |
| 3 | B | 1 | Total | C | N | O | P | 9 | 0 |
| | | | 44 | 21 | 7 | 14 | 2 | | |
| 3 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 44 | 21 | 7 | 14 | 2 | | |
| 3 | C | 1 | Total | C | N | O | P | 9 | 0 |
| | | | 44 | 21 | 7 | 14 | 2 | | |
| 3 | D | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 44 | 21 | 7 | 14 | 2 | | |
| 3 | D | 1 | Total | C | N | O | P | 9 | 0 |
| | | | 44 | 21 | 7 | 14 | 2 | | |

- Molecule 4 is TARTRONATE (three-letter code: TTN) (formula: C₃H₂O₅).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4 | A | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 3 | 5 | | |
| 4 | B | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 3 | 5 | | |
| 4 | C | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 3 | 5 | | |
| 4 | D | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 3 | 5 | | |

- Molecule 5 is water.

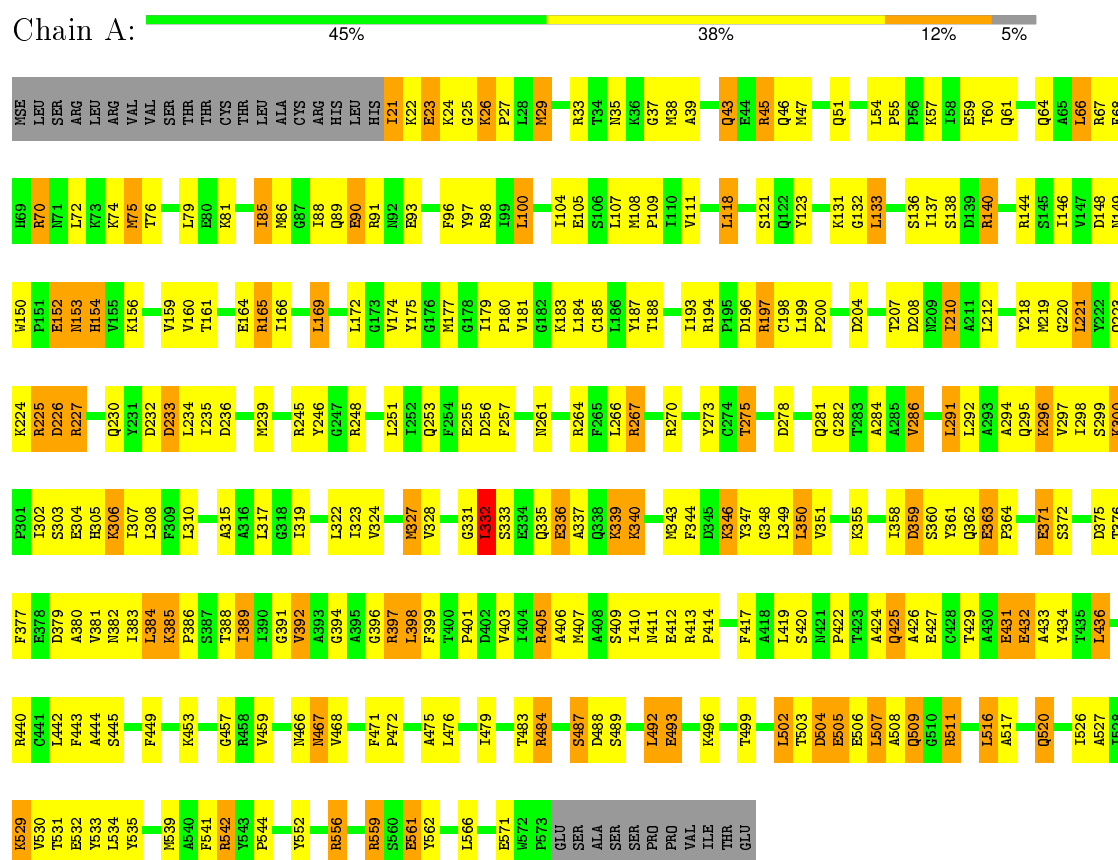
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5 | A | 24 | Total | O | 0 | 0 |
| | | | 24 | 24 | | |
| 5 | B | 17 | Total | O | 0 | 0 |
| | | | 17 | 17 | | |
| 5 | C | 23 | Total | O | 0 | 0 |
| | | | 23 | 23 | | |
| 5 | D | 27 | Total | O | 0 | 0 |
| | | | 27 | 27 | | |

3 Residue-property plots

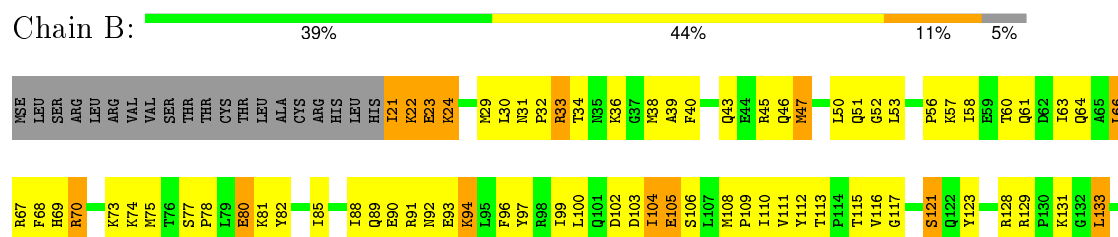
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

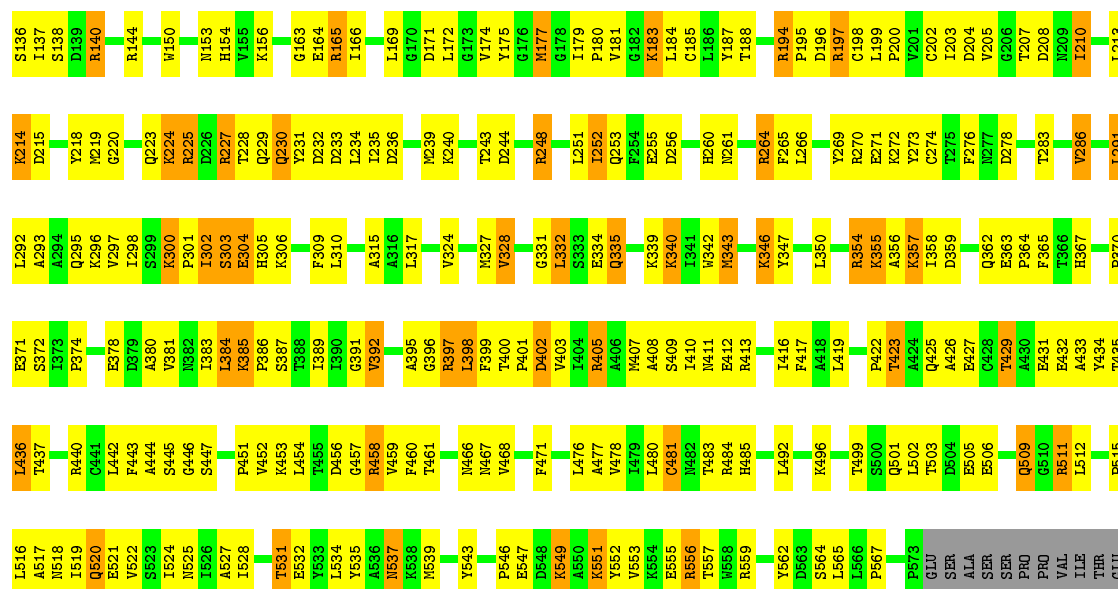
Note EDS was not executed.

• Molecule 1: MALIC ENZYME



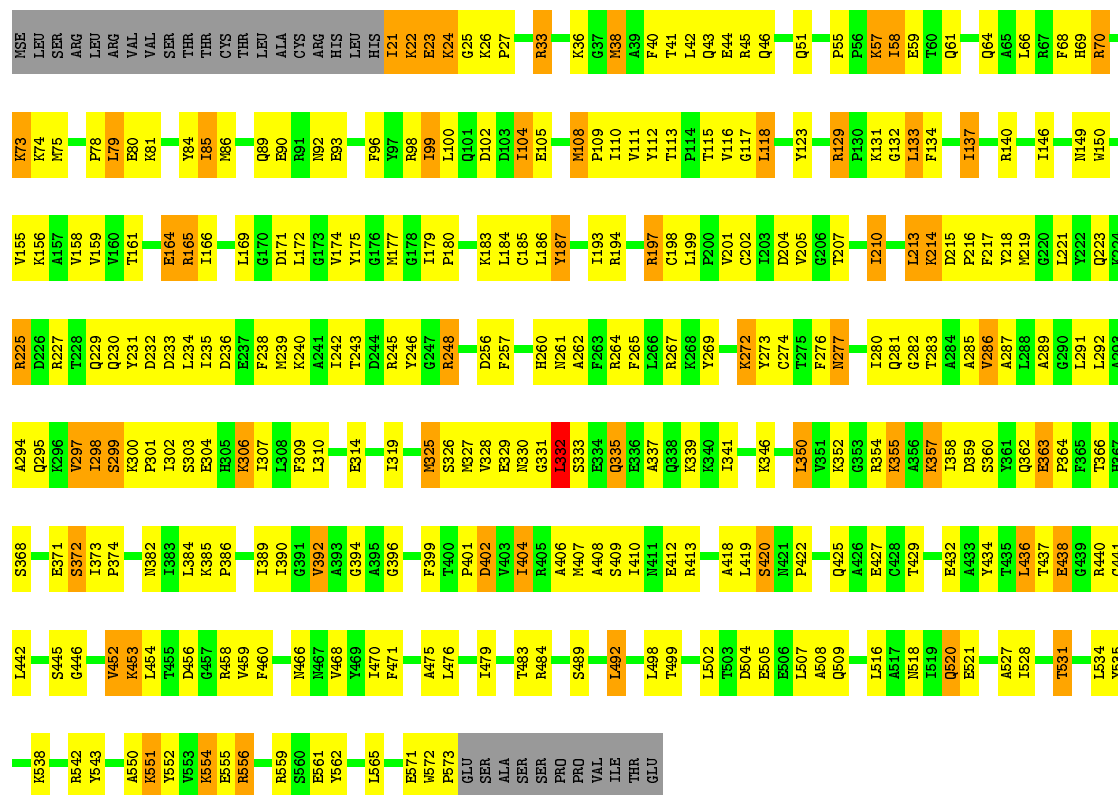
• Molecule 1: MALIC ENZYME





• Molecule 1: MALIC ENZYME

Chain C: 45% 40% 10% 5%



• Molecule 1: MALIC ENZYME

Chain D: 43% 42% 9% 5%



| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| T531 | E532 | L533 | L534 | Y535 | A536 | N537 | A540 | F541 | B542 | Y543 | P544 | E545 | D548 | K549 | A550 | K551 | K554 | E555 | B556 | B559 | S560 | E561 | Y562 | D563 | S564 | L565 | L566 | N572 | P573 | GLU | SER | ALA | SER | SER | PRO | VAL | ILE | THR | GLU | | | | | | | | | | | | | | | |
| Q457 | R458 | V459 | F460 | N466 | N467 | V468 | V469 | I470 | F471 | P472 | A475 | L476 | A477 | V478 | I479 | L480 | C481 | N482 | T483 | R484 | H485 | I486 | S489 | L492 | K496 | L497 | L498 | T499 | S500 | Q501 | L502 | T503 | D504 | E505 | E506 | L507 | A508 | Q509 | G510 | R511 | P515 | L516 | A517 | N518 | I519 | Q520 | E521 | I526 | A527 | K528 | V530 | | | |
| F377 | E378 | D379 | A380 | V381 | N382 | T383 | L384 | K385 | P386 | S387 | T388 | L389 | G390 | G391 | V392 | G393 | G394 | R397 | L398 | F399 | T400 | D402 | V403 | L404 | R405 | A406 | N407 | A408 | S409 | I410 | P411 | R413 | P414 | V415 | L416 | F417 | S420 | T423 | E427 | E432 | L436 | T437 | R440 | C441 | L442 | F443 | S447 | D456 | | | | | | |
| A294 | Q295 | R296 | V297 | I298 | S299 | K300 | F301 | L302 | S303 | E304 | K305 | K306 | I307 | F309 | L310 | E314 | A315 | A316 | T319 | V324 | M327 | V328 | L351 | G331 | L332 | S333 | E334 | Q335 | E336 | A337 | M342 | M343 | K346 | Y347 | L350 | K355 | A356 | K357 | L358 | D359 | S360 | Y361 | Q362 | T366 | E371 | S372 | I373 | | | | | | | |
| L221 | T222 | Q223 | K224 | R225 | D226 | R227 | T228 | Q229 | Q230 | D233 | L234 | T235 | D236 | E237 | F238 | N239 | K240 | L241 | T242 | T243 | D244 | R245 | Y246 | N249 | T250 | L251 | T252 | Q253 | D256 | N261 | A262 | F263 | R264 | F265 | L266 | R267 | K268 | Y269 | R270 | E271 | K272 | Y273 | C274 | T275 | F276 | A285 | Y286 | A287 | L288 | A289 | G290 | L291 | L292 | A293 |
| R144 | S145 | I146 | V147 | D148 | N149 | W150 | F151 | E152 | N153 | K156 | R165 | I166 | L169 | V174 | Y175 | G176 | M177 | G178 | I179 | P180 | K183 | L184 | F186 | A189 | Y197 | C190 | A191 | G192 | I193 | R194 | P195 | D196 | R197 | C198 | P199 | P200 | V201 | C202 | I203 | D204 | T207 | D208 | N209 | I210 | A211 | L212 | K214 | D215 | P216 | F217 | Y218 | M219 | G220 | |
| L65 | L66 | R67 | F68 | B69 | R70 | N71 | L72 | K73 | K74 | M75 | T76 | S77 | F78 | L79 | E80 | K81 | Y82 | L83 | T84 | L85 | R86 | R91 | N92 | E93 | R94 | L95 | F96 | Y97 | R98 | I99 | L100 | Q101 | I104 | L107 | M108 | P109 | I110 | V111 | Y112 | T115 | H125 | R128 | K131 | G132 | L133 | S136 | I137 | S138 | D139 | R140 | | | | |

4 Data and refinement statistics

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

| Property | Value | Source |
|--|---|-----------|
| Space group | C 1 2 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 228.80 Å 117.00 Å 114.30 Å 90.00° 109.20° 90.00° | Depositor |
| Resolution (Å) | 20.00 – 2.60 | Depositor |
| % Data completeness (in resolution range) | (Not available) (20.00-2.60) | Depositor |
| R_{merge} | 0.07 | Depositor |
| R_{sym} | (Not available) | Depositor |
| Refinement program | X-PLOR 3.851 | Depositor |
| R, R_{free} | 0.206 , 0.285 | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 17947 | wwPDB-VP |
| Average B, all atoms (Å ²) | 21.0 | wwPDB-VP |

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, TTN, NAD

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------|-------------|----------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | A | 0.46 | 0/4447 | 0.65 | 0/5998 |
| 1 | B | 0.46 | 0/4447 | 0.66 | 0/5998 |
| 1 | C | 0.45 | 0/4447 | 0.65 | 1/5998 (0.0%) |
| 1 | D | 0.46 | 0/4447 | 0.65 | 0/5998 |
| All | All | 0.46 | 0/17788 | 0.65 | 1/23992 (0.0%) |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | C | 310 | LEU | N-CA-C | -5.09 | 97.27 | 111.00 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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 | 4367 | 0 | 4407 | 333 | 0 |
| 1 | B | 4367 | 0 | 4407 | 331 | 0 |
| 1 | C | 4367 | 0 | 4407 | 252 | 0 |
| 1 | D | 4367 | 0 | 4407 | 314 | 0 |
| 2 | A | 1 | 0 | 0 | 0 | 0 |
| 2 | B | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | C | 1 | 0 | 0 | 0 | 0 |
| 2 | D | 1 | 0 | 0 | 0 | 0 |
| 3 | A | 88 | 0 | 52 | 6 | 0 |
| 3 | B | 88 | 0 | 52 | 2 | 0 |
| 3 | C | 88 | 0 | 52 | 5 | 0 |
| 3 | D | 88 | 0 | 52 | 4 | 0 |
| 4 | A | 8 | 0 | 1 | 0 | 0 |
| 4 | B | 8 | 0 | 1 | 1 | 0 |
| 4 | C | 8 | 0 | 1 | 2 | 0 |
| 4 | D | 8 | 0 | 2 | 1 | 0 |
| 5 | A | 24 | 0 | 0 | 5 | 0 |
| 5 | B | 17 | 0 | 0 | 9 | 0 |
| 5 | C | 23 | 0 | 0 | 5 | 0 |
| 5 | D | 27 | 0 | 0 | 3 | 0 |
| All | All | 17947 | 0 | 17841 | 1185 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (1185) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:227:ARG:HH11 | 1:A:227:ARG:HG2 | 1.03 | 1.11 |
| 1:D:520:GLN:HE22 | 1:D:521:GLU:HG2 | 1.13 | 1.07 |
| 1:A:511:ARG:HB3 | 1:A:511:ARG:HH11 | 1.20 | 1.02 |
| 1:C:355:LYS:HA | 1:C:355:LYS:HE2 | 1.42 | 1.01 |
| 1:B:227:ARG:HH11 | 1:B:227:ARG:HG2 | 1.24 | 1.00 |
| 1:D:520:GLN:NE2 | 1:D:521:GLU:HG2 | 1.75 | 1.00 |
| 1:D:298:ILE:HG22 | 1:D:300:LYS:H | 1.27 | 0.99 |
| 1:A:327:MSE:HE3 | 1:A:337:ALA:HB1 | 1.45 | 0.97 |
| 1:A:108:MSE:HE3 | 1:A:516:LEU:HD11 | 1.46 | 0.97 |
| 1:C:327:MSE:HE3 | 1:C:337:ALA:HB1 | 1.45 | 0.96 |
| 3:B:1602:NAD:H51N | 5:C:4090:HOH:O | 1.64 | 0.96 |
| 1:A:324:VAL:HA | 1:A:327:MSE:HE2 | 1.48 | 0.95 |
| 1:D:520:GLN:NE2 | 1:D:521:GLU:H | 1.66 | 0.94 |
| 1:D:481:CYS:SG | 1:D:531:THR:HB | 2.08 | 0.94 |
| 1:B:527:ALA:O | 1:B:531:THR:HG22 | 1.66 | 0.94 |
| 1:D:211:ALA:HA | 1:D:214:LYS:HE2 | 1.51 | 0.93 |
| 1:B:300:LYS:HZ2 | 1:B:300:LYS:HB3 | 1.33 | 0.93 |
| 1:C:184:LEU:HD13 | 1:C:198:CYS:HB3 | 1.50 | 0.92 |
| 1:D:327:MSE:HE3 | 1:D:337:ALA:HB1 | 1.52 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:197:ARG:HH11 | 1:C:197:ARG:HG3 | 1.35 | 0.92 |
| 1:A:425:GLN:HE21 | 1:A:425:GLN:N | 1.67 | 0.91 |
| 1:C:325:MSE:HE2 | 1:C:492:LEU:HD12 | 1.53 | 0.91 |
| 1:C:194:ARG:HB2 | 1:C:197:ARG:HG2 | 1.51 | 0.91 |
| 1:D:47:MSE:HE3 | 1:D:566:LEU:HD22 | 1.53 | 0.91 |
| 1:A:468:VAL:HA | 1:A:471:PHE:CE2 | 2.06 | 0.91 |
| 1:D:286:VAL:HG21 | 1:D:467:ASN:HA | 1.53 | 0.90 |
| 1:A:405:ARG:HH11 | 1:A:405:ARG:HB2 | 1.34 | 0.90 |
| 1:B:184:LEU:HD22 | 1:B:198:CYS:HB3 | 1.53 | 0.90 |
| 1:A:397:ARG:HH11 | 1:A:397:ARG:HG3 | 1.36 | 0.89 |
| 1:A:371:GLU:H | 1:A:371:GLU:CD | 1.75 | 0.87 |
| 1:B:47:MSE:HE2 | 1:B:567:PRO:HG2 | 1.54 | 0.87 |
| 1:B:61:GLN:HA | 1:B:64:GLN:HE21 | 1.38 | 0.87 |
| 1:A:227:ARG:NH1 | 1:A:227:ARG:HG2 | 1.82 | 0.86 |
| 1:C:85:ILE:HD12 | 1:C:96:PHE:HE1 | 1.39 | 0.86 |
| 1:B:453:LYS:HG2 | 1:B:459:VAL:HG12 | 1.57 | 0.86 |
| 1:D:381:VAL:HG13 | 1:D:407:MSE:HE1 | 1.58 | 0.86 |
| 1:D:300:LYS:HB3 | 1:D:300:LYS:HZ2 | 1.39 | 0.85 |
| 1:A:220:GLY:HA2 | 1:B:56:PRO:HG2 | 1.58 | 0.85 |
| 1:A:520:GLN:HE21 | 1:A:520:GLN:H | 1.24 | 0.85 |
| 1:D:315:ALA:O | 1:D:319:ILE:HG13 | 1.77 | 0.85 |
| 1:B:453:LYS:HE3 | 1:B:457:GLY:HA2 | 1.58 | 0.84 |
| 1:B:378:GLU:O | 1:B:381:VAL:HG12 | 1.77 | 0.83 |
| 1:A:23:GLU:HA | 1:A:23:GLU:OE1 | 1.76 | 0.83 |
| 1:A:108:MSE:HB3 | 1:A:109:PRO:HD3 | 1.58 | 0.83 |
| 1:A:286:VAL:HG21 | 1:A:467:ASN:HA | 1.59 | 0.83 |
| 1:B:29:MSE:HE1 | 1:B:53:LEU:HB2 | 1.59 | 0.83 |
| 1:B:422:PRO:HD2 | 1:B:425:GLN:CG | 2.09 | 0.83 |
| 1:B:397:ARG:NH2 | 1:B:423:THR:O | 2.12 | 0.82 |
| 1:A:166:ILE:HD12 | 1:A:179:ILE:HG13 | 1.61 | 0.82 |
| 1:B:300:LYS:NZ | 1:B:300:LYS:HB3 | 1.93 | 0.82 |
| 1:A:47:MSE:HE3 | 1:A:566:LEU:HD22 | 1.62 | 0.82 |
| 1:B:532:GLU:HG2 | 1:B:549:LYS:HG2 | 1.62 | 0.82 |
| 1:D:23:GLU:HA | 1:D:23:GLU:OE2 | 1.80 | 0.82 |
| 1:D:286:VAL:HG22 | 1:D:470:ILE:HG13 | 1.61 | 0.81 |
| 1:D:107:LEU:O | 1:D:111:VAL:HG12 | 1.78 | 0.81 |
| 1:D:509:GLN:HB2 | 5:D:4058:HOH:O | 1.80 | 0.81 |
| 1:D:261:ASN:ND2 | 1:D:264:ARG:HH21 | 1.78 | 0.81 |
| 1:A:381:VAL:HG13 | 1:A:407:MSE:HE3 | 1.60 | 0.81 |
| 1:B:77:SER:O | 1:B:81:LYS:HG3 | 1.80 | 0.81 |
| 1:D:144:ARG:HD2 | 1:D:147:VAL:CG2 | 2.11 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:300:LYS:HE3 | 1:D:305:HIS:ND1 | 1.95 | 0.81 |
| 1:B:67:ARG:HD2 | 5:B:4079:HOH:O | 1.80 | 0.80 |
| 1:D:22:LYS:HD2 | 1:D:22:LYS:O | 1.81 | 0.80 |
| 1:A:487:SER:HB3 | 1:A:539:MSE:HE1 | 1.61 | 0.80 |
| 1:D:559:ARG:HG3 | 1:D:561:GLU:OE1 | 1.80 | 0.80 |
| 1:A:425:GLN:HE21 | 1:A:425:GLN:H | 1.27 | 0.80 |
| 1:D:184:LEU:HD22 | 1:D:198:CYS:HB3 | 1.64 | 0.80 |
| 1:B:306:LYS:HG2 | 1:B:386:PRO:HA | 1.64 | 0.80 |
| 1:A:407:MSE:HE2 | 1:A:407:MSE:HA | 1.63 | 0.79 |
| 1:A:425:GLN:NE2 | 1:A:425:GLN:N | 2.31 | 0.79 |
| 1:D:43:GLN:HG2 | 1:D:566:LEU:HD11 | 1.64 | 0.79 |
| 1:A:335:GLN:O | 1:A:339:LYS:HD2 | 1.83 | 0.79 |
| 1:D:328:VAL:HA | 1:D:332:LEU:O | 1.83 | 0.79 |
| 1:B:108:MSE:HE3 | 1:B:516:LEU:HD11 | 1.64 | 0.78 |
| 1:B:371:GLU:CD | 1:B:371:GLU:H | 1.87 | 0.78 |
| 1:B:422:PRO:HD2 | 1:B:425:GLN:HG3 | 1.65 | 0.78 |
| 1:A:511:ARG:NH1 | 1:A:511:ARG:HB3 | 1.98 | 0.78 |
| 1:D:177:MSE:HE1 | 1:D:180:PRO:HB2 | 1.66 | 0.78 |
| 1:D:194:ARG:HE | 1:D:197:ARG:NE | 1.82 | 0.78 |
| 1:B:343:MSE:HE3 | 1:B:350:LEU:HD12 | 1.66 | 0.77 |
| 1:A:21:ILE:HD13 | 1:A:21:ILE:N | 1.99 | 0.77 |
| 1:B:29:MSE:HE2 | 1:B:50:LEU:HD22 | 1.64 | 0.77 |
| 1:B:483:THR:HG21 | 1:B:534:LEU:HD13 | 1.67 | 0.77 |
| 1:D:324:VAL:HA | 1:D:327:MSE:HE2 | 1.67 | 0.77 |
| 1:D:310:LEU:HB3 | 1:D:391:GLY:HA2 | 1.65 | 0.77 |
| 1:B:431:GLU:O | 1:B:435:THR:HG23 | 1.85 | 0.77 |
| 1:A:24:LYS:HE2 | 1:C:22:LYS:HD2 | 1.67 | 0.77 |
| 1:C:179:ILE:HB | 1:C:180:PRO:HD3 | 1.66 | 0.76 |
| 1:D:466:ASN:HB3 | 1:D:468:VAL:HG12 | 1.68 | 0.76 |
| 1:B:29:MSE:HE2 | 1:B:50:LEU:HB3 | 1.65 | 0.76 |
| 1:A:511:ARG:HH11 | 1:A:511:ARG:CB | 1.99 | 0.76 |
| 1:C:85:ILE:HG13 | 1:C:86:MSE:N | 1.98 | 0.76 |
| 1:B:335:GLN:O | 1:B:339:LYS:HG3 | 1.85 | 0.76 |
| 1:A:175:TYR:CD2 | 1:A:219:MSE:HE2 | 2.19 | 0.76 |
| 1:A:38:MSE:HE3 | 1:A:59:GLU:CD | 2.07 | 0.76 |
| 1:B:395:ALA:HB3 | 1:B:398:LEU:HD21 | 1.68 | 0.76 |
| 1:D:359:ASP:OD2 | 1:D:362:GLN:HG3 | 1.85 | 0.76 |
| 1:B:401:PRO:O | 1:B:405:ARG:HG3 | 1.86 | 0.75 |
| 1:D:298:ILE:CG2 | 1:D:300:LYS:HB2 | 2.16 | 0.75 |
| 1:B:227:ARG:CG | 1:B:227:ARG:HH11 | 1.98 | 0.75 |
| 1:A:154:HIS:O | 1:A:197:ARG:HG3 | 1.87 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:47:MSE:HE3 | 1:D:47:MSE:SE | 2.38 | 0.74 |
| 1:D:383:ILE:HG22 | 1:D:384:LEU:HD13 | 1.69 | 0.74 |
| 1:B:177:MSE:O | 1:B:180:PRO:HD2 | 1.87 | 0.74 |
| 1:D:207:THR:O | 1:D:224:LYS:HA | 1.87 | 0.74 |
| 1:A:405:ARG:NH1 | 1:A:405:ARG:HB2 | 2.02 | 0.73 |
| 1:D:33:ARG:HD3 | 1:D:196:ASP:HB3 | 1.71 | 0.73 |
| 1:A:47:MSE:CE | 1:A:566:LEU:HD22 | 2.19 | 0.73 |
| 1:C:551:LYS:O | 1:C:555:GLU:HB2 | 1.88 | 0.73 |
| 1:D:400:THR:OG1 | 1:D:403:VAL:HG23 | 1.89 | 0.72 |
| 1:A:227:ARG:CG | 1:A:227:ARG:HH11 | 1.90 | 0.72 |
| 1:B:105:GLU:HB2 | 5:B:4016:HOH:O | 1.89 | 0.72 |
| 1:D:548:ASP:OD1 | 1:D:551:LYS:HB2 | 1.90 | 0.72 |
| 1:B:137:ILE:O | 1:B:140:ARG:HG2 | 1.89 | 0.72 |
| 1:B:332:LEU:HD21 | 1:B:340:LYS:HE3 | 1.71 | 0.72 |
| 1:D:392:VAL:O | 1:D:392:VAL:HG13 | 1.89 | 0.72 |
| 1:B:385:LYS:HA | 1:B:410:ILE:HD13 | 1.70 | 0.72 |
| 1:A:123:TYR:HD2 | 1:A:219:MSE:HE1 | 1.53 | 0.71 |
| 1:C:432:GLU:O | 1:C:436:LEU:HB2 | 1.90 | 0.71 |
| 1:D:468:VAL:HA | 1:D:471:PHE:CE2 | 2.26 | 0.71 |
| 1:D:240:LYS:HE3 | 1:D:273:TYR:OH | 1.90 | 0.71 |
| 1:B:22:LYS:NZ | 1:D:27:PRO:HG2 | 2.05 | 0.71 |
| 1:B:408:ALA:HB1 | 1:B:440:ARG:NH2 | 2.06 | 0.71 |
| 1:B:22:LYS:HZ3 | 1:D:27:PRO:HG2 | 1.54 | 0.71 |
| 1:B:324:VAL:O | 1:B:328:VAL:HG13 | 1.91 | 0.71 |
| 1:C:306:LYS:HG2 | 1:C:386:PRO:HA | 1.72 | 0.71 |
| 1:D:381:VAL:CG1 | 1:D:407:MSE:HE1 | 2.20 | 0.70 |
| 1:C:289:ALA:CB | 1:C:498:LEU:HD23 | 2.21 | 0.70 |
| 1:C:355:LYS:CA | 1:C:355:LYS:HE2 | 2.19 | 0.70 |
| 1:D:194:ARG:HB2 | 1:D:197:ARG:HG3 | 1.72 | 0.70 |
| 1:A:392:VAL:HG13 | 1:A:392:VAL:O | 1.89 | 0.70 |
| 1:A:81:LYS:O | 1:A:85:ILE:HG23 | 1.91 | 0.70 |
| 1:D:177:MSE:CE | 1:D:180:PRO:HB2 | 2.22 | 0.70 |
| 1:D:520:GLN:HE22 | 1:D:521:GLU:CG | 1.99 | 0.70 |
| 1:B:166:ILE:HG21 | 1:B:172:LEU:HD12 | 1.73 | 0.70 |
| 1:A:177:MSE:HE1 | 1:A:180:PRO:HB2 | 1.72 | 0.70 |
| 1:B:354:ARG:HE | 1:B:358:ILE:HD11 | 1.55 | 0.70 |
| 1:B:90:GLU:OE1 | 1:B:131:LYS:HG3 | 1.92 | 0.70 |
| 1:D:253:GLN:HB2 | 1:D:276:PHE:CE2 | 2.26 | 0.70 |
| 1:D:194:ARG:HG2 | 1:D:194:ARG:HH11 | 1.55 | 0.70 |
| 1:B:335:GLN:HG3 | 1:B:339:LYS:HE3 | 1.74 | 0.70 |
| 1:B:302:ILE:HA | 1:B:305:HIS:ND1 | 2.07 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:261:ASN:ND2 | 1:B:264:ARG:CZ | 2.55 | 0.70 |
| 1:A:401:PRO:HB3 | 1:A:436:LEU:HD21 | 1.72 | 0.69 |
| 1:A:520:GLN:H | 1:A:520:GLN:NE2 | 1.88 | 0.69 |
| 1:B:433:ALA:O | 1:B:437:THR:HG23 | 1.92 | 0.69 |
| 1:C:197:ARG:HG3 | 1:C:197:ARG:NH1 | 1.98 | 0.69 |
| 1:B:24:LYS:O | 1:D:22:LYS:HE3 | 1.91 | 0.69 |
| 1:D:415:VAL:HG22 | 1:D:442:LEU:HD12 | 1.74 | 0.69 |
| 1:C:520:GLN:H | 1:C:520:GLN:HE21 | 1.40 | 0.69 |
| 1:C:434:TYR:CD1 | 1:C:452:VAL:HG11 | 2.28 | 0.69 |
| 1:C:81:LYS:O | 1:C:85:ILE:HG23 | 1.92 | 0.69 |
| 1:A:405:ARG:HH11 | 1:A:405:ARG:CB | 2.06 | 0.69 |
| 1:D:551:LYS:O | 1:D:555:GLU:HB2 | 1.93 | 0.68 |
| 1:B:537:ASN:HD22 | 1:B:537:ASN:N | 1.91 | 0.68 |
| 1:B:305:HIS:HB2 | 1:B:340:LYS:HZ1 | 1.58 | 0.68 |
| 1:A:91:ARG:NE | 5:A:4055:HOH:O | 2.26 | 0.68 |
| 1:B:347:TYR:HB2 | 1:B:354:ARG:HH12 | 1.58 | 0.68 |
| 1:D:211:ALA:HA | 1:D:214:LYS:CE | 2.22 | 0.68 |
| 1:D:43:GLN:OE1 | 1:D:47:MSE:HE2 | 1.93 | 0.68 |
| 1:C:133:LEU:HB2 | 1:C:199:LEU:HD11 | 1.75 | 0.68 |
| 1:C:357:LYS:HD2 | 1:C:357:LYS:H | 1.59 | 0.68 |
| 1:B:328:VAL:HA | 1:B:332:LEU:O | 1.93 | 0.68 |
| 1:B:60:THR:OG1 | 1:B:63:ILE:HG13 | 1.93 | 0.68 |
| 1:B:528:ILE:O | 1:B:532:GLU:HG3 | 1.94 | 0.68 |
| 1:B:205:VAL:HG11 | 1:B:231:TYR:HD1 | 1.59 | 0.67 |
| 1:A:79:LEU:HB2 | 1:A:118:LEU:HD21 | 1.76 | 0.67 |
| 1:D:64:GLN:NE2 | 1:D:562:TYR:OH | 2.25 | 0.67 |
| 1:D:306:LYS:CG | 1:D:386:PRO:HA | 2.23 | 0.67 |
| 1:A:398:LEU:HD23 | 1:A:398:LEU:N | 2.09 | 0.67 |
| 1:C:23:GLU:OE1 | 1:C:23:GLU:HA | 1.93 | 0.67 |
| 1:D:550:ALA:O | 1:D:554:LYS:HG2 | 1.95 | 0.67 |
| 1:A:45:ARG:HB3 | 1:A:51:GLN:HG2 | 1.76 | 0.67 |
| 1:D:31:ASN:ND2 | 1:D:34:THR:HG23 | 2.09 | 0.67 |
| 1:B:75:MSE:HG2 | 1:B:80:GLU:CD | 2.15 | 0.67 |
| 1:B:81:LYS:O | 1:B:85:ILE:HG13 | 1.94 | 0.67 |
| 1:B:291:LEU:HD13 | 1:B:417:PHE:CE2 | 2.29 | 0.67 |
| 1:A:108:MSE:CE | 1:A:516:LEU:HD11 | 2.24 | 0.67 |
| 1:B:91:ARG:HH11 | 1:B:91:ARG:HG2 | 1.60 | 0.67 |
| 1:A:137:ILE:HD12 | 1:A:234:LEU:HD22 | 1.77 | 0.67 |
| 1:C:85:ILE:HD11 | 1:C:111:VAL:HG23 | 1.76 | 0.67 |
| 1:B:253:GLN:HB2 | 1:B:276:PHE:CE2 | 2.30 | 0.67 |
| 1:A:177:MSE:HE2 | 1:A:181:VAL:HG23 | 1.78 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:140:ARG:HH22 | 1:A:233:ASP:HB3 | 1.57 | 0.66 |
| 1:A:453:LYS:CG | 1:A:459:VAL:HG22 | 2.24 | 0.66 |
| 1:A:401:PRO:HB2 | 1:A:405:ARG:HH22 | 1.59 | 0.66 |
| 1:B:422:PRO:HD2 | 1:B:425:GLN:HG2 | 1.77 | 0.66 |
| 1:C:75:MSE:HG2 | 1:C:80:GLU:CD | 2.15 | 0.66 |
| 1:A:397:ARG:HG3 | 1:A:397:ARG:NH1 | 2.09 | 0.66 |
| 1:C:298:ILE:HD13 | 1:C:413:ARG:HB2 | 1.76 | 0.66 |
| 1:A:453:LYS:HG3 | 1:A:459:VAL:HG22 | 1.77 | 0.66 |
| 1:B:503:THR:HB | 1:B:505:GLU:OE2 | 1.94 | 0.66 |
| 1:B:240:LYS:HE3 | 1:B:244:ASP:OD2 | 1.94 | 0.66 |
| 1:D:327:MSE:CE | 1:D:337:ALA:HB1 | 2.24 | 0.66 |
| 1:B:51:GLN:NE2 | 5:B:4050:HOH:O | 2.28 | 0.66 |
| 1:D:51:GLN:HA | 1:D:51:GLN:HE21 | 1.61 | 0.66 |
| 1:C:79:LEU:HD22 | 1:C:118:LEU:HG | 1.78 | 0.66 |
| 1:B:60:THR:H | 1:B:63:ILE:HD12 | 1.60 | 0.66 |
| 1:A:335:GLN:CD | 1:A:339:LYS:HZ3 | 1.99 | 0.66 |
| 1:D:137:ILE:O | 1:D:140:ARG:HG2 | 1.95 | 0.66 |
| 1:C:357:LYS:HD2 | 1:C:357:LYS:N | 2.11 | 0.66 |
| 1:A:324:VAL:HA | 1:A:327:MSE:CE | 2.22 | 0.66 |
| 1:B:395:ALA:HB3 | 1:B:398:LEU:CD2 | 2.26 | 0.66 |
| 1:A:156:LYS:HE3 | 1:A:479:ILE:HG23 | 1.77 | 0.66 |
| 1:A:140:ARG:NH2 | 1:A:230:GLN:O | 2.29 | 0.65 |
| 1:D:505:GLU:O | 1:D:508:ALA:HB3 | 1.96 | 0.65 |
| 1:D:437:THR:O | 1:D:440:ARG:HG3 | 1.95 | 0.65 |
| 1:D:85:ILE:HD11 | 1:D:100:LEU:HD11 | 1.78 | 0.65 |
| 1:B:22:LYS:O | 1:D:24:LYS:HE3 | 1.97 | 0.65 |
| 1:D:166:ILE:HD12 | 1:D:179:ILE:HG13 | 1.77 | 0.65 |
| 1:D:327:MSE:HE3 | 1:D:337:ALA:CB | 2.25 | 0.65 |
| 1:A:371:GLU:CD | 1:A:371:GLU:N | 2.47 | 0.65 |
| 1:A:392:VAL:CG1 | 1:A:392:VAL:O | 2.44 | 0.65 |
| 1:C:314:GLU:HB2 | 3:C:2601:NAD:O1N | 1.96 | 0.65 |
| 1:B:492:LEU:CD2 | 1:B:496:LYS:HE3 | 2.27 | 0.65 |
| 1:D:346:LYS:HE2 | 1:D:347:TYR:CZ | 2.31 | 0.65 |
| 1:D:350:LEU:HD23 | 1:D:350:LEU:N | 2.11 | 0.65 |
| 1:B:518:ASN:O | 1:B:522:VAL:HG23 | 1.96 | 0.65 |
| 1:D:502:LEU:HD13 | 1:D:507:LEU:CD1 | 2.27 | 0.65 |
| 1:D:407:MSE:CA | 1:D:407:MSE:HE2 | 2.27 | 0.65 |
| 1:D:509:GLN:HG3 | 1:D:511:ARG:HG3 | 1.77 | 0.65 |
| 1:B:81:LYS:HD2 | 5:B:4051:HOH:O | 1.97 | 0.65 |
| 1:B:309:PHE:HB2 | 1:B:343:MSE:HG3 | 1.79 | 0.65 |
| 1:D:520:GLN:NE2 | 1:D:521:GLU:N | 2.43 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:467:ASN:H | 1:A:467:ASN:ND2 | 1.94 | 0.64 |
| 1:B:374:PRO:HG3 | 1:B:383:ILE:HD12 | 1.78 | 0.64 |
| 1:A:310:LEU:HD21 | 1:A:398:LEU:HB2 | 1.79 | 0.64 |
| 1:B:423:THR:HG23 | 1:B:447:SER:HB3 | 1.79 | 0.64 |
| 1:A:358:ILE:HG23 | 1:A:362:GLN:HB2 | 1.79 | 0.64 |
| 1:B:61:GLN:HG3 | 1:B:562:TYR:CE1 | 2.32 | 0.64 |
| 1:A:328:VAL:HA | 1:A:332:LEU:O | 1.96 | 0.64 |
| 1:D:385:LYS:HA | 1:D:410:ILE:HD13 | 1.80 | 0.64 |
| 1:D:300:LYS:CB | 1:D:300:LYS:HZ2 | 2.11 | 0.64 |
| 1:D:286:VAL:HG11 | 1:D:466:ASN:O | 1.98 | 0.64 |
| 1:D:68:PHE:CE2 | 1:D:99:ILE:HG21 | 2.33 | 0.64 |
| 1:A:487:SER:HB3 | 1:A:539:MSE:CE | 2.26 | 0.64 |
| 1:A:177:MSE:HE3 | 1:A:180:PRO:HD2 | 1.80 | 0.64 |
| 1:B:305:HIS:HB2 | 1:B:340:LYS:NZ | 2.12 | 0.64 |
| 1:B:492:LEU:HD21 | 1:B:496:LYS:HE3 | 1.80 | 0.63 |
| 1:D:210:ILE:HG12 | 1:D:211:ALA:N | 2.14 | 0.63 |
| 1:C:159:VAL:HG23 | 1:C:184:LEU:HD21 | 1.79 | 0.63 |
| 1:A:204:ASP:OD2 | 1:B:56:PRO:HG3 | 1.98 | 0.63 |
| 1:B:273:TYR:O | 1:B:485:HIS:HD2 | 1.81 | 0.63 |
| 1:A:111:VAL:O | 5:A:4046:HOH:O | 2.15 | 0.63 |
| 1:B:110:ILE:O | 1:B:115:THR:HB | 1.98 | 0.63 |
| 1:B:116:VAL:HG13 | 1:B:117:GLY:N | 2.14 | 0.63 |
| 1:A:504:ASP:OD2 | 1:A:504:ASP:N | 2.31 | 0.63 |
| 1:C:70:ARG:HH11 | 1:C:70:ARG:HG2 | 1.64 | 0.63 |
| 1:B:501:GLN:HE22 | 1:B:525:ASN:HB3 | 1.63 | 0.63 |
| 1:B:261:ASN:ND2 | 1:B:264:ARG:NH1 | 2.47 | 0.63 |
| 1:A:88:ILE:HD13 | 1:A:91:ARG:HH21 | 1.64 | 0.63 |
| 1:A:298:ILE:HG22 | 1:A:300:LYS:HB2 | 1.81 | 0.63 |
| 1:A:61:GLN:HA | 1:A:64:GLN:HE21 | 1.64 | 0.63 |
| 1:D:153:ASN:ND2 | 1:D:153:ASN:H | 1.97 | 0.63 |
| 1:C:90:GLU:OE1 | 1:C:131:LYS:HG3 | 1.98 | 0.63 |
| 1:C:550:ALA:O | 1:C:554:LYS:HG2 | 1.98 | 0.63 |
| 1:B:197:ARG:NH1 | 1:B:197:ARG:HG3 | 2.12 | 0.63 |
| 1:B:468:VAL:HA | 1:B:471:PHE:CE2 | 2.34 | 0.63 |
| 1:B:346:LYS:HB2 | 1:B:346:LYS:NZ | 2.14 | 0.63 |
| 1:B:517:ALA:O | 1:B:520:GLN:OE1 | 2.16 | 0.63 |
| 1:A:310:LEU:HB3 | 1:A:391:GLY:HA2 | 1.81 | 0.62 |
| 1:C:172:LEU:O | 1:C:175:TYR:HB2 | 1.98 | 0.62 |
| 1:B:197:ARG:HG3 | 1:B:197:ARG:HH11 | 1.64 | 0.62 |
| 1:D:300:LYS:HB3 | 1:D:300:LYS:NZ | 2.04 | 0.62 |
| 1:D:481:CYS:HB3 | 1:D:540:ALA:HB1 | 1.79 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:306:LYS:HG2 | 1:D:386:PRO:HA | 1.82 | 0.62 |
| 1:C:110:ILE:O | 1:C:115:THR:HB | 2.00 | 0.62 |
| 1:D:95:LEU:O | 1:D:99:ILE:HG12 | 1.99 | 0.62 |
| 1:A:233:ASP:OD2 | 1:A:233:ASP:C | 2.38 | 0.62 |
| 1:A:483:THR:OG1 | 1:A:534:LEU:HD13 | 1.99 | 0.62 |
| 1:A:177:MSE:CE | 1:A:180:PRO:HB2 | 2.29 | 0.62 |
| 1:B:23:GLU:HA | 1:B:23:GLU:OE1 | 1.99 | 0.62 |
| 1:C:302:ILE:CD1 | 1:C:332:LEU:HD22 | 2.30 | 0.62 |
| 1:B:515:PRO:HB2 | 1:B:518:ASN:HD22 | 1.65 | 0.62 |
| 1:D:270:ARG:HG3 | 1:D:271:GLU:OE2 | 2.00 | 0.62 |
| 1:D:286:VAL:HG21 | 1:D:467:ASN:CA | 2.29 | 0.62 |
| 1:A:29:MSE:HA | 1:A:35:ASN:OD1 | 2.00 | 0.62 |
| 1:D:108:MSE:HB3 | 1:D:109:PRO:HD3 | 1.80 | 0.61 |
| 1:B:295:GLN:HA | 1:B:295:GLN:OE1 | 1.99 | 0.61 |
| 1:D:33:ARG:NH1 | 1:D:93:GLU:OE1 | 2.33 | 0.61 |
| 1:C:112:TYR:CD2 | 1:C:113:THR:HG22 | 2.35 | 0.61 |
| 1:A:307:ILE:HG13 | 1:A:388:THR:HB | 1.81 | 0.61 |
| 1:D:286:VAL:CG2 | 1:D:467:ASN:HA | 2.27 | 0.61 |
| 1:A:132:GLY:HA2 | 1:A:200:PRO:HG2 | 1.81 | 0.61 |
| 1:A:123:TYR:CD2 | 1:A:219:MSE:HE1 | 2.35 | 0.61 |
| 1:C:406:ALA:O | 1:C:410:ILE:HG13 | 2.01 | 0.61 |
| 1:D:391:GLY:HA3 | 1:D:427:GLU:HG2 | 1.82 | 0.61 |
| 1:C:221:LEU:HB3 | 1:C:223:GLN:HG2 | 1.82 | 0.61 |
| 1:D:298:ILE:HD11 | 1:D:442:LEU:CD1 | 2.30 | 0.61 |
| 1:A:475:ALA:O | 1:A:479:ILE:HD12 | 2.00 | 0.61 |
| 1:D:70:ARG:HG2 | 1:D:70:ARG:NH1 | 2.14 | 0.61 |
| 1:B:47:MSE:HE2 | 1:B:567:PRO:CG | 2.29 | 0.61 |
| 1:A:55:PRO:HG3 | 1:B:219:MSE:HE3 | 1.83 | 0.61 |
| 1:C:21:ILE:HD12 | 1:C:22:LYS:N | 2.16 | 0.61 |
| 1:A:29:MSE:HE1 | 1:A:54:LEU:HD21 | 1.83 | 0.61 |
| 1:D:298:ILE:HG22 | 1:D:300:LYS:HB2 | 1.81 | 0.61 |
| 1:A:210:ILE:H | 1:A:210:ILE:HD13 | 1.66 | 0.61 |
| 1:C:61:GLN:HA | 1:C:64:GLN:HE21 | 1.66 | 0.61 |
| 1:C:434:TYR:HD1 | 1:C:452:VAL:HG11 | 1.64 | 0.60 |
| 1:C:454:LEU:HD11 | 1:C:460:PHE:HE2 | 1.64 | 0.60 |
| 1:D:179:ILE:HB | 1:D:180:PRO:HD3 | 1.82 | 0.60 |
| 1:D:70:ARG:CG | 1:D:70:ARG:HH11 | 2.15 | 0.60 |
| 1:B:177:MSE:O | 1:B:181:VAL:HG23 | 2.00 | 0.60 |
| 1:D:243:THR:HG21 | 1:D:273:TYR:CD2 | 2.36 | 0.60 |
| 1:D:407:MSE:HA | 1:D:407:MSE:HE2 | 1.82 | 0.60 |
| 1:A:443:PHE:CZ | 1:A:445:SER:HB3 | 2.37 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:203:ILE:HD13 | 1:D:235:ILE:CD1 | 2.31 | 0.60 |
| 1:D:306:LYS:HE2 | 1:D:342:TRP:NE1 | 2.17 | 0.60 |
| 1:C:70:ARG:HH11 | 1:C:70:ARG:CG | 2.14 | 0.60 |
| 1:B:532:GLU:HG2 | 1:B:549:LYS:CG | 2.31 | 0.60 |
| 1:A:535:TYR:OH | 1:A:542:ARG:HB3 | 2.01 | 0.60 |
| 1:C:326:SER:O | 1:C:329:GLU:HG2 | 2.02 | 0.60 |
| 1:C:483:THR:OG1 | 1:C:534:LEU:HD13 | 2.01 | 0.60 |
| 1:C:165:ARG:NH2 | 1:C:256:ASP:OD1 | 2.34 | 0.59 |
| 1:B:506:GLU:O | 1:B:511:ARG:HB2 | 2.02 | 0.59 |
| 1:B:297:VAL:HG22 | 1:B:298:ILE:N | 2.16 | 0.59 |
| 1:C:68:PHE:CD2 | 1:C:99:ILE:HG13 | 2.37 | 0.59 |
| 1:A:225:ARG:CG | 1:A:225:ARG:HH11 | 2.16 | 0.59 |
| 1:B:24:LYS:NZ | 1:D:22:LYS:HD3 | 2.17 | 0.59 |
| 1:D:243:THR:HG21 | 1:D:273:TYR:CE2 | 2.37 | 0.59 |
| 1:A:233:ASP:OD2 | 1:A:234:LEU:N | 2.35 | 0.59 |
| 1:C:248:ARG:HH22 | 1:C:272:LYS:HZ2 | 1.49 | 0.59 |
| 1:A:179:ILE:HB | 1:A:180:PRO:HD3 | 1.83 | 0.59 |
| 1:D:397:ARG:NH2 | 1:D:423:THR:O | 2.35 | 0.59 |
| 1:C:21:ILE:HD12 | 1:C:22:LYS:H | 1.67 | 0.59 |
| 1:B:397:ARG:NH2 | 1:B:426:ALA:HB3 | 2.17 | 0.59 |
| 1:A:333:SER:OG | 1:A:336:GLU:HG3 | 2.02 | 0.59 |
| 1:A:286:VAL:CG2 | 1:A:467:ASN:HA | 2.32 | 0.59 |
| 1:B:543:TYR:CZ | 1:C:484:ARG:HG2 | 2.38 | 0.59 |
| 1:A:57:LYS:HD3 | 1:B:218:TYR:O | 2.02 | 0.59 |
| 1:B:205:VAL:HG11 | 1:B:231:TYR:CD1 | 2.38 | 0.59 |
| 1:C:307:ILE:N | 1:C:307:ILE:HD12 | 2.18 | 0.59 |
| 1:A:221:LEU:HB3 | 1:A:223:GLN:HG2 | 1.84 | 0.59 |
| 1:A:132:GLY:CA | 1:A:200:PRO:HG2 | 2.33 | 0.59 |
| 1:A:150:TRP:NE1 | 1:A:152:GLU:HB2 | 2.18 | 0.59 |
| 1:D:36:LYS:HE2 | 1:D:562:TYR:HB3 | 1.85 | 0.58 |
| 1:D:140:ARG:NH2 | 1:D:230:GLN:HG2 | 2.17 | 0.58 |
| 1:B:46:GLN:HG3 | 1:B:51:GLN:HG3 | 1.84 | 0.58 |
| 1:B:346:LYS:HB2 | 1:B:346:LYS:HZ3 | 1.68 | 0.58 |
| 1:C:552:TYR:O | 1:C:556:ARG:HG2 | 2.02 | 0.58 |
| 1:D:389:ILE:HG23 | 1:D:399:PHE:CZ | 2.38 | 0.58 |
| 1:A:105:GLU:HG3 | 1:A:516:LEU:HB3 | 1.86 | 0.58 |
| 1:C:453:LYS:HB2 | 1:C:459:VAL:HG22 | 1.85 | 0.58 |
| 1:A:350:LEU:HD11 | 1:A:362:GLN:NE2 | 2.17 | 0.58 |
| 1:C:328:VAL:HA | 1:C:332:LEU:O | 2.02 | 0.58 |
| 1:A:476:LEU:HD23 | 1:A:527:ALA:CB | 2.34 | 0.58 |
| 1:D:293:ALA:O | 1:D:296:LYS:HB2 | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:33:ARG:HD2 | 1:B:93:GLU:OE1 | 2.04 | 0.58 |
| 1:A:493:GLU:HG2 | 1:A:533:TYR:CD1 | 2.39 | 0.58 |
| 1:A:207:THR:O | 1:A:224:LYS:HA | 2.04 | 0.58 |
| 1:D:518:ASN:HA | 1:D:520:GLN:OE1 | 2.02 | 0.58 |
| 1:B:301:PRO:HG2 | 1:B:304:GLU:OE2 | 2.03 | 0.58 |
| 1:B:389:ILE:HG23 | 1:B:399:PHE:CZ | 2.38 | 0.58 |
| 1:C:85:ILE:HD12 | 1:C:96:PHE:CE1 | 2.31 | 0.58 |
| 1:A:177:MSE:HE1 | 1:A:200:PRO:HB2 | 1.86 | 0.58 |
| 1:D:38:MSE:SE | 1:D:55:PRO:HG2 | 2.54 | 0.58 |
| 1:A:397:ARG:HD2 | 1:A:426:ALA:O | 2.03 | 0.58 |
| 1:D:285:ALA:HB1 | 1:D:470:ILE:HD12 | 1.84 | 0.58 |
| 1:A:57:LYS:HZ3 | 1:A:59:GLU:HG2 | 1.68 | 0.57 |
| 1:A:152:GLU:N | 1:A:152:GLU:OE1 | 2.36 | 0.57 |
| 1:B:128:ARG:HH11 | 1:B:128:ARG:HG3 | 1.69 | 0.57 |
| 1:A:424:ALA:HB3 | 1:A:425:GLN:HE22 | 1.68 | 0.57 |
| 1:B:515:PRO:HB2 | 1:B:518:ASN:ND2 | 2.19 | 0.57 |
| 1:C:420:SER:HA | 3:C:2601:NAD:H1D | 1.86 | 0.57 |
| 1:B:128:ARG:NE | 5:B:4056:HOH:O | 2.20 | 0.57 |
| 1:B:354:ARG:HE | 1:B:358:ILE:CD1 | 2.17 | 0.57 |
| 1:D:306:LYS:HG3 | 1:D:386:PRO:HA | 1.85 | 0.57 |
| 1:A:350:LEU:HD13 | 1:A:358:ILE:CD1 | 2.34 | 0.57 |
| 1:A:55:PRO:CG | 1:B:219:MSE:HE3 | 2.34 | 0.57 |
| 1:B:128:ARG:NH1 | 1:B:128:ARG:HG3 | 2.18 | 0.57 |
| 1:C:231:TYR:CE2 | 1:C:265:PHE:HZ | 2.23 | 0.57 |
| 1:D:535:TYR:OH | 1:D:542:ARG:HB3 | 2.05 | 0.57 |
| 1:D:43:GLN:HG2 | 1:D:566:LEU:CD1 | 2.32 | 0.57 |
| 1:B:552:TYR:O | 1:B:556:ARG:HG3 | 2.05 | 0.57 |
| 1:B:227:ARG:HG2 | 1:B:227:ARG:NH1 | 2.04 | 0.57 |
| 1:D:481:CYS:HB3 | 1:D:540:ALA:CB | 2.34 | 0.57 |
| 1:B:22:LYS:HZ3 | 1:D:27:PRO:CG | 2.18 | 0.57 |
| 1:D:86:MSE:HG3 | 1:D:131:LYS:HZ1 | 1.69 | 0.57 |
| 1:B:29:MSE:CE | 1:B:50:LEU:HD22 | 2.35 | 0.57 |
| 1:B:343:MSE:HB3 | 1:B:350:LEU:HG | 1.85 | 0.57 |
| 1:D:456:ASP:OD2 | 1:D:458:ARG:NH1 | 2.37 | 0.57 |
| 1:B:456:ASP:OD2 | 1:B:458:ARG:NH1 | 2.37 | 0.57 |
| 1:B:183:LYS:NZ | 1:B:255:GLU:OE1 | 2.38 | 0.57 |
| 1:C:446:GLY:N | 5:C:4012:HOH:O | 2.24 | 0.57 |
| 1:C:261:ASN:HD21 | 1:C:264:ARG:HH21 | 1.52 | 0.57 |
| 1:D:526:ILE:O | 1:D:530:VAL:HG23 | 2.05 | 0.57 |
| 1:D:394:GLY:HA2 | 1:D:420:SER:HB3 | 1.87 | 0.57 |
| 1:C:412:GLU:O | 1:C:440:ARG:NH1 | 2.37 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:551:LYS:O | 1:B:555:GLU:HB2 | 2.05 | 0.57 |
| 1:C:41:THR:OG1 | 1:C:44:GLU:HG3 | 2.04 | 0.57 |
| 1:B:274:CYS:HB2 | 1:B:484:ARG:O | 2.04 | 0.57 |
| 1:D:381:VAL:CG2 | 1:D:389:ILE:HD11 | 2.35 | 0.56 |
| 1:C:437:THR:C | 1:C:438:GLU:HG2 | 2.25 | 0.56 |
| 1:A:503:THR:OG1 | 1:A:505:GLU:HG2 | 2.04 | 0.56 |
| 1:B:227:ARG:CG | 1:B:227:ARG:NH1 | 2.61 | 0.56 |
| 1:A:467:ASN:HD22 | 1:A:467:ASN:H | 1.52 | 0.56 |
| 1:C:392:VAL:HG13 | 1:C:392:VAL:O | 2.05 | 0.56 |
| 1:C:40:PHE:HE2 | 1:C:565:LEU:CD1 | 2.17 | 0.56 |
| 1:B:184:LEU:HD12 | 1:B:200:PRO:HB3 | 1.88 | 0.56 |
| 1:B:396:GLY:O | 1:B:427:GLU:HA | 2.06 | 0.56 |
| 1:A:91:ARG:HD2 | 5:A:4055:HOH:O | 2.04 | 0.56 |
| 1:D:81:LYS:O | 1:D:85:ILE:HG22 | 2.06 | 0.56 |
| 1:A:61:GLN:OE1 | 1:A:98:ARG:HD3 | 2.05 | 0.56 |
| 1:B:552:TYR:CD1 | 1:B:556:ARG:NH1 | 2.73 | 0.56 |
| 1:C:350:LEU:HD22 | 1:C:354:ARG:CZ | 2.35 | 0.56 |
| 1:A:520:GLN:HE21 | 1:A:520:GLN:N | 1.99 | 0.56 |
| 1:B:478:VAL:HG13 | 1:B:483:THR:OG1 | 2.05 | 0.56 |
| 1:D:86:MSE:HG3 | 1:D:131:LYS:NZ | 2.20 | 0.56 |
| 1:A:527:ALA:O | 1:A:531:THR:HG23 | 2.05 | 0.56 |
| 1:A:144:ARG:NE | 1:A:148:ASP:OD1 | 2.38 | 0.56 |
| 1:D:85:ILE:HG23 | 1:D:86:MSE:HE2 | 1.88 | 0.56 |
| 1:D:432:GLU:OE2 | 5:D:4048:HOH:O | 2.17 | 0.56 |
| 1:A:398:LEU:CD2 | 1:A:398:LEU:N | 2.68 | 0.56 |
| 1:A:306:LYS:HG2 | 1:A:386:PRO:HA | 1.87 | 0.56 |
| 1:A:484:ARG:HG2 | 1:D:543:TYR:CE1 | 2.40 | 0.56 |
| 1:D:72:LEU:HA | 1:D:75:MSE:HG3 | 1.87 | 0.56 |
| 1:C:79:LEU:HB2 | 1:C:118:LEU:HD21 | 1.88 | 0.56 |
| 1:C:61:GLN:OE1 | 1:C:98:ARG:HD3 | 2.06 | 0.56 |
| 1:B:286:VAL:HG21 | 1:B:467:ASN:HA | 1.87 | 0.56 |
| 1:D:441:CYS:O | 1:D:442:LEU:HD23 | 2.06 | 0.56 |
| 1:C:248:ARG:NH1 | 1:C:273:TYR:CD2 | 2.74 | 0.56 |
| 1:D:201:VAL:HG11 | 1:D:238:PHE:CE1 | 2.41 | 0.56 |
| 1:C:535:TYR:OH | 1:C:542:ARG:HB3 | 2.06 | 0.56 |
| 1:B:297:VAL:CG2 | 1:B:298:ILE:N | 2.68 | 0.56 |
| 1:A:212:LEU:HD22 | 1:A:218:TYR:CD2 | 2.41 | 0.56 |
| 1:D:309:PHE:HB2 | 1:D:343:MSE:HG2 | 1.88 | 0.56 |
| 1:B:347:TYR:HB2 | 1:B:354:ARG:NH1 | 2.21 | 0.55 |
| 1:A:91:ARG:CD | 5:A:4055:HOH:O | 2.53 | 0.55 |
| 1:C:371:GLU:HG2 | 1:C:372:SER:N | 2.21 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:85:ILE:HG13 | 1:C:86:MSE:H | 1.71 | 0.55 |
| 1:A:177:MSE:O | 1:A:177:MSE:HG3 | 2.06 | 0.55 |
| 1:A:38:MSE:HE3 | 1:A:59:GLU:CG | 2.36 | 0.55 |
| 1:A:153:ASN:N | 1:A:153:ASN:HD22 | 2.03 | 0.55 |
| 1:A:225:ARG:O | 1:A:227:ARG:HD2 | 2.06 | 0.55 |
| 1:B:29:MSE:HE2 | 1:B:50:LEU:CD2 | 2.33 | 0.55 |
| 1:C:42:LEU:O | 1:C:46:GLN:HG3 | 2.05 | 0.55 |
| 1:D:36:LYS:HB3 | 1:D:39:ALA:HB3 | 1.88 | 0.55 |
| 1:A:66:LEU:HD22 | 1:A:70:ARG:CD | 2.37 | 0.55 |
| 1:B:357:LYS:HD3 | 1:B:357:LYS:N | 2.22 | 0.55 |
| 1:D:261:ASN:HD21 | 1:D:264:ARG:HH21 | 1.53 | 0.55 |
| 1:C:302:ILE:HG23 | 1:C:303:SER:N | 2.22 | 0.55 |
| 1:B:556:ARG:HH11 | 1:B:556:ARG:CG | 2.19 | 0.55 |
| 1:A:502:LEU:HD13 | 1:A:507:LEU:HD13 | 1.87 | 0.55 |
| 1:B:476:LEU:HD23 | 1:B:527:ALA:CB | 2.37 | 0.55 |
| 1:A:64:GLN:NE2 | 1:A:562:TYR:OH | 2.37 | 0.55 |
| 1:C:205:VAL:HG11 | 1:C:231:TYR:HD1 | 1.72 | 0.55 |
| 1:C:242:ILE:CG2 | 1:C:243:THR:N | 2.69 | 0.55 |
| 1:B:75:MSE:HG2 | 1:B:80:GLU:OE1 | 2.07 | 0.55 |
| 1:B:105:GLU:HG2 | 1:B:516:LEU:HB3 | 1.89 | 0.55 |
| 1:B:350:LEU:HD22 | 1:B:354:ARG:NH2 | 2.22 | 0.55 |
| 1:B:154:HIS:O | 1:B:197:ARG:HD2 | 2.07 | 0.55 |
| 1:C:45:ARG:HB3 | 1:C:51:GLN:HG2 | 1.89 | 0.55 |
| 1:A:331:GLY:O | 1:A:332:LEU:C | 2.45 | 0.55 |
| 1:A:104:ILE:HG13 | 1:A:108:MSE:HE2 | 1.89 | 0.55 |
| 1:A:305:HIS:O | 1:A:340:LYS:HD3 | 2.07 | 0.55 |
| 1:B:446:GLY:O | 1:B:466:ASN:ND2 | 2.38 | 0.55 |
| 1:A:431:GLU:OE2 | 1:A:431:GLU:HA | 2.07 | 0.55 |
| 1:C:108:MSE:HB3 | 1:C:109:PRO:HD3 | 1.89 | 0.55 |
| 1:D:287:ALA:CB | 1:D:319:ILE:HD13 | 2.37 | 0.54 |
| 1:D:144:ARG:HA | 1:D:147:VAL:HG22 | 1.89 | 0.54 |
| 1:B:432:GLU:O | 1:B:436:LEU:HB2 | 2.07 | 0.54 |
| 1:B:179:ILE:HB | 1:B:180:PRO:HD3 | 1.89 | 0.54 |
| 1:C:389:ILE:HB | 1:C:407:MSE:HE2 | 1.88 | 0.54 |
| 1:C:264:ARG:HG2 | 1:C:264:ARG:HH11 | 1.72 | 0.54 |
| 1:A:146:ILE:O | 1:A:149:ASN:HB2 | 2.08 | 0.54 |
| 1:A:315:ALA:O | 1:A:319:ILE:HG13 | 2.07 | 0.54 |
| 1:C:325:MSE:HE1 | 1:C:489:SER:HA | 1.88 | 0.54 |
| 1:D:68:PHE:CE2 | 1:D:72:LEU:HD22 | 2.42 | 0.54 |
| 1:A:140:ARG:NH2 | 1:A:233:ASP:HB3 | 2.22 | 0.54 |
| 1:A:175:TYR:CE2 | 1:A:219:MSE:HE2 | 2.42 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:153:ASN:ND2 | 1:A:153:ASN:N | 2.55 | 0.54 |
| 1:D:300:LYS:CB | 1:D:300:LYS:NZ | 2.65 | 0.54 |
| 1:B:300:LYS:NZ | 1:B:300:LYS:CB | 2.62 | 0.54 |
| 1:D:194:ARG:HE | 1:D:197:ARG:CZ | 2.20 | 0.54 |
| 1:A:298:ILE:CG2 | 1:A:300:LYS:HB2 | 2.37 | 0.54 |
| 1:C:112:TYR:CD1 | 1:C:186:LEU:HD11 | 2.43 | 0.54 |
| 1:D:379:ASP:O | 1:D:383:ILE:HD13 | 2.07 | 0.54 |
| 1:A:261:ASN:ND2 | 1:A:264:ARG:HE | 2.06 | 0.54 |
| 1:D:401:PRO:O | 1:D:405:ARG:HG3 | 2.07 | 0.54 |
| 1:A:177:MSE:CE | 1:A:200:PRO:HB2 | 2.37 | 0.54 |
| 1:A:137:ILE:HA | 1:A:234:LEU:HD22 | 1.89 | 0.54 |
| 1:C:46:GLN:HG2 | 1:C:51:GLN:HG3 | 1.90 | 0.54 |
| 1:C:300:LYS:HG3 | 1:C:301:PRO:HD2 | 1.90 | 0.54 |
| 1:D:475:ALA:O | 1:D:479:ILE:HD12 | 2.08 | 0.54 |
| 1:D:307:ILE:HG13 | 1:D:388:THR:HB | 1.90 | 0.54 |
| 1:A:24:LYS:HG3 | 1:C:22:LYS:HE2 | 1.89 | 0.54 |
| 1:D:242:ILE:HG22 | 1:D:243:THR:N | 2.23 | 0.54 |
| 1:C:287:ALA:O | 1:C:291:LEU:HD13 | 2.06 | 0.54 |
| 1:A:22:LYS:NZ | 1:C:27:PRO:HG2 | 2.23 | 0.54 |
| 1:B:29:MSE:HE3 | 1:B:53:LEU:HD12 | 1.90 | 0.54 |
| 1:B:29:MSE:HE1 | 1:B:53:LEU:CB | 2.34 | 0.54 |
| 1:C:552:TYR:CD1 | 1:C:556:ARG:NH1 | 2.75 | 0.54 |
| 1:D:460:PHE:CD2 | 1:D:460:PHE:N | 2.76 | 0.54 |
| 1:D:486:ILE:HD12 | 1:D:486:ILE:N | 2.22 | 0.54 |
| 1:A:282:GLY:O | 1:A:286:VAL:HG23 | 2.07 | 0.54 |
| 1:A:219:MSE:HG2 | 1:B:38:MSE:HE1 | 1.88 | 0.54 |
| 1:B:331:GLY:O | 1:B:332:LEU:O | 2.26 | 0.54 |
| 1:B:91:ARG:NH1 | 1:B:91:ARG:HG2 | 2.23 | 0.54 |
| 1:C:358:ILE:HG23 | 1:C:362:GLN:HB2 | 1.88 | 0.54 |
| 1:D:298:ILE:HG22 | 1:D:300:LYS:N | 2.10 | 0.54 |
| 1:C:354:ARG:HG2 | 1:C:358:ILE:HD11 | 1.90 | 0.54 |
| 1:B:431:GLU:OE2 | 1:B:452:VAL:HG13 | 2.07 | 0.53 |
| 1:B:374:PRO:HB3 | 1:B:380:ALA:N | 2.22 | 0.53 |
| 1:A:68:PHE:HZ | 1:A:85:ILE:HG22 | 1.71 | 0.53 |
| 1:C:286:VAL:HG11 | 1:C:466:ASN:O | 2.08 | 0.53 |
| 1:C:335:GLN:NE2 | 1:C:339:LYS:NZ | 2.56 | 0.53 |
| 1:D:21:ILE:HD12 | 1:D:21:ILE:N | 2.24 | 0.53 |
| 1:B:310:LEU:HB3 | 1:B:391:GLY:HA2 | 1.90 | 0.53 |
| 1:A:25:GLY:HA3 | 1:C:22:LYS:HE3 | 1.90 | 0.53 |
| 1:D:414:PRO:HD2 | 1:D:441:CYS:HA | 1.89 | 0.53 |
| 1:A:397:ARG:HD3 | 1:A:397:ARG:N | 2.24 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:22:LYS:HD2 | 1:D:24:LYS:HE3 | 1.90 | 0.53 |
| 1:B:77:SER:OG | 1:B:80:GLU:HB3 | 2.08 | 0.53 |
| 1:B:58:ILE:O | 1:B:58:ILE:HG22 | 2.07 | 0.53 |
| 1:B:401:PRO:HB3 | 1:B:436:LEU:HD21 | 1.90 | 0.53 |
| 1:C:527:ALA:O | 1:C:531:THR:CG2 | 2.56 | 0.53 |
| 1:D:70:ARG:CG | 1:D:70:ARG:NH1 | 2.71 | 0.53 |
| 1:C:227:ARG:HG2 | 1:C:227:ARG:NH1 | 2.23 | 0.53 |
| 1:B:546:PRO:HG2 | 1:B:549:LYS:HD2 | 1.90 | 0.53 |
| 1:A:210:ILE:CD1 | 1:A:210:ILE:H | 2.22 | 0.53 |
| 1:A:434:TYR:CZ | 1:A:443:PHE:HB3 | 2.44 | 0.53 |
| 1:A:505:GLU:O | 1:A:508:ALA:HB3 | 2.08 | 0.53 |
| 1:B:24:LYS:HZ3 | 1:D:22:LYS:HD3 | 1.74 | 0.53 |
| 1:D:556:ARG:HG2 | 1:D:556:ARG:NH1 | 2.24 | 0.53 |
| 1:D:294:ALA:O | 1:D:297:VAL:HG22 | 2.09 | 0.53 |
| 1:C:227:ARG:HG2 | 1:C:227:ARG:HH11 | 1.72 | 0.53 |
| 1:B:133:LEU:HB2 | 1:B:199:LEU:HD11 | 1.90 | 0.53 |
| 1:D:245:ARG:HD3 | 1:D:246:TYR:CZ | 2.44 | 0.53 |
| 1:B:453:LYS:CG | 1:B:459:VAL:HG12 | 2.36 | 0.53 |
| 1:D:427:GLU:N | 1:D:427:GLU:OE1 | 2.41 | 0.53 |
| 1:B:137:ILE:HA | 1:B:234:LEU:HD22 | 1.90 | 0.53 |
| 1:B:261:ASN:HA | 1:B:264:ARG:HG2 | 1.91 | 0.53 |
| 1:A:300:LYS:HZ2 | 1:A:300:LYS:HB3 | 1.73 | 0.53 |
| 1:C:331:GLY:O | 1:C:332:LEU:O | 2.27 | 0.53 |
| 1:D:412:GLU:HG3 | 1:D:413:ARG:CD | 2.38 | 0.53 |
| 1:B:363:GLU:HB3 | 1:B:364:PRO:HD3 | 1.91 | 0.53 |
| 1:C:194:ARG:CB | 1:C:197:ARG:HG2 | 2.32 | 0.53 |
| 1:D:37:GLY:C | 1:D:39:ALA:H | 2.12 | 0.53 |
| 1:D:274:CYS:SG | 1:D:486:ILE:HD11 | 2.49 | 0.53 |
| 1:B:177:MSE:HG2 | 1:B:202:CYS:HB2 | 1.91 | 0.53 |
| 1:A:411:ASN:HB2 | 1:A:414:PRO:HG3 | 1.90 | 0.53 |
| 1:B:45:ARG:HB3 | 1:B:51:GLN:HG2 | 1.91 | 0.53 |
| 1:C:116:VAL:HG13 | 1:C:117:GLY:N | 2.23 | 0.53 |
| 1:C:505:GLU:H | 1:C:505:GLU:CD | 2.11 | 0.53 |
| 1:B:30:LEU:O | 1:B:32:PRO:HD3 | 2.09 | 0.53 |
| 1:B:402:ASP:OD2 | 1:B:402:ASP:N | 2.42 | 0.53 |
| 1:B:184:LEU:O | 1:B:187:TYR:HB2 | 2.09 | 0.52 |
| 1:B:239:MSE:CE | 1:B:252:ILE:HD12 | 2.39 | 0.52 |
| 1:A:300:LYS:NZ | 1:A:305:HIS:HD2 | 2.07 | 0.52 |
| 1:C:527:ALA:O | 1:C:531:THR:HG23 | 2.09 | 0.52 |
| 1:D:70:ARG:HH11 | 1:D:70:ARG:HG2 | 1.74 | 0.52 |
| 1:B:400:THR:OG1 | 1:B:403:VAL:HG23 | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:354:ARG:NH1 | 1:B:356:ALA:HB3 | 2.24 | 0.52 |
| 1:B:484:ARG:HG2 | 1:C:543:TYR:CZ | 2.44 | 0.52 |
| 1:B:197:ARG:CG | 1:B:197:ARG:HH11 | 2.22 | 0.52 |
| 1:B:466:ASN:HB3 | 1:B:468:VAL:HG12 | 1.92 | 0.52 |
| 1:A:359:ASP:OD2 | 1:A:361:TYR:N | 2.41 | 0.52 |
| 1:A:382:ASN:O | 1:A:385:LYS:HD2 | 2.09 | 0.52 |
| 1:C:89:GLN:NE2 | 1:C:185:CYS:SG | 2.82 | 0.52 |
| 1:B:358:ILE:HG23 | 1:B:362:GLN:HB2 | 1.92 | 0.52 |
| 1:B:261:ASN:HD21 | 1:B:264:ARG:CZ | 2.21 | 0.52 |
| 1:B:239:MSE:HE1 | 1:B:252:ILE:HD12 | 1.92 | 0.52 |
| 1:B:88:ILE:HD13 | 1:B:99:ILE:HD13 | 1.91 | 0.52 |
| 1:D:194:ARG:HE | 1:D:197:ARG:HE | 1.57 | 0.52 |
| 1:B:293:ALA:O | 1:B:296:LYS:HB2 | 2.10 | 0.52 |
| 1:D:295:GLN:OE1 | 1:D:295:GLN:HA | 2.10 | 0.52 |
| 1:C:454:LEU:CD1 | 1:C:460:PHE:HE2 | 2.22 | 0.52 |
| 1:B:343:MSE:HE3 | 1:B:350:LEU:CD1 | 2.39 | 0.52 |
| 1:B:215:ASP:OD2 | 1:B:218:TYR:N | 2.42 | 0.52 |
| 1:D:350:LEU:CD2 | 1:D:350:LEU:N | 2.72 | 0.52 |
| 1:C:248:ARG:HH22 | 1:C:272:LYS:NZ | 2.08 | 0.52 |
| 1:A:146:ILE:HG23 | 1:B:52:GLY:HA3 | 1.91 | 0.52 |
| 1:D:165:ARG:NH2 | 4:D:3603:TTN:O1 | 2.43 | 0.52 |
| 1:D:194:ARG:NH1 | 1:D:194:ARG:HG2 | 2.25 | 0.52 |
| 1:C:298:ILE:HD11 | 1:C:442:LEU:HD12 | 1.91 | 0.51 |
| 1:C:221:LEU:HD23 | 1:C:223:GLN:CD | 2.30 | 0.51 |
| 1:A:96:PHE:O | 1:A:100:LEU:HD22 | 2.10 | 0.51 |
| 1:B:528:ILE:O | 1:B:531:THR:HG23 | 2.10 | 0.51 |
| 1:D:184:LEU:HD12 | 1:D:200:PRO:HB3 | 1.91 | 0.51 |
| 1:B:260:HIS:CD2 | 1:B:264:ARG:HH11 | 2.28 | 0.51 |
| 1:A:261:ASN:HA | 1:A:264:ARG:HG2 | 1.92 | 0.51 |
| 1:D:300:LYS:HE3 | 1:D:305:HIS:CE1 | 2.45 | 0.51 |
| 1:C:429:THR:HG23 | 1:C:432:GLU:OE2 | 2.10 | 0.51 |
| 1:D:191:ALA:HB3 | 1:D:193:ILE:HD12 | 1.93 | 0.51 |
| 1:C:357:LYS:CD | 1:C:357:LYS:N | 2.73 | 0.51 |
| 1:B:452:VAL:O | 1:B:459:VAL:HA | 2.11 | 0.51 |
| 1:C:150:TRP:CE2 | 1:C:199:LEU:HD13 | 2.46 | 0.51 |
| 1:B:116:VAL:CG1 | 1:B:117:GLY:N | 2.73 | 0.51 |
| 1:B:31:ASN:HB3 | 1:B:34:THR:OG1 | 2.10 | 0.51 |
| 1:C:327:MSE:HE3 | 1:C:337:ALA:CB | 2.29 | 0.51 |
| 1:B:228:THR:OG1 | 1:B:230:GLN:HB2 | 2.10 | 0.51 |
| 1:D:306:LYS:HE2 | 1:D:342:TRP:HE1 | 1.75 | 0.51 |
| 1:C:132:GLY:HA3 | 1:C:177:MSE:HE3 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:175:TYR:CE2 | 1:A:218:TYR:HA | 2.45 | 0.51 |
| 1:A:307:ILE:HD12 | 1:A:307:ILE:N | 2.25 | 0.51 |
| 1:B:88:ILE:HG22 | 1:B:96:PHE:HB2 | 1.92 | 0.51 |
| 1:A:61:GLN:HG3 | 1:A:562:TYR:CE1 | 2.46 | 0.51 |
| 1:D:309:PHE:CE1 | 1:D:316:ALA:HA | 2.46 | 0.51 |
| 1:C:137:ILE:HA | 1:C:234:LEU:HD22 | 1.93 | 0.51 |
| 1:B:374:PRO:HG3 | 1:B:383:ILE:CD1 | 2.40 | 0.50 |
| 1:D:397:ARG:HA | 1:D:427:GLU:O | 2.11 | 0.50 |
| 1:C:520:GLN:H | 1:C:520:GLN:NE2 | 2.05 | 0.50 |
| 1:A:300:LYS:NZ | 1:A:305:HIS:CD2 | 2.79 | 0.50 |
| 1:B:194:ARG:NH2 | 1:B:196:ASP:OD2 | 2.44 | 0.50 |
| 1:C:454:LEU:HD11 | 1:C:460:PHE:CE2 | 2.45 | 0.50 |
| 1:B:150:TRP:CE2 | 1:B:199:LEU:HD13 | 2.45 | 0.50 |
| 1:C:164:GLU:HG3 | 1:C:225:ARG:NE | 2.26 | 0.50 |
| 1:B:261:ASN:CG | 1:B:264:ARG:NH1 | 2.64 | 0.50 |
| 1:C:207:THR:CG2 | 1:C:213:LEU:HD13 | 2.41 | 0.50 |
| 1:A:184:LEU:HD13 | 1:A:198:CYS:HB3 | 1.94 | 0.50 |
| 1:D:208:ASP:CG | 1:D:227:ARG:HH22 | 2.14 | 0.50 |
| 1:A:267:ARG:HG3 | 1:A:267:ARG:O | 2.11 | 0.50 |
| 1:C:57:LYS:HG3 | 1:C:58:ILE:N | 2.25 | 0.50 |
| 1:C:401:PRO:HA | 1:C:404:ILE:HG13 | 1.92 | 0.50 |
| 1:A:506:GLU:O | 1:A:511:ARG:HG3 | 2.11 | 0.50 |
| 1:A:346:LYS:HD3 | 1:A:347:TYR:CE1 | 2.47 | 0.50 |
| 1:D:68:PHE:CD2 | 1:D:99:ILE:HG21 | 2.47 | 0.50 |
| 1:D:86:MSE:N | 1:D:86:MSE:HE2 | 2.26 | 0.50 |
| 1:D:291:LEU:HD13 | 1:D:417:PHE:CE2 | 2.45 | 0.50 |
| 1:D:144:ARG:HG2 | 1:D:144:ARG:HH11 | 1.76 | 0.50 |
| 1:B:534:LEU:CD2 | 1:B:539:MSE:HE2 | 2.42 | 0.50 |
| 1:D:392:VAL:O | 1:D:392:VAL:CG1 | 2.58 | 0.50 |
| 1:D:61:GLN:HG3 | 1:D:562:TYR:CE1 | 2.47 | 0.50 |
| 1:B:505:GLU:O | 1:B:509:GLN:HG2 | 2.12 | 0.50 |
| 1:D:482:ASN:HD21 | 3:D:3602:NAD:H4B | 1.76 | 0.50 |
| 1:A:319:ILE:O | 1:A:323:ILE:HG13 | 2.12 | 0.50 |
| 1:A:43:GLN:O | 1:A:47:MSE:HB2 | 2.11 | 0.50 |
| 1:B:327:MSE:HG2 | 1:B:332:LEU:HD22 | 1.94 | 0.50 |
| 1:D:25:GLY:C | 1:D:27:PRO:HD2 | 2.32 | 0.50 |
| 1:A:59:GLU:CD | 1:A:67:ARG:HH12 | 2.14 | 0.50 |
| 1:B:315:ALA:HB3 | 1:B:392:VAL:HG21 | 1.94 | 0.50 |
| 1:A:57:LYS:NZ | 1:A:59:GLU:HG2 | 2.26 | 0.50 |
| 1:B:239:MSE:HE2 | 1:B:273:TYR:CD1 | 2.47 | 0.50 |
| 1:B:68:PHE:CD2 | 1:B:99:ILE:HG12 | 2.46 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:210:ILE:O | 1:D:214:LYS:HG3 | 2.12 | 0.49 |
| 1:A:407:MSE:CE | 1:A:407:MSE:HA | 2.38 | 0.49 |
| 1:D:346:LYS:HE2 | 1:D:347:TYR:OH | 2.12 | 0.49 |
| 1:C:350:LEU:HD22 | 1:C:354:ARG:NH2 | 2.27 | 0.49 |
| 1:B:286:VAL:CG2 | 1:B:467:ASN:HA | 2.42 | 0.49 |
| 1:A:472:PRO:HD2 | 5:A:4029:HOH:O | 2.10 | 0.49 |
| 1:D:527:ALA:O | 1:D:531:THR:CG2 | 2.60 | 0.49 |
| 1:B:297:VAL:HG21 | 1:B:442:LEU:HD21 | 1.94 | 0.49 |
| 1:D:177:MSE:HE3 | 1:D:180:PRO:HD2 | 1.94 | 0.49 |
| 1:C:286:VAL:HG13 | 1:C:470:ILE:HG12 | 1.93 | 0.49 |
| 1:C:217:PHE:HZ | 1:D:66:LEU:HD13 | 1.76 | 0.49 |
| 1:A:412:GLU:HG3 | 1:A:413:ARG:HG2 | 1.93 | 0.49 |
| 1:A:38:MSE:HE3 | 1:A:59:GLU:HG3 | 1.94 | 0.49 |
| 1:B:93:GLU:OE1 | 1:B:195:PRO:HB2 | 2.12 | 0.49 |
| 1:C:276:PHE:HB2 | 1:C:281:GLN:OE1 | 2.12 | 0.49 |
| 1:A:273:TYR:HB2 | 1:A:275:THR:CG2 | 2.42 | 0.49 |
| 1:A:376:THR:O | 1:A:379:ASP:HB2 | 2.11 | 0.49 |
| 1:C:146:ILE:O | 1:C:149:ASN:HB2 | 2.13 | 0.49 |
| 1:C:36:LYS:HE2 | 1:C:562:TYR:HB3 | 1.93 | 0.49 |
| 1:B:248:ARG:HB3 | 1:C:543:TYR:CZ | 2.48 | 0.49 |
| 1:D:212:LEU:HD22 | 1:D:218:TYR:CD2 | 2.48 | 0.49 |
| 1:A:140:ARG:NH2 | 1:A:230:GLN:HA | 2.27 | 0.49 |
| 1:C:408:ALA:HB1 | 1:C:440:ARG:NH2 | 2.28 | 0.49 |
| 1:C:298:ILE:HD11 | 1:C:442:LEU:CD1 | 2.43 | 0.49 |
| 1:C:79:LEU:HD22 | 1:C:118:LEU:CG | 2.41 | 0.49 |
| 1:D:556:ARG:NE | 3:D:3602:NAD:O2A | 2.46 | 0.49 |
| 1:A:24:LYS:O | 1:C:22:LYS:HE2 | 2.12 | 0.49 |
| 1:B:140:ARG:CZ | 1:B:230:GLN:HG3 | 2.43 | 0.49 |
| 1:D:502:LEU:HD13 | 1:D:507:LEU:HD12 | 1.95 | 0.49 |
| 1:A:184:LEU:O | 1:A:187:TYR:HB2 | 2.12 | 0.49 |
| 1:D:239:MSE:O | 1:D:243:THR:HG23 | 2.13 | 0.49 |
| 1:C:418:ALA:O | 5:C:4012:HOH:O | 2.18 | 0.49 |
| 1:D:405:ARG:HH11 | 1:D:405:ARG:HG3 | 1.78 | 0.49 |
| 1:D:208:ASP:OD2 | 1:D:227:ARG:NH2 | 2.34 | 0.49 |
| 1:A:310:LEU:HD22 | 1:A:399:PHE:CE2 | 2.48 | 0.49 |
| 1:A:89:GLN:HB2 | 1:A:96:PHE:CD2 | 2.48 | 0.49 |
| 1:B:521:GLU:HG2 | 1:B:525:ASN:ND2 | 2.28 | 0.49 |
| 1:A:467:ASN:O | 1:A:471:PHE:HD2 | 1.95 | 0.49 |
| 1:A:397:ARG:NH1 | 1:A:397:ARG:CG | 2.75 | 0.49 |
| 1:A:396:GLY:C | 1:A:398:LEU:HD23 | 2.34 | 0.49 |
| 1:B:207:THR:O | 1:B:224:LYS:HA | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:327:MSE:CE | 1:A:337:ALA:HB1 | 2.30 | 0.48 |
| 1:C:197:ARG:CG | 1:C:197:ARG:HH11 | 2.13 | 0.48 |
| 1:B:518:ASN:HA | 1:B:520:GLN:OE1 | 2.13 | 0.48 |
| 1:C:165:ARG:NH2 | 4:C:2603:TTN:O1 | 2.46 | 0.48 |
| 1:B:451:PRO:HG3 | 1:B:461:THR:HG23 | 1.94 | 0.48 |
| 1:D:144:ARG:HD2 | 1:D:147:VAL:HG21 | 1.91 | 0.48 |
| 1:C:116:VAL:CG1 | 1:C:117:GLY:N | 2.75 | 0.48 |
| 1:A:385:LYS:HA | 1:A:410:ILE:HD13 | 1.95 | 0.48 |
| 1:A:245:ARG:HD3 | 1:A:246:TYR:CE1 | 2.48 | 0.48 |
| 1:A:37:GLY:C | 1:A:39:ALA:H | 2.17 | 0.48 |
| 1:B:266:LEU:O | 1:B:270:ARG:HB3 | 2.12 | 0.48 |
| 1:A:72:LEU:HA | 1:A:75:MSE:HG3 | 1.94 | 0.48 |
| 1:B:29:MSE:CE | 1:B:50:LEU:HB3 | 2.40 | 0.48 |
| 1:A:194:ARG:HG3 | 3:A:602:NAD:C6A | 2.43 | 0.48 |
| 1:D:314:GLU:HB2 | 3:D:3601:NAD:O1N | 2.12 | 0.48 |
| 1:D:333:SER:H | 1:D:336:GLU:CG | 2.26 | 0.48 |
| 1:B:453:LYS:HG2 | 1:B:459:VAL:CG1 | 2.34 | 0.48 |
| 1:B:235:ILE:O | 1:B:239:MSE:HG2 | 2.14 | 0.48 |
| 1:A:29:MSE:HE1 | 1:A:54:LEU:CD2 | 2.43 | 0.48 |
| 1:D:156:LYS:HD3 | 1:D:479:ILE:HG23 | 1.94 | 0.48 |
| 1:D:45:ARG:CZ | 1:D:58:ILE:HD13 | 2.43 | 0.48 |
| 1:A:225:ARG:HG2 | 1:A:225:ARG:HH11 | 1.79 | 0.48 |
| 1:B:339:LYS:HA | 1:B:367:HIS:CE1 | 2.49 | 0.48 |
| 1:A:377:PHE:CZ | 1:A:389:ILE:HD12 | 2.49 | 0.48 |
| 1:C:309:PHE:HE2 | 1:C:341:ILE:HG23 | 1.79 | 0.48 |
| 1:D:371:GLU:HG3 | 1:D:371:GLU:H | 1.39 | 0.48 |
| 1:A:248:ARG:HG2 | 1:A:248:ARG:HH11 | 1.79 | 0.48 |
| 1:D:381:VAL:CG1 | 1:D:407:MSE:CE | 2.91 | 0.48 |
| 1:A:300:LYS:NZ | 1:A:300:LYS:HB3 | 2.29 | 0.48 |
| 1:D:506:GLU:O | 1:D:509:GLN:HG2 | 2.12 | 0.48 |
| 1:D:140:ARG:CZ | 1:D:230:GLN:HG2 | 2.44 | 0.48 |
| 1:B:389:ILE:HG22 | 1:B:416:ILE:HA | 1.95 | 0.48 |
| 1:B:501:GLN:NE2 | 1:B:525:ASN:HB3 | 2.28 | 0.48 |
| 1:A:394:GLY:HA2 | 1:A:420:SER:HB3 | 1.96 | 0.48 |
| 1:B:412:GLU:O | 1:B:440:ARG:NH1 | 2.46 | 0.48 |
| 1:D:306:LYS:HZ2 | 1:D:306:LYS:HB2 | 1.79 | 0.48 |
| 1:A:294:ALA:O | 1:A:297:VAL:HG22 | 2.13 | 0.48 |
| 1:A:502:LEU:CD1 | 1:A:507:LEU:HD13 | 2.44 | 0.48 |
| 1:C:468:VAL:HA | 1:C:471:PHE:CE2 | 2.49 | 0.48 |
| 1:B:520:GLN:O | 1:B:524:ILE:HD12 | 2.13 | 0.48 |
| 1:B:231:TYR:HE2 | 1:B:261:ASN:ND2 | 2.12 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:542:ARG:HH12 | 1:A:544:PRO:HD2 | 1.78 | 0.48 |
| 1:C:235:ILE:HG13 | 1:C:265:PHE:CZ | 2.49 | 0.48 |
| 1:B:255:GLU:OE2 | 1:B:278:ASP:CB | 2.62 | 0.48 |
| 1:A:559:ARG:HB3 | 1:A:561:GLU:HG2 | 1.95 | 0.48 |
| 1:D:520:GLN:CD | 1:D:520:GLN:H | 2.17 | 0.48 |
| 1:A:397:ARG:HA | 1:A:427:GLU:O | 2.14 | 0.48 |
| 1:C:166:ILE:HD12 | 1:C:179:ILE:HG13 | 1.95 | 0.48 |
| 1:C:396:GLY:O | 1:C:427:GLU:HA | 2.14 | 0.48 |
| 1:A:26:LYS:N | 1:A:27:PRO:CD | 2.77 | 0.48 |
| 1:C:301:PRO:HG2 | 1:C:304:GLU:CD | 2.34 | 0.48 |
| 1:A:194:ARG:HG3 | 3:A:602:NAD:N1A | 2.29 | 0.47 |
| 1:B:537:ASN:ND2 | 1:B:537:ASN:N | 2.59 | 0.47 |
| 1:A:137:ILE:HG13 | 1:A:137:ILE:O | 2.13 | 0.47 |
| 1:B:556:ARG:NH1 | 1:B:556:ARG:CG | 2.74 | 0.47 |
| 1:D:415:VAL:CG2 | 1:D:442:LEU:HD12 | 2.44 | 0.47 |
| 1:B:169:LEU:HD13 | 1:B:422:PRO:HD3 | 1.95 | 0.47 |
| 1:D:24:LYS:HA | 1:D:28:LEU:CD1 | 2.44 | 0.47 |
| 1:D:177:MSE:CE | 1:D:200:PRO:HB2 | 2.44 | 0.47 |
| 3:C:2602:NAD:O3B | 5:C:4060:HOH:O | 2.10 | 0.47 |
| 1:C:335:GLN:NE2 | 1:C:339:LYS:HZ1 | 2.12 | 0.47 |
| 1:D:377:PHE:CE2 | 1:D:399:PHE:CE2 | 3.02 | 0.47 |
| 1:A:468:VAL:HA | 1:A:471:PHE:HE2 | 1.72 | 0.47 |
| 1:B:163:GLY:HA2 | 1:B:166:ILE:HD11 | 1.96 | 0.47 |
| 1:D:239:MSE:HE3 | 1:D:252:ILE:HD13 | 1.96 | 0.47 |
| 1:C:294:ALA:O | 1:C:297:VAL:HG13 | 2.13 | 0.47 |
| 1:A:150:TRP:CD1 | 1:A:152:GLU:HB2 | 2.49 | 0.47 |
| 1:A:159:VAL:HG13 | 1:A:253:GLN:NE2 | 2.29 | 0.47 |
| 1:B:92:ASN:HB2 | 5:B:4003:HOH:O | 2.14 | 0.47 |
| 1:D:174:VAL:C | 1:D:176:GLY:H | 2.18 | 0.47 |
| 1:A:25:GLY:HA3 | 1:C:22:LYS:CE | 2.45 | 0.47 |
| 1:A:150:TRP:HE1 | 1:A:152:GLU:HB2 | 1.78 | 0.47 |
| 1:B:165:ARG:NH2 | 4:B:1603:TTN:O1 | 2.48 | 0.47 |
| 1:B:443:PHE:CZ | 1:B:445:SER:HB3 | 2.50 | 0.47 |
| 1:A:417:PHE:CD1 | 1:A:444:ALA:HB3 | 2.50 | 0.47 |
| 1:D:389:ILE:HG23 | 1:D:399:PHE:CE1 | 2.50 | 0.47 |
| 1:D:527:ALA:O | 1:D:531:THR:HG23 | 2.15 | 0.47 |
| 1:D:23:GLU:O | 1:D:28:LEU:HD11 | 2.15 | 0.47 |
| 1:D:152:GLU:HG2 | 1:D:196:ASP:O | 2.14 | 0.47 |
| 1:B:140:ARG:NH2 | 1:B:230:GLN:HG3 | 2.30 | 0.47 |
| 1:A:137:ILE:HA | 1:A:234:LEU:CD2 | 2.45 | 0.47 |
| 1:A:363:GLU:HB3 | 1:A:364:PRO:CD | 2.44 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:194:ARG:HB2 | 1:B:197:ARG:CG | 2.44 | 0.47 |
| 1:A:208:ASP:O | 1:A:210:ILE:HD13 | 2.14 | 0.47 |
| 1:C:264:ARG:NH1 | 1:C:264:ARG:HG2 | 2.29 | 0.47 |
| 1:A:484:ARG:HD2 | 1:A:541:PHE:CD1 | 2.48 | 0.47 |
| 1:D:405:ARG:HG3 | 1:D:405:ARG:NH1 | 2.30 | 0.47 |
| 1:A:559:ARG:HG3 | 1:A:561:GLU:OE1 | 2.15 | 0.47 |
| 1:A:85:ILE:CG1 | 1:A:86:MSE:N | 2.77 | 0.47 |
| 1:A:184:LEU:HD22 | 1:A:198:CYS:HB3 | 1.95 | 0.47 |
| 1:A:225:ARG:NH1 | 1:A:225:ARG:CG | 2.73 | 0.47 |
| 1:D:542:ARG:NH1 | 1:D:544:PRO:HD2 | 2.30 | 0.47 |
| 1:C:210:ILE:O | 1:C:214:LYS:HG3 | 2.15 | 0.47 |
| 1:B:434:TYR:HD1 | 1:B:452:VAL:HG21 | 1.78 | 0.47 |
| 1:A:221:LEU:HD13 | 1:B:56:PRO:HB2 | 1.97 | 0.47 |
| 1:B:75:MSE:HG2 | 1:B:80:GLU:CG | 2.45 | 0.47 |
| 1:B:208:ASP:OD1 | 1:B:224:LYS:HD3 | 2.15 | 0.47 |
| 1:A:174:VAL:HG21 | 1:A:220:GLY:CA | 2.45 | 0.46 |
| 1:B:166:ILE:O | 1:B:169:LEU:HB2 | 2.15 | 0.46 |
| 1:A:381:VAL:CG1 | 1:A:407:MSE:HE3 | 2.41 | 0.46 |
| 1:B:57:LYS:HG3 | 1:B:58:ILE:N | 2.30 | 0.46 |
| 1:C:70:ARG:NH1 | 1:C:70:ARG:CG | 2.76 | 0.46 |
| 1:C:61:GLN:HG3 | 1:C:562:TYR:CE1 | 2.50 | 0.46 |
| 1:A:484:ARG:HD2 | 1:A:541:PHE:CE1 | 2.51 | 0.46 |
| 1:D:165:ARG:NH2 | 1:D:256:ASP:OD1 | 2.48 | 0.46 |
| 1:C:137:ILE:HG13 | 1:C:137:ILE:O | 2.15 | 0.46 |
| 1:D:520:GLN:HE21 | 1:D:521:GLU:N | 2.12 | 0.46 |
| 1:D:298:ILE:HG21 | 1:D:300:LYS:HB2 | 1.94 | 0.46 |
| 1:D:406:ALA:O | 1:D:410:ILE:HG13 | 2.16 | 0.46 |
| 1:C:422:PRO:HD2 | 1:C:425:GLN:HE21 | 1.81 | 0.46 |
| 1:A:487:SER:CB | 1:A:539:MSE:HE1 | 2.41 | 0.46 |
| 1:C:302:ILE:CG2 | 1:C:303:SER:N | 2.78 | 0.46 |
| 1:C:363:GLU:N | 1:C:364:PRO:CD | 2.77 | 0.46 |
| 1:D:407:MSE:HG3 | 1:D:414:PRO:CB | 2.45 | 0.46 |
| 1:A:286:VAL:HG21 | 1:A:467:ASN:CA | 2.39 | 0.46 |
| 1:A:24:LYS:C | 1:C:22:LYS:HE2 | 2.35 | 0.46 |
| 1:D:385:LYS:HG3 | 1:D:410:ILE:HD13 | 1.98 | 0.46 |
| 1:D:79:LEU:O | 1:D:83:ILE:HG13 | 2.14 | 0.46 |
| 1:B:549:LYS:O | 1:B:553:VAL:HG23 | 2.16 | 0.46 |
| 1:A:29:MSE:HE2 | 1:A:29:MSE:HB3 | 1.89 | 0.46 |
| 1:A:484:ARG:HG2 | 1:D:543:TYR:CZ | 2.51 | 0.46 |
| 1:C:129:ARG:NH2 | 1:D:91:ARG:HB2 | 2.31 | 0.46 |
| 1:D:112:TYR:OH | 1:D:183:LYS:HE2 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:289:ALA:CB | 1:D:498:LEU:HD23 | 2.45 | 0.46 |
| 1:A:424:ALA:HB3 | 1:A:425:GLN:NE2 | 2.30 | 0.46 |
| 1:B:29:MSE:HE2 | 1:B:50:LEU:CB | 2.40 | 0.46 |
| 1:A:46:GLN:CG | 1:A:51:GLN:HG3 | 2.46 | 0.46 |
| 1:D:100:LEU:HD23 | 1:D:189:ALA:HB2 | 1.98 | 0.46 |
| 1:A:306:LYS:C | 1:A:307:ILE:HD12 | 2.36 | 0.46 |
| 1:C:61:GLN:HA | 1:C:64:GLN:NE2 | 2.29 | 0.46 |
| 1:D:401:PRO:HA | 1:D:436:LEU:HD13 | 1.98 | 0.46 |
| 1:B:387:SER:HA | 1:B:411:ASN:OD1 | 2.16 | 0.46 |
| 1:D:476:LEU:HD23 | 1:D:527:ALA:CB | 2.46 | 0.46 |
| 1:D:331:GLY:O | 1:D:332:LEU:C | 2.53 | 0.46 |
| 1:A:363:GLU:N | 1:A:364:PRO:HD2 | 2.31 | 0.46 |
| 1:A:152:GLU:HG3 | 1:A:196:ASP:O | 2.16 | 0.46 |
| 1:C:355:LYS:HZ3 | 1:C:357:LYS:NZ | 2.14 | 0.46 |
| 1:B:109:PRO:HA | 1:B:113:THR:O | 2.15 | 0.46 |
| 1:B:335:GLN:O | 1:B:339:LYS:CG | 2.59 | 0.46 |
| 1:A:144:ARG:HE | 1:A:148:ASP:CG | 2.19 | 0.46 |
| 1:D:78:PRO:HB3 | 1:D:110:ILE:HD12 | 1.97 | 0.46 |
| 1:D:398:LEU:N | 1:D:398:LEU:HD12 | 2.29 | 0.46 |
| 1:A:389:ILE:HD13 | 1:A:389:ILE:HA | 1.76 | 0.46 |
| 1:D:484:ARG:HG3 | 1:D:541:PHE:CE1 | 2.50 | 0.46 |
| 1:D:533:TYR:CZ | 1:D:537:ASN:ND2 | 2.84 | 0.46 |
| 1:B:298:ILE:HG22 | 1:B:300:LYS:H | 1.80 | 0.46 |
| 1:D:144:ARG:NH1 | 1:D:244:ASP:HB3 | 2.31 | 0.46 |
| 1:C:394:GLY:HA2 | 1:C:420:SER:HB3 | 1.98 | 0.46 |
| 1:A:96:PHE:CZ | 1:A:100:LEU:HD21 | 2.50 | 0.46 |
| 1:D:204:ASP:OD2 | 1:D:221:LEU:N | 2.44 | 0.46 |
| 1:A:136:SER:HB2 | 1:A:221:LEU:CD2 | 2.46 | 0.45 |
| 1:D:253:GLN:HG2 | 1:D:253:GLN:O | 2.16 | 0.45 |
| 1:A:343:MSE:HB2 | 1:A:350:LEU:HG | 1.98 | 0.45 |
| 1:A:210:ILE:N | 1:A:210:ILE:HD13 | 2.30 | 0.45 |
| 1:C:155:VAL:HB | 1:C:246:TYR:CD1 | 2.51 | 0.45 |
| 1:A:397:ARG:CD | 1:A:397:ARG:N | 2.80 | 0.45 |
| 1:B:22:LYS:HA | 1:D:24:LYS:CE | 2.46 | 0.45 |
| 1:D:21:ILE:HG21 | 1:D:28:LEU:HD21 | 1.98 | 0.45 |
| 1:B:85:ILE:CD1 | 1:B:110:ILE:HG21 | 2.46 | 0.45 |
| 1:A:21:ILE:N | 1:A:21:ILE:CD1 | 2.68 | 0.45 |
| 1:A:266:LEU:O | 1:A:270:ARG:HB3 | 2.16 | 0.45 |
| 1:A:403:VAL:O | 1:A:406:ALA:HB3 | 2.16 | 0.45 |
| 1:A:105:GLU:OE2 | 1:A:517:ALA:HB2 | 2.15 | 0.45 |
| 1:B:310:LEU:HD21 | 1:B:398:LEU:CB | 2.46 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:359:ASP:OD2 | 1:D:359:ASP:C | 2.55 | 0.45 |
| 1:A:492:LEU:HD22 | 1:A:496:LYS:HD2 | 1.97 | 0.45 |
| 1:C:69:HIS:HE1 | 1:C:102:ASP:OD2 | 1.98 | 0.45 |
| 1:B:24:LYS:NZ | 1:D:22:LYS:CD | 2.79 | 0.45 |
| 1:D:412:GLU:HG3 | 1:D:413:ARG:HD2 | 1.99 | 0.45 |
| 1:D:175:TYR:CD1 | 1:D:212:LEU:HD21 | 2.52 | 0.45 |
| 1:D:496:LYS:HA | 1:D:499:THR:HG22 | 1.99 | 0.45 |
| 1:A:327:MSE:HG2 | 1:A:332:LEU:HD23 | 1.98 | 0.45 |
| 1:C:289:ALA:HB2 | 1:C:498:LEU:HD23 | 1.98 | 0.45 |
| 1:D:36:LYS:O | 1:D:39:ALA:HB3 | 2.16 | 0.45 |
| 1:C:297:VAL:HG22 | 1:C:298:ILE:HG12 | 1.97 | 0.45 |
| 1:A:26:LYS:HA | 1:A:29:MSE:HG3 | 1.98 | 0.45 |
| 1:C:229:GLN:HG3 | 1:C:233:ASP:OD2 | 2.16 | 0.45 |
| 1:A:509:GLN:HG2 | 1:A:511:ARG:HG3 | 1.99 | 0.45 |
| 1:A:327:MSE:HE3 | 1:A:337:ALA:CB | 2.32 | 0.45 |
| 1:C:194:ARG:HB2 | 1:C:197:ARG:CG | 2.36 | 0.45 |
| 1:A:23:GLU:CA | 1:A:23:GLU:OE1 | 2.57 | 0.45 |
| 1:B:177:MSE:C | 1:B:180:PRO:HD2 | 2.36 | 0.45 |
| 1:C:26:LYS:N | 1:C:27:PRO:CD | 2.80 | 0.45 |
| 1:D:545:GLU:OE2 | 1:D:549:LYS:NZ | 2.37 | 0.45 |
| 1:C:184:LEU:O | 1:C:187:TYR:HB2 | 2.17 | 0.45 |
| 1:D:61:GLN:OE1 | 1:D:98:ARG:HD3 | 2.17 | 0.45 |
| 1:A:156:LYS:HB3 | 1:A:156:LYS:HE3 | 1.73 | 0.45 |
| 1:C:392:VAL:O | 3:C:2601:NAD:H51N | 2.15 | 0.45 |
| 1:C:78:PRO:HB3 | 1:C:110:ILE:CD1 | 2.47 | 0.45 |
| 1:C:104:ILE:HG12 | 1:C:108:MSE:CE | 2.46 | 0.45 |
| 1:A:529:LYS:HE3 | 1:A:529:LYS:HA | 1.99 | 0.45 |
| 1:A:227:ARG:CG | 1:A:227:ARG:NH1 | 2.56 | 0.45 |
| 1:D:517:ALA:O | 1:D:520:GLN:OE1 | 2.35 | 0.45 |
| 1:B:343:MSE:HE2 | 1:B:343:MSE:HB2 | 1.81 | 0.45 |
| 1:B:343:MSE:HE1 | 1:B:365:PHE:HB2 | 1.99 | 0.45 |
| 1:C:25:GLY:C | 1:C:27:PRO:HD2 | 2.37 | 0.45 |
| 1:A:359:ASP:OD2 | 1:A:361:TYR:HD1 | 2.00 | 0.45 |
| 1:C:285:ALA:HB3 | 1:C:470:ILE:HG13 | 1.99 | 0.45 |
| 1:C:373:ILE:O | 1:C:373:ILE:CG2 | 2.65 | 0.45 |
| 1:A:226:ASP:OD1 | 1:A:226:ASP:C | 2.55 | 0.45 |
| 1:B:535:TYR:CZ | 1:B:546:PRO:HD2 | 2.52 | 0.45 |
| 1:A:46:GLN:HG3 | 1:A:51:GLN:HG3 | 1.99 | 0.45 |
| 1:D:298:ILE:HD11 | 1:D:442:LEU:HD12 | 1.99 | 0.44 |
| 1:B:172:LEU:O | 1:B:175:TYR:HB2 | 2.17 | 0.44 |
| 1:A:194:ARG:HD3 | 1:A:197:ARG:NE | 2.32 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:552:TYR:CE1 | 1:C:556:ARG:NH1 | 2.85 | 0.44 |
| 1:A:165:ARG:O | 1:A:256:ASP:HB3 | 2.17 | 0.44 |
| 1:B:342:TRP:CH2 | 1:B:370:PRO:HD3 | 2.52 | 0.44 |
| 1:A:297:VAL:CG2 | 1:A:442:LEU:HD11 | 2.47 | 0.44 |
| 1:B:444:ALA:HB2 | 1:B:512:LEU:HD12 | 2.00 | 0.44 |
| 1:B:36:LYS:HB3 | 1:B:39:ALA:HB3 | 1.98 | 0.44 |
| 1:D:150:TRP:CE2 | 1:D:199:LEU:HD13 | 2.52 | 0.44 |
| 1:B:261:ASN:ND2 | 1:B:265:PHE:CE1 | 2.86 | 0.44 |
| 1:B:255:GLU:OE2 | 1:B:278:ASP:HB3 | 2.17 | 0.44 |
| 1:C:217:PHE:CZ | 1:D:66:LEU:HD13 | 2.52 | 0.44 |
| 1:A:33:ARG:HD2 | 1:A:93:GLU:OE1 | 2.18 | 0.44 |
| 1:A:166:ILE:HG21 | 1:A:172:LEU:HD12 | 2.00 | 0.44 |
| 1:B:395:ALA:CB | 1:B:398:LEU:HD21 | 2.43 | 0.44 |
| 1:B:408:ALA:HB1 | 1:B:440:ARG:HH22 | 1.78 | 0.44 |
| 1:A:156:LYS:CE | 1:A:479:ILE:HG23 | 2.47 | 0.44 |
| 1:C:282:GLY:O | 1:C:286:VAL:HG22 | 2.18 | 0.44 |
| 1:D:212:LEU:HD13 | 1:D:218:TYR:CE2 | 2.52 | 0.44 |
| 1:B:229:GLN:HG3 | 1:B:229:GLN:O | 2.16 | 0.44 |
| 1:B:332:LEU:HD21 | 1:B:340:LYS:CE | 2.46 | 0.44 |
| 1:A:412:GLU:O | 1:A:440:ARG:HD2 | 2.18 | 0.44 |
| 1:A:235:ILE:O | 1:A:239:MSE:HG2 | 2.18 | 0.44 |
| 1:A:346:LYS:HD2 | 3:A:601:NAD:O2B | 2.18 | 0.44 |
| 1:A:429:THR:OG1 | 1:A:432:GLU:HG2 | 2.17 | 0.44 |
| 1:B:359:ASP:OD1 | 1:B:362:GLN:HG3 | 2.17 | 0.44 |
| 1:A:24:LYS:HE2 | 1:C:22:LYS:HA | 1.99 | 0.44 |
| 1:B:346:LYS:CB | 1:B:346:LYS:NZ | 2.74 | 0.44 |
| 1:C:205:VAL:HG11 | 1:C:231:TYR:CD1 | 2.53 | 0.44 |
| 1:C:505:GLU:O | 1:C:508:ALA:HB3 | 2.18 | 0.44 |
| 1:C:92:ASN:HB2 | 5:C:4011:HOH:O | 2.16 | 0.44 |
| 1:A:552:TYR:O | 1:A:556:ARG:NH1 | 2.51 | 0.44 |
| 1:C:352:LYS:N | 1:C:366:THR:HG22 | 2.32 | 0.44 |
| 1:D:226:ASP:C | 1:D:226:ASP:OD1 | 2.55 | 0.44 |
| 1:D:43:GLN:O | 1:D:47:MSE:HG3 | 2.16 | 0.44 |
| 1:B:481:CYS:HB3 | 1:B:483:THR:CG2 | 2.47 | 0.44 |
| 1:A:333:SER:H | 1:A:336:GLU:CD | 2.21 | 0.44 |
| 1:C:231:TYR:HE2 | 1:C:265:PHE:HZ | 1.65 | 0.44 |
| 1:D:174:VAL:C | 1:D:176:GLY:N | 2.71 | 0.44 |
| 1:A:429:THR:HA | 1:A:449:PHE:CE1 | 2.53 | 0.44 |
| 1:B:343:MSE:CE | 1:B:350:LEU:HD12 | 2.41 | 0.44 |
| 1:B:261:ASN:HD21 | 1:B:264:ARG:NH2 | 2.14 | 0.44 |
| 1:A:453:LYS:HG2 | 1:A:459:VAL:HG22 | 1.97 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:317:LEU:HD21 | 1:A:343:MSE:HE1 | 2.00 | 0.44 |
| 1:A:261:ASN:HD22 | 1:A:264:ARG:HE | 1.65 | 0.44 |
| 1:C:57:LYS:HD3 | 1:D:218:TYR:O | 2.17 | 0.44 |
| 1:A:401:PRO:HB2 | 1:A:405:ARG:NH2 | 2.31 | 0.44 |
| 1:A:391:GLY:HA3 | 1:A:427:GLU:HG2 | 2.00 | 0.44 |
| 1:B:108:MSE:HB3 | 1:B:109:PRO:CD | 2.48 | 0.44 |
| 1:B:317:LEU:HD21 | 1:B:362:GLN:HG2 | 2.00 | 0.44 |
| 1:D:310:LEU:HD21 | 1:D:398:LEU:HB2 | 2.00 | 0.44 |
| 1:C:75:MSE:HG2 | 1:C:80:GLU:CG | 2.48 | 0.44 |
| 1:C:420:SER:OG | 1:C:427:GLU:OE2 | 2.36 | 0.44 |
| 1:A:384:LEU:O | 1:A:385:LYS:HB2 | 2.18 | 0.44 |
| 1:C:164:GLU:HG3 | 1:C:225:ARG:CZ | 2.47 | 0.44 |
| 1:B:174:VAL:HG12 | 1:B:174:VAL:O | 2.18 | 0.44 |
| 1:C:174:VAL:CG1 | 1:C:174:VAL:O | 2.65 | 0.44 |
| 1:B:397:ARG:HA | 1:B:427:GLU:O | 2.18 | 0.43 |
| 1:D:85:ILE:HD11 | 1:D:100:LEU:CD1 | 2.46 | 0.43 |
| 1:D:215:ASP:OD1 | 1:D:216:PRO:HD2 | 2.18 | 0.43 |
| 1:C:559:ARG:HG2 | 1:C:561:GLU:HG2 | 2.00 | 0.43 |
| 1:C:382:ASN:O | 1:C:385:LYS:NZ | 2.48 | 0.43 |
| 1:B:306:LYS:HD3 | 1:B:384:LEU:O | 2.18 | 0.43 |
| 1:D:253:GLN:HB2 | 1:D:276:PHE:HE2 | 1.81 | 0.43 |
| 1:C:335:GLN:HB3 | 1:C:335:GLN:HE21 | 1.57 | 0.43 |
| 1:B:97:TYR:CE2 | 1:B:188:THR:HB | 2.53 | 0.43 |
| 1:C:73:LYS:HE2 | 1:C:73:LYS:HA | 2.00 | 0.43 |
| 1:D:358:ILE:HG12 | 1:D:366:THR:OG1 | 2.18 | 0.43 |
| 1:B:298:ILE:HG22 | 1:B:300:LYS:HB2 | 2.00 | 0.43 |
| 1:B:423:THR:HG23 | 1:B:447:SER:CB | 2.48 | 0.43 |
| 1:B:370:PRO:O | 1:B:371:GLU:C | 2.57 | 0.43 |
| 1:D:556:ARG:HG2 | 1:D:556:ARG:HH11 | 1.82 | 0.43 |
| 1:B:392:VAL:HG13 | 1:B:392:VAL:O | 2.18 | 0.43 |
| 1:A:468:VAL:HA | 1:A:471:PHE:CD2 | 2.51 | 0.43 |
| 1:D:554:LYS:HG2 | 1:D:554:LYS:H | 1.50 | 0.43 |
| 1:A:350:LEU:N | 1:A:350:LEU:HD23 | 2.33 | 0.43 |
| 1:C:164:GLU:HG3 | 1:C:225:ARG:CD | 2.48 | 0.43 |
| 1:D:136:SER:HA | 1:D:204:ASP:O | 2.18 | 0.43 |
| 1:C:174:VAL:CG2 | 1:C:204:ASP:HB2 | 2.49 | 0.43 |
| 1:C:382:ASN:OD1 | 1:C:382:ASN:N | 2.51 | 0.43 |
| 1:C:218:TYR:O | 1:D:57:LYS:HE3 | 2.17 | 0.43 |
| 1:D:298:ILE:HD11 | 1:D:442:LEU:HD11 | 1.99 | 0.43 |
| 1:B:525:ASN:HA | 1:B:528:ILE:HD12 | 2.00 | 0.43 |
| 1:A:419:LEU:O | 3:A:601:NAD:H2N | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:556:ARG:CG | 1:D:556:ARG:HH11 | 2.32 | 0.43 |
| 1:B:128:ARG:CD | 5:B:4056:HOH:O | 2.64 | 0.43 |
| 1:A:308:LEU:HB3 | 1:A:389:ILE:HD13 | 1.99 | 0.43 |
| 1:D:60:THR:OG1 | 1:D:63:ILE:HG12 | 2.17 | 0.43 |
| 1:B:21:ILE:HD12 | 1:B:21:ILE:HA | 1.77 | 0.43 |
| 1:A:164:GLU:OE1 | 1:A:225:ARG:HD3 | 2.17 | 0.43 |
| 1:B:24:LYS:HZ2 | 1:D:22:LYS:CD | 2.32 | 0.43 |
| 1:C:248:ARG:NH2 | 1:C:272:LYS:NZ | 2.66 | 0.43 |
| 1:D:110:ILE:O | 1:D:115:THR:HB | 2.18 | 0.43 |
| 1:A:284:ALA:CB | 1:A:322:LEU:HD12 | 2.48 | 0.43 |
| 1:B:429:THR:HG23 | 1:B:432:GLU:OE2 | 2.19 | 0.43 |
| 1:D:306:LYS:HG3 | 1:D:306:LYS:O | 2.18 | 0.43 |
| 1:C:75:MSE:HG2 | 1:C:80:GLU:HG2 | 2.01 | 0.43 |
| 1:B:174:VAL:HG21 | 1:B:220:GLY:HA3 | 2.00 | 0.43 |
| 1:C:134:PHE:HB3 | 1:D:56:PRO:HD3 | 2.01 | 0.43 |
| 1:A:420:SER:HA | 3:A:601:NAD:H1D | 2.01 | 0.43 |
| 1:A:401:PRO:HA | 1:A:436:LEU:HD23 | 2.01 | 0.43 |
| 1:B:359:ASP:C | 1:B:359:ASP:OD1 | 2.57 | 0.43 |
| 1:B:165:ARG:NH2 | 1:B:256:ASP:OD1 | 2.52 | 0.43 |
| 1:D:146:ILE:O | 1:D:149:ASN:HB2 | 2.19 | 0.43 |
| 1:D:23:GLU:CA | 1:D:23:GLU:OE2 | 2.61 | 0.43 |
| 1:D:26:LYS:N | 1:D:27:PRO:CD | 2.82 | 0.43 |
| 1:B:343:MSE:CE | 1:B:365:PHE:HB2 | 2.49 | 0.43 |
| 1:B:477:ALA:O | 1:B:481:CYS:HB2 | 2.18 | 0.43 |
| 1:C:133:LEU:HD23 | 1:D:53:LEU:HD23 | 2.01 | 0.43 |
| 1:D:61:GLN:HG3 | 1:D:562:TYR:CZ | 2.54 | 0.43 |
| 1:B:243:THR:HG21 | 1:B:273:TYR:CD2 | 2.54 | 0.43 |
| 1:C:528:ILE:HA | 1:C:531:THR:HG23 | 2.00 | 0.43 |
| 1:B:213:LEU:CD1 | 1:B:224:LYS:HZ2 | 2.31 | 0.43 |
| 1:C:55:PRO:CG | 1:D:219:MSE:HE3 | 2.49 | 0.43 |
| 1:A:302:ILE:HG23 | 1:A:332:LEU:HD22 | 2.01 | 0.43 |
| 1:B:77:SER:HA | 1:B:78:PRO:HD3 | 1.86 | 0.43 |
| 1:D:502:LEU:HD13 | 1:D:507:LEU:HD11 | 2.01 | 0.43 |
| 1:A:362:GLN:O | 1:A:363:GLU:C | 2.57 | 0.43 |
| 1:C:329:GLU:HG3 | 1:C:330:ASN:ND2 | 2.34 | 0.43 |
| 1:A:153:ASN:H | 1:A:153:ASN:HD22 | 1.66 | 0.43 |
| 1:C:38:MSE:HB3 | 1:C:59:GLU:HG3 | 2.01 | 0.43 |
| 1:B:40:PHE:HE2 | 1:B:565:LEU:CD1 | 2.31 | 0.43 |
| 1:D:373:ILE:O | 1:D:373:ILE:HG22 | 2.18 | 0.43 |
| 1:D:305:HIS:HD2 | 1:D:307:ILE:HD11 | 1.84 | 0.42 |
| 1:D:177:MSE:HE1 | 1:D:200:PRO:HB2 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:358:ILE:CG2 | 1:B:359:ASP:N | 2.81 | 0.42 |
| 1:B:260:HIS:CD2 | 1:B:264:ARG:NH1 | 2.87 | 0.42 |
| 1:A:160:VAL:HG22 | 1:A:161:THR:N | 2.34 | 0.42 |
| 1:A:429:THR:HG22 | 1:A:449:PHE:CZ | 2.54 | 0.42 |
| 1:B:302:ILE:CG2 | 1:B:303:SER:N | 2.82 | 0.42 |
| 1:A:300:LYS:HZ1 | 1:A:304:GLU:C | 2.22 | 0.42 |
| 1:C:99:ILE:HA | 1:C:99:ILE:HD13 | 1.69 | 0.42 |
| 1:C:238:PHE:CE1 | 1:C:242:ILE:HD13 | 2.55 | 0.42 |
| 1:C:242:ILE:HG22 | 1:C:243:THR:N | 2.33 | 0.42 |
| 1:C:108:MSE:HE3 | 1:C:108:MSE:HB2 | 1.77 | 0.42 |
| 1:C:164:GLU:HG3 | 1:C:225:ARG:HD3 | 2.01 | 0.42 |
| 1:C:38:MSE:HG2 | 1:C:57:LYS:O | 2.18 | 0.42 |
| 1:C:373:ILE:HA | 1:C:374:PRO:HD2 | 1.90 | 0.42 |
| 1:C:161:THR:HA | 1:C:257:PHE:CE1 | 2.54 | 0.42 |
| 1:C:402:ASP:OD1 | 1:C:402:ASP:N | 2.52 | 0.42 |
| 1:C:295:GLN:OE1 | 1:C:295:GLN:HA | 2.18 | 0.42 |
| 1:D:377:PHE:CE2 | 1:D:399:PHE:HE2 | 2.37 | 0.42 |
| 1:B:22:LYS:HA | 1:D:24:LYS:HE2 | 2.01 | 0.42 |
| 1:C:171:ASP:OD2 | 1:C:225:ARG:NE | 2.36 | 0.42 |
| 1:B:297:VAL:HG22 | 1:B:298:ILE:H | 1.83 | 0.42 |
| 1:A:467:ASN:ND2 | 3:A:601:NAD:O7N | 2.45 | 0.42 |
| 1:A:529:LYS:HA | 1:A:532:GLU:HG3 | 2.01 | 0.42 |
| 1:D:483:THR:OG1 | 1:D:534:LEU:HD13 | 2.19 | 0.42 |
| 1:B:354:ARG:CZ | 1:B:356:ALA:HB3 | 2.49 | 0.42 |
| 1:C:452:VAL:O | 1:C:452:VAL:HG22 | 2.18 | 0.42 |
| 1:C:528:ILE:HG12 | 1:C:550:ALA:HA | 2.01 | 0.42 |
| 1:C:239:MSE:HE2 | 1:C:269:TYR:CD1 | 2.55 | 0.42 |
| 1:D:59:GLU:HB3 | 1:D:63:ILE:HG13 | 2.01 | 0.42 |
| 1:B:419:LEU:O | 3:B:1601:NAD:H2N | 2.19 | 0.42 |
| 1:C:572:TRP:HA | 1:C:573:PRO:HD3 | 1.90 | 0.42 |
| 1:B:300:LYS:HE2 | 1:B:304:GLU:O | 2.19 | 0.42 |
| 1:C:158:VAL:HA | 1:C:199:LEU:O | 2.20 | 0.42 |
| 1:C:104:ILE:HG12 | 1:C:108:MSE:HE1 | 2.02 | 0.42 |
| 1:C:104:ILE:CG2 | 1:C:105:GLU:N | 2.83 | 0.42 |
| 1:C:475:ALA:O | 1:C:479:ILE:HD12 | 2.20 | 0.42 |
| 1:A:509:GLN:HE21 | 1:A:509:GLN:HB3 | 1.64 | 0.42 |
| 1:A:85:ILE:HG12 | 1:A:86:MSE:N | 2.34 | 0.42 |
| 1:D:297:VAL:HG12 | 1:D:507:LEU:HD23 | 2.00 | 0.42 |
| 1:C:283:THR:O | 1:C:286:VAL:HG23 | 2.20 | 0.42 |
| 1:A:165:ARG:NH2 | 1:A:256:ASP:OD1 | 2.52 | 0.42 |
| 1:A:344:PHE:CZ | 1:A:348:GLY:HA2 | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:443:PHE:O | 5:D:4062:HOH:O | 2.22 | 0.42 |
| 1:A:286:VAL:HG11 | 1:A:466:ASN:O | 2.18 | 0.42 |
| 1:D:64:GLN:HB3 | 1:D:95:LEU:CD2 | 2.50 | 0.42 |
| 1:A:453:LYS:NZ | 1:A:457:GLY:HA2 | 2.34 | 0.42 |
| 1:C:534:LEU:HA | 1:C:534:LEU:HD23 | 1.80 | 0.42 |
| 1:B:389:ILE:HB | 1:B:407:MSE:HE2 | 2.02 | 0.42 |
| 1:D:82:TYR:C | 1:D:82:TYR:CD2 | 2.93 | 0.42 |
| 1:A:174:VAL:HG21 | 1:A:220:GLY:HA3 | 2.02 | 0.42 |
| 1:C:453:LYS:CB | 1:C:459:VAL:HG22 | 2.49 | 0.42 |
| 1:C:108:MSE:SE | 1:C:516:LEU:HD21 | 2.69 | 0.42 |
| 1:C:335:GLN:O | 1:C:339:LYS:HE3 | 2.19 | 0.42 |
| 1:A:349:LEU:HD23 | 1:A:351:VAL:CG1 | 2.50 | 0.42 |
| 1:D:515:PRO:HG2 | 1:D:518:ASN:OD1 | 2.20 | 0.42 |
| 1:A:432:GLU:O | 1:A:436:LEU:HB2 | 2.19 | 0.42 |
| 1:D:197:ARG:NH1 | 3:D:3602:NAD:O2B | 2.53 | 0.42 |
| 1:A:218:TYR:O | 1:B:57:LYS:HD3 | 2.20 | 0.42 |
| 1:B:492:LEU:HD23 | 1:B:496:LYS:HE3 | 2.00 | 0.42 |
| 1:C:213:LEU:HA | 1:C:213:LEU:HD12 | 1.83 | 0.42 |
| 1:A:255:GLU:OE2 | 1:A:278:ASP:HB3 | 2.20 | 0.42 |
| 1:D:229:GLN:NE2 | 1:D:229:GLN:HA | 2.34 | 0.42 |
| 1:C:277:ASN:HD22 | 1:C:277:ASN:C | 2.24 | 0.42 |
| 1:A:399:PHE:CG | 1:A:427:GLU:HB3 | 2.54 | 0.41 |
| 1:D:144:ARG:O | 1:D:147:VAL:CG2 | 2.68 | 0.41 |
| 1:C:133:LEU:HD11 | 1:C:146:ILE:HG22 | 2.01 | 0.41 |
| 1:D:85:ILE:HG12 | 1:D:96:PHE:HE1 | 1.85 | 0.41 |
| 1:D:263:PHE:CZ | 1:D:314:GLU:HA | 2.55 | 0.41 |
| 1:A:344:PHE:CE2 | 1:A:348:GLY:HA2 | 2.55 | 0.41 |
| 1:A:291:LEU:HA | 1:A:291:LEU:HD12 | 1.81 | 0.41 |
| 1:A:174:VAL:CG2 | 1:A:220:GLY:HA3 | 2.50 | 0.41 |
| 1:D:26:LYS:HD3 | 1:D:26:LYS:O | 2.20 | 0.41 |
| 1:D:132:GLY:CA | 1:D:200:PRO:HG2 | 2.50 | 0.41 |
| 1:D:239:MSE:HE1 | 1:D:252:ILE:HG21 | 2.02 | 0.41 |
| 1:D:269:TYR:O | 1:D:271:GLU:N | 2.53 | 0.41 |
| 1:C:359:ASP:OD1 | 1:C:362:GLN:CD | 2.59 | 0.41 |
| 1:C:171:ASP:CG | 1:C:225:ARG:HH21 | 2.23 | 0.41 |
| 1:A:561:GLU:CD | 1:A:561:GLU:H | 2.24 | 0.41 |
| 1:C:174:VAL:HG12 | 1:C:174:VAL:O | 2.20 | 0.41 |
| 1:A:161:THR:HA | 1:A:257:PHE:CE1 | 2.56 | 0.41 |
| 1:B:144:ARG:HD2 | 1:B:144:ARG:HA | 1.94 | 0.41 |
| 1:B:210:ILE:O | 1:B:214:LYS:HG2 | 2.20 | 0.41 |
| 1:D:381:VAL:HG22 | 1:D:389:ILE:HD11 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:407:MSE:HG3 | 1:D:414:PRO:HB2 | 2.02 | 0.41 |
| 1:A:108:MSE:HB3 | 1:A:109:PRO:CD | 2.40 | 0.41 |
| 1:B:331:GLY:O | 1:B:332:LEU:C | 2.57 | 0.41 |
| 1:B:194:ARG:NH2 | 1:B:196:ASP:CG | 2.74 | 0.41 |
| 1:D:478:VAL:HG13 | 1:D:483:THR:HB | 2.01 | 0.41 |
| 1:B:103:ASP:OD2 | 1:B:106:SER:HB3 | 2.20 | 0.41 |
| 1:D:389:ILE:HD12 | 1:D:407:MSE:SE | 2.70 | 0.41 |
| 1:B:521:GLU:HG2 | 1:B:525:ASN:HD22 | 1.84 | 0.41 |
| 1:A:401:PRO:HB3 | 1:A:436:LEU:CD2 | 2.47 | 0.41 |
| 1:B:105:GLU:HG3 | 1:B:517:ALA:N | 2.36 | 0.41 |
| 1:B:225:ARG:HG2 | 1:B:225:ARG:HH11 | 1.85 | 0.41 |
| 1:B:520:GLN:CD | 1:B:520:GLN:H | 2.23 | 0.41 |
| 1:C:389:ILE:HG23 | 1:C:399:PHE:CZ | 2.55 | 0.41 |
| 1:B:128:ARG:HD3 | 5:B:4056:HOH:O | 2.20 | 0.41 |
| 1:C:287:ALA:HB3 | 1:C:319:ILE:HG12 | 2.02 | 0.41 |
| 1:B:68:PHE:CD1 | 1:B:88:ILE:HD11 | 2.55 | 0.41 |
| 1:D:496:LYS:O | 1:D:500:SER:HB3 | 2.20 | 0.41 |
| 1:A:429:THR:H | 1:A:432:GLU:CG | 2.32 | 0.41 |
| 1:B:94:LYS:HB3 | 1:B:562:TYR:CE2 | 2.56 | 0.41 |
| 1:D:261:ASN:HD22 | 1:D:264:ARG:HE | 1.68 | 0.41 |
| 1:B:82:TYR:HA | 1:B:85:ILE:HD12 | 2.03 | 0.41 |
| 1:C:183:LYS:NZ | 4:C:2603:TTN:C3 | 2.83 | 0.41 |
| 1:B:174:VAL:HG22 | 1:B:204:ASP:HB2 | 2.02 | 0.41 |
| 1:A:322:LEU:HD23 | 1:A:322:LEU:HA | 1.77 | 0.41 |
| 1:B:454:LEU:CD1 | 1:B:460:PHE:HE2 | 2.34 | 0.41 |
| 1:A:296:LYS:HE2 | 1:A:296:LYS:HB2 | 1.75 | 0.41 |
| 1:A:401:PRO:O | 1:A:405:ARG:NH1 | 2.53 | 0.41 |
| 1:A:219:MSE:HB2 | 1:A:219:MSE:HE3 | 1.86 | 0.41 |
| 1:B:235:ILE:HG22 | 1:B:269:TYR:OH | 2.21 | 0.41 |
| 1:C:274:CYS:HB2 | 1:C:484:ARG:O | 2.20 | 0.41 |
| 1:A:284:ALA:HB1 | 1:A:322:LEU:HD12 | 2.02 | 0.41 |
| 1:D:29:MSE:HE3 | 1:D:54:LEU:HG | 2.02 | 0.41 |
| 1:C:215:ASP:HA | 1:C:216:PRO:HD3 | 1.83 | 0.41 |
| 1:A:90:GLU:OE2 | 1:A:131:LYS:HD2 | 2.21 | 0.41 |
| 1:D:383:ILE:HG22 | 1:D:384:LEU:N | 2.35 | 0.41 |
| 1:C:260:HIS:CD2 | 1:C:264:ARG:HE | 2.39 | 0.41 |
| 1:A:66:LEU:HD22 | 1:A:70:ARG:NE | 2.36 | 0.41 |
| 1:D:104:ILE:HG21 | 1:D:519:ILE:HG22 | 2.03 | 0.41 |
| 1:A:396:GLY:O | 1:A:398:LEU:HD23 | 2.21 | 0.41 |
| 1:B:112:TYR:CD2 | 1:B:113:THR:HG22 | 2.56 | 0.41 |
| 1:D:77:SER:O | 1:D:81:LYS:HG3 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:26:LYS:HD3 | 1:A:29:MSE:HG3 | 2.03 | 0.41 |
| 1:A:434:TYR:OH | 1:A:443:PHE:HB3 | 2.21 | 0.41 |
| 1:D:456:ASP:OD1 | 1:D:458:ARG:HB2 | 2.20 | 0.41 |
| 1:C:418:ALA:O | 1:C:445:SER:HA | 2.21 | 0.41 |
| 1:A:308:LEU:HB3 | 1:A:389:ILE:CD1 | 2.51 | 0.41 |
| 1:A:169:LEU:HD22 | 1:A:422:PRO:HD3 | 2.03 | 0.41 |
| 1:A:372:SER:O | 1:A:383:ILE:HD13 | 2.21 | 0.41 |
| 1:C:33:ARG:HD2 | 1:C:93:GLU:OE2 | 2.21 | 0.41 |
| 1:D:407:MSE:CA | 1:D:407:MSE:CE | 2.98 | 0.41 |
| 1:B:104:ILE:HG23 | 1:B:105:GLU:N | 2.35 | 0.41 |
| 1:D:380:ALA:O | 1:D:384:LEU:HB2 | 2.21 | 0.41 |
| 1:D:408:ALA:HB2 | 1:D:437:THR:HG22 | 2.02 | 0.41 |
| 1:C:419:LEU:O | 3:C:2601:NAD:H2N | 2.21 | 0.41 |
| 1:B:194:ARG:NH2 | 1:B:196:ASP:OD1 | 2.54 | 0.41 |
| 1:A:22:LYS:HE3 | 1:C:24:LYS:O | 2.20 | 0.41 |
| 1:B:315:ALA:CB | 1:B:392:VAL:HG21 | 2.51 | 0.41 |
| 1:C:262:ALA:HB1 | 1:C:280:ILE:HD11 | 2.03 | 0.41 |
| 1:A:133:LEU:HB2 | 1:A:199:LEU:HD11 | 2.03 | 0.41 |
| 1:C:79:LEU:HD12 | 1:C:79:LEU:O | 2.21 | 0.40 |
| 1:C:550:ALA:O | 1:C:554:LYS:CG | 2.69 | 0.40 |
| 1:B:194:ARG:HB3 | 1:B:194:ARG:HE | 1.34 | 0.40 |
| 1:B:543:TYR:CE1 | 1:C:484:ARG:HG2 | 2.55 | 0.40 |
| 1:D:174:VAL:HG12 | 1:D:174:VAL:O | 2.21 | 0.40 |
| 1:C:295:GLN:O | 1:C:299:SER:N | 2.43 | 0.40 |
| 1:D:302:ILE:HG22 | 1:D:303:SER:N | 2.37 | 0.40 |
| 1:B:355:LYS:HE2 | 1:B:355:LYS:HB2 | 1.97 | 0.40 |
| 1:B:60:THR:O | 1:B:64:GLN:HG3 | 2.22 | 0.40 |
| 1:B:380:ALA:O | 1:B:384:LEU:HB2 | 2.21 | 0.40 |
| 1:C:235:ILE:O | 1:C:239:MSE:HG2 | 2.21 | 0.40 |
| 1:A:380:ALA:O | 1:A:384:LEU:HB2 | 2.21 | 0.40 |
| 1:A:526:ILE:O | 1:A:530:VAL:HG23 | 2.22 | 0.40 |
| 1:C:193:ILE:HD11 | 1:C:476:LEU:HB2 | 2.03 | 0.40 |
| 1:B:89:GLN:NE2 | 1:B:185:CYS:SG | 2.95 | 0.40 |
| 1:B:66:LEU:O | 1:B:70:ARG:HB2 | 2.21 | 0.40 |
| 1:C:201:VAL:HG12 | 1:C:202:CYS:N | 2.35 | 0.40 |
| 1:A:332:LEU:HA | 1:A:332:LEU:HD12 | 1.83 | 0.40 |
| 1:B:298:ILE:CG2 | 1:B:300:LYS:HB2 | 2.51 | 0.40 |
| 1:D:177:MSE:O | 1:D:180:PRO:HD2 | 2.21 | 0.40 |
| 1:A:24:LYS:O | 1:C:22:LYS:CE | 2.69 | 0.40 |
| 1:A:123:TYR:HB3 | 1:A:219:MSE:HE1 | 2.02 | 0.40 |
| 1:A:297:VAL:CG2 | 1:A:298:ILE:N | 2.84 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:128:ARG:HH11 | 1:B:128:ARG:CG | 2.29 | 0.40 |
| 1:A:559:ARG:HD3 | 1:A:559:ARG:HA | 1.92 | 0.40 |
| 1:D:221:LEU:HB3 | 1:D:223:GLN:HG2 | 2.03 | 0.40 |
| 1:B:171:ASP:CG | 1:B:225:ARG:HE | 2.23 | 0.40 |
| 1:A:97:TYR:CE2 | 1:A:188:THR:HB | 2.56 | 0.40 |
| 1:D:441:CYS:C | 1:D:442:LEU:HD23 | 2.42 | 0.40 |
| 1:B:358:ILE:HG22 | 1:B:359:ASP:N | 2.36 | 0.40 |
| 1:C:399:PHE:CG | 1:C:427:GLU:HB3 | 2.56 | 0.40 |
| 1:B:552:TYR:CE1 | 1:B:556:ARG:CZ | 3.05 | 0.40 |
| 1:B:174:VAL:CG2 | 1:B:220:GLY:HA3 | 2.50 | 0.40 |
| 1:B:66:LEU:HA | 1:B:66:LEU:HD23 | 1.89 | 0.40 |
| 1:B:69:HIS:HE1 | 1:B:102:ASP:OD2 | 2.05 | 0.40 |
| 1:A:177:MSE:CE | 1:A:177:MSE:O | 2.70 | 0.40 |
| 1:D:398:LEU:N | 1:D:398:LEU:CD1 | 2.84 | 0.40 |
| 1:D:33:ARG:HG3 | 1:D:33:ARG:NH1 | 2.36 | 0.40 |
| 1:C:75:MSE:HE1 | 1:C:84:TYR:CG | 2.56 | 0.40 |
| 1:B:248:ARG:HB3 | 1:C:543:TYR:OH | 2.22 | 0.40 |
| 5:B:4078:HOH:O | 1:C:543:TYR:HD1 | 2.05 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1 | A | 551/584 (94%) | 516 (94%) | 33 (6%) | 2 (0%) | 39 | 65 |
| 1 | B | 551/584 (94%) | 513 (93%) | 35 (6%) | 3 (0%) | 34 | 60 |
| 1 | C | 551/584 (94%) | 525 (95%) | 23 (4%) | 3 (0%) | 34 | 60 |
| 1 | D | 551/584 (94%) | 515 (94%) | 32 (6%) | 4 (1%) | 26 | 51 |
| All | All | 2204/2336 (94%) | 2069 (94%) | 123 (6%) | 12 (0%) | 34 | 60 |

All (12) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 332 | LEU |
| 1 | C | 332 | LEU |
| 1 | C | 392 | VAL |
| 1 | A | 332 | LEU |
| 1 | D | 270 | ARG |
| 1 | D | 332 | LEU |
| 1 | A | 433 | ALA |
| 1 | B | 121 | SER |
| 1 | C | 441 | CYS |
| 1 | D | 392 | VAL |
| 1 | B | 392 | VAL |
| 1 | D | 472 | PRO |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|---|
| 1 | A | 469/483 (97%) | 371 (79%) | 98 (21%) | 1 | 2 |
| 1 | B | 469/483 (97%) | 373 (80%) | 96 (20%) | 1 | 2 |
| 1 | C | 469/483 (97%) | 379 (81%) | 90 (19%) | 2 | 3 |
| 1 | D | 469/483 (97%) | 384 (82%) | 85 (18%) | 2 | 3 |
| All | All | 1876/1932 (97%) | 1507 (80%) | 369 (20%) | 1 | 2 |

All (369) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 21 | ILE |
| 1 | A | 23 | GLU |
| 1 | A | 26 | LYS |
| 1 | A | 29 | MSE |
| 1 | A | 43 | GLN |
| 1 | A | 45 | ARG |
| 1 | A | 60 | THR |
| 1 | A | 66 | LEU |
| 1 | A | 70 | ARG |
| 1 | A | 74 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 75 | MSE |
| 1 | A | 76 | THR |
| 1 | A | 85 | ILE |
| 1 | A | 90 | GLU |
| 1 | A | 100 | LEU |
| 1 | A | 107 | LEU |
| 1 | A | 118 | LEU |
| 1 | A | 121 | SER |
| 1 | A | 133 | LEU |
| 1 | A | 138 | SER |
| 1 | A | 140 | ARG |
| 1 | A | 152 | GLU |
| 1 | A | 153 | ASN |
| 1 | A | 154 | HIS |
| 1 | A | 165 | ARG |
| 1 | A | 169 | LEU |
| 1 | A | 183 | LYS |
| 1 | A | 185 | CYS |
| 1 | A | 193 | ILE |
| 1 | A | 197 | ARG |
| 1 | A | 210 | ILE |
| 1 | A | 221 | LEU |
| 1 | A | 225 | ARG |
| 1 | A | 226 | ASP |
| 1 | A | 227 | ARG |
| 1 | A | 232 | ASP |
| 1 | A | 233 | ASP |
| 1 | A | 236 | ASP |
| 1 | A | 251 | LEU |
| 1 | A | 267 | ARG |
| 1 | A | 275 | THR |
| 1 | A | 281 | GLN |
| 1 | A | 286 | VAL |
| 1 | A | 291 | LEU |
| 1 | A | 292 | LEU |
| 1 | A | 295 | GLN |
| 1 | A | 296 | LYS |
| 1 | A | 299 | SER |
| 1 | A | 300 | LYS |
| 1 | A | 303 | SER |
| 1 | A | 306 | LYS |
| 1 | A | 327 | MSE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 332 | LEU |
| 1 | A | 336 | GLU |
| 1 | A | 339 | LYS |
| 1 | A | 340 | LYS |
| 1 | A | 346 | LYS |
| 1 | A | 350 | LEU |
| 1 | A | 355 | LYS |
| 1 | A | 359 | ASP |
| 1 | A | 360 | SER |
| 1 | A | 363 | GLU |
| 1 | A | 371 | GLU |
| 1 | A | 375 | ASP |
| 1 | A | 384 | LEU |
| 1 | A | 385 | LYS |
| 1 | A | 389 | ILE |
| 1 | A | 392 | VAL |
| 1 | A | 397 | ARG |
| 1 | A | 398 | LEU |
| 1 | A | 405 | ARG |
| 1 | A | 409 | SER |
| 1 | A | 425 | GLN |
| 1 | A | 431 | GLU |
| 1 | A | 432 | GLU |
| 1 | A | 436 | LEU |
| 1 | A | 467 | ASN |
| 1 | A | 484 | ARG |
| 1 | A | 487 | SER |
| 1 | A | 488 | ASP |
| 1 | A | 489 | SER |
| 1 | A | 492 | LEU |
| 1 | A | 493 | GLU |
| 1 | A | 499 | THR |
| 1 | A | 502 | LEU |
| 1 | A | 504 | ASP |
| 1 | A | 505 | GLU |
| 1 | A | 507 | LEU |
| 1 | A | 509 | GLN |
| 1 | A | 511 | ARG |
| 1 | A | 516 | LEU |
| 1 | A | 520 | GLN |
| 1 | A | 529 | LYS |
| 1 | A | 542 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 556 | ARG |
| 1 | A | 559 | ARG |
| 1 | A | 561 | GLU |
| 1 | A | 571 | GLU |
| 1 | B | 21 | ILE |
| 1 | B | 22 | LYS |
| 1 | B | 23 | GLU |
| 1 | B | 24 | LYS |
| 1 | B | 33 | ARG |
| 1 | B | 43 | GLN |
| 1 | B | 47 | MSE |
| 1 | B | 66 | LEU |
| 1 | B | 70 | ARG |
| 1 | B | 73 | LYS |
| 1 | B | 74 | LYS |
| 1 | B | 80 | GLU |
| 1 | B | 94 | LYS |
| 1 | B | 100 | LEU |
| 1 | B | 104 | ILE |
| 1 | B | 105 | GLU |
| 1 | B | 111 | VAL |
| 1 | B | 121 | SER |
| 1 | B | 123 | TYR |
| 1 | B | 129 | ARG |
| 1 | B | 133 | LEU |
| 1 | B | 136 | SER |
| 1 | B | 138 | SER |
| 1 | B | 140 | ARG |
| 1 | B | 153 | ASN |
| 1 | B | 156 | LYS |
| 1 | B | 164 | GLU |
| 1 | B | 165 | ARG |
| 1 | B | 177 | MSE |
| 1 | B | 183 | LYS |
| 1 | B | 194 | ARG |
| 1 | B | 197 | ARG |
| 1 | B | 203 | ILE |
| 1 | B | 210 | ILE |
| 1 | B | 214 | LYS |
| 1 | B | 223 | GLN |
| 1 | B | 224 | LYS |
| 1 | B | 225 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 227 | ARG |
| 1 | B | 230 | GLN |
| 1 | B | 232 | ASP |
| 1 | B | 233 | ASP |
| 1 | B | 236 | ASP |
| 1 | B | 248 | ARG |
| 1 | B | 251 | LEU |
| 1 | B | 252 | ILE |
| 1 | B | 264 | ARG |
| 1 | B | 271 | GLU |
| 1 | B | 272 | LYS |
| 1 | B | 283 | THR |
| 1 | B | 286 | VAL |
| 1 | B | 291 | LEU |
| 1 | B | 292 | LEU |
| 1 | B | 300 | LYS |
| 1 | B | 302 | ILE |
| 1 | B | 303 | SER |
| 1 | B | 304 | GLU |
| 1 | B | 328 | VAL |
| 1 | B | 334 | GLU |
| 1 | B | 335 | GLN |
| 1 | B | 340 | LYS |
| 1 | B | 343 | MSE |
| 1 | B | 346 | LYS |
| 1 | B | 354 | ARG |
| 1 | B | 355 | LYS |
| 1 | B | 357 | LYS |
| 1 | B | 372 | SER |
| 1 | B | 384 | LEU |
| 1 | B | 385 | LYS |
| 1 | B | 397 | ARG |
| 1 | B | 398 | LEU |
| 1 | B | 402 | ASP |
| 1 | B | 405 | ARG |
| 1 | B | 409 | SER |
| 1 | B | 413 | ARG |
| 1 | B | 423 | THR |
| 1 | B | 429 | THR |
| 1 | B | 436 | LEU |
| 1 | B | 458 | ARG |
| 1 | B | 480 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 481 | CYS |
| 1 | B | 499 | THR |
| 1 | B | 502 | LEU |
| 1 | B | 509 | GLN |
| 1 | B | 511 | ARG |
| 1 | B | 519 | ILE |
| 1 | B | 520 | GLN |
| 1 | B | 531 | THR |
| 1 | B | 537 | ASN |
| 1 | B | 547 | GLU |
| 1 | B | 549 | LYS |
| 1 | B | 551 | LYS |
| 1 | B | 556 | ARG |
| 1 | B | 557 | THR |
| 1 | B | 559 | ARG |
| 1 | B | 564 | SER |
| 1 | C | 21 | ILE |
| 1 | C | 22 | LYS |
| 1 | C | 23 | GLU |
| 1 | C | 24 | LYS |
| 1 | C | 33 | ARG |
| 1 | C | 38 | MSE |
| 1 | C | 43 | GLN |
| 1 | C | 57 | LYS |
| 1 | C | 58 | ILE |
| 1 | C | 66 | LEU |
| 1 | C | 70 | ARG |
| 1 | C | 73 | LYS |
| 1 | C | 74 | LYS |
| 1 | C | 79 | LEU |
| 1 | C | 85 | ILE |
| 1 | C | 99 | ILE |
| 1 | C | 100 | LEU |
| 1 | C | 104 | ILE |
| 1 | C | 108 | MSE |
| 1 | C | 118 | LEU |
| 1 | C | 123 | TYR |
| 1 | C | 129 | ARG |
| 1 | C | 133 | LEU |
| 1 | C | 137 | ILE |
| 1 | C | 140 | ARG |
| 1 | C | 156 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 164 | GLU |
| 1 | C | 165 | ARG |
| 1 | C | 169 | LEU |
| 1 | C | 187 | TYR |
| 1 | C | 197 | ARG |
| 1 | C | 210 | ILE |
| 1 | C | 213 | LEU |
| 1 | C | 214 | LYS |
| 1 | C | 219 | MSE |
| 1 | C | 225 | ARG |
| 1 | C | 230 | GLN |
| 1 | C | 232 | ASP |
| 1 | C | 236 | ASP |
| 1 | C | 240 | LYS |
| 1 | C | 245 | ARG |
| 1 | C | 248 | ARG |
| 1 | C | 267 | ARG |
| 1 | C | 272 | LYS |
| 1 | C | 277 | ASN |
| 1 | C | 286 | VAL |
| 1 | C | 292 | LEU |
| 1 | C | 297 | VAL |
| 1 | C | 298 | ILE |
| 1 | C | 299 | SER |
| 1 | C | 306 | LYS |
| 1 | C | 325 | MSE |
| 1 | C | 332 | LEU |
| 1 | C | 333 | SER |
| 1 | C | 335 | GLN |
| 1 | C | 346 | LYS |
| 1 | C | 350 | LEU |
| 1 | C | 355 | LYS |
| 1 | C | 357 | LYS |
| 1 | C | 360 | SER |
| 1 | C | 363 | GLU |
| 1 | C | 368 | SER |
| 1 | C | 372 | SER |
| 1 | C | 384 | LEU |
| 1 | C | 390 | ILE |
| 1 | C | 402 | ASP |
| 1 | C | 404 | ILE |
| 1 | C | 409 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 420 | SER |
| 1 | C | 436 | LEU |
| 1 | C | 438 | GLU |
| 1 | C | 452 | VAL |
| 1 | C | 453 | LYS |
| 1 | C | 456 | ASP |
| 1 | C | 458 | ARG |
| 1 | C | 492 | LEU |
| 1 | C | 499 | THR |
| 1 | C | 502 | LEU |
| 1 | C | 504 | ASP |
| 1 | C | 507 | LEU |
| 1 | C | 509 | GLN |
| 1 | C | 518 | ASN |
| 1 | C | 520 | GLN |
| 1 | C | 521 | GLU |
| 1 | C | 531 | THR |
| 1 | C | 538 | LYS |
| 1 | C | 551 | LYS |
| 1 | C | 554 | LYS |
| 1 | C | 556 | ARG |
| 1 | C | 571 | GLU |
| 1 | D | 22 | LYS |
| 1 | D | 23 | GLU |
| 1 | D | 24 | LYS |
| 1 | D | 26 | LYS |
| 1 | D | 33 | ARG |
| 1 | D | 43 | GLN |
| 1 | D | 51 | GLN |
| 1 | D | 57 | LYS |
| 1 | D | 62 | ASP |
| 1 | D | 63 | ILE |
| 1 | D | 66 | LEU |
| 1 | D | 70 | ARG |
| 1 | D | 73 | LYS |
| 1 | D | 75 | MSE |
| 1 | D | 76 | THR |
| 1 | D | 85 | ILE |
| 1 | D | 91 | ARG |
| 1 | D | 101 | GLN |
| 1 | D | 104 | ILE |
| 1 | D | 125 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 128 | ARG |
| 1 | D | 133 | LEU |
| 1 | D | 138 | SER |
| 1 | D | 140 | ARG |
| 1 | D | 153 | ASN |
| 1 | D | 156 | LYS |
| 1 | D | 165 | ARG |
| 1 | D | 169 | LEU |
| 1 | D | 210 | ILE |
| 1 | D | 214 | LYS |
| 1 | D | 221 | LEU |
| 1 | D | 225 | ARG |
| 1 | D | 229 | GLN |
| 1 | D | 230 | GLN |
| 1 | D | 233 | ASP |
| 1 | D | 236 | ASP |
| 1 | D | 240 | LYS |
| 1 | D | 249 | ASN |
| 1 | D | 251 | LEU |
| 1 | D | 266 | LEU |
| 1 | D | 268 | LYS |
| 1 | D | 271 | GLU |
| 1 | D | 272 | LYS |
| 1 | D | 286 | VAL |
| 1 | D | 291 | LEU |
| 1 | D | 292 | LEU |
| 1 | D | 296 | LYS |
| 1 | D | 297 | VAL |
| 1 | D | 300 | LYS |
| 1 | D | 302 | ILE |
| 1 | D | 305 | HIS |
| 1 | D | 306 | LYS |
| 1 | D | 332 | LEU |
| 1 | D | 335 | GLN |
| 1 | D | 350 | LEU |
| 1 | D | 355 | LYS |
| 1 | D | 357 | LYS |
| 1 | D | 358 | ILE |
| 1 | D | 360 | SER |
| 1 | D | 371 | GLU |
| 1 | D | 373 | ILE |
| 1 | D | 384 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 389 | ILE |
| 1 | D | 392 | VAL |
| 1 | D | 409 | SER |
| 1 | D | 447 | SER |
| 1 | D | 458 | ARG |
| 1 | D | 489 | SER |
| 1 | D | 492 | LEU |
| 1 | D | 500 | SER |
| 1 | D | 502 | LEU |
| 1 | D | 504 | ASP |
| 1 | D | 507 | LEU |
| 1 | D | 520 | GLN |
| 1 | D | 529 | LYS |
| 1 | D | 531 | THR |
| 1 | D | 542 | ARG |
| 1 | D | 543 | TYR |
| 1 | D | 551 | LYS |
| 1 | D | 554 | LYS |
| 1 | D | 556 | ARG |
| 1 | D | 559 | ARG |
| 1 | D | 561 | GLU |
| 1 | D | 564 | SER |
| 1 | D | 572 | TRP |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 51 | GLN |
| 1 | A | 64 | GLN |
| 1 | A | 89 | GLN |
| 1 | A | 101 | GLN |
| 1 | A | 153 | ASN |
| 1 | A | 261 | ASN |
| 1 | A | 281 | GLN |
| 1 | A | 305 | HIS |
| 1 | A | 425 | GLN |
| 1 | A | 482 | ASN |
| 1 | A | 520 | GLN |
| 1 | B | 43 | GLN |
| 1 | B | 64 | GLN |
| 1 | B | 69 | HIS |
| 1 | B | 229 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 260 | HIS |
| 1 | B | 261 | ASN |
| 1 | B | 330 | ASN |
| 1 | B | 335 | GLN |
| 1 | B | 482 | ASN |
| 1 | B | 485 | HIS |
| 1 | B | 501 | GLN |
| 1 | B | 518 | ASN |
| 1 | B | 525 | ASN |
| 1 | B | 537 | ASN |
| 1 | C | 43 | GLN |
| 1 | C | 64 | GLN |
| 1 | C | 69 | HIS |
| 1 | C | 229 | GLN |
| 1 | C | 230 | GLN |
| 1 | C | 261 | ASN |
| 1 | C | 277 | ASN |
| 1 | C | 321 | ASN |
| 1 | C | 330 | ASN |
| 1 | C | 335 | GLN |
| 1 | C | 425 | GLN |
| 1 | C | 482 | ASN |
| 1 | C | 509 | GLN |
| 1 | C | 520 | GLN |
| 1 | D | 51 | GLN |
| 1 | D | 64 | GLN |
| 1 | D | 153 | ASN |
| 1 | D | 154 | HIS |
| 1 | D | 223 | GLN |
| 1 | D | 229 | GLN |
| 1 | D | 230 | GLN |
| 1 | D | 261 | ASN |
| 1 | D | 330 | ASN |
| 1 | D | 482 | ASN |
| 1 | D | 485 | HIS |
| 1 | D | 520 | GLN |
| 1 | D | 537 | ASN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | # $ Z > 2$ | Counts | RMSZ | # $ Z > 2$ |
| 3 | NAD | A | 601 | - | 38,48,48 | 1.69 | 8 (21%) | 47,73,73 | 2.07 | 7 (14%) |
| 3 | NAD | A | 602 | - | 38,48,48 | 1.96 | 9 (23%) | 47,73,73 | 1.98 | 5 (10%) |
| 4 | TTN | A | 603 | 2 | 1,7,7 | 0.34 | 0 | 2,9,9 | 0.36 | 0 |
| 3 | NAD | B | 1601 | - | 38,48,48 | 1.75 | 9 (23%) | 47,73,73 | 2.07 | 8 (17%) |
| 3 | NAD | B | 1602 | - | 38,48,48 | 1.90 | 10 (26%) | 47,73,73 | 1.88 | 5 (10%) |
| 4 | TTN | B | 1603 | 2 | 1,7,7 | 0.37 | 0 | 2,9,9 | 0.70 | 0 |
| 3 | NAD | C | 2601 | - | 38,48,48 | 1.75 | 9 (23%) | 47,73,73 | 2.10 | 6 (12%) |
| 3 | NAD | C | 2602 | - | 38,48,48 | 2.09 | 11 (28%) | 47,73,73 | 1.86 | 5 (10%) |
| 4 | TTN | C | 2603 | 2 | 1,7,7 | 0.13 | 0 | 2,9,9 | 0.95 | 0 |
| 3 | NAD | D | 3601 | - | 38,48,48 | 1.84 | 9 (23%) | 47,73,73 | 2.02 | 7 (14%) |
| 3 | NAD | D | 3602 | - | 38,48,48 | 2.01 | 11 (28%) | 47,73,73 | 1.94 | 4 (8%) |
| 4 | TTN | D | 3603 | 2 | 1,7,7 | 0.40 | 0 | 2,9,9 | 0.58 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 3 | NAD | A | 601 | - | - | 0/22/62/62 | 0/5/5/5 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 3 | NAD | A | 602 | - | - | 0/22/62/62 | 0/5/5/5 |
| 4 | TTN | A | 603 | 2 | - | 0/0/8/8 | 0/0/0/0 |
| 3 | NAD | B | 1601 | - | - | 0/22/62/62 | 0/5/5/5 |
| 3 | NAD | B | 1602 | - | - | 0/22/62/62 | 0/5/5/5 |
| 4 | TTN | B | 1603 | 2 | - | 0/0/8/8 | 0/0/0/0 |
| 3 | NAD | C | 2601 | - | - | 0/22/62/62 | 0/5/5/5 |
| 3 | NAD | C | 2602 | - | - | 0/22/62/62 | 0/5/5/5 |
| 4 | TTN | C | 2603 | 2 | - | 0/0/8/8 | 0/0/0/0 |
| 3 | NAD | D | 3601 | - | - | 0/22/62/62 | 0/5/5/5 |
| 3 | NAD | D | 3602 | - | - | 0/22/62/62 | 0/5/5/5 |
| 4 | TTN | D | 3603 | 2 | - | 0/0/8/8 | 0/0/0/0 |

All (76) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3 | C | 2601 | NAD | C5A-C4A | -3.50 | 1.32 | 1.40 |
| 3 | A | 601 | NAD | C5A-C4A | -3.29 | 1.33 | 1.40 |
| 3 | A | 602 | NAD | C5A-C4A | -3.10 | 1.33 | 1.40 |
| 3 | B | 1602 | NAD | C5A-C4A | -3.03 | 1.33 | 1.40 |
| 3 | B | 1601 | NAD | C5A-C4A | -2.91 | 1.33 | 1.40 |
| 3 | C | 2602 | NAD | C5A-C4A | -2.88 | 1.34 | 1.40 |
| 3 | D | 3601 | NAD | C5A-C4A | -2.79 | 1.34 | 1.40 |
| 3 | D | 3602 | NAD | C5A-C4A | -2.62 | 1.34 | 1.40 |
| 3 | B | 1601 | NAD | C5A-N7A | -2.54 | 1.30 | 1.39 |
| 3 | D | 3602 | NAD | C5A-N7A | -2.43 | 1.31 | 1.39 |
| 3 | C | 2601 | NAD | C5A-N7A | -2.30 | 1.31 | 1.39 |
| 3 | D | 3601 | NAD | C5A-N7A | -2.29 | 1.31 | 1.39 |
| 3 | A | 601 | NAD | C5A-N7A | -2.26 | 1.31 | 1.39 |
| 3 | C | 2602 | NAD | C5A-N7A | -2.24 | 1.31 | 1.39 |
| 3 | A | 602 | NAD | C5A-N7A | -2.21 | 1.31 | 1.39 |
| 3 | B | 1602 | NAD | C5A-N7A | -2.18 | 1.32 | 1.39 |
| 3 | B | 1602 | NAD | O4D-C4D | 2.01 | 1.49 | 1.45 |
| 3 | D | 3602 | NAD | C2A-N1A | 2.05 | 1.37 | 1.33 |
| 3 | D | 3602 | NAD | C2N-C3N | 2.05 | 1.42 | 1.39 |
| 3 | C | 2602 | NAD | C2N-C3N | 2.06 | 1.42 | 1.39 |
| 3 | B | 1601 | NAD | C4N-C3N | 2.08 | 1.42 | 1.39 |
| 3 | B | 1602 | NAD | C2A-N1A | 2.09 | 1.37 | 1.33 |
| 3 | C | 2602 | NAD | C4N-C3N | 2.11 | 1.42 | 1.39 |
| 3 | A | 602 | NAD | O4D-C4D | 2.12 | 1.49 | 1.45 |
| 3 | A | 602 | NAD | C4N-C3N | 2.13 | 1.42 | 1.39 |
| 3 | C | 2601 | NAD | C4N-C3N | 2.13 | 1.42 | 1.39 |
| 3 | C | 2602 | NAD | PN-O5D | 2.16 | 1.68 | 1.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 3 | B | 1602 | NAD | C4N-C3N | 2.16 | 1.43 | 1.39 |
| 3 | D | 3602 | NAD | C4N-C3N | 2.16 | 1.43 | 1.39 |
| 3 | A | 601 | NAD | C2A-N1A | 2.17 | 1.38 | 1.33 |
| 3 | C | 2601 | NAD | C5N-C4N | 2.26 | 1.43 | 1.38 |
| 3 | D | 3602 | NAD | O4D-C4D | 2.32 | 1.50 | 1.45 |
| 3 | C | 2601 | NAD | O4D-C1D | 2.39 | 1.44 | 1.41 |
| 3 | D | 3601 | NAD | C4N-C3N | 2.55 | 1.43 | 1.39 |
| 3 | B | 1601 | NAD | C2A-N3A | 2.58 | 1.36 | 1.32 |
| 3 | B | 1601 | NAD | C2A-N1A | 2.59 | 1.38 | 1.33 |
| 3 | A | 601 | NAD | O4D-C1D | 2.62 | 1.44 | 1.41 |
| 3 | D | 3601 | NAD | C2A-N1A | 2.67 | 1.39 | 1.33 |
| 3 | D | 3602 | NAD | C3N-C7N | 2.72 | 1.54 | 1.50 |
| 3 | C | 2602 | NAD | C2A-N3A | 2.79 | 1.37 | 1.32 |
| 3 | A | 601 | NAD | C3N-C7N | 2.93 | 1.55 | 1.50 |
| 3 | A | 601 | NAD | C6N-N1N | 2.99 | 1.43 | 1.35 |
| 3 | A | 602 | NAD | C3N-C7N | 3.04 | 1.55 | 1.50 |
| 3 | C | 2602 | NAD | C3N-C7N | 3.04 | 1.55 | 1.50 |
| 3 | A | 602 | NAD | C2A-N3A | 3.06 | 1.37 | 1.32 |
| 3 | C | 2602 | NAD | O4D-C4D | 3.12 | 1.52 | 1.45 |
| 3 | B | 1602 | NAD | C2A-N3A | 3.13 | 1.37 | 1.32 |
| 3 | C | 2601 | NAD | C2A-N3A | 3.15 | 1.37 | 1.32 |
| 3 | B | 1602 | NAD | C3N-C7N | 3.18 | 1.55 | 1.50 |
| 3 | B | 1601 | NAD | C3N-C7N | 3.25 | 1.55 | 1.50 |
| 3 | B | 1601 | NAD | C6N-N1N | 3.27 | 1.44 | 1.35 |
| 3 | A | 601 | NAD | C2A-N3A | 3.27 | 1.38 | 1.32 |
| 3 | B | 1602 | NAD | C6N-N1N | 3.29 | 1.44 | 1.35 |
| 3 | D | 3602 | NAD | C2A-N3A | 3.32 | 1.38 | 1.32 |
| 3 | D | 3601 | NAD | C2A-N3A | 3.36 | 1.38 | 1.32 |
| 3 | C | 2602 | NAD | C6N-N1N | 3.37 | 1.44 | 1.35 |
| 3 | D | 3601 | NAD | C3N-C7N | 3.46 | 1.56 | 1.50 |
| 3 | D | 3602 | NAD | C6N-N1N | 3.46 | 1.44 | 1.35 |
| 3 | C | 2601 | NAD | C6N-N1N | 3.50 | 1.44 | 1.35 |
| 3 | A | 602 | NAD | C6N-N1N | 3.50 | 1.44 | 1.35 |
| 3 | B | 1602 | NAD | O4B-C1B | 3.65 | 1.45 | 1.41 |
| 3 | D | 3601 | NAD | C6N-N1N | 3.77 | 1.45 | 1.35 |
| 3 | B | 1601 | NAD | O4D-C1D | 3.85 | 1.46 | 1.41 |
| 3 | D | 3601 | NAD | O4D-C1D | 3.87 | 1.46 | 1.41 |
| 3 | C | 2601 | NAD | O4B-C1B | 3.96 | 1.46 | 1.41 |
| 3 | D | 3602 | NAD | O4B-C1B | 4.05 | 1.46 | 1.41 |
| 3 | C | 2601 | NAD | C3N-C7N | 4.11 | 1.57 | 1.50 |
| 3 | C | 2602 | NAD | O4B-C1B | 4.37 | 1.46 | 1.41 |
| 3 | A | 602 | NAD | O4B-C1B | 4.44 | 1.46 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 3 | B | 1601 | NAD | O4B-C1B | 4.51 | 1.46 | 1.41 |
| 3 | D | 3601 | NAD | O4B-C1B | 4.90 | 1.47 | 1.41 |
| 3 | A | 601 | NAD | O4B-C1B | 4.98 | 1.47 | 1.41 |
| 3 | A | 602 | NAD | O4D-C1D | 6.22 | 1.49 | 1.41 |
| 3 | B | 1602 | NAD | O4D-C1D | 6.40 | 1.49 | 1.41 |
| 3 | D | 3602 | NAD | O4D-C1D | 7.12 | 1.50 | 1.41 |
| 3 | C | 2602 | NAD | O4D-C1D | 7.41 | 1.50 | 1.41 |

All (47) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 3 | C | 2601 | NAD | N3A-C2A-N1A | -11.20 | 120.32 | 128.89 |
| 3 | A | 602 | NAD | N3A-C2A-N1A | -10.87 | 120.57 | 128.89 |
| 3 | A | 601 | NAD | N3A-C2A-N1A | -10.79 | 120.64 | 128.89 |
| 3 | B | 1601 | NAD | N3A-C2A-N1A | -10.64 | 120.75 | 128.89 |
| 3 | D | 3601 | NAD | N3A-C2A-N1A | -10.60 | 120.78 | 128.89 |
| 3 | D | 3602 | NAD | N3A-C2A-N1A | -10.47 | 120.88 | 128.89 |
| 3 | B | 1602 | NAD | N3A-C2A-N1A | -10.26 | 121.04 | 128.89 |
| 3 | C | 2602 | NAD | N3A-C2A-N1A | -10.00 | 121.24 | 128.89 |
| 3 | C | 2601 | NAD | C4B-O4B-C1B | -2.75 | 106.70 | 109.72 |
| 3 | C | 2601 | NAD | C4D-O4D-C1D | -2.64 | 106.82 | 109.72 |
| 3 | D | 3601 | NAD | C4D-O4D-C1D | -2.64 | 106.82 | 109.72 |
| 3 | B | 1601 | NAD | C3N-C7N-N7N | -2.59 | 114.98 | 117.82 |
| 3 | A | 601 | NAD | C4D-O4D-C1D | -2.44 | 107.03 | 109.72 |
| 3 | B | 1601 | NAD | C4D-O4D-C1D | -2.41 | 107.07 | 109.72 |
| 3 | D | 3601 | NAD | C3N-C7N-N7N | -2.32 | 115.28 | 117.82 |
| 3 | A | 601 | NAD | C3N-C7N-N7N | -2.31 | 115.29 | 117.82 |
| 3 | A | 601 | NAD | C4B-O4B-C1B | -2.30 | 107.19 | 109.72 |
| 3 | B | 1601 | NAD | C4B-O4B-C1B | -2.28 | 107.21 | 109.72 |
| 3 | D | 3601 | NAD | C4B-O4B-C1B | -2.19 | 107.31 | 109.72 |
| 3 | C | 2602 | NAD | C3N-C7N-N7N | -2.19 | 115.42 | 117.82 |
| 3 | A | 602 | NAD | C3N-C7N-N7N | -2.19 | 115.42 | 117.82 |
| 3 | B | 1602 | NAD | C3N-C7N-N7N | -2.14 | 115.47 | 117.82 |
| 3 | B | 1601 | NAD | C1B-N9A-C4A | -2.05 | 123.85 | 126.94 |
| 3 | B | 1602 | NAD | C2D-C3D-C4D | 2.03 | 106.79 | 102.61 |
| 3 | C | 2602 | NAD | C2D-C3D-C4D | 2.04 | 106.81 | 102.61 |
| 3 | C | 2601 | NAD | O4B-C1B-N9A | 2.04 | 112.37 | 108.10 |
| 3 | A | 602 | NAD | C2D-C3D-C4D | 2.09 | 106.91 | 102.61 |
| 3 | D | 3602 | NAD | C2D-C3D-C4D | 2.12 | 106.97 | 102.61 |
| 3 | D | 3601 | NAD | O4B-C1B-N9A | 2.35 | 113.03 | 108.10 |
| 3 | A | 601 | NAD | O4B-C1B-N9A | 2.41 | 113.14 | 108.10 |
| 3 | B | 1601 | NAD | O4B-C1B-N9A | 2.87 | 114.10 | 108.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 3 | A | 602 | NAD | O4D-C1D-N1N | 3.23 | 111.68 | 108.13 |
| 3 | D | 3601 | NAD | O4D-C1D-N1N | 3.36 | 111.83 | 108.13 |
| 3 | A | 601 | NAD | O4D-C1D-N1N | 3.47 | 111.95 | 108.13 |
| 3 | C | 2602 | NAD | O4D-C1D-N1N | 3.53 | 112.01 | 108.13 |
| 3 | C | 2601 | NAD | O4D-C1D-N1N | 3.61 | 112.10 | 108.13 |
| 3 | D | 3602 | NAD | O4D-C1D-N1N | 3.79 | 112.29 | 108.13 |
| 3 | B | 1602 | NAD | C4A-C5A-N7A | 3.88 | 113.05 | 109.48 |
| 3 | B | 1602 | NAD | O4D-C1D-N1N | 3.92 | 112.43 | 108.13 |
| 3 | B | 1601 | NAD | O4D-C1D-N1N | 3.95 | 112.47 | 108.13 |
| 3 | C | 2602 | NAD | C4A-C5A-N7A | 4.11 | 113.26 | 109.48 |
| 3 | D | 3602 | NAD | C4A-C5A-N7A | 4.15 | 113.30 | 109.48 |
| 3 | A | 602 | NAD | C4A-C5A-N7A | 4.52 | 113.64 | 109.48 |
| 3 | D | 3601 | NAD | C4A-C5A-N7A | 4.72 | 113.82 | 109.48 |
| 3 | C | 2601 | NAD | C4A-C5A-N7A | 4.73 | 113.83 | 109.48 |
| 3 | B | 1601 | NAD | C4A-C5A-N7A | 4.74 | 113.84 | 109.48 |
| 3 | A | 601 | NAD | C4A-C5A-N7A | 4.75 | 113.85 | 109.48 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 21 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3 | A | 601 | NAD | 4 | 0 |
| 3 | A | 602 | NAD | 2 | 0 |
| 3 | B | 1601 | NAD | 1 | 0 |
| 3 | B | 1602 | NAD | 1 | 0 |
| 4 | B | 1603 | TTN | 1 | 0 |
| 3 | C | 2601 | NAD | 4 | 0 |
| 3 | C | 2602 | NAD | 1 | 0 |
| 4 | C | 2603 | TTN | 2 | 0 |
| 3 | D | 3601 | NAD | 1 | 0 |
| 3 | D | 3602 | NAD | 3 | 0 |
| 4 | D | 3603 | TTN | 1 | 0 |

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.