



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2020 – 02:21 PM BST

PDB ID : 2GR9
Title : Crystal structure of P5CR complexed with NADH
Authors : Meng, Z.; Lou, Z.; Liu, Z.; Rao, Z.
Deposited on : 2006-04-23
Resolution : 3.10 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.2

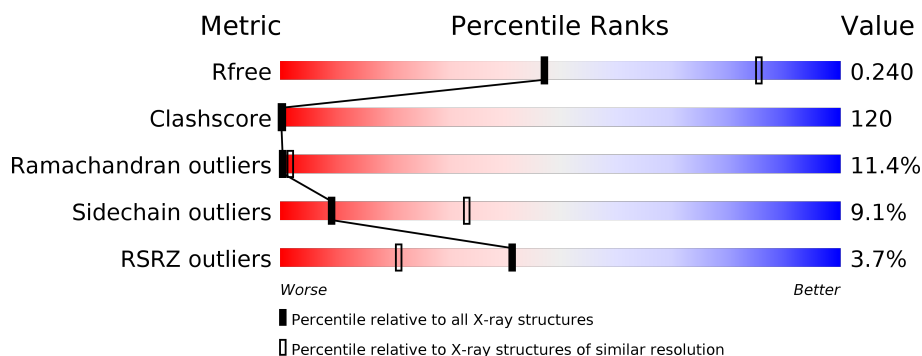
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 1094 (3.10-3.10) |
| Clashscore | 141614 | 1184 (3.10-3.10) |
| Ramachandran outliers | 138981 | 1141 (3.10-3.10) |
| Sidechain outliers | 138945 | 1141 (3.10-3.10) |
| RSRZ outliers | 127900 | 1067 (3.10-3.10) |

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 277 | <div> <div>19%</div> <div>63%</div> <div>16%</div> <div>.</div> </div> |
| 1 | B | 277 | <div> <div>8%</div> <div>18%</div> <div>65%</div> <div>14%</div> <div>.</div> </div> |
| 1 | C | 277 | <div> <div>7%</div> <div>19%</div> <div>68%</div> <div>13%</div> </div> |
| 1 | D | 277 | <div> <div>%</div> <div>21%</div> <div>67%</div> <div>11%</div> <div>.</div> </div> |
| 1 | E | 277 | <div> <div>2%</div> <div>17%</div> <div>67%</div> <div>15%</div> <div>.</div> </div> |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 2 | NAI | A | 1300 | X | - | X | X |
| 2 | NAI | B | 2300 | X | - | X | X |
| 2 | NAI | C | 3300 | X | - | X | X |
| 2 | NAI | D | 4300 | X | - | X | X |
| 2 | NAI | E | 5300 | X | - | X | - |
| 3 | GLU | A | 1301 | - | - | X | X |
| 3 | GLU | B | 2301 | - | - | X | X |
| 3 | GLU | C | 3301 | - | - | X | X |
| 3 | GLU | D | 4301 | - | - | X | X |
| 3 | GLU | E | 5301 | - | - | X | X |

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11077 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.

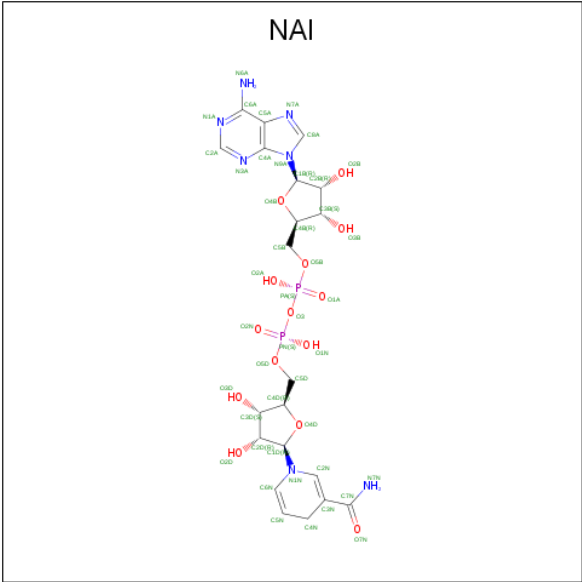
- Molecule 1 is a protein called Pyrroline-5-carboxylate reductase 1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 277 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2038 | 1279 | 363 | 383 | 13 | | | |
| 1 | B | 276 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2023 | 1270 | 358 | 382 | 13 | | | |
| 1 | C | 277 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2032 | 1276 | 360 | 383 | 13 | | | |
| 1 | D | 277 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2038 | 1279 | 363 | 383 | 13 | | | |
| 1 | E | 277 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2038 | 1279 | 363 | 383 | 13 | | | |

There are 10 discrepancies between the modelled and reference sequences:

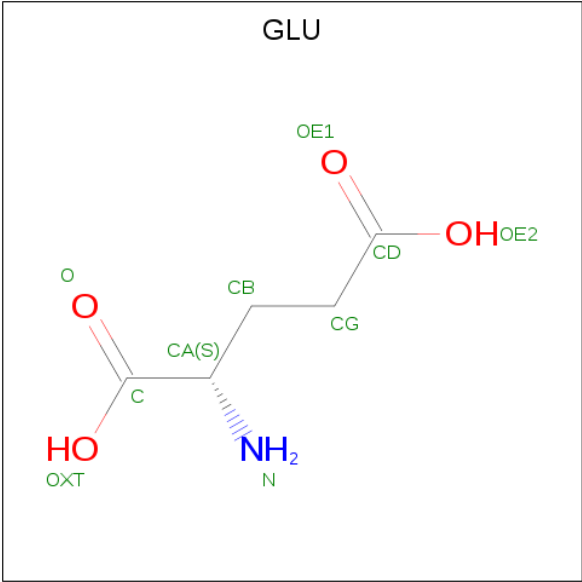
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------------|------------|
| A | -1 | ARG | - | cloning artifact | UNP P32322 |
| A | 0 | GLY | - | cloning artifact | UNP P32322 |
| B | -1 | ARG | - | cloning artifact | UNP P32322 |
| B | 0 | GLY | - | cloning artifact | UNP P32322 |
| C | -1 | ARG | - | cloning artifact | UNP P32322 |
| C | 0 | GLY | - | cloning artifact | UNP P32322 |
| D | -1 | ARG | - | cloning artifact | UNP P32322 |
| D | 0 | GLY | - | cloning artifact | UNP P32322 |
| E | -1 | ARG | - | cloning artifact | UNP P32322 |
| E | 0 | GLY | - | cloning artifact | UNP P32322 |

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 2 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 43 | 21 | 6 | 14 | 2 | | |
| 2 | B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 43 | 21 | 6 | 14 | 2 | | |
| 2 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 43 | 21 | 6 | 14 | 2 | | |
| 2 | D | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 43 | 21 | 6 | 14 | 2 | | |
| 2 | E | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 43 | 21 | 6 | 14 | 2 | | |

- Molecule 3 is GLUTAMIC ACID (three-letter code: GLU) (formula: C₅H₉NO₄).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 3 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 10 | 5 | 1 | 4 | | |
| 3 | B | 1 | Total | C | N | O | 0 | 0 |
| | | | 10 | 5 | 1 | 4 | | |
| 3 | C | 1 | Total | C | N | O | 0 | 0 |
| | | | 10 | 5 | 1 | 4 | | |
| 3 | D | 1 | Total | C | N | O | 0 | 0 |
| | | | 10 | 5 | 1 | 4 | | |
| 3 | E | 1 | Total | C | N | O | 0 | 0 |
| | | | 10 | 5 | 1 | 4 | | |

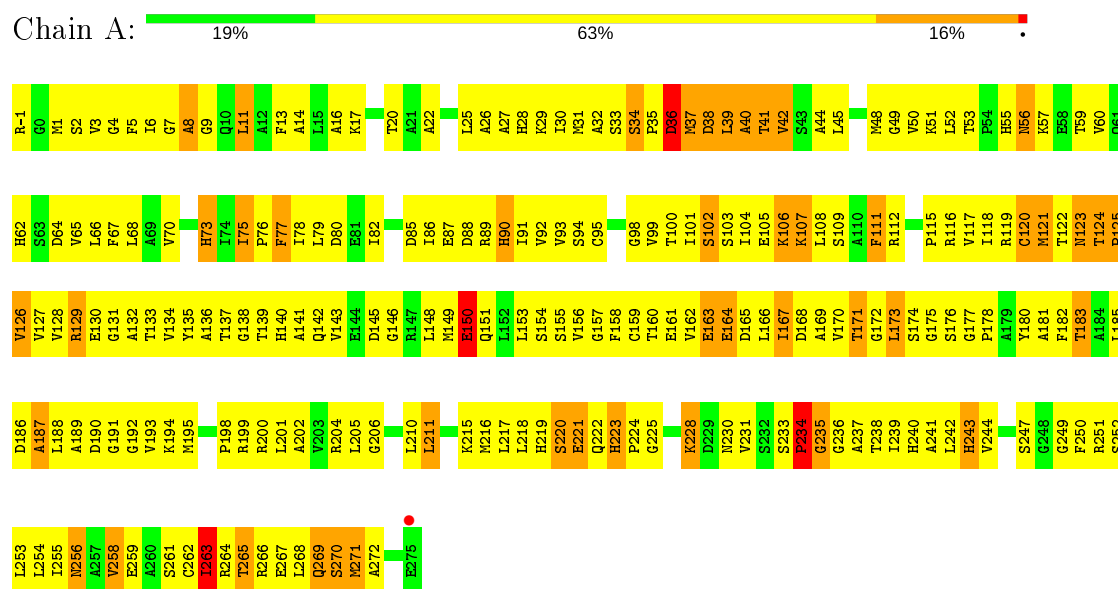
- Molecule 4 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 4 | A | 141 | Total | O | 0 | 0 |
| | | | 141 | 141 | | |
| 4 | B | 93 | Total | O | 0 | 0 |
| | | | 93 | 93 | | |
| 4 | C | 116 | Total | O | 0 | 0 |
| | | | 116 | 116 | | |
| 4 | D | 155 | Total | O | 0 | 0 |
| | | | 155 | 155 | | |
| 4 | E | 138 | Total | O | 0 | 0 |
| | | | 138 | 138 | | |

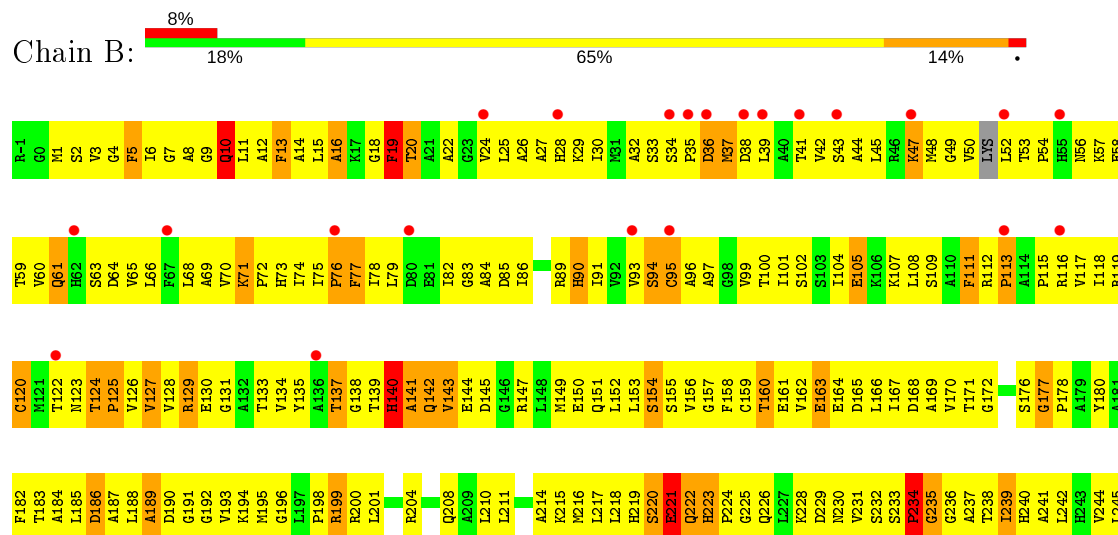
3 Residue-property plots

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

• Molecule 1: Pyrroline-5-carboxylate reductase 1



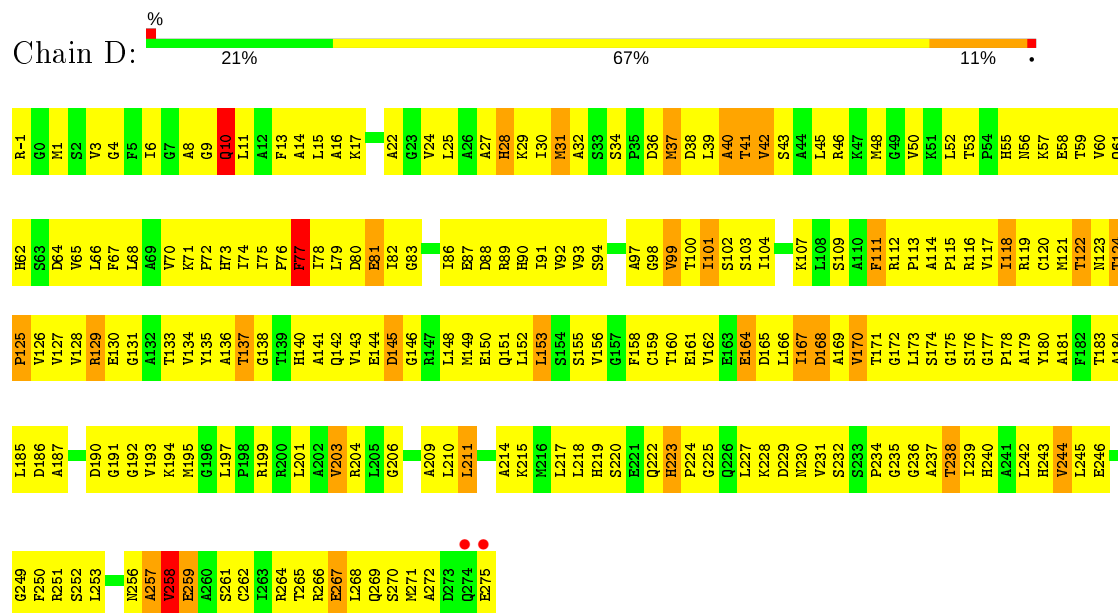
• Molecule 1: Pyrroline-5-carboxylate reductase 1



- Molecule 1: Pyrroline-5-carboxylate reductase 1



- Molecule 1: Pyrroline-5-carboxylate reductase 1



- Molecule 1: Pyrroline-5-carboxylate reductase 1



| | | | | |
|------|------|------|------|-----|
| L245 | T183 | M121 | Q61 | R-1 |
| E246 | A184 | T122 | H62 | G0 |
| S247 | L185 | M123 | S63 | M1 |
| | D186 | T124 | D64 | S2 |
| F250 | A187 | P125 | V65 | V3 |
| R251 | L188 | V126 | L66 | G4 |
| S252 | A189 | V127 | F67 | F5 |
| L253 | D190 | V128 | L68 | T6 |
| L254 | G191 | R129 | A69 | G7 |
| T255 | G192 | E130 | V70 | A8 |
| M256 | V193 | G131 | K71 | G9 |
| A257 | K194 | A132 | F72 | G10 |
| V258 | M195 | T133 | H73 | L11 |
| E259 | | V134 | I74 | A12 |
| A260 | P198 | V135 | I75 | F13 |
| S261 | R199 | A136 | P76 | A14 |
| C262 | R200 | T137 | F77 | L15 |
| I263 | L201 | G138 | I78 | A16 |
| R264 | A202 | T139 | L79 | K17 |
| T265 | V203 | H140 | D80 | G18 |
| R266 | | A141 | B81 | F19 |
| | G206 | G142 | I82 | T20 |
| Q269 | A207 | V143 | G83 | A21 |
| A272 | Q268 | | H84 | A22 |
| D273 | A209 | R147 | D85 | |
| Q274 | L210 | L148 | I86 | L25 |
| E275 | G211 | M149 | B87 | |
| | G212 | E150 | D88 | H28 |
| | A213 | O151 | R89 | K29 |
| | A214 | L152 | H90 | I30 |
| | R215 | L153 | I91 | M31 |
| | L216 | S154 | V92 | A32 |
| | L217 | G155 | V93 | S33 |
| | L218 | V156 | S94 | S34 |
| | R219 | G157 | C95 | P35 |
| S220 | | F158 | A96 | D86 |
| E221 | Q221 | C159 | A97 | K37 |
| Q222 | R222 | T160 | G98 | D38 |
| R223 | G223 | E161 | V99 | L39 |
| P224 | P224 | V162 | T100 | A40 |
| G225 | G225 | E163 | T101 | T41 |
| Q226 | Q226 | E164 | S102 | V42 |
| L227 | L227 | D165 | S103 | S43 |
| K228 | K228 | L166 | T104 | A44 |
| D229 | D229 | I167 | E105 | L45 |
| M230 | M230 | D168 | K106 | R46 |
| V231 | V231 | A169 | K107 | K47 |
| S232 | S232 | V170 | L108 | K48 |
| S233 | S233 | T171 | S109 | G49 |
| P234 | P234 | G172 | F110 | V50 |
| G235 | G235 | L173 | F111 | K51 |
| Q236 | Q236 | S174 | R112 | L52 |
| A237 | A237 | G175 | P113 | T53 |
| T238 | T238 | S176 | A114 | P54 |
| I239 | I239 | G177 | P115 | H55 |
| H240 | H240 | P178 | R116 | N56 |
| A241 | A241 | A179 | V117 | K57 |
| L242 | L242 | V180 | I118 | E58 |
| H243 | H243 | A181 | T119 | T59 |
| T244 | T244 | F182 | C120 | V60 |

4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | C 1 2 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 208.18Å 122.64Å 120.71Å 90.00° 122.03° 90.00° | Depositor |
| Resolution (Å) | 50.00 – 3.10 28.96 – 2.80 | Depositor EDS |
| % Data completeness (in resolution range) | (Not available) (50.00-3.10) 94.9 (28.96-2.80) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.71 (at 2.80Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, R_{free} | 0.241 , 0.278 0.236 , 0.240 | Depositor DCC |
| R_{free} test set | 3139 reflections (5.05%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 61.4 | Xtriage |
| Anisotropy | 0.443 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.31 , 96.4 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$ | Xtriage |
| Estimated twinning fraction | 0.017 for $-1/2^*h+1/2^*k+1, 1/2^*h-1/2^*k+1, 1/2^*h+1/2^*k$ 0.026 for $-1/2^*h-1/2^*k+1, -1/2^*h-1/2^*k-1, 1/2^*h-1/2^*k$ | Xtriage |
| F_o, F_c correlation | 0.91 | EDS |
| Total number of atoms | 11077 | wwPDB-VP |
| Average B, all atoms (Å ²) | 97.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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 | 0.41 | 0/2069 | 0.72 | 1/2800 (0.0%) |
| 1 | B | 0.37 | 0/2053 | 0.71 | 1/2779 (0.0%) |
| 1 | C | 0.38 | 0/2063 | 0.70 | 1/2793 (0.0%) |
| 1 | D | 0.42 | 0/2069 | 0.69 | 0/2800 |
| 1 | E | 0.49 | 2/2069 (0.1%) | 0.86 | 6/2800 (0.2%) |
| All | All | 0.41 | 2/10323 (0.0%) | 0.74 | 9/13972 (0.1%) |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | E | 129 | ARG | C-N | 11.03 | 1.59 | 1.34 |
| 1 | E | 128 | VAL | C-N | -5.02 | 1.22 | 1.34 |

All (9) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1 | E | 128 | VAL | O-C-N | 14.89 | 146.53 | 122.70 |
| 1 | E | 128 | VAL | CA-C-N | -11.74 | 91.36 | 117.20 |
| 1 | E | 129 | ARG | O-C-N | -10.77 | 105.48 | 122.70 |
| 1 | E | 128 | VAL | C-N-CA | -8.96 | 99.30 | 121.70 |
| 1 | E | 129 | ARG | CA-C-N | 6.87 | 132.32 | 117.20 |
| 1 | A | 221 | GLU | CB-CA-C | 5.99 | 122.37 | 110.40 |
| 1 | B | 221 | GLU | CB-CA-C | 5.31 | 121.02 | 110.40 |
| 1 | E | 129 | ARG | C-N-CA | 5.28 | 134.90 | 121.70 |
| 1 | C | 191 | GLY | N-CA-C | -5.04 | 100.49 | 113.10 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 2038 | 0 | 2084 | 489 | 6 |
| 1 | B | 2023 | 0 | 2059 | 491 | 5 |
| 1 | C | 2032 | 0 | 2072 | 530 | 2 |
| 1 | D | 2038 | 0 | 2084 | 436 | 2 |
| 1 | E | 2038 | 0 | 2084 | 492 | 1 |
| 2 | A | 43 | 0 | 23 | 26 | 0 |
| 2 | B | 43 | 0 | 24 | 67 | 5 |
| 2 | C | 43 | 0 | 23 | 39 | 4 |
| 2 | D | 43 | 0 | 24 | 40 | 0 |
| 2 | E | 43 | 0 | 21 | 32 | 1 |
| 3 | A | 10 | 0 | 5 | 8 | 0 |
| 3 | B | 10 | 0 | 5 | 17 | 0 |
| 3 | C | 10 | 0 | 5 | 12 | 0 |
| 3 | D | 10 | 0 | 5 | 21 | 0 |
| 3 | E | 10 | 0 | 5 | 11 | 0 |
| 4 | A | 141 | 0 | 0 | 262 | 6 |
| 4 | B | 93 | 0 | 0 | 169 | 3 |
| 4 | C | 116 | 0 | 0 | 256 | 4 |
| 4 | D | 155 | 0 | 0 | 247 | 2 |
| 4 | E | 138 | 0 | 0 | 298 | 1 |
| All | All | 11077 | 0 | 10523 | 2520 | 22 |

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 120.

All (2520) 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) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:1300:NAI:C1D | 2:A:1300:NAI:N1N | 1.68 | 1.55 |
| 2:E:5300:NAI:O3 | 2:E:5300:NAI:PN | 1.13 | 1.50 |
| 1:B:129:ARG:CZ | 2:B:2300:NAI:H2N | 1.48 | 1.40 |
| 2:E:5300:NAI:O5B | 2:E:5300:NAI:C5B | 1.71 | 1.36 |
| 2:D:4300:NAI:H1D | 3:D:4301:GLU:N | 1.41 | 1.36 |
| 1:E:199:ARG:HG3 | 4:E:5320:HOH:O | 1.21 | 1.35 |
| 1:B:129:ARG:HH22 | 3:B:2301:GLU:CB | 1.40 | 1.35 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:251:ARG:HB3 | 4:E:5348:HOH:O | 1.27 | 1.34 |
| 1:A:42:VAL:HG23 | 4:A:1349:HOH:O | 1.19 | 1.33 |
| 1:E:111:PHE:HB3 | 4:E:5422:HOH:O | 1.26 | 1.32 |
| 1:D:265:THR:HB | 4:D:4360:HOH:O | 1.23 | 1.31 |
| 1:E:150:GLU:HB3 | 4:E:5327:HOH:O | 1.15 | 1.31 |
| 1:B:129:ARG:NH1 | 2:B:2300:NAI:H2N | 1.42 | 1.31 |
| 1:A:141:ALA:HA | 4:A:1390:HOH:O | 1.25 | 1.30 |
| 1:E:38:ASP:HA | 4:E:5427:HOH:O | 1.27 | 1.30 |
| 1:B:129:ARG:NH2 | 2:B:2300:NAI:O7N | 1.65 | 1.29 |
| 1:B:37:MET:HB2 | 4:B:2393:HOH:O | 1.12 | 1.28 |
| 1:D:214:ALA:HA | 4:D:4323:HOH:O | 1.29 | 1.28 |
| 1:C:259:GLU:HB3 | 4:C:3381:HOH:O | 1.33 | 1.28 |
| 1:A:82:ILE:HA | 4:A:1437:HOH:O | 1.30 | 1.28 |
| 1:A:11:LEU:HB2 | 4:A:1389:HOH:O | 1.30 | 1.27 |
| 1:B:99:VAL:HG21 | 4:B:2309:HOH:O | 1.33 | 1.26 |
| 1:E:185:LEU:HG | 4:E:5383:HOH:O | 1.29 | 1.26 |
| 1:E:91:ILE:HB | 4:E:5344:HOH:O | 1.30 | 1.26 |
| 1:A:258:VAL:HA | 4:A:1302:HOH:O | 1.19 | 1.26 |
| 1:C:180:TYR:HB2 | 4:C:3336:HOH:O | 1.28 | 1.26 |
| 1:E:188:LEU:HD23 | 4:E:5343:HOH:O | 1.12 | 1.25 |
| 2:A:1300:NAI:C2N | 3:A:1301:GLU:HB3 | 1.65 | 1.24 |
| 1:B:238:THR:HG22 | 4:B:2352:HOH:O | 1.37 | 1.24 |
| 2:B:2300:NAI:C2N | 3:B:2301:GLU:HB3 | 1.65 | 1.24 |
| 1:C:31:MET:HE2 | 4:C:3362:HOH:O | 1.32 | 1.24 |
| 2:C:3300:NAI:C2N | 3:C:3301:GLU:HB3 | 1.65 | 1.24 |
| 1:E:134:VAL:HG13 | 4:E:5413:HOH:O | 1.36 | 1.24 |
| 1:A:182:PHE:HA | 4:A:1419:HOH:O | 1.38 | 1.24 |
| 1:D:227:LEU:HB2 | 4:D:4363:HOH:O | 1.28 | 1.24 |
| 1:D:126:VAL:HA | 4:D:4331:HOH:O | 1.11 | 1.24 |
| 1:D:195:MET:HE2 | 4:D:4366:HOH:O | 1.32 | 1.23 |
| 1:A:157:GLY:O | 2:A:1300:NAI:H42N | 1.32 | 1.23 |
| 2:E:5300:NAI:O5D | 3:E:5301:GLU:O | 1.54 | 1.22 |
| 1:A:272:ALA:HB3 | 4:A:1407:HOH:O | 1.35 | 1.22 |
| 1:B:158:PHE:CZ | 2:B:2300:NAI:H4B | 1.73 | 1.22 |
| 2:E:5300:NAI:O1N | 3:E:5301:GLU:HA | 1.38 | 1.22 |
| 1:E:179:ALA:HA | 4:E:5369:HOH:O | 1.38 | 1.22 |
| 1:E:163:GLU:HG3 | 4:E:5399:HOH:O | 1.39 | 1.22 |
| 1:D:186:ASP:HA | 4:D:4361:HOH:O | 1.34 | 1.21 |
| 1:B:129:ARG:NH2 | 3:B:2301:GLU:CB | 2.02 | 1.21 |
| 1:B:129:ARG:NH2 | 2:B:2300:NAI:H2N | 1.55 | 1.20 |
| 1:C:122:THR:HB | 4:C:3317:HOH:O | 1.41 | 1.20 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:240:HIS:HA | 4:D:4320:HOH:O | 1.37 | 1.20 |
| 1:C:29:LYS:HG3 | 4:C:3344:HOH:O | 1.39 | 1.19 |
| 1:A:199:ARG:HA | 4:A:1369:HOH:O | 1.38 | 1.19 |
| 1:A:171:THR:HA | 4:A:1402:HOH:O | 1.36 | 1.19 |
| 1:D:231:VAL:HG12 | 4:D:4401:HOH:O | 1.37 | 1.19 |
| 1:C:180:TYR:HA | 4:C:3302:HOH:O | 1.43 | 1.18 |
| 1:C:257:ALA:HA | 4:C:3378:HOH:O | 1.39 | 1.18 |
| 1:C:261:SER:HA | 4:C:3354:HOH:O | 1.40 | 1.18 |
| 1:E:251:ARG:HG2 | 4:E:5317:HOH:O | 1.43 | 1.17 |
| 1:A:191:GLY:HA2 | 4:A:1420:HOH:O | 1.44 | 1.17 |
| 1:B:129:ARG:HH22 | 3:B:2301:GLU:HB3 | 1.00 | 1.17 |
| 1:D:167:ILE:HG22 | 4:D:4440:HOH:O | 1.40 | 1.17 |
| 1:A:217:LEU:HB3 | 4:A:1312:HOH:O | 1.43 | 1.16 |
| 1:C:122:THR:HB | 4:C:3331:HOH:O | 1.37 | 1.16 |
| 1:D:99:VAL:HA | 4:D:4445:HOH:O | 1.41 | 1.16 |
| 1:E:176:SER:HA | 4:E:5333:HOH:O | 1.44 | 1.16 |
| 1:B:129:ARG:CZ | 2:B:2300:NAI:O7N | 1.92 | 1.16 |
| 1:B:119:ARG:HG3 | 4:B:2333:HOH:O | 1.42 | 1.16 |
| 1:D:122:THR:HG23 | 1:D:133:THR:HB | 1.25 | 1.16 |
| 1:D:217:LEU:HD13 | 4:D:4372:HOH:O | 1.45 | 1.16 |
| 1:E:158:PHE:HA | 4:E:5425:HOH:O | 1.43 | 1.15 |
| 1:E:229:ASP:HA | 4:E:5337:HOH:O | 1.46 | 1.15 |
| 1:A:254:LEU:HB3 | 4:A:1360:HOH:O | 1.47 | 1.15 |
| 1:C:157:GLY:O | 2:C:3300:NAI:H42N | 1.45 | 1.15 |
| 1:B:129:ARG:NH2 | 2:B:2300:NAI:C2N | 2.09 | 1.15 |
| 1:D:119:ARG:HD2 | 4:D:4422:HOH:O | 1.47 | 1.15 |
| 1:D:239:ILE:HG13 | 4:D:4429:HOH:O | 1.45 | 1.15 |
| 1:E:80:ASP:HB2 | 4:E:5336:HOH:O | 1.47 | 1.14 |
| 1:D:180:TYR:HA | 4:D:4308:HOH:O | 1.45 | 1.14 |
| 1:C:255:ILE:HB | 4:C:3364:HOH:O | 1.48 | 1.14 |
| 1:C:158:PHE:CZ | 2:C:3300:NAI:O3B | 1.99 | 1.14 |
| 1:E:238:THR:HG21 | 4:E:5321:HOH:O | 1.45 | 1.14 |
| 1:A:162:VAL:HA | 4:A:1355:HOH:O | 1.46 | 1.14 |
| 1:D:267:GLU:HB2 | 4:D:4338:HOH:O | 1.46 | 1.14 |
| 1:D:251:ARG:HB2 | 4:D:4342:HOH:O | 1.46 | 1.13 |
| 1:A:86:ILE:HD12 | 1:A:108:LEU:HD11 | 1.28 | 1.13 |
| 1:A:40:ALA:HB3 | 4:A:1336:HOH:O | 1.49 | 1.12 |
| 1:E:194:LYS:HA | 4:E:5303:HOH:O | 1.48 | 1.12 |
| 1:C:244:VAL:HA | 4:C:3321:HOH:O | 1.44 | 1.12 |
| 1:D:224:PRO:HD2 | 4:D:4355:HOH:O | 1.47 | 1.12 |
| 1:B:129:ARG:CZ | 2:B:2300:NAI:C2N | 2.27 | 1.12 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:105:GLU:HB2 | 4:A:1344:HOH:O | 1.43 | 1.12 |
| 1:B:228:LYS:HA | 4:B:2364:HOH:O | 1.50 | 1.12 |
| 1:C:126:VAL:HA | 4:C:3307:HOH:O | 1.46 | 1.12 |
| 1:C:48:MET:HB2 | 4:C:3371:HOH:O | 1.49 | 1.12 |
| 2:E:5300:NAI:PN | 3:E:5301:GLU:O | 2.07 | 1.12 |
| 1:B:259:GLU:HB3 | 4:B:2381:HOH:O | 1.46 | 1.11 |
| 1:B:228:LYS:HE3 | 4:B:2386:HOH:O | 1.48 | 1.11 |
| 4:A:1352:HOH:O | 1:C:194:LYS:HG3 | 1.48 | 1.10 |
| 1:A:259:GLU:HA | 4:A:1366:HOH:O | 1.51 | 1.10 |
| 1:C:75:ILE:HD12 | 4:C:3415:HOH:O | 1.51 | 1.09 |
| 2:D:4300:NAI:H4N | 3:D:4301:GLU:O | 1.50 | 1.09 |
| 2:E:5300:NAI:H8A | 2:E:5300:NAI:O2B | 1.36 | 1.09 |
| 1:D:135:TYR:HE1 | 4:D:4398:HOH:O | 1.36 | 1.09 |
| 1:C:218:LEU:HD13 | 2:C:3300:NAI:C5D | 1.83 | 1.09 |
| 1:E:262:CYS:SG | 4:E:5342:HOH:O | 2.09 | 1.09 |
| 1:E:134:VAL:HB | 4:E:5407:HOH:O | 1.50 | 1.08 |
| 1:A:210:LEU:HD21 | 4:A:1380:HOH:O | 1.52 | 1.08 |
| 1:A:218:LEU:HD22 | 2:A:1300:NAI:H52A | 1.31 | 1.07 |
| 1:A:1:MET:HB3 | 4:A:1427:HOH:O | 1.53 | 1.07 |
| 1:D:124:THR:HG23 | 4:D:4375:HOH:O | 1.53 | 1.07 |
| 2:D:4300:NAI:N1N | 3:D:4301:GLU:N | 2.01 | 1.07 |
| 1:D:218:LEU:HD22 | 2:D:4300:NAI:H52A | 1.29 | 1.07 |
| 1:D:229:ASP:HB2 | 4:D:4393:HOH:O | 1.55 | 1.06 |
| 2:D:4300:NAI:C4N | 3:D:4301:GLU:O | 2.02 | 1.06 |
| 1:D:91:ILE:HA | 4:D:4455:HOH:O | 1.55 | 1.06 |
| 1:B:142:GLN:HG2 | 1:B:143:VAL:H | 1.14 | 1.06 |
| 1:D:185:LEU:HG | 4:D:4330:HOH:O | 1.52 | 1.06 |
| 1:A:182:PHE:CE1 | 4:A:1324:HOH:O | 2.08 | 1.06 |
| 1:D:37:MET:HG2 | 4:D:4306:HOH:O | 1.51 | 1.06 |
| 2:D:4300:NAI:C2N | 3:D:4301:GLU:CA | 2.34 | 1.06 |
| 1:C:129:ARG:HH12 | 3:C:3301:GLU:HG3 | 1.17 | 1.06 |
| 1:C:218:LEU:HD22 | 2:C:3300:NAI:PA | 1.96 | 1.05 |
| 1:C:60:VAL:HG23 | 4:C:3383:HOH:O | 1.51 | 1.05 |
| 2:D:4300:NAI:C1D | 3:D:4301:GLU:N | 2.20 | 1.05 |
| 1:B:29:LYS:HB3 | 4:B:2332:HOH:O | 1.56 | 1.05 |
| 2:A:1300:NAI:C6N | 3:A:1301:GLU:OXT | 2.04 | 1.05 |
| 1:A:133:THR:HG21 | 1:A:153:LEU:HD13 | 1.37 | 1.04 |
| 1:B:129:ARG:NH2 | 2:B:2300:NAI:C7N | 2.19 | 1.04 |
| 1:B:154:SER:O | 2:B:2300:NAI:N7N | 1.91 | 1.04 |
| 1:D:64:ASP:HB3 | 4:D:4353:HOH:O | 1.55 | 1.04 |
| 1:D:78:ILE:HD11 | 4:D:4446:HOH:O | 1.55 | 1.04 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:95:CYS:HB2 | 4:A:1337:HOH:O | 1.56 | 1.04 |
| 1:C:218:LEU:HD13 | 2:C:3300:NAI:H52N | 1.40 | 1.04 |
| 2:E:5300:NAI:C5B | 2:E:5300:NAI:PA | 2.45 | 1.04 |
| 1:D:141:ALA:HB2 | 4:D:4364:HOH:O | 1.58 | 1.04 |
| 1:B:129:ARG:NE | 2:B:2300:NAI:O7N | 1.89 | 1.04 |
| 1:A:183:THR:HA | 4:A:1354:HOH:O | 1.58 | 1.03 |
| 1:A:95:CYS:CB | 4:A:1337:HOH:O | 2.07 | 1.03 |
| 1:B:129:ARG:NH2 | 3:B:2301:GLU:HB3 | 1.64 | 1.03 |
| 1:B:259:GLU:HA | 4:B:2307:HOH:O | 1.58 | 1.03 |
| 1:B:219:HIS:CE1 | 2:B:2300:NAI:O5D | 2.12 | 1.03 |
| 1:C:29:LYS:CD | 4:C:3404:HOH:O | 2.06 | 1.03 |
| 1:E:122:THR:HB | 1:E:133:THR:HG22 | 1.41 | 1.03 |
| 1:A:178:PRO:HD2 | 4:A:1436:HOH:O | 1.59 | 1.02 |
| 1:C:70:VAL:HB | 4:C:3407:HOH:O | 1.58 | 1.02 |
| 1:D:107:LYS:HD2 | 4:D:4370:HOH:O | 1.59 | 1.02 |
| 1:B:176:SER:HB2 | 4:B:2324:HOH:O | 1.55 | 1.02 |
| 1:B:158:PHE:CE1 | 2:B:2300:NAI:H4B | 1.93 | 1.02 |
| 1:B:158:PHE:CE2 | 2:B:2300:NAI:O3B | 2.12 | 1.01 |
| 1:D:30:ILE:HB | 4:D:4425:HOH:O | 1.62 | 1.00 |
| 1:C:237:ALA:HA | 4:C:3411:HOH:O | 1.59 | 1.00 |
| 1:E:187:ALA:HB2 | 4:E:5363:HOH:O | 1.58 | 1.00 |
| 1:A:112:ARG:CD | 4:A:1392:HOH:O | 2.08 | 1.00 |
| 1:B:75:ILE:HB | 1:B:76:PRO:HD3 | 1.40 | 1.00 |
| 2:A:1300:NAI:H5N | 4:A:1412:HOH:O | 1.61 | 1.00 |
| 2:C:3300:NAI:C6N | 3:C:3301:GLU:OXT | 2.10 | 1.00 |
| 1:A:16:ALA:HB3 | 4:A:1387:HOH:O | 1.62 | 1.00 |
| 2:E:5300:NAI:C8A | 2:E:5300:NAI:O2B | 2.08 | 0.99 |
| 2:D:4300:NAI:C3N | 3:D:4301:GLU:O | 2.10 | 0.99 |
| 2:B:2300:NAI:C6N | 3:B:2301:GLU:OXT | 2.10 | 0.99 |
| 1:A:161:GLU:HB3 | 4:A:1364:HOH:O | 1.61 | 0.99 |
| 1:B:71:LYS:HB3 | 1:B:72:PRO:HD2 | 1.43 | 0.99 |
| 1:C:168:ASP:HA | 4:C:3380:HOH:O | 1.61 | 0.99 |
| 1:E:112:ARG:HG3 | 4:E:5328:HOH:O | 1.61 | 0.99 |
| 2:D:4300:NAI:C2N | 3:D:4301:GLU:HA | 1.92 | 0.99 |
| 1:C:129:ARG:HD2 | 2:C:3300:NAI:O7N | 1.62 | 0.99 |
| 1:C:213:ALA:HB2 | 4:C:3386:HOH:O | 1.63 | 0.99 |
| 1:C:22:ALA:HB3 | 4:C:3369:HOH:O | 1.61 | 0.99 |
| 1:B:155:SER:HA | 2:B:2300:NAI:H72N | 1.25 | 0.98 |
| 1:E:185:LEU:HA | 4:E:5323:HOH:O | 1.61 | 0.98 |
| 1:C:129:ARG:NH1 | 3:C:3301:GLU:HG3 | 1.76 | 0.98 |
| 1:B:189:ALA:C | 4:B:2302:HOH:O | 2.00 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:178:PRO:HB2 | 4:D:4454:HOH:O | 1.62 | 0.98 |
| 1:A:98:GLY:HA2 | 4:A:1328:HOH:O | 1.62 | 0.98 |
| 1:E:17:LYS:HB2 | 4:E:5306:HOH:O | 1.61 | 0.98 |
| 1:A:234:PRO:HB3 | 1:C:196:GLY:O | 1.62 | 0.98 |
| 1:C:151:GLN:HA | 4:C:3319:HOH:O | 1.64 | 0.98 |
| 1:B:183:THR:HA | 4:B:2305:HOH:O | 1.61 | 0.97 |
| 1:B:129:ARG:NH1 | 2:B:2300:NAI:C2N | 2.27 | 0.97 |
| 1:D:122:THR:CG2 | 1:D:133:THR:HB | 1.93 | 0.97 |
| 1:B:158:PHE:CZ | 2:B:2300:NAI:O3B | 2.18 | 0.97 |
| 1:D:194:LYS:HB3 | 4:D:4366:HOH:O | 1.64 | 0.96 |
| 2:E:5300:NAI:H51N | 4:E:5404:HOH:O | 1.63 | 0.96 |
| 1:C:176:SER:HA | 4:C:3330:HOH:O | 1.66 | 0.96 |
| 1:E:188:LEU:HA | 4:E:5343:HOH:O | 1.65 | 0.96 |
| 1:E:9:GLY:H | 1:E:41:THR:HG21 | 1.28 | 0.96 |
| 1:B:218:LEU:HD22 | 2:B:2300:NAI:PA | 2.04 | 0.96 |
| 1:C:48:MET:CB | 4:C:3371:HOH:O | 2.06 | 0.96 |
| 1:D:122:THR:HG23 | 1:D:133:THR:CB | 1.96 | 0.96 |
| 1:B:45:LEU:HD11 | 4:B:2314:HOH:O | 1.62 | 0.96 |
| 1:C:112:ARG:HH11 | 1:C:113:PRO:HD2 | 1.27 | 0.96 |
| 1:E:163:GLU:CG | 4:E:5399:HOH:O | 2.02 | 0.96 |
| 1:C:108:LEU:HB3 | 4:C:3358:HOH:O | 1.65 | 0.96 |
| 1:B:218:LEU:HD13 | 2:B:2300:NAI:H52N | 1.46 | 0.95 |
| 1:B:33:SER:HB2 | 1:B:59:THR:OG1 | 1.66 | 0.95 |
| 1:D:219:HIS:HE1 | 2:D:4300:NAI:C5D | 1.79 | 0.95 |
| 1:E:17:LYS:CB | 4:E:5306:HOH:O | 2.14 | 0.95 |
| 1:A:13:PHE:HA | 4:A:1387:HOH:O | 1.64 | 0.95 |
| 1:D:165:ASP:HB2 | 4:D:4368:HOH:O | 1.67 | 0.95 |
| 1:A:182:PHE:CA | 4:A:1419:HOH:O | 2.01 | 0.95 |
| 1:E:188:LEU:HD12 | 4:E:5439:HOH:O | 1.65 | 0.95 |
| 1:E:47:LYS:HE2 | 4:E:5338:HOH:O | 1.65 | 0.95 |
| 1:B:9:GLY:H | 1:B:12:ALA:HB3 | 1.28 | 0.95 |
| 1:E:225:GLY:CA | 4:E:5353:HOH:O | 2.14 | 0.95 |
| 1:C:178:PRO:HB2 | 4:C:3396:HOH:O | 1.65 | 0.94 |
| 1:C:122:THR:CB | 4:C:3317:HOH:O | 2.03 | 0.94 |
| 1:C:29:LYS:HD3 | 4:C:3404:HOH:O | 1.65 | 0.94 |
| 1:D:180:TYR:CA | 4:D:4308:HOH:O | 2.09 | 0.94 |
| 1:C:101:ILE:HG12 | 4:C:3394:HOH:O | 1.66 | 0.94 |
| 1:D:118:ILE:HB | 4:D:4408:HOH:O | 1.67 | 0.94 |
| 1:B:14:ALA:HA | 1:B:127:VAL:HG22 | 1.49 | 0.94 |
| 1:E:101:ILE:HG13 | 4:E:5418:HOH:O | 1.66 | 0.94 |
| 1:C:213:ALA:N | 4:C:3386:HOH:O | 2.01 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:-1:ARG:HG3 | 4:D:4424:HOH:O | 1.68 | 0.94 |
| 1:C:266:ARG:HD2 | 4:C:3303:HOH:O | 1.68 | 0.94 |
| 1:E:132:ALA:HB3 | 4:E:5335:HOH:O | 1.67 | 0.94 |
| 1:C:89:ARG:HD2 | 1:C:90:HIS:N | 1.83 | 0.94 |
| 1:B:155:SER:CA | 2:B:2300:NAI:H72N | 1.81 | 0.94 |
| 1:C:122:THR:HB | 1:C:133:THR:HG22 | 1.48 | 0.94 |
| 1:C:179:ALA:N | 4:C:3396:HOH:O | 2.01 | 0.94 |
| 1:B:236:GLY:HA2 | 1:B:239:ILE:HG22 | 1.49 | 0.93 |
| 1:B:89:ARG:NH2 | 4:B:2325:HOH:O | 2.00 | 0.93 |
| 1:E:132:ALA:HB1 | 4:E:5391:HOH:O | 1.67 | 0.93 |
| 1:A:250:PHE:N | 4:A:1314:HOH:O | 2.02 | 0.93 |
| 1:A:9:GLY:H | 1:A:41:THR:HG21 | 1.33 | 0.93 |
| 4:C:3375:HOH:O | 1:D:199:ARG:HD3 | 1.67 | 0.93 |
| 1:A:186:ASP:N | 4:A:1370:HOH:O | 2.01 | 0.93 |
| 1:C:237:ALA:CB | 4:C:3411:HOH:O | 2.16 | 0.93 |
| 1:A:121:MET:HB2 | 4:A:1327:HOH:O | 1.68 | 0.92 |
| 1:C:167:ILE:CG2 | 4:C:3345:HOH:O | 2.16 | 0.92 |
| 1:D:98:GLY:N | 4:D:4333:HOH:O | 2.01 | 0.92 |
| 1:A:210:LEU:HG | 4:A:1421:HOH:O | 1.68 | 0.92 |
| 1:E:-1:ARG:CD | 4:E:5319:HOH:O | 2.17 | 0.92 |
| 1:E:63:SER:N | 4:E:5372:HOH:O | 2.00 | 0.92 |
| 1:A:266:ARG:CD | 4:A:1331:HOH:O | 2.16 | 0.92 |
| 1:A:95:CYS:N | 4:A:1337:HOH:O | 2.03 | 0.92 |
| 1:D:62:HIS:C | 4:D:4448:HOH:O | 2.08 | 0.92 |
| 1:E:3:VAL:N | 4:E:5387:HOH:O | 2.01 | 0.92 |
| 1:B:247:SER:HA | 4:B:2350:HOH:O | 1.70 | 0.92 |
| 1:D:174:SER:C | 4:D:4315:HOH:O | 2.07 | 0.92 |
| 1:A:222:GLN:HG2 | 4:A:1441:HOH:O | 1.69 | 0.92 |
| 1:C:4:GLY:N | 4:C:3356:HOH:O | 2.02 | 0.92 |
| 1:C:108:LEU:HD23 | 4:C:3329:HOH:O | 1.70 | 0.92 |
| 1:E:107:LYS:N | 4:E:5384:HOH:O | 2.01 | 0.92 |
| 1:E:69:ALA:HB3 | 4:E:5379:HOH:O | 1.70 | 0.92 |
| 1:B:153:LEU:CA | 4:B:2392:HOH:O | 2.16 | 0.92 |
| 1:C:7:GLY:N | 4:C:3322:HOH:O | 2.03 | 0.92 |
| 1:E:241:ALA:O | 1:E:244:VAL:HG12 | 1.69 | 0.92 |
| 1:B:29:LYS:HE2 | 4:B:2332:HOH:O | 1.68 | 0.91 |
| 1:C:129:ARG:HH12 | 3:C:3301:GLU:CG | 1.83 | 0.91 |
| 1:C:45:LEU:HA | 4:C:3371:HOH:O | 1.71 | 0.91 |
| 1:E:63:SER:C | 4:E:5417:HOH:O | 2.08 | 0.91 |
| 1:B:5:PHE:HZ | 1:B:15:LEU:HB2 | 1.34 | 0.91 |
| 1:C:171:THR:O | 1:C:175:GLY:HA3 | 1.71 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:130:GLU:N | 4:E:5401:HOH:O | 2.02 | 0.91 |
| 1:C:49:GLY:C | 4:C:3363:HOH:O | 2.09 | 0.91 |
| 1:C:259:GLU:N | 4:C:3391:HOH:O | 2.03 | 0.91 |
| 1:C:266:ARG:CD | 4:C:3303:HOH:O | 2.19 | 0.91 |
| 1:D:225:GLY:HA2 | 4:D:4397:HOH:O | 1.68 | 0.91 |
| 1:A:119:ARG:CG | 4:A:1372:HOH:O | 2.18 | 0.90 |
| 1:A:119:ARG:NH2 | 4:A:1328:HOH:O | 2.03 | 0.90 |
| 1:D:219:HIS:CE1 | 2:D:4300:NAI:O5D | 2.24 | 0.90 |
| 1:E:122:THR:HB | 4:E:5385:HOH:O | 1.70 | 0.90 |
| 1:B:176:SER:CB | 4:B:2324:HOH:O | 2.14 | 0.90 |
| 2:B:2300:NAI:C3N | 3:B:2301:GLU:HB3 | 2.00 | 0.90 |
| 1:E:215:LYS:CE | 4:E:5430:HOH:O | 2.18 | 0.90 |
| 1:E:185:LEU:HD23 | 4:E:5323:HOH:O | 1.71 | 0.90 |
| 1:A:29:LYS:NZ | 4:A:1400:HOH:O | 2.04 | 0.90 |
| 2:E:5300:NAI:O1N | 3:E:5301:GLU:CA | 2.18 | 0.90 |
| 1:A:121:MET:HE1 | 4:A:1346:HOH:O | 1.70 | 0.90 |
| 1:B:153:LEU:C | 4:B:2392:HOH:O | 2.10 | 0.90 |
| 2:C:3300:NAI:C3N | 3:C:3301:GLU:HB3 | 2.00 | 0.90 |
| 1:B:218:LEU:HD13 | 2:B:2300:NAI:C5D | 2.01 | 0.90 |
| 1:D:1:MET:HE2 | 1:D:25:LEU:HD21 | 1.54 | 0.90 |
| 1:D:78:ILE:CD1 | 4:D:4446:HOH:O | 2.14 | 0.90 |
| 1:B:129:ARG:HH12 | 2:B:2300:NAI:H2N | 1.30 | 0.90 |
| 1:B:129:ARG:NH2 | 3:B:2301:GLU:HB2 | 1.86 | 0.90 |
| 1:D:141:ALA:HA | 4:D:4386:HOH:O | 1.69 | 0.90 |
| 4:B:2308:HOH:O | 1:D:239:ILE:CG2 | 2.18 | 0.89 |
| 1:C:105:GLU:HG2 | 4:C:3315:HOH:O | 1.71 | 0.89 |
| 1:D:87:GLU:HB3 | 4:D:4322:HOH:O | 1.71 | 0.89 |
| 1:A:239:ILE:HG12 | 4:C:3309:HOH:O | 1.73 | 0.89 |
| 1:A:7:GLY:N | 4:A:1305:HOH:O | 2.05 | 0.89 |
| 1:A:88:ASP:HB2 | 1:A:112:ARG:HH21 | 1.38 | 0.89 |
| 1:E:122:THR:HG22 | 1:E:133:THR:HB | 1.54 | 0.89 |
| 1:E:246:GLU:HB3 | 4:E:5312:HOH:O | 1.70 | 0.89 |
| 1:A:256:ASN:N | 4:A:1335:HOH:O | 2.06 | 0.89 |
| 1:C:237:ALA:N | 4:C:3398:HOH:O | 2.06 | 0.89 |
| 1:C:266:ARG:HA | 4:C:3340:HOH:O | 1.72 | 0.89 |
| 1:C:129:ARG:CZ | 2:C:3300:NAI:H2N | 2.02 | 0.89 |
| 1:E:162:VAL:HG13 | 1:E:166:LEU:HD12 | 1.55 | 0.89 |
| 1:E:65:VAL:HA | 4:E:5344:HOH:O | 1.72 | 0.89 |
| 1:C:133:THR:HG22 | 4:C:3317:HOH:O | 1.71 | 0.88 |
| 1:C:203:VAL:HA | 4:C:3355:HOH:O | 1.73 | 0.88 |
| 1:B:129:ARG:NH1 | 2:B:2300:NAI:O2D | 2.07 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:73:HIS:CD2 | 4:B:2320:HOH:O | 2.26 | 0.88 |
| 1:D:53:THR:HB | 4:D:4404:HOH:O | 1.73 | 0.88 |
| 1:A:102:SER:HB2 | 4:A:1358:HOH:O | 1.72 | 0.88 |
| 1:E:187:ALA:HA | 4:E:5381:HOH:O | 1.70 | 0.88 |
| 1:B:73:HIS:HD2 | 4:B:2320:HOH:O | 1.56 | 0.88 |
| 1:E:122:THR:CB | 4:E:5385:HOH:O | 2.21 | 0.88 |
| 1:A:154:SER:O | 2:A:1300:NAI:N7N | 2.05 | 0.88 |
| 1:B:50:VAL:HB | 4:B:2385:HOH:O | 1.73 | 0.88 |
| 1:C:160:THR:CG2 | 4:C:3323:HOH:O | 2.22 | 0.88 |
| 2:E:5300:NAI:O5D | 2:E:5300:NAI:O3 | 1.92 | 0.88 |
| 1:C:192:GLY:CA | 4:C:3367:HOH:O | 2.20 | 0.88 |
| 1:E:200:ARG:HG3 | 4:E:5416:HOH:O | 1.74 | 0.87 |
| 1:B:129:ARG:NH2 | 2:B:2300:NAI:C3N | 2.36 | 0.87 |
| 1:B:95:CYS:HA | 4:B:2349:HOH:O | 1.73 | 0.87 |
| 1:E:123:ASN:ND2 | 4:E:5335:HOH:O | 2.07 | 0.87 |
| 2:E:5300:NAI:C5D | 3:E:5301:GLU:O | 2.22 | 0.87 |
| 1:A:112:ARG:NE | 4:A:1392:HOH:O | 2.08 | 0.87 |
| 1:C:112:ARG:HG3 | 1:C:113:PRO:HD2 | 1.54 | 0.87 |
| 1:A:124:THR:O | 1:A:127:VAL:HG23 | 1.75 | 0.87 |
| 1:B:122:THR:HG22 | 1:B:133:THR:CB | 2.04 | 0.87 |
| 1:D:272:ALA:HB1 | 4:D:4328:HOH:O | 1.71 | 0.87 |
| 1:D:64:ASP:CB | 4:D:4353:HOH:O | 2.15 | 0.87 |
| 1:B:158:PHE:CZ | 2:B:2300:NAI:C4B | 2.57 | 0.87 |
| 1:B:12:ALA:HB3 | 4:B:2314:HOH:O | 1.75 | 0.87 |
| 1:B:190:ASP:N | 4:B:2302:HOH:O | 2.06 | 0.86 |
| 1:C:33:SER:HB2 | 1:C:59:THR:OG1 | 1.75 | 0.86 |
| 1:B:236:GLY:HA3 | 4:B:2318:HOH:O | 1.75 | 0.86 |
| 1:A:102:SER:N | 4:A:1358:HOH:O | 2.08 | 0.86 |
| 1:B:228:LYS:CE | 4:B:2386:HOH:O | 2.12 | 0.86 |
| 1:C:155:SER:HA | 2:C:3300:NAI:H72N | 1.37 | 0.86 |
| 1:C:28:HIS:HA | 1:C:51:LYS:HE3 | 1.58 | 0.86 |
| 1:B:73:HIS:CE1 | 4:B:2390:HOH:O | 2.28 | 0.86 |
| 1:D:224:PRO:CD | 4:D:4355:HOH:O | 2.14 | 0.86 |
| 1:D:30:ILE:HB | 1:D:50:VAL:HG22 | 1.55 | 0.86 |
| 1:C:69:ALA:N | 4:C:3322:HOH:O | 2.07 | 0.86 |
| 1:B:228:LYS:CA | 4:B:2364:HOH:O | 2.12 | 0.86 |
| 1:E:73:HIS:HB2 | 4:E:5415:HOH:O | 1.75 | 0.86 |
| 1:E:88:ASP:N | 4:E:5318:HOH:O | 2.03 | 0.86 |
| 1:A:122:THR:C | 4:A:1428:HOH:O | 2.14 | 0.86 |
| 1:A:259:GLU:CA | 4:A:1366:HOH:O | 2.17 | 0.86 |
| 1:E:53:THR:HG22 | 1:E:55:HIS:H | 1.38 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:102:SER:CB | 4:A:1358:HOH:O | 2.24 | 0.85 |
| 1:B:129:ARG:HH22 | 3:B:2301:GLU:CG | 1.89 | 0.85 |
| 1:C:247:SER:C | 4:C:3402:HOH:O | 2.15 | 0.85 |
| 1:D:57:LYS:CE | 4:D:4376:HOH:O | 2.21 | 0.85 |
| 1:E:115:PRO:HA | 4:E:5436:HOH:O | 1.76 | 0.85 |
| 1:C:251:ARG:HA | 4:C:3359:HOH:O | 1.76 | 0.85 |
| 1:B:193:VAL:HG12 | 1:D:239:ILE:HD13 | 1.58 | 0.85 |
| 1:E:53:THR:HG21 | 4:E:5332:HOH:O | 1.75 | 0.85 |
| 1:B:10:GLN:NE2 | 4:B:2354:HOH:O | 2.08 | 0.85 |
| 1:B:185:LEU:HD21 | 1:B:210:LEU:HD12 | 1.58 | 0.85 |
| 1:E:174:SER:HB2 | 4:E:5335:HOH:O | 1.76 | 0.85 |
| 1:E:111:PHE:HE1 | 4:E:5326:HOH:O | 1.58 | 0.85 |
| 1:E:55:HIS:HB2 | 4:E:5332:HOH:O | 1.75 | 0.85 |
| 1:A:138:GLY:HA3 | 4:A:1310:HOH:O | 1.75 | 0.85 |
| 1:D:219:HIS:CE1 | 2:D:4300:NAI:C5D | 2.59 | 0.85 |
| 1:D:39:LEU:HD23 | 4:D:4405:HOH:O | 1.77 | 0.85 |
| 1:C:123:ASN:HD21 | 1:C:132:ALA:HB3 | 1.42 | 0.85 |
| 1:C:237:ALA:CA | 4:C:3411:HOH:O | 2.21 | 0.85 |
| 1:C:53:THR:HG21 | 1:C:58:GLU:HB2 | 1.58 | 0.85 |
| 1:B:155:SER:HA | 2:B:2300:NAI:N7N | 1.90 | 0.85 |
| 1:A:266:ARG:CZ | 4:A:1440:HOH:O | 2.24 | 0.84 |
| 1:B:241:ALA:HA | 4:B:2329:HOH:O | 1.75 | 0.84 |
| 1:B:95:CYS:N | 4:B:2349:HOH:O | 2.09 | 0.84 |
| 1:E:231:VAL:HG12 | 4:E:5321:HOH:O | 1.77 | 0.84 |
| 1:C:236:GLY:C | 4:C:3398:HOH:O | 2.14 | 0.84 |
| 1:E:183:THR:CB | 4:E:5370:HOH:O | 2.24 | 0.84 |
| 1:A:259:GLU:O | 1:A:263:ILE:HD13 | 1.76 | 0.84 |
| 1:D:178:PRO:C | 4:D:4454:HOH:O | 2.16 | 0.84 |
| 1:E:96:ALA:N | 4:E:5423:HOH:O | 2.07 | 0.84 |
| 1:A:118:ILE:HG22 | 1:A:137:THR:HA | 1.60 | 0.84 |
| 1:A:119:ARG:HG3 | 4:A:1372:HOH:O | 1.77 | 0.84 |
| 1:B:129:ARG:HH22 | 2:B:2300:NAI:C2N | 1.86 | 0.84 |
| 1:B:160:THR:CG2 | 4:B:2360:HOH:O | 2.26 | 0.84 |
| 1:E:183:THR:HG22 | 4:E:5370:HOH:O | 1.76 | 0.84 |
| 1:A:210:LEU:CD2 | 4:A:1380:HOH:O | 2.16 | 0.84 |
| 1:B:74:ILE:HG13 | 4:B:2309:HOH:O | 1.77 | 0.84 |
| 1:C:162:VAL:HB | 1:C:166:LEU:HD12 | 1.57 | 0.84 |
| 1:E:188:LEU:CA | 4:E:5343:HOH:O | 2.21 | 0.84 |
| 1:B:138:GLY:HA3 | 4:B:2370:HOH:O | 1.77 | 0.84 |
| 1:E:243:HIS:CE1 | 4:E:5357:HOH:O | 2.30 | 0.84 |
| 1:C:247:SER:HA | 4:C:3402:HOH:O | 1.76 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:118:ILE:HG23 | 1:D:137:THR:HA | 1.60 | 0.84 |
| 1:D:53:THR:HG22 | 1:D:55:HIS:H | 1.41 | 0.84 |
| 1:B:129:ARG:HH22 | 2:B:2300:NAI:H2N | 1.43 | 0.84 |
| 1:B:45:LEU:HB2 | 1:B:52:LEU:HD21 | 1.58 | 0.84 |
| 1:C:194:LYS:HA | 4:C:3309:HOH:O | 1.77 | 0.84 |
| 1:A:-1:ARG:CG | 4:A:1332:HOH:O | 2.26 | 0.83 |
| 1:E:182:PHE:HB2 | 4:E:5369:HOH:O | 1.77 | 0.83 |
| 1:A:28:HIS:ND1 | 4:A:1382:HOH:O | 2.10 | 0.83 |
| 1:D:228:LYS:HE2 | 4:D:4414:HOH:O | 1.78 | 0.83 |
| 1:D:9:GLY:N | 1:D:41:THR:HG21 | 1.93 | 0.83 |
| 1:A:255:ILE:HG22 | 4:A:1335:HOH:O | 1.79 | 0.83 |
| 1:B:11:LEU:HD23 | 4:B:2343:HOH:O | 1.78 | 0.83 |
| 1:B:160:THR:HG23 | 4:B:2360:HOH:O | 1.79 | 0.83 |
| 1:B:250:PHE:HB2 | 4:B:2353:HOH:O | 1.77 | 0.83 |
| 1:C:171:THR:CA | 4:C:3351:HOH:O | 2.26 | 0.83 |
| 1:D:126:VAL:HG13 | 1:D:156:VAL:HG11 | 1.60 | 0.83 |
| 2:D:4300:NAI:C4N | 3:D:4301:GLU:C | 2.45 | 0.83 |
| 1:C:199:ARG:CD | 4:C:3392:HOH:O | 2.27 | 0.83 |
| 1:C:133:THR:CG2 | 4:C:3317:HOH:O | 2.25 | 0.83 |
| 1:E:212:GLY:HA2 | 4:E:5314:HOH:O | 1.76 | 0.83 |
| 1:B:245:LEU:HA | 4:B:2353:HOH:O | 1.79 | 0.83 |
| 1:C:89:ARG:HD2 | 1:C:90:HIS:H | 1.39 | 0.83 |
| 1:C:213:ALA:CA | 4:C:3386:HOH:O | 2.27 | 0.83 |
| 1:D:136:ALA:HA | 4:D:4394:HOH:O | 1.78 | 0.83 |
| 1:A:194:LYS:NZ | 4:A:1381:HOH:O | 2.12 | 0.82 |
| 1:A:161:GLU:CD | 4:A:1364:HOH:O | 2.16 | 0.82 |
| 1:C:171:THR:N | 4:C:3351:HOH:O | 2.11 | 0.82 |
| 1:E:-1:ARG:HD3 | 4:E:5319:HOH:O | 1.76 | 0.82 |
| 1:B:79:LEU:HD11 | 1:B:104:ILE:HG12 | 1.61 | 0.82 |
| 1:D:251:ARG:NH1 | 4:D:4427:HOH:O | 2.12 | 0.82 |
| 1:D:123:ASN:HB3 | 4:D:4309:HOH:O | 1.78 | 0.82 |
| 1:D:211:LEU:HD12 | 4:D:4406:HOH:O | 1.79 | 0.82 |
| 1:E:274:GLN:HG3 | 1:E:275:GLU:H | 1.41 | 0.82 |
| 1:A:120:CYS:HA | 4:A:1368:HOH:O | 1.79 | 0.82 |
| 1:D:228:LYS:C | 4:D:4310:HOH:O | 2.16 | 0.82 |
| 1:D:266:ARG:NH2 | 4:D:4378:HOH:O | 2.05 | 0.82 |
| 1:E:31:MET:HG2 | 1:E:51:LYS:HB2 | 1.61 | 0.82 |
| 1:D:107:LYS:CD | 4:D:4370:HOH:O | 2.22 | 0.82 |
| 1:E:262:CYS:SG | 4:E:5375:HOH:O | 2.38 | 0.82 |
| 1:D:246:GLU:HG3 | 4:D:4383:HOH:O | 1.80 | 0.82 |
| 1:B:164:GLU:HG3 | 1:B:167:ILE:HD12 | 1.62 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:C:131:GLY:HA3 | 4:C:3307:HOH:O | 1.78 | 0.82 |
| 1:A:258:VAL:CG2 | 4:A:1302:HOH:O | 2.27 | 0.81 |
| 1:C:134:VAL:HB | 4:C:3327:HOH:O | 1.80 | 0.81 |
| 1:C:258:VAL:O | 1:C:258:VAL:HG12 | 1.79 | 0.81 |
| 1:C:7:GLY:CA | 4:C:3322:HOH:O | 2.25 | 0.81 |
| 1:D:158:PHE:CZ | 2:D:4300:NAI:O3B | 2.33 | 0.81 |
| 1:D:223:HIS:N | 4:D:4384:HOH:O | 2.01 | 0.81 |
| 2:A:1300:NAI:H51N | 4:A:1431:HOH:O | 1.78 | 0.81 |
| 1:B:82:ILE:HA | 4:B:2376:HOH:O | 1.78 | 0.81 |
| 1:B:82:ILE:HG22 | 1:B:86:ILE:HD11 | 1.61 | 0.81 |
| 1:D:272:ALA:HA | 4:D:4400:HOH:O | 1.80 | 0.81 |
| 1:B:142:GLN:HG2 | 1:B:143:VAL:N | 1.94 | 0.81 |
| 1:B:7:GLY:O | 1:B:12:ALA:HB2 | 1.80 | 0.81 |
| 1:C:247:SER:CA | 4:C:3402:HOH:O | 2.27 | 0.81 |
| 1:C:7:GLY:HA3 | 4:C:3322:HOH:O | 1.80 | 0.81 |
| 1:A:266:ARG:NH1 | 4:A:1308:HOH:O | 2.14 | 0.81 |
| 1:A:9:GLY:N | 1:A:41:THR:HG21 | 1.94 | 0.81 |
| 1:D:257:ALA:C | 4:D:4349:HOH:O | 2.17 | 0.81 |
| 1:D:31:MET:HG2 | 1:D:59:THR:HA | 1.62 | 0.81 |
| 1:D:121:MET:HG2 | 4:D:4324:HOH:O | 1.79 | 0.81 |
| 1:B:122:THR:HG22 | 1:B:133:THR:HB | 1.59 | 0.81 |
| 1:B:6:ILE:HD12 | 1:B:56:ASN:O | 1.81 | 0.81 |
| 1:C:240:HIS:HB2 | 4:C:3398:HOH:O | 1.80 | 0.81 |
| 1:A:239:ILE:HG21 | 4:C:3309:HOH:O | 1.81 | 0.81 |
| 1:A:202:ALA:HB3 | 4:A:1369:HOH:O | 1.80 | 0.81 |
| 1:B:63:SER:HB2 | 1:B:89:ARG:HH12 | 1.45 | 0.81 |
| 1:D:133:THR:O | 1:D:159:CYS:HA | 1.81 | 0.81 |
| 1:E:153:LEU:HB2 | 4:E:5432:HOH:O | 1.80 | 0.81 |
| 2:A:1300:NAI:N1N | 3:A:1301:GLU:OXT | 2.14 | 0.81 |
| 1:D:211:LEU:HD12 | 1:D:211:LEU:O | 1.80 | 0.81 |
| 1:C:262:CYS:SG | 4:C:3320:HOH:O | 2.39 | 0.80 |
| 1:E:138:GLY:HA2 | 4:E:5418:HOH:O | 1.79 | 0.80 |
| 1:E:183:THR:HB | 4:E:5370:HOH:O | 1.80 | 0.80 |
| 1:B:5:PHE:CZ | 1:B:15:LEU:HB2 | 2.16 | 0.80 |
| 1:A:123:ASN:HD21 | 1:A:132:ALA:H | 1.30 | 0.80 |
| 1:B:251:ARG:HD3 | 4:B:2330:HOH:O | 1.80 | 0.80 |
| 1:D:60:VAL:HG21 | 1:D:82:ILE:HG23 | 1.63 | 0.80 |
| 1:E:60:VAL:HG21 | 1:E:82:ILE:HD12 | 1.63 | 0.80 |
| 1:C:218:LEU:CD1 | 2:C:3300:NAI:C5D | 2.59 | 0.80 |
| 1:C:87:GLU:HG3 | 4:C:3382:HOH:O | 1.80 | 0.80 |
| 1:D:91:ILE:CA | 4:D:4455:HOH:O | 2.19 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:215:LYS:HE2 | 4:E:5430:HOH:O | 1.77 | 0.80 |
| 1:C:192:GLY:C | 4:C:3367:HOH:O | 2.19 | 0.80 |
| 4:B:2308:HOH:O | 1:D:239:ILE:HG23 | 1.82 | 0.80 |
| 1:A:181:ALA:C | 4:A:1419:HOH:O | 2.20 | 0.80 |
| 1:C:236:GLY:CA | 4:C:3398:HOH:O | 2.30 | 0.80 |
| 1:C:158:PHE:CE1 | 2:C:3300:NAI:H4B | 2.17 | 0.80 |
| 1:D:124:THR:CB | 4:D:4375:HOH:O | 2.30 | 0.80 |
| 2:A:1300:NAI:C2N | 2:A:1300:NAI:C1D | 2.60 | 0.80 |
| 1:C:218:LEU:CD1 | 2:C:3300:NAI:H52N | 2.12 | 0.80 |
| 1:D:219:HIS:HE1 | 2:D:4300:NAI:H51N | 1.45 | 0.80 |
| 1:D:88:ASP:CA | 4:D:4432:HOH:O | 2.29 | 0.80 |
| 1:C:226:GLN:HG2 | 4:C:3366:HOH:O | 1.82 | 0.79 |
| 1:E:9:GLY:N | 1:E:41:THR:HG21 | 1.96 | 0.79 |
| 1:A:79:LEU:HD11 | 1:A:104:ILE:HD12 | 1.63 | 0.79 |
| 1:A:94:SER:O | 4:A:1372:HOH:O | 2.00 | 0.79 |
| 1:C:167:ILE:HG21 | 4:C:3345:HOH:O | 1.80 | 0.79 |
| 1:D:118:ILE:CB | 4:D:4408:HOH:O | 2.27 | 0.79 |
| 1:B:142:GLN:HB2 | 4:B:2339:HOH:O | 1.83 | 0.79 |
| 1:C:178:PRO:HG3 | 4:C:3346:HOH:O | 1.83 | 0.79 |
| 1:C:199:ARG:HD3 | 4:C:3392:HOH:O | 1.81 | 0.79 |
| 2:D:4300:NAI:C3N | 3:D:4301:GLU:C | 2.50 | 0.79 |
| 1:E:183:THR:CG2 | 4:E:5370:HOH:O | 2.28 | 0.79 |
| 1:E:199:ARG:C | 4:E:5320:HOH:O | 2.21 | 0.79 |
| 1:A:8:ALA:O | 4:A:1333:HOH:O | 2.01 | 0.79 |
| 1:E:121:MET:HE2 | 1:E:122:THR:N | 1.98 | 0.79 |
| 1:B:95:CYS:CA | 4:B:2349:HOH:O | 2.27 | 0.79 |
| 1:A:45:LEU:HD11 | 4:A:1379:HOH:O | 1.82 | 0.79 |
| 1:D:113:PRO:N | 4:D:4329:HOH:O | 2.15 | 0.79 |
| 1:C:266:ARG:HG2 | 1:C:266:ARG:HH11 | 1.47 | 0.79 |
| 1:A:178:PRO:O | 4:A:1324:HOH:O | 2.01 | 0.79 |
| 1:A:37:MET:HA | 1:A:42:VAL:HG21 | 1.64 | 0.79 |
| 1:C:266:ARG:CA | 4:C:3340:HOH:O | 2.29 | 0.79 |
| 1:D:56:ASN:ND2 | 4:D:4446:HOH:O | 2.16 | 0.79 |
| 1:E:94:SER:C | 4:E:5423:HOH:O | 2.20 | 0.79 |
| 1:B:60:VAL:HG12 | 1:B:89:ARG:HH22 | 1.49 | 0.79 |
| 1:C:129:ARG:NH1 | 3:C:3301:GLU:CG | 2.45 | 0.79 |
| 1:D:112:ARG:HD2 | 4:D:4347:HOH:O | 1.81 | 0.79 |
| 1:E:132:ALA:HA | 4:E:5351:HOH:O | 1.82 | 0.79 |
| 1:E:159:CYS:SG | 4:E:5432:HOH:O | 2.41 | 0.78 |
| 1:E:179:ALA:HB1 | 4:E:5322:HOH:O | 1.81 | 0.78 |
| 1:E:188:LEU:N | 4:E:5343:HOH:O | 2.15 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:61:GLN:O | 4:E:5324:HOH:O | 2.00 | 0.78 |
| 1:C:98:GLY:HA2 | 4:C:3310:HOH:O | 1.83 | 0.78 |
| 1:A:120:CYS:CA | 4:A:1368:HOH:O | 2.31 | 0.78 |
| 1:A:238:THR:N | 4:A:1391:HOH:O | 2.14 | 0.78 |
| 1:B:187:ALA:HA | 4:B:2341:HOH:O | 1.83 | 0.78 |
| 1:D:162:VAL:HG13 | 1:D:166:LEU:HD12 | 1.63 | 0.78 |
| 1:D:94:SER:OG | 4:D:4344:HOH:O | 2.01 | 0.78 |
| 1:C:48:MET:HG3 | 4:C:3363:HOH:O | 1.83 | 0.78 |
| 2:D:4300:NAI:H3D | 4:D:4410:HOH:O | 1.82 | 0.78 |
| 2:D:4300:NAI:O1N | 3:D:4301:GLU:N | 2.15 | 0.78 |
| 2:E:5300:NAI:C1D | 3:E:5301:GLU:N | 2.47 | 0.78 |
| 1:B:228:LYS:O | 4:B:2364:HOH:O | 2.02 | 0.78 |
| 1:C:128:VAL:HG12 | 1:C:129:ARG:H | 1.49 | 0.78 |
| 1:E:185:LEU:CA | 4:E:5323:HOH:O | 2.25 | 0.78 |
| 1:D:275:GLU:O | 4:D:4456:HOH:O | 2.00 | 0.78 |
| 1:E:-1:ARG:NE | 4:E:5319:HOH:O | 2.14 | 0.78 |
| 2:A:1300:NAI:H2N | 3:A:1301:GLU:HB3 | 1.63 | 0.78 |
| 1:B:108:LEU:O | 4:B:2328:HOH:O | 2.02 | 0.78 |
| 1:B:129:ARG:HH21 | 2:B:2300:NAI:C7N | 1.91 | 0.78 |
| 1:B:256:ASN:HB3 | 4:B:2369:HOH:O | 1.82 | 0.78 |
| 1:D:179:ALA:O | 4:D:4335:HOH:O | 2.01 | 0.78 |
| 1:D:158:PHE:CE2 | 2:D:4300:NAI:O3B | 2.36 | 0.78 |
| 1:E:207:ALA:N | 4:E:5408:HOH:O | 2.15 | 0.78 |
| 1:A:155:SER:O | 4:A:1425:HOH:O | 2.01 | 0.78 |
| 1:D:223:HIS:CD2 | 4:D:4321:HOH:O | 2.37 | 0.78 |
| 1:B:161:GLU:OE2 | 4:B:2346:HOH:O | 2.00 | 0.77 |
| 1:A:112:ARG:HD3 | 4:A:1392:HOH:O | 1.77 | 0.77 |
| 1:C:53:THR:HG22 | 1:C:55:HIS:H | 1.46 | 0.77 |
| 1:D:146:GLY:O | 4:D:4443:HOH:O | 2.01 | 0.77 |
| 1:E:53:THR:CG2 | 4:E:5332:HOH:O | 2.29 | 0.77 |
| 1:B:141:ALA:O | 1:B:145:ASP:HB3 | 1.85 | 0.77 |
| 1:B:155:SER:CA | 2:B:2300:NAI:N7N | 2.47 | 0.77 |
| 1:D:4:GLY:O | 4:D:4327:HOH:O | 2.02 | 0.77 |
| 1:D:43:SER:HB2 | 4:D:4405:HOH:O | 1.83 | 0.77 |
| 1:E:105:GLU:OE1 | 4:E:5437:HOH:O | 2.02 | 0.77 |
| 1:A:102:SER:CA | 4:A:1358:HOH:O | 2.33 | 0.77 |
| 1:B:135:TYR:CE1 | 1:B:161:GLU:HB3 | 2.20 | 0.77 |
| 1:B:153:LEU:HA | 4:B:2392:HOH:O | 1.80 | 0.77 |
| 1:C:160:THR:HG22 | 4:C:3323:HOH:O | 1.82 | 0.77 |
| 1:D:204:ARG:NH2 | 4:D:4411:HOH:O | 2.17 | 0.77 |
| 1:E:137:THR:HG23 | 4:E:5426:HOH:O | 1.84 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:185:LEU:C | 4:A:1370:HOH:O | 2.21 | 0.77 |
| 1:C:271:MET:HA | 1:C:274:GLN:HB3 | 1.67 | 0.77 |
| 1:D:30:ILE:HA | 4:D:4365:HOH:O | 1.83 | 0.77 |
| 1:D:88:ASP:O | 4:D:4432:HOH:O | 2.02 | 0.77 |
| 1:E:172:GLY:HA2 | 1:E:261:SER:OG | 1.85 | 0.77 |
| 2:E:5300:NAI:O2A | 2:E:5300:NAI:C5B | 2.32 | 0.77 |
| 1:E:80:ASP:CB | 4:E:5336:HOH:O | 2.18 | 0.77 |
| 1:E:59:THR:O | 4:E:5372:HOH:O | 2.03 | 0.77 |
| 1:B:11:LEU:N | 4:B:2343:HOH:O | 2.18 | 0.76 |
| 1:C:248:GLY:N | 4:C:3402:HOH:O | 2.16 | 0.76 |
| 1:C:255:ILE:HA | 4:C:3332:HOH:O | 1.85 | 0.76 |
| 1:C:86:ILE:C | 4:C:3382:HOH:O | 2.24 | 0.76 |
| 1:D:115:PRO:HA | 4:D:4374:HOH:O | 1.85 | 0.76 |
| 1:B:74:ILE:HD12 | 4:B:2306:HOH:O | 1.84 | 0.76 |
| 1:D:115:PRO:O | 4:D:4304:HOH:O | 2.02 | 0.76 |
| 1:D:64:ASP:OD2 | 4:D:4353:HOH:O | 2.03 | 0.76 |
| 1:E:129:ARG:HB3 | 4:E:5401:HOH:O | 1.85 | 0.76 |
| 1:A:168:ASP:OD1 | 4:A:1328:HOH:O | 2.03 | 0.76 |
| 1:A:75:ILE:HG22 | 1:A:76:PRO:HD3 | 1.67 | 0.76 |
| 1:D:27:ALA:O | 4:D:4425:HOH:O | 2.02 | 0.76 |
| 3:A:1301:GLU:HB2 | 4:A:1408:HOH:O | 1.86 | 0.76 |
| 1:B:1:MET:O | 4:B:2332:HOH:O | 2.04 | 0.76 |
| 1:A:122:THR:HG22 | 1:A:123:ASN:N | 1.99 | 0.76 |
| 1:B:251:ARG:CD | 4:B:2330:HOH:O | 2.34 | 0.76 |
| 1:D:156:VAL:O | 1:D:156:VAL:HG12 | 1.83 | 0.76 |
| 1:D:57:LYS:HE2 | 4:D:4376:HOH:O | 1.79 | 0.76 |
| 1:E:185:LEU:N | 4:E:5323:HOH:O | 2.19 | 0.76 |
| 1:A:218:LEU:HD22 | 2:A:1300:NAI:C5B | 2.14 | 0.76 |
| 1:C:15:LEU:CD1 | 4:C:3348:HOH:O | 2.34 | 0.76 |
| 1:C:71:LYS:HD3 | 1:C:71:LYS:H | 1.48 | 0.76 |
| 1:E:236:GLY:O | 4:E:5307:HOH:O | 2.03 | 0.76 |
| 1:D:220:SER:HB2 | 4:D:4419:HOH:O | 1.83 | 0.76 |
| 1:E:199:ARG:O | 4:E:5320:HOH:O | 2.02 | 0.76 |
| 1:E:58:GLU:HB2 | 4:E:5332:HOH:O | 1.85 | 0.76 |
| 1:A:-1:ARG:HG3 | 4:A:1424:HOH:O | 1.85 | 0.76 |
| 1:D:224:PRO:CG | 4:D:4355:HOH:O | 2.33 | 0.76 |
| 1:E:169:ALA:CA | 4:E:5375:HOH:O | 2.34 | 0.76 |
| 2:A:1300:NAI:C3N | 3:A:1301:GLU:HB3 | 2.15 | 0.76 |
| 1:A:89:ARG:NH1 | 4:A:1316:HOH:O | 2.18 | 0.76 |
| 1:B:45:LEU:O | 4:B:2385:HOH:O | 2.03 | 0.76 |
| 1:C:163:GLU:HB2 | 4:C:3397:HOH:O | 1.86 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:184:ALA:C | 4:C:3352:HOH:O | 2.24 | 0.76 |
| 2:C:3300:NAI:PN | 2:C:3300:NAI:O4D | 2.44 | 0.76 |
| 1:E:231:VAL:O | 4:E:5321:HOH:O | 2.03 | 0.76 |
| 1:E:263:ILE:N | 4:E:5342:HOH:O | 2.18 | 0.76 |
| 2:E:5300:NAI:O1N | 3:E:5301:GLU:O | 2.03 | 0.76 |
| 1:A:130:GLU:OE1 | 2:A:1300:NAI:H2D | 1.85 | 0.76 |
| 1:B:152:LEU:O | 4:B:2392:HOH:O | 2.04 | 0.76 |
| 1:B:129:ARG:HH22 | 3:B:2301:GLU:HG3 | 1.51 | 0.76 |
| 1:B:6:ILE:HA | 1:B:33:SER:HB3 | 1.66 | 0.76 |
| 1:C:198:PRO:N | 4:C:3361:HOH:O | 2.19 | 0.76 |
| 1:D:9:GLY:H | 1:D:41:THR:HG21 | 1.48 | 0.76 |
| 1:A:3:VAL:HG22 | 1:A:65:VAL:HB | 1.66 | 0.75 |
| 1:B:10:GLN:HB3 | 4:B:2343:HOH:O | 1.85 | 0.75 |
| 1:B:195:MET:HA | 1:B:195:MET:HE2 | 1.67 | 0.75 |
| 1:E:206:GLY:HA3 | 4:E:5408:HOH:O | 1.85 | 0.75 |
| 1:C:217:LEU:CD1 | 4:C:3417:HOH:O | 2.33 | 0.75 |
| 1:D:223:HIS:C | 4:D:4372:HOH:O | 2.24 | 0.75 |
| 1:E:134:VAL:CG1 | 4:E:5413:HOH:O | 2.11 | 0.75 |
| 1:B:259:GLU:HA | 4:B:2382:HOH:O | 1.83 | 0.75 |
| 1:C:252:SER:O | 1:C:254:LEU:N | 2.18 | 0.75 |
| 1:D:3:VAL:O | 4:D:4365:HOH:O | 2.03 | 0.75 |
| 1:A:-1:ARG:HG3 | 4:A:1332:HOH:O | 1.87 | 0.75 |
| 1:B:232:SER:OG | 4:B:2352:HOH:O | 2.03 | 0.75 |
| 1:C:154:SER:O | 2:C:3300:NAI:N7N | 2.19 | 0.75 |
| 1:E:91:ILE:CA | 4:E:5344:HOH:O | 2.28 | 0.75 |
| 1:E:178:PRO:N | 4:E:5315:HOH:O | 2.19 | 0.75 |
| 1:D:257:ALA:O | 4:D:4349:HOH:O | 2.03 | 0.75 |
| 1:E:158:PHE:HB3 | 4:E:5351:HOH:O | 1.86 | 0.75 |
| 1:A:183:THR:CA | 4:A:1354:HOH:O | 2.21 | 0.75 |
| 1:D:218:LEU:CD2 | 2:D:4300:NAI:H52A | 2.13 | 0.75 |
| 2:D:4300:NAI:C2N | 3:D:4301:GLU:N | 2.47 | 0.75 |
| 1:B:178:PRO:C | 4:B:2373:HOH:O | 2.25 | 0.75 |
| 1:E:121:MET:HB3 | 4:E:5407:HOH:O | 1.85 | 0.75 |
| 1:A:33:SER:O | 1:A:35:PRO:HD3 | 1.87 | 0.75 |
| 1:D:223:HIS:NE2 | 4:D:4321:HOH:O | 2.18 | 0.75 |
| 1:E:253:LEU:HD23 | 4:E:5364:HOH:O | 1.85 | 0.75 |
| 1:A:64:ASP:OD2 | 4:A:1403:HOH:O | 2.03 | 0.74 |
| 1:B:9:GLY:N | 4:B:2314:HOH:O | 2.19 | 0.74 |
| 1:C:82:ILE:HG22 | 1:C:86:ILE:HD13 | 1.68 | 0.74 |
| 1:E:221:GLU:O | 1:E:223:HIS:N | 2.19 | 0.74 |
| 1:A:186:ASP:CA | 4:A:1370:HOH:O | 2.34 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:29:LYS:HA | 4:A:1329:HOH:O | 1.88 | 0.74 |
| 2:B:2300:NAI:O4D | 2:B:2300:NAI:PN | 2.44 | 0.74 |
| 1:B:228:LYS:C | 4:B:2364:HOH:O | 2.26 | 0.74 |
| 1:C:163:GLU:CB | 4:C:3397:HOH:O | 2.36 | 0.74 |
| 1:C:195:MET:HA | 1:C:195:MET:HE2 | 1.70 | 0.74 |
| 1:D:124:THR:OG1 | 4:D:4312:HOH:O | 2.04 | 0.74 |
| 1:D:173:LEU:O | 4:D:4315:HOH:O | 2.05 | 0.74 |
| 1:A:182:PHE:N | 4:A:1419:HOH:O | 2.13 | 0.74 |
| 1:C:137:THR:OG1 | 4:C:3384:HOH:O | 2.04 | 0.74 |
| 1:E:162:VAL:HB | 4:E:5413:HOH:O | 1.87 | 0.74 |
| 1:E:183:THR:OG1 | 4:E:5390:HOH:O | 2.04 | 0.74 |
| 1:A:188:LEU:N | 4:A:1303:HOH:O | 2.21 | 0.74 |
| 1:A:199:ARG:HD3 | 4:A:1351:HOH:O | 1.87 | 0.74 |
| 1:C:158:PHE:CE2 | 2:C:3300:NAI:O3B | 2.39 | 0.74 |
| 1:E:162:VAL:N | 4:E:5413:HOH:O | 2.19 | 0.74 |
| 1:A:77:PHE:C | 4:A:1356:HOH:O | 2.25 | 0.74 |
| 1:B:12:ALA:CB | 4:B:2314:HOH:O | 2.32 | 0.74 |
| 1:B:129:ARG:CZ | 2:B:2300:NAI:C7N | 2.63 | 0.74 |
| 1:E:111:PHE:CE1 | 4:E:5326:HOH:O | 2.36 | 0.74 |
| 1:C:178:PRO:CB | 4:C:3396:HOH:O | 2.29 | 0.74 |
| 1:A:13:PHE:HB2 | 4:A:1379:HOH:O | 1.87 | 0.74 |
| 1:B:239:ILE:HG21 | 4:E:5303:HOH:O | 1.87 | 0.74 |
| 1:D:229:ASP:CB | 4:D:4393:HOH:O | 2.22 | 0.74 |
| 1:B:258:VAL:C | 4:B:2382:HOH:O | 2.25 | 0.73 |
| 1:B:45:LEU:HA | 1:B:48:MET:SD | 2.28 | 0.73 |
| 1:A:163:GLU:HG3 | 4:A:1417:HOH:O | 1.87 | 0.73 |
| 1:A:186:ASP:HB3 | 4:A:1354:HOH:O | 1.89 | 0.73 |
| 1:B:222:GLN:O | 1:B:223:HIS:HB2 | 1.88 | 0.73 |
| 2:D:4300:NAI:O4D | 2:D:4300:NAI:PN | 2.44 | 0.73 |
| 1:A:137:THR:O | 4:A:1367:HOH:O | 2.05 | 0.73 |
| 1:B:75:ILE:H | 1:B:75:ILE:HD12 | 1.53 | 0.73 |
| 1:C:75:ILE:HD13 | 4:C:3377:HOH:O | 1.87 | 0.73 |
| 1:A:171:THR:CA | 4:A:1402:HOH:O | 2.11 | 0.73 |
| 1:C:1:MET:O | 4:C:3306:HOH:O | 2.06 | 0.73 |
| 1:C:29:LYS:HE3 | 4:C:3404:HOH:O | 1.88 | 0.73 |
| 1:A:122:THR:O | 4:A:1428:HOH:O | 2.05 | 0.73 |
| 1:A:35:PRO:O | 1:A:36:ASP:HB2 | 1.88 | 0.73 |
| 1:D:112:ARG:HB3 | 4:D:4329:HOH:O | 1.88 | 0.73 |
| 1:E:179:ALA:CA | 4:E:5369:HOH:O | 2.14 | 0.73 |
| 1:A:125:PRO:HG2 | 1:A:131:GLY:HA2 | 1.68 | 0.73 |
| 1:C:123:ASN:HB2 | 1:C:125:PRO:HD2 | 1.69 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:62:HIS:ND1 | 4:C:3362:HOH:O | 2.21 | 0.73 |
| 1:A:183:THR:O | 4:A:1354:HOH:O | 2.07 | 0.73 |
| 1:A:266:ARG:HG2 | 1:A:266:ARG:HH11 | 1.54 | 0.73 |
| 1:A:2:SER:OG | 4:A:1403:HOH:O | 2.07 | 0.73 |
| 1:A:269:GLN:HG2 | 1:A:270:SER:N | 2.02 | 0.73 |
| 1:B:120:CYS:N | 4:B:2349:HOH:O | 2.10 | 0.73 |
| 1:B:153:LEU:O | 4:B:2392:HOH:O | 2.07 | 0.73 |
| 1:B:85:ASP:HB2 | 4:B:2376:HOH:O | 1.89 | 0.73 |
| 1:B:65:VAL:HG22 | 1:B:91:ILE:HD13 | 1.70 | 0.73 |
| 1:D:246:GLU:OE2 | 4:D:4417:HOH:O | 2.07 | 0.73 |
| 2:D:4300:NAI:C2N | 3:D:4301:GLU:C | 2.57 | 0.73 |
| 1:D:178:PRO:CB | 4:D:4454:HOH:O | 2.27 | 0.72 |
| 1:E:73:HIS:CB | 4:E:5415:HOH:O | 2.30 | 0.72 |
| 1:B:157:GLY:O | 2:B:2300:NAI:H42N | 1.89 | 0.72 |
| 1:C:135:TYR:CE1 | 1:C:161:GLU:HB3 | 2.23 | 0.72 |
| 1:C:193:VAL:HG12 | 4:C:3309:HOH:O | 1.88 | 0.72 |
| 1:D:180:TYR:N | 4:D:4308:HOH:O | 2.18 | 0.72 |
| 1:B:60:VAL:HG12 | 1:B:89:ARG:NH2 | 2.03 | 0.72 |
| 2:D:4300:NAI:C5N | 3:D:4301:GLU:C | 2.57 | 0.72 |
| 1:E:211:LEU:O | 4:E:5314:HOH:O | 2.08 | 0.72 |
| 1:A:126:VAL:HG22 | 1:A:156:VAL:HG12 | 1.71 | 0.72 |
| 1:B:160:THR:HG22 | 1:B:161:GLU:N | 2.04 | 0.72 |
| 1:B:4:GLY:HA3 | 1:B:66:LEU:HD23 | 1.72 | 0.72 |
| 2:E:5300:NAI:PA | 2:E:5300:NAI:C4B | 2.78 | 0.72 |
| 1:D:100:THR:HA | 4:D:4422:HOH:O | 1.89 | 0.72 |
| 1:E:234:PRO:O | 4:E:5309:HOH:O | 2.08 | 0.72 |
| 1:B:186:ASP:OD2 | 4:B:2356:HOH:O | 2.07 | 0.72 |
| 1:C:209:ALA:O | 4:C:3386:HOH:O | 2.08 | 0.72 |
| 1:D:231:VAL:HB | 4:D:4402:HOH:O | 1.89 | 0.72 |
| 1:E:126:VAL:HG21 | 4:E:5385:HOH:O | 1.88 | 0.72 |
| 1:A:186:ASP:HA | 4:A:1370:HOH:O | 1.88 | 0.72 |
| 1:D:101:ILE:HB | 1:D:164:GLU:OE1 | 1.90 | 0.72 |
| 1:C:171:THR:OG1 | 4:C:3351:HOH:O | 2.08 | 0.72 |
| 1:E:153:LEU:CB | 4:E:5432:HOH:O | 2.38 | 0.72 |
| 1:A:201:LEU:O | 1:A:205:LEU:HG | 1.89 | 0.72 |
| 1:B:142:GLN:CG | 1:B:143:VAL:H | 1.91 | 0.72 |
| 1:D:100:THR:HG22 | 1:D:102:SER:H | 1.55 | 0.72 |
| 1:D:246:GLU:OE1 | 4:D:4383:HOH:O | 2.08 | 0.72 |
| 1:E:246:GLU:OE2 | 4:E:5312:HOH:O | 2.07 | 0.72 |
| 1:E:91:ILE:CB | 4:E:5344:HOH:O | 2.02 | 0.72 |
| 1:C:163:GLU:HG3 | 4:C:3397:HOH:O | 1.89 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:211:LEU:O | 4:D:4406:HOH:O | 2.07 | 0.71 |
| 1:D:6:ILE:HD12 | 1:D:66:LEU:HD21 | 1.71 | 0.71 |
| 1:E:141:ALA:HB2 | 4:E:5388:HOH:O | 1.89 | 0.71 |
| 1:E:158:PHE:CD1 | 2:E:5300:NAI:H4B | 2.25 | 0.71 |
| 1:E:251:ARG:NH1 | 4:E:5366:HOH:O | 2.22 | 0.71 |
| 1:B:150:GLU:OE1 | 4:B:2312:HOH:O | 2.08 | 0.71 |
| 1:D:11:LEU:N | 4:D:4387:HOH:O | 2.23 | 0.71 |
| 1:D:174:SER:CA | 4:D:4315:HOH:O | 2.39 | 0.71 |
| 1:E:130:GLU:OE2 | 2:E:5300:NAI:H2D | 1.90 | 0.71 |
| 1:D:124:THR:O | 1:D:127:VAL:HG23 | 1.89 | 0.71 |
| 1:D:97:ALA:HB1 | 1:D:265:THR:HG23 | 1.72 | 0.71 |
| 1:E:57:LYS:HD3 | 1:E:57:LYS:H | 1.56 | 0.71 |
| 1:E:58:GLU:OE1 | 4:E:5332:HOH:O | 2.07 | 0.71 |
| 1:A:27:ALA:N | 4:A:1382:HOH:O | 2.21 | 0.71 |
| 1:A:89:ARG:NH2 | 4:A:1395:HOH:O | 2.23 | 0.71 |
| 1:B:28:HIS:O | 4:B:2344:HOH:O | 2.08 | 0.71 |
| 1:A:2:SER:HB3 | 4:A:1334:HOH:O | 1.89 | 0.71 |
| 1:C:126:VAL:HG11 | 4:C:3317:HOH:O | 1.89 | 0.71 |
| 1:D:83:GLY:O | 1:D:86:ILE:HG22 | 1.89 | 0.71 |
| 1:E:206:GLY:CA | 4:E:5408:HOH:O | 2.36 | 0.71 |
| 1:D:37:MET:CG | 4:D:4306:HOH:O | 2.22 | 0.71 |
| 1:E:70:VAL:N | 4:E:5305:HOH:O | 2.15 | 0.71 |
| 1:A:88:ASP:HB2 | 1:A:112:ARG:NH2 | 2.05 | 0.71 |
| 1:A:3:VAL:N | 4:A:1334:HOH:O | 2.22 | 0.71 |
| 1:B:2:SER:HA | 1:B:30:ILE:HG12 | 1.72 | 0.71 |
| 1:D:124:THR:CA | 4:D:4375:HOH:O | 2.39 | 0.71 |
| 1:A:86:ILE:CD1 | 1:A:108:LEU:HD11 | 2.15 | 0.71 |
| 1:E:199:ARG:HB3 | 4:E:5416:HOH:O | 1.90 | 0.71 |
| 1:B:117:VAL:O | 4:B:2370:HOH:O | 2.09 | 0.71 |
| 1:C:222:GLN:HA | 4:C:3304:HOH:O | 1.89 | 0.71 |
| 1:D:161:GLU:OE2 | 4:D:4398:HOH:O | 2.08 | 0.71 |
| 1:C:3:VAL:HB | 1:C:30:ILE:CG1 | 2.21 | 0.71 |
| 1:D:185:LEU:HD21 | 1:D:210:LEU:HD12 | 1.72 | 0.71 |
| 1:C:91:ILE:HG23 | 1:C:116:ARG:HB2 | 1.73 | 0.70 |
| 1:D:150:GLU:OE2 | 4:D:4390:HOH:O | 2.09 | 0.70 |
| 1:D:32:ALA:HB3 | 1:D:52:LEU:HD23 | 1.72 | 0.70 |
| 1:E:121:MET:HE2 | 1:E:122:THR:H | 1.55 | 0.70 |
| 1:E:153:LEU:CA | 4:E:5432:HOH:O | 2.39 | 0.70 |
| 1:E:215:LYS:HE3 | 4:E:5430:HOH:O | 1.84 | 0.70 |
| 1:A:190:ASP:O | 4:A:1420:HOH:O | 2.09 | 0.70 |
| 1:A:269:GLN:HA | 4:A:1407:HOH:O | 1.91 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:-1:ARG:HB3 | 4:A:1342:HOH:O | 1.90 | 0.70 |
| 1:C:126:VAL:HG12 | 4:C:3307:HOH:O | 1.89 | 0.70 |
| 1:C:218:LEU:HB3 | 2:C:3300:NAI:H52N | 1.73 | 0.70 |
| 1:C:264:ARG:NE | 4:C:3353:HOH:O | 2.10 | 0.70 |
| 1:A:75:ILE:HG22 | 1:A:76:PRO:CD | 2.21 | 0.70 |
| 1:B:100:THR:HG22 | 1:B:101:ILE:N | 2.06 | 0.70 |
| 1:B:187:ALA:O | 1:B:190:ASP:HB2 | 1.91 | 0.70 |
| 1:B:19:PHE:HA | 1:B:22:ALA:HB3 | 1.73 | 0.70 |
| 1:C:122:THR:CB | 1:C:133:THR:HG22 | 2.19 | 0.70 |
| 1:C:6:ILE:HD12 | 1:C:56:ASN:HB3 | 1.73 | 0.70 |
| 1:D:128:VAL:O | 1:D:129:ARG:HB2 | 1.92 | 0.70 |
| 1:A:122:THR:CG2 | 1:A:123:ASN:H | 2.04 | 0.70 |
| 1:A:124:THR:N | 4:A:1325:HOH:O | 2.15 | 0.70 |
| 1:A:158:PHE:HA | 4:A:1412:HOH:O | 1.91 | 0.70 |
| 1:A:266:ARG:HD2 | 4:A:1331:HOH:O | 1.82 | 0.70 |
| 1:D:116:ARG:HA | 4:D:4389:HOH:O | 1.91 | 0.70 |
| 1:D:168:ASP:OD1 | 4:D:4337:HOH:O | 2.09 | 0.70 |
| 1:E:100:THR:HG22 | 1:E:102:SER:H | 1.56 | 0.70 |
| 1:B:218:LEU:CD2 | 2:B:2300:NAI:H52A | 2.21 | 0.70 |
| 1:C:15:LEU:HD11 | 4:C:3348:HOH:O | 1.88 | 0.70 |
| 1:C:274:GLN:NE2 | 4:C:3339:HOH:O | 2.22 | 0.70 |
| 1:D:184:ALA:HB2 | 4:D:4340:HOH:O | 1.92 | 0.70 |
| 1:E:165:ASP:O | 4:E:5349:HOH:O | 2.09 | 0.70 |
| 1:E:57:LYS:HD3 | 1:E:57:LYS:N | 2.07 | 0.70 |
| 1:A:161:GLU:CB | 4:A:1364:HOH:O | 2.26 | 0.70 |
| 1:C:195:MET:HA | 1:C:195:MET:CE | 2.21 | 0.70 |
| 1:C:29:LYS:CB | 4:C:3306:HOH:O | 2.39 | 0.70 |
| 1:E:156:VAL:HG12 | 1:E:156:VAL:O | 1.90 | 0.70 |
| 1:A:130:GLU:O | 4:A:1307:HOH:O | 2.10 | 0.70 |
| 1:C:266:ARG:NE | 4:C:3303:HOH:O | 2.24 | 0.70 |
| 1:E:60:VAL:HG21 | 1:E:82:ILE:HG23 | 1.71 | 0.70 |
| 1:C:165:ASP:O | 4:C:3311:HOH:O | 2.10 | 0.70 |
| 1:C:7:GLY:HA2 | 1:C:70:VAL:HG22 | 1.74 | 0.70 |
| 1:E:194:LYS:CA | 4:E:5303:HOH:O | 2.19 | 0.70 |
| 1:B:208:GLN:OE1 | 4:B:2359:HOH:O | 2.09 | 0.70 |
| 1:D:56:ASN:ND2 | 4:D:4369:HOH:O | 2.25 | 0.70 |
| 1:E:174:SER:CB | 4:E:5391:HOH:O | 2.40 | 0.70 |
| 1:B:208:GLN:HB2 | 4:B:2359:HOH:O | 1.91 | 0.69 |
| 1:C:27:ALA:HB1 | 4:C:3363:HOH:O | 1.92 | 0.69 |
| 1:D:103:SER:HA | 4:D:4449:HOH:O | 1.91 | 0.69 |
| 1:D:97:ALA:HA | 4:D:4333:HOH:O | 1.91 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:136:ALA:O | 4:E:5434:HOH:O | 2.09 | 0.69 |
| 1:B:100:THR:HG22 | 1:B:101:ILE:H | 1.55 | 0.69 |
| 1:C:56:ASN:O | 4:C:3383:HOH:O | 2.10 | 0.69 |
| 1:C:85:ASP:O | 4:C:3382:HOH:O | 2.10 | 0.69 |
| 1:A:106:LYS:O | 4:A:1432:HOH:O | 2.09 | 0.69 |
| 1:C:10:GLN:NE2 | 4:C:3390:HOH:O | 2.25 | 0.69 |
| 1:C:198:PRO:HG2 | 1:C:201:LEU:HB3 | 1.75 | 0.69 |
| 1:D:231:VAL:O | 4:D:4401:HOH:O | 2.09 | 0.69 |
| 1:B:8:ALA:HA | 1:B:12:ALA:CB | 2.22 | 0.69 |
| 1:D:124:THR:CG2 | 4:D:4375:HOH:O | 2.20 | 0.69 |
| 1:E:169:ALA:HA | 4:E:5375:HOH:O | 1.92 | 0.69 |
| 1:E:91:ILE:N | 4:E:5344:HOH:O | 2.26 | 0.69 |
| 1:A:130:GLU:OE2 | 2:A:1300:NAI:H2D | 1.92 | 0.69 |
| 1:A:168:ASP:HB2 | 4:A:1338:HOH:O | 1.92 | 0.69 |
| 1:C:115:PRO:HB3 | 4:C:3358:HOH:O | 1.93 | 0.69 |
| 1:A:162:VAL:HG13 | 1:A:166:LEU:HD12 | 1.75 | 0.69 |
| 1:B:37:MET:HE3 | 4:B:2393:HOH:O | 1.92 | 0.69 |
| 1:E:102:SER:HB3 | 4:E:5347:HOH:O | 1.91 | 0.69 |
| 2:E:5300:NAI:O2A | 2:E:5300:NAI:O4B | 2.11 | 0.69 |
| 2:E:5300:NAI:PA | 2:E:5300:NAI:PN | 2.89 | 0.69 |
| 1:A:193:VAL:CG2 | 4:A:1369:HOH:O | 2.40 | 0.69 |
| 1:C:128:VAL:HG12 | 1:C:129:ARG:N | 2.06 | 0.69 |
| 1:D:125:PRO:O | 1:D:128:VAL:HG12 | 1.92 | 0.69 |
| 1:A:122:THR:CG2 | 1:A:123:ASN:N | 2.56 | 0.69 |
| 1:B:231:VAL:CG1 | 4:B:2363:HOH:O | 2.40 | 0.69 |
| 1:C:100:THR:HG22 | 1:C:102:SER:H | 1.57 | 0.69 |
| 1:C:118:ILE:H | 1:C:118:ILE:HD13 | 1.57 | 0.69 |
| 1:C:140:HIS:HB2 | 4:C:3385:HOH:O | 1.91 | 0.69 |
| 1:E:164:GLU:O | 4:E:5395:HOH:O | 2.11 | 0.69 |
| 1:A:29:LYS:CA | 4:A:1329:HOH:O | 2.41 | 0.69 |
| 1:D:61:GLN:O | 4:D:4430:HOH:O | 2.11 | 0.69 |
| 1:E:253:LEU:N | 4:E:5364:HOH:O | 2.25 | 0.69 |
| 1:E:262:CYS:CB | 4:E:5342:HOH:O | 2.37 | 0.69 |
| 1:E:80:ASP:OD1 | 4:E:5326:HOH:O | 2.10 | 0.69 |
| 1:C:203:VAL:CA | 4:C:3355:HOH:O | 2.34 | 0.68 |
| 1:D:67:PHE:N | 4:D:4327:HOH:O | 2.26 | 0.68 |
| 1:E:133:THR:CG2 | 4:E:5385:HOH:O | 2.40 | 0.68 |
| 4:A:1315:HOH:O | 1:E:228:LYS:HE2 | 1.92 | 0.68 |
| 1:A:183:THR:C | 4:A:1354:HOH:O | 2.32 | 0.68 |
| 1:A:230:ASN:CB | 4:A:1317:HOH:O | 2.40 | 0.68 |
| 1:B:229:ASP:OD1 | 4:B:2386:HOH:O | 2.09 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:101:ILE:CG1 | 4:C:3394:HOH:O | 2.32 | 0.68 |
| 1:D:3:VAL:HB | 1:D:30:ILE:CD1 | 2.22 | 0.68 |
| 1:E:11:LEU:O | 1:E:15:LEU:HD12 | 1.93 | 0.68 |
| 1:E:175:GLY:O | 4:E:5397:HOH:O | 2.10 | 0.68 |
| 1:E:251:ARG:CD | 4:E:5330:HOH:O | 2.40 | 0.68 |
| 1:C:257:ALA:O | 4:C:3378:HOH:O | 2.11 | 0.68 |
| 1:C:266:ARG:HG2 | 4:C:3340:HOH:O | 1.92 | 0.68 |
| 1:C:129:ARG:CD | 2:C:3300:NAI:O7N | 2.41 | 0.68 |
| 1:D:133:THR:HG21 | 1:D:153:LEU:HD12 | 1.75 | 0.68 |
| 1:E:2:SER:HB3 | 4:E:5387:HOH:O | 1.93 | 0.68 |
| 1:A:-1:ARG:HG2 | 4:A:1332:HOH:O | 1.87 | 0.68 |
| 1:D:175:GLY:O | 4:D:4309:HOH:O | 2.10 | 0.68 |
| 1:E:251:ARG:N | 4:E:5317:HOH:O | 2.26 | 0.68 |
| 1:A:150:GLU:OE2 | 4:A:1383:HOH:O | 2.11 | 0.68 |
| 1:B:6:ILE:CD1 | 1:B:59:THR:HB | 2.24 | 0.68 |
| 1:C:124:THR:N | 1:C:125:PRO:HD2 | 2.08 | 0.68 |
| 1:D:251:ARG:HD3 | 4:D:4427:HOH:O | 1.94 | 0.68 |
| 1:D:88:ASP:HA | 4:D:4432:HOH:O | 1.91 | 0.68 |
| 1:A:194:LYS:HE2 | 1:E:240:HIS:CE1 | 2.29 | 0.68 |
| 1:A:130:GLU:CD | 2:A:1300:NAI:H2D | 2.13 | 0.68 |
| 1:E:48:MET:O | 1:E:48:MET:HG2 | 1.94 | 0.68 |
| 1:B:6:ILE:HD13 | 1:B:59:THR:HB | 1.75 | 0.68 |
| 1:C:252:SER:OG | 4:C:3308:HOH:O | 2.07 | 0.68 |
| 1:E:225:GLY:HA2 | 4:E:5353:HOH:O | 1.86 | 0.68 |
| 1:E:251:ARG:HD2 | 4:E:5330:HOH:O | 1.94 | 0.68 |
| 1:C:185:LEU:CD2 | 4:C:3324:HOH:O | 2.42 | 0.68 |
| 1:B:124:THR:N | 1:B:125:PRO:HD2 | 2.09 | 0.68 |
| 1:C:180:TYR:HD2 | 4:C:3302:HOH:O | 1.76 | 0.68 |
| 1:C:203:VAL:HG13 | 4:C:3355:HOH:O | 1.92 | 0.68 |
| 1:D:150:GLU:HB2 | 4:D:4443:HOH:O | 1.94 | 0.68 |
| 1:E:114:ALA:O | 4:E:5436:HOH:O | 2.11 | 0.68 |
| 1:A:22:ALA:CB | 4:A:1425:HOH:O | 2.41 | 0.67 |
| 1:D:181:ALA:O | 4:D:4330:HOH:O | 2.11 | 0.67 |
| 1:E:190:ASP:OD1 | 4:E:5381:HOH:O | 2.12 | 0.67 |
| 1:A:266:ARG:NE | 4:A:1331:HOH:O | 2.21 | 0.67 |
| 1:B:124:THR:O | 1:B:127:VAL:HG23 | 1.94 | 0.67 |
| 1:B:50:VAL:HA | 4:B:2378:HOH:O | 1.95 | 0.67 |
| 1:D:148:LEU:HB2 | 4:D:4348:HOH:O | 1.93 | 0.67 |
| 1:E:147:ARG:O | 1:E:151:GLN:HB2 | 1.94 | 0.67 |
| 1:B:101:ILE:O | 1:B:105:GLU:HB2 | 1.93 | 0.67 |
| 1:C:29:LYS:HB3 | 4:C:3306:HOH:O | 1.93 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:229:ASP:N | 4:D:4310:HOH:O | 2.25 | 0.67 |
| 1:C:150:GLU:O | 4:C:3319:HOH:O | 2.13 | 0.67 |
| 1:E:199:ARG:NH2 | 4:E:5316:HOH:O | 2.28 | 0.67 |
| 1:A:76:PRO:O | 4:A:1356:HOH:O | 2.12 | 0.67 |
| 1:B:61:GLN:HA | 4:B:2325:HOH:O | 1.94 | 0.67 |
| 1:B:71:LYS:HB3 | 1:B:72:PRO:CD | 2.22 | 0.67 |
| 1:D:30:ILE:CB | 4:D:4425:HOH:O | 2.28 | 0.67 |
| 1:E:123:ASN:HB3 | 4:E:5397:HOH:O | 1.94 | 0.67 |
| 1:C:223:HIS:N | 4:C:3304:HOH:O | 2.21 | 0.67 |
| 1:C:66:LEU:HD23 | 1:C:67:PHE:N | 2.10 | 0.67 |
| 1:A:158:PHE:CZ | 2:A:1300:NAI:O3B | 2.48 | 0.67 |
| 1:A:165:ASP:O | 4:A:1393:HOH:O | 2.12 | 0.67 |
| 1:B:129:ARG:C | 4:B:2372:HOH:O | 2.33 | 0.67 |
| 1:E:122:THR:CB | 1:E:133:THR:HG22 | 2.23 | 0.67 |
| 1:A:124:THR:OG1 | 4:A:1325:HOH:O | 2.13 | 0.66 |
| 1:B:178:PRO:O | 4:B:2373:HOH:O | 2.13 | 0.66 |
| 1:C:231:VAL:O | 1:C:231:VAL:HG12 | 1.95 | 0.66 |
| 1:C:260:ALA:HB3 | 4:C:3378:HOH:O | 1.94 | 0.66 |
| 1:C:273:ASP:C | 4:C:3393:HOH:O | 2.33 | 0.66 |
| 1:C:275:GLU:N | 4:C:3393:HOH:O | 2.23 | 0.66 |
| 1:C:29:LYS:CE | 4:C:3404:HOH:O | 2.33 | 0.66 |
| 1:E:179:ALA:O | 4:E:5322:HOH:O | 2.14 | 0.66 |
| 1:E:75:ILE:HG21 | 1:E:104:ILE:HD11 | 1.78 | 0.66 |
| 1:C:75:ILE:HA | 4:C:3407:HOH:O | 1.94 | 0.66 |
| 1:D:161:GLU:CD | 4:D:4398:HOH:O | 2.33 | 0.66 |
| 1:D:62:HIS:ND1 | 1:D:62:HIS:O | 2.27 | 0.66 |
| 1:A:120:CYS:CB | 4:A:1368:HOH:O | 2.42 | 0.66 |
| 1:A:187:ALA:C | 4:A:1303:HOH:O | 2.34 | 0.66 |
| 1:B:255:ILE:HG12 | 4:B:2303:HOH:O | 1.96 | 0.66 |
| 1:E:185:LEU:HD21 | 1:E:210:LEU:HD12 | 1.76 | 0.66 |
| 1:A:79:LEU:HD11 | 1:A:104:ILE:CD1 | 2.24 | 0.66 |
| 1:C:251:ARG:O | 1:C:252:SER:O | 2.13 | 0.66 |
| 1:D:266:ARG:NE | 4:D:4378:HOH:O | 2.27 | 0.66 |
| 1:D:32:ALA:HB3 | 1:D:52:LEU:CD2 | 2.25 | 0.66 |
| 1:C:198:PRO:CD | 4:C:3361:HOH:O | 2.42 | 0.66 |
| 1:C:265:THR:HG22 | 4:C:3340:HOH:O | 1.94 | 0.66 |
| 1:D:151:GLN:HB3 | 4:D:4444:HOH:O | 1.94 | 0.66 |
| 1:D:61:GLN:O | 4:D:4415:HOH:O | 2.13 | 0.66 |
| 1:A:253:LEU:HD23 | 4:A:1405:HOH:O | 1.95 | 0.66 |
| 1:A:26:ALA:HB1 | 4:A:1382:HOH:O | 1.96 | 0.66 |
| 1:B:129:ARG:CA | 4:B:2372:HOH:O | 2.42 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:182:PHE:CD1 | 4:B:2373:HOH:O | 2.47 | 0.66 |
| 1:B:219:HIS:HE1 | 2:B:2300:NAI:O5D | 1.73 | 0.66 |
| 1:D:232:SER:HB3 | 1:D:239:ILE:HG12 | 1.78 | 0.66 |
| 1:A:124:THR:N | 1:A:125:PRO:HD2 | 2.10 | 0.66 |
| 1:C:101:ILE:HD11 | 1:C:117:VAL:O | 1.95 | 0.66 |
| 1:A:193:VAL:HG23 | 4:A:1369:HOH:O | 1.96 | 0.66 |
| 1:B:129:ARG:HH21 | 3:B:2301:GLU:HB2 | 1.59 | 0.66 |
| 1:D:251:ARG:CZ | 4:D:4427:HOH:O | 2.42 | 0.66 |
| 1:E:220:SER:O | 1:E:221:GLU:HB2 | 1.95 | 0.66 |
| 1:B:168:ASP:CB | 4:B:2357:HOH:O | 2.43 | 0.66 |
| 1:D:93:VAL:HA | 4:D:4408:HOH:O | 1.95 | 0.66 |
| 1:E:193:VAL:O | 4:E:5303:HOH:O | 2.12 | 0.66 |
| 1:D:256:ASN:O | 4:D:4318:HOH:O | 2.13 | 0.66 |
| 1:D:3:VAL:HB | 1:D:30:ILE:HD12 | 1.78 | 0.66 |
| 1:E:55:HIS:HB3 | 1:E:57:LYS:HE2 | 1.78 | 0.66 |
| 1:A:120:CYS:C | 4:A:1327:HOH:O | 2.35 | 0.65 |
| 1:A:206:GLY:O | 4:A:1421:HOH:O | 2.14 | 0.65 |
| 1:A:1:MET:CB | 4:A:1427:HOH:O | 2.25 | 0.65 |
| 1:B:189:ALA:CA | 4:B:2302:HOH:O | 2.35 | 0.65 |
| 1:C:118:ILE:HG22 | 1:C:137:THR:HA | 1.76 | 0.65 |
| 1:E:114:ALA:HB1 | 1:E:140:HIS:CG | 2.31 | 0.65 |
| 1:B:94:SER:HB2 | 4:B:2306:HOH:O | 1.95 | 0.65 |
| 1:C:192:GLY:HA3 | 4:C:3367:HOH:O | 1.88 | 0.65 |
| 1:C:50:VAL:N | 4:C:3363:HOH:O | 2.27 | 0.65 |
| 1:B:195:MET:HA | 1:B:195:MET:CE | 2.26 | 0.65 |
| 1:D:264:ARG:NH2 | 4:D:4380:HOH:O | 2.15 | 0.65 |
| 1:D:3:VAL:HG22 | 1:D:65:VAL:CG1 | 2.27 | 0.65 |
| 1:D:90:HIS:O | 4:D:4455:HOH:O | 2.14 | 0.65 |
| 1:C:29:LYS:C | 1:C:30:ILE:HD12 | 2.17 | 0.65 |
| 2:D:4300:NAI:N1N | 3:D:4301:GLU:CA | 2.55 | 0.65 |
| 1:E:118:ILE:O | 4:E:5325:HOH:O | 2.13 | 0.65 |
| 1:A:240:HIS:HA | 4:A:1352:HOH:O | 1.97 | 0.65 |
| 1:A:85:ASP:HB2 | 4:A:1437:HOH:O | 1.95 | 0.65 |
| 1:B:160:THR:N | 4:B:2311:HOH:O | 2.23 | 0.65 |
| 1:B:172:GLY:HA2 | 1:B:261:SER:OG | 1.96 | 0.65 |
| 1:C:29:LYS:CG | 4:C:3404:HOH:O | 2.39 | 0.65 |
| 1:C:29:LYS:N | 4:C:3404:HOH:O | 2.29 | 0.65 |
| 1:A:182:PHE:O | 4:A:1354:HOH:O | 2.13 | 0.65 |
| 1:A:187:ALA:HB1 | 4:A:1303:HOH:O | 1.97 | 0.65 |
| 1:A:198:PRO:HG2 | 1:A:201:LEU:HB3 | 1.77 | 0.65 |
| 1:B:3:VAL:H | 1:B:30:ILE:HG23 | 1.61 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:57:LYS:NZ | 4:D:4438:HOH:O | 2.28 | 0.65 |
| 1:E:178:PRO:CD | 4:E:5315:HOH:O | 2.44 | 0.65 |
| 1:A:238:THR:OG1 | 4:A:1320:HOH:O | 2.14 | 0.65 |
| 1:B:218:LEU:CD1 | 2:B:2300:NAI:H52N | 2.25 | 0.65 |
| 1:C:171:THR:OG1 | 4:C:3380:HOH:O | 2.15 | 0.65 |
| 1:A:142:GLN:N | 4:A:1390:HOH:O | 2.05 | 0.65 |
| 1:A:240:HIS:NE2 | 4:A:1375:HOH:O | 2.22 | 0.65 |
| 1:C:251:ARG:CA | 4:C:3359:HOH:O | 2.40 | 0.65 |
| 1:A:198:PRO:HD2 | 1:A:201:LEU:HD23 | 1.77 | 0.65 |
| 1:D:222:GLN:O | 1:D:223:HIS:CB | 2.44 | 0.65 |
| 1:D:53:THR:HG22 | 1:D:55:HIS:N | 2.11 | 0.65 |
| 1:E:163:GLU:OE2 | 4:E:5399:HOH:O | 2.14 | 0.65 |
| 2:E:5300:NAI:O2A | 2:E:5300:NAI:C4B | 2.45 | 0.65 |
| 1:E:83:GLY:HA2 | 1:E:86:ILE:HD12 | 1.79 | 0.65 |
| 1:A:135:TYR:OH | 1:A:150:GLU:HG3 | 1.97 | 0.64 |
| 1:B:133:THR:O | 4:B:2311:HOH:O | 2.15 | 0.64 |
| 1:B:73:HIS:ND1 | 4:B:2390:HOH:O | 2.26 | 0.64 |
| 1:B:74:ILE:HG23 | 1:B:78:ILE:HG21 | 1.79 | 0.64 |
| 1:B:63:SER:HB2 | 1:B:89:ARG:NH1 | 2.13 | 0.64 |
| 1:B:9:GLY:H | 1:B:12:ALA:CB | 2.05 | 0.64 |
| 1:A:126:VAL:HG22 | 1:A:156:VAL:CG1 | 2.26 | 0.64 |
| 1:B:126:VAL:HA | 4:B:2372:HOH:O | 1.98 | 0.64 |
| 1:B:185:LEU:O | 1:B:187:ALA:N | 2.30 | 0.64 |
| 1:D:224:PRO:N | 4:D:4372:HOH:O | 2.29 | 0.64 |
| 1:E:220:SER:HB2 | 1:E:222:GLN:HG2 | 1.79 | 0.64 |
| 1:A:138:GLY:CA | 4:A:1310:HOH:O | 2.39 | 0.64 |
| 1:B:128:VAL:O | 1:B:129:ARG:HB2 | 1.97 | 0.64 |
| 1:D:223:HIS:CE1 | 4:D:4355:HOH:O | 2.51 | 0.64 |
| 2:D:4300:NAI:C6N | 3:D:4301:GLU:C | 2.65 | 0.64 |
| 1:A:181:ALA:O | 4:A:1419:HOH:O | 2.12 | 0.64 |
| 1:B:134:VAL:HA | 4:B:2311:HOH:O | 1.98 | 0.64 |
| 1:C:131:GLY:CA | 4:C:3307:HOH:O | 2.41 | 0.64 |
| 1:C:43:SER:O | 1:C:46:ARG:HB2 | 1.97 | 0.64 |
| 1:D:125:PRO:HB2 | 1:D:131:GLY:HA2 | 1.80 | 0.64 |
| 1:A:128:VAL:O | 1:A:129:ARG:HB2 | 1.97 | 0.64 |
| 1:B:95:CYS:HA | 1:B:120:CYS:O | 1.97 | 0.64 |
| 1:C:124:THR:O | 1:C:127:VAL:HG23 | 1.97 | 0.64 |
| 1:C:169:ALA:HB2 | 4:C:3320:HOH:O | 1.97 | 0.64 |
| 1:C:24:VAL:N | 4:C:3369:HOH:O | 2.09 | 0.64 |
| 1:E:178:PRO:HB2 | 4:E:5393:HOH:O | 1.96 | 0.64 |
| 1:A:11:LEU:HD12 | 4:A:1399:HOH:O | 1.97 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:94:SER:CA | 4:A:1321:HOH:O | 2.45 | 0.64 |
| 1:E:0:GLY:O | 4:E:5371:HOH:O | 2.13 | 0.64 |
| 1:E:124:THR:O | 1:E:127:VAL:HG23 | 1.96 | 0.64 |
| 1:E:151:GLN:HB3 | 4:E:5428:HOH:O | 1.98 | 0.64 |
| 1:A:111:PHE:O | 4:A:1365:HOH:O | 2.14 | 0.64 |
| 1:A:194:LYS:O | 1:A:195:MET:SD | 2.55 | 0.64 |
| 1:C:185:LEU:N | 4:C:3352:HOH:O | 2.31 | 0.64 |
| 1:C:198:PRO:HD3 | 4:C:3361:HOH:O | 1.98 | 0.64 |
| 3:A:1301:GLU:HG2 | 4:A:1408:HOH:O | 1.97 | 0.64 |
| 1:A:26:ALA:HB3 | 1:A:29:LYS:HB2 | 1.78 | 0.64 |
| 1:C:178:PRO:CA | 4:C:3396:HOH:O | 2.46 | 0.64 |
| 1:C:62:HIS:CE1 | 4:C:3362:HOH:O | 2.50 | 0.64 |
| 1:D:99:VAL:O | 4:D:4317:HOH:O | 2.15 | 0.64 |
| 1:A:135:TYR:CE2 | 1:A:150:GLU:HG2 | 2.33 | 0.64 |
| 4:B:2308:HOH:O | 1:D:239:ILE:HG21 | 1.92 | 0.64 |
| 1:E:130:GLU:OE2 | 2:E:5300:NAI:C2D | 2.46 | 0.64 |
| 1:E:13:PHE:CE1 | 4:E:5306:HOH:O | 2.51 | 0.64 |
| 1:E:232:SER:HB2 | 4:E:5345:HOH:O | 1.97 | 0.64 |
| 1:E:56:ASN:O | 1:E:60:VAL:HG23 | 1.98 | 0.64 |
| 1:A:156:VAL:O | 1:A:156:VAL:HG12 | 1.98 | 0.64 |
| 1:C:223:HIS:ND1 | 1:C:224:PRO:HD2 | 2.13 | 0.64 |
| 1:D:115:PRO:HA | 4:D:4307:HOH:O | 1.98 | 0.64 |
| 1:D:22:ALA:HB3 | 1:D:24:VAL:HG23 | 1.80 | 0.64 |
| 1:E:203:VAL:HG23 | 4:E:5320:HOH:O | 1.98 | 0.64 |
| 1:E:218:LEU:HD22 | 2:E:5300:NAI:H52A | 1.79 | 0.64 |
| 1:E:63:SER:CA | 4:E:5417:HOH:O | 2.43 | 0.64 |
| 1:A:119:ARG:HG2 | 4:A:1372:HOH:O | 1.90 | 0.63 |
| 1:C:112:ARG:HG3 | 1:C:112:ARG:HH11 | 1.63 | 0.63 |
| 1:A:269:GLN:C | 1:A:271:MET:H | 2.02 | 0.63 |
| 1:A:33:SER:OG | 1:A:56:ASN:HB3 | 1.98 | 0.63 |
| 1:A:36:ASP:O | 1:A:37:MET:HB2 | 1.98 | 0.63 |
| 1:B:4:GLY:HA2 | 1:B:59:THR:HG22 | 1.79 | 0.63 |
| 1:B:73:HIS:O | 1:B:78:ILE:HD13 | 1.98 | 0.63 |
| 1:C:117:VAL:HG23 | 4:C:3315:HOH:O | 1.98 | 0.63 |
| 1:C:213:ALA:CB | 4:C:3386:HOH:O | 2.24 | 0.63 |
| 1:A:129:ARG:HD2 | 4:A:1371:HOH:O | 1.98 | 0.63 |
| 1:B:182:PHE:CE1 | 4:B:2373:HOH:O | 2.51 | 0.63 |
| 1:B:259:GLU:CA | 4:B:2382:HOH:O | 2.43 | 0.63 |
| 1:C:155:SER:HA | 2:C:3300:NAI:N7N | 2.09 | 0.63 |
| 1:C:160:THR:HG22 | 1:C:161:GLU:N | 2.13 | 0.63 |
| 1:C:29:LYS:HG2 | 4:C:3404:HOH:O | 1.98 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:217:LEU:HB3 | 4:D:4323:HOH:O | 1.98 | 0.63 |
| 1:A:164:GLU:HA | 1:A:167:ILE:HG12 | 1.80 | 0.63 |
| 1:A:271:MET:HG2 | 1:A:271:MET:O | 1.98 | 0.63 |
| 1:B:155:SER:C | 2:B:2300:NAI:H72N | 2.02 | 0.63 |
| 1:C:123:ASN:N | 4:C:3331:HOH:O | 2.17 | 0.63 |
| 1:C:172:GLY:HA2 | 1:C:261:SER:OG | 1.98 | 0.63 |
| 1:A:17:LYS:HA | 1:A:48:MET:HE3 | 1.81 | 0.63 |
| 1:E:198:PRO:HG2 | 1:E:201:LEU:HB3 | 1.81 | 0.63 |
| 1:B:94:SER:C | 4:B:2349:HOH:O | 2.36 | 0.63 |
| 1:D:87:GLU:CB | 4:D:4322:HOH:O | 2.34 | 0.63 |
| 1:E:190:ASP:CG | 4:E:5381:HOH:O | 2.35 | 0.63 |
| 1:A:89:ARG:HG3 | 1:A:90:HIS:N | 2.14 | 0.63 |
| 1:B:158:PHE:CZ | 2:B:2300:NAI:C3B | 2.82 | 0.63 |
| 1:D:168:ASP:CG | 4:D:4337:HOH:O | 2.37 | 0.63 |
| 1:E:177:GLY:HA2 | 1:E:180:TYR:CD1 | 2.34 | 0.63 |
| 1:E:211:LEU:CD1 | 4:E:5314:HOH:O | 2.46 | 0.63 |
| 1:E:229:ASP:CA | 4:E:5337:HOH:O | 2.20 | 0.63 |
| 1:E:158:PHE:CE2 | 2:E:5300:NAI:O3B | 2.52 | 0.63 |
| 1:A:55:HIS:HB3 | 1:A:57:LYS:HD2 | 1.80 | 0.63 |
| 1:B:256:ASN:CB | 4:B:2369:HOH:O | 2.42 | 0.63 |
| 1:A:100:THR:HG22 | 1:A:102:SER:H | 1.64 | 0.63 |
| 1:C:114:ALA:HB1 | 1:C:140:HIS:ND1 | 2.14 | 0.63 |
| 1:E:30:ILE:HB | 1:E:50:VAL:HG22 | 1.79 | 0.63 |
| 1:E:94:SER:N | 4:E:5325:HOH:O | 2.05 | 0.63 |
| 1:A:123:ASN:HB2 | 4:A:1325:HOH:O | 1.98 | 0.62 |
| 1:B:160:THR:HG22 | 1:B:161:GLU:H | 1.62 | 0.62 |
| 1:C:172:GLY:O | 1:C:258:VAL:HG22 | 1.99 | 0.62 |
| 1:C:266:ARG:HG2 | 1:C:266:ARG:NH1 | 2.14 | 0.62 |
| 1:E:225:GLY:O | 4:E:5353:HOH:O | 2.16 | 0.62 |
| 1:A:139:THR:N | 4:A:1310:HOH:O | 2.31 | 0.62 |
| 1:C:3:VAL:O | 1:C:30:ILE:HA | 1.98 | 0.62 |
| 1:E:169:ALA:C | 1:E:171:THR:H | 2.01 | 0.62 |
| 1:A:174:SER:CB | 4:A:1339:HOH:O | 2.46 | 0.62 |
| 1:C:218:LEU:CB | 2:C:3300:NAI:H52N | 2.28 | 0.62 |
| 1:E:153:LEU:C | 4:E:5432:HOH:O | 2.37 | 0.62 |
| 1:E:17:LYS:HB3 | 4:E:5306:HOH:O | 1.90 | 0.62 |
| 1:B:109:SER:OG | 1:B:115:PRO:HD2 | 1.98 | 0.62 |
| 1:B:129:ARG:N | 4:B:2372:HOH:O | 2.32 | 0.62 |
| 1:C:19:PHE:O | 4:C:3369:HOH:O | 2.15 | 0.62 |
| 1:C:218:LEU:HB3 | 2:C:3300:NAI:C5D | 2.30 | 0.62 |
| 1:C:155:SER:CA | 2:C:3300:NAI:H72N | 2.10 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:101:ILE:HG12 | 1:A:119:ARG:HB2 | 1.81 | 0.62 |
| 1:B:259:GLU:N | 4:B:2382:HOH:O | 2.33 | 0.62 |
| 1:D:103:SER:CA | 4:D:4449:HOH:O | 2.45 | 0.62 |
| 1:A:121:MET:N | 4:A:1327:HOH:O | 2.33 | 0.62 |
| 1:D:266:ARG:C | 1:D:268:LEU:H | 2.03 | 0.62 |
| 1:D:176:SER:O | 1:D:179:ALA:HB3 | 1.99 | 0.62 |
| 1:A:78:ILE:N | 4:A:1356:HOH:O | 2.31 | 0.62 |
| 1:B:162:VAL:HG12 | 1:B:163:GLU:HG2 | 1.82 | 0.62 |
| 1:B:264:ARG:O | 1:B:268:LEU:HG | 2.00 | 0.62 |
| 1:C:25:LEU:HD11 | 1:C:30:ILE:HD11 | 1.81 | 0.62 |
| 1:D:71:LYS:O | 1:D:75:ILE:HD12 | 1.99 | 0.62 |
| 2:D:4300:NAI:H3D | 4:D:4423:HOH:O | 2.00 | 0.62 |
| 1:E:193:VAL:C | 4:E:5303:HOH:O | 2.37 | 0.62 |
| 1:B:141:ALA:HB1 | 1:B:145:ASP:OD2 | 2.00 | 0.62 |
| 1:B:225:GLY:O | 1:B:228:LYS:HB3 | 1.99 | 0.62 |
| 1:C:258:VAL:CG1 | 1:C:258:VAL:O | 2.47 | 0.62 |
| 1:A:118:ILE:HD12 | 1:A:149:MET:SD | 2.39 | 0.61 |
| 1:A:172:GLY:HA2 | 1:A:261:SER:HB3 | 1.82 | 0.61 |
| 1:B:122:THR:HG22 | 1:B:133:THR:OG1 | 1.99 | 0.61 |
| 1:B:200:ARG:NH1 | 1:B:204:ARG:HH21 | 1.98 | 0.61 |
| 1:C:185:LEU:HD23 | 4:C:3324:HOH:O | 1.99 | 0.61 |
| 1:C:71:LYS:HB2 | 1:C:73:HIS:CE1 | 2.35 | 0.61 |
| 1:D:30:ILE:CA | 4:D:4365:HOH:O | 2.41 | 0.61 |
| 1:A:123:ASN:HD21 | 1:A:132:ALA:N | 1.97 | 0.61 |
| 1:A:13:PHE:CA | 4:A:1379:HOH:O | 2.47 | 0.61 |
| 1:A:193:VAL:C | 1:A:195:MET:H | 2.04 | 0.61 |
| 1:B:125:PRO:HG2 | 1:B:131:GLY:HA2 | 1.82 | 0.61 |
| 1:E:122:THR:HG22 | 1:E:133:THR:CB | 2.28 | 0.61 |
| 1:A:258:VAL:HG23 | 4:A:1302:HOH:O | 1.94 | 0.61 |
| 1:C:250:PHE:N | 4:C:3312:HOH:O | 2.33 | 0.61 |
| 1:C:68:LEU:HD11 | 1:C:78:ILE:HG21 | 1.82 | 0.61 |
| 1:D:53:THR:HG21 | 1:D:58:GLU:OE1 | 2.00 | 0.61 |
| 1:D:58:GLU:HB3 | 4:D:4358:HOH:O | 1.99 | 0.61 |
| 1:E:209:ALA:C | 4:E:5360:HOH:O | 2.37 | 0.61 |
| 1:A:2:SER:CB | 4:A:1403:HOH:O | 2.47 | 0.61 |
| 1:C:3:VAL:HB | 1:C:30:ILE:HG12 | 1.82 | 0.61 |
| 1:A:93:VAL:HG13 | 1:A:118:ILE:HG13 | 1.82 | 0.61 |
| 1:B:119:ARG:HD2 | 1:B:164:GLU:OE2 | 2.00 | 0.61 |
| 1:C:208:GLN:OE1 | 4:C:3395:HOH:O | 2.16 | 0.61 |
| 1:C:37:MET:HA | 1:C:42:VAL:HG11 | 1.82 | 0.61 |
| 1:E:86:ILE:HD12 | 1:E:108:LEU:HD22 | 1.81 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:263:ILE:H | 1:A:263:ILE:CD1 | 2.14 | 0.61 |
| 1:B:129:ARG:CZ | 2:B:2300:NAI:C3N | 2.78 | 0.61 |
| 1:B:231:VAL:HG13 | 4:B:2363:HOH:O | 1.99 | 0.61 |
| 1:C:119:ARG:NH2 | 4:C:3310:HOH:O | 2.31 | 0.61 |
| 1:D:229:ASP:HA | 4:D:4316:HOH:O | 2.01 | 0.61 |
| 1:A:241:ALA:O | 1:A:244:VAL:HG22 | 2.01 | 0.61 |
| 1:B:14:ALA:CA | 1:B:127:VAL:HG22 | 2.28 | 0.61 |
| 2:B:2300:NAI:N1N | 3:B:2301:GLU:OXT | 2.33 | 0.61 |
| 1:C:122:THR:CB | 4:C:3331:HOH:O | 2.15 | 0.61 |
| 2:C:3300:NAI:N1N | 3:C:3301:GLU:OXT | 2.33 | 0.61 |
| 1:A:68:LEU:HD12 | 1:A:94:SER:HB2 | 1.82 | 0.61 |
| 1:C:133:THR:HG22 | 4:C:3331:HOH:O | 2.00 | 0.61 |
| 1:E:106:LYS:CB | 4:E:5384:HOH:O | 2.47 | 0.61 |
| 1:B:129:ARG:NH2 | 3:B:2301:GLU:HG3 | 2.14 | 0.61 |
| 1:B:64:ASP:O | 1:B:90:HIS:HA | 1.99 | 0.61 |
| 1:B:70:VAL:HG23 | 4:B:2368:HOH:O | 2.01 | 0.61 |
| 1:D:220:SER:HB2 | 1:D:222:GLN:HG2 | 1.82 | 0.61 |
| 1:E:113:PRO:HD2 | 4:E:5367:HOH:O | 2.01 | 0.61 |
| 1:A:220:SER:HB2 | 4:A:1441:HOH:O | 2.00 | 0.61 |
| 1:A:259:GLU:N | 4:A:1366:HOH:O | 2.29 | 0.61 |
| 1:B:133:THR:HG22 | 4:B:2387:HOH:O | 2.01 | 0.61 |
| 1:B:256:ASN:C | 4:B:2381:HOH:O | 2.38 | 0.61 |
| 1:A:115:PRO:HD2 | 1:A:140:HIS:CD2 | 2.36 | 0.60 |
| 1:B:266:ARG:O | 1:B:269:GLN:HG2 | 2.01 | 0.60 |
| 1:C:48:MET:HB3 | 4:C:3371:HOH:O | 1.89 | 0.60 |
| 1:D:30:ILE:CG1 | 4:D:4425:HOH:O | 2.48 | 0.60 |
| 1:D:38:ASP:OD2 | 1:D:40:ALA:HB3 | 2.01 | 0.60 |
| 1:E:135:TYR:CE1 | 1:E:161:GLU:HB3 | 2.36 | 0.60 |
| 1:E:251:ARG:NE | 4:E:5348:HOH:O | 2.34 | 0.60 |
| 1:A:79:LEU:HD11 | 1:A:104:ILE:HG23 | 1.83 | 0.60 |
| 1:B:245:LEU:CA | 4:B:2353:HOH:O | 2.40 | 0.60 |
| 1:C:49:GLY:CA | 4:C:3363:HOH:O | 2.47 | 0.60 |
| 1:E:77:PHE:HD1 | 1:E:77:PHE:H | 1.47 | 0.60 |
| 1:B:178:PRO:HG2 | 4:B:2345:HOH:O | 2.02 | 0.60 |
| 1:C:264:ARG:NH2 | 4:C:3353:HOH:O | 2.23 | 0.60 |
| 1:D:168:ASP:HA | 4:D:4337:HOH:O | 2.01 | 0.60 |
| 1:D:266:ARG:CZ | 4:D:4378:HOH:O | 2.46 | 0.60 |
| 1:A:45:LEU:HD21 | 4:A:1379:HOH:O | 2.01 | 0.60 |
| 1:B:218:LEU:HD22 | 2:B:2300:NAI:O5B | 2.00 | 0.60 |
| 1:C:93:VAL:CG1 | 1:C:118:ILE:HD11 | 2.30 | 0.60 |
| 1:C:45:LEU:O | 1:C:48:MET:HB3 | 2.02 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:126:VAL:HG13 | 1:D:156:VAL:CG1 | 2.30 | 0.60 |
| 1:D:246:GLU:CG | 4:D:4383:HOH:O | 2.44 | 0.60 |
| 1:D:266:ARG:CD | 4:D:4311:HOH:O | 2.49 | 0.60 |
| 1:A:123:ASN:C | 1:A:125:PRO:HD2 | 2.22 | 0.60 |
| 1:A:222:GLN:O | 1:A:223:HIS:CB | 2.49 | 0.60 |
| 2:B:2300:NAI:H2N | 3:B:2301:GLU:HB3 | 1.78 | 0.60 |
| 1:B:70:VAL:HG12 | 1:B:71:LYS:H | 1.66 | 0.60 |
| 1:D:185:LEU:CG | 4:D:4330:HOH:O | 2.28 | 0.60 |
| 1:D:203:VAL:HG12 | 1:D:204:ARG:N | 2.17 | 0.60 |
| 1:D:78:ILE:HG23 | 1:D:82:ILE:HD13 | 1.83 | 0.60 |
| 1:A:186:ASP:CB | 4:A:1354:HOH:O | 2.45 | 0.60 |
| 1:B:188:LEU:C | 1:B:190:ASP:H | 2.05 | 0.60 |
| 1:D:265:THR:CB | 4:D:4360:HOH:O | 2.06 | 0.60 |
| 1:E:128:VAL:O | 1:E:129:ARG:C | 2.39 | 0.60 |
| 1:E:133:THR:HG21 | 4:E:5385:HOH:O | 2.01 | 0.60 |
| 1:A:106:LYS:HG3 | 4:A:1344:HOH:O | 2.02 | 0.60 |
| 1:A:95:CYS:N | 4:A:1321:HOH:O | 2.33 | 0.60 |
| 1:B:102:SER:HA | 1:B:105:GLU:HB2 | 1.82 | 0.60 |
| 1:B:223:HIS:ND1 | 1:B:224:PRO:HD2 | 2.16 | 0.60 |
| 1:C:249:GLY:O | 1:C:252:SER:HB3 | 2.02 | 0.60 |
| 1:E:86:ILE:CD1 | 1:E:108:LEU:HD22 | 2.32 | 0.60 |
| 1:B:258:VAL:HG22 | 4:B:2382:HOH:O | 2.02 | 0.60 |
| 1:C:105:GLU:CG | 4:C:3315:HOH:O | 2.41 | 0.60 |
| 1:C:3:VAL:HB | 1:C:30:ILE:HG13 | 1.84 | 0.60 |
| 1:E:133:THR:HG22 | 4:E:5385:HOH:O | 2.01 | 0.60 |
| 1:E:22:ALA:HA | 1:E:129:ARG:NH2 | 2.17 | 0.60 |
| 1:B:129:ARG:NH2 | 3:B:2301:GLU:CG | 2.56 | 0.60 |
| 1:A:55:HIS:C | 1:A:57:LYS:H | 2.05 | 0.59 |
| 1:C:115:PRO:HG3 | 4:C:3358:HOH:O | 2.01 | 0.59 |
| 1:C:169:ALA:CA | 4:C:3320:HOH:O | 2.49 | 0.59 |
| 1:C:51:LYS:NZ | 1:C:51:LYS:HB2 | 2.17 | 0.59 |
| 1:D:116:ARG:O | 4:D:4455:HOH:O | 2.16 | 0.59 |
| 1:D:151:GLN:C | 4:D:4444:HOH:O | 2.41 | 0.59 |
| 1:D:174:SER:HA | 4:D:4315:HOH:O | 1.98 | 0.59 |
| 1:D:211:LEU:CD1 | 4:D:4406:HOH:O | 2.42 | 0.59 |
| 1:A:123:ASN:ND2 | 1:A:132:ALA:H | 2.00 | 0.59 |
| 1:A:182:PHE:CD1 | 4:A:1324:HOH:O | 2.45 | 0.59 |
| 1:B:82:ILE:HG22 | 1:B:86:ILE:CD1 | 2.31 | 0.59 |
| 1:C:125:PRO:HB2 | 1:C:130:GLU:O | 2.02 | 0.59 |
| 1:C:238:THR:O | 1:C:241:ALA:N | 2.35 | 0.59 |
| 1:D:222:GLN:N | 4:D:4384:HOH:O | 2.35 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:162:VAL:CB | 4:E:5413:HOH:O | 2.47 | 0.59 |
| 1:A:239:ILE:N | 4:A:1391:HOH:O | 2.34 | 0.59 |
| 1:A:26:ALA:C | 4:A:1382:HOH:O | 2.40 | 0.59 |
| 1:A:28:HIS:CD2 | 4:A:1329:HOH:O | 2.56 | 0.59 |
| 1:B:235:GLY:O | 4:B:2318:HOH:O | 2.17 | 0.59 |
| 1:E:64:ASP:N | 4:E:5417:HOH:O | 2.31 | 0.59 |
| 1:E:70:VAL:O | 1:E:71:LYS:HB2 | 2.02 | 0.59 |
| 1:B:94:SER:O | 1:B:96:ALA:N | 2.35 | 0.59 |
| 1:C:266:ARG:NH2 | 4:C:3311:HOH:O | 2.15 | 0.59 |
| 1:A:94:SER:OG | 4:A:1321:HOH:O | 2.15 | 0.59 |
| 1:B:129:ARG:HH12 | 2:B:2300:NAI:C2N | 2.06 | 0.59 |
| 1:B:251:ARG:O | 1:B:254:LEU:N | 2.31 | 0.59 |
| 1:B:269:GLN:C | 1:B:271:MET:H | 2.06 | 0.59 |
| 1:B:41:THR:O | 1:B:45:LEU:HG | 2.02 | 0.59 |
| 1:C:35:PRO:O | 1:C:36:ASP:HB2 | 2.02 | 0.59 |
| 1:E:136:ALA:HB3 | 4:E:5434:HOH:O | 2.01 | 0.59 |
| 1:A:122:THR:HG22 | 1:A:123:ASN:H | 1.64 | 0.59 |
| 1:B:101:ILE:HG13 | 1:B:102:SER:N | 2.17 | 0.59 |
| 1:B:11:LEU:CD2 | 4:B:2343:HOH:O | 2.43 | 0.59 |
| 1:B:231:VAL:O | 4:B:2363:HOH:O | 2.17 | 0.59 |
| 1:D:123:ASN:CB | 4:D:4309:HOH:O | 2.43 | 0.59 |
| 1:E:185:LEU:CG | 4:E:5383:HOH:O | 2.11 | 0.59 |
| 1:B:168:ASP:HB3 | 4:B:2357:HOH:O | 2.00 | 0.59 |
| 1:D:116:ARG:HB2 | 4:D:4455:HOH:O | 2.03 | 0.59 |
| 1:E:176:SER:CA | 4:E:5333:HOH:O | 2.20 | 0.59 |
| 2:A:1300:NAI:C5D | 4:A:1431:HOH:O | 2.44 | 0.59 |
| 1:A:223:HIS:ND1 | 1:A:224:PRO:HD2 | 2.16 | 0.59 |
| 1:B:189:ALA:HA | 4:B:2302:HOH:O | 1.99 | 0.59 |
| 1:E:168:ASP:OD2 | 1:E:266:ARG:HG3 | 2.03 | 0.59 |
| 1:E:223:HIS:ND1 | 1:E:224:PRO:HD2 | 2.18 | 0.59 |
| 1:A:112:ARG:HD3 | 4:A:1365:HOH:O | 2.02 | 0.59 |
| 1:B:240:HIS:C | 4:B:2329:HOH:O | 2.40 | 0.59 |
| 1:C:156:VAL:HG12 | 1:C:156:VAL:O | 2.02 | 0.59 |
| 1:D:13:PHE:HA | 1:D:16:ALA:HB3 | 1.85 | 0.59 |
| 1:D:197:LEU:HD22 | 1:D:201:LEU:HD23 | 1.85 | 0.59 |
| 1:A:133:THR:HG21 | 1:A:153:LEU:CD1 | 2.25 | 0.59 |
| 1:A:68:LEU:HB2 | 4:A:1321:HOH:O | 2.02 | 0.59 |
| 1:C:177:GLY:HA2 | 1:C:180:TYR:CD1 | 2.37 | 0.59 |
| 1:D:6:ILE:CD1 | 1:D:66:LEU:HD21 | 2.32 | 0.59 |
| 1:A:268:LEU:HD21 | 4:A:1322:HOH:O | 2.03 | 0.58 |
| 1:A:60:VAL:HG21 | 1:A:82:ILE:HD12 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:215:LYS:NZ | 4:B:2394:HOH:O | 2.29 | 0.58 |
| 1:B:53:THR:HG23 | 1:B:58:GLU:OE2 | 2.03 | 0.58 |
| 1:A:22:ALA:HB2 | 4:A:1425:HOH:O | 2.02 | 0.58 |
| 1:B:176:SER:HB3 | 1:B:180:TYR:CE2 | 2.37 | 0.58 |
| 1:C:246:GLU:O | 4:C:3402:HOH:O | 2.17 | 0.58 |
| 1:A:190:ASP:N | 1:A:199:ARG:HH12 | 2.00 | 0.58 |
| 1:C:266:ARG:CG | 4:C:3340:HOH:O | 2.50 | 0.58 |
| 1:D:117:VAL:O | 1:D:138:GLY:HA3 | 2.02 | 0.58 |
| 1:D:266:ARG:O | 1:D:268:LEU:N | 2.36 | 0.58 |
| 1:D:264:ARG:O | 1:D:268:LEU:HB2 | 2.03 | 0.58 |
| 1:E:122:THR:CG2 | 1:E:133:THR:HB | 2.30 | 0.58 |
| 1:E:37:MET:O | 4:E:5392:HOH:O | 2.16 | 0.58 |
| 1:E:89:ARG:NH2 | 4:E:5324:HOH:O | 2.36 | 0.58 |
| 1:B:123:ASN:HB2 | 1:B:125:PRO:HD2 | 1.84 | 0.58 |
| 1:D:275:GLU:C | 4:D:4456:HOH:O | 2.41 | 0.58 |
| 1:D:88:ASP:C | 4:D:4432:HOH:O | 2.37 | 0.58 |
| 1:E:222:GLN:O | 1:E:223:HIS:CB | 2.51 | 0.58 |
| 1:B:215:LYS:HG3 | 4:B:2377:HOH:O | 2.03 | 0.58 |
| 1:C:250:PHE:O | 4:C:3359:HOH:O | 2.17 | 0.58 |
| 1:D:97:ALA:CA | 4:D:4333:HOH:O | 2.50 | 0.58 |
| 1:E:123:ASN:HB2 | 4:E:5310:HOH:O | 2.04 | 0.58 |
| 1:E:274:GLN:HG3 | 1:E:275:GLU:N | 2.17 | 0.58 |
| 1:B:13:PHE:HB2 | 1:B:41:THR:HG21 | 1.86 | 0.58 |
| 1:D:113:PRO:CD | 4:D:4329:HOH:O | 2.49 | 0.58 |
| 1:D:75:ILE:HG21 | 1:D:104:ILE:HD11 | 1.86 | 0.58 |
| 1:E:188:LEU:HB3 | 4:E:5396:HOH:O | 2.02 | 0.58 |
| 1:E:75:ILE:HG13 | 1:E:99:VAL:HG21 | 1.85 | 0.58 |
| 1:A:138:GLY:C | 4:A:1310:HOH:O | 2.42 | 0.58 |
| 1:A:267:GLU:O | 1:A:271:MET:HB3 | 2.03 | 0.58 |
| 1:B:8:ALA:HB1 | 1:B:45:LEU:CD1 | 2.34 | 0.58 |
| 1:C:194:LYS:N | 4:C:3309:HOH:O | 2.35 | 0.58 |
| 1:D:258:VAL:HG12 | 1:D:259:GLU:N | 2.18 | 0.58 |
| 1:D:264:ARG:NE | 4:D:4380:HOH:O | 2.26 | 0.58 |
| 1:E:62:HIS:ND1 | 4:E:5372:HOH:O | 2.31 | 0.58 |
| 1:A:175:GLY:O | 4:A:1436:HOH:O | 2.16 | 0.58 |
| 1:B:221:GLU:O | 1:B:223:HIS:N | 2.37 | 0.58 |
| 1:C:131:GLY:N | 4:C:3307:HOH:O | 2.37 | 0.58 |
| 1:C:79:LEU:HD22 | 1:C:108:LEU:HD11 | 1.85 | 0.58 |
| 1:A:136:ALA:HA | 4:A:1404:HOH:O | 2.02 | 0.58 |
| 1:D:98:GLY:HA3 | 1:D:269:GLN:HB2 | 1.86 | 0.58 |
| 1:D:57:LYS:HD3 | 4:D:4438:HOH:O | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:100:THR:HG22 | 1:E:101:ILE:N | 2.19 | 0.57 |
| 1:E:125:PRO:CG | 4:E:5302:HOH:O | 2.52 | 0.57 |
| 1:E:251:ARG:CZ | 4:E:5366:HOH:O | 2.52 | 0.57 |
| 1:B:71:LYS:HB2 | 1:B:73:HIS:CE1 | 2.39 | 0.57 |
| 1:E:117:VAL:O | 1:E:138:GLY:HA3 | 2.03 | 0.57 |
| 1:A:264:ARG:NE | 4:A:1322:HOH:O | 2.12 | 0.57 |
| 1:B:159:CYS:HA | 4:B:2311:HOH:O | 2.03 | 0.57 |
| 1:C:101:ILE:CD1 | 4:C:3394:HOH:O | 2.52 | 0.57 |
| 1:A:68:LEU:HB2 | 1:A:94:SER:HA | 1.87 | 0.57 |
| 1:B:192:GLY:N | 4:B:2355:HOH:O | 2.37 | 0.57 |
| 1:D:169:ALA:C | 1:D:171:THR:H | 2.07 | 0.57 |
| 1:E:106:LYS:HA | 4:E:5398:HOH:O | 2.04 | 0.57 |
| 1:E:159:CYS:N | 4:E:5425:HOH:O | 2.35 | 0.57 |
| 1:A:231:VAL:O | 1:A:231:VAL:HG12 | 2.04 | 0.57 |
| 1:B:160:THR:CG2 | 1:B:161:GLU:H | 2.17 | 0.57 |
| 1:C:124:THR:C | 1:C:126:VAL:H | 2.07 | 0.57 |
| 1:D:177:GLY:HA2 | 1:D:180:TYR:CD1 | 2.40 | 0.57 |
| 1:E:195:MET:CE | 1:E:195:MET:HA | 2.35 | 0.57 |
| 1:A:259:GLU:OE1 | 4:A:1330:HOH:O | 2.18 | 0.57 |
| 1:C:185:LEU:CA | 4:C:3352:HOH:O | 2.53 | 0.57 |
| 1:C:221:GLU:OE2 | 1:C:221:GLU:HA | 2.02 | 0.57 |
| 1:D:130:GLU:OE2 | 2:D:4300:NAI:H2D | 2.05 | 0.57 |
| 1:C:121:MET:HG3 | 4:C:3351:HOH:O | 2.04 | 0.57 |
| 1:B:1:MET:HB2 | 1:B:64:ASP:HB2 | 1.85 | 0.57 |
| 1:B:70:VAL:HG12 | 1:B:71:LYS:N | 2.18 | 0.57 |
| 1:C:45:LEU:O | 1:C:45:LEU:HD23 | 2.05 | 0.57 |
| 1:C:55:HIS:C | 1:C:57:LYS:H | 2.09 | 0.57 |
| 1:E:169:ALA:O | 1:E:171:THR:N | 2.38 | 0.57 |
| 1:E:73:HIS:CD2 | 4:E:5429:HOH:O | 2.56 | 0.57 |
| 1:C:185:LEU:HA | 4:C:3352:HOH:O | 2.04 | 0.57 |
| 1:E:141:ALA:CB | 4:E:5388:HOH:O | 2.52 | 0.57 |
| 1:E:172:GLY:HA2 | 1:E:261:SER:HG | 1.69 | 0.57 |
| 1:A:187:ALA:CB | 4:A:1303:HOH:O | 2.52 | 0.57 |
| 1:A:29:LYS:CG | 4:A:1329:HOH:O | 2.52 | 0.57 |
| 1:B:101:ILE:HG23 | 1:B:164:GLU:OE2 | 2.05 | 0.57 |
| 1:D:1:MET:CE | 1:D:25:LEU:HD21 | 2.33 | 0.57 |
| 1:E:47:LYS:CE | 4:E:5338:HOH:O | 2.37 | 0.57 |
| 1:A:89:ARG:HG3 | 1:A:90:HIS:H | 1.69 | 0.56 |
| 1:B:160:THR:CG2 | 1:B:161:GLU:N | 2.67 | 0.56 |
| 1:C:264:ARG:O | 1:C:268:LEU:HG | 2.05 | 0.56 |
| 1:E:229:ASP:HA | 4:E:5340:HOH:O | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:163:GLU:N | 4:A:1355:HOH:O | 2.32 | 0.56 |
| 1:A:264:ARG:NH2 | 4:A:1322:HOH:O | 2.36 | 0.56 |
| 1:B:219:HIS:CE1 | 2:B:2300:NAI:PN | 2.99 | 0.56 |
| 1:B:74:ILE:O | 1:B:79:LEU:HG | 2.06 | 0.56 |
| 1:B:82:ILE:CA | 4:B:2376:HOH:O | 2.44 | 0.56 |
| 1:C:203:VAL:CG1 | 4:C:3355:HOH:O | 2.49 | 0.56 |
| 2:A:1300:NAI:C6N | 2:A:1300:NAI:C1D | 2.78 | 0.56 |
| 1:B:153:LEU:C | 1:B:155:SER:H | 2.07 | 0.56 |
| 1:B:220:SER:C | 4:B:2322:HOH:O | 2.42 | 0.56 |
| 1:E:22:ALA:HA | 1:E:129:ARG:HH21 | 1.69 | 0.56 |
| 1:A:249:GLY:HA2 | 4:A:1318:HOH:O | 2.04 | 0.56 |
| 1:B:176:SER:HA | 4:B:2327:HOH:O | 2.05 | 0.56 |
| 2:B:2300:NAI:C5N | 3:B:2301:GLU:OXT | 2.53 | 0.56 |
| 1:C:169:ALA:HA | 4:C:3320:HOH:O | 2.05 | 0.56 |
| 1:C:197:LEU:HD12 | 4:C:3367:HOH:O | 2.04 | 0.56 |
| 1:D:80:ASP:CG | 4:D:4370:HOH:O | 2.43 | 0.56 |
| 1:E:119:ARG:HA | 4:E:5325:HOH:O | 2.04 | 0.56 |
| 1:E:179:ALA:C | 4:E:5369:HOH:O | 2.39 | 0.56 |
| 1:E:222:GLN:HG3 | 1:E:227:LEU:HD21 | 1.87 | 0.56 |
| 1:B:74:ILE:O | 1:B:78:ILE:HB | 2.05 | 0.56 |
| 1:D:229:ASP:CA | 4:D:4310:HOH:O | 2.54 | 0.56 |
| 1:D:62:HIS:HA | 4:D:4415:HOH:O | 2.05 | 0.56 |
| 1:A:70:VAL:HG22 | 1:A:75:ILE:HD12 | 1.86 | 0.56 |
| 1:B:115:PRO:HB3 | 4:B:2328:HOH:O | 2.05 | 0.56 |
| 1:B:231:VAL:HG12 | 4:B:2363:HOH:O | 2.02 | 0.56 |
| 1:B:259:GLU:OE1 | 4:B:2334:HOH:O | 2.17 | 0.56 |
| 1:C:236:GLY:HA2 | 4:C:3398:HOH:O | 1.98 | 0.56 |
| 1:C:269:GLN:C | 1:C:271:MET:H | 2.08 | 0.56 |
| 1:E:163:GLU:CD | 4:E:5399:HOH:O | 2.36 | 0.56 |
| 1:B:222:GLN:O | 1:B:223:HIS:CB | 2.52 | 0.56 |
| 1:B:236:GLY:HA2 | 1:B:239:ILE:CG2 | 2.30 | 0.56 |
| 1:B:94:SER:OG | 1:B:119:ARG:HA | 2.06 | 0.56 |
| 1:C:163:GLU:CG | 4:C:3397:HOH:O | 2.45 | 0.56 |
| 1:C:194:LYS:CA | 4:C:3309:HOH:O | 2.44 | 0.56 |
| 1:C:260:ALA:N | 4:C:3381:HOH:O | 2.39 | 0.56 |
| 1:D:103:SER:N | 4:D:4449:HOH:O | 2.38 | 0.56 |
| 1:E:170:VAL:HG12 | 1:E:170:VAL:O | 2.06 | 0.56 |
| 1:E:228:LYS:C | 4:E:5337:HOH:O | 2.44 | 0.56 |
| 1:B:184:ALA:O | 1:B:188:LEU:HG | 2.06 | 0.56 |
| 1:C:114:ALA:HB1 | 1:C:140:HIS:CE1 | 2.41 | 0.56 |
| 1:C:181:ALA:N | 4:C:3336:HOH:O | 2.39 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:169:ALA:O | 1:D:171:THR:N | 2.39 | 0.56 |
| 1:D:82:ILE:N | 1:D:82:ILE:HD12 | 2.20 | 0.56 |
| 1:E:33:SER:O | 1:E:35:PRO:HD3 | 2.06 | 0.56 |
| 1:E:63:SER:HB3 | 4:E:5372:HOH:O | 2.06 | 0.56 |
| 1:C:75:ILE:HB | 1:C:76:PRO:HD3 | 1.88 | 0.56 |
| 1:D:141:ALA:CA | 4:D:4386:HOH:O | 2.38 | 0.56 |
| 1:D:269:GLN:C | 1:D:271:MET:H | 2.10 | 0.56 |
| 1:E:162:VAL:CG1 | 1:E:166:LEU:HB2 | 2.35 | 0.56 |
| 1:B:198:PRO:HD2 | 1:B:201:LEU:HD23 | 1.87 | 0.56 |
| 1:B:241:ALA:CA | 4:B:2329:HOH:O | 2.44 | 0.56 |
| 1:E:151:GLN:N | 4:E:5327:HOH:O | 2.30 | 0.56 |
| 1:C:141:ALA:HA | 1:C:145:ASP:OD1 | 2.05 | 0.56 |
| 1:C:75:ILE:HG13 | 1:C:99:VAL:HG21 | 1.87 | 0.56 |
| 1:D:113:PRO:HD2 | 4:D:4329:HOH:O | 2.06 | 0.56 |
| 1:D:164:GLU:HA | 1:D:167:ILE:HG12 | 1.87 | 0.56 |
| 1:E:105:GLU:HB2 | 4:E:5437:HOH:O | 2.06 | 0.56 |
| 1:A:135:TYR:HE2 | 1:A:150:GLU:HG2 | 1.70 | 0.55 |
| 1:A:2:SER:HB2 | 4:A:1403:HOH:O | 2.04 | 0.55 |
| 1:B:200:ARG:O | 1:B:204:ARG:HG2 | 2.06 | 0.55 |
| 1:C:118:ILE:N | 1:C:118:ILE:HD13 | 2.19 | 0.55 |
| 1:C:249:GLY:O | 1:C:253:LEU:HD13 | 2.06 | 0.55 |
| 1:D:136:ALA:HB3 | 4:D:4367:HOH:O | 2.05 | 0.55 |
| 1:D:269:GLN:O | 1:D:271:MET:N | 2.39 | 0.55 |
| 1:A:172:GLY:HA2 | 1:A:261:SER:CB | 2.35 | 0.55 |
| 1:A:116:ARG:NH2 | 1:A:145:ASP:OD1 | 2.38 | 0.55 |
| 1:B:251:ARG:C | 4:B:2303:HOH:O | 2.44 | 0.55 |
| 1:B:35:PRO:HG2 | 1:B:71:LYS:NZ | 2.21 | 0.55 |
| 1:C:86:ILE:HG22 | 1:C:87:GLU:N | 2.21 | 0.55 |
| 1:E:218:LEU:CD2 | 4:E:5424:HOH:O | 2.54 | 0.55 |
| 1:B:198:PRO:HG2 | 1:B:201:LEU:HB3 | 1.88 | 0.55 |
| 1:C:124:THR:O | 1:C:126:VAL:N | 2.39 | 0.55 |
| 1:C:218:LEU:CB | 2:C:3300:NAI:C5D | 2.84 | 0.55 |
| 1:C:45:LEU:HD21 | 1:C:50:VAL:HB | 1.87 | 0.55 |
| 1:D:180:TYR:HD2 | 4:D:4308:HOH:O | 1.88 | 0.55 |
| 1:D:57:LYS:HE3 | 4:D:4376:HOH:O | 1.97 | 0.55 |
| 1:D:81:GLU:HB3 | 1:D:82:ILE:HD12 | 1.89 | 0.55 |
| 1:E:91:ILE:O | 4:E:5344:HOH:O | 2.18 | 0.55 |
| 1:B:231:VAL:HB | 4:B:2364:HOH:O | 2.05 | 0.55 |
| 1:C:53:THR:CG2 | 1:C:58:GLU:HB2 | 2.35 | 0.55 |
| 1:D:252:SER:N | 4:D:4342:HOH:O | 2.39 | 0.55 |
| 1:A:230:ASN:ND2 | 4:A:1317:HOH:O | 2.11 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:266:ARG:NH2 | 4:A:1440:HOH:O | 2.36 | 0.55 |
| 1:B:102:SER:HA | 1:B:105:GLU:CB | 2.37 | 0.55 |
| 1:B:220:SER:O | 1:B:221:GLU:CB | 2.55 | 0.55 |
| 1:B:68:LEU:HB3 | 4:B:2368:HOH:O | 2.05 | 0.55 |
| 1:C:258:VAL:C | 4:C:3391:HOH:O | 2.38 | 0.55 |
| 1:C:275:GLU:C | 4:C:3401:HOH:O | 2.45 | 0.55 |
| 1:E:125:PRO:O | 1:E:129:ARG:O | 2.25 | 0.55 |
| 1:E:75:ILE:O | 1:E:79:LEU:HG | 2.05 | 0.55 |
| 1:A:120:CYS:N | 4:A:1372:HOH:O | 2.40 | 0.55 |
| 1:C:185:LEU:HD21 | 1:C:210:LEU:HD12 | 1.88 | 0.55 |
| 1:C:236:GLY:O | 1:C:237:ALA:HB3 | 2.06 | 0.55 |
| 1:C:253:LEU:HD12 | 1:C:253:LEU:H | 1.71 | 0.55 |
| 1:C:29:LYS:NZ | 4:C:3344:HOH:O | 2.25 | 0.55 |
| 2:C:3300:NAI:H2N | 3:C:3301:GLU:HB3 | 1.79 | 0.55 |
| 1:D:101:ILE:HD11 | 1:D:117:VAL:O | 2.07 | 0.55 |
| 1:D:128:VAL:O | 1:D:129:ARG:CB | 2.55 | 0.55 |
| 1:D:170:VAL:HG12 | 1:D:170:VAL:O | 2.07 | 0.55 |
| 1:E:106:LYS:HB2 | 4:E:5384:HOH:O | 2.06 | 0.55 |
| 1:A:182:PHE:CZ | 4:A:1324:HOH:O | 2.48 | 0.55 |
| 1:A:219:HIS:O | 1:A:220:SER:HB3 | 2.06 | 0.55 |
| 1:B:235:GLY:C | 4:B:2318:HOH:O | 2.44 | 0.55 |
| 2:C:3300:NAI:C5N | 3:C:3301:GLU:OXT | 2.53 | 0.55 |
| 1:D:62:HIS:CA | 4:D:4448:HOH:O | 2.53 | 0.55 |
| 1:D:183:THR:HG21 | 4:D:4428:HOH:O | 2.07 | 0.55 |
| 1:D:211:LEU:HD12 | 1:D:211:LEU:C | 2.27 | 0.55 |
| 1:D:231:VAL:CG1 | 4:D:4401:HOH:O | 2.16 | 0.55 |
| 1:A:221:GLU:N | 4:A:1441:HOH:O | 2.11 | 0.55 |
| 1:E:101:ILE:O | 1:E:105:GLU:HG3 | 2.06 | 0.55 |
| 1:E:225:GLY:C | 4:E:5353:HOH:O | 2.40 | 0.55 |
| 1:D:167:ILE:HG23 | 4:D:4324:HOH:O | 2.06 | 0.54 |
| 1:D:229:ASP:HA | 4:D:4310:HOH:O | 2.07 | 0.54 |
| 1:E:179:ALA:C | 4:E:5322:HOH:O | 2.44 | 0.54 |
| 1:E:16:ALA:O | 1:E:20:THR:HG23 | 2.07 | 0.54 |
| 1:E:60:VAL:CG2 | 1:E:82:ILE:HD12 | 2.34 | 0.54 |
| 1:B:186:ASP:HB3 | 4:B:2305:HOH:O | 2.06 | 0.54 |
| 1:C:4:GLY:C | 1:C:66:LEU:HG | 2.27 | 0.54 |
| 2:D:4300:NAI:N1N | 3:D:4301:GLU:C | 2.60 | 0.54 |
| 1:D:78:ILE:O | 1:D:82:ILE:HD13 | 2.07 | 0.54 |
| 1:A:178:PRO:C | 4:A:1324:HOH:O | 2.42 | 0.54 |
| 1:B:129:ARG:O | 1:B:157:GLY:HA2 | 2.07 | 0.54 |
| 1:B:82:ILE:O | 1:B:86:ILE:HG13 | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:237:ALA:HB2 | 4:C:3411:HOH:O | 1.93 | 0.54 |
| 1:E:126:VAL:HG13 | 1:E:156:VAL:HG11 | 1.89 | 0.54 |
| 1:A:129:ARG:HA | 1:A:156:VAL:O | 2.08 | 0.54 |
| 1:A:230:ASN:HB3 | 4:A:1317:HOH:O | 2.05 | 0.54 |
| 1:B:178:PRO:CG | 4:B:2345:HOH:O | 2.56 | 0.54 |
| 1:B:77:PHE:C | 1:B:78:ILE:HD12 | 2.27 | 0.54 |
| 1:B:60:VAL:O | 1:B:89:ARG:NH2 | 2.39 | 0.54 |
| 1:C:266:ARG:NH2 | 4:C:3320:HOH:O | 2.40 | 0.54 |
| 1:C:87:GLU:N | 1:C:90:HIS:HE1 | 2.06 | 0.54 |
| 1:A:133:THR:O | 1:A:159:CYS:HA | 2.07 | 0.54 |
| 1:B:27:ALA:O | 4:B:2378:HOH:O | 2.19 | 0.54 |
| 1:C:51:LYS:H | 1:C:51:LYS:HD3 | 1.72 | 0.54 |
| 1:E:9:GLY:O | 1:E:12:ALA:HB3 | 2.06 | 0.54 |
| 1:E:169:ALA:C | 1:E:171:THR:N | 2.61 | 0.54 |
| 1:E:45:LEU:HD23 | 1:E:48:MET:HE1 | 1.89 | 0.54 |
| 1:B:101:ILE:HD12 | 1:B:138:GLY:HA2 | 1.89 | 0.54 |
| 1:C:7:GLY:CA | 1:C:70:VAL:HG22 | 2.38 | 0.54 |
| 1:E:181:ALA:O | 1:E:184:ALA:N | 2.39 | 0.54 |
| 1:E:45:LEU:HA | 1:E:48:MET:HE3 | 1.90 | 0.54 |
| 1:E:68:LEU:HB2 | 1:E:94:SER:HA | 1.90 | 0.54 |
| 1:A:99:VAL:HG11 | 1:A:104:ILE:HD11 | 1.90 | 0.54 |
| 1:A:266:ARG:NE | 4:A:1440:HOH:O | 2.35 | 0.54 |
| 1:B:158:PHE:O | 4:B:2387:HOH:O | 2.18 | 0.54 |
| 1:C:93:VAL:HG13 | 1:C:118:ILE:HD11 | 1.89 | 0.54 |
| 1:C:89:ARG:HE | 1:C:90:HIS:CD2 | 2.26 | 0.54 |
| 1:D:39:LEU:HA | 4:D:4405:HOH:O | 2.06 | 0.54 |
| 1:A:-1:ARG:N | 4:A:1427:HOH:O | 2.08 | 0.54 |
| 1:A:91:ILE:H | 1:A:91:ILE:HD12 | 1.72 | 0.54 |
| 1:B:238:THR:O | 1:B:240:HIS:N | 2.41 | 0.54 |
| 1:B:259:GLU:CA | 4:B:2307:HOH:O | 2.34 | 0.54 |
| 1:B:99:VAL:CG2 | 4:B:2309:HOH:O | 2.15 | 0.54 |
| 1:C:122:THR:CG2 | 1:C:133:THR:HG22 | 2.37 | 0.54 |
| 2:C:3300:NAI:C3N | 3:C:3301:GLU:CB | 2.81 | 0.54 |
| 1:C:87:GLU:H | 1:C:90:HIS:HE1 | 1.55 | 0.54 |
| 1:C:91:ILE:N | 1:C:91:ILE:HD12 | 2.23 | 0.54 |
| 1:E:105:GLU:CB | 4:E:5437:HOH:O | 2.56 | 0.54 |
| 1:E:185:LEU:CD1 | 4:E:5383:HOH:O | 2.51 | 0.54 |
| 1:A:178:PRO:CD | 4:A:1436:HOH:O | 2.32 | 0.54 |
| 1:A:255:ILE:C | 4:A:1335:HOH:O | 2.42 | 0.54 |
| 1:B:258:VAL:HG13 | 1:B:259:GLU:H | 1.72 | 0.54 |
| 1:D:93:VAL:HG13 | 4:D:4408:HOH:O | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:125:PRO:HG3 | 4:E:5302:HOH:O | 2.07 | 0.54 |
| 1:E:14:ALA:HA | 1:E:127:VAL:HG22 | 1.89 | 0.54 |
| 1:E:211:LEU:HD12 | 4:E:5314:HOH:O | 2.05 | 0.54 |
| 1:E:218:LEU:HA | 4:E:5424:HOH:O | 2.08 | 0.54 |
| 1:E:82:ILE:O | 1:E:85:ASP:N | 2.37 | 0.54 |
| 1:B:137:THR:HG21 | 4:B:2339:HOH:O | 2.07 | 0.54 |
| 1:B:162:VAL:HB | 1:B:166:LEU:HD12 | 1.90 | 0.54 |
| 1:B:218:LEU:CD1 | 2:B:2300:NAI:C5D | 2.81 | 0.54 |
| 1:B:78:ILE:N | 1:B:78:ILE:HD12 | 2.23 | 0.54 |
| 1:C:164:GLU:HG2 | 4:C:3372:HOH:O | 2.07 | 0.54 |
| 1:C:49:GLY:N | 4:C:3363:HOH:O | 2.40 | 0.54 |
| 1:D:3:VAL:HG22 | 1:D:65:VAL:HG13 | 1.90 | 0.54 |
| 1:E:169:ALA:N | 4:E:5375:HOH:O | 2.37 | 0.54 |
| 1:E:130:GLU:OE2 | 2:E:5300:NAI:C1D | 2.55 | 0.54 |
| 1:A:100:THR:HG22 | 1:A:102:SER:N | 2.22 | 0.53 |
| 1:B:153:LEU:O | 1:B:155:SER:N | 2.41 | 0.53 |
| 1:B:82:ILE:CG2 | 1:B:86:ILE:HD11 | 2.36 | 0.53 |
| 1:B:93:VAL:HG12 | 1:B:95:CYS:SG | 2.48 | 0.53 |
| 1:C:129:ARG:NH2 | 2:C:3300:NAI:H2N | 2.23 | 0.53 |
| 1:D:183:THR:CG2 | 4:D:4428:HOH:O | 2.55 | 0.53 |
| 1:D:77:PHE:HD1 | 1:D:77:PHE:H | 1.56 | 0.53 |
| 1:A:101:ILE:HG13 | 1:A:164:GLU:OE1 | 2.09 | 0.53 |
| 1:B:91:ILE:N | 1:B:91:ILE:HD12 | 2.24 | 0.53 |
| 1:C:112:ARG:HH11 | 1:C:113:PRO:CD | 2.09 | 0.53 |
| 1:C:122:THR:HG22 | 1:C:133:THR:HB | 1.90 | 0.53 |
| 1:C:134:VAL:CG1 | 1:C:162:VAL:HG22 | 2.38 | 0.53 |
| 1:C:116:ARG:HA | 1:C:140:HIS:HB2 | 1.90 | 0.53 |
| 1:A:26:ALA:CB | 1:A:29:LYS:HE3 | 2.38 | 0.53 |
| 1:B:158:PHE:CE1 | 2:B:2300:NAI:C4B | 2.82 | 0.53 |
| 1:B:169:ALA:O | 1:B:171:THR:N | 2.42 | 0.53 |
| 1:B:45:LEU:HB3 | 4:B:2385:HOH:O | 2.08 | 0.53 |
| 1:C:123:ASN:ND2 | 1:C:132:ALA:HB3 | 2.20 | 0.53 |
| 1:C:50:VAL:CG2 | 4:C:3363:HOH:O | 2.55 | 0.53 |
| 1:C:82:ILE:HG22 | 1:C:86:ILE:CD1 | 2.36 | 0.53 |
| 1:D:134:VAL:CG2 | 1:D:162:VAL:HB | 2.37 | 0.53 |
| 1:D:72:PRO:HA | 1:D:75:ILE:HD13 | 1.90 | 0.53 |
| 1:A:255:ILE:CG2 | 4:A:1335:HOH:O | 2.47 | 0.53 |
| 1:A:50:VAL:HG12 | 1:A:51:LYS:N | 2.23 | 0.53 |
| 1:C:19:PHE:O | 1:C:22:ALA:HB3 | 2.09 | 0.53 |
| 1:D:57:LYS:CD | 4:D:4438:HOH:O | 2.55 | 0.53 |
| 1:E:60:VAL:HG21 | 1:E:82:ILE:CG2 | 2.37 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:93:VAL:HG22 | 1:A:118:ILE:HD11 | 1.91 | 0.53 |
| 1:A:115:PRO:O | 1:A:140:HIS:HB2 | 2.08 | 0.53 |
| 1:B:139:THR:O | 1:B:139:THR:HG22 | 2.09 | 0.53 |
| 1:B:190:ASP:OD2 | 1:D:228:LYS:NZ | 2.41 | 0.53 |
| 1:C:180:TYR:CA | 4:C:3302:HOH:O | 2.20 | 0.53 |
| 1:B:196:GLY:O | 1:D:234:PRO:HB3 | 2.09 | 0.53 |
| 1:E:178:PRO:HD3 | 4:E:5315:HOH:O | 2.06 | 0.53 |
| 1:E:269:GLN:OE1 | 4:E:5400:HOH:O | 2.19 | 0.53 |
| 1:E:98:GLY:O | 4:E:5400:HOH:O | 2.19 | 0.53 |
| 1:C:6:ILE:H | 1:C:66:LEU:HD21 | 1.74 | 0.53 |
| 1:D:79:LEU:HD22 | 1:D:104:ILE:HD13 | 1.89 | 0.53 |
| 1:E:231:VAL:O | 1:E:231:VAL:HG12 | 2.08 | 0.53 |
| 1:C:104:ILE:HG22 | 1:C:117:VAL:HG21 | 1.90 | 0.53 |
| 1:C:236:GLY:HA2 | 1:C:239:ILE:HG22 | 1.91 | 0.53 |
| 1:C:261:SER:CA | 4:C:3354:HOH:O | 2.21 | 0.53 |
| 1:C:3:VAL:HA | 1:C:65:VAL:O | 2.08 | 0.53 |
| 1:D:119:ARG:CD | 4:D:4422:HOH:O | 2.24 | 0.53 |
| 2:D:4300:NAI:C3D | 4:D:4410:HOH:O | 2.47 | 0.53 |
| 1:E:3:VAL:O | 1:E:30:ILE:HA | 2.09 | 0.53 |
| 1:A:106:LYS:HB3 | 4:A:1432:HOH:O | 2.09 | 0.53 |
| 1:A:258:VAL:C | 4:A:1366:HOH:O | 2.46 | 0.53 |
| 1:A:29:LYS:N | 4:A:1329:HOH:O | 2.41 | 0.53 |
| 1:B:188:LEU:O | 1:B:190:ASP:N | 2.42 | 0.53 |
| 1:D:31:MET:N | 4:D:4365:HOH:O | 2.42 | 0.53 |
| 1:A:178:PRO:CG | 4:A:1436:HOH:O | 2.55 | 0.53 |
| 1:B:199:ARG:HD3 | 4:B:2340:HOH:O | 2.08 | 0.53 |
| 1:B:45:LEU:HD23 | 1:B:48:MET:SD | 2.48 | 0.53 |
| 1:B:75:ILE:HD12 | 1:B:75:ILE:N | 2.22 | 0.53 |
| 1:C:115:PRO:CB | 4:C:3358:HOH:O | 2.51 | 0.53 |
| 1:C:257:ALA:CA | 4:C:3378:HOH:O | 2.17 | 0.53 |
| 1:C:39:LEU:HA | 1:C:43:SER:CB | 2.39 | 0.53 |
| 1:E:75:ILE:CG2 | 1:E:104:ILE:HD11 | 2.39 | 0.53 |
| 1:E:124:THR:N | 1:E:125:PRO:HD2 | 2.24 | 0.53 |
| 1:E:7:GLY:H | 1:E:33:SER:HB2 | 1.73 | 0.53 |
| 1:A:135:TYR:OH | 1:A:161:GLU:HG3 | 2.09 | 0.53 |
| 1:B:185:LEU:O | 1:B:186:ASP:C | 2.47 | 0.53 |
| 1:C:261:SER:N | 4:C:3391:HOH:O | 2.41 | 0.53 |
| 1:D:31:MET:CE | 4:D:4358:HOH:O | 2.55 | 0.53 |
| 1:E:150:GLU:O | 1:E:152:LEU:N | 2.41 | 0.53 |
| 1:E:228:LYS:HE3 | 1:E:242:LEU:HD13 | 1.91 | 0.53 |
| 1:A:143:VAL:O | 1:A:143:VAL:HG12 | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:192:GLY:O | 1:A:195:MET:HB2 | 2.09 | 0.52 |
| 1:A:6:ILE:HD11 | 1:A:66:LEU:HD11 | 1.91 | 0.52 |
| 1:B:157:GLY:O | 2:B:2300:NAI:C4N | 2.56 | 0.52 |
| 2:B:2300:NAI:C3N | 3:B:2301:GLU:CB | 2.81 | 0.52 |
| 1:C:25:LEU:HD11 | 1:C:30:ILE:CD1 | 2.38 | 0.52 |
| 1:E:55:HIS:CB | 1:E:57:LYS:HE2 | 2.38 | 0.52 |
| 1:A:236:GLY:HA2 | 1:A:239:ILE:HG22 | 1.91 | 0.52 |
| 1:B:130:GLU:OE2 | 2:B:2300:NAI:H2D | 2.09 | 0.52 |
| 1:B:8:ALA:HA | 1:B:12:ALA:HB2 | 1.90 | 0.52 |
| 1:B:94:SER:OG | 4:B:2333:HOH:O | 2.03 | 0.52 |
| 1:E:177:GLY:O | 1:E:180:TYR:N | 2.42 | 0.52 |
| 1:E:45:LEU:HA | 1:E:48:MET:CE | 2.39 | 0.52 |
| 1:A:149:MET:CE | 1:A:153:LEU:HG | 2.39 | 0.52 |
| 1:A:198:PRO:HG2 | 1:A:201:LEU:CB | 2.40 | 0.52 |
| 1:A:-1:ARG:CB | 4:A:1342:HOH:O | 2.52 | 0.52 |
| 1:B:176:SER:O | 1:B:177:GLY:C | 2.46 | 0.52 |
| 1:C:24:VAL:O | 1:C:24:VAL:HG12 | 2.09 | 0.52 |
| 2:C:3300:NAI:O2B | 4:C:3408:HOH:O | 2.18 | 0.52 |
| 1:D:266:ARG:C | 1:D:268:LEU:N | 2.62 | 0.52 |
| 1:E:112:ARG:NE | 4:E:5328:HOH:O | 2.41 | 0.52 |
| 1:A:218:LEU:CD2 | 2:A:1300:NAI:H52A | 2.22 | 0.52 |
| 1:B:12:ALA:O | 1:B:16:ALA:HB2 | 2.08 | 0.52 |
| 1:B:5:PHE:HZ | 1:B:15:LEU:CB | 2.15 | 0.52 |
| 1:B:73:HIS:HB2 | 4:B:2320:HOH:O | 2.09 | 0.52 |
| 1:C:199:ARG:O | 1:C:203:VAL:HG23 | 2.09 | 0.52 |
| 1:E:185:LEU:HD22 | 4:E:5408:HOH:O | 2.09 | 0.52 |
| 1:A:251:ARG:HG3 | 4:A:1314:HOH:O | 2.08 | 0.52 |
| 1:A:62:HIS:ND1 | 1:A:62:HIS:O | 2.43 | 0.52 |
| 1:C:147:ARG:O | 1:C:151:GLN:HG3 | 2.10 | 0.52 |
| 1:D:123:ASN:HB2 | 1:D:125:PRO:HD2 | 1.91 | 0.52 |
| 1:D:232:SER:HA | 4:D:4343:HOH:O | 2.08 | 0.52 |
| 1:E:221:GLU:HG3 | 4:E:5350:HOH:O | 2.09 | 0.52 |
| 1:E:97:ALA:CB | 4:E:5358:HOH:O | 2.58 | 0.52 |
| 1:A:70:VAL:CG2 | 1:A:75:ILE:HD12 | 2.40 | 0.52 |
| 1:A:91:ILE:N | 1:A:91:ILE:HD12 | 2.24 | 0.52 |
| 1:B:18:GLY:O | 1:B:20:THR:N | 2.43 | 0.52 |
| 1:C:33:SER:OG | 1:C:56:ASN:HA | 2.09 | 0.52 |
| 1:D:252:SER:OG | 1:D:253:LEU:N | 2.43 | 0.52 |
| 1:E:3:VAL:HG12 | 1:E:4:GLY:N | 2.23 | 0.52 |
| 1:A:249:GLY:C | 4:A:1314:HOH:O | 2.41 | 0.52 |
| 1:B:245:LEU:O | 1:B:247:SER:N | 2.43 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:34:SER:C | 1:B:36:ASP:H | 2.12 | 0.52 |
| 1:C:158:PHE:CD1 | 2:C:3300:NAI:H4B | 2.44 | 0.52 |
| 2:A:1300:NAI:C4D | 4:A:1435:HOH:O | 2.58 | 0.52 |
| 1:A:256:ASN:HA | 4:A:1335:HOH:O | 2.10 | 0.52 |
| 1:A:36:ASP:O | 1:A:37:MET:CB | 2.56 | 0.52 |
| 1:B:68:LEU:C | 4:B:2368:HOH:O | 2.48 | 0.52 |
| 1:C:56:ASN:C | 4:C:3383:HOH:O | 2.48 | 0.52 |
| 1:D:224:PRO:HB2 | 4:D:4355:HOH:O | 2.10 | 0.52 |
| 1:A:32:ALA:O | 1:A:52:LEU:HA | 2.10 | 0.52 |
| 1:B:13:PHE:HB2 | 1:B:41:THR:CG2 | 2.40 | 0.52 |
| 1:E:242:LEU:HD11 | 4:E:5345:HOH:O | 2.09 | 0.52 |
| 1:A:6:ILE:CD1 | 1:A:66:LEU:HD11 | 2.39 | 0.52 |
| 1:C:169:ALA:CB | 4:C:3320:HOH:O | 2.55 | 0.52 |
| 1:C:51:LYS:H | 1:C:51:LYS:HZ2 | 1.56 | 0.52 |
| 1:D:169:ALA:C | 1:D:171:THR:N | 2.63 | 0.52 |
| 1:B:75:ILE:CB | 1:B:76:PRO:HD3 | 2.26 | 0.51 |
| 1:C:218:LEU:HD13 | 2:C:3300:NAI:C4D | 2.39 | 0.51 |
| 1:C:242:LEU:O | 1:C:245:LEU:N | 2.40 | 0.51 |
| 1:D:181:ALA:C | 4:D:4330:HOH:O | 2.48 | 0.51 |
| 1:D:60:VAL:O | 1:D:90:HIS:NE2 | 2.39 | 0.51 |
| 1:D:73:HIS:O | 1:D:76:PRO:HD2 | 2.10 | 0.51 |
| 1:E:121:MET:HE2 | 1:E:122:THR:O | 2.10 | 0.51 |
| 1:E:183:THR:C | 4:E:5370:HOH:O | 2.48 | 0.51 |
| 1:E:206:GLY:O | 1:E:209:ALA:HB3 | 2.10 | 0.51 |
| 1:A:121:MET:HG3 | 4:A:1402:HOH:O | 2.09 | 0.51 |
| 1:A:191:GLY:CA | 4:A:1420:HOH:O | 2.24 | 0.51 |
| 1:A:94:SER:CB | 4:A:1321:HOH:O | 2.58 | 0.51 |
| 1:B:118:ILE:HG21 | 1:B:149:MET:SD | 2.50 | 0.51 |
| 1:B:156:VAL:HG12 | 1:B:156:VAL:O | 2.11 | 0.51 |
| 1:B:195:MET:CE | 1:B:195:MET:CA | 2.88 | 0.51 |
| 1:C:122:THR:CG2 | 4:C:3317:HOH:O | 2.50 | 0.51 |
| 1:C:266:ARG:N | 4:C:3340:HOH:O | 2.42 | 0.51 |
| 1:D:141:ALA:CB | 4:D:4386:HOH:O | 2.57 | 0.51 |
| 1:A:79:LEU:CD1 | 1:A:104:ILE:HG23 | 2.40 | 0.51 |
| 1:B:158:PHE:CE1 | 2:B:2300:NAI:O1A | 2.64 | 0.51 |
| 1:B:159:CYS:CA | 4:B:2311:HOH:O | 2.56 | 0.51 |
| 1:C:100:THR:HG22 | 1:C:101:ILE:N | 2.25 | 0.51 |
| 1:C:15:LEU:HD12 | 4:C:3348:HOH:O | 2.01 | 0.51 |
| 1:C:251:ARG:HD2 | 4:C:3376:HOH:O | 2.09 | 0.51 |
| 1:C:29:LYS:HG3 | 4:C:3306:HOH:O | 2.11 | 0.51 |
| 1:D:166:LEU:O | 1:D:168:ASP:N | 2.44 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:218:LEU:CA | 4:E:5424:HOH:O | 2.57 | 0.51 |
| 1:A:11:LEU:O | 1:A:11:LEU:HD23 | 2.10 | 0.51 |
| 1:B:2:SER:OG | 1:B:30:ILE:HA | 2.10 | 0.51 |
| 1:E:136:ALA:CB | 4:E:5434:HOH:O | 2.58 | 0.51 |
| 1:E:34:SER:HB3 | 1:E:54:PRO:HA | 1.91 | 0.51 |
| 1:B:168:ASP:HB2 | 4:B:2357:HOH:O | 2.06 | 0.51 |
| 1:C:51:LYS:HZ2 | 1:C:51:LYS:HB2 | 1.74 | 0.51 |
| 1:D:228:LYS:HB2 | 4:D:4397:HOH:O | 2.11 | 0.51 |
| 1:E:136:ALA:HB2 | 1:E:167:ILE:HD11 | 1.93 | 0.51 |
| 1:E:262:CYS:HB3 | 4:E:5342:HOH:O | 2.06 | 0.51 |
| 1:E:39:LEU:HA | 1:E:43:SER:HB2 | 1.93 | 0.51 |
| 1:E:94:SER:HB3 | 4:E:5325:HOH:O | 2.09 | 0.51 |
| 1:A:215:LYS:O | 1:A:216:MET:C | 2.49 | 0.51 |
| 2:B:2300:NAI:H2A | 4:B:2380:HOH:O | 2.09 | 0.51 |
| 1:E:225:GLY:HA3 | 4:E:5353:HOH:O | 1.98 | 0.51 |
| 1:E:89:ARG:HH11 | 1:E:89:ARG:HG2 | 1.76 | 0.51 |
| 1:A:141:ALA:CA | 4:A:1390:HOH:O | 2.04 | 0.51 |
| 1:A:30:ILE:HG22 | 1:A:31:MET:N | 2.26 | 0.51 |
| 1:B:140:HIS:O | 1:B:141:ALA:HB2 | 2.11 | 0.51 |
| 1:B:9:GLY:O | 1:B:41:THR:HG21 | 2.11 | 0.51 |
| 1:E:118:ILE:HD12 | 1:E:118:ILE:N | 2.26 | 0.51 |
| 1:E:168:ASP:HB2 | 4:E:5349:HOH:O | 2.10 | 0.51 |
| 1:A:163:GLU:O | 1:A:165:ASP:N | 2.43 | 0.51 |
| 1:B:188:LEU:O | 4:B:2302:HOH:O | 2.19 | 0.51 |
| 1:C:86:ILE:HB | 1:C:112:ARG:HB2 | 1.93 | 0.51 |
| 1:C:122:THR:CA | 4:C:3331:HOH:O | 2.51 | 0.51 |
| 1:E:114:ALA:N | 4:E:5367:HOH:O | 2.39 | 0.51 |
| 1:A:236:GLY:O | 1:A:237:ALA:HB3 | 2.10 | 0.51 |
| 1:A:38:ASP:O | 1:A:39:LEU:C | 2.49 | 0.51 |
| 1:C:11:LEU:HD12 | 1:C:14:ALA:HB3 | 1.92 | 0.51 |
| 1:C:218:LEU:CD1 | 2:C:3300:NAI:H51N | 2.40 | 0.51 |
| 1:C:237:ALA:HB3 | 4:C:3406:HOH:O | 2.11 | 0.51 |
| 1:D:224:PRO:CB | 4:D:4355:HOH:O | 2.58 | 0.51 |
| 1:D:266:ARG:NH1 | 4:D:4442:HOH:O | 2.01 | 0.51 |
| 1:D:75:ILE:HB | 1:D:76:PRO:HD3 | 1.92 | 0.51 |
| 1:A:219:HIS:NE2 | 2:A:1300:NAI:H51N | 2.25 | 0.51 |
| 1:C:269:GLN:HG3 | 1:C:270:SER:H | 1.76 | 0.51 |
| 1:A:156:VAL:CG1 | 1:A:156:VAL:O | 2.59 | 0.50 |
| 1:A:121:MET:CG | 1:A:171:THR:HG23 | 2.41 | 0.50 |
| 1:C:255:ILE:CA | 4:C:3332:HOH:O | 2.53 | 0.50 |
| 1:C:270:SER:O | 1:C:274:GLN:HB2 | 2.10 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:215:LYS:HG3 | 1:D:219:HIS:CE1 | 2.46 | 0.50 |
| 1:E:74:ILE:C | 1:E:76:PRO:HD2 | 2.31 | 0.50 |
| 1:A:60:VAL:HG21 | 1:A:82:ILE:HG23 | 1.92 | 0.50 |
| 1:C:185:LEU:HD22 | 4:C:3324:HOH:O | 2.07 | 0.50 |
| 1:E:102:SER:CB | 4:E:5347:HOH:O | 2.52 | 0.50 |
| 1:E:121:MET:CE | 1:E:122:THR:H | 2.21 | 0.50 |
| 1:E:158:PHE:CD2 | 2:E:5300:NAI:O3B | 2.64 | 0.50 |
| 1:A:76:PRO:C | 1:A:78:ILE:H | 2.14 | 0.50 |
| 1:B:215:LYS:HE3 | 4:B:2377:HOH:O | 2.12 | 0.50 |
| 1:A:6:ILE:HD11 | 1:A:60:VAL:HG22 | 1.93 | 0.50 |
| 1:C:218:LEU:CG | 2:C:3300:NAI:H52N | 2.40 | 0.50 |
| 1:D:123:ASN:HB2 | 4:D:4312:HOH:O | 2.11 | 0.50 |
| 1:D:194:LYS:NZ | 4:D:4319:HOH:O | 2.06 | 0.50 |
| 1:E:112:ARG:CG | 4:E:5328:HOH:O | 2.36 | 0.50 |
| 1:E:132:ALA:CB | 4:E:5391:HOH:O | 2.41 | 0.50 |
| 1:A:11:LEU:CB | 4:A:1389:HOH:O | 2.15 | 0.50 |
| 1:C:274:GLN:HG2 | 1:C:274:GLN:O | 2.12 | 0.50 |
| 1:C:26:ALA:C | 1:C:28:HIS:H | 2.15 | 0.50 |
| 1:D:251:ARG:HH11 | 1:D:251:ARG:HG2 | 1.77 | 0.50 |
| 1:D:73:HIS:CE1 | 1:D:74:ILE:HG12 | 2.46 | 0.50 |
| 1:A:112:ARG:CD | 4:A:1365:HOH:O | 2.57 | 0.50 |
| 1:A:194:LYS:C | 4:E:5309:HOH:O | 2.50 | 0.50 |
| 1:B:180:TYR:O | 1:B:183:THR:HB | 2.11 | 0.50 |
| 1:B:251:ARG:O | 1:B:252:SER:C | 2.50 | 0.50 |
| 1:D:101:ILE:HG22 | 1:D:102:SER:N | 2.26 | 0.50 |
| 1:D:143:VAL:C | 1:D:145:ASP:H | 2.13 | 0.50 |
| 1:D:229:ASP:CG | 4:D:4393:HOH:O | 2.49 | 0.50 |
| 1:A:174:SER:HB2 | 4:A:1339:HOH:O | 2.08 | 0.50 |
| 1:B:123:ASN:O | 1:B:126:VAL:HG23 | 2.12 | 0.50 |
| 1:C:160:THR:CG2 | 1:C:161:GLU:N | 2.74 | 0.50 |
| 1:D:135:TYR:CE1 | 4:D:4398:HOH:O | 2.27 | 0.50 |
| 1:A:115:PRO:HD2 | 1:A:140:HIS:HD2 | 1.75 | 0.50 |
| 1:A:134:VAL:HG13 | 1:A:162:VAL:CG2 | 2.42 | 0.50 |
| 1:B:79:LEU:HD12 | 1:B:107:LYS:HD3 | 1.94 | 0.50 |
| 1:D:121:MET:HE3 | 1:D:171:THR:HG23 | 1.92 | 0.50 |
| 1:D:30:ILE:HG12 | 4:D:4425:HOH:O | 2.11 | 0.50 |
| 1:E:25:LEU:HD23 | 1:E:25:LEU:N | 2.26 | 0.50 |
| 1:A:130:GLU:OE2 | 2:A:1300:NAI:C2D | 2.60 | 0.50 |
| 1:C:187:ALA:O | 1:C:190:ASP:HB2 | 2.12 | 0.50 |
| 1:E:177:GLY:C | 4:E:5315:HOH:O | 2.47 | 0.50 |
| 1:E:198:PRO:HD2 | 1:E:201:LEU:HD23 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:E:45:LEU:HD23 | 1:E:48:MET:CE | 2.42 | 0.50 |
| 1:A:123:ASN:HB2 | 4:A:1436:HOH:O | 2.12 | 0.49 |
| 1:A:238:THR:C | 4:A:1391:HOH:O | 2.50 | 0.49 |
| 1:A:253:LEU:CD2 | 4:A:1405:HOH:O | 2.54 | 0.49 |
| 1:A:45:LEU:HD21 | 4:A:1387:HOH:O | 2.10 | 0.49 |
| 1:B:264:ARG:HD2 | 1:B:264:ARG:O | 2.11 | 0.49 |
| 1:B:25:LEU:HD22 | 1:B:30:ILE:HD11 | 1.93 | 0.49 |
| 1:C:211:LEU:C | 1:C:211:LEU:HD13 | 2.32 | 0.49 |
| 1:C:82:ILE:HA | 1:C:85:ASP:HB2 | 1.93 | 0.49 |
| 1:D:124:THR:O | 1:D:126:VAL:N | 2.45 | 0.49 |
| 1:E:19:PHE:CE2 | 1:E:152:LEU:HG | 2.47 | 0.49 |
| 1:A:13:PHE:N | 4:A:1379:HOH:O | 2.45 | 0.49 |
| 1:A:29:LYS:HG3 | 4:A:1329:HOH:O | 2.11 | 0.49 |
| 1:B:100:THR:CG2 | 1:B:101:ILE:N | 2.76 | 0.49 |
| 1:B:91:ILE:H | 1:B:91:ILE:HD12 | 1.77 | 0.49 |
| 1:C:108:LEU:C | 4:C:3358:HOH:O | 2.51 | 0.49 |
| 1:D:97:ALA:HA | 4:D:4435:HOH:O | 2.11 | 0.49 |
| 1:E:70:VAL:CA | 4:E:5305:HOH:O | 2.56 | 0.49 |
| 1:B:135:TYR:O | 1:B:161:GLU:HB2 | 2.13 | 0.49 |
| 1:B:58:GLU:O | 1:B:61:GLN:HG3 | 2.12 | 0.49 |
| 1:C:79:LEU:O | 4:C:3329:HOH:O | 2.20 | 0.49 |
| 1:E:232:SER:OG | 1:E:239:ILE:HB | 2.12 | 0.49 |
| 1:E:98:GLY:HA2 | 4:E:5400:HOH:O | 2.10 | 0.49 |
| 2:A:1300:NAI:H52N | 4:A:1435:HOH:O | 2.12 | 0.49 |
| 1:B:147:ARG:HG3 | 1:B:147:ARG:O | 2.11 | 0.49 |
| 1:C:115:PRO:CG | 4:C:3358:HOH:O | 2.57 | 0.49 |
| 1:C:197:LEU:CG | 4:C:3367:HOH:O | 2.60 | 0.49 |
| 1:C:74:ILE:O | 1:C:74:ILE:HG22 | 2.12 | 0.49 |
| 1:E:134:VAL:CG1 | 1:E:162:VAL:HB | 2.42 | 0.49 |
| 1:E:13:PHE:CZ | 4:E:5306:HOH:O | 2.66 | 0.49 |
| 1:E:228:LYS:O | 4:E:5337:HOH:O | 2.19 | 0.49 |
| 1:E:95:CYS:N | 4:E:5423:HOH:O | 2.42 | 0.49 |
| 1:B:100:THR:CG2 | 1:B:101:ILE:H | 2.24 | 0.49 |
| 1:B:74:ILE:HD11 | 1:B:96:ALA:HB3 | 1.94 | 0.49 |
| 1:A:31:MET:HA | 1:A:51:LYS:O | 2.12 | 0.49 |
| 1:A:6:ILE:HD13 | 1:A:59:THR:CG2 | 2.43 | 0.49 |
| 1:A:94:SER:C | 4:A:1321:HOH:O | 2.50 | 0.49 |
| 1:B:152:LEU:C | 4:B:2392:HOH:O | 2.47 | 0.49 |
| 1:C:104:ILE:HG21 | 1:C:117:VAL:HG11 | 1.94 | 0.49 |
| 1:C:9:GLY:O | 1:C:12:ALA:HB3 | 2.13 | 0.49 |
| 1:C:45:LEU:CD2 | 1:C:50:VAL:HB | 2.42 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:222:GLN:O | 1:D:223:HIS:HB3 | 2.12 | 0.49 |
| 1:A:117:VAL:HG12 | 4:A:1343:HOH:O | 2.11 | 0.49 |
| 1:A:178:PRO:CB | 4:A:1324:HOH:O | 2.61 | 0.49 |
| 1:D:58:GLU:CB | 4:D:4358:HOH:O | 2.57 | 0.49 |
| 1:D:70:VAL:HG12 | 1:D:74:ILE:HB | 1.95 | 0.49 |
| 1:E:190:ASP:HB2 | 4:E:5381:HOH:O | 2.12 | 0.49 |
| 1:E:70:VAL:O | 1:E:70:VAL:HG12 | 2.13 | 0.49 |
| 1:B:160:THR:HA | 4:B:2312:HOH:O | 2.12 | 0.49 |
| 1:E:222:GLN:O | 1:E:223:HIS:HB2 | 2.12 | 0.49 |
| 1:E:236:GLY:HA2 | 1:E:239:ILE:HG22 | 1.93 | 0.49 |
| 1:E:36:ASP:OD1 | 1:E:37:MET:N | 2.46 | 0.49 |
| 1:B:71:LYS:H | 1:B:71:LYS:HD2 | 1.76 | 0.49 |
| 1:C:75:ILE:N | 1:C:76:PRO:CD | 2.75 | 0.49 |
| 1:C:72:PRO:HG2 | 1:C:97:ALA:O | 2.13 | 0.49 |
| 1:E:124:THR:O | 1:E:126:VAL:N | 2.45 | 0.49 |
| 1:A:41:THR:O | 1:A:44:ALA:HB3 | 2.12 | 0.49 |
| 1:B:105:GLU:HA | 1:B:105:GLU:OE1 | 2.13 | 0.49 |
| 1:C:119:ARG:NE | 4:C:3345:HOH:O | 2.46 | 0.49 |
| 1:C:240:HIS:N | 4:C:3398:HOH:O | 2.34 | 0.49 |
| 1:D:121:MET:CE | 1:D:171:THR:HG23 | 2.42 | 0.49 |
| 1:D:242:LEU:O | 1:D:243:HIS:C | 2.51 | 0.49 |
| 1:D:68:LEU:HD12 | 1:D:94:SER:HB2 | 1.94 | 0.49 |
| 1:A:101:ILE:CG1 | 1:A:119:ARG:HB2 | 2.43 | 0.48 |
| 1:B:137:THR:CG2 | 4:B:2339:HOH:O | 2.59 | 0.48 |
| 1:B:155:SER:C | 2:B:2300:NAI:N7N | 2.66 | 0.48 |
| 1:B:79:LEU:HD22 | 1:B:104:ILE:HG23 | 1.95 | 0.48 |
| 1:C:26:ALA:O | 1:C:28:HIS:N | 2.46 | 0.48 |
| 2:D:4300:NAI:C3N | 4:D:4413:HOH:O | 2.61 | 0.48 |
| 2:D:4300:NAI:H2N | 4:D:4436:HOH:O | 2.11 | 0.48 |
| 1:E:113:PRO:HD2 | 4:E:5328:HOH:O | 2.12 | 0.48 |
| 1:E:251:ARG:NH2 | 4:E:5366:HOH:O | 2.45 | 0.48 |
| 1:A:171:THR:N | 4:A:1402:HOH:O | 2.34 | 0.48 |
| 1:A:45:LEU:CD2 | 4:A:1387:HOH:O | 2.60 | 0.48 |
| 1:B:134:VAL:HG13 | 1:B:160:THR:O | 2.12 | 0.48 |
| 1:B:75:ILE:HB | 1:B:76:PRO:CD | 2.27 | 0.48 |
| 1:C:61:GLN:C | 1:C:63:SER:N | 2.66 | 0.48 |
| 1:D:231:VAL:O | 1:D:231:VAL:HG12 | 2.13 | 0.48 |
| 2:E:5300:NAI:N1N | 3:E:5301:GLU:N | 2.61 | 0.48 |
| 1:A:178:PRO:HG2 | 4:A:1436:HOH:O | 2.13 | 0.48 |
| 1:B:74:ILE:HD11 | 1:B:96:ALA:CB | 2.43 | 0.48 |
| 1:B:122:THR:CG2 | 1:B:133:THR:HB | 2.40 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:238:THR:C | 1:B:240:HIS:N | 2.66 | 0.48 |
| 1:C:140:HIS:CB | 4:C:3385:HOH:O | 2.56 | 0.48 |
| 1:C:147:ARG:HG2 | 1:C:151:GLN:OE1 | 2.13 | 0.48 |
| 1:C:3:VAL:O | 1:C:30:ILE:HG13 | 2.12 | 0.48 |
| 1:D:22:ALA:HA | 1:D:129:ARG:CZ | 2.44 | 0.48 |
| 1:D:80:ASP:OD2 | 1:D:107:LYS:NZ | 2.45 | 0.48 |
| 1:E:221:GLU:N | 4:E:5350:HOH:O | 2.47 | 0.48 |
| 1:A:14:ALA:HA | 1:A:127:VAL:HG22 | 1.94 | 0.48 |
| 1:C:122:THR:HG22 | 1:C:133:THR:CB | 2.43 | 0.48 |
| 1:C:257:ALA:C | 1:C:259:GLU:H | 2.17 | 0.48 |
| 1:D:118:ILE:CG1 | 4:D:4408:HOH:O | 2.57 | 0.48 |
| 1:D:231:VAL:CG2 | 4:D:4402:HOH:O | 2.61 | 0.48 |
| 1:A:42:VAL:CG2 | 4:A:1349:HOH:O | 2.05 | 0.48 |
| 1:C:222:GLN:CA | 4:C:3304:HOH:O | 2.56 | 0.48 |
| 1:E:68:LEU:HD12 | 1:E:94:SER:HB2 | 1.96 | 0.48 |
| 1:A:6:ILE:HG22 | 1:A:6:ILE:O | 2.13 | 0.48 |
| 1:B:180:TYR:CD2 | 1:B:180:TYR:N | 2.77 | 0.48 |
| 1:B:221:GLU:HB2 | 4:B:2322:HOH:O | 2.13 | 0.48 |
| 1:B:231:VAL:HG12 | 1:B:231:VAL:O | 2.12 | 0.48 |
| 1:C:112:ARG:CG | 1:C:113:PRO:HD2 | 2.34 | 0.48 |
| 1:C:72:PRO:HA | 1:C:75:ILE:HG13 | 1.95 | 0.48 |
| 1:C:7:GLY:HA3 | 1:C:69:ALA:O | 2.12 | 0.48 |
| 1:D:223:HIS:ND1 | 1:D:224:PRO:HD2 | 2.29 | 0.48 |
| 1:D:60:VAL:HG21 | 1:D:82:ILE:CG2 | 2.39 | 0.48 |
| 1:E:187:ALA:CB | 4:E:5363:HOH:O | 2.34 | 0.48 |
| 1:E:46:ARG:HG3 | 1:E:46:ARG:NH1 | 2.28 | 0.48 |
| 1:A:194:LYS:HA | 4:E:5309:HOH:O | 2.13 | 0.48 |
| 1:A:222:GLN:O | 1:A:223:HIS:HB3 | 2.13 | 0.48 |
| 1:B:178:PRO:HD2 | 4:B:2345:HOH:O | 2.13 | 0.48 |
| 1:C:27:ALA:CB | 4:C:3363:HOH:O | 2.58 | 0.48 |
| 1:C:33:SER:HA | 1:C:53:THR:O | 2.14 | 0.48 |
| 1:D:15:LEU:HA | 1:D:126:VAL:HG11 | 1.96 | 0.48 |
| 1:E:106:LYS:CG | 4:E:5398:HOH:O | 2.62 | 0.48 |
| 1:E:112:ARG:CD | 4:E:5328:HOH:O | 2.62 | 0.48 |
| 1:E:123:ASN:CB | 4:E:5310:HOH:O | 2.59 | 0.48 |
| 1:E:134:VAL:HG21 | 1:E:170:VAL:HG11 | 1.96 | 0.48 |
| 1:E:199:ARG:NE | 4:E:5346:HOH:O | 2.26 | 0.48 |
| 1:A:112:ARG:HG2 | 4:A:1392:HOH:O | 2.13 | 0.48 |
| 1:A:28:HIS:N | 4:A:1382:HOH:O | 2.47 | 0.48 |
| 1:C:126:VAL:C | 1:C:128:VAL:N | 2.67 | 0.48 |
| 1:C:83:GLY:CA | 4:C:3329:HOH:O | 2.60 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:161:GLU:HG3 | 4:D:4394:HOH:O | 2.14 | 0.48 |
| 1:D:37:MET:HA | 1:D:37:MET:HE3 | 1.96 | 0.48 |
| 1:D:16:ALA:HB1 | 1:D:48:MET:HE1 | 1.96 | 0.48 |
| 1:E:179:ALA:CB | 4:E:5322:HOH:O | 2.51 | 0.48 |
| 1:E:55:HIS:HB3 | 1:E:57:LYS:HG2 | 1.95 | 0.48 |
| 1:A:149:MET:HE2 | 1:A:153:LEU:HG | 1.96 | 0.48 |
| 1:A:240:HIS:HD2 | 4:A:1352:HOH:O | 1.95 | 0.48 |
| 1:B:112:ARG:HG3 | 1:B:113:PRO:HD2 | 1.95 | 0.48 |
| 1:B:124:THR:O | 1:B:126:VAL:N | 2.47 | 0.48 |
| 1:C:29:LYS:HB2 | 1:C:30:ILE:HD12 | 1.96 | 0.48 |
| 1:C:39:LEU:HA | 1:C:43:SER:HB3 | 1.96 | 0.48 |
| 1:E:91:ILE:CG2 | 1:E:118:ILE:HD13 | 2.44 | 0.48 |
| 1:E:193:VAL:HG21 | 1:E:199:ARG:HD2 | 1.96 | 0.48 |
| 1:B:147:ARG:HG3 | 1:B:151:GLN:HE21 | 1.79 | 0.47 |
| 1:B:101:ILE:HG12 | 1:B:164:GLU:OE1 | 2.14 | 0.47 |
| 1:B:84:ALA:H | 1:B:111:PHE:HD2 | 1.62 | 0.47 |
| 1:C:134:VAL:HG11 | 1:C:162:VAL:HG22 | 1.95 | 0.47 |
| 1:C:240:HIS:CE1 | 1:D:194:LYS:HE2 | 2.49 | 0.47 |
| 1:C:25:LEU:HD21 | 1:C:30:ILE:CD1 | 2.44 | 0.47 |
| 1:D:119:ARG:NH1 | 4:D:4422:HOH:O | 2.46 | 0.47 |
| 1:D:228:LYS:HG2 | 4:D:4310:HOH:O | 2.13 | 0.47 |
| 1:D:262:CYS:O | 4:D:4360:HOH:O | 2.20 | 0.47 |
| 1:E:123:ASN:HB2 | 1:E:125:PRO:HD2 | 1.96 | 0.47 |
| 1:E:91:ILE:C | 4:E:5344:HOH:O | 2.50 | 0.47 |
| 1:A:64:ASP:O | 1:A:90:HIS:CB | 2.62 | 0.47 |
| 1:C:82:ILE:O | 1:C:86:ILE:HG12 | 2.14 | 0.47 |
| 1:E:118:ILE:HG21 | 1:E:149:MET:HG2 | 1.96 | 0.47 |
| 1:A:123:ASN:H | 1:A:123:ASN:HD22 | 1.62 | 0.47 |
| 1:A:242:LEU:O | 1:A:243:HIS:C | 2.51 | 0.47 |
| 1:B:115:PRO:CG | 4:B:2328:HOH:O | 2.61 | 0.47 |
| 1:D:184:ALA:CA | 4:D:4340:HOH:O | 2.63 | 0.47 |
| 1:D:79:LEU:HD21 | 1:D:104:ILE:HA | 1.95 | 0.47 |
| 1:E:226:GLN:NE2 | 1:E:226:GLN:HA | 2.29 | 0.47 |
| 1:E:46:ARG:HH11 | 1:E:46:ARG:HG3 | 1.79 | 0.47 |
| 1:C:199:ARG:HD2 | 4:C:3392:HOH:O | 2.05 | 0.47 |
| 1:C:8:ALA:HB3 | 1:C:34:SER:HB2 | 1.96 | 0.47 |
| 1:D:143:VAL:C | 1:D:145:ASP:N | 2.67 | 0.47 |
| 1:D:146:GLY:O | 1:D:149:MET:HB3 | 2.14 | 0.47 |
| 1:D:70:VAL:O | 1:D:75:ILE:HD11 | 2.15 | 0.47 |
| 1:E:109:SER:C | 1:E:111:PHE:H | 2.18 | 0.47 |
| 1:E:15:LEU:HB3 | 1:E:19:PHE:CE1 | 2.50 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:134:VAL:HG12 | 1:A:167:ILE:CD1 | 2.44 | 0.47 |
| 1:A:82:ILE:CA | 4:A:1437:HOH:O | 2.14 | 0.47 |
| 1:C:89:ARG:NE | 1:C:90:HIS:CD2 | 2.82 | 0.47 |
| 1:D:172:GLY:HA2 | 1:D:261:SER:OG | 2.14 | 0.47 |
| 1:E:112:ARG:N | 4:E:5422:HOH:O | 2.47 | 0.47 |
| 1:E:184:ALA:N | 4:E:5370:HOH:O | 2.47 | 0.47 |
| 1:E:67:PHE:HA | 1:E:93:VAL:O | 2.14 | 0.47 |
| 1:A:13:PHE:CB | 4:A:1379:HOH:O | 2.53 | 0.47 |
| 1:A:82:ILE:O | 1:A:85:ASP:N | 2.48 | 0.47 |
| 1:D:88:ASP:CB | 4:D:4432:HOH:O | 2.60 | 0.47 |
| 1:E:123:ASN:O | 1:E:126:VAL:HB | 2.15 | 0.47 |
| 1:A:193:VAL:C | 1:A:195:MET:N | 2.68 | 0.47 |
| 1:A:4:GLY:HA2 | 1:A:31:MET:O | 2.15 | 0.47 |
| 1:A:75:ILE:HG22 | 1:A:76:PRO:N | 2.29 | 0.47 |
| 1:B:236:GLY:CA | 4:B:2318:HOH:O | 2.48 | 0.47 |
| 1:C:101:ILE:HD11 | 4:C:3394:HOH:O | 2.14 | 0.47 |
| 1:D:217:LEU:CD1 | 4:D:4372:HOH:O | 2.26 | 0.47 |
| 1:D:251:ARG:CB | 4:D:4342:HOH:O | 2.28 | 0.47 |
| 1:B:245:LEU:C | 1:B:247:SER:H | 2.16 | 0.47 |
| 1:B:172:GLY:O | 1:B:258:VAL:HA | 2.13 | 0.47 |
| 1:B:2:SER:O | 1:B:3:VAL:HG23 | 2.15 | 0.47 |
| 1:C:218:LEU:CD2 | 2:C:3300:NAI:H52A | 2.45 | 0.47 |
| 1:C:3:VAL:HG12 | 1:C:4:GLY:N | 2.30 | 0.47 |
| 1:D:115:PRO:CA | 4:D:4374:HOH:O | 2.52 | 0.47 |
| 1:D:34:SER:HB2 | 1:D:36:ASP:O | 2.14 | 0.47 |
| 1:E:124:THR:C | 1:E:126:VAL:H | 2.16 | 0.47 |
| 1:E:124:THR:C | 1:E:126:VAL:N | 2.68 | 0.47 |
| 2:E:5300:NAI:O1N | 3:E:5301:GLU:C | 2.53 | 0.47 |
| 1:E:82:ILE:HG22 | 1:E:86:ILE:HG13 | 1.97 | 0.47 |
| 1:A:11:LEU:N | 4:A:1389:HOH:O | 2.35 | 0.47 |
| 1:B:241:ALA:N | 4:B:2329:HOH:O | 2.47 | 0.47 |
| 1:B:245:LEU:C | 1:B:247:SER:N | 2.67 | 0.47 |
| 1:C:168:ASP:HB2 | 1:C:266:ARG:NH1 | 2.30 | 0.47 |
| 1:C:251:ARG:C | 1:C:252:SER:O | 2.53 | 0.47 |
| 1:C:50:VAL:HG23 | 4:C:3363:HOH:O | 2.14 | 0.47 |
| 1:D:238:THR:HG22 | 1:D:239:ILE:N | 2.30 | 0.47 |
| 1:D:88:ASP:HB3 | 4:D:4432:HOH:O | 2.14 | 0.47 |
| 1:E:158:PHE:CA | 4:E:5425:HOH:O | 2.23 | 0.47 |
| 1:A:239:ILE:C | 4:A:1352:HOH:O | 2.52 | 0.47 |
| 1:A:55:HIS:O | 1:A:57:LYS:N | 2.40 | 0.47 |
| 1:B:158:PHE:CE2 | 2:B:2300:NAI:H4B | 2.43 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:168:ASP:HB2 | 1:C:266:ARG:HH12 | 1.80 | 0.47 |
| 1:C:231:VAL:O | 1:C:231:VAL:CG1 | 2.62 | 0.47 |
| 1:D:156:VAL:HG12 | 4:D:4331:HOH:O | 2.15 | 0.47 |
| 1:D:193:VAL:C | 1:D:195:MET:H | 2.17 | 0.47 |
| 1:E:123:ASN:CA | 4:E:5310:HOH:O | 2.63 | 0.47 |
| 1:E:95:CYS:CA | 4:E:5423:HOH:O | 2.63 | 0.47 |
| 1:A:264:ARG:CZ | 4:A:1322:HOH:O | 2.59 | 0.47 |
| 1:A:45:LEU:HB2 | 1:A:52:LEU:HD11 | 1.96 | 0.47 |
| 1:C:128:VAL:CG1 | 1:C:129:ARG:N | 2.78 | 0.47 |
| 1:D:179:ALA:C | 4:D:4308:HOH:O | 2.49 | 0.47 |
| 1:D:185:LEU:HD21 | 1:D:210:LEU:CD1 | 2.42 | 0.47 |
| 1:E:162:VAL:HG11 | 1:E:166:LEU:HB2 | 1.95 | 0.47 |
| 1:E:243:HIS:ND1 | 4:E:5357:HOH:O | 2.35 | 0.47 |
| 1:E:46:ARG:C | 1:E:48:MET:H | 2.17 | 0.47 |
| 1:A:128:VAL:HG12 | 1:A:129:ARG:N | 2.30 | 0.46 |
| 1:A:238:THR:C | 1:A:240:HIS:N | 2.65 | 0.46 |
| 1:B:115:PRO:HD3 | 4:B:2328:HOH:O | 2.13 | 0.46 |
| 1:B:153:LEU:C | 1:B:155:SER:N | 2.69 | 0.46 |
| 1:B:129:ARG:NH1 | 2:B:2300:NAI:C2D | 2.77 | 0.46 |
| 1:B:29:LYS:C | 1:B:30:ILE:HG13 | 2.35 | 0.46 |
| 1:C:53:THR:HG23 | 1:C:58:GLU:OE2 | 2.15 | 0.46 |
| 1:D:191:GLY:O | 1:D:192:GLY:C | 2.53 | 0.46 |
| 1:B:195:MET:N | 1:B:195:MET:HE3 | 2.31 | 0.46 |
| 1:B:73:HIS:C | 1:B:75:ILE:H | 2.19 | 0.46 |
| 1:C:143:VAL:HG12 | 1:C:143:VAL:O | 2.15 | 0.46 |
| 1:D:266:ARG:HD2 | 4:D:4311:HOH:O | 2.13 | 0.46 |
| 1:E:79:LEU:HD21 | 1:E:104:ILE:HG12 | 1.96 | 0.46 |
| 1:E:87:GLU:O | 1:E:89:ARG:N | 2.49 | 0.46 |
| 1:A:111:PHE:CD1 | 1:A:111:PHE:N | 2.84 | 0.46 |
| 1:B:112:ARG:CD | 1:B:113:PRO:HD2 | 2.45 | 0.46 |
| 1:B:143:VAL:HG12 | 1:B:144:GLU:N | 2.30 | 0.46 |
| 1:C:169:ALA:O | 1:C:172:GLY:N | 2.38 | 0.46 |
| 1:C:233:SER:N | 4:C:3374:HOH:O | 2.47 | 0.46 |
| 1:C:269:GLN:HG3 | 1:C:270:SER:N | 2.30 | 0.46 |
| 1:C:28:HIS:HB2 | 4:C:3404:HOH:O | 2.15 | 0.46 |
| 1:D:39:LEU:O | 1:D:40:ALA:O | 2.34 | 0.46 |
| 1:E:113:PRO:CD | 4:E:5367:HOH:O | 2.60 | 0.46 |
| 1:B:119:ARG:HD3 | 1:B:167:ILE:HD13 | 1.98 | 0.46 |
| 1:B:105:GLU:OE2 | 1:B:139:THR:HB | 2.15 | 0.46 |
| 2:B:2300:NAI:O4D | 2:B:2300:NAI:O3 | 2.34 | 0.46 |
| 1:E:73:HIS:HB3 | 4:E:5415:HOH:O | 2.08 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:75:ILE:N | 1:E:76:PRO:CD | 2.79 | 0.46 |
| 1:A:26:ALA:HB3 | 1:A:29:LYS:HE3 | 1.97 | 0.46 |
| 1:B:105:GLU:HG2 | 1:B:139:THR:OG1 | 2.15 | 0.46 |
| 1:B:36:ASP:O | 1:B:37:MET:HB2 | 2.15 | 0.46 |
| 1:B:7:GLY:HA3 | 1:B:69:ALA:C | 2.35 | 0.46 |
| 1:C:52:LEU:HD23 | 1:C:52:LEU:C | 2.35 | 0.46 |
| 1:C:6:ILE:HG21 | 1:C:78:ILE:HG21 | 1.96 | 0.46 |
| 1:D:265:THR:CG2 | 4:D:4360:HOH:O | 2.51 | 0.46 |
| 1:E:206:GLY:C | 4:E:5408:HOH:O | 2.48 | 0.46 |
| 1:B:70:VAL:CB | 4:B:2368:HOH:O | 2.63 | 0.46 |
| 1:C:240:HIS:CB | 4:C:3398:HOH:O | 2.52 | 0.46 |
| 1:D:112:ARG:HB3 | 4:D:4347:HOH:O | 2.14 | 0.46 |
| 1:D:17:LYS:HD2 | 1:D:127:VAL:CG1 | 2.45 | 0.46 |
| 1:D:70:VAL:HG12 | 1:D:71:LYS:N | 2.31 | 0.46 |
| 1:E:129:ARG:C | 4:E:5401:HOH:O | 2.49 | 0.46 |
| 1:E:218:LEU:HD23 | 4:E:5424:HOH:O | 2.15 | 0.46 |
| 1:E:97:ALA:N | 4:E:5358:HOH:O | 2.23 | 0.46 |
| 1:A:160:THR:HG22 | 1:A:161:GLU:O | 2.15 | 0.46 |
| 1:A:62:HIS:HE1 | 4:A:1334:HOH:O | 1.98 | 0.46 |
| 1:C:112:ARG:HG3 | 1:C:112:ARG:NH1 | 2.30 | 0.46 |
| 1:C:109:SER:OG | 1:C:115:PRO:HD2 | 2.16 | 0.46 |
| 1:D:114:ALA:HB1 | 1:D:140:HIS:CG | 2.51 | 0.46 |
| 1:D:97:ALA:C | 4:D:4333:HOH:O | 2.43 | 0.46 |
| 1:E:229:ASP:N | 4:E:5337:HOH:O | 2.43 | 0.46 |
| 2:E:5300:NAI:C6N | 4:E:5402:HOH:O | 2.64 | 0.46 |
| 1:A:55:HIS:C | 1:A:57:LYS:N | 2.69 | 0.46 |
| 1:A:62:HIS:CE1 | 4:A:1334:HOH:O | 2.69 | 0.46 |
| 1:B:218:LEU:CD2 | 2:B:2300:NAI:C5B | 2.93 | 0.46 |
| 1:B:52:LEU:O | 1:B:54:PRO:HD3 | 2.16 | 0.46 |
| 1:C:121:MET:CB | 4:C:3327:HOH:O | 2.64 | 0.46 |
| 1:C:193:VAL:C | 4:C:3309:HOH:O | 2.54 | 0.46 |
| 1:C:45:LEU:C | 1:C:45:LEU:HD23 | 2.36 | 0.46 |
| 1:C:7:GLY:HA3 | 1:C:69:ALA:C | 2.35 | 0.46 |
| 1:E:106:LYS:HG2 | 4:E:5398:HOH:O | 2.15 | 0.46 |
| 1:E:115:PRO:O | 1:E:140:HIS:HB2 | 2.16 | 0.46 |
| 1:E:62:HIS:C | 4:E:5372:HOH:O | 2.43 | 0.46 |
| 1:A:189:ALA:O | 1:A:190:ASP:C | 2.54 | 0.46 |
| 1:A:263:ILE:CD1 | 1:A:263:ILE:N | 2.78 | 0.46 |
| 1:B:233:SER:O | 1:B:234:PRO:C | 2.54 | 0.46 |
| 1:C:149:MET:C | 1:C:151:GLN:H | 2.18 | 0.46 |
| 1:C:223:HIS:C | 4:C:3417:HOH:O | 2.54 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:253:LEU:HD12 | 1:C:253:LEU:N | 2.30 | 0.46 |
| 1:E:33:SER:O | 1:E:35:PRO:CD | 2.64 | 0.46 |
| 1:E:62:HIS:CE1 | 4:E:5387:HOH:O | 2.69 | 0.46 |
| 1:A:79:LEU:HD22 | 1:A:108:LEU:HD13 | 1.96 | 0.46 |
| 1:B:6:ILE:CD1 | 1:B:56:ASN:O | 2.60 | 0.46 |
| 1:C:163:GLU:HB2 | 1:C:165:ASP:OD2 | 2.16 | 0.46 |
| 1:D:16:ALA:HB1 | 1:D:48:MET:CE | 2.46 | 0.46 |
| 1:E:135:TYR:CZ | 1:E:161:GLU:HB3 | 2.51 | 0.46 |
| 1:E:194:LYS:N | 4:E:5303:HOH:O | 2.41 | 0.46 |
| 1:E:215:LYS:O | 1:E:219:HIS:HD2 | 1.99 | 0.46 |
| 1:A:132:ALA:HB3 | 4:A:1339:HOH:O | 2.16 | 0.45 |
| 1:A:178:PRO:HB3 | 4:A:1324:HOH:O | 2.14 | 0.45 |
| 1:C:178:PRO:N | 4:C:3396:HOH:O | 2.49 | 0.45 |
| 1:C:218:LEU:HD22 | 2:C:3300:NAI:O5B | 2.16 | 0.45 |
| 1:D:29:LYS:O | 1:D:30:ILE:HD13 | 2.16 | 0.45 |
| 2:D:4300:NAI:O4D | 2:D:4300:NAI:O3 | 2.34 | 0.45 |
| 1:E:143:VAL:HG12 | 1:E:143:VAL:O | 2.16 | 0.45 |
| 1:E:126:VAL:O | 1:E:156:VAL:CG1 | 2.65 | 0.45 |
| 1:A:33:SER:HA | 1:A:53:THR:O | 2.16 | 0.45 |
| 2:C:3300:NAI:O4D | 2:C:3300:NAI:O3 | 2.34 | 0.45 |
| 1:C:61:GLN:C | 1:C:63:SER:H | 2.19 | 0.45 |
| 1:E:89:ARG:HG3 | 1:E:90:HIS:N | 2.30 | 0.45 |
| 1:A:136:ALA:CA | 4:A:1404:HOH:O | 2.63 | 0.45 |
| 1:A:27:ALA:HB1 | 1:A:49:GLY:HA3 | 1.99 | 0.45 |
| 1:B:15:LEU:O | 1:B:19:PHE:CE1 | 2.69 | 0.45 |
| 1:B:238:THR:HG22 | 1:B:239:ILE:N | 2.30 | 0.45 |
| 1:C:14:ALA:HB1 | 1:C:126:VAL:HG23 | 1.98 | 0.45 |
| 1:C:237:ALA:CB | 4:C:3406:HOH:O | 2.64 | 0.45 |
| 1:C:9:GLY:O | 1:C:10:GLN:C | 2.55 | 0.45 |
| 1:D:232:SER:HB3 | 1:D:239:ILE:CG1 | 2.44 | 0.45 |
| 1:B:101:ILE:CD1 | 1:B:138:GLY:HA2 | 2.46 | 0.45 |
| 2:B:2300:NAI:H1D | 2:B:2300:NAI:O1N | 2.17 | 0.45 |
| 1:B:239:ILE:N | 4:B:2352:HOH:O | 2.49 | 0.45 |
| 1:B:35:PRO:HG2 | 1:B:71:LYS:HZ2 | 1.82 | 0.45 |
| 1:C:118:ILE:HG12 | 1:C:118:ILE:O | 2.17 | 0.45 |
| 2:C:3300:NAI:H1D | 2:C:3300:NAI:O1N | 2.17 | 0.45 |
| 1:C:73:HIS:CE1 | 1:C:74:ILE:HG12 | 2.51 | 0.45 |
| 1:B:124:THR:C | 1:B:126:VAL:H | 2.20 | 0.45 |
| 1:C:176:SER:O | 1:C:177:GLY:C | 2.53 | 0.45 |
| 2:D:4300:NAI:O1N | 2:D:4300:NAI:H1D | 2.16 | 0.45 |
| 1:E:28:HIS:C | 1:E:28:HIS:CD2 | 2.88 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:39:LEU:H | 1:E:39:LEU:HD23 | 1.81 | 0.45 |
| 1:A:9:GLY:CA | 1:A:41:THR:HG21 | 2.46 | 0.45 |
| 1:C:187:ALA:O | 1:C:188:LEU:C | 2.55 | 0.45 |
| 1:D:100:THR:HG22 | 1:D:101:ILE:N | 2.31 | 0.45 |
| 1:D:237:ALA:O | 1:D:240:HIS:HB2 | 2.17 | 0.45 |
| 1:D:257:ALA:O | 1:D:258:VAL:C | 2.55 | 0.45 |
| 1:E:154:SER:O | 2:E:5300:NAI:H42N | 2.17 | 0.45 |
| 1:E:175:GLY:C | 4:E:5333:HOH:O | 2.54 | 0.45 |
| 1:B:83:GLY:C | 1:B:85:ASP:H | 2.19 | 0.45 |
| 1:B:84:ALA:N | 1:B:111:PHE:HD2 | 2.15 | 0.45 |
| 1:C:171:THR:HA | 4:C:3351:HOH:O | 2.00 | 0.45 |
| 1:C:255:ILE:HG23 | 4:C:3332:HOH:O | 2.16 | 0.45 |
| 1:C:45:LEU:CA | 4:C:3371:HOH:O | 2.44 | 0.45 |
| 1:D:242:LEU:O | 1:D:244:VAL:N | 2.50 | 0.45 |
| 1:E:106:LYS:HB3 | 4:E:5384:HOH:O | 2.14 | 0.45 |
| 1:E:190:ASP:CB | 4:E:5381:HOH:O | 2.65 | 0.45 |
| 1:E:1:MET:HG2 | 1:E:2:SER:N | 2.31 | 0.45 |
| 1:E:254:LEU:O | 1:E:257:ALA:HB3 | 2.17 | 0.45 |
| 1:E:74:ILE:CG2 | 1:E:78:ILE:HD11 | 2.46 | 0.45 |
| 2:A:1300:NAI:C3N | 3:A:1301:GLU:CB | 2.91 | 0.45 |
| 1:A:95:CYS:SG | 4:A:1337:HOH:O | 2.61 | 0.45 |
| 1:B:18:GLY:O | 1:B:19:PHE:C | 2.55 | 0.45 |
| 1:B:222:GLN:OE1 | 1:B:226:GLN:HG2 | 2.15 | 0.45 |
| 1:C:189:ALA:HB2 | 1:C:203:VAL:HA | 1.97 | 0.45 |
| 2:D:4300:NAI:C5N | 3:D:4301:GLU:OXT | 2.64 | 0.45 |
| 1:D:77:PHE:N | 1:D:77:PHE:CD1 | 2.83 | 0.45 |
| 1:E:137:THR:O | 1:E:137:THR:HG23 | 2.17 | 0.45 |
| 1:E:70:VAL:O | 1:E:71:LYS:CB | 2.65 | 0.45 |
| 1:A:124:THR:O | 1:A:126:VAL:N | 2.50 | 0.45 |
| 1:B:190:ASP:O | 4:B:2308:HOH:O | 2.21 | 0.45 |
| 1:B:245:LEU:O | 4:B:2353:HOH:O | 2.21 | 0.45 |
| 1:B:258:VAL:HG13 | 1:B:259:GLU:N | 2.31 | 0.45 |
| 1:D:133:THR:HG21 | 1:D:153:LEU:CD1 | 2.45 | 0.45 |
| 1:D:184:ALA:N | 4:D:4340:HOH:O | 2.50 | 0.45 |
| 1:D:37:MET:HE3 | 1:D:42:VAL:HB | 1.99 | 0.45 |
| 2:D:4300:NAI:C3N | 3:D:4301:GLU:CA | 2.91 | 0.45 |
| 2:D:4300:NAI:H2N | 3:D:4301:GLU:HA | 1.89 | 0.45 |
| 1:E:262:CYS:O | 1:E:263:ILE:C | 2.54 | 0.45 |
| 1:E:46:ARG:C | 1:E:48:MET:N | 2.70 | 0.45 |
| 1:A:225:GLY:O | 1:A:228:LYS:HB3 | 2.17 | 0.45 |
| 1:B:135:TYR:HE1 | 1:B:161:GLU:OE1 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:236:GLY:C | 1:B:238:THR:H | 2.20 | 0.45 |
| 1:B:66:LEU:N | 1:B:91:ILE:O | 2.50 | 0.45 |
| 1:C:206:GLY:O | 1:C:209:ALA:HB3 | 2.17 | 0.45 |
| 1:C:60:VAL:N | 4:C:3383:HOH:O | 2.47 | 0.45 |
| 1:D:14:ALA:HA | 1:D:127:VAL:HG22 | 1.98 | 0.45 |
| 1:E:177:GLY:HA2 | 1:E:180:TYR:HD1 | 1.81 | 0.45 |
| 1:E:211:LEU:HD13 | 4:E:5314:HOH:O | 2.13 | 0.45 |
| 1:E:251:ARG:CG | 4:E:5304:HOH:O | 2.64 | 0.45 |
| 1:E:47:LYS:NZ | 4:E:5338:HOH:O | 2.47 | 0.45 |
| 1:E:53:THR:HG21 | 1:E:58:GLU:CB | 2.47 | 0.45 |
| 1:A:233:SER:O | 1:A:235:GLY:N | 2.50 | 0.44 |
| 1:A:236:GLY:C | 4:A:1391:HOH:O | 2.54 | 0.44 |
| 1:A:258:VAL:HG13 | 4:A:1366:HOH:O | 2.16 | 0.44 |
| 1:B:199:ARG:NH1 | 4:B:2340:HOH:O | 2.22 | 0.44 |
| 1:C:126:VAL:CG1 | 4:C:3307:HOH:O | 2.57 | 0.44 |
| 1:C:19:PHE:HE2 | 1:C:153:LEU:HD23 | 1.82 | 0.44 |
| 1:C:160:THR:CG2 | 1:C:161:GLU:H | 2.30 | 0.44 |
| 1:D:227:LEU:HD12 | 4:D:4363:HOH:O | 2.16 | 0.44 |
| 1:D:269:GLN:C | 1:D:271:MET:N | 2.70 | 0.44 |
| 1:D:64:ASP:CG | 4:D:4353:HOH:O | 2.34 | 0.44 |
| 1:E:177:GLY:O | 1:E:180:TYR:HB2 | 2.17 | 0.44 |
| 1:E:43:SER:O | 1:E:46:ARG:HB2 | 2.17 | 0.44 |
| 1:A:120:CYS:HB2 | 4:A:1368:HOH:O | 2.12 | 0.44 |
| 1:A:219:HIS:CE1 | 4:A:1431:HOH:O | 2.69 | 0.44 |
| 1:A:6:ILE:HD13 | 1:A:59:THR:HG21 | 2.00 | 0.44 |
| 1:B:129:ARG:HH12 | 2:B:2300:NAI:C2D | 2.29 | 0.44 |
| 1:C:275:GLU:C | 4:C:3393:HOH:O | 2.56 | 0.44 |
| 1:C:61:GLN:O | 1:C:89:ARG:NH2 | 2.49 | 0.44 |
| 1:D:195:MET:HG2 | 4:D:4366:HOH:O | 2.16 | 0.44 |
| 1:A:123:ASN:HD22 | 1:A:123:ASN:N | 2.16 | 0.44 |
| 1:A:135:TYR:OH | 1:A:150:GLU:CG | 2.64 | 0.44 |
| 1:A:195:MET:N | 4:E:5309:HOH:O | 2.50 | 0.44 |
| 1:A:252:SER:HA | 1:A:255:ILE:HD12 | 1.99 | 0.44 |
| 1:A:269:GLN:C | 1:A:271:MET:N | 2.70 | 0.44 |
| 1:B:47:LYS:NZ | 1:B:47:LYS:HB3 | 2.33 | 0.44 |
| 1:C:101:ILE:HB | 1:C:164:GLU:OE1 | 2.17 | 0.44 |
| 1:C:93:VAL:HG12 | 1:C:118:ILE:HD11 | 1.99 | 0.44 |
| 1:C:124:THR:C | 1:C:126:VAL:N | 2.71 | 0.44 |
| 1:C:9:GLY:H | 1:C:12:ALA:HB3 | 1.81 | 0.44 |
| 1:D:10:GLN:N | 4:D:4387:HOH:O | 2.50 | 0.44 |
| 2:D:4300:NAI:C3N | 3:D:4301:GLU:HA | 2.47 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:104:ILE:HG22 | 1:E:117:VAL:HG21 | 1.99 | 0.44 |
| 1:E:150:GLU:O | 1:E:151:GLN:C | 2.56 | 0.44 |
| 1:E:172:GLY:HA2 | 1:E:261:SER:CB | 2.47 | 0.44 |
| 1:E:38:ASP:H | 1:E:42:VAL:CG2 | 2.29 | 0.44 |
| 1:E:62:HIS:HE1 | 4:E:5387:HOH:O | 2.00 | 0.44 |
| 1:A:200:ARG:O | 1:A:204:ARG:HG2 | 2.17 | 0.44 |
| 1:A:256:ASN:CA | 4:A:1335:HOH:O | 2.53 | 0.44 |
| 1:B:169:ALA:C | 1:B:171:THR:N | 2.70 | 0.44 |
| 1:B:251:ARG:HD2 | 4:B:2330:HOH:O | 2.11 | 0.44 |
| 1:D:92:VAL:HB | 1:D:117:VAL:HG22 | 1.99 | 0.44 |
| 1:D:30:ILE:C | 4:D:4365:HOH:O | 2.56 | 0.44 |
| 1:A:255:ILE:O | 1:A:258:VAL:N | 2.48 | 0.44 |
| 1:B:221:GLU:N | 4:B:2322:HOH:O | 2.50 | 0.44 |
| 1:C:124:THR:N | 1:C:125:PRO:CD | 2.79 | 0.44 |
| 1:C:167:ILE:HG22 | 4:C:3345:HOH:O | 2.03 | 0.44 |
| 1:C:61:GLN:O | 1:C:63:SER:N | 2.51 | 0.44 |
| 1:C:8:ALA:HB3 | 1:C:34:SER:CB | 2.48 | 0.44 |
| 1:E:184:ALA:O | 1:E:187:ALA:HB3 | 2.17 | 0.44 |
| 1:A:11:LEU:CD1 | 4:A:1399:HOH:O | 2.59 | 0.44 |
| 1:A:266:ARG:HG2 | 1:A:266:ARG:NH1 | 2.24 | 0.44 |
| 1:C:199:ARG:NH1 | 4:C:3392:HOH:O | 2.48 | 0.44 |
| 1:A:211:LEU:CD1 | 1:A:211:LEU:C | 2.86 | 0.44 |
| 1:A:28:HIS:C | 4:A:1329:HOH:O | 2.56 | 0.44 |
| 1:A:1:MET:HG2 | 1:A:2:SER:N | 2.33 | 0.44 |
| 1:C:3:VAL:C | 4:C:3356:HOH:O | 2.49 | 0.44 |
| 1:E:220:SER:O | 4:E:5362:HOH:O | 2.21 | 0.44 |
| 1:E:251:ARG:HG2 | 4:E:5304:HOH:O | 2.17 | 0.44 |
| 1:E:264:ARG:O | 1:E:265:THR:C | 2.55 | 0.44 |
| 1:A:172:GLY:C | 4:A:1302:HOH:O | 2.55 | 0.44 |
| 1:C:261:SER:HB3 | 4:C:3391:HOH:O | 2.18 | 0.44 |
| 1:C:71:LYS:HB2 | 1:C:73:HIS:HE1 | 1.80 | 0.44 |
| 1:D:100:THR:HG22 | 1:D:102:SER:N | 2.30 | 0.44 |
| 1:D:249:GLY:O | 1:D:250:PHE:C | 2.56 | 0.44 |
| 1:D:219:HIS:CE1 | 2:D:4300:NAI:H51N | 2.37 | 0.44 |
| 1:A:121:MET:N | 4:A:1368:HOH:O | 2.49 | 0.44 |
| 1:A:101:ILE:HG21 | 1:A:138:GLY:HA2 | 2.00 | 0.44 |
| 1:A:190:ASP:N | 1:A:199:ARG:NH1 | 2.65 | 0.44 |
| 1:B:218:LEU:HB3 | 2:B:2300:NAI:H52N | 2.00 | 0.44 |
| 1:B:60:VAL:O | 1:B:89:ARG:NH1 | 2.51 | 0.44 |
| 1:C:13:PHE:O | 1:C:16:ALA:HB3 | 2.18 | 0.44 |
| 1:C:266:ARG:O | 1:C:269:GLN:HG2 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:26:ALA:HB3 | 1:C:29:LYS:HE3 | 1.99 | 0.44 |
| 1:C:30:ILE:N | 1:C:30:ILE:HD12 | 2.32 | 0.44 |
| 1:C:75:ILE:CA | 4:C:3407:HOH:O | 2.60 | 0.44 |
| 1:D:115:PRO:CB | 4:D:4374:HOH:O | 2.65 | 0.44 |
| 1:D:222:GLN:O | 1:D:223:HIS:HB2 | 2.18 | 0.44 |
| 1:D:266:ARG:HD3 | 4:D:4311:HOH:O | 2.13 | 0.44 |
| 1:E:211:LEU:C | 4:E:5314:HOH:O | 2.55 | 0.44 |
| 1:E:228:LYS:CE | 1:E:242:LEU:HD13 | 2.48 | 0.44 |
| 1:A:169:ALA:O | 1:A:170:VAL:C | 2.57 | 0.43 |
| 1:A:176:SER:HB3 | 1:A:180:TYR:CE2 | 2.54 | 0.43 |
| 1:A:194:LYS:CB | 4:A:1420:HOH:O | 2.65 | 0.43 |
| 1:A:238:THR:CG2 | 4:A:1320:HOH:O | 2.66 | 0.43 |
| 1:A:258:VAL:HG22 | 4:A:1302:HOH:O | 2.09 | 0.43 |
| 1:A:3:VAL:HG11 | 1:A:67:PHE:HE1 | 1.82 | 0.43 |
| 1:B:142:GLN:CG | 1:B:143:VAL:N | 2.64 | 0.43 |
| 1:B:236:GLY:O | 1:B:237:ALA:HB3 | 2.17 | 0.43 |
| 1:C:140:HIS:N | 4:C:3385:HOH:O | 2.51 | 0.43 |
| 1:C:262:CYS:O | 1:C:265:THR:HB | 2.18 | 0.43 |
| 1:C:269:GLN:O | 1:C:271:MET:N | 2.45 | 0.43 |
| 1:C:39:LEU:HA | 1:C:43:SER:HB2 | 2.00 | 0.43 |
| 1:C:91:ILE:HG23 | 1:C:116:ARG:CB | 2.43 | 0.43 |
| 1:D:124:THR:N | 4:D:4375:HOH:O | 2.50 | 0.43 |
| 1:D:92:VAL:N | 4:D:4455:HOH:O | 2.51 | 0.43 |
| 1:E:242:LEU:O | 1:E:244:VAL:N | 2.50 | 0.43 |
| 1:E:259:GLU:O | 1:E:262:CYS:N | 2.50 | 0.43 |
| 1:A:218:LEU:CD1 | 4:A:1435:HOH:O | 2.65 | 0.43 |
| 1:A:231:VAL:O | 1:A:231:VAL:CG1 | 2.65 | 0.43 |
| 1:B:163:GLU:HG3 | 1:B:165:ASP:OD1 | 2.18 | 0.43 |
| 1:B:214:ALA:O | 1:B:217:LEU:N | 2.50 | 0.43 |
| 1:B:74:ILE:HG22 | 1:B:74:ILE:O | 2.18 | 0.43 |
| 1:C:123:ASN:O | 1:C:126:VAL:HG22 | 2.17 | 0.43 |
| 1:C:138:GLY:HA3 | 4:C:3394:HOH:O | 2.18 | 0.43 |
| 1:C:233:SER:O | 1:C:234:PRO:C | 2.56 | 0.43 |
| 1:C:29:LYS:CG | 4:C:3306:HOH:O | 2.65 | 0.43 |
| 1:D:124:THR:N | 1:D:125:PRO:CD | 2.80 | 0.43 |
| 1:D:121:MET:O | 1:D:133:THR:HA | 2.19 | 0.43 |
| 1:D:135:TYR:HE2 | 1:D:150:GLU:HG3 | 1.83 | 0.43 |
| 1:D:224:PRO:HG2 | 4:D:4355:HOH:O | 2.12 | 0.43 |
| 1:E:238:THR:CG2 | 4:E:5321:HOH:O | 2.25 | 0.43 |
| 1:A:123:ASN:CB | 4:A:1436:HOH:O | 2.67 | 0.43 |
| 1:A:123:ASN:N | 1:A:123:ASN:ND2 | 2.64 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:211:LEU:HD12 | 1:A:211:LEU:C | 2.39 | 0.43 |
| 1:A:64:ASP:O | 1:A:90:HIS:HB3 | 2.18 | 0.43 |
| 1:C:150:GLU:C | 1:C:154:SER:HB2 | 2.38 | 0.43 |
| 1:D:193:VAL:C | 1:D:195:MET:N | 2.71 | 0.43 |
| 1:E:126:VAL:HG22 | 1:E:156:VAL:HG12 | 2.01 | 0.43 |
| 1:E:53:THR:HG22 | 1:E:55:HIS:N | 2.19 | 0.43 |
| 1:E:94:SER:O | 4:E:5423:HOH:O | 2.19 | 0.43 |
| 1:A:139:THR:HG23 | 4:A:1430:HOH:O | 2.18 | 0.43 |
| 1:A:193:VAL:O | 1:A:195:MET:N | 2.48 | 0.43 |
| 1:B:164:GLU:O | 1:B:167:ILE:HB | 2.18 | 0.43 |
| 1:C:93:VAL:HG12 | 1:C:118:ILE:CG1 | 2.48 | 0.43 |
| 1:C:15:LEU:O | 1:C:19:PHE:CD1 | 2.71 | 0.43 |
| 1:C:240:HIS:CE1 | 4:C:3365:HOH:O | 2.71 | 0.43 |
| 1:D:245:LEU:HA | 1:D:245:LEU:HD23 | 1.87 | 0.43 |
| 1:E:233:SER:O | 1:E:235:GLY:N | 2.52 | 0.43 |
| 1:E:41:THR:O | 1:E:42:VAL:C | 2.57 | 0.43 |
| 1:A:119:ARG:HA | 4:A:1372:HOH:O | 2.18 | 0.43 |
| 1:A:221:GLU:O | 1:A:222:GLN:HB2 | 2.18 | 0.43 |
| 1:A:60:VAL:HG21 | 1:A:82:ILE:CG2 | 2.49 | 0.43 |
| 1:A:86:ILE:O | 1:A:86:ILE:HG22 | 2.19 | 0.43 |
| 1:B:185:LEU:CD2 | 1:B:210:LEU:HD12 | 2.40 | 0.43 |
| 1:C:60:VAL:HG12 | 1:C:60:VAL:O | 2.18 | 0.43 |
| 1:C:83:GLY:O | 1:C:86:ILE:HG12 | 2.18 | 0.43 |
| 1:D:112:ARG:C | 4:D:4329:HOH:O | 2.54 | 0.43 |
| 1:D:185:LEU:O | 4:D:4361:HOH:O | 2.21 | 0.43 |
| 1:E:107:LYS:HG3 | 4:E:5384:HOH:O | 2.18 | 0.43 |
| 1:E:212:GLY:O | 1:E:213:ALA:C | 2.56 | 0.43 |
| 2:E:5300:NAI:O2D | 3:E:5301:GLU:N | 2.51 | 0.43 |
| 1:B:79:LEU:CD2 | 1:B:104:ILE:HG23 | 2.48 | 0.43 |
| 1:B:83:GLY:HA3 | 1:B:111:PHE:CD2 | 2.54 | 0.43 |
| 1:C:112:ARG:NH1 | 1:C:113:PRO:HD2 | 2.11 | 0.43 |
| 1:C:51:LYS:N | 1:C:51:LYS:HD3 | 2.32 | 0.43 |
| 1:C:89:ARG:CD | 1:C:90:HIS:N | 2.68 | 0.43 |
| 1:D:42:VAL:HA | 1:D:45:LEU:HD12 | 2.00 | 0.43 |
| 1:E:136:ALA:C | 4:E:5434:HOH:O | 2.55 | 0.43 |
| 1:E:191:GLY:O | 1:E:192:GLY:C | 2.56 | 0.43 |
| 1:A:262:CYS:O | 1:A:265:THR:N | 2.52 | 0.43 |
| 1:A:34:SER:HB2 | 1:A:37:MET:HG2 | 2.01 | 0.43 |
| 1:B:32:ALA:O | 1:B:53:THR:HB | 2.18 | 0.43 |
| 1:C:38:ASP:H | 1:C:42:VAL:HB | 1.84 | 0.43 |
| 1:D:128:VAL:HG13 | 1:D:129:ARG:N | 2.33 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:162:VAL:CG1 | 1:D:166:LEU:HB2 | 2.48 | 0.43 |
| 1:E:223:HIS:O | 1:E:224:PRO:C | 2.57 | 0.43 |
| 1:A:194:LYS:HE2 | 1:E:240:HIS:ND1 | 2.34 | 0.43 |
| 1:B:128:VAL:O | 1:B:129:ARG:CB | 2.66 | 0.43 |
| 1:B:256:ASN:O | 4:B:2381:HOH:O | 2.21 | 0.43 |
| 1:D:73:HIS:ND1 | 1:D:74:ILE:HG12 | 2.34 | 0.43 |
| 1:E:106:LYS:CA | 4:E:5398:HOH:O | 2.66 | 0.43 |
| 1:E:129:ARG:HA | 1:E:156:VAL:HG13 | 2.01 | 0.43 |
| 1:A:56:ASN:O | 1:A:82:ILE:HD11 | 2.19 | 0.43 |
| 1:B:260:ALA:N | 4:B:2381:HOH:O | 2.50 | 0.43 |
| 1:B:26:ALA:HB3 | 1:B:29:LYS:HB2 | 2.00 | 0.43 |
| 1:C:35:PRO:O | 1:C:36:ASP:CB | 2.66 | 0.43 |
| 1:C:75:ILE:HG21 | 1:C:99:VAL:HG11 | 2.01 | 0.43 |
| 1:A:73:HIS:O | 1:A:76:PRO:HD2 | 2.19 | 0.43 |
| 1:B:133:THR:N | 4:B:2387:HOH:O | 2.51 | 0.43 |
| 1:B:147:ARG:NH1 | 1:B:150:GLU:OE2 | 2.52 | 0.43 |
| 1:C:112:ARG:HG3 | 1:C:113:PRO:CD | 2.39 | 0.43 |
| 1:E:125:PRO:HB2 | 1:E:130:GLU:O | 2.19 | 0.43 |
| 1:E:131:GLY:O | 1:E:157:GLY:HA3 | 2.19 | 0.43 |
| 1:A:6:ILE:HG23 | 1:A:56:ASN:HB2 | 2.00 | 0.42 |
| 1:B:111:PHE:N | 1:B:111:PHE:CD1 | 2.87 | 0.42 |
| 1:B:238:THR:O | 1:B:241:ALA:N | 2.51 | 0.42 |
| 1:B:269:GLN:O | 1:B:271:MET:N | 2.47 | 0.42 |
| 1:C:79:LEU:HD11 | 1:C:104:ILE:CG1 | 2.48 | 0.42 |
| 1:C:252:SER:HA | 4:C:3364:HOH:O | 2.19 | 0.42 |
| 1:C:24:VAL:O | 1:C:25:LEU:HB2 | 2.16 | 0.42 |
| 1:C:46:ARG:O | 1:C:48:MET:N | 2.52 | 0.42 |
| 1:D:121:MET:HE3 | 1:D:171:THR:HA | 2.00 | 0.42 |
| 1:D:89:ARG:CZ | 1:D:90:HIS:CE1 | 3.02 | 0.42 |
| 1:B:105:GLU:O | 1:B:109:SER:HB2 | 2.18 | 0.42 |
| 1:B:154:SER:C | 2:B:2300:NAI:N7N | 2.66 | 0.42 |
| 1:C:123:ASN:HD21 | 1:C:132:ALA:CB | 2.22 | 0.42 |
| 1:D:142:GLN:C | 1:D:145:ASP:HB2 | 2.40 | 0.42 |
| 1:D:134:VAL:HG23 | 1:D:160:THR:O | 2.19 | 0.42 |
| 1:D:203:VAL:CG1 | 1:D:204:ARG:N | 2.82 | 0.42 |
| 1:E:115:PRO:CA | 4:E:5436:HOH:O | 2.52 | 0.42 |
| 1:E:136:ALA:HB2 | 1:E:167:ILE:CD1 | 2.49 | 0.42 |
| 1:E:195:MET:HE2 | 1:E:195:MET:HA | 2.01 | 0.42 |
| 1:E:243:HIS:O | 1:E:247:SER:OG | 2.35 | 0.42 |
| 1:B:124:THR:N | 1:B:125:PRO:CD | 2.80 | 0.42 |
| 1:B:204:ARG:HD3 | 1:B:204:ARG:N | 2.35 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:125:PRO:HG3 | 4:C:3346:HOH:O | 2.19 | 0.42 |
| 1:C:185:LEU:HG | 4:C:3352:HOH:O | 2.19 | 0.42 |
| 1:D:109:SER:C | 1:D:111:PHE:H | 2.22 | 0.42 |
| 1:D:39:LEU:O | 1:D:43:SER:HB3 | 2.19 | 0.42 |
| 1:D:57:LYS:O | 1:D:61:GLN:HG3 | 2.19 | 0.42 |
| 1:E:238:THR:CB | 4:E:5321:HOH:O | 2.60 | 0.42 |
| 1:A:119:ARG:O | 1:A:135:TYR:HA | 2.19 | 0.42 |
| 1:A:92:VAL:O | 1:A:117:VAL:HG23 | 2.20 | 0.42 |
| 1:B:165:ASP:OD1 | 1:B:166:LEU:N | 2.53 | 0.42 |
| 1:B:218:LEU:CB | 2:B:2300:NAI:H52N | 2.50 | 0.42 |
| 1:B:39:LEU:HA | 1:B:43:SER:HB2 | 2.01 | 0.42 |
| 1:C:129:ARG:NH1 | 3:C:3301:GLU:HG2 | 2.32 | 0.42 |
| 1:E:259:GLU:O | 1:E:260:ALA:C | 2.57 | 0.42 |
| 1:E:31:MET:HE3 | 1:E:51:LYS:HD3 | 2.01 | 0.42 |
| 1:A:169:ALA:O | 1:A:172:GLY:N | 2.51 | 0.42 |
| 1:A:258:VAL:HG12 | 1:A:259:GLU:N | 2.34 | 0.42 |
| 1:A:269:GLN:O | 1:A:271:MET:N | 2.52 | 0.42 |
| 1:B:172:GLY:HA2 | 1:B:261:SER:CB | 2.49 | 0.42 |
| 1:B:188:LEU:C | 1:B:190:ASP:N | 2.71 | 0.42 |
| 1:D:111:PHE:O | 1:D:112:ARG:C | 2.57 | 0.42 |
| 1:E:132:ALA:CA | 4:E:5351:HOH:O | 2.52 | 0.42 |
| 1:E:246:GLU:CA | 4:E:5312:HOH:O | 2.66 | 0.42 |
| 1:A:105:GLU:O | 1:A:107:LYS:N | 2.45 | 0.42 |
| 1:A:119:ARG:CA | 4:A:1372:HOH:O | 2.68 | 0.42 |
| 1:A:149:MET:O | 1:A:151:GLN:N | 2.52 | 0.42 |
| 1:A:219:HIS:NE2 | 2:A:1300:NAI:C5D | 2.82 | 0.42 |
| 1:A:249:GLY:O | 1:A:252:SER:HB3 | 2.20 | 0.42 |
| 1:B:75:ILE:H | 1:B:75:ILE:CD1 | 2.27 | 0.42 |
| 1:C:11:LEU:O | 1:C:15:LEU:HG | 2.20 | 0.42 |
| 1:C:22:ALA:CB | 4:C:3369:HOH:O | 2.40 | 0.42 |
| 1:E:111:PHE:O | 1:E:112:ARG:C | 2.56 | 0.42 |
| 1:E:199:ARG:NH2 | 4:E:5346:HOH:O | 2.49 | 0.42 |
| 1:E:211:LEU:HD13 | 1:E:211:LEU:O | 2.19 | 0.42 |
| 1:E:89:ARG:NH2 | 1:E:90:HIS:HE1 | 2.17 | 0.42 |
| 1:A:173:LEU:HB3 | 1:A:174:SER:H | 1.55 | 0.42 |
| 1:A:50:VAL:CG1 | 1:A:51:LYS:N | 2.83 | 0.42 |
| 1:B:274:GLN:HG2 | 1:B:275:GLU:HG3 | 2.01 | 0.42 |
| 1:D:133:THR:HG22 | 1:D:158:PHE:O | 2.19 | 0.42 |
| 1:D:28:HIS:CD2 | 1:D:28:HIS:C | 2.93 | 0.42 |
| 1:E:260:ALA:HA | 4:E:5329:HOH:O | 2.20 | 0.42 |
| 1:E:62:HIS:O | 4:E:5417:HOH:O | 2.22 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:102:SER:O | 1:A:104:ILE:N | 2.53 | 0.42 |
| 1:A:109:SER:C | 1:A:111:PHE:H | 2.23 | 0.42 |
| 1:A:166:LEU:O | 1:A:168:ASP:N | 2.52 | 0.42 |
| 1:A:194:LYS:CA | 4:E:5309:HOH:O | 2.66 | 0.42 |
| 1:A:249:GLY:CA | 4:A:1318:HOH:O | 2.66 | 0.42 |
| 1:B:158:PHE:HE2 | 2:B:2300:NAI:O3B | 1.85 | 0.42 |
| 1:C:177:GLY:O | 1:C:180:TYR:N | 2.45 | 0.42 |
| 1:C:185:LEU:HA | 1:C:185:LEU:HD23 | 1.90 | 0.42 |
| 1:D:30:ILE:CB | 1:D:50:VAL:HG22 | 2.40 | 0.42 |
| 1:D:70:VAL:CG1 | 1:D:74:ILE:HB | 2.50 | 0.42 |
| 1:A:162:VAL:CG1 | 1:A:166:LEU:HD12 | 2.45 | 0.42 |
| 1:A:267:GLU:O | 1:A:268:LEU:C | 2.57 | 0.42 |
| 1:A:80:ASP:OD2 | 1:A:107:LYS:NZ | 2.42 | 0.42 |
| 1:B:176:SER:HB2 | 1:B:180:TYR:OH | 2.20 | 0.42 |
| 1:B:191:GLY:O | 1:B:194:LYS:HB3 | 2.20 | 0.42 |
| 1:C:57:LYS:C | 4:C:3383:HOH:O | 2.58 | 0.42 |
| 1:C:86:ILE:HG22 | 1:C:87:GLU:H | 1.84 | 0.42 |
| 1:D:251:ARG:NH1 | 1:D:251:ARG:HG2 | 2.35 | 0.42 |
| 1:D:62:HIS:HA | 4:D:4448:HOH:O | 2.16 | 0.42 |
| 1:E:39:LEU:HA | 1:E:43:SER:CB | 2.50 | 0.42 |
| 1:A:106:LYS:CB | 4:A:1432:HOH:O | 2.67 | 0.42 |
| 1:B:164:GLU:HA | 1:B:167:ILE:CD1 | 2.49 | 0.42 |
| 1:B:89:ARG:O | 1:B:89:ARG:HD2 | 2.20 | 0.42 |
| 1:D:119:ARG:CZ | 4:D:4422:HOH:O | 2.68 | 0.42 |
| 1:E:78:ILE:O | 1:E:81:GLU:HB2 | 2.19 | 0.42 |
| 1:A:119:ARG:HH11 | 1:A:164:GLU:HG2 | 1.85 | 0.41 |
| 1:B:250:PHE:N | 4:B:2361:HOH:O | 2.53 | 0.41 |
| 1:B:57:LYS:HG3 | 1:B:58:GLU:N | 2.35 | 0.41 |
| 1:C:133:THR:O | 1:C:159:CYS:HA | 2.19 | 0.41 |
| 1:C:197:LEU:CD1 | 4:C:3367:HOH:O | 2.66 | 0.41 |
| 1:D:219:HIS:NE2 | 2:D:4300:NAI:O5D | 2.52 | 0.41 |
| 1:E:116:ARG:HA | 4:E:5388:HOH:O | 2.20 | 0.41 |
| 1:E:121:MET:HA | 1:E:121:MET:HE3 | 2.02 | 0.41 |
| 1:E:218:LEU:CB | 4:E:5424:HOH:O | 2.68 | 0.41 |
| 1:A:146:GLY:O | 1:A:150:GLU:HB2 | 2.20 | 0.41 |
| 1:A:187:ALA:O | 1:A:190:ASP:HB2 | 2.20 | 0.41 |
| 1:B:228:LYS:NZ | 4:E:5316:HOH:O | 2.32 | 0.41 |
| 1:B:45:LEU:CA | 4:B:2385:HOH:O | 2.69 | 0.41 |
| 1:B:5:PHE:CE1 | 1:B:12:ALA:HA | 2.55 | 0.41 |
| 1:C:240:HIS:HE1 | 4:C:3365:HOH:O | 2.03 | 0.41 |
| 1:D:172:GLY:HA2 | 1:D:261:SER:CB | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:17:LYS:HD2 | 1:D:127:VAL:HG12 | 2.01 | 0.41 |
| 1:D:98:GLY:O | 1:D:99:VAL:C | 2.58 | 0.41 |
| 1:E:229:ASP:O | 1:E:231:VAL:N | 2.52 | 0.41 |
| 1:E:180:TYR:CE2 | 1:E:257:ALA:HB1 | 2.55 | 0.41 |
| 1:A:223:HIS:ND1 | 1:A:224:PRO:CD | 2.83 | 0.41 |
| 1:B:101:ILE:HG23 | 1:B:164:GLU:CD | 2.41 | 0.41 |
| 1:C:87:GLU:HB2 | 1:C:90:HIS:CE1 | 2.55 | 0.41 |
| 1:D:227:LEU:HA | 1:D:230:ASN:HB2 | 2.02 | 0.41 |
| 1:D:43:SER:CB | 4:D:4405:HOH:O | 2.56 | 0.41 |
| 1:E:6:ILE:HG12 | 1:E:66:LEU:HD11 | 2.02 | 0.41 |
| 1:A:123:ASN:HD21 | 1:A:131:GLY:CA | 2.34 | 0.41 |
| 1:A:73:HIS:HE1 | 4:E:5334:HOH:O | 2.03 | 0.41 |
| 1:B:86:ILE:HD12 | 1:B:108:LEU:HD22 | 2.03 | 0.41 |
| 1:C:12:ALA:HA | 1:C:15:LEU:HD12 | 2.02 | 0.41 |
| 1:C:133:THR:HG21 | 4:C:3317:HOH:O | 2.04 | 0.41 |
| 1:C:173:LEU:HD12 | 1:C:173:LEU:HA | 1.85 | 0.41 |
| 1:C:213:ALA:O | 1:C:216:MET:HB2 | 2.19 | 0.41 |
| 1:E:94:SER:CA | 4:E:5325:HOH:O | 2.60 | 0.41 |
| 1:A:171:THR:O | 1:A:175:GLY:HA3 | 2.21 | 0.41 |
| 1:A:263:ILE:H | 1:A:263:ILE:HD13 | 1.81 | 0.41 |
| 1:B:70:VAL:HB | 4:B:2368:HOH:O | 2.19 | 0.41 |
| 1:C:16:ALA:O | 1:C:18:GLY:N | 2.53 | 0.41 |
| 1:C:15:LEU:HB3 | 1:C:19:PHE:CE1 | 2.55 | 0.41 |
| 1:D:166:LEU:O | 1:D:167:ILE:C | 2.59 | 0.41 |
| 1:D:229:ASP:O | 4:D:4316:HOH:O | 2.22 | 0.41 |
| 1:E:69:ALA:CB | 4:E:5379:HOH:O | 2.48 | 0.41 |
| 1:A:149:MET:CE | 1:A:149:MET:HA | 2.51 | 0.41 |
| 1:B:218:LEU:HD21 | 2:B:2300:NAI:H52A | 2.02 | 0.41 |
| 1:B:233:SER:O | 1:B:235:GLY:N | 2.53 | 0.41 |
| 1:B:42:VAL:C | 1:B:44:ALA:H | 2.23 | 0.41 |
| 1:C:123:ASN:OD1 | 1:C:132:ALA:N | 2.53 | 0.41 |
| 1:C:134:VAL:O | 4:C:3327:HOH:O | 2.22 | 0.41 |
| 1:C:4:GLY:CA | 1:C:66:LEU:HG | 2.51 | 0.41 |
| 1:C:74:ILE:HG22 | 1:C:78:ILE:HG12 | 2.03 | 0.41 |
| 1:D:89:ARG:CZ | 1:D:90:HIS:HE1 | 2.34 | 0.41 |
| 1:E:57:LYS:CD | 1:E:57:LYS:N | 2.74 | 0.41 |
| 1:A:149:MET:HE1 | 1:A:153:LEU:HG | 2.03 | 0.41 |
| 1:A:167:ILE:HG22 | 1:A:167:ILE:O | 2.21 | 0.41 |
| 1:A:22:ALA:HB1 | 4:A:1425:HOH:O | 2.15 | 0.41 |
| 1:A:38:ASP:O | 1:A:40:ALA:N | 2.54 | 0.41 |
| 1:A:41:THR:HG22 | 1:A:42:VAL:N | 2.36 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:140:HIS:O | 1:B:141:ALA:CB | 2.68 | 0.41 |
| 1:B:229:ASP:C | 1:B:231:VAL:H | 2.23 | 0.41 |
| 1:B:53:THR:HG21 | 1:B:58:GLU:HB2 | 2.03 | 0.41 |
| 1:B:89:ARG:NH1 | 1:B:90:HIS:HD1 | 2.18 | 0.41 |
| 1:C:19:PHE:CE2 | 1:C:153:LEU:HD23 | 2.55 | 0.41 |
| 1:D:164:GLU:OE2 | 4:D:4422:HOH:O | 2.21 | 0.41 |
| 1:D:210:LEU:O | 1:D:211:LEU:C | 2.58 | 0.41 |
| 1:D:220:SER:C | 1:D:222:GLN:H | 2.24 | 0.41 |
| 1:D:236:GLY:O | 1:D:237:ALA:HB3 | 2.21 | 0.41 |
| 1:E:129:ARG:CB | 4:E:5401:HOH:O | 2.56 | 0.41 |
| 1:A:116:ARG:HG3 | 4:A:1416:HOH:O | 2.19 | 0.41 |
| 1:C:119:ARG:NH1 | 4:C:3372:HOH:O | 2.53 | 0.41 |
| 1:C:252:SER:O | 1:C:253:LEU:C | 2.58 | 0.41 |
| 1:C:6:ILE:HD12 | 1:C:56:ASN:CB | 2.46 | 0.41 |
| 1:D:161:GLU:O | 1:D:162:VAL:HG23 | 2.21 | 0.41 |
| 1:D:67:PHE:O | 4:D:4327:HOH:O | 2.21 | 0.41 |
| 1:D:80:ASP:O | 1:D:82:ILE:N | 2.54 | 0.41 |
| 1:E:117:VAL:O | 1:E:138:GLY:CA | 2.67 | 0.41 |
| 1:E:134:VAL:CG2 | 1:E:170:VAL:HG11 | 2.51 | 0.41 |
| 1:A:11:LEU:HD11 | 4:A:1346:HOH:O | 2.20 | 0.41 |
| 1:A:7:GLY:CA | 4:A:1305:HOH:O | 2.59 | 0.41 |
| 1:B:28:HIS:CD2 | 1:B:49:GLY:O | 2.73 | 0.41 |
| 1:B:8:ALA:HB1 | 1:B:45:LEU:HD12 | 2.03 | 0.41 |
| 1:C:222:GLN:HG3 | 1:C:227:LEU:HD21 | 2.02 | 0.41 |
| 1:D:121:MET:CE | 1:D:171:THR:HA | 2.50 | 0.41 |
| 1:D:269:GLN:NE2 | 4:D:4445:HOH:O | 2.52 | 0.41 |
| 1:D:46:ARG:HG3 | 1:D:52:LEU:HD12 | 2.02 | 0.41 |
| 1:E:100:THR:HG22 | 1:E:101:ILE:H | 1.86 | 0.41 |
| 1:E:242:LEU:O | 1:E:245:LEU:N | 2.54 | 0.41 |
| 1:E:75:ILE:HG21 | 1:E:99:VAL:HG11 | 2.02 | 0.41 |
| 1:A:13:PHE:HA | 1:A:45:LEU:HD21 | 2.03 | 0.41 |
| 1:B:164:GLU:CG | 1:B:167:ILE:HD12 | 2.42 | 0.41 |
| 1:B:241:ALA:O | 1:B:242:LEU:C | 2.57 | 0.41 |
| 1:C:137:THR:O | 4:C:3414:HOH:O | 2.22 | 0.41 |
| 1:A:240:HIS:CD2 | 1:C:194:LYS:HE3 | 2.56 | 0.41 |
| 1:C:158:PHE:HZ | 2:C:3300:NAI:HO2A | 1.66 | 0.41 |
| 1:D:165:ASP:O | 4:D:4368:HOH:O | 2.22 | 0.41 |
| 1:D:187:ALA:O | 1:D:190:ASP:HB2 | 2.20 | 0.41 |
| 1:D:24:VAL:HG11 | 1:D:152:LEU:CD2 | 2.51 | 0.41 |
| 1:A:185:LEU:HG | 4:A:1419:HOH:O | 2.21 | 0.41 |
| 1:A:98:GLY:CA | 4:A:1328:HOH:O | 2.39 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:107:LYS:HE2 | 1:B:107:LYS:HB3 | 1.91 | 0.41 |
| 1:B:91:ILE:HG23 | 1:B:116:ARG:HB3 | 2.03 | 0.41 |
| 1:B:134:VAL:HG12 | 1:B:135:TYR:N | 2.36 | 0.41 |
| 1:B:16:ALA:C | 1:B:18:GLY:N | 2.72 | 0.41 |
| 1:C:104:ILE:CG2 | 1:C:117:VAL:HG11 | 2.51 | 0.41 |
| 1:C:119:ARG:NH2 | 4:C:3345:HOH:O | 2.53 | 0.41 |
| 1:D:193:VAL:HA | 1:D:197:LEU:O | 2.21 | 0.41 |
| 1:D:89:ARG:NH1 | 1:D:90:HIS:CE1 | 2.89 | 0.41 |
| 1:E:3:VAL:HG22 | 1:E:65:VAL:HB | 2.03 | 0.41 |
| 1:A:242:LEU:O | 1:A:244:VAL:N | 2.53 | 0.40 |
| 1:A:77:PHE:CD1 | 1:A:77:PHE:N | 2.89 | 0.40 |
| 1:B:228:LYS:HE2 | 1:B:229:ASP:OD1 | 2.21 | 0.40 |
| 1:C:129:ARG:O | 1:C:157:GLY:HA2 | 2.21 | 0.40 |
| 1:C:160:THR:HG22 | 1:C:161:GLU:H | 1.81 | 0.40 |
| 1:C:233:SER:N | 4:C:3313:HOH:O | 2.45 | 0.40 |
| 1:E:215:LYS:O | 1:E:219:HIS:CD2 | 2.74 | 0.40 |
| 1:E:255:ILE:O | 1:E:256:ASN:C | 2.59 | 0.40 |
| 1:A:26:ALA:HB2 | 1:A:29:LYS:HE3 | 2.03 | 0.40 |
| 1:B:12:ALA:HB1 | 4:B:2314:HOH:O | 2.13 | 0.40 |
| 1:B:12:ALA:O | 1:B:16:ALA:CB | 2.69 | 0.40 |
| 1:B:194:LYS:HG2 | 1:B:195:MET:HE3 | 2.02 | 0.40 |
| 1:B:76:PRO:HB2 | 1:B:77:PHE:CD1 | 2.56 | 0.40 |
| 1:C:82:ILE:O | 1:C:82:ILE:HG22 | 2.21 | 0.40 |
| 1:D:156:VAL:CG1 | 1:D:156:VAL:O | 2.56 | 0.40 |
| 1:D:206:GLY:O | 1:D:209:ALA:HB3 | 2.22 | 0.40 |
| 1:D:251:ARG:CD | 4:D:4427:HOH:O | 2.59 | 0.40 |
| 1:E:133:THR:O | 1:E:159:CYS:HA | 2.21 | 0.40 |
| 2:E:5300:NAI:C2D | 3:E:5301:GLU:N | 2.85 | 0.40 |
| 1:A:124:THR:C | 1:A:126:VAL:H | 2.24 | 0.40 |
| 1:A:240:HIS:HD2 | 1:C:194:LYS:HG3 | 1.86 | 0.40 |
| 1:A:62:HIS:O | 1:A:62:HIS:CG | 2.74 | 0.40 |
| 1:B:160:THR:HG22 | 4:B:2360:HOH:O | 2.07 | 0.40 |
| 1:B:269:GLN:C | 1:B:271:MET:N | 2.74 | 0.40 |
| 1:C:128:VAL:CG1 | 1:C:129:ARG:H | 2.26 | 0.40 |
| 1:C:50:VAL:HG22 | 4:C:3363:HOH:O | 2.18 | 0.40 |
| 1:D:129:ARG:HD3 | 1:D:155:SER:O | 2.21 | 0.40 |
| 1:E:113:PRO:N | 4:E:5367:HOH:O | 2.55 | 0.40 |
| 1:E:63:SER:CB | 4:E:5372:HOH:O | 2.67 | 0.40 |
| 1:E:77:PHE:N | 1:E:77:PHE:CD1 | 2.86 | 0.40 |
| 1:A:100:THR:HG22 | 1:A:101:ILE:N | 2.37 | 0.40 |
| 1:A:26:ALA:O | 1:A:27:ALA:C | 2.60 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:40:ALA:O | 1:A:44:ALA:HB2 | 2.22 | 0.40 |
| 1:B:216:MET:CE | 4:B:2315:HOH:O | 2.69 | 0.40 |
| 1:B:73:HIS:C | 1:B:75:ILE:N | 2.74 | 0.40 |
| 1:B:77:PHE:N | 1:B:77:PHE:CD1 | 2.85 | 0.40 |
| 1:B:89:ARG:C | 1:B:89:ARG:HD2 | 2.41 | 0.40 |
| 1:C:176:SER:HB2 | 1:C:180:TYR:CZ | 2.56 | 0.40 |
| 1:C:228:LYS:NZ | 1:C:229:ASP:OD1 | 2.55 | 0.40 |
| 1:C:79:LEU:HD11 | 1:C:104:ILE:HG12 | 2.04 | 0.40 |
| 1:D:251:ARG:NH1 | 4:D:4447:HOH:O | 2.28 | 0.40 |
| 1:E:181:ALA:C | 4:E:5383:HOH:O | 2.58 | 0.40 |
| 1:A:5:PHE:C | 1:A:7:GLY:N | 2.74 | 0.40 |
| 1:E:135:TYR:N | 4:E:5413:HOH:O | 2.54 | 0.40 |

All (22) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------------|--------------------------|-------------------|
| 1:B:200:ARG:NH1 | 2:B:2300:NAI:N7A[2_555] | 1.66 | 0.54 |
| 1:A:204:ARG:CB | 2:C:3300:NAI:C3B[2_555] | 1.75 | 0.45 |
| 1:B:204:ARG:CB | 2:B:2300:NAI:C3B[2_555] | 1.76 | 0.44 |
| 2:B:2300:NAI:O5B | 4:B:2359:HOH:O[2_555] | 1.88 | 0.32 |
| 1:D:204:ARG:CB | 2:E:5300:NAI:C2B[2_555] | 1.94 | 0.26 |
| 1:B:204:ARG:CG | 2:B:2300:NAI:C2B[2_555] | 2.01 | 0.19 |
| 1:E:250:PHE:CE2 | 4:D:4340:HOH:O[2_555] | 2.03 | 0.17 |
| 1:B:204:ARG:NE | 2:B:2300:NAI:C8A[2_555] | 2.03 | 0.17 |
| 4:A:1320:HOH:O | 4:C:3330:HOH:O[2_555] | 2.04 | 0.16 |
| 1:A:243:HIS:NE2 | 4:A:1335:HOH:O[2_555] | 2.07 | 0.13 |
| 4:B:2337:HOH:O | 4:B:2363:HOH:O[2_555] | 2.09 | 0.11 |
| 4:A:1398:HOH:O | 4:C:3376:HOH:O[2_555] | 2.09 | 0.11 |
| 1:A:251:ARG:NH1 | 1:A:251:ARG:NH1[2_555] | 2.09 | 0.11 |
| 1:C:231:VAL:CG1 | 4:A:1347:HOH:O[2_555] | 2.10 | 0.10 |
| 1:C:255:ILE:CG2 | 4:E:5357:HOH:O[2_555] | 2.11 | 0.09 |
| 4:A:1380:HOH:O | 4:C:3336:HOH:O[2_555] | 2.11 | 0.09 |
| 1:A:204:ARG:CG | 2:C:3300:NAI:C2B[2_555] | 2.15 | 0.05 |
| 1:A:204:ARG:CG | 2:C:3300:NAI:O4B[2_555] | 2.16 | 0.04 |
| 1:D:29:LYS:CE | 4:D:4430:HOH:O[2_556] | 2.16 | 0.04 |
| 1:B:258:VAL:CG2 | 4:B:2355:HOH:O[2_555] | 2.17 | 0.03 |
| 4:A:1442:HOH:O | 4:C:3379:HOH:O[2_555] | 2.17 | 0.03 |
| 1:A:204:ARG:CB | 2:C:3300:NAI:O4B[2_555] | 2.18 | 0.02 |

5.3 Torsion angles

5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|-----------|-----------|-----------|-------------|---|
| 1 | A | 275/277 (99%) | 189 (69%) | 54 (20%) | 32 (12%) | 0 | 2 |
| 1 | B | 272/277 (98%) | 168 (62%) | 62 (23%) | 42 (15%) | 0 | 0 |
| 1 | C | 275/277 (99%) | 198 (72%) | 49 (18%) | 28 (10%) | 0 | 3 |
| 1 | D | 275/277 (99%) | 190 (69%) | 64 (23%) | 21 (8%) | 1 | 5 |
| 1 | E | 275/277 (99%) | 178 (65%) | 64 (23%) | 33 (12%) | 0 | 1 |
| All | All | 1372/1385 (99%) | 923 (67%) | 293 (21%) | 156 (11%) | 0 | 2 |

All (156) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 8 | ALA |
| 1 | A | 36 | ASP |
| 1 | A | 39 | LEU |
| 1 | A | 107 | LYS |
| 1 | A | 129 | ARG |
| 1 | A | 164 | GLU |
| 1 | A | 173 | LEU |
| 1 | B | 10 | GLN |
| 1 | B | 19 | PHE |
| 1 | B | 36 | ASP |
| 1 | B | 37 | MET |
| 1 | B | 76 | PRO |
| 1 | B | 95 | CYS |
| 1 | B | 97 | ALA |
| 1 | B | 129 | ARG |
| 1 | B | 137 | THR |
| 1 | B | 140 | HIS |
| 1 | B | 141 | ALA |
| 1 | B | 142 | GLN |
| 1 | B | 221 | GLU |
| 1 | B | 222 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 223 | HIS |
| 1 | C | 10 | GLN |
| 1 | C | 27 | ALA |
| 1 | C | 63 | SER |
| 1 | C | 65 | VAL |
| 1 | C | 113 | PRO |
| 1 | C | 252 | SER |
| 1 | C | 253 | LEU |
| 1 | D | 40 | ALA |
| 1 | D | 99 | VAL |
| 1 | D | 129 | ARG |
| 1 | D | 164 | GLU |
| 1 | D | 223 | HIS |
| 1 | E | 88 | ASP |
| 1 | E | 164 | GLU |
| 1 | E | 222 | GLN |
| 1 | E | 223 | HIS |
| 1 | E | 274 | GLN |
| 1 | A | 41 | THR |
| 1 | A | 42 | VAL |
| 1 | A | 235 | GLY |
| 1 | B | 61 | GLN |
| 1 | B | 77 | PHE |
| 1 | B | 113 | PRO |
| 1 | B | 154 | SER |
| 1 | B | 160 | THR |
| 1 | B | 170 | VAL |
| 1 | B | 177 | GLY |
| 1 | B | 186 | ASP |
| 1 | B | 189 | ALA |
| 1 | C | 16 | ALA |
| 1 | C | 36 | ASP |
| 1 | C | 64 | ASP |
| 1 | C | 107 | LYS |
| 1 | D | 8 | ALA |
| 1 | D | 167 | ILE |
| 1 | D | 267 | GLU |
| 1 | D | 270 | SER |
| 1 | E | 41 | THR |
| 1 | E | 42 | VAL |
| 1 | E | 50 | VAL |
| 1 | E | 78 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 90 | HIS |
| 1 | E | 151 | GLN |
| 1 | E | 170 | VAL |
| 1 | E | 230 | ASN |
| 1 | E | 235 | GLY |
| 1 | E | 260 | ALA |
| 1 | A | 37 | MET |
| 1 | A | 77 | PHE |
| 1 | A | 103 | SER |
| 1 | A | 106 | LYS |
| 1 | A | 167 | ILE |
| 1 | A | 223 | HIS |
| 1 | A | 243 | HIS |
| 1 | A | 256 | ASN |
| 1 | A | 270 | SER |
| 1 | B | 38 | ASP |
| 1 | B | 94 | SER |
| 1 | B | 143 | VAL |
| 1 | B | 163 | GLU |
| 1 | B | 199 | ARG |
| 1 | B | 220 | SER |
| 1 | B | 230 | ASN |
| 1 | B | 270 | SER |
| 1 | C | 17 | LYS |
| 1 | C | 20 | THR |
| 1 | C | 47 | LYS |
| 1 | C | 56 | ASN |
| 1 | C | 125 | PRO |
| 1 | C | 139 | THR |
| 1 | C | 197 | LEU |
| 1 | C | 258 | VAL |
| 1 | D | 10 | GLN |
| 1 | D | 41 | THR |
| 1 | D | 81 | GLU |
| 1 | D | 170 | VAL |
| 1 | D | 258 | VAL |
| 1 | E | 243 | HIS |
| 1 | E | 250 | PHE |
| 1 | A | 40 | ALA |
| 1 | A | 87 | GLU |
| 1 | A | 102 | SER |
| 1 | A | 150 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 163 | GLU |
| 1 | A | 187 | ALA |
| 1 | A | 220 | SER |
| 1 | B | 16 | ALA |
| 1 | B | 20 | THR |
| 1 | B | 125 | PRO |
| 1 | B | 246 | GLU |
| 1 | C | 46 | ARG |
| 1 | C | 72 | PRO |
| 1 | C | 173 | LEU |
| 1 | D | 235 | GLY |
| 1 | D | 257 | ALA |
| 1 | E | 36 | ASP |
| 1 | E | 77 | PHE |
| 1 | E | 130 | GLU |
| 1 | E | 163 | GLU |
| 1 | E | 221 | GLU |
| 1 | E | 237 | ALA |
| 1 | E | 259 | GLU |
| 1 | A | 177 | GLY |
| 1 | A | 234 | PRO |
| 1 | B | 71 | LYS |
| 1 | C | 11 | LEU |
| 1 | C | 40 | ALA |
| 1 | C | 62 | HIS |
| 1 | C | 150 | GLU |
| 1 | C | 270 | SER |
| 1 | D | 77 | PHE |
| 1 | D | 125 | PRO |
| 1 | D | 238 | THR |
| 1 | E | 113 | PRO |
| 1 | E | 143 | VAL |
| 1 | A | 56 | ASN |
| 1 | A | 263 | ILE |
| 1 | C | 177 | GLY |
| 1 | D | 42 | VAL |
| 1 | D | 111 | PHE |
| 1 | E | 81 | GLU |
| 1 | A | 125 | PRO |
| 1 | B | 239 | ILE |
| 1 | E | 74 | ILE |
| 1 | E | 125 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 34 | SER |
| 1 | B | 24 | VAL |
| 1 | B | 235 | GLY |
| 1 | E | 234 | PRO |
| 1 | B | 234 | PRO |
| 1 | B | 127 | VAL |
| 1 | E | 34 | SER |
| 1 | E | 71 | LYS |
| 1 | E | 167 | ILE |

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 | 215/215 (100%) | 188 (87%) | 27 (13%) | 4 | 18 |
| 1 | B | 213/215 (99%) | 197 (92%) | 16 (8%) | 13 | 42 |
| 1 | C | 214/215 (100%) | 197 (92%) | 17 (8%) | 12 | 40 |
| 1 | D | 215/215 (100%) | 195 (91%) | 20 (9%) | 9 | 32 |
| 1 | E | 215/215 (100%) | 200 (93%) | 15 (7%) | 15 | 45 |
| All | All | 1072/1075 (100%) | 977 (91%) | 95 (9%) | 9 | 34 |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 11 | LEU |
| 1 | A | 20 | THR |
| 1 | A | 25 | LEU |
| 1 | A | 36 | ASP |
| 1 | A | 38 | ASP |
| 1 | A | 73 | HIS |
| 1 | A | 75 | ILE |
| 1 | A | 90 | HIS |
| 1 | A | 111 | PHE |
| 1 | A | 120 | CYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 121 | MET |
| 1 | A | 123 | ASN |
| 1 | A | 124 | THR |
| 1 | A | 126 | VAL |
| 1 | A | 148 | LEU |
| 1 | A | 150 | GLU |
| 1 | A | 171 | THR |
| 1 | A | 183 | THR |
| 1 | A | 211 | LEU |
| 1 | A | 228 | LYS |
| 1 | A | 234 | PRO |
| 1 | A | 247 | SER |
| 1 | A | 258 | VAL |
| 1 | A | 263 | ILE |
| 1 | A | 265 | THR |
| 1 | A | 269 | GLN |
| 1 | A | 271 | MET |
| 1 | B | 5 | PHE |
| 1 | B | 10 | GLN |
| 1 | B | 13 | PHE |
| 1 | B | 19 | PHE |
| 1 | B | 47 | LYS |
| 1 | B | 90 | HIS |
| 1 | B | 105 | GLU |
| 1 | B | 111 | PHE |
| 1 | B | 120 | CYS |
| 1 | B | 124 | THR |
| 1 | B | 140 | HIS |
| 1 | B | 211 | LEU |
| 1 | B | 234 | PRO |
| 1 | B | 244 | VAL |
| 1 | B | 247 | SER |
| 1 | B | 265 | THR |
| 1 | C | 13 | PHE |
| 1 | C | 51 | LYS |
| 1 | C | 61 | GLN |
| 1 | C | 72 | PRO |
| 1 | C | 89 | ARG |
| 1 | C | 90 | HIS |
| 1 | C | 118 | ILE |
| 1 | C | 120 | CYS |
| 1 | C | 121 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 123 | ASN |
| 1 | C | 124 | THR |
| 1 | C | 190 | ASP |
| 1 | C | 195 | MET |
| 1 | C | 216 | MET |
| 1 | C | 244 | VAL |
| 1 | C | 265 | THR |
| 1 | C | 273 | ASP |
| 1 | D | 10 | GLN |
| 1 | D | 28 | HIS |
| 1 | D | 31 | MET |
| 1 | D | 37 | MET |
| 1 | D | 77 | PHE |
| 1 | D | 101 | ILE |
| 1 | D | 118 | ILE |
| 1 | D | 120 | CYS |
| 1 | D | 122 | THR |
| 1 | D | 124 | THR |
| 1 | D | 137 | THR |
| 1 | D | 144 | GLU |
| 1 | D | 145 | ASP |
| 1 | D | 153 | LEU |
| 1 | D | 168 | ASP |
| 1 | D | 203 | VAL |
| 1 | D | 211 | LEU |
| 1 | D | 244 | VAL |
| 1 | D | 258 | VAL |
| 1 | D | 259 | GLU |
| 1 | E | 28 | HIS |
| 1 | E | 57 | LYS |
| 1 | E | 77 | PHE |
| 1 | E | 90 | HIS |
| 1 | E | 101 | ILE |
| 1 | E | 120 | CYS |
| 1 | E | 124 | THR |
| 1 | E | 160 | THR |
| 1 | E | 168 | ASP |
| 1 | E | 176 | SER |
| 1 | E | 178 | PRO |
| 1 | E | 195 | MET |
| 1 | E | 211 | LEU |
| 1 | E | 216 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 233 | SER |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 73 | HIS |
| 1 | A | 90 | HIS |
| 1 | A | 123 | ASN |
| 1 | A | 140 | HIS |
| 1 | A | 226 | GLN |
| 1 | A | 240 | HIS |
| 1 | B | 151 | GLN |
| 1 | C | 73 | HIS |
| 1 | C | 90 | HIS |
| 1 | C | 240 | HIS |
| 1 | C | 243 | HIS |
| 1 | D | 28 | HIS |
| 1 | D | 55 | HIS |
| 1 | D | 140 | HIS |
| 1 | D | 219 | HIS |
| 1 | E | 28 | HIS |
| 1 | E | 142 | GLN |
| 1 | E | 219 | HIS |
| 1 | E | 226 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

10 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | NAI | D | 4300 | - | 40,47,48 | 5.42 | 23 (57%) | 43,71,73 | 4.67 | 21 (48%) |
| 2 | NAI | B | 2300 | - | 40,47,48 | 5.41 | 23 (57%) | 43,71,73 | 4.66 | 21 (48%) |
| 2 | NAI | C | 3300 | - | 40,47,48 | 5.41 | 22 (55%) | 43,71,73 | 4.67 | 21 (48%) |
| 2 | NAI | E | 5300 | - | 40,47,48 | 5.83 | 25 (62%) | 43,71,73 | 6.29 | 31 (72%) |
| 2 | NAI | A | 1300 | - | 40,47,48 | 6.28 | 27 (67%) | 43,71,73 | 5.94 | 24 (55%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|-------------|---------|
| 2 | NAI | D | 4300 | - | 1/1/13/16 | 12/25/72/72 | 0/5/5/5 |
| 2 | NAI | B | 2300 | - | 1/1/13/16 | 12/25/72/72 | 0/5/5/5 |
| 2 | NAI | C | 3300 | - | 1/1/13/16 | 12/25/72/72 | 0/5/5/5 |
| 2 | NAI | E | 5300 | - | 3/3/13/16 | 11/25/72/72 | 0/5/5/5 |
| 2 | NAI | A | 1300 | - | 2/2/13/16 | 14/25/72/72 | 0/5/5/5 |

All (120) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 2 | C | 3300 | NAI | C8A-N7A | 16.62 | 1.64 | 1.34 |
| 2 | B | 2300 | NAI | C8A-N7A | 16.61 | 1.64 | 1.34 |
| 2 | D | 4300 | NAI | C8A-N7A | 16.58 | 1.64 | 1.34 |
| 2 | E | 5300 | NAI | C8A-N7A | 16.55 | 1.64 | 1.34 |
| 2 | A | 1300 | NAI | O7N-C7N | 15.71 | 1.61 | 1.24 |
| 2 | A | 1300 | NAI | O4D-C4D | -14.41 | 1.12 | 1.45 |
| 2 | D | 4300 | NAI | O4D-C4D | -14.40 | 1.12 | 1.45 |
| 2 | C | 3300 | NAI | O4D-C4D | -14.40 | 1.12 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 2 | B | 2300 | NAI | O4D-C4D | -14.39 | 1.12 | 1.45 |
| 2 | A | 1300 | NAI | O4B-C1B | 14.05 | 1.60 | 1.41 |
| 2 | A | 1300 | NAI | C2B-C1B | -13.33 | 1.33 | 1.53 |
| 2 | E | 5300 | NAI | C3D-C4D | -12.48 | 1.21 | 1.53 |
| 2 | E | 5300 | NAI | C1D-N1N | 12.24 | 1.81 | 1.46 |
| 2 | D | 4300 | NAI | O4B-C1B | 12.14 | 1.58 | 1.41 |
| 2 | C | 3300 | NAI | O4B-C1B | 12.11 | 1.58 | 1.41 |
| 2 | E | 5300 | NAI | O4B-C1B | 12.08 | 1.57 | 1.41 |
| 2 | B | 2300 | NAI | O4B-C1B | 12.08 | 1.57 | 1.41 |
| 2 | E | 5300 | NAI | O7N-C7N | 10.88 | 1.50 | 1.24 |
| 2 | A | 1300 | NAI | C7N-C3N | -9.74 | 1.27 | 1.48 |
| 2 | A | 1300 | NAI | C4A-N3A | 9.14 | 1.48 | 1.35 |
| 2 | D | 4300 | NAI | C3D-C4D | -9.09 | 1.29 | 1.53 |
| 2 | A | 1300 | NAI | O4D-C1D | -9.07 | 1.20 | 1.42 |
| 2 | D | 4300 | NAI | O4D-C1D | -9.07 | 1.20 | 1.42 |
| 2 | C | 3300 | NAI | O4D-C1D | -9.06 | 1.20 | 1.42 |
| 2 | C | 3300 | NAI | C3D-C4D | -9.06 | 1.29 | 1.53 |
| 2 | A | 1300 | NAI | C3D-C4D | -9.05 | 1.29 | 1.53 |
| 2 | B | 2300 | NAI | C3D-C4D | -9.04 | 1.29 | 1.53 |
| 2 | B | 2300 | NAI | O4D-C1D | -9.03 | 1.20 | 1.42 |
| 2 | C | 3300 | NAI | PA-O1A | 8.99 | 1.82 | 1.50 |
| 2 | D | 4300 | NAI | PA-O1A | 8.98 | 1.82 | 1.50 |
| 2 | A | 1300 | NAI | PA-O1A | 8.97 | 1.82 | 1.50 |
| 2 | B | 2300 | NAI | PA-O1A | 8.96 | 1.82 | 1.50 |
| 2 | E | 5300 | NAI | C2A-N3A | 8.93 | 1.46 | 1.32 |
| 2 | A | 1300 | NAI | C1D-N1N | 7.86 | 1.68 | 1.46 |
| 2 | E | 5300 | NAI | O3D-C3D | -7.81 | 1.24 | 1.43 |
| 2 | C | 3300 | NAI | C7N-N7N | 7.55 | 1.53 | 1.33 |
| 2 | B | 2300 | NAI | C7N-N7N | 7.55 | 1.53 | 1.33 |
| 2 | E | 5300 | NAI | C7N-N7N | 7.54 | 1.53 | 1.33 |
| 2 | D | 4300 | NAI | C7N-N7N | 7.50 | 1.53 | 1.33 |
| 2 | E | 5300 | NAI | O5B-C5B | 6.95 | 1.71 | 1.44 |
| 2 | A | 1300 | NAI | PN-O2N | 6.81 | 1.75 | 1.50 |
| 2 | E | 5300 | NAI | PA-O1A | -6.33 | 1.28 | 1.50 |
| 2 | C | 3300 | NAI | C1D-N1N | 6.32 | 1.64 | 1.46 |
| 2 | D | 4300 | NAI | C1D-N1N | 6.28 | 1.64 | 1.46 |
| 2 | B | 2300 | NAI | C1D-N1N | 6.27 | 1.64 | 1.46 |
| 2 | E | 5300 | NAI | C2D-C1D | -6.23 | 1.33 | 1.53 |
| 2 | B | 2300 | NAI | PA-O2A | 5.72 | 1.82 | 1.55 |
| 2 | D | 4300 | NAI | PA-O2A | 5.71 | 1.82 | 1.55 |
| 2 | A | 1300 | NAI | PA-O2A | 5.71 | 1.82 | 1.55 |
| 2 | C | 3300 | NAI | PA-O2A | 5.70 | 1.82 | 1.55 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2 | E | 5300 | NAI | PN-O5D | -5.51 | 1.37 | 1.59 |
| 2 | E | 5300 | NAI | PN-O2N | 5.03 | 1.68 | 1.50 |
| 2 | A | 1300 | NAI | C8A-N7A | 5.01 | 1.43 | 1.34 |
| 2 | C | 3300 | NAI | PN-O5D | -4.85 | 1.39 | 1.59 |
| 2 | D | 4300 | NAI | PN-O5D | -4.84 | 1.39 | 1.59 |
| 2 | B | 2300 | NAI | PN-O5D | -4.83 | 1.39 | 1.59 |
| 2 | A | 1300 | NAI | PN-O1N | 4.74 | 1.77 | 1.55 |
| 2 | C | 3300 | NAI | C4A-N3A | -4.49 | 1.29 | 1.35 |
| 2 | A | 1300 | NAI | C6N-C5N | 4.48 | 1.41 | 1.33 |
| 2 | E | 5300 | NAI | C4A-N3A | -4.48 | 1.29 | 1.35 |
| 2 | B | 2300 | NAI | C4A-N3A | -4.45 | 1.29 | 1.35 |
| 2 | D | 4300 | NAI | C4A-N3A | -4.43 | 1.29 | 1.35 |
| 2 | D | 4300 | NAI | O5B-C5B | 4.36 | 1.61 | 1.44 |
| 2 | B | 2300 | NAI | O5B-C5B | 4.35 | 1.61 | 1.44 |
| 2 | C | 3300 | NAI | O5B-C5B | 4.33 | 1.61 | 1.44 |
| 2 | E | 5300 | NAI | O2D-C2D | -4.30 | 1.32 | 1.43 |
| 2 | C | 3300 | NAI | O7N-C7N | -4.16 | 1.14 | 1.24 |
| 2 | B | 2300 | NAI | O7N-C7N | -4.14 | 1.14 | 1.24 |
| 2 | D | 4300 | NAI | O7N-C7N | -4.14 | 1.14 | 1.24 |
| 2 | A | 1300 | NAI | C4N-C5N | -4.06 | 1.38 | 1.48 |
| 2 | E | 5300 | NAI | C5D-C4D | -4.04 | 1.39 | 1.51 |
| 2 | A | 1300 | NAI | C5A-C4A | -3.84 | 1.30 | 1.40 |
| 2 | B | 2300 | NAI | C6N-N1N | 3.77 | 1.46 | 1.37 |
| 2 | C | 3300 | NAI | C6N-N1N | 3.77 | 1.46 | 1.37 |
| 2 | D | 4300 | NAI | C6N-N1N | 3.76 | 1.46 | 1.37 |
| 2 | E | 5300 | NAI | C6N-N1N | 3.71 | 1.46 | 1.37 |
| 2 | D | 4300 | NAI | PA-O5B | -3.59 | 1.44 | 1.59 |
| 2 | B | 2300 | NAI | PA-O5B | -3.58 | 1.44 | 1.59 |
| 2 | C | 3300 | NAI | PA-O5B | -3.57 | 1.44 | 1.59 |
| 2 | A | 1300 | NAI | PA-O5B | -3.47 | 1.45 | 1.59 |
| 2 | A | 1300 | NAI | C6N-N1N | 3.40 | 1.45 | 1.37 |
| 2 | A | 1300 | NAI | C7N-N7N | 3.21 | 1.41 | 1.33 |
| 2 | A | 1300 | NAI | C4N-C3N | -2.86 | 1.44 | 1.49 |
| 2 | E | 5300 | NAI | C5A-N7A | 2.80 | 1.47 | 1.38 |
| 2 | C | 3300 | NAI | C5A-N7A | 2.80 | 1.47 | 1.38 |
| 2 | D | 4300 | NAI | C5A-N7A | 2.78 | 1.47 | 1.38 |
| 2 | B | 2300 | NAI | C5A-N7A | 2.76 | 1.47 | 1.38 |
| 2 | D | 4300 | NAI | C2N-C3N | 2.73 | 1.42 | 1.34 |
| 2 | C | 3300 | NAI | C2N-C3N | 2.73 | 1.42 | 1.34 |
| 2 | E | 5300 | NAI | O4D-C4D | -2.73 | 1.38 | 1.45 |
| 2 | B | 2300 | NAI | C2N-C3N | 2.72 | 1.42 | 1.34 |
| 2 | E | 5300 | NAI | C2N-C3N | 2.71 | 1.42 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2 | E | 5300 | NAI | PA-O5B | 2.70 | 1.70 | 1.59 |
| 2 | D | 4300 | NAI | C2A-N3A | 2.65 | 1.36 | 1.32 |
| 2 | B | 2300 | NAI | C2A-N3A | 2.64 | 1.36 | 1.32 |
| 2 | A | 1300 | NAI | C2A-N3A | 2.61 | 1.36 | 1.32 |
| 2 | C | 3300 | NAI | C2A-N3A | 2.61 | 1.36 | 1.32 |
| 2 | B | 2300 | NAI | O4B-C4B | 2.44 | 1.50 | 1.45 |
| 2 | A | 1300 | NAI | O4B-C4B | 2.43 | 1.50 | 1.45 |
| 2 | C | 3300 | NAI | C2D-C3D | -2.42 | 1.46 | 1.53 |
| 2 | D | 4300 | NAI | O4B-C4B | 2.40 | 1.50 | 1.45 |
| 2 | B | 2300 | NAI | C2D-C3D | -2.40 | 1.46 | 1.53 |
| 2 | E | 5300 | NAI | O4B-C4B | 2.39 | 1.50 | 1.45 |
| 2 | C | 3300 | NAI | O4B-C4B | 2.39 | 1.50 | 1.45 |
| 2 | A | 1300 | NAI | C2D-C3D | -2.38 | 1.46 | 1.53 |
| 2 | C | 3300 | NAI | C2B-C3B | -2.36 | 1.46 | 1.53 |
| 2 | D | 4300 | NAI | C2D-C3D | -2.36 | 1.46 | 1.53 |
| 2 | A | 1300 | NAI | C2B-C3B | -2.35 | 1.46 | 1.53 |
| 2 | B | 2300 | NAI | C2B-C3B | -2.33 | 1.47 | 1.53 |
| 2 | D | 4300 | NAI | C2B-C3B | -2.31 | 1.47 | 1.53 |
| 2 | E | 5300 | NAI | C2B-C3B | -2.30 | 1.47 | 1.53 |
| 2 | D | 4300 | NAI | C5D-C4D | 2.29 | 1.58 | 1.51 |
| 2 | E | 5300 | NAI | PN-O1N | 2.20 | 1.65 | 1.55 |
| 2 | D | 4300 | NAI | C6A-N1A | 2.13 | 1.36 | 1.32 |
| 2 | C | 3300 | NAI | C6A-N1A | 2.11 | 1.36 | 1.32 |
| 2 | A | 1300 | NAI | C6A-N1A | 2.09 | 1.36 | 1.32 |
| 2 | B | 2300 | NAI | C6A-N1A | 2.07 | 1.36 | 1.32 |
| 2 | B | 2300 | NAI | O5D-C5D | 2.04 | 1.52 | 1.44 |
| 2 | A | 1300 | NAI | O5B-C5B | -2.02 | 1.37 | 1.44 |
| 2 | E | 5300 | NAI | C6A-N1A | 2.01 | 1.36 | 1.32 |

All (118) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 2 | A | 1300 | NAI | C1B-N9A-C4A | 20.66 | 162.94 | 126.64 |
| 2 | E | 5300 | NAI | C1D-N1N-C6N | -19.23 | 79.40 | 120.83 |
| 2 | E | 5300 | NAI | C1D-N1N-C2N | 18.54 | 151.99 | 121.11 |
| 2 | E | 5300 | NAI | O4D-C1D-N1N | 15.13 | 137.63 | 108.06 |
| 2 | A | 1300 | NAI | O4D-C1D-N1N | 14.55 | 136.50 | 108.06 |
| 2 | C | 3300 | NAI | O4B-C1B-C2B | -12.81 | 88.20 | 106.93 |
| 2 | B | 2300 | NAI | O4B-C1B-C2B | -12.81 | 88.21 | 106.93 |
| 2 | E | 5300 | NAI | O4B-C1B-C2B | -12.78 | 88.24 | 106.93 |
| 2 | D | 4300 | NAI | O4B-C1B-C2B | -12.77 | 88.26 | 106.93 |
| 2 | A | 1300 | NAI | O7N-C7N-N7N | -12.54 | 93.56 | 122.88 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2 | A | 1300 | NAI | C3N-C7N-N7N | 11.70 | 138.46 | 117.67 |
| 2 | B | 2300 | NAI | O4D-C1D-N1N | 11.04 | 129.64 | 108.06 |
| 2 | D | 4300 | NAI | O4D-C1D-N1N | 11.03 | 129.63 | 108.06 |
| 2 | C | 3300 | NAI | O4D-C1D-N1N | 11.02 | 129.61 | 108.06 |
| 2 | A | 1300 | NAI | O4B-C1B-C2B | -9.23 | 93.44 | 106.93 |
| 2 | E | 5300 | NAI | PN-O3-PA | 9.00 | 163.71 | 132.83 |
| 2 | B | 2300 | NAI | PN-O3-PA | 8.30 | 161.32 | 132.83 |
| 2 | C | 3300 | NAI | PN-O3-PA | 8.30 | 161.31 | 132.83 |
| 2 | D | 4300 | NAI | PN-O3-PA | 8.28 | 161.25 | 132.83 |
| 2 | D | 4300 | NAI | O2A-PA-O5B | 8.13 | 145.51 | 107.75 |
| 2 | B | 2300 | NAI | O2A-PA-O5B | 8.12 | 145.46 | 107.75 |
| 2 | C | 3300 | NAI | O2A-PA-O5B | 8.12 | 145.45 | 107.75 |
| 2 | A | 1300 | NAI | O4B-C4B-C3B | -8.09 | 89.11 | 105.11 |
| 2 | B | 2300 | NAI | O4B-C4B-C3B | -8.07 | 89.14 | 105.11 |
| 2 | C | 3300 | NAI | O4B-C4B-C3B | -8.05 | 89.19 | 105.11 |
| 2 | E | 5300 | NAI | O4B-C4B-C3B | -8.04 | 89.21 | 105.11 |
| 2 | D | 4300 | NAI | O4B-C4B-C3B | -8.03 | 89.21 | 105.11 |
| 2 | D | 4300 | NAI | O5B-C5B-C4B | 7.78 | 135.77 | 108.99 |
| 2 | B | 2300 | NAI | O5B-C5B-C4B | 7.77 | 135.75 | 108.99 |
| 2 | C | 3300 | NAI | O5B-C5B-C4B | 7.77 | 135.73 | 108.99 |
| 2 | A | 1300 | NAI | C4D-O4D-C1D | 7.68 | 126.43 | 109.47 |
| 2 | D | 4300 | NAI | C4D-O4D-C1D | 7.67 | 126.39 | 109.47 |
| 2 | B | 2300 | NAI | C4D-O4D-C1D | 7.66 | 126.38 | 109.47 |
| 2 | C | 3300 | NAI | C4D-O4D-C1D | 7.64 | 126.34 | 109.47 |
| 2 | B | 2300 | NAI | C1B-N9A-C4A | -7.60 | 113.28 | 126.64 |
| 2 | C | 3300 | NAI | C1B-N9A-C4A | -7.60 | 113.30 | 126.64 |
| 2 | D | 4300 | NAI | C1B-N9A-C4A | -7.58 | 113.32 | 126.64 |
| 2 | A | 1300 | NAI | O2A-PA-O5B | 7.47 | 142.46 | 107.75 |
| 2 | A | 1300 | NAI | C2D-C1D-N1N | 7.12 | 131.15 | 113.30 |
| 2 | E | 5300 | NAI | O5B-PA-O1A | 6.69 | 135.21 | 109.07 |
| 2 | D | 4300 | NAI | O4D-C1D-C2D | -6.58 | 92.31 | 106.64 |
| 2 | A | 1300 | NAI | O4D-C1D-C2D | -6.57 | 92.32 | 106.64 |
| 2 | B | 2300 | NAI | O4D-C1D-C2D | -6.57 | 92.32 | 106.64 |
| 2 | C | 3300 | NAI | O4D-C1D-C2D | -6.57 | 92.32 | 106.64 |
| 2 | C | 3300 | NAI | C5B-C4B-C3B | 6.41 | 139.20 | 115.18 |
| 2 | B | 2300 | NAI | C5B-C4B-C3B | 6.41 | 139.18 | 115.18 |
| 2 | D | 4300 | NAI | C5B-C4B-C3B | 6.40 | 139.18 | 115.18 |
| 2 | E | 5300 | NAI | C5D-C4D-C3D | 6.30 | 138.80 | 115.18 |
| 2 | E | 5300 | NAI | O4B-C4B-C5B | -6.27 | 88.75 | 109.37 |
| 2 | E | 5300 | NAI | O1N-PN-O2N | -5.81 | 83.50 | 112.24 |
| 2 | E | 5300 | NAI | PN-O5D-C5D | 5.48 | 153.84 | 121.68 |
| 2 | E | 5300 | NAI | O5B-C5B-C4B | 5.39 | 127.53 | 108.99 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2 | E | 5300 | NAI | N1A-C2A-N3A | -5.15 | 121.06 | 127.65 |
| 2 | E | 5300 | NAI | PA-O5B-C5B | -5.09 | 91.82 | 121.68 |
| 2 | E | 5300 | NAI | C1B-N9A-C4A | 5.08 | 135.56 | 126.64 |
| 2 | D | 4300 | NAI | O5D-C5D-C4D | -5.06 | 91.57 | 108.99 |
| 2 | C | 3300 | NAI | C5D-C4D-C3D | 4.98 | 133.84 | 115.18 |
| 2 | D | 4300 | NAI | C5D-C4D-C3D | 4.92 | 133.60 | 115.18 |
| 2 | C | 3300 | NAI | O2A-PA-O1A | -4.82 | 88.42 | 112.24 |
| 2 | B | 2300 | NAI | O2A-PA-O1A | -4.82 | 88.42 | 112.24 |
| 2 | D | 4300 | NAI | O2A-PA-O1A | -4.82 | 88.43 | 112.24 |
| 2 | A | 1300 | NAI | O2A-PA-O1A | -4.82 | 88.43 | 112.24 |
| 2 | A | 1300 | NAI | O5B-PA-O1A | -4.69 | 90.75 | 109.07 |
| 2 | C | 3300 | NAI | O5D-C5D-C4D | -4.68 | 92.90 | 108.99 |
| 2 | B | 2300 | NAI | C5D-C4D-C3D | 4.62 | 132.49 | 115.18 |
| 2 | D | 4300 | NAI | O5B-PA-O1A | -4.47 | 91.61 | 109.07 |
| 2 | C | 3300 | NAI | O5B-PA-O1A | -4.46 | 91.63 | 109.07 |
| 2 | B | 2300 | NAI | O5B-PA-O1A | -4.46 | 91.63 | 109.07 |
| 2 | A | 1300 | NAI | O1N-PN-O2N | -4.41 | 90.44 | 112.24 |
| 2 | E | 5300 | NAI | C5B-C4B-C3B | -4.40 | 98.70 | 115.18 |
| 2 | A | 1300 | NAI | O4D-C4D-C5D | 4.31 | 123.57 | 109.37 |
| 2 | A | 1300 | NAI | C3B-C2B-C1B | 4.26 | 107.39 | 100.98 |
| 2 | B | 2300 | NAI | O4B-C4B-C5B | -4.20 | 95.55 | 109.37 |
| 2 | D | 4300 | NAI | O4B-C4B-C5B | -4.20 | 95.57 | 109.37 |
| 2 | C | 3300 | NAI | O4B-C4B-C5B | -4.19 | 95.58 | 109.37 |
| 2 | B | 2300 | NAI | O5D-C5D-C4D | -4.14 | 94.75 | 108.99 |
| 2 | C | 3300 | NAI | O1N-PN-O5D | 4.13 | 126.93 | 107.75 |
| 2 | D | 4300 | NAI | O1N-PN-O5D | 4.12 | 126.90 | 107.75 |
| 2 | B | 2300 | NAI | O1N-PN-O5D | 4.12 | 126.90 | 107.75 |
| 2 | E | 5300 | NAI | O7N-C7N-N7N | -3.88 | 113.81 | 122.88 |
| 2 | A | 1300 | NAI | C1D-N1N-C2N | -3.80 | 114.79 | 121.11 |
| 2 | A | 1300 | NAI | PA-O5B-C5B | -3.66 | 100.20 | 121.68 |
| 2 | B | 2300 | NAI | O1N-PN-O2N | -3.61 | 94.41 | 112.24 |
| 2 | C | 3300 | NAI | O1N-PN-O2N | -3.61 | 94.41 | 112.24 |
| 2 | D | 4300 | NAI | O1N-PN-O2N | -3.60 | 94.47 | 112.24 |
| 2 | A | 1300 | NAI | O7N-C7N-C3N | 3.54 | 127.57 | 120.90 |
| 2 | A | 1300 | NAI | O5B-C5B-C4B | 3.48 | 120.96 | 108.99 |
| 2 | E | 5300 | NAI | C6A-N1A-C2A | 3.40 | 120.71 | 115.84 |
| 2 | E | 5300 | NAI | O2A-PA-O5B | -3.36 | 92.14 | 107.75 |
| 2 | A | 1300 | NAI | PN-O5D-C5D | 3.32 | 141.13 | 121.68 |
| 2 | E | 5300 | NAI | O4D-C4D-C3D | 3.20 | 111.44 | 105.11 |
| 2 | A | 1300 | NAI | C5D-C4D-C3D | 3.19 | 127.14 | 115.18 |
| 2 | A | 1300 | NAI | C5B-C4B-C3B | 2.98 | 126.35 | 115.18 |
| 2 | E | 5300 | NAI | O2A-PA-O1A | 2.94 | 126.79 | 112.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2 | C | 3300 | NAI | C3N-C2N-N1N | -2.90 | 118.95 | 123.10 |
| 2 | D | 4300 | NAI | C3N-C2N-N1N | -2.88 | 118.99 | 123.10 |
| 2 | B | 2300 | NAI | C3N-C2N-N1N | -2.87 | 119.00 | 123.10 |
| 2 | B | 2300 | NAI | O4D-C4D-C5D | 2.85 | 118.77 | 109.37 |
| 2 | E | 5300 | NAI | C3N-C2N-N1N | -2.85 | 119.03 | 123.10 |
| 2 | C | 3300 | NAI | C1D-N1N-C6N | -2.83 | 114.74 | 120.83 |
| 2 | B | 2300 | NAI | C1D-N1N-C6N | -2.82 | 114.75 | 120.83 |
| 2 | D | 4300 | NAI | C1D-N1N-C6N | -2.80 | 114.80 | 120.83 |
| 2 | A | 1300 | NAI | O1N-PN-O5D | -2.62 | 95.56 | 107.75 |
| 2 | E | 5300 | NAI | C3D-C2D-C1D | 2.55 | 106.28 | 101.43 |
| 2 | E | 5300 | NAI | O7N-C7N-C3N | 2.52 | 125.65 | 120.90 |
| 2 | D | 4300 | NAI | O4D-C4D-C5D | 2.49 | 117.58 | 109.37 |
| 2 | E | 5300 | NAI | O3D-C3D-C4D | -2.48 | 103.87 | 111.05 |
| 2 | E | 5300 | NAI | O5D-C5D-C4D | 2.47 | 117.50 | 108.99 |
| 2 | E | 5300 | NAI | O3D-C3D-C2D | 2.45 | 119.73 | 111.82 |
| 2 | C | 3300 | NAI | O4D-C4D-C5D | 2.44 | 117.41 | 109.37 |
| 2 | E | 5300 | NAI | O2D-C2D-C3D | -2.38 | 104.11 | 111.82 |
| 2 | E | 5300 | NAI | O2D-C2D-C1D | 2.38 | 117.97 | 110.02 |
| 2 | C | 3300 | NAI | C3B-C2B-C1B | 2.32 | 104.47 | 100.98 |
| 2 | E | 5300 | NAI | C3B-C2B-C1B | 2.32 | 104.47 | 100.98 |
| 2 | D | 4300 | NAI | C3B-C2B-C1B | 2.31 | 104.45 | 100.98 |
| 2 | B | 2300 | NAI | C3B-C2B-C1B | 2.30 | 104.44 | 100.98 |
| 2 | E | 5300 | NAI | C2D-C3D-C4D | 2.04 | 106.60 | 102.64 |
| 2 | A | 1300 | NAI | O4B-C4B-C5B | -2.01 | 102.76 | 109.37 |

All (8) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 2 | A | 1300 | NAI | C1D |
| 2 | A | 1300 | NAI | C4D |
| 2 | D | 4300 | NAI | C4D |
| 2 | E | 5300 | NAI | C1D |
| 2 | E | 5300 | NAI | C4D |
| 2 | E | 5300 | NAI | C1B |
| 2 | B | 2300 | NAI | C4D |
| 2 | C | 3300 | NAI | C4D |

All (61) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|----------------|
| 2 | A | 1300 | NAI | C5B-O5B-PA-O2A |
| 2 | A | 1300 | NAI | C5B-O5B-PA-O3 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 2 | A | 1300 | NAI | O4B-C4B-C5B-O5B |
| 2 | A | 1300 | NAI | C3B-C4B-C5B-O5B |
| 2 | A | 1300 | NAI | C5D-O5D-PN-O3 |
| 2 | A | 1300 | NAI | C5D-O5D-PN-O1N |
| 2 | A | 1300 | NAI | C4D-C5D-O5D-PN |
| 2 | A | 1300 | NAI | C3D-C4D-C5D-O5D |
| 2 | A | 1300 | NAI | C2D-C1D-N1N-C2N |
| 2 | D | 4300 | NAI | C5B-O5B-PA-O1A |
| 2 | D | 4300 | NAI | C5B-O5B-PA-O2A |
| 2 | D | 4300 | NAI | C4B-C5B-O5B-PA |
| 2 | D | 4300 | NAI | C5D-O5D-PN-O3 |
| 2 | D | 4300 | NAI | C5D-O5D-PN-O1N |
| 2 | D | 4300 | NAI | C5D-O5D-PN-O2N |
| 2 | D | 4300 | NAI | C4D-C5D-O5D-PN |
| 2 | D | 4300 | NAI | C3D-C4D-C5D-O5D |
| 2 | E | 5300 | NAI | C4B-C5B-O5B-PA |
| 2 | B | 2300 | NAI | C5B-O5B-PA-O1A |
| 2 | B | 2300 | NAI | C5B-O5B-PA-O2A |
| 2 | B | 2300 | NAI | C4B-C5B-O5B-PA |
| 2 | B | 2300 | NAI | C5D-O5D-PN-O3 |
| 2 | B | 2300 | NAI | C5D-O5D-PN-O1N |
| 2 | B | 2300 | NAI | C5D-O5D-PN-O2N |
| 2 | B | 2300 | NAI | C4D-C5D-O5D-PN |
| 2 | B | 2300 | NAI | C3D-C4D-C5D-O5D |
| 2 | C | 3300 | NAI | C5B-O5B-PA-O1A |
| 2 | C | 3300 | NAI | C5B-O5B-PA-O2A |
| 2 | C | 3300 | NAI | C4B-C5B-O5B-PA |
| 2 | C | 3300 | NAI | C5D-O5D-PN-O3 |
| 2 | C | 3300 | NAI | C5D-O5D-PN-O1N |
| 2 | C | 3300 | NAI | C5D-O5D-PN-O2N |
| 2 | C | 3300 | NAI | C4D-C5D-O5D-PN |
| 2 | C | 3300 | NAI | C3D-C4D-C5D-O5D |
| 2 | A | 1300 | NAI | O4D-C1D-N1N-C2N |
| 2 | D | 4300 | NAI | O4D-C1D-N1N-C2N |
| 2 | B | 2300 | NAI | O4D-C1D-N1N-C2N |
| 2 | C | 3300 | NAI | O4D-C1D-N1N-C2N |
| 2 | A | 1300 | NAI | C2D-C1D-N1N-C6N |
| 2 | E | 5300 | NAI | C2D-C1D-N1N-C6N |
| 2 | E | 5300 | NAI | O4B-C4B-C5B-O5B |
| 2 | E | 5300 | NAI | C3D-C4D-C5D-O5D |
| 2 | E | 5300 | NAI | C4D-C5D-O5D-PN |
| 2 | D | 4300 | NAI | O4B-C4B-C5B-O5B |

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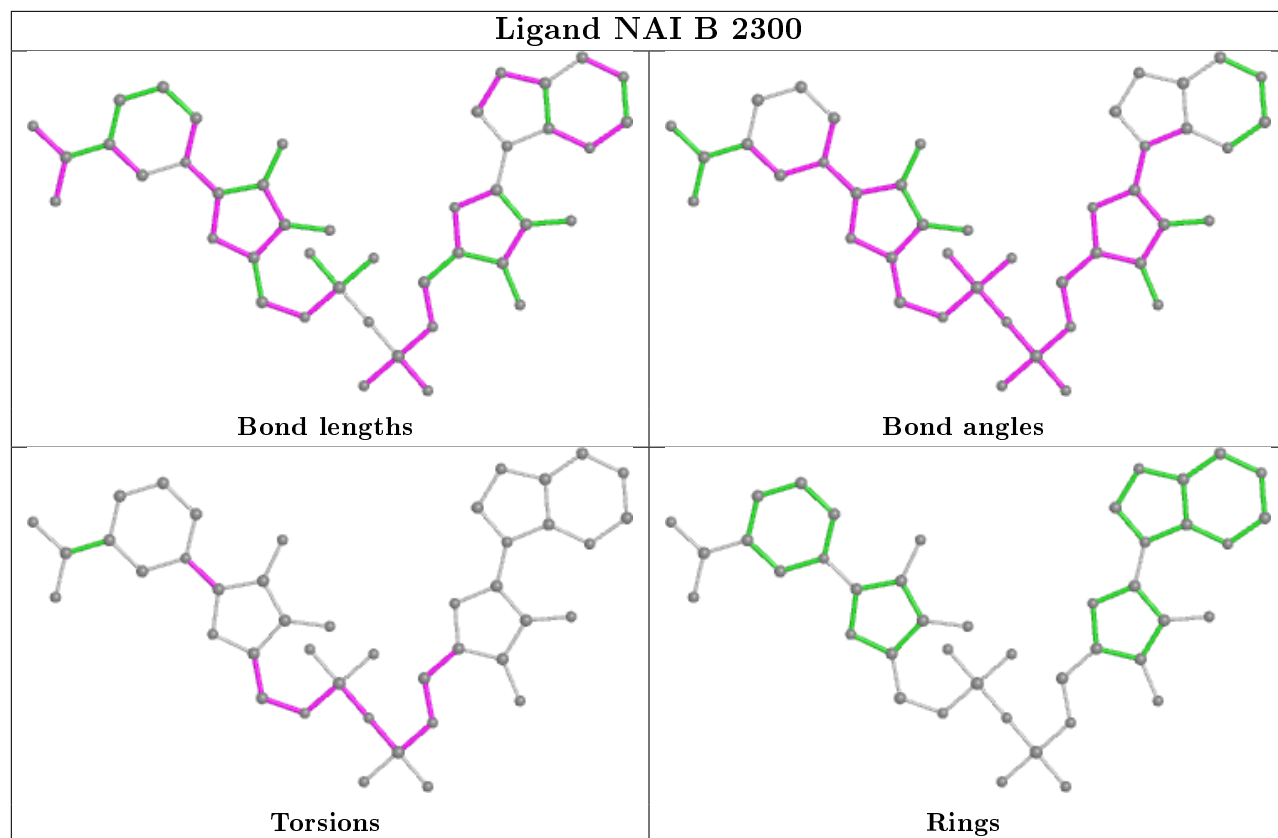
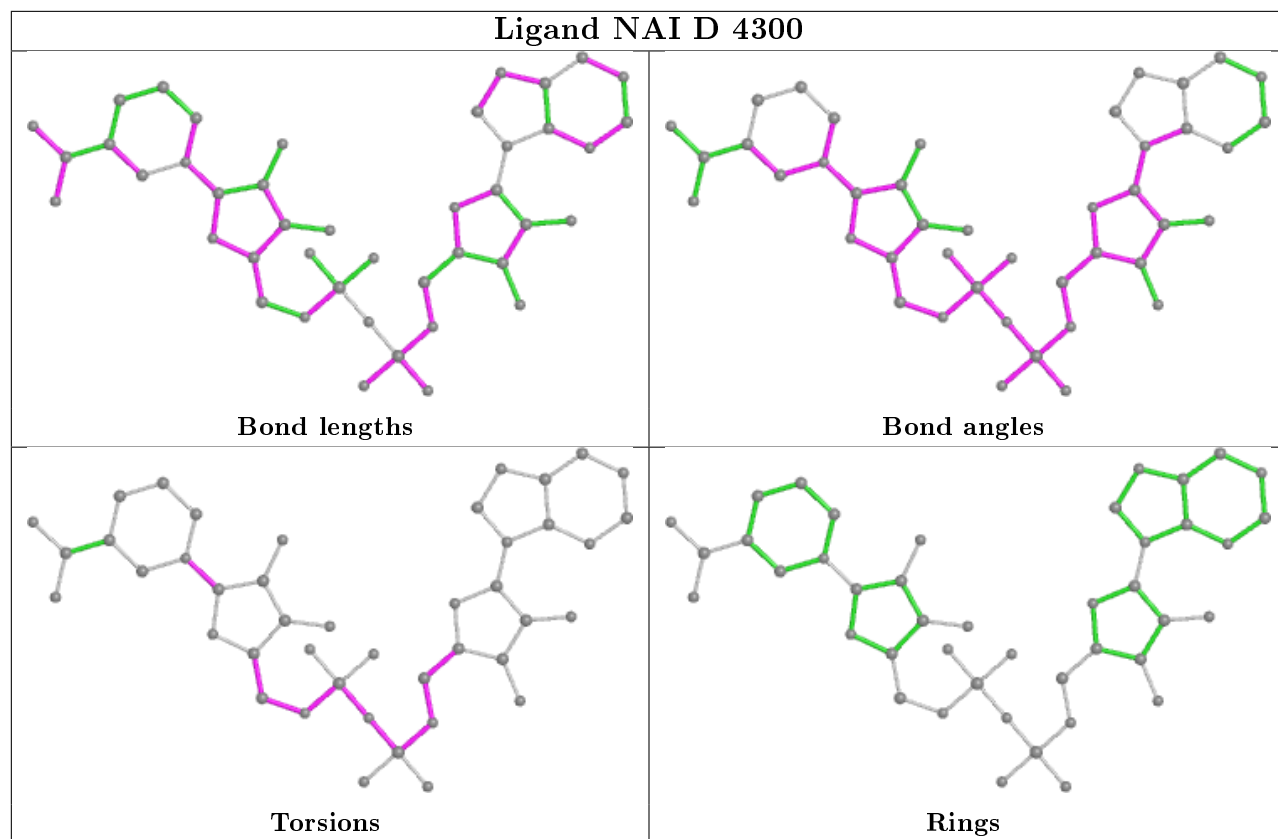
| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 2 | E | 5300 | NAI | O4D-C4D-C5D-O5D |
| 2 | B | 2300 | NAI | O4B-C4B-C5B-O5B |
| 2 | C | 3300 | NAI | O4B-C4B-C5B-O5B |
| 2 | E | 5300 | NAI | O4D-C1D-N1N-C2N |
| 2 | A | 1300 | NAI | C4B-C5B-O5B-PA |
| 2 | D | 4300 | NAI | PN-O3-PA-O2A |
| 2 | B | 2300 | NAI | PN-O3-PA-O2A |
| 2 | C | 3300 | NAI | PN-O3-PA-O2A |
| 2 | A | 1300 | NAI | C5B-O5B-PA-O1A |
| 2 | E | 5300 | NAI | C5B-O5B-PA-O1A |
| 2 | E | 5300 | NAI | PA-O3-PN-O1N |
| 2 | E | 5300 | NAI | C5B-O5B-PA-O3 |
| 2 | E | 5300 | NAI | C3B-C4B-C5B-O5B |
| 2 | D | 4300 | NAI | PA-O3-PN-O1N |
| 2 | B | 2300 | NAI | PA-O3-PN-O1N |
| 2 | C | 3300 | NAI | PA-O3-PN-O1N |
| 2 | A | 1300 | NAI | C5D-O5D-PN-O2N |

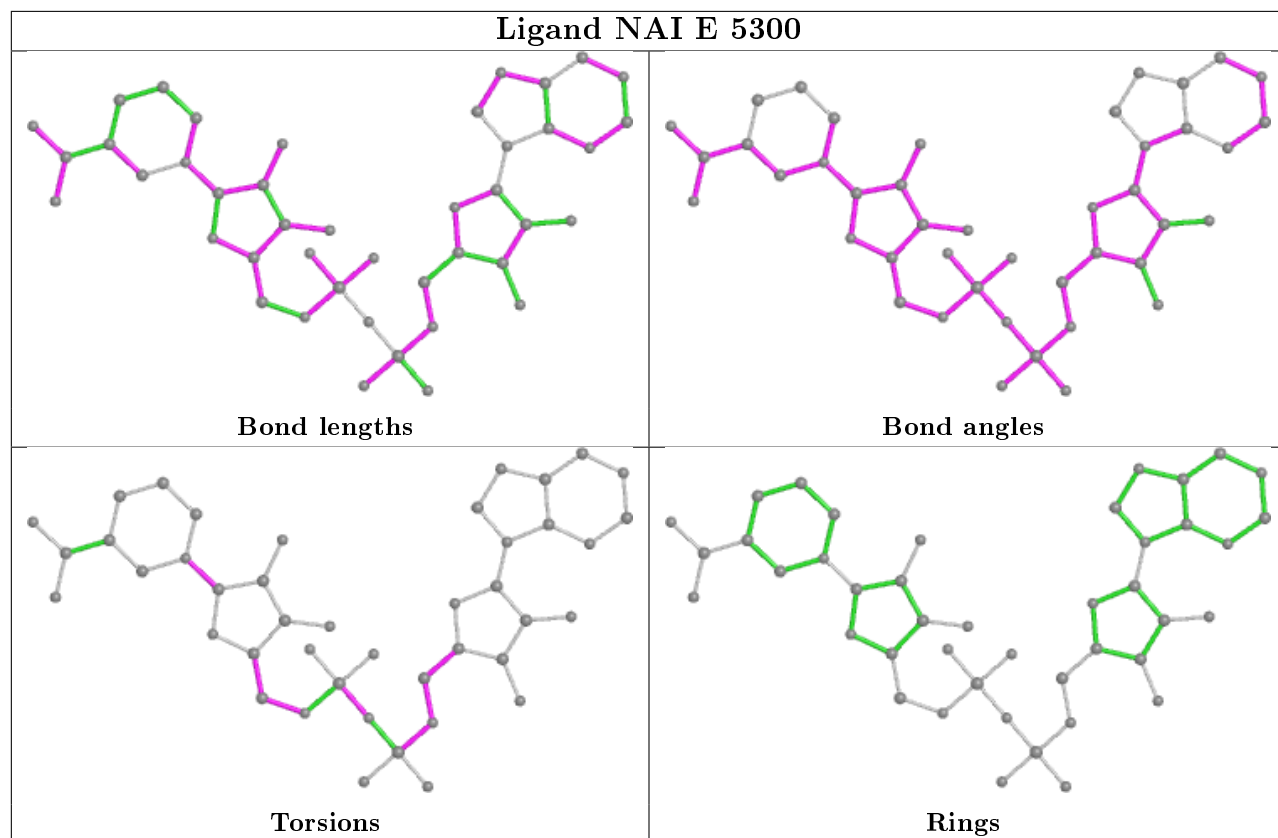
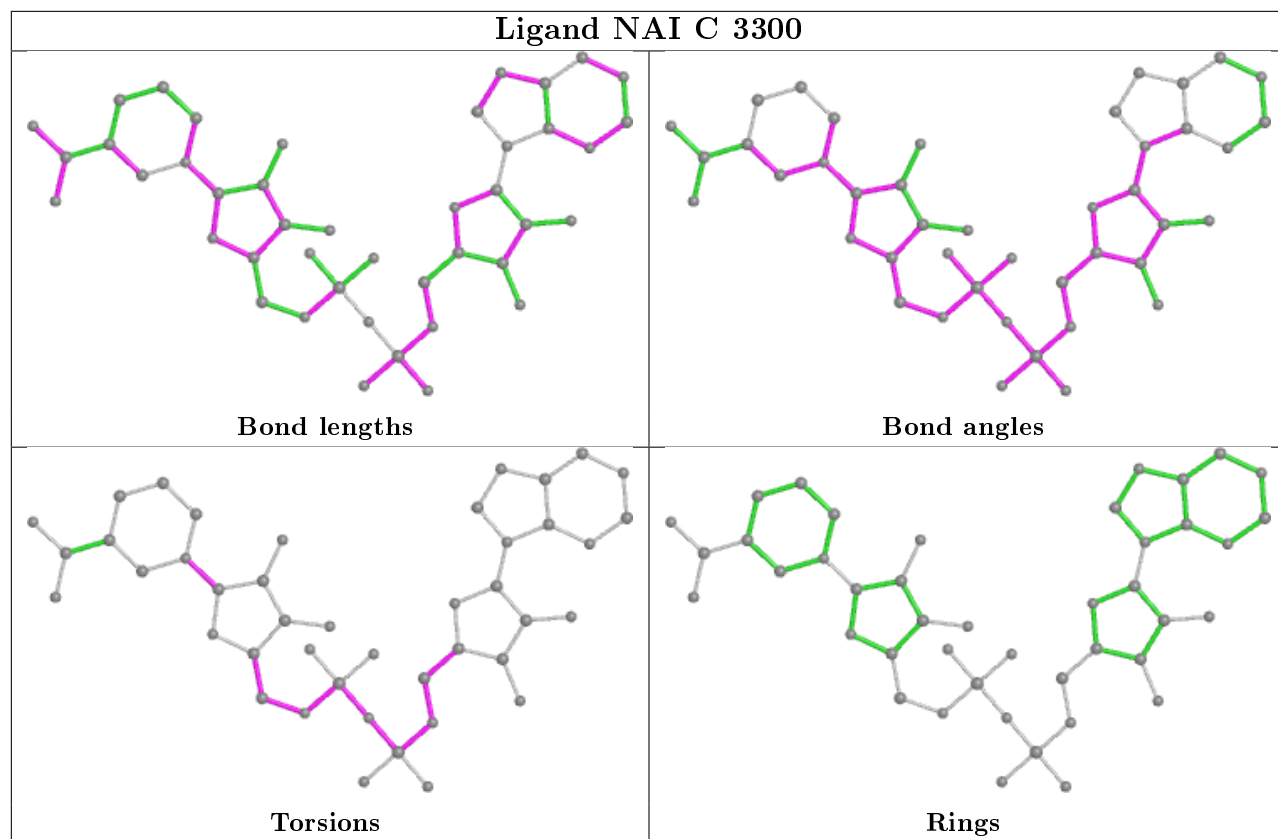
There are no ring outliers.

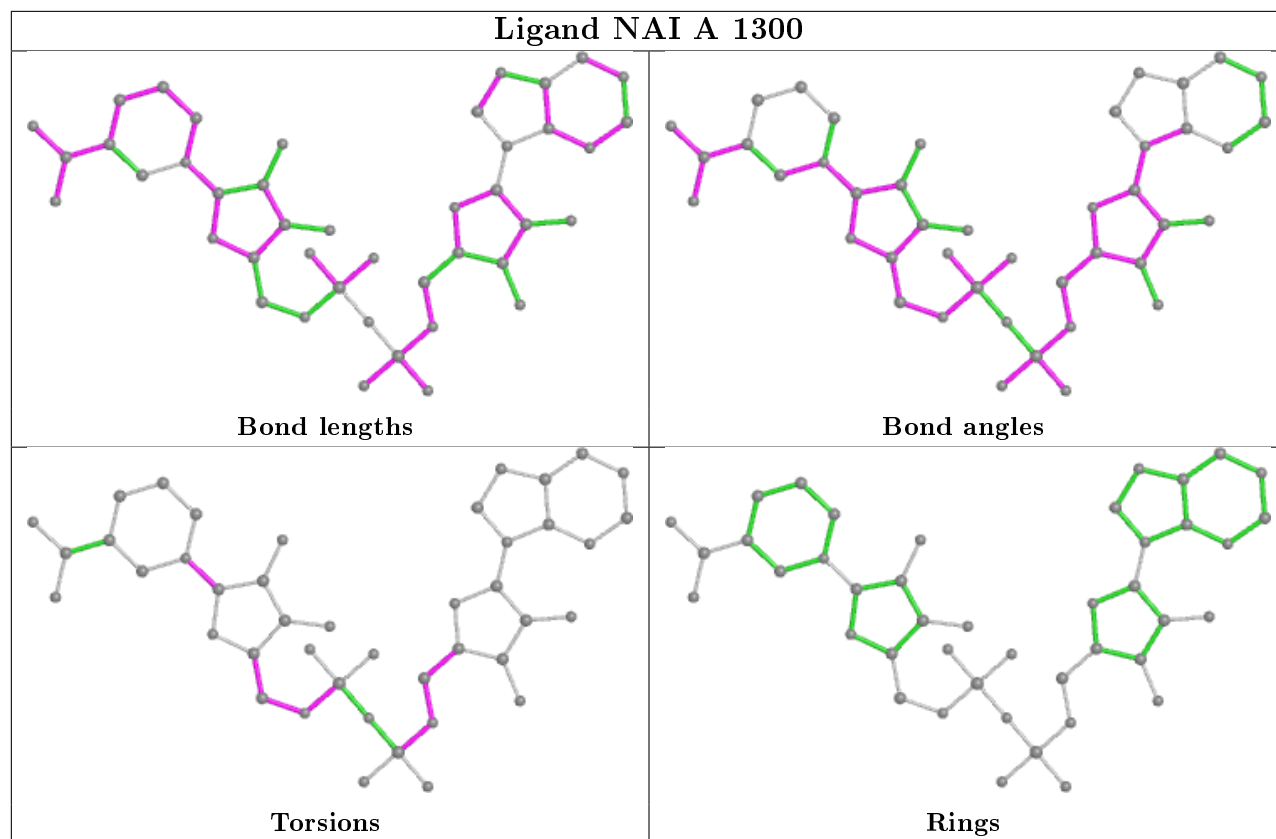
5 monomers are involved in 214 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2 | D | 4300 | NAI | 40 | 0 |
| 2 | B | 2300 | NAI | 67 | 5 |
| 2 | C | 3300 | NAI | 39 | 4 |
| 2 | E | 5300 | NAI | 32 | 1 |
| 2 | A | 1300 | NAI | 26 | 0 |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ > 2 | OWAB(Å ²) | Q < 0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|---------|
| 1 | A | 277/277 (100%) | -0.36 | 1 (0%) 92 84 | 32, 82, 117, 153 | 0 |
| 1 | B | 276/277 (99%) | 0.11 | 23 (8%) 11 4 | 39, 129, 183, 200 | 0 |
| 1 | C | 277/277 (100%) | 0.12 | 20 (7%) 15 6 | 31, 125, 181, 195 | 0 |
| 1 | D | 277/277 (100%) | -0.43 | 2 (0%) 87 75 | 34, 76, 118, 191 | 0 |
| 1 | E | 277/277 (100%) | -0.40 | 5 (1%) 68 47 | 24, 80, 128, 142 | 0 |
| All | All | 1384/1385 (99%) | -0.19 | 51 (3%) 41 21 | 24, 87, 168, 200 | 0 |

All (51) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | D | 275 | GLU | 4.8 |
| 1 | C | 95 | CYS | 4.7 |
| 1 | C | 36 | ASP | 4.7 |
| 1 | C | 32 | ALA | 4.6 |
| 1 | C | 274 | GLN | 3.7 |
| 1 | B | 52 | LEU | 3.6 |
| 1 | C | 275 | GLU | 3.6 |
| 1 | B | 93 | VAL | 3.6 |
| 1 | B | 38 | ASP | 3.5 |
| 1 | B | 24 | VAL | 3.5 |
| 1 | C | 94 | SER | 3.4 |
| 1 | B | 39 | LEU | 3.3 |
| 1 | B | 36 | ASP | 3.3 |
| 1 | C | 39 | LEU | 3.2 |
| 1 | B | 62 | HIS | 3.0 |
| 1 | B | 41 | THR | 3.0 |
| 1 | C | 93 | VAL | 2.8 |
| 1 | E | 39 | LEU | 2.7 |
| 1 | C | 96 | ALA | 2.7 |
| 1 | C | 64 | ASP | 2.6 |

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Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | C | 66 | LEU | 2.6 |
| 1 | C | 54 | PRO | 2.6 |
| 1 | C | 146 | GLY | 2.6 |
| 1 | B | 136 | ALA | 2.5 |
| 1 | B | 47 | LYS | 2.5 |
| 1 | E | 272 | ALA | 2.5 |
| 1 | B | 67 | PHE | 2.4 |
| 1 | C | 25 | LEU | 2.4 |
| 1 | B | 35 | PRO | 2.4 |
| 1 | B | 34 | SER | 2.4 |
| 1 | C | 47 | LYS | 2.4 |
| 1 | A | 275 | GLU | 2.4 |
| 1 | E | 73 | HIS | 2.4 |
| 1 | B | 116 | ARG | 2.3 |
| 1 | B | 28 | HIS | 2.3 |
| 1 | C | 52 | LEU | 2.3 |
| 1 | B | 80 | ASP | 2.3 |
| 1 | C | 143 | VAL | 2.3 |
| 1 | C | 138 | GLY | 2.3 |
| 1 | E | 95 | CYS | 2.2 |
| 1 | E | 143 | VAL | 2.2 |
| 1 | B | 43 | SER | 2.2 |
| 1 | B | 55 | HIS | 2.1 |
| 1 | B | 122 | THR | 2.1 |
| 1 | C | 78 | ILE | 2.1 |
| 1 | C | 145 | ASP | 2.1 |
| 1 | B | 113 | PRO | 2.1 |
| 1 | B | 95 | CYS | 2.1 |
| 1 | D | 274 | GLN | 2.0 |
| 1 | B | 76 | PRO | 2.0 |
| 1 | B | 274 | GLN | 2.0 |

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

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

6.3 Carbohydrates ⓘ

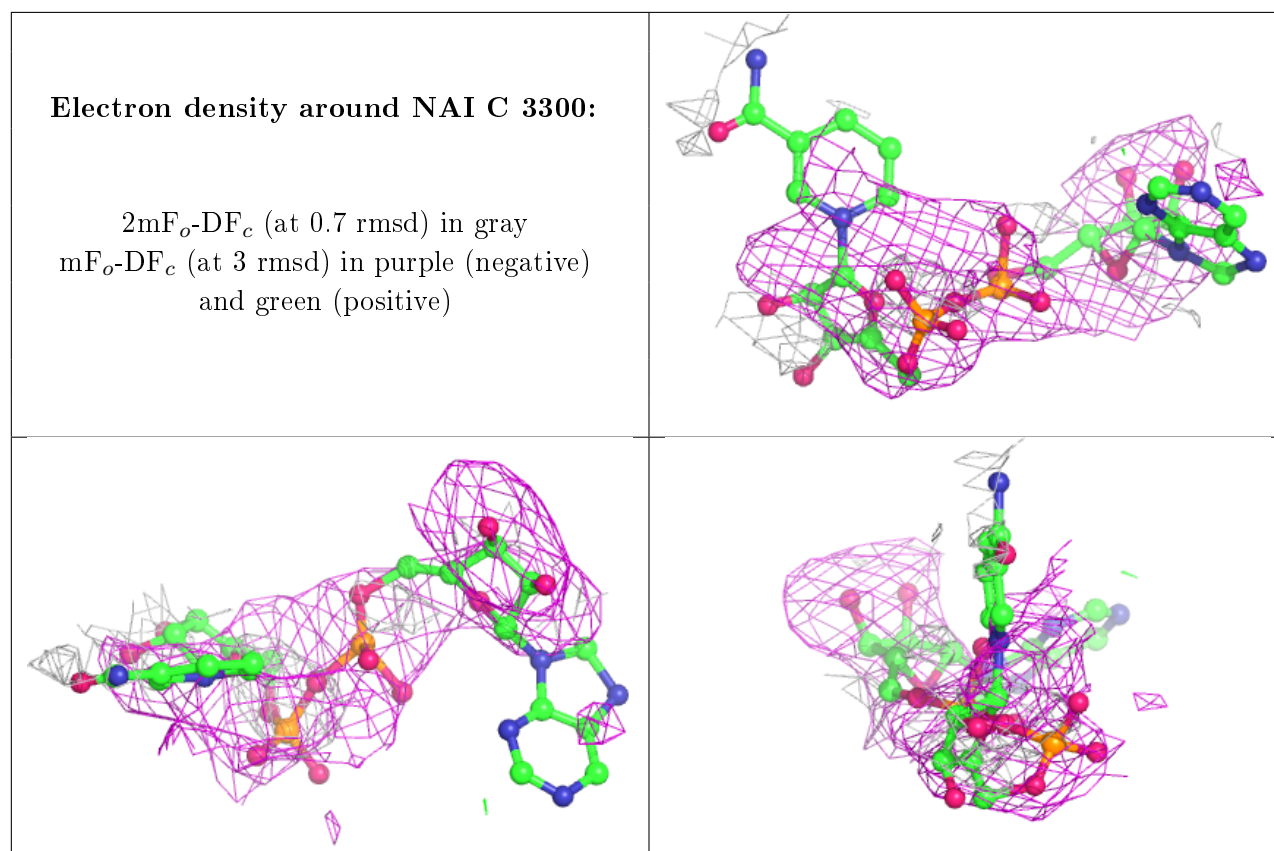
There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

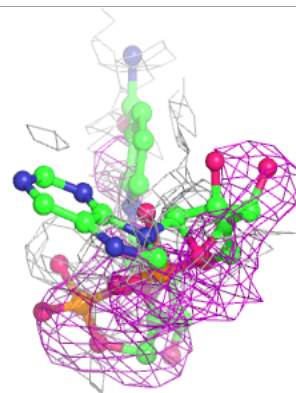
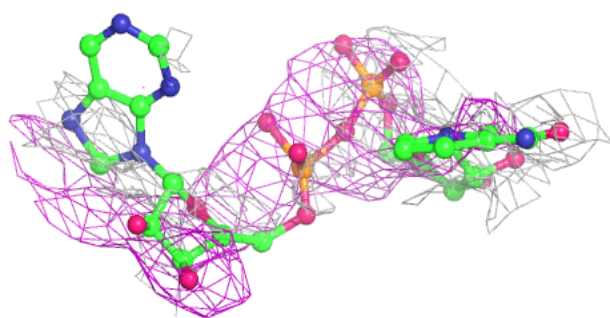
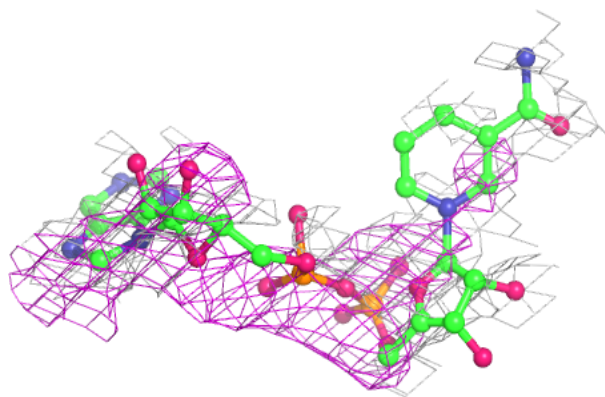
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 3 | GLU | C | 3301 | 10/10 | 0.09 | 1.45 | 200,200,200,200 | 0 |
| 3 | GLU | B | 2301 | 10/10 | 0.41 | 0.87 | 192,200,200,200 | 0 |
| 2 | NAI | C | 3300 | 43/44 | 0.54 | 0.97 | 189,195,195,195 | 0 |
| 3 | GLU | D | 4301 | 10/10 | 0.58 | 0.73 | 182,193,196,198 | 0 |
| 3 | GLU | A | 1301 | 10/10 | 0.64 | 0.61 | 120,131,140,140 | 0 |
| 2 | NAI | B | 2300 | 43/44 | 0.66 | 0.73 | 192,195,195,195 | 0 |
| 2 | NAI | D | 4300 | 43/44 | 0.74 | 0.65 | 81,91,95,95 | 0 |
| 3 | GLU | E | 5301 | 10/10 | 0.78 | 0.56 | 195,200,200,200 | 0 |
| 2 | NAI | A | 1300 | 43/44 | 0.78 | 0.57 | 63,93,95,95 | 0 |
| 2 | NAI | E | 5300 | 43/44 | 0.80 | 0.54 | 69,94,95,95 | 0 |

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

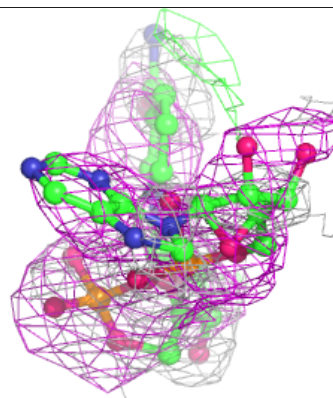
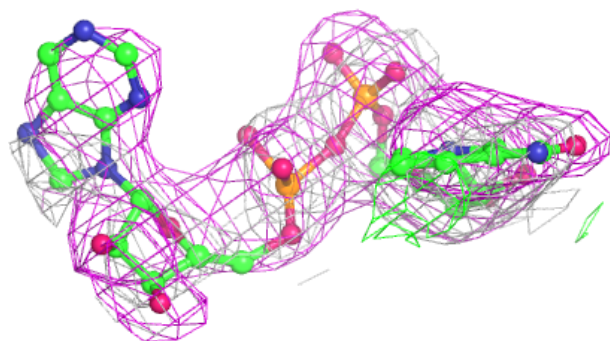
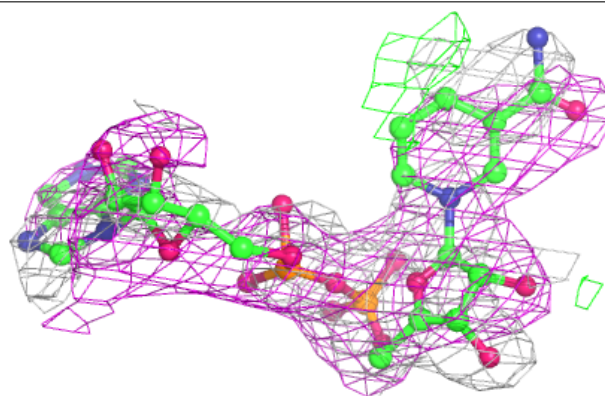


Electron density around NAI B 2300:

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

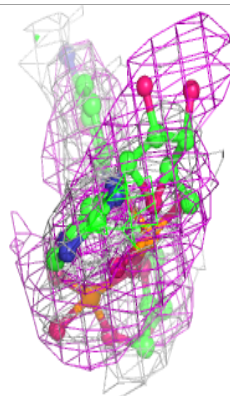
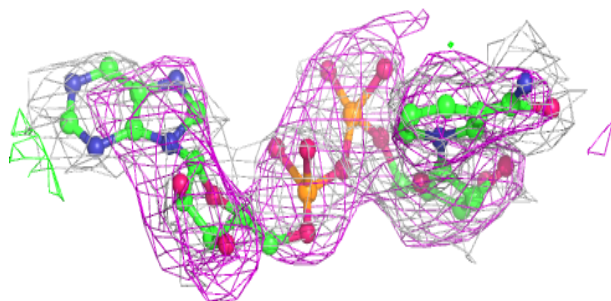
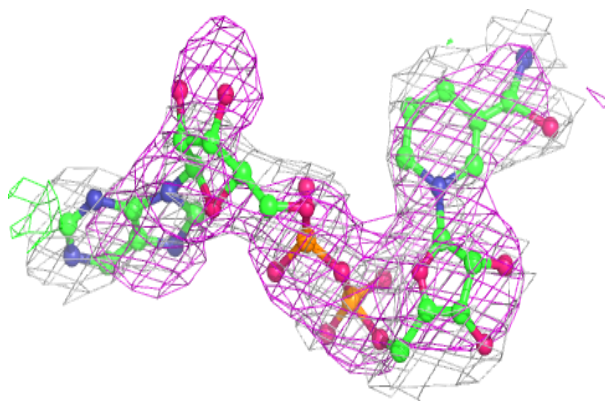
**Electron density around NAI D 4300:**

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

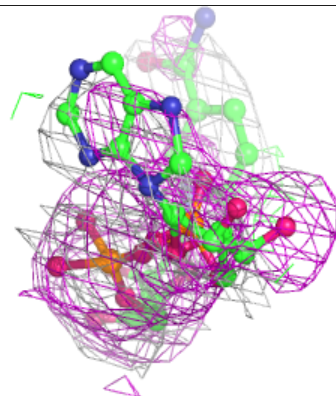
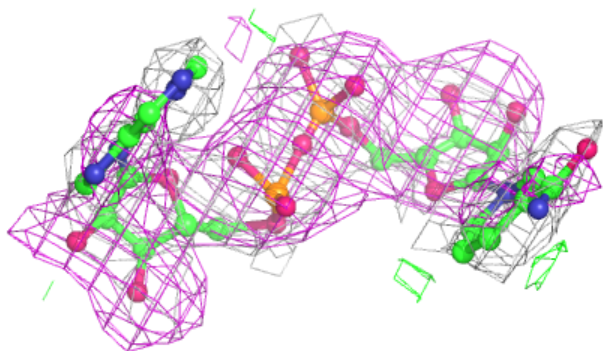
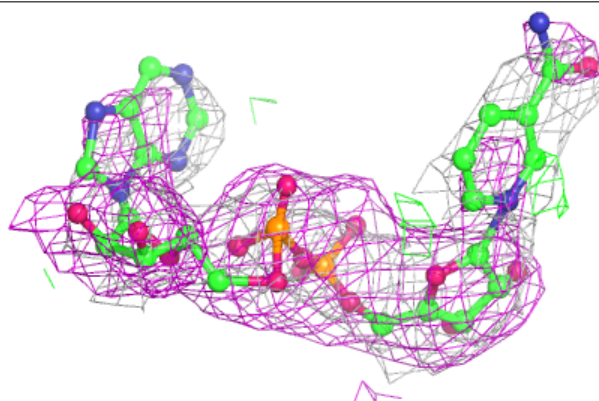


Electron density around NAI A 1300:

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

**Electron density around NAI E 5300:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.