



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 01:46 pm BST

PDB ID : 1H6V
Title : Mammalian thioredoxin reductase
Authors : Sandalova, T.; Zhong, L.; Lindqvist, Y.; Holmgren, A.; Schneider, G.
Deposited on : 2001-06-27
Resolution : 3.00 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 : 2.11
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) : 2.11

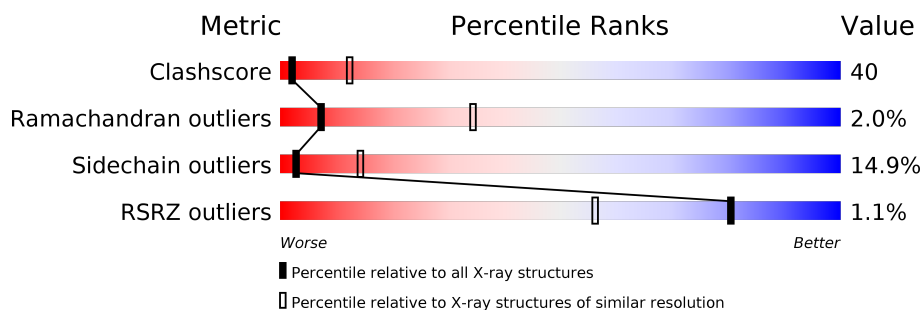
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore | 141614 | 2416 (3.00-3.00) |
| Ramachandran outliers | 138981 | 2333 (3.00-3.00) |
| Sidechain outliers | 138945 | 2336 (3.00-3.00) |
| RSRZ outliers | 127900 | 1990 (3.00-3.00) |

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 | 499 | |
| 1 | B | 499 | |
| 1 | C | 499 | |
| 1 | D | 499 | |
| 1 | E | 499 | |
| 1 | F | 499 | |

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23075 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 THIOREDOXIN REDUCTASE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 490 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3764 | 2391 | 635 | 716 | 22 | | | |
| 1 | B | 487 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3753 | 2387 | 633 | 713 | 20 | | | |
| 1 | C | 482 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3707 | 2356 | 627 | 704 | 20 | | | |
| 1 | D | 487 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3753 | 2387 | 633 | 713 | 20 | | | |
| 1 | E | 491 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3773 | 2397 | 637 | 717 | 22 | | | |
| 1 | F | 490 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3764 | 2391 | 635 | 716 | 22 | | | |

There are 11 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| A | 52 | ASN | ARG | conflict | UNP O89049 |
| B | 52 | ASN | ARG | conflict | UNP O89049 |
| C | 52 | ASN | ARG | conflict | UNP O89049 |
| D | 52 | ASN | ARG | conflict | UNP O89049 |
| E | 52 | ASN | ARG | conflict | UNP O89049 |
| F | 52 | ASN | ARG | conflict | UNP O89049 |
| A | 497 | CYS | SEL | engineered mutation | UNP O89049 |
| B | 497 | CYS | SEL | engineered mutation | UNP O89049 |
| C | 497 | CYS | SEL | engineered mutation | UNP O89049 |
| D | 497 | CYS | SEL | engineered mutation | UNP O89049 |
| E | 497 | CYS | SEL | engineered mutation | UNP O89049 |

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



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

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|---------|
| 3 | A | 1 | Total 39 | C 15 | N 5 | O 16 | P 3 | 0 | 0 |
| 3 | B | 1 | Total 39 | C 15 | N 5 | O 16 | P 3 | 0 | 0 |
| 3 | C | 1 | Total 39 | C 15 | N 5 | O 16 | P 3 | 0 | 0 |
| 3 | D | 1 | Total 39 | C 15 | N 5 | O 16 | P 3 | 0 | 0 |
| 3 | E | 1 | Total 39 | C 15 | N 5 | O 16 | P 3 | 0 | 0 |
| 3 | F | 1 | Total 39 | C 15 | N 5 | O 16 | P 3 | 0 | 0 |

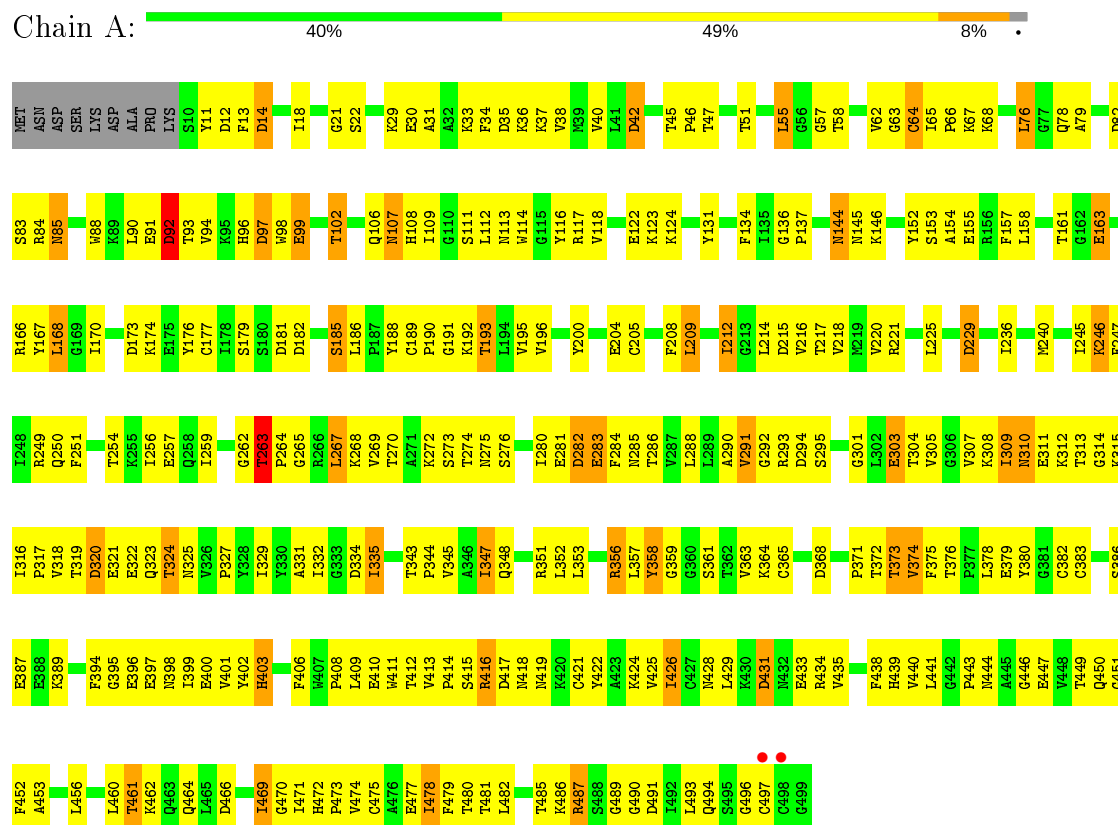
- Molecule 4 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 4 | A | 1 | Total O 1 1 | 0 | 0 |
| 4 | B | 1 | Total O 1 1 | 0 | 0 |
| 4 | C | 3 | Total O 3 3 | 0 | 0 |
| 4 | D | 1 | Total O 1 1 | 0 | 0 |
| 4 | E | 2 | Total O 2 2 | 0 | 0 |
| 4 | F | 1 | Total O 1 1 | 0 | 0 |

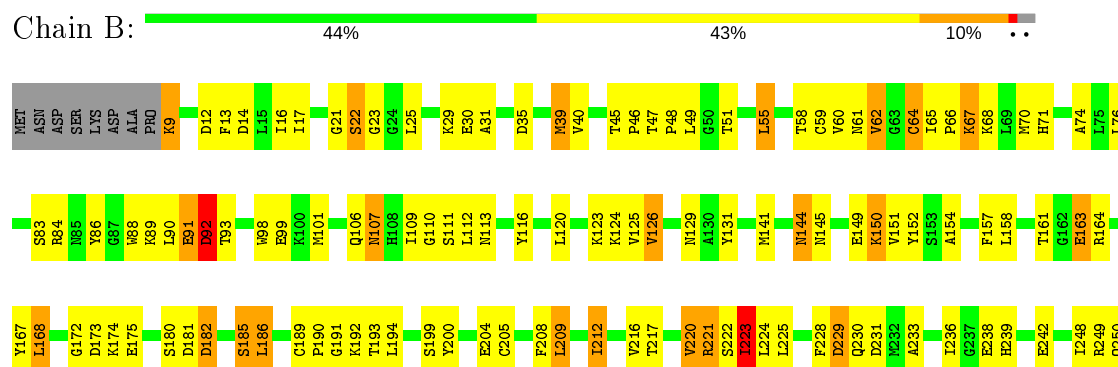
3 Residue-property plots

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

• Molecule 1: THIOREDOXIN REDUCTASE



• Molecule 1: THIOREDOXIN REDUCTASE





| | | | | | | |
|------|------|------|------|------|------|-----|
| I469 | V391 | K345 | E242 | L168 | D82 | MET |
| G470 | E392 | V318 | K246 | G169 | S83 | ASN |
| I471 | | T319 | | I170 | R84 | ASP |
| H472 | G395 | D320 | R349 | P471 | | SER |
| P473 | E396 | E321 | Q250 | G172 | K89 | LYS |
| V474 | | E322 | Q251 | D173 | L90 | ASP |
| C475 | E400 | Q323 | V252 | K174 | E91 | ALA |
| A476 | | Q324 | V253 | E175 | D92 | PRO |
| I477 | H403 | T324 | P253 | | T93 | LYS |
| E478 | S404 | N325 | T254 | I178 | V94 | S10 |
| F479 | F405 | | K255 | S179 | G95 | Y11 |
| T480 | F406 | | I256 | S180 | H96 | D12 |
| | | I329 | E257 | D181 | D97 | F13 |
| K486 | W411 | A331 | Q258 | D182 | E99 | D14 |
| R487 | T412 | I332 | | | | L15 |
| S488 | V413 | D334 | A261 | S185 | K100 | |
| G489 | P414 | I335 | G262 | L186 | M101 | G20 |
| A490 | S415 | I336 | T263 | P187 | T102 | G21 |
| D491 | R416 | | P264 | I188 | E103 | S22 |
| I492 | D417 | K339 | G265 | C189 | S104 | |
| L493 | N418 | R266 | R266 | P190 | V105 | K29 |
| Q494 | N419 | L340 | L267 | G191 | Q106 | E39 |
| S495 | K420 | | | K192 | N107 | A31 |
| G496 | C421 | T343 | T270 | T193 | H108 | A32 |
| C497 | Y422 | P344 | | L194 | I109 | K33 |
| C498 | K423 | I347 | S273 | V195 | G110 | F34 |
| G499 | A424 | Q348 | T274 | V196 | L112 | D85 |
| | V425 | | N275 | | N113 | |
| | I426 | | S276 | L203 | | V38 |
| | C427 | R351 | E277 | | | K39 |
| | N428 | L352 | | F208 | Y116 | V40 |
| | | L353 | I280 | L209 | | L41 |
| | D431 | A354 | E281 | | K123 | D42 |
| | | Q355 | D282 | I212 | K124 | |
| | R434 | R356 | E283 | G213 | | T47 |
| | V435 | | F284 | L214 | Y131 | P48 |
| | V436 | S361 | N285 | T217 | | L49 |
| | G437 | T362 | T286 | | P137 | |
| | F438 | V363 | V287 | H138 | | L55 |
| | H439 | K364 | L288 | K139 | G139 | G56 |
| | V440 | C365 | L289 | R221 | T140 | G57 |
| | L441 | | A290 | S222 | M141 | T58 |
| | G442 | D368 | V291 | I223 | A142 | C59 |
| | | N369 | G292 | L224 | N144 | |
| | G446 | V370 | R293 | T143 | | V62 |
| | E447 | P371 | D294 | L225 | | G63 |
| | V448 | T372 | S295 | | | C64 |
| | T449 | T373 | C296 | F228 | K150 | |
| | Q450 | V374 | T297 | D229 | Y151 | G63 |
| | | F375 | | Q230 | S153 | C64 |
| | | | | D231 | A154 | |
| | K457 | L302 | | N232 | | P66 |
| | C458 | L378 | E303 | L233 | | K67 |
| | | F379 | T304 | A233 | | K68 |
| | T461 | X380 | V305 | N234 | L158 | L69 |
| | K462 | G381 | | K235 | I159 | H70 |
| | Q463 | | | L236 | | H71 |
| | Q464 | | K308 | G237 | G162 | Q72 |
| | L465 | E387 | I309 | E238 | E163 | |
| | D466 | K389 | | H239 | | L76 |
| | | I390 | | N240 | | |
| | | | T313 | E240 | R166 | |
| | | | C314 | E241 | Y165 | V31 |

4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 78.92Å 140.46Å 170.83Å 90.00° 94.64° 90.00° | Depositor |
| Resolution (Å) | 30.00 – 3.00 29.86 – 2.99 | Depositor EDS |
| % Data completeness (in resolution range) | 92.4 (30.00-3.00) 92.5 (29.86-2.99) | Depositor EDS |
| R_{merge} | 0.10 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.35 (at 3.00Å) | Xtriage |
| Refinement program | REFMAC | Depositor |
| R, R_{free} | 0.224 , 0.263 0.257 , (Not available) | Depositor DCC |
| R_{free} test set | No test flags present. | wwPDB-VP |
| Wilson B-factor (Å ²) | 61.1 | Xtriage |
| Anisotropy | 0.096 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.27 , 4.8 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.89 | EDS |
| Total number of atoms | 23075 | wwPDB-VP |
| Average B, all atoms (Å ²) | 14.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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

5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|-----------------|
| | | RMSZ | # $ Z > 5$ | RMSZ | # $ Z > 5$ |
| 1 | A | 0.92 | 0/3838 | 1.07 | 15/5193 (0.3%) |
| 1 | B | 0.90 | 0/3827 | 1.04 | 14/5178 (0.3%) |
| 1 | C | 0.82 | 1/3779 (0.0%) | 1.03 | 15/5114 (0.3%) |
| 1 | D | 0.97 | 3/3827 (0.1%) | 1.08 | 16/5178 (0.3%) |
| 1 | E | 0.99 | 2/3847 (0.1%) | 1.11 | 16/5204 (0.3%) |
| 1 | F | 0.80 | 0/3838 | 1.03 | 14/5193 (0.3%) |
| All | All | 0.90 | 6/22956 (0.0%) | 1.06 | 90/31060 (0.3%) |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | E | 489 | GLY | C-O | -6.05 | 1.14 | 1.23 |
| 1 | D | 410 | GLU | CD-OE1 | 5.80 | 1.32 | 1.25 |
| 1 | D | 114 | TRP | CB-CG | -5.08 | 1.41 | 1.50 |
| 1 | C | 300 | ILE | C-O | -5.07 | 1.13 | 1.23 |
| 1 | D | 88 | TRP | CB-CG | -5.03 | 1.41 | 1.50 |
| 1 | E | 116 | TYR | CG-CD2 | -5.01 | 1.32 | 1.39 |

All (90) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 1 | C | 82 | ASP | CB-CG-OD2 | 9.47 | 126.82 | 118.30 |
| 1 | F | 229 | ASP | CB-CG-OD2 | 9.21 | 126.59 | 118.30 |
| 1 | F | 417 | ASP | CB-CG-OD2 | 8.16 | 125.65 | 118.30 |
| 1 | E | 282 | ASP | CB-CG-OD2 | 7.91 | 125.42 | 118.30 |
| 1 | F | 466 | ASP | CB-CG-OD2 | 7.83 | 125.35 | 118.30 |
| 1 | A | 368 | ASP | CB-CG-OD2 | 7.77 | 125.30 | 118.30 |
| 1 | E | 320 | ASP | CB-CG-OD2 | 7.54 | 125.08 | 118.30 |
| 1 | D | 35 | ASP | CB-CG-OD2 | 7.46 | 125.02 | 118.30 |
| 1 | E | 417 | ASP | CB-CG-OD2 | 7.45 | 125.00 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | D | 334 | ASP | CB-CG-OD2 | 7.34 | 124.91 | 118.30 |
| 1 | A | 417 | ASP | CB-CG-OD2 | 7.34 | 124.91 | 118.30 |
| 1 | F | 368 | ASP | CB-CG-OD2 | 7.17 | 124.75 | 118.30 |
| 1 | D | 182 | ASP | CB-CG-OD2 | 7.03 | 124.63 | 118.30 |
| 1 | D | 14 | ASP | CB-CG-OD2 | 7.02 | 124.62 | 118.30 |
| 1 | E | 173 | ASP | CB-CG-OD2 | 6.88 | 124.49 | 118.30 |
| 1 | B | 35 | ASP | CB-CG-OD2 | 6.86 | 124.47 | 118.30 |
| 1 | B | 417 | ASP | CB-CG-OD2 | 6.71 | 124.34 | 118.30 |
| 1 | A | 320 | ASP | CB-CG-OD2 | 6.65 | 124.28 | 118.30 |
| 1 | F | 495 | SER | C-N-CA | -6.64 | 108.35 | 122.30 |
| 1 | C | 42 | ASP | CB-CG-OD2 | 6.64 | 124.28 | 118.30 |
| 1 | C | 92 | ASP | CB-CG-OD2 | 6.55 | 124.19 | 118.30 |
| 1 | B | 282 | ASP | CB-CG-OD2 | 6.50 | 124.15 | 118.30 |
| 1 | B | 466 | ASP | CB-CG-OD2 | 6.45 | 124.11 | 118.30 |
| 1 | F | 35 | ASP | CB-CG-OD2 | 6.33 | 123.99 | 118.30 |
| 1 | E | 229 | ASP | CB-CG-OD2 | 6.31 | 123.97 | 118.30 |
| 1 | D | 215 | ASP | CB-CG-OD2 | 6.24 | 123.92 | 118.30 |
| 1 | C | 14 | ASP | CB-CG-OD2 | 6.20 | 123.88 | 118.30 |
| 1 | B | 223 | ILE | CG1-CB-CG2 | -6.19 | 97.78 | 111.40 |
| 1 | E | 181 | ASP | CB-CG-OD2 | 6.17 | 123.86 | 118.30 |
| 1 | F | 182 | ASP | CB-CG-OD2 | 6.14 | 123.83 | 118.30 |
| 1 | A | 92 | ASP | CB-CG-OD2 | 6.11 | 123.80 | 118.30 |
| 1 | D | 274 | THR | CB-CA-C | -6.10 | 95.12 | 111.60 |
| 1 | F | 371 | PRO | N-CD-CG | -6.09 | 94.06 | 103.20 |
| 1 | E | 293 | ARG | NE-CZ-NH2 | 6.04 | 123.32 | 120.30 |
| 1 | F | 496 | GLY | N-CA-C | 6.04 | 128.20 | 113.10 |
| 1 | F | 168 | LEU | CA-CB-CG | 6.04 | 129.19 | 115.30 |
| 1 | A | 97 | ASP | CB-CG-OD2 | 5.96 | 123.66 | 118.30 |
| 1 | A | 182 | ASP | CB-CG-OD2 | 5.93 | 123.63 | 118.30 |
| 1 | E | 431 | ASP | CB-CG-OD2 | 5.91 | 123.62 | 118.30 |
| 1 | E | 490 | GLY | N-CA-C | -5.88 | 98.39 | 113.10 |
| 1 | C | 294 | ASP | CB-CG-OD2 | 5.85 | 123.56 | 118.30 |
| 1 | D | 282 | ASP | CB-CG-OD2 | 5.85 | 123.56 | 118.30 |
| 1 | E | 97 | ASP | CB-CG-OD2 | 5.84 | 123.55 | 118.30 |
| 1 | B | 340 | LEU | CA-CB-CG | 5.83 | 128.71 | 115.30 |
| 1 | B | 489 | GLY | N-CA-C | 5.79 | 127.58 | 113.10 |
| 1 | D | 80 | LEU | CB-CG-CD1 | -5.75 | 101.23 | 111.00 |
| 1 | B | 182 | ASP | CB-CG-OD2 | 5.72 | 123.45 | 118.30 |
| 1 | D | 368 | ASP | CB-CG-OD2 | 5.67 | 123.40 | 118.30 |
| 1 | C | 229 | ASP | CB-CG-OD2 | 5.58 | 123.32 | 118.30 |
| 1 | E | 313 | THR | OG1-CB-CG2 | -5.58 | 97.16 | 110.00 |
| 1 | D | 273 | SER | N-CA-CB | 5.54 | 118.81 | 110.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 263 | THR | N-CA-C | -5.50 | 96.16 | 111.00 |
| 1 | C | 215 | ASP | CB-CG-OD2 | 5.47 | 123.22 | 118.30 |
| 1 | A | 42 | ASP | CB-CG-OD2 | 5.46 | 123.22 | 118.30 |
| 1 | A | 431 | ASP | CB-CG-OD2 | 5.44 | 123.20 | 118.30 |
| 1 | A | 181 | ASP | CB-CG-OD2 | 5.44 | 123.19 | 118.30 |
| 1 | F | 497 | CYS | N-CA-C | -5.43 | 96.35 | 111.00 |
| 1 | C | 181 | ASP | CB-CG-OD2 | 5.36 | 123.12 | 118.30 |
| 1 | D | 65 | ILE | CG1-CB-CG2 | -5.36 | 99.62 | 111.40 |
| 1 | C | 378 | LEU | CA-CB-CG | 5.35 | 127.60 | 115.30 |
| 1 | E | 488 | SER | CB-CA-C | -5.35 | 99.94 | 110.10 |
| 1 | A | 290 | ALA | CB-CA-C | 5.35 | 118.12 | 110.10 |
| 1 | D | 229 | ASP | CB-CG-OD2 | 5.33 | 123.09 | 118.30 |
| 1 | B | 126 | VAL | CB-CA-C | -5.32 | 101.29 | 111.40 |
| 1 | F | 92 | ASP | CB-CG-OD2 | 5.32 | 123.09 | 118.30 |
| 1 | B | 368 | ASP | CB-CG-OD2 | 5.29 | 123.06 | 118.30 |
| 1 | D | 320 | ASP | CB-CG-OD2 | 5.29 | 123.06 | 118.30 |
| 1 | E | 366 | ASP | CB-CG-OD2 | 5.28 | 123.05 | 118.30 |
| 1 | C | 18 | ILE | CG1-CB-CG2 | -5.25 | 99.85 | 111.40 |
| 1 | C | 466 | ASP | CB-CG-OD2 | 5.24 | 123.02 | 118.30 |
| 1 | B | 14 | ASP | CB-CG-OD2 | 5.23 | 123.01 | 118.30 |
| 1 | C | 320 | ASP | CB-CG-OD2 | 5.22 | 123.00 | 118.30 |
| 1 | E | 489 | GLY | N-CA-C | 5.21 | 126.13 | 113.10 |
| 1 | A | 215 | ASP | CB-CG-OD2 | 5.20 | 122.98 | 118.30 |
| 1 | D | 431 | ASP | CB-CG-OD2 | 5.18 | 122.96 | 118.30 |
| 1 | B | 12 | ASP | CB-CG-OD2 | 5.17 | 122.96 | 118.30 |
| 1 | F | 62 | VAL | CB-CA-C | -5.17 | 101.57 | 111.40 |
| 1 | A | 490 | GLY | N-CA-C | -5.14 | 100.24 | 113.10 |
| 1 | D | 293 | ARG | NE-CZ-NH2 | 5.14 | 122.87 | 120.30 |
| 1 | B | 224 | LEU | CB-CG-CD1 | -5.14 | 102.26 | 111.00 |
| 1 | E | 195 | VAL | CB-CA-C | -5.13 | 101.66 | 111.40 |
| 1 | C | 327 | PRO | N-CA-C | 5.12 | 125.42 | 112.10 |
| 1 | B | 431 | ASP | CB-CG-OD2 | 5.10 | 122.89 | 118.30 |
| 1 | A | 466 | ASP | CB-CG-OD2 | 5.09 | 122.88 | 118.30 |
| 1 | F | 320 | ASP | CB-CG-OD2 | 5.08 | 122.87 | 118.30 |
| 1 | E | 495 | SER | C-N-CA | -5.08 | 111.64 | 122.30 |
| 1 | A | 374 | VAL | CB-CA-C | -5.05 | 101.80 | 111.40 |
| 1 | D | 466 | ASP | CB-CG-OD2 | 5.04 | 122.84 | 118.30 |
| 1 | C | 417 | ASP | CB-CG-OD2 | 5.04 | 122.83 | 118.30 |
| 1 | C | 182 | ASP | CB-CG-OD2 | 5.01 | 122.81 | 118.30 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 3764 | 0 | 3764 | 309 | 0 |
| 1 | B | 3753 | 0 | 3763 | 287 | 0 |
| 1 | C | 3707 | 0 | 3721 | 463 | 0 |
| 1 | D | 3753 | 0 | 3761 | 294 | 0 |
| 1 | E | 3773 | 0 | 3777 | 257 | 0 |
| 1 | F | 3764 | 0 | 3764 | 300 | 0 |
| 2 | A | 53 | 0 | 31 | 5 | 0 |
| 2 | B | 53 | 0 | 31 | 10 | 0 |
| 2 | C | 53 | 0 | 31 | 17 | 0 |
| 2 | D | 53 | 0 | 31 | 4 | 0 |
| 2 | E | 53 | 0 | 31 | 3 | 0 |
| 2 | F | 53 | 0 | 31 | 5 | 0 |
| 3 | A | 39 | 0 | 18 | 2 | 0 |
| 3 | B | 39 | 0 | 18 | 8 | 0 |
| 3 | C | 39 | 0 | 18 | 6 | 0 |
| 3 | D | 39 | 0 | 18 | 6 | 0 |
| 3 | E | 39 | 0 | 18 | 1 | 0 |
| 3 | F | 39 | 0 | 18 | 4 | 0 |
| 4 | A | 1 | 0 | 0 | 0 | 0 |
| 4 | B | 1 | 0 | 0 | 0 | 0 |
| 4 | C | 3 | 0 | 0 | 2 | 0 |
| 4 | D | 1 | 0 | 0 | 0 | 0 |
| 4 | E | 2 | 0 | 0 | 1 | 0 |
| 4 | F | 1 | 0 | 0 | 0 | 0 |
| All | All | 23075 | 0 | 22844 | 1832 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 40.

All (1832) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------|--------------------------|-------------------|
| 1:C:98:TRP:NE1 | 1:C:190:PRO:HD2 | 1.54 | 1.21 |
| 1:C:98:TRP:CD1 | 1:C:189:CYS:HA | 1.76 | 1.20 |
| 1:D:477:GLU:O | 1:D:480:THR:HG22 | 1.49 | 1.13 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:378:LEU:HD13 | 1:C:441:LEU:HD11 | 1.13 | 1.12 |
| 1:C:98:TRP:CZ3 | 1:C:102:THR:HG23 | 1.85 | 1.12 |
| 1:F:478:ILE:HD12 | 1:F:478:ILE:N | 1.62 | 1.11 |
| 1:C:98:TRP:HZ3 | 1:C:102:THR:HG23 | 1.00 | 1.11 |
| 1:C:18:ILE:HG13 | 1:C:18:ILE:O | 1.47 | 1.10 |
| 1:D:303:GLU:OE1 | 1:D:303:GLU:N | 1.84 | 1.10 |
| 1:B:371:PRO:HG3 | 1:B:453:ALA:HB2 | 1.34 | 1.10 |
| 1:F:168:LEU:HB3 | 1:F:170:ILE:HG23 | 1.35 | 1.04 |
| 1:A:263:THR:OG1 | 1:A:264:PRO:CD | 2.07 | 1.03 |
| 1:C:378:LEU:HD13 | 1:C:441:LEU:CD1 | 1.90 | 1.01 |
| 1:C:72:GLN:HE21 | 1:D:410:GLU:HB3 | 1.18 | 1.01 |
| 1:C:172:GLY:HA2 | 1:C:175:GLU:HG3 | 1.36 | 1.01 |
| 1:D:251:PHE:HD1 | 1:D:273:SER:HB2 | 1.22 | 1.00 |
| 1:C:255:LYS:HD2 | 1:C:270:THR:OG1 | 1.62 | 1.00 |
| 1:C:320:ASP:O | 1:C:364:LYS:HG3 | 1.62 | 1.00 |
| 1:A:98:TRP:NE1 | 1:A:102:THR:HG21 | 1.76 | 0.99 |
| 1:C:98:TRP:HE3 | 1:C:102:THR:HG1 | 1.02 | 0.99 |
| 1:A:378:LEU:HG | 1:A:441:LEU:HD11 | 1.44 | 0.98 |
| 1:D:320:ASP:OD2 | 1:D:364:LYS:NZ | 1.97 | 0.98 |
| 1:E:289:LEU:O | 1:E:291:VAL:HG22 | 1.64 | 0.97 |
| 1:B:67:LYS:HE2 | 1:B:204:GLU:OE1 | 1.63 | 0.97 |
| 1:F:238:GLU:O | 1:F:242:GLU:HG3 | 1.64 | 0.97 |
| 1:E:263:THR:HB | 1:E:264:PRO:HD3 | 1.46 | 0.97 |
| 1:F:426:ILE:HD11 | 1:F:436:VAL:HG23 | 1.43 | 0.97 |
| 1:F:361:SER:OG | 1:F:363:VAL:HG23 | 1.63 | 0.96 |
| 1:D:325:ASN:N | 1:D:325:ASN:HD22 | 1.62 | 0.96 |
| 1:C:272:LYS:HE3 | 1:C:276:SER:HA | 1.49 | 0.95 |
| 1:C:461:THR:OG1 | 1:C:464:GLN:HG3 | 1.66 | 0.94 |
| 1:C:426:ILE:HG22 | 1:C:437:GLY:HA3 | 1.49 | 0.94 |
| 1:A:478:ILE:HD12 | 1:A:478:ILE:N | 1.83 | 0.94 |
| 1:E:256:ILE:HD13 | 1:E:269:VAL:HG22 | 1.47 | 0.94 |
| 1:C:224:LEU:H | 1:C:224:LEU:HD12 | 1.32 | 0.93 |
| 1:A:114:TRP:HB3 | 1:D:114:TRP:NE1 | 1.82 | 0.93 |
| 1:A:263:THR:OG1 | 1:A:264:PRO:HD3 | 1.66 | 0.93 |
| 1:A:353:LEU:HD12 | 1:A:356:ARG:HH21 | 1.34 | 0.92 |
| 1:B:65:ILE:HG22 | 1:B:66:PRO:HD3 | 1.51 | 0.92 |
| 1:C:403:HIS:CE1 | 1:C:492:ILE:HD11 | 2.05 | 0.92 |
| 1:A:348:GLN:HE22 | 1:A:351:ARG:NH1 | 1.66 | 0.92 |
| 1:C:258:GLN:HE22 | 1:C:261:ALA:HB2 | 1.33 | 0.92 |
| 1:E:303:GLU:OE2 | 1:E:304:THR:HG23 | 1.69 | 0.92 |
| 1:F:192:LYS:N | 1:F:285:ASN:HD22 | 1.67 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:331:ALA:O | 1:F:332:ILE:HD12 | 1.70 | 0.91 |
| 1:F:478:ILE:HD12 | 1:F:478:ILE:H | 1.24 | 0.91 |
| 1:B:426:ILE:HG12 | 1:B:437:GLY:HA3 | 1.52 | 0.91 |
| 1:D:325:ASN:ND2 | 1:D:325:ASN:H | 1.64 | 0.91 |
| 1:C:418:ASN:ND2 | 1:C:419:ASN:H | 1.68 | 0.90 |
| 1:D:389:LYS:NZ | 1:D:392:GLU:OE1 | 2.05 | 0.90 |
| 1:A:78:GLN:HE21 | 1:A:416:ARG:NH1 | 1.69 | 0.90 |
| 1:B:67:LYS:HE2 | 1:B:204:GLU:CD | 1.90 | 0.90 |
| 1:B:193:THR:HG22 | 1:B:286:THR:HB | 1.51 | 0.89 |
| 1:C:220:VAL:HG21 | 1:C:249:ARG:NE | 1.87 | 0.89 |
| 1:F:223:ILE:HD11 | 1:F:230:GLN:CD | 1.93 | 0.89 |
| 1:E:497:CYS:SG | 1:F:116:TYR:CE2 | 2.66 | 0.89 |
| 1:B:313:THR:O | 1:B:315:LYS:N | 2.04 | 0.89 |
| 1:F:313:THR:O | 1:F:315:LYS:N | 2.05 | 0.88 |
| 1:D:270:THR:HG22 | 1:D:280:ILE:HA | 1.55 | 0.88 |
| 1:E:263:THR:CB | 1:E:264:PRO:CD | 2.51 | 0.88 |
| 1:F:191:GLY:O | 1:F:193:THR:HG22 | 1.74 | 0.88 |
| 1:A:394:PHE:O | 1:A:398:ASN:ND2 | 2.06 | 0.88 |
| 1:B:371:PRO:CG | 1:B:453:ALA:CB | 2.52 | 0.88 |
| 1:D:325:ASN:HD22 | 1:D:325:ASN:H | 0.88 | 0.87 |
| 1:C:192:LYS:HE2 | 1:C:215:ASP:OD2 | 1.73 | 0.87 |
| 1:D:313:THR:O | 1:D:315:LYS:N | 2.06 | 0.87 |
| 1:A:318:VAL:CG1 | 1:A:322:GLU:HA | 2.04 | 0.87 |
| 1:D:250:GLN:O | 1:D:273:SER:CB | 2.23 | 0.87 |
| 1:C:256:ILE:HD11 | 1:C:267:LEU:CD1 | 2.05 | 0.87 |
| 1:C:291:VAL:O | 1:C:291:VAL:HG12 | 1.74 | 0.87 |
| 1:E:406:PHE:CZ | 1:E:421:CYS:HB3 | 2.09 | 0.86 |
| 1:E:308:LYS:H | 1:E:325:ASN:HD21 | 1.18 | 0.86 |
| 1:C:285:ASN:H | 1:C:285:ASN:HD22 | 1.21 | 0.86 |
| 1:E:343:THR:HB | 1:E:344:PRO:HD3 | 1.55 | 0.86 |
| 1:D:144:ASN:HD22 | 1:D:146:LYS:H | 1.24 | 0.86 |
| 1:F:434:ARG:HG2 | 1:F:434:ARG:HH11 | 1.40 | 0.86 |
| 1:C:164:ARG:HB3 | 1:C:165:PRO:HD2 | 1.56 | 0.85 |
| 1:B:262:GLY:O | 1:B:263:THR:O | 1.93 | 0.85 |
| 1:A:373:THR:HG23 | 1:B:471:ILE:HG21 | 1.58 | 0.85 |
| 1:C:46:PRO:HB3 | 1:C:50:GLY:HA2 | 1.59 | 0.85 |
| 1:E:144:ASN:OD1 | 1:E:145:ASN:N | 2.09 | 0.85 |
| 1:E:263:THR:OG1 | 1:E:264:PRO:HD2 | 1.75 | 0.85 |
| 1:B:192:LYS:H | 1:B:285:ASN:HD22 | 1.25 | 0.85 |
| 1:C:96:HIS:HE1 | 1:D:86:TYR:O | 1.58 | 0.85 |
| 1:E:434:ARG:HG2 | 1:E:434:ARG:HH11 | 1.41 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:318:VAL:HG11 | 1:A:322:GLU:HA | 1.57 | 0.85 |
| 1:B:371:PRO:HG3 | 1:B:453:ALA:CB | 2.06 | 0.85 |
| 1:B:371:PRO:CG | 1:B:453:ALA:HB2 | 2.07 | 0.85 |
| 1:C:196:VAL:O | 1:C:291:VAL:CG2 | 2.25 | 0.84 |
| 1:C:313:THR:OG1 | 1:C:315:LYS:HG3 | 1.77 | 0.84 |
| 1:A:66:PRO:HG3 | 1:A:109:ILE:HD11 | 1.59 | 0.84 |
| 1:B:66:PRO:HG3 | 1:B:109:ILE:HD11 | 1.59 | 0.84 |
| 1:C:96:HIS:CD2 | 1:C:212:ILE:HG13 | 2.11 | 0.84 |
| 1:F:325:ASN:H | 1:F:325:ASN:ND2 | 1.73 | 0.84 |
| 1:A:220:VAL:HG21 | 1:A:249:ARG:HE | 1.40 | 0.84 |
| 1:B:295:SER:HB3 | 1:B:335:ILE:HD12 | 1.57 | 0.84 |
| 1:A:308:LYS:H | 1:A:325:ASN:ND2 | 1.75 | 0.83 |
| 1:D:407:TRP:CG | 1:D:418:ASN:ND2 | 2.45 | 0.83 |
| 1:A:98:TRP:O | 1:A:102:THR:HG23 | 1.79 | 0.83 |
| 1:F:478:ILE:CD1 | 1:F:478:ILE:N | 2.39 | 0.83 |
| 1:C:196:VAL:HG12 | 1:C:291:VAL:HG21 | 1.59 | 0.83 |
| 1:C:447:GLU:OE2 | 1:D:474:VAL:HG13 | 1.78 | 0.83 |
| 1:A:493:LEU:O | 1:A:494:GLN:HG2 | 1.79 | 0.83 |
| 1:B:131:TYR:CZ | 2:B:600:FAD:N6A | 2.46 | 0.83 |
| 1:F:223:ILE:HD11 | 1:F:230:GLN:NE2 | 1.94 | 0.83 |
| 1:F:275:ASN:ND2 | 1:F:275:ASN:O | 2.12 | 0.83 |
| 1:E:232:MET:HE1 | 1:E:441:LEU:HB2 | 1.60 | 0.82 |
| 1:C:98:TRP:CZ3 | 1:C:102:THR:CG2 | 2.61 | 0.82 |
| 1:E:374:VAL:HG12 | 1:E:376:THR:HG23 | 1.58 | 0.82 |
| 1:C:185:SER:O | 1:C:187:PRO:HD3 | 1.79 | 0.82 |
| 1:C:208:PHE:CE1 | 1:C:209:LEU:HD22 | 2.13 | 0.82 |
| 1:C:383:CYS:SG | 1:C:456:LEU:HD12 | 2.18 | 0.82 |
| 1:E:313:THR:O | 1:E:315:LYS:N | 2.12 | 0.82 |
| 1:C:403:HIS:NE2 | 1:C:492:ILE:HD11 | 1.94 | 0.82 |
| 1:D:98:TRP:NE1 | 1:D:102:THR:HG21 | 1.94 | 0.82 |
| 1:E:263:THR:HB | 1:E:264:PRO:CD | 2.10 | 0.82 |
| 1:E:490:GLY:N | 4:E:2002:HOH:O | 2.11 | 0.82 |
| 1:D:144:ASN:ND2 | 1:D:146:LYS:H | 1.78 | 0.82 |
| 1:A:99:GLU:HG2 | 1:D:146:LYS:HD3 | 1.59 | 0.81 |
| 1:D:52:ASN:N | 1:D:52:ASN:HD22 | 1.78 | 0.81 |
| 1:A:353:LEU:HA | 1:A:356:ARG:NH2 | 1.95 | 0.81 |
| 1:A:65:ILE:HB | 1:A:66:PRO:CD | 2.09 | 0.81 |
| 1:C:18:ILE:O | 1:C:18:ILE:CG1 | 2.27 | 0.81 |
| 1:C:196:VAL:O | 1:C:291:VAL:HG23 | 1.81 | 0.81 |
| 1:F:256:ILE:HD11 | 1:F:267:LEU:HB3 | 1.61 | 0.81 |
| 1:F:422:TYR:HD1 | 1:F:423:ALA:N | 1.77 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:493:LEU:C | 1:B:494:GLN:HG3 | 2.00 | 0.81 |
| 1:C:230:GLN:O | 1:C:234:ASN:ND2 | 2.13 | 0.81 |
| 1:B:223:ILE:HG13 | 1:B:230:GLN:OE1 | 1.81 | 0.81 |
| 1:C:418:ASN:HD22 | 1:C:419:ASN:H | 1.28 | 0.81 |
| 1:E:426:ILE:HG12 | 1:E:437:GLY:HA3 | 1.62 | 0.81 |
| 1:A:397:GLU:CD | 1:A:397:GLU:H | 1.81 | 0.81 |
| 1:D:251:PHE:HA | 1:D:273:SER:HB2 | 1.61 | 0.81 |
| 1:F:469:ILE:N | 1:F:469:ILE:HD12 | 1.95 | 0.80 |
| 1:A:295:SER:HB3 | 1:A:335:ILE:HD12 | 1.62 | 0.80 |
| 1:B:426:ILE:CG1 | 1:B:437:GLY:HA3 | 2.12 | 0.80 |
| 1:A:353:LEU:HD12 | 1:A:356:ARG:NH2 | 1.96 | 0.80 |
| 1:A:478:ILE:H | 1:A:478:ILE:HD12 | 1.43 | 0.80 |
| 1:C:168:LEU:HD22 | 1:C:289:LEU:HD21 | 1.61 | 0.80 |
| 1:C:98:TRP:HZ3 | 1:C:102:THR:CG2 | 1.90 | 0.80 |
| 1:B:150:LYS:HG2 | 1:B:152:TYR:CE1 | 2.17 | 0.80 |
| 1:C:477:GLU:HA | 1:D:450:GLN:NE2 | 1.96 | 0.80 |
| 1:D:114:TRP:HZ3 | 1:D:118:VAL:HG21 | 1.47 | 0.80 |
| 1:A:358:TYR:N | 1:A:358:TYR:CD1 | 2.49 | 0.79 |
| 1:D:114:TRP:CZ3 | 1:D:118:VAL:HG21 | 2.17 | 0.79 |
| 1:D:251:PHE:HD1 | 1:D:273:SER:CB | 1.94 | 0.79 |
| 1:E:173:ASP:OD1 | 1:E:174:LYS:N | 2.16 | 0.79 |
| 1:A:308:LYS:H | 1:A:325:ASN:HD21 | 1.28 | 0.79 |
| 1:A:272:LYS:HE3 | 1:A:276:SER:HA | 1.64 | 0.79 |
| 1:C:318:VAL:HG13 | 1:C:319:THR:O | 1.81 | 0.79 |
| 1:C:239:HIS:ND1 | 1:C:378:LEU:HB2 | 1.97 | 0.79 |
| 1:C:378:LEU:CD1 | 1:C:441:LEU:HD11 | 2.05 | 0.79 |
| 1:E:431:ASP:OD2 | 1:E:434:ARG:NH1 | 2.14 | 0.79 |
| 1:B:493:LEU:N | 1:B:493:LEU:HD23 | 1.97 | 0.78 |
| 1:C:163:GLU:HB3 | 1:C:294:ASP:C | 2.03 | 0.78 |
| 1:C:58:THR:O | 1:C:63:GLY:N | 2.16 | 0.78 |
| 1:E:150:LYS:HD3 | 1:E:152:TYR:OH | 1.83 | 0.78 |
| 1:E:471:ILE:HG21 | 1:F:373:THR:HG23 | 1.66 | 0.78 |
| 1:A:67:LYS:NZ | 1:A:204:GLU:OE1 | 2.16 | 0.78 |
| 1:C:310:ASN:ND2 | 1:C:312:LYS:H | 1.82 | 0.78 |
| 1:E:320:ASP:OD2 | 1:E:364:LYS:NZ | 2.15 | 0.78 |
| 1:F:422:TYR:CD1 | 1:F:423:ALA:N | 2.52 | 0.78 |
| 1:F:313:THR:OG1 | 1:F:313:THR:O | 1.94 | 0.78 |
| 1:C:106:GLN:O | 1:C:109:ILE:HB | 1.83 | 0.78 |
| 1:C:426:ILE:CG2 | 1:C:437:GLY:HA3 | 2.13 | 0.78 |
| 1:C:98:TRP:HD1 | 1:C:189:CYS:HA | 1.45 | 0.78 |
| 1:C:472:HIS:HD2 | 1:C:477:GLU:OE2 | 1.67 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:67:LYS:CE | 1:B:204:GLU:OE1 | 2.31 | 0.77 |
| 1:F:428:ASN:HD22 | 1:F:431:ASP:CB | 1.96 | 0.77 |
| 1:A:418:ASN:HD22 | 1:A:419:ASN:H | 1.33 | 0.77 |
| 1:F:305:VAL:HG11 | 1:F:329:ILE:HD11 | 1.66 | 0.77 |
| 1:B:291:VAL:HG22 | 3:B:601:NDP:C4A | 2.15 | 0.77 |
| 1:C:67:LYS:HD3 | 1:C:204:GLU:HG2 | 1.66 | 0.77 |
| 1:A:262:GLY:O | 1:A:263:THR:O | 2.03 | 0.76 |
| 1:C:98:TRP:HE1 | 1:C:190:PRO:HD2 | 1.45 | 0.76 |
| 1:C:20:GLY:HA3 | 1:C:42:ASP:CG | 2.06 | 0.76 |
| 1:E:371:PRO:HB2 | 1:F:471:ILE:HD11 | 1.67 | 0.76 |
| 1:F:192:LYS:H | 1:F:285:ASN:HD22 | 1.31 | 0.76 |
| 1:D:51:THR:C | 1:D:52:ASN:HD22 | 1.89 | 0.76 |
| 1:C:179:SER:H | 1:C:182:ASP:HB2 | 1.49 | 0.76 |
| 1:D:168:LEU:HB3 | 1:D:170:ILE:HG23 | 1.66 | 0.76 |
| 1:A:84:ARG:HH11 | 1:A:84:ARG:HG3 | 1.51 | 0.76 |
| 1:D:473:PRO:O | 1:D:473:PRO:HG2 | 1.84 | 0.76 |
| 1:F:493:LEU:O | 1:F:494:GLN:HG2 | 1.85 | 0.76 |
| 1:D:407:TRP:HB2 | 1:D:418:ASN:HD21 | 1.51 | 0.76 |
| 1:C:161:THR:HG23 | 1:C:335:ILE:CD1 | 2.16 | 0.76 |
| 1:D:418:ASN:ND2 | 1:D:419:ASN:H | 1.84 | 0.76 |
| 1:D:250:GLN:O | 1:D:273:SER:HB2 | 1.85 | 0.75 |
| 1:F:20:GLY:N | 1:F:42:ASP:OD1 | 2.15 | 0.75 |
| 1:F:380:TYR:OH | 1:F:439:HIS:HD2 | 1.69 | 0.75 |
| 1:F:323:GLN:HA | 1:F:330:TYR:CD1 | 2.20 | 0.75 |
| 1:B:373:THR:HG21 | 1:B:446:GLY:HA2 | 1.69 | 0.75 |
| 1:A:374:VAL:HG12 | 1:A:376:THR:HG23 | 1.68 | 0.75 |
| 1:A:378:LEU:HG | 1:A:441:LEU:CD1 | 2.15 | 0.75 |
| 1:C:325:ASN:O | 1:C:327:PRO:HD3 | 1.87 | 0.75 |
| 1:E:426:ILE:CG1 | 1:E:437:GLY:HA3 | 2.16 | 0.75 |
| 1:A:291:VAL:O | 1:A:291:VAL:HG12 | 1.87 | 0.75 |
| 1:A:418:ASN:ND2 | 1:A:419:ASN:H | 1.84 | 0.74 |
| 1:A:373:THR:HG21 | 1:A:446:GLY:HA2 | 1.66 | 0.74 |
| 1:D:291:VAL:O | 1:D:291:VAL:HG13 | 1.87 | 0.74 |
| 1:C:263:THR:OG1 | 1:C:264:PRO:HD3 | 1.87 | 0.74 |
| 1:C:471:ILE:HG21 | 1:D:373:THR:HG23 | 1.69 | 0.74 |
| 1:E:192:LYS:H | 1:E:285:ASN:HD22 | 1.35 | 0.74 |
| 1:F:373:THR:HG21 | 1:F:446:GLY:HA2 | 1.69 | 0.74 |
| 1:A:36:LYS:HG3 | 1:A:358:TYR:CD2 | 2.22 | 0.74 |
| 1:C:59:CYS:HA | 1:C:63:GLY:HA3 | 1.69 | 0.74 |
| 1:E:374:VAL:CG1 | 1:E:376:THR:HG23 | 2.16 | 0.74 |
| 1:E:86:TYR:O | 1:F:96:HIS:HE1 | 1.71 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:115:GLY:HA3 | 1:F:497:CYS:SG | 2.27 | 0.74 |
| 1:D:418:ASN:HD22 | 1:D:419:ASN:H | 1.33 | 0.74 |
| 1:B:192:LYS:N | 1:B:285:ASN:HD22 | 1.86 | 0.74 |
| 1:E:272:LYS:HE2 | 1:E:276:SER:HA | 1.70 | 0.74 |
| 1:F:110:GLY:HA2 | 1:F:113:ASN:HD22 | 1.52 | 0.74 |
| 1:B:65:ILE:CG2 | 1:B:66:PRO:HD3 | 2.18 | 0.74 |
| 1:C:98:TRP:CE2 | 1:C:190:PRO:HD2 | 2.23 | 0.73 |
| 1:C:163:GLU:OE2 | 1:C:334:ASP:HB3 | 1.88 | 0.73 |
| 1:C:256:ILE:HD11 | 1:C:267:LEU:HD13 | 1.68 | 0.73 |
| 1:A:471:ILE:HG21 | 1:B:373:THR:HG23 | 1.70 | 0.73 |
| 1:C:178:ILE:N | 1:C:178:ILE:HD13 | 2.04 | 0.73 |
| 1:C:258:GLN:NE2 | 1:C:261:ALA:HB2 | 2.02 | 0.73 |
| 1:E:282:ASP:N | 1:E:282:ASP:OD1 | 2.20 | 0.73 |
| 1:A:65:ILE:HB | 1:A:66:PRO:HD2 | 1.71 | 0.73 |
| 1:C:220:VAL:HG23 | 1:C:249:ARG:HA | 1.68 | 0.73 |
| 1:F:71:HIS:CD2 | 1:F:375:PHE:HB3 | 2.23 | 0.73 |
| 1:F:325:ASN:H | 1:F:325:ASN:HD22 | 1.35 | 0.73 |
| 1:A:114:TRP:O | 1:A:118:VAL:HG23 | 1.89 | 0.73 |
| 1:B:256:ILE:HD11 | 1:B:267:LEU:HD13 | 1.71 | 0.73 |
| 1:C:55:LEU:CD1 | 1:C:116:TYR:HB3 | 2.18 | 0.73 |
| 1:D:30:GLU:OE2 | 1:D:33:LYS:HE3 | 1.89 | 0.73 |
| 1:D:352:LEU:HD12 | 1:D:365:CYS:HB2 | 1.71 | 0.73 |
| 1:D:163:GLU:HB3 | 1:D:295:SER:HA | 1.71 | 0.72 |
| 1:A:310:ASN:C | 1:A:310:ASN:HD22 | 1.92 | 0.72 |
| 1:B:310:ASN:ND2 | 1:B:313:THR:H | 1.87 | 0.72 |
| 1:F:39:MET:CE | 1:F:41:LEU:HD21 | 2.20 | 0.72 |
| 1:B:39:MET:HB2 | 1:B:126:VAL:HB | 1.72 | 0.72 |
| 1:C:343:THR:N | 2:C:600:FAD:O3' | 2.23 | 0.72 |
| 1:C:285:ASN:HD22 | 1:C:285:ASN:N | 1.87 | 0.72 |
| 1:D:373:THR:HG21 | 1:D:446:GLY:HA2 | 1.69 | 0.72 |
| 1:D:394:PHE:HB2 | 1:D:399:ILE:HD11 | 1.70 | 0.72 |
| 1:D:119:ALA:O | 1:D:123:LYS:HG3 | 1.88 | 0.72 |
| 1:B:191:GLY:O | 1:B:193:THR:HG23 | 1.90 | 0.72 |
| 1:B:356:ARG:NH1 | 1:B:364:LYS:HA | 2.05 | 0.72 |
| 1:C:188:TYR:CD2 | 1:C:263:THR:HG22 | 2.25 | 0.72 |
| 1:F:389:LYS:HD2 | 1:F:392:GLU:OE1 | 1.90 | 0.72 |
| 1:F:425:VAL:HG13 | 1:F:435:VAL:HG13 | 1.70 | 0.72 |
| 1:B:295:SER:HB3 | 1:B:335:ILE:CD1 | 2.19 | 0.72 |
| 1:C:178:ILE:HD13 | 1:C:178:ILE:H | 1.54 | 0.72 |
| 1:E:404:SER:HB3 | 1:E:478:ILE:HD11 | 1.72 | 0.72 |
| 1:A:263:THR:OG1 | 1:A:264:PRO:HD2 | 1.89 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:251:PHE:CD1 | 1:D:273:SER:HB2 | 2.15 | 0.71 |
| 1:E:410:GLU:OE2 | 1:F:68:LYS:NZ | 2.22 | 0.71 |
| 1:A:189:CYS:SG | 1:A:214:LEU:HD21 | 2.30 | 0.71 |
| 1:F:263:THR:HB | 1:F:264:PRO:HD3 | 1.72 | 0.71 |
| 1:A:310:ASN:ND2 | 1:A:312:LYS:H | 1.88 | 0.71 |
| 1:B:64:CYS:SG | 2:B:600:FAD:C4X | 2.78 | 0.71 |
| 1:D:82:ASP:OD2 | 1:D:416:ARG:NH1 | 2.23 | 0.71 |
| 1:B:403:HIS:CD2 | 1:B:492:ILE:HD13 | 2.25 | 0.71 |
| 1:C:309:ILE:HG22 | 1:C:316:ILE:HG12 | 1.71 | 0.71 |
| 1:A:167:TYR:CE2 | 1:A:174:LYS:HA | 2.26 | 0.71 |
| 1:F:192:LYS:H | 1:F:285:ASN:ND2 | 1.87 | 0.71 |
| 1:A:22:SER:OG | 1:A:343:THR:HG23 | 1.90 | 0.71 |
| 1:A:379:GLU:O | 1:A:441:LEU:HD12 | 1.91 | 0.71 |
| 1:D:67:LYS:NZ | 1:D:204:GLU:OE1 | 2.21 | 0.71 |
| 1:C:19:GLY:HA2 | 2:C:600:FAD:N3A | 2.05 | 0.71 |
| 1:B:281:GLU:O | 1:B:282:ASP:C | 2.29 | 0.71 |
| 1:C:425:VAL:HG13 | 1:C:435:VAL:HG13 | 1.71 | 0.71 |
| 1:E:373:THR:CG2 | 1:F:471:ILE:HG21 | 2.21 | 0.71 |
| 1:C:23:GLY:N | 2:C:600:FAD:O1P | 2.22 | 0.71 |
| 1:D:254:THR:HG23 | 1:D:271:ALA:HA | 1.72 | 0.71 |
| 1:E:263:THR:OG1 | 1:E:264:PRO:CD | 2.39 | 0.71 |
| 1:B:425:VAL:HG13 | 1:B:435:VAL:HG13 | 1.72 | 0.70 |
| 1:F:406:PHE:CE1 | 1:F:421:CYS:HB3 | 2.26 | 0.70 |
| 1:C:404:SER:HA | 1:C:492:ILE:CG2 | 2.21 | 0.70 |
| 1:E:262:GLY:O | 1:E:263:THR:O | 2.09 | 0.70 |
| 1:B:282:ASP:OD1 | 1:B:282:ASP:N | 2.23 | 0.70 |
| 1:E:461:THR:OG1 | 1:E:464:GLN:HG3 | 1.91 | 0.70 |
| 1:F:15:LEU:HB3 | 1:F:38:VAL:HG12 | 1.73 | 0.70 |
| 1:F:426:ILE:CD1 | 1:F:436:VAL:HG23 | 2.19 | 0.70 |
| 1:A:310:ASN:HD22 | 1:A:311:GLU:N | 1.90 | 0.70 |
| 1:C:258:GLN:HE22 | 1:C:261:ALA:CB | 2.03 | 0.70 |
| 1:F:256:ILE:HD12 | 1:F:257:GLU:N | 2.07 | 0.70 |
| 1:F:426:ILE:HD11 | 1:F:436:VAL:CG2 | 2.21 | 0.70 |
| 1:D:431:ASP:O | 1:D:432:ASN:HB2 | 1.92 | 0.70 |
| 1:A:267:LEU:N | 1:A:267:LEU:HD22 | 2.07 | 0.70 |
| 1:B:163:GLU:HB3 | 1:B:295:SER:HA | 1.73 | 0.70 |
| 1:C:477:GLU:HA | 1:D:450:GLN:HE21 | 1.54 | 0.70 |
| 1:A:471:ILE:HD11 | 1:B:371:PRO:HB3 | 1.74 | 0.69 |
| 1:A:90:LEU:HD21 | 1:B:90:LEU:HD21 | 1.73 | 0.69 |
| 1:B:474:VAL:O | 1:B:477:GLU:HG2 | 1.91 | 0.69 |
| 1:E:14:ASP:OD2 | 1:E:37:LYS:N | 2.24 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:158:LEU:HD11 | 1:A:332:ILE:CG1 | 2.21 | 0.69 |
| 1:D:400:GLU:OE2 | 1:D:487:ARG:HD2 | 1.92 | 0.69 |
| 1:B:401:VAL:HG22 | 1:B:426:ILE:HG22 | 1.72 | 0.69 |
| 1:B:291:VAL:HG22 | 3:B:601:NDP:N9A | 2.07 | 0.69 |
| 1:C:186:LEU:HD12 | 1:C:190:PRO:HG3 | 1.72 | 0.69 |
| 1:C:67:LYS:HD3 | 1:C:204:GLU:CD | 2.12 | 0.69 |
| 1:E:450:GLN:HE22 | 1:F:470:GLY:HA2 | 1.57 | 0.69 |
| 1:A:263:THR:O | 1:A:265:GLY:N | 2.25 | 0.69 |
| 1:E:289:LEU:O | 1:E:291:VAL:CG2 | 2.40 | 0.69 |
| 1:C:67:LYS:HD3 | 1:C:204:GLU:CG | 2.22 | 0.69 |
| 1:C:21:GLY:O | 1:C:25:LEU:HG | 1.92 | 0.69 |
| 1:C:438:PHE:CE2 | 1:C:452:PHE:CG | 2.80 | 0.69 |
| 1:E:473:PRO:O | 1:F:68:LYS:HE3 | 1.93 | 0.69 |
| 1:A:373:THR:CG2 | 1:B:471:ILE:HG21 | 2.23 | 0.69 |
| 1:C:256:ILE:HD11 | 1:C:267:LEU:HD12 | 1.72 | 0.69 |
| 1:A:470:GLY:HA2 | 1:B:450:GLN:HE22 | 1.57 | 0.69 |
| 1:F:223:ILE:CG1 | 1:F:230:GLN:NE2 | 2.56 | 0.69 |
| 1:C:220:VAL:CG2 | 1:C:249:ARG:HA | 2.22 | 0.69 |
| 1:A:78:GLN:NE2 | 1:A:416:ARG:NH1 | 2.40 | 0.69 |
| 1:A:65:ILE:CB | 1:A:66:PRO:CD | 2.71 | 0.69 |
| 1:C:42:ASP:OD1 | 1:C:43:PHE:N | 2.25 | 0.69 |
| 1:D:266:ARG:HD2 | 1:D:283:GLU:OE1 | 1.93 | 0.68 |
| 1:C:418:ASN:ND2 | 1:C:419:ASN:N | 2.38 | 0.68 |
| 1:C:315:LYS:HD3 | 1:C:337:GLU:HA | 1.75 | 0.68 |
| 1:D:96:HIS:CD2 | 1:D:212:ILE:HG13 | 2.29 | 0.68 |
| 1:D:400:GLU:HG2 | 1:D:429:LEU:HD11 | 1.74 | 0.68 |
| 1:C:153:SER:HB3 | 4:C:2002:HOH:O | 1.93 | 0.68 |
| 1:C:190:PRO:O | 1:C:191:GLY:O | 2.11 | 0.68 |
| 1:C:20:GLY:HA3 | 1:C:42:ASP:OD2 | 1.92 | 0.68 |
| 1:C:65:ILE:HG22 | 1:C:66:PRO:N | 2.09 | 0.68 |
| 1:C:98:TRP:HE3 | 1:C:102:THR:OG1 | 1.75 | 0.68 |
| 1:E:323:GLN:HA | 1:E:330:TYR:CD1 | 2.29 | 0.68 |
| 1:A:282:ASP:N | 1:A:282:ASP:OD1 | 2.27 | 0.68 |
| 1:A:357:LEU:HB3 | 1:A:358:TYR:CE1 | 2.27 | 0.68 |
| 1:C:220:VAL:HG21 | 1:C:249:ARG:CZ | 2.23 | 0.68 |
| 1:C:225:LEU:HD23 | 1:C:228:PHE:CD2 | 2.29 | 0.68 |
| 1:C:252:VAL:HG13 | 1:C:253:PRO:HD2 | 1.76 | 0.68 |
| 1:F:63:GLY:O | 1:F:66:PRO:HD2 | 1.93 | 0.68 |
| 1:C:426:ILE:HG22 | 1:C:437:GLY:CA | 2.23 | 0.68 |
| 1:E:308:LYS:H | 1:E:325:ASN:ND2 | 1.90 | 0.68 |
| 1:F:263:THR:CB | 1:F:264:PRO:CD | 2.71 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:371:PRO:HG2 | 1:B:453:ALA:CB | 2.24 | 0.68 |
| 1:C:31:ALA:O | 1:C:33:LYS:N | 2.27 | 0.68 |
| 1:A:250:GLN:O | 1:A:273:SER:HB2 | 1.94 | 0.67 |
| 1:B:91:GLU:O | 1:B:93:THR:N | 2.27 | 0.67 |
| 1:C:188:TYR:CE1 | 1:C:263:THR:O | 2.48 | 0.67 |
| 1:A:461:THR:HG23 | 1:A:464:GLN:OE1 | 1.94 | 0.67 |
| 1:C:161:THR:O | 2:C:600:FAD:H52A | 1.93 | 0.67 |
| 1:C:36:LYS:O | 1:C:38:VAL:HG13 | 1.94 | 0.67 |
| 1:F:422:TYR:HD1 | 1:F:422:TYR:C | 1.97 | 0.67 |
| 1:B:291:VAL:CG2 | 3:B:601:NDP:C4A | 2.73 | 0.67 |
| 1:E:275:ASN:O | 1:E:276:SER:HB2 | 1.95 | 0.67 |
| 1:B:200:TYR:O | 1:B:204:GLU:HG3 | 1.92 | 0.67 |
| 1:B:233:ALA:HA | 1:B:236:ILE:HD12 | 1.76 | 0.67 |
| 1:B:238:GLU:O | 1:B:242:GLU:HG3 | 1.95 | 0.67 |
| 1:A:318:VAL:HG12 | 1:A:319:THR:O | 1.95 | 0.67 |
| 1:B:229:ASP:C | 1:B:229:ASP:OD1 | 2.32 | 0.67 |
| 1:B:319:THR:HG23 | 1:B:323:GLN:O | 1.95 | 0.67 |
| 1:F:49:LEU:N | 1:F:49:LEU:HD22 | 2.09 | 0.67 |
| 1:B:250:GLN:O | 1:B:273:SER:CB | 2.43 | 0.67 |
| 1:C:188:TYR:O | 1:C:190:PRO:HD3 | 1.94 | 0.67 |
| 1:D:38:VAL:HG23 | 1:D:125:VAL:HG13 | 1.77 | 0.67 |
| 1:D:167:TYR:HB3 | 1:D:173:ASP:OD2 | 1.95 | 0.67 |
| 1:F:150:LYS:HD3 | 1:F:152:TYR:OH | 1.95 | 0.67 |
| 1:F:422:TYR:HE1 | 1:F:424:LYS:HB3 | 1.59 | 0.67 |
| 1:B:167:TYR:HB3 | 1:B:173:ASP:OD2 | 1.95 | 0.66 |
| 1:C:400:GLU:HA | 1:C:400:GLU:OE1 | 1.94 | 0.66 |
| 1:E:473:PRO:O | 1:E:473:PRO:HG2 | 1.94 | 0.66 |
| 1:F:428:ASN:HD22 | 1:F:431:ASP:HB2 | 1.59 | 0.66 |
| 1:A:114:TRP:HB3 | 1:D:114:TRP:HE1 | 1.59 | 0.66 |
| 1:A:378:LEU:CG | 1:A:441:LEU:HD11 | 2.23 | 0.66 |
| 1:B:260:GLU:OE1 | 1:B:266:ARG:NH1 | 2.28 | 0.66 |
| 1:B:374:VAL:O | 1:B:374:VAL:HG13 | 1.94 | 0.66 |
| 1:C:208:PHE:CD1 | 1:C:209:LEU:N | 2.64 | 0.66 |
| 1:F:250:GLN:O | 1:F:273:SER:HB3 | 1.94 | 0.66 |
| 1:D:480:THR:HG23 | 1:D:481:THR:HG23 | 1.76 | 0.66 |
| 1:F:380:TYR:OH | 1:F:439:HIS:CD2 | 2.47 | 0.66 |
| 1:A:418:ASN:ND2 | 1:A:419:ASN:N | 2.43 | 0.66 |
| 1:B:64:CYS:SG | 2:B:600:FAD:C10 | 2.84 | 0.66 |
| 1:D:85:ASN:HB2 | 1:D:413:VAL:HG12 | 1.77 | 0.66 |
| 1:F:361:SER:HG | 1:F:363:VAL:HG23 | 1.59 | 0.66 |
| 1:F:422:TYR:C | 1:F:422:TYR:CD1 | 2.69 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:84:ARG:HB2 | 1:F:84:ARG:HH11 | 1.60 | 0.66 |
| 1:B:66:PRO:CG | 1:B:109:ILE:HD11 | 2.26 | 0.66 |
| 1:E:168:LEU:HD11 | 1:E:291:VAL:HG21 | 1.78 | 0.66 |
| 1:E:280:ILE:HG13 | 1:E:280:ILE:O | 1.96 | 0.66 |
| 1:E:98:TRP:CE2 | 1:E:102:THR:HG21 | 2.31 | 0.66 |
| 1:F:324:THR:OG1 | 1:F:329:ILE:O | 2.10 | 0.66 |
| 1:C:208:PHE:HE1 | 1:C:209:LEU:HD22 | 1.55 | 0.66 |
| 1:D:411:TRP:C | 1:D:414:PRO:HD2 | 2.15 | 0.66 |
| 1:C:159:ILE:HG12 | 1:C:330:TYR:O | 1.95 | 0.66 |
| 1:C:325:ASN:HD22 | 1:C:325:ASN:H | 1.41 | 0.66 |
| 1:A:313:THR:OG1 | 1:A:313:THR:O | 2.11 | 0.66 |
| 1:B:144:ASN:OD1 | 1:B:145:ASN:N | 2.29 | 0.66 |
| 1:A:192:LYS:H | 1:A:285:ASN:HD22 | 1.44 | 0.65 |
| 1:E:281:GLU:O | 1:E:282:ASP:C | 2.34 | 0.65 |
| 1:C:310:ASN:OD1 | 1:C:313:THR:HG23 | 1.96 | 0.65 |
| 1:E:49:LEU:HD22 | 1:E:49:LEU:N | 2.12 | 0.65 |
| 1:C:176:TYR:CE2 | 1:C:258:GLN:HB3 | 2.31 | 0.65 |
| 1:C:191:GLY:O | 1:C:193:THR:HG22 | 1.96 | 0.65 |
| 1:D:220:VAL:HG21 | 1:D:249:ARG:HE | 1.61 | 0.65 |
| 1:B:120:LEU:HD22 | 1:B:125:VAL:HG11 | 1.79 | 0.65 |
| 1:C:170:ILE:HB | 1:C:254:THR:O | 1.97 | 0.65 |
| 1:C:492:ILE:O | 1:C:492:ILE:HG22 | 1.97 | 0.65 |
| 1:D:343:THR:HB | 1:D:344:PRO:CD | 2.27 | 0.65 |
| 1:F:223:ILE:CD1 | 1:F:230:GLN:NE2 | 2.60 | 0.65 |
| 1:B:399:ILE:HD12 | 1:B:427:CYS:O | 1.96 | 0.65 |
| 1:B:91:GLU:OE1 | 1:B:92:ASP:N | 2.30 | 0.65 |
| 1:F:428:ASN:HD22 | 1:F:431:ASP:HB3 | 1.60 | 0.65 |
| 1:A:68:LYS:HG2 | 1:B:409:LEU:HD23 | 1.77 | 0.65 |
| 1:B:65:ILE:HG22 | 1:B:66:PRO:CD | 2.26 | 0.65 |
| 1:E:343:THR:CB | 1:E:344:PRO:HD3 | 2.26 | 0.65 |
| 1:B:308:LYS:H | 1:B:325:ASN:HD21 | 1.43 | 0.65 |
| 1:A:281:GLU:O | 1:A:282:ASP:C | 2.35 | 0.65 |
| 1:C:96:HIS:CE1 | 1:D:86:TYR:O | 2.46 | 0.64 |
| 1:E:98:TRP:NE1 | 1:E:102:THR:HG21 | 2.12 | 0.64 |
| 1:E:67:LYS:NZ | 1:E:204:GLU:OE1 | 2.26 | 0.64 |
| 1:E:423:ALA:HB3 | 1:E:478:ILE:HD13 | 1.79 | 0.64 |
| 1:A:373:THR:HG23 | 1:B:471:ILE:CG2 | 2.26 | 0.64 |
| 1:A:98:TRP:CD1 | 1:A:102:THR:HG21 | 2.31 | 0.64 |
| 1:A:291:VAL:CG1 | 3:A:601:NDP:C4A | 2.75 | 0.64 |
| 1:B:263:THR:O | 1:B:265:GLY:N | 2.31 | 0.64 |
| 1:B:378:LEU:CD1 | 1:B:441:LEU:HG | 2.27 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:291:VAL:HG13 | 3:C:601:NDP:N9A | 2.12 | 0.64 |
| 1:D:262:GLY:O | 1:D:263:THR:O | 2.15 | 0.64 |
| 1:F:256:ILE:C | 1:F:256:ILE:HD12 | 2.17 | 0.64 |
| 1:A:450:GLN:HE22 | 1:B:470:GLY:HA2 | 1.61 | 0.64 |
| 1:A:34:PHE:CE2 | 1:A:359:GLY:HA2 | 2.33 | 0.64 |
| 1:B:487:ARG:O | 1:B:487:ARG:HG3 | 1.97 | 0.64 |
| 1:C:411:TRP:C | 1:C:414:PRO:HD2 | 2.17 | 0.64 |
| 1:C:133:LYS:HD3 | 1:C:301:GLY:N | 2.12 | 0.64 |
| 1:C:189:CYS:O | 1:C:191:GLY:N | 2.31 | 0.64 |
| 1:D:419:ASN:O | 1:D:420:LYS:HD3 | 1.98 | 0.64 |
| 1:F:321:GLU:O | 1:F:322:GLU:HB2 | 1.98 | 0.64 |
| 1:A:82:ASP:OD1 | 1:A:416:ARG:NH1 | 2.31 | 0.64 |
| 1:E:138:HIS:HD2 | 1:E:154:ALA:O | 1.80 | 0.64 |
| 1:A:249:ARG:HB3 | 1:A:250:GLN:NE2 | 2.14 | 0.64 |
| 1:D:371:PRO:C | 1:D:372:THR:HG22 | 2.18 | 0.64 |
| 1:F:22:SER:HB3 | 1:F:343:THR:HG23 | 1.80 | 0.64 |
| 1:B:55:LEU:HD13 | 1:B:116:TYR:HB3 | 1.80 | 0.63 |
| 1:C:323:GLN:HB2 | 1:C:330:TYR:CE2 | 2.33 | 0.63 |
| 1:F:230:GLN:O | 1:F:234:ASN:ND2 | 2.31 | 0.63 |
| 1:F:489:GLY:O | 1:F:490:GLY:C | 2.34 | 0.63 |
| 1:E:186:LEU:HD22 | 1:E:188:TYR:CZ | 2.34 | 0.63 |
| 1:C:374:VAL:O | 1:C:374:VAL:HG12 | 1.97 | 0.63 |
| 1:E:98:TRP:O | 1:E:102:THR:HG23 | 1.97 | 0.63 |
| 1:E:378:LEU:HD23 | 1:E:441:LEU:HD21 | 1.81 | 0.63 |
| 1:E:38:VAL:CG2 | 1:E:125:VAL:HG13 | 2.27 | 0.63 |
| 1:E:72:GLN:HG3 | 1:E:76:LEU:HD22 | 1.80 | 0.63 |
| 1:F:291:VAL:HG13 | 1:F:291:VAL:O | 1.99 | 0.63 |
| 1:B:308:LYS:H | 1:B:325:ASN:ND2 | 1.97 | 0.63 |
| 1:F:30:GLU:OE2 | 1:F:33:LYS:NZ | 2.29 | 0.63 |
| 1:F:472:HIS:ND1 | 1:F:473:PRO:HA | 2.12 | 0.63 |
| 1:C:343:THR:HB | 1:C:344:PRO:HD3 | 1.78 | 0.63 |
| 1:F:167:TYR:HB3 | 1:F:173:ASP:OD2 | 1.99 | 0.63 |
| 1:C:161:THR:HG23 | 1:C:335:ILE:HD11 | 1.80 | 0.63 |
| 1:E:91:GLU:O | 1:E:93:THR:N | 2.31 | 0.63 |
| 1:F:217:THR:HG23 | 1:F:246:LYS:HB2 | 1.81 | 0.63 |
| 1:C:173:ASP:O | 1:C:177:CYS:HB2 | 1.99 | 0.62 |
| 1:C:291:VAL:O | 1:C:291:VAL:CG1 | 2.47 | 0.62 |
| 1:D:284:PHE:CD1 | 1:D:284:PHE:N | 2.67 | 0.62 |
| 1:C:135:ILE:HG12 | 1:C:136:GLY:N | 2.14 | 0.62 |
| 1:C:322:GLU:OE1 | 1:C:356:ARG:NH2 | 2.32 | 0.62 |
| 1:D:258:GLN:NE2 | 1:D:261:ALA:HB2 | 2.15 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:471:ILE:CG2 | 1:F:373:THR:HG23 | 2.28 | 0.62 |
| 1:F:84:ARG:NH1 | 1:F:84:ARG:HB2 | 2.13 | 0.62 |
| 1:B:110:GLY:HA2 | 1:B:113:ASN:HD22 | 1.64 | 0.62 |
| 1:B:204:GLU:OE2 | 1:B:375:PHE:N | 2.26 | 0.62 |
| 1:D:418:ASN:HD22 | 1:D:419:ASN:N | 1.97 | 0.62 |
| 1:D:177:CYS:SG | 1:D:256:ILE:HD13 | 2.40 | 0.62 |
| 1:D:448:VAL:HG22 | 1:D:476:ALA:HB2 | 1.82 | 0.62 |
| 1:E:9:LYS:HG3 | 1:E:10:SER:N | 2.15 | 0.62 |
| 1:F:108:HIS:O | 1:F:111:SER:HB3 | 1.99 | 0.62 |
| 1:D:208:PHE:CE1 | 1:D:209:LEU:HD13 | 2.35 | 0.62 |
| 1:E:108:HIS:O | 1:E:111:SER:HB3 | 2.00 | 0.62 |
| 1:E:434:ARG:CG | 1:E:434:ARG:HH11 | 2.11 | 0.62 |
| 1:F:343:THR:HB | 1:F:344:PRO:HD3 | 1.80 | 0.62 |
| 1:A:378:LEU:HD23 | 1:A:441:LEU:HD21 | 1.82 | 0.62 |
| 1:C:176:TYR:CD2 | 1:C:258:GLN:HB3 | 2.35 | 0.62 |
| 1:C:18:ILE:HG12 | 1:C:159:ILE:HA | 1.80 | 0.62 |
| 1:C:234:ASN:HD22 | 1:C:234:ASN:N | 1.97 | 0.62 |
| 1:C:47:THR:HB | 1:C:48:PRO:HD2 | 1.81 | 0.62 |
| 1:F:98:TRP:O | 1:F:102:THR:HG23 | 2.00 | 0.62 |
| 1:F:70:MET:HG2 | 1:F:101:MET:HE3 | 1.82 | 0.62 |
| 1:B:313:THR:O | 1:B:313:THR:OG1 | 2.12 | 0.61 |
| 1:C:18:ILE:HD11 | 1:C:159:ILE:HG23 | 1.81 | 0.61 |
| 1:C:406:PHE:CZ | 1:C:421:CYS:HB3 | 2.35 | 0.61 |
| 1:C:404:SER:HA | 1:C:492:ILE:HG23 | 1.82 | 0.61 |
| 1:E:321:GLU:O | 1:E:322:GLU:HB2 | 1.99 | 0.61 |
| 1:A:65:ILE:HG22 | 1:A:66:PRO:HD3 | 1.83 | 0.61 |
| 1:C:98:TRP:CD1 | 1:C:190:PRO:HD2 | 2.33 | 0.61 |
| 1:C:472:HIS:CD2 | 1:C:473:PRO:HA | 2.35 | 0.61 |
| 1:D:222:SER:OG | 3:D:601:NDP:O3X | 2.15 | 0.61 |
| 1:F:281:GLU:O | 1:F:282:ASP:C | 2.36 | 0.61 |
| 1:A:84:ARG:NH1 | 1:A:84:ARG:HG3 | 2.13 | 0.61 |
| 1:E:58:THR:HG21 | 1:E:293:ARG:NH2 | 2.16 | 0.61 |
| 1:C:234:ASN:H | 1:C:234:ASN:HD22 | 1.47 | 0.61 |
| 1:C:328:TYR:CD1 | 1:C:329:ILE:HG13 | 2.35 | 0.61 |
| 1:E:373:THR:HG21 | 1:E:446:GLY:HA2 | 1.82 | 0.61 |
| 1:F:262:GLY:O | 1:F:263:THR:O | 2.18 | 0.61 |
| 1:C:193:THR:HB | 1:C:286:THR:HB | 1.82 | 0.61 |
| 1:C:98:TRP:CD1 | 1:C:189:CYS:CA | 2.69 | 0.61 |
| 1:E:411:TRP:C | 1:E:414:PRO:HD2 | 2.21 | 0.61 |
| 1:B:250:GLN:O | 1:B:273:SER:HB2 | 2.00 | 0.61 |
| 1:F:370:VAL:O | 1:F:370:VAL:HG23 | 2.01 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:29:LYS:CG | 1:B:30:GLU:N | 2.64 | 0.61 |
| 1:A:410:GLU:OE2 | 1:B:68:LYS:NZ | 2.34 | 0.61 |
| 1:A:411:TRP:C | 1:A:414:PRO:HD2 | 2.21 | 0.61 |
| 1:B:431:ASP:O | 1:B:432:ASN:HB2 | 2.00 | 0.61 |
| 1:B:59:CYS:HG | 1:B:64:CYS:CB | 2.13 | 0.61 |
| 1:A:478:ILE:CD1 | 1:A:478:ILE:N | 2.54 | 0.61 |
| 1:B:13:PHE:O | 1:B:154:ALA:HA | 2.00 | 0.61 |
| 1:B:256:ILE:CD1 | 1:B:267:LEU:HB3 | 2.31 | 0.61 |
| 1:C:163:GLU:HB3 | 1:C:294:ASP:O | 2.00 | 0.61 |
| 1:C:418:ASN:HD22 | 1:C:419:ASN:N | 1.98 | 0.61 |
| 1:E:477:GLU:O | 1:E:480:THR:HB | 2.01 | 0.61 |
| 1:A:374:VAL:CG1 | 1:A:376:THR:HG23 | 2.30 | 0.60 |
| 1:B:221:ARG:HD2 | 1:B:252:VAL:HG21 | 1.82 | 0.60 |
| 1:D:323:GLN:HG3 | 1:D:330:TYR:CE1 | 2.36 | 0.60 |
| 1:F:163:GLU:HB3 | 1:F:295:SER:HA | 1.83 | 0.60 |
| 1:C:427:CYS:HB3 | 1:C:433:GLU:O | 2.01 | 0.60 |
| 1:C:72:GLN:NE2 | 1:D:410:GLU:HB3 | 2.03 | 0.60 |
| 1:E:322:GLU:HG2 | 1:E:332:ILE:CD1 | 2.31 | 0.60 |
| 1:F:431:ASP:OD1 | 1:F:434:ARG:NH1 | 2.34 | 0.60 |
| 1:F:62:VAL:HG23 | 1:F:62:VAL:O | 2.01 | 0.60 |
| 1:A:144:ASN:CG | 1:A:145:ASN:N | 2.54 | 0.60 |
| 1:C:183:LEU:C | 1:C:185:SER:H | 2.05 | 0.60 |
| 1:C:398:ASN:OD1 | 1:C:430:LYS:HG3 | 2.00 | 0.60 |
| 1:C:55:LEU:HD13 | 1:C:116:TYR:HB3 | 1.82 | 0.60 |
| 1:C:68:LYS:O | 1:C:71:HIS:HB3 | 2.01 | 0.60 |
| 1:D:323:GLN:HA | 1:D:330:TYR:CD1 | 2.37 | 0.60 |
| 1:E:431:ASP:CG | 1:E:434:ARG:NH1 | 2.54 | 0.60 |
| 1:F:461:THR:OG1 | 1:F:464:GLN:HG3 | 2.01 | 0.60 |
| 1:A:348:GLN:NE2 | 1:A:351:ARG:NH1 | 2.45 | 0.60 |
| 1:C:198:ALA:HB2 | 1:C:220:VAL:HG12 | 1.82 | 0.60 |
| 1:C:318:VAL:HG13 | 1:C:319:THR:N | 2.15 | 0.60 |
| 1:C:31:ALA:C | 1:C:33:LYS:H | 2.05 | 0.60 |
| 1:C:405:PHE:H | 1:C:492:ILE:HG22 | 1.66 | 0.60 |
| 1:C:222:SER:OG | 3:C:601:NDP:O3X | 2.16 | 0.60 |
| 1:D:321:GLU:O | 1:D:322:GLU:HB2 | 1.99 | 0.60 |
| 1:B:291:VAL:O | 1:B:291:VAL:HG13 | 2.01 | 0.60 |
| 1:C:275:ASN:O | 1:C:276:SER:HB2 | 2.00 | 0.60 |
| 1:F:426:ILE:HD12 | 1:F:426:ILE:C | 2.22 | 0.60 |
| 1:A:324:THR:OG1 | 1:A:329:ILE:O | 2.18 | 0.60 |
| 1:A:440:VAL:HB | 1:A:479:PHE:HZ | 1.67 | 0.60 |
| 1:D:77:GLY:O | 1:D:80:LEU:HB2 | 2.02 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:58:THR:OG1 | 2:E:600:FAD:O1A | 2.19 | 0.60 |
| 1:E:72:GLN:HE21 | 1:E:72:GLN:HA | 1.67 | 0.60 |
| 1:B:16:ILE:HB | 1:B:157:PHE:CE1 | 2.37 | 0.60 |
| 1:B:263:THR:CB | 1:B:264:PRO:CD | 2.80 | 0.60 |
| 1:F:411:TRP:C | 1:F:414:PRO:HD2 | 2.22 | 0.60 |
| 1:B:193:THR:CG2 | 1:B:286:THR:HB | 2.28 | 0.59 |
| 1:B:492:ILE:C | 1:B:493:LEU:HD23 | 2.22 | 0.59 |
| 3:B:601:NDP:O1A | 3:B:601:NDP:H52N | 2.02 | 0.59 |
| 1:A:96:HIS:HE1 | 1:B:86:TYR:O | 1.84 | 0.59 |
| 1:C:223:ILE:O | 1:C:223:ILE:HG13 | 2.02 | 0.59 |
| 1:C:336:LEU:HB3 | 1:C:339:LYS:HG3 | 1.84 | 0.59 |
| 1:C:36:LYS:HE3 | 1:C:358:TYR:HD2 | 1.67 | 0.59 |
| 1:D:236:ILE:HG13 | 1:D:441:LEU:HD11 | 1.83 | 0.59 |
| 1:A:373:THR:HG21 | 1:A:446:GLY:CA | 2.32 | 0.59 |
| 1:F:263:THR:OG1 | 1:F:264:PRO:HD2 | 2.02 | 0.59 |
| 1:F:30:GLU:O | 1:F:31:ALA:C | 2.39 | 0.59 |
| 1:A:220:VAL:HG22 | 1:A:249:ARG:HA | 1.84 | 0.59 |
| 1:C:133:LYS:HD3 | 1:C:300:ILE:C | 2.23 | 0.59 |
| 1:C:47:THR:HB | 1:C:48:PRO:CD | 2.33 | 0.59 |
| 1:F:434:ARG:HE | 1:F:461:THR:HG22 | 1.67 | 0.59 |
| 1:A:477:GLU:O | 1:A:480:THR:HG22 | 2.03 | 0.59 |
| 1:C:302:LEU:HD21 | 1:C:309:ILE:HG12 | 1.85 | 0.59 |
| 1:C:58:THR:CB | 2:C:600:FAD:O2A | 2.51 | 0.59 |
| 1:E:221:ARG:NH1 | 3:E:601:NDP:O3X | 2.36 | 0.59 |
| 1:E:30:GLU:O | 1:E:31:ALA:C | 2.40 | 0.59 |
| 1:F:173:ASP:OD1 | 1:F:174:LYS:N | 2.34 | 0.59 |
| 1:F:203:LEU:HD12 | 1:F:225:LEU:HD21 | 1.84 | 0.59 |
| 1:D:473:PRO:O | 1:D:473:PRO:CG | 2.47 | 0.59 |
| 1:E:272:LYS:HG2 | 1:E:273:SER:N | 2.17 | 0.59 |
| 1:F:55:LEU:HD13 | 1:F:116:TYR:HB3 | 1.83 | 0.59 |
| 1:A:65:ILE:HB | 1:A:66:PRO:HD3 | 1.85 | 0.59 |
| 1:C:255:LYS:O | 1:C:255:LYS:HD3 | 2.02 | 0.59 |
| 1:E:266:ARG:C | 1:E:267:LEU:HD13 | 2.22 | 0.59 |
| 1:A:65:ILE:CG2 | 1:A:66:PRO:HD3 | 2.33 | 0.59 |
| 1:B:167:TYR:CE2 | 1:B:174:LYS:HA | 2.38 | 0.59 |
| 1:B:250:GLN:O | 1:B:273:SER:HB3 | 2.02 | 0.59 |
| 1:C:263:THR:CB | 1:C:264:PRO:HD3 | 2.32 | 0.59 |
| 1:C:438:PHE:HE2 | 1:C:452:PHE:CG | 2.20 | 0.59 |
| 1:D:431:ASP:OD2 | 1:D:434:ARG:NH1 | 2.36 | 0.59 |
| 1:E:203:LEU:HD22 | 1:E:240:MET:CE | 2.33 | 0.59 |
| 1:A:295:SER:CB | 1:A:335:ILE:HD12 | 2.31 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:272:LYS:HE3 | 1:D:276:SER:HA | 1.84 | 0.59 |
| 1:D:281:GLU:O | 1:D:282:ASP:C | 2.39 | 0.59 |
| 1:E:418:ASN:ND2 | 1:E:419:ASN:H | 1.99 | 0.59 |
| 1:A:123:LYS:O | 1:A:124:LYS:HB2 | 2.02 | 0.59 |
| 1:C:167:TYR:CE2 | 1:C:174:LYS:HA | 2.38 | 0.59 |
| 1:A:114:TRP:CB | 1:D:114:TRP:NE1 | 2.60 | 0.59 |
| 1:F:336:LEU:HD23 | 1:F:339:LYS:HG3 | 1.85 | 0.59 |
| 1:C:167:TYR:HB3 | 1:C:173:ASP:OD2 | 2.03 | 0.58 |
| 1:C:183:LEU:O | 1:C:185:SER:N | 2.36 | 0.58 |
| 1:C:401:VAL:HG21 | 1:C:486:LYS:HD2 | 1.85 | 0.58 |
| 1:C:150:LYS:HD2 | 1:C:152:TYR:OH | 2.03 | 0.58 |
| 1:C:325:ASN:ND2 | 1:C:325:ASN:H | 2.00 | 0.58 |
| 1:C:328:TYR:CE1 | 1:C:329:ILE:HG13 | 2.38 | 0.58 |
| 1:A:357:LEU:C | 1:A:358:TYR:HD1 | 2.07 | 0.58 |
| 1:B:356:ARG:HH11 | 1:B:364:LYS:HA | 1.67 | 0.58 |
| 1:C:22:SER:HB3 | 1:C:343:THR:HG23 | 1.85 | 0.58 |
| 1:C:441:LEU:HD12 | 1:C:441:LEU:C | 2.23 | 0.58 |
| 1:D:158:LEU:HD11 | 1:D:332:ILE:HB | 1.85 | 0.58 |
| 1:D:220:VAL:HG21 | 1:D:249:ARG:NE | 2.17 | 0.58 |
| 1:F:263:THR:HB | 1:F:264:PRO:CD | 2.32 | 0.58 |
| 1:A:240:MET:HE2 | 1:A:247:PHE:HZ | 1.69 | 0.58 |
| 1:B:200:TYR:HB2 | 1:B:374:VAL:HG23 | 1.85 | 0.58 |
| 1:D:413:VAL:N | 1:D:414:PRO:CD | 2.66 | 0.58 |
| 1:E:322:GLU:HG2 | 1:E:332:ILE:HD12 | 1.85 | 0.58 |
| 1:F:203:LEU:HD12 | 1:F:225:LEU:CD2 | 2.33 | 0.58 |
| 1:B:426:ILE:HG12 | 1:B:437:GLY:CA | 2.31 | 0.58 |
| 1:C:285:ASN:ND2 | 1:C:285:ASN:H | 1.98 | 0.58 |
| 1:D:162:GLY:O | 1:D:335:ILE:HD11 | 2.03 | 0.58 |
| 1:F:168:LEU:HB3 | 1:F:170:ILE:CG2 | 2.24 | 0.58 |
| 1:F:315:LYS:HE3 | 1:F:336:LEU:O | 2.04 | 0.58 |
| 1:D:98:TRP:O | 1:D:102:THR:HG23 | 2.03 | 0.58 |
| 1:D:402:TYR:OH | 1:D:433:GLU:OE1 | 2.19 | 0.58 |
| 1:D:52:ASN:N | 1:D:52:ASN:ND2 | 2.49 | 0.58 |
| 1:E:158:LEU:HD11 | 1:E:332:ILE:HB | 1.85 | 0.58 |
| 1:A:158:LEU:HD11 | 1:A:332:ILE:HG13 | 1.84 | 0.58 |
| 1:C:208:PHE:O | 1:C:209:LEU:C | 2.42 | 0.58 |
| 1:D:251:PHE:CD1 | 1:D:273:SER:CB | 2.82 | 0.58 |
| 1:D:263:THR:HB | 1:D:264:PRO:HD3 | 1.86 | 0.58 |
| 1:E:40:VAL:O | 1:E:40:VAL:HG22 | 2.03 | 0.58 |
| 1:F:193:THR:HB | 1:F:286:THR:HB | 1.86 | 0.58 |
| 1:F:67:LYS:HE2 | 2:F:600:FAD:H6 | 1.86 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:250:GLN:O | 1:A:251:PHE:CD1 | 2.57 | 0.58 |
| 1:A:30:GLU:O | 1:A:31:ALA:C | 2.41 | 0.58 |
| 1:A:358:TYR:N | 1:A:358:TYR:HD1 | 2.02 | 0.58 |
| 1:B:22:SER:OG | 1:B:343:THR:HG23 | 2.03 | 0.58 |
| 1:C:342:LEU:HB2 | 1:C:345:VAL:CG2 | 2.33 | 0.58 |
| 1:E:223:ILE:HD11 | 1:E:230:GLN:HG3 | 1.84 | 0.58 |
| 1:F:380:TYR:CD1 | 1:F:380:TYR:C | 2.72 | 0.58 |
| 1:B:387:GLU:OE1 | 1:B:424:LYS:NZ | 2.33 | 0.58 |
| 1:C:473:PRO:O | 1:C:473:PRO:HG2 | 2.04 | 0.58 |
| 1:D:425:VAL:HG13 | 1:D:435:VAL:HG13 | 1.86 | 0.58 |
| 1:F:318:VAL:CG2 | 1:F:322:GLU:C | 2.73 | 0.58 |
| 1:B:394:PHE:CE2 | 1:B:428:ASN:ND2 | 2.72 | 0.57 |
| 1:B:431:ASP:OD2 | 1:B:434:ARG:NH1 | 2.37 | 0.57 |
| 1:C:318:VAL:CG1 | 1:C:319:THR:O | 2.52 | 0.57 |
| 1:F:321:GLU:HG2 | 1:F:356:ARG:HH11 | 1.69 | 0.57 |
| 1:E:336:LEU:HB3 | 1:E:339:LYS:CG | 2.34 | 0.57 |
| 1:F:232:MET:O | 1:F:236:ILE:HG13 | 2.04 | 0.57 |
| 1:B:131:TYR:CE1 | 2:B:600:FAD:N6A | 2.71 | 0.57 |
| 1:C:168:LEU:HD23 | 1:C:170:ILE:HD13 | 1.86 | 0.57 |
| 1:D:63:GLY:O | 1:D:66:PRO:HD2 | 2.04 | 0.57 |
| 1:B:263:THR:OG1 | 1:B:264:PRO:HD2 | 2.04 | 0.57 |
| 1:F:186:LEU:HD12 | 1:F:188:TYR:O | 2.04 | 0.57 |
| 1:E:410:GLU:HG2 | 1:F:72:GLN:NE2 | 2.19 | 0.57 |
| 1:A:406:PHE:CZ | 1:A:421:CYS:HB3 | 2.39 | 0.57 |
| 1:F:323:GLN:HG3 | 1:F:330:TYR:CE1 | 2.39 | 0.57 |
| 1:F:97:ASP:C | 1:F:97:ASP:OD1 | 2.43 | 0.57 |
| 1:A:189:CYS:SG | 1:A:190:PRO:HD2 | 2.45 | 0.57 |
| 1:A:205:CYS:HA | 1:A:208:PHE:CE2 | 2.40 | 0.57 |
| 1:E:410:GLU:CG | 1:F:72:GLN:NE2 | 2.67 | 0.57 |
| 1:F:396:GLU:C | 1:F:396:GLU:CD | 2.62 | 0.57 |
| 1:F:400:GLU:OE1 | 1:F:487:ARG:NH1 | 2.38 | 0.57 |
| 1:B:368:ASP:O | 1:B:369:ASN:HB2 | 2.05 | 0.57 |
| 1:D:178:ILE:HB | 1:D:182:ASP:HB2 | 1.85 | 0.57 |
| 1:D:325:ASN:N | 1:D:325:ASN:ND2 | 2.34 | 0.57 |
| 1:C:225:LEU:HB3 | 1:C:228:PHE:HB2 | 1.86 | 0.57 |
| 1:F:39:MET:HE3 | 1:F:41:LEU:HD21 | 1.87 | 0.57 |
| 1:A:418:ASN:HD22 | 1:A:419:ASN:N | 1.99 | 0.56 |
| 1:A:76:LEU:O | 1:A:79:ALA:HB3 | 2.05 | 0.56 |
| 1:C:178:ILE:HB | 1:C:182:ASP:HB2 | 1.86 | 0.56 |
| 1:C:223:ILE:CG1 | 1:C:223:ILE:O | 2.52 | 0.56 |
| 1:D:30:GLU:O | 1:D:33:LYS:HG3 | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:220:VAL:HG21 | 1:A:249:ARG:NE | 2.17 | 0.56 |
| 1:A:90:LEU:HD21 | 1:B:90:LEU:CD2 | 2.35 | 0.56 |
| 1:C:195:VAL:HB | 1:C:218:VAL:HG22 | 1.87 | 0.56 |
| 1:D:426:ILE:HD12 | 1:D:427:CYS:N | 2.20 | 0.56 |
| 1:F:258:GLN:HE22 | 1:F:261:ALA:HB2 | 1.69 | 0.56 |
| 1:F:440:VAL:O | 1:F:440:VAL:HG13 | 2.04 | 0.56 |
| 1:D:62:VAL:HG23 | 1:D:62:VAL:O | 2.04 | 0.56 |
| 1:E:411:TRP:O | 1:E:414:PRO:HD2 | 2.06 | 0.56 |
| 1:F:82:ASP:OD1 | 1:F:416:ARG:NH1 | 2.38 | 0.56 |
| 1:C:137:PRO:O | 1:C:138:HIS:HB2 | 2.05 | 0.56 |
| 1:F:168:LEU:HD23 | 1:F:170:ILE:HD13 | 1.87 | 0.56 |
| 1:E:471:ILE:HG21 | 1:F:373:THR:CG2 | 2.34 | 0.56 |
| 1:B:173:ASP:OD1 | 1:B:174:LYS:N | 2.34 | 0.56 |
| 1:B:25:LEU:HD13 | 1:B:116:TYR:CD1 | 2.41 | 0.56 |
| 1:B:403:HIS:NE2 | 1:B:492:ILE:HD13 | 2.21 | 0.56 |
| 1:C:194:LEU:HD23 | 1:C:194:LEU:C | 2.25 | 0.56 |
| 1:C:493:LEU:HD12 | 1:C:493:LEU:N | 2.19 | 0.56 |
| 1:D:108:HIS:CE1 | 1:D:112:LEU:HD11 | 2.40 | 0.56 |
| 1:F:34:PHE:HZ | 1:F:355:GLN:NE2 | 2.03 | 0.56 |
| 1:A:188:TYR:CD2 | 1:A:263:THR:HB | 2.40 | 0.56 |
| 1:B:325:ASN:H | 1:B:325:ASN:ND2 | 2.03 | 0.56 |
| 1:B:65:ILE:CB | 1:B:66:PRO:CD | 2.82 | 0.56 |
| 1:D:250:GLN:O | 1:D:251:PHE:CD1 | 2.59 | 0.56 |
| 1:D:91:GLU:O | 1:D:93:THR:N | 2.39 | 0.56 |
| 1:C:172:GLY:CA | 1:C:175:GLU:HG3 | 2.24 | 0.56 |
| 1:D:434:ARG:HG2 | 1:D:434:ARG:HH11 | 1.71 | 0.56 |
| 1:E:170:ILE:HD11 | 1:E:253:PRO:HB2 | 1.86 | 0.56 |
| 1:F:291:VAL:CG1 | 1:F:291:VAL:O | 2.53 | 0.56 |
| 1:D:83:SER:HB2 | 1:D:88:TRP:HB2 | 1.87 | 0.56 |
| 1:E:215:ASP:C | 1:E:215:ASP:OD1 | 2.44 | 0.56 |
| 1:F:96:HIS:CD2 | 1:F:212:ILE:HG13 | 2.41 | 0.56 |
| 1:B:263:THR:HB | 1:B:264:PRO:HD3 | 1.88 | 0.56 |
| 1:B:239:HIS:CE1 | 1:B:378:LEU:HB2 | 2.41 | 0.56 |
| 1:D:51:THR:C | 1:D:52:ASN:ND2 | 2.59 | 0.56 |
| 1:E:373:THR:HG23 | 1:F:471:ILE:CG2 | 2.36 | 0.56 |
| 1:F:221:ARG:HH11 | 1:F:221:ARG:CG | 2.19 | 0.56 |
| 1:A:343:THR:HB | 1:A:344:PRO:HD3 | 1.88 | 0.55 |
| 1:B:70:MET:SD | 1:B:101:MET:CE | 2.94 | 0.55 |
| 1:B:321:GLU:O | 1:B:322:GLU:HB2 | 2.04 | 0.55 |
| 1:C:200:TYR:O | 1:C:204:GLU:HB2 | 2.06 | 0.55 |
| 1:C:259:ILE:HG23 | 1:C:259:ILE:O | 2.06 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:321:GLU:HG3 | 1:C:356:ARG:NH1 | 2.21 | 0.55 |
| 1:D:316:ILE:HG13 | 1:D:335:ILE:HG22 | 1.88 | 0.55 |
| 1:F:474:VAL:O | 1:F:477:GLU:HG2 | 2.06 | 0.55 |
| 1:B:199:SER:HA | 1:B:225:LEU:HD23 | 1.88 | 0.55 |
| 1:D:406:PHE:CZ | 1:D:421:CYS:HB3 | 2.41 | 0.55 |
| 1:E:267:LEU:HD13 | 1:E:267:LEU:N | 2.21 | 0.55 |
| 1:C:133:LYS:C | 1:C:140:ILE:HG13 | 2.26 | 0.55 |
| 1:D:163:GLU:OE2 | 1:D:334:ASP:HB3 | 2.07 | 0.55 |
| 1:E:38:VAL:HG23 | 1:E:125:VAL:HG13 | 1.87 | 0.55 |
| 1:A:400:GLU:OE1 | 1:A:400:GLU:HA | 2.06 | 0.55 |
| 1:A:401:VAL:HG12 | 1:A:401:VAL:O | 2.07 | 0.55 |
| 1:C:15:LEU:HD12 | 1:C:156:ARG:O | 2.07 | 0.55 |
| 1:A:47:THR:HG21 | 1:A:51:THR:OG1 | 2.07 | 0.55 |
| 1:C:66:PRO:HG3 | 1:C:109:ILE:HD11 | 1.88 | 0.55 |
| 1:D:324:THR:HG23 | 1:D:329:ILE:O | 2.07 | 0.55 |
| 1:E:256:ILE:CD1 | 1:E:269:VAL:HG22 | 2.28 | 0.55 |
| 1:A:173:ASP:O | 1:A:177:CYS:HB2 | 2.06 | 0.55 |
| 1:C:340:LEU:HG | 1:C:370:VAL:HG21 | 1.88 | 0.55 |
| 1:D:175:GLU:N | 1:D:175:GLU:OE1 | 2.39 | 0.55 |
| 1:F:158:LEU:HD12 | 1:F:159:ILE:N | 2.22 | 0.55 |
| 1:A:108:HIS:O | 1:A:111:SER:HB3 | 2.06 | 0.55 |
| 1:B:192:LYS:H | 1:B:285:ASN:ND2 | 2.01 | 0.55 |
| 1:B:65:ILE:HB | 1:B:66:PRO:CD | 2.37 | 0.55 |
| 1:C:310:ASN:HD22 | 1:C:311:GLU:N | 2.04 | 0.55 |
| 1:D:114:TRP:CZ3 | 1:D:118:VAL:CG2 | 2.90 | 0.55 |
| 1:D:407:TRP:CD1 | 1:D:418:ASN:HA | 2.41 | 0.55 |
| 1:D:67:LYS:HD3 | 1:D:204:GLU:OE1 | 2.05 | 0.55 |
| 1:E:373:THR:HG23 | 1:F:471:ILE:HG21 | 1.89 | 0.55 |
| 1:C:21:GLY:HA2 | 1:C:57:GLY:HA3 | 1.88 | 0.55 |
| 1:D:194:LEU:HB2 | 1:D:284:PHE:CE2 | 2.42 | 0.55 |
| 1:E:141:MET:CE | 1:E:149:GLU:OE2 | 2.55 | 0.55 |
| 1:E:497:CYS:SG | 1:F:116:TYR:CD2 | 2.98 | 0.55 |
| 1:A:168:LEU:O | 1:A:173:ASP:OD2 | 2.25 | 0.55 |
| 1:F:428:ASN:ND2 | 1:F:431:ASP:HB2 | 2.21 | 0.55 |
| 1:B:419:ASN:O | 1:B:420:LYS:HD3 | 2.07 | 0.54 |
| 1:B:461:THR:OG1 | 1:B:464:GLN:HG3 | 2.07 | 0.54 |
| 1:A:447:GLU:CD | 1:B:474:VAL:HG13 | 2.28 | 0.54 |
| 1:E:192:LYS:N | 1:E:285:ASN:HD22 | 2.02 | 0.54 |
| 1:C:319:THR:C | 1:C:321:GLU:H | 2.08 | 0.54 |
| 1:C:72:GLN:HE21 | 1:D:410:GLU:CB | 2.05 | 0.54 |
| 1:D:221:ARG:NH1 | 3:D:601:NDP:P2B | 2.80 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:61:ASN:HA | 1:E:109:ILE:HD13 | 1.88 | 0.54 |
| 1:F:343:THR:O | 1:F:347:ILE:HG23 | 2.07 | 0.54 |
| 1:F:68:LYS:HE2 | 1:F:375:PHE:CE2 | 2.43 | 0.54 |
| 1:A:196:VAL:O | 1:A:291:VAL:HG22 | 2.07 | 0.54 |
| 1:A:65:ILE:CB | 1:A:66:PRO:HD3 | 2.37 | 0.54 |
| 1:C:190:PRO:O | 1:C:191:GLY:C | 2.46 | 0.54 |
| 1:C:47:THR:CB | 1:C:48:PRO:CD | 2.85 | 0.54 |
| 1:F:60:VAL:HG13 | 1:F:112:LEU:HD13 | 1.89 | 0.54 |
| 1:F:318:VAL:HG21 | 1:F:322:GLU:C | 2.28 | 0.54 |
| 1:C:308:LYS:H | 1:C:325:ASN:ND2 | 2.06 | 0.54 |
| 1:C:309:ILE:HG13 | 1:C:309:ILE:O | 2.07 | 0.54 |
| 1:E:70:MET:HG2 | 1:E:101:MET:CE | 2.38 | 0.54 |
| 1:E:185:SER:O | 1:E:186:LEU:C | 2.43 | 0.54 |
| 1:E:272:LYS:CE | 1:E:276:SER:HA | 2.37 | 0.54 |
| 1:E:38:VAL:HG22 | 1:E:125:VAL:HG22 | 1.89 | 0.54 |
| 1:F:13:PHE:O | 1:F:154:ALA:HA | 2.08 | 0.54 |
| 1:F:277:GLU:OE1 | 1:F:277:GLU:HA | 2.07 | 0.54 |
| 1:A:272:LYS:CE | 1:A:276:SER:HA | 2.36 | 0.54 |
| 1:A:98:TRP:CD1 | 1:A:102:THR:CG2 | 2.90 | 0.54 |
| 1:B:402:TYR:CE2 | 1:B:462:LYS:HE3 | 2.41 | 0.54 |
| 1:C:343:THR:N | 2:C:600:FAD:HO3' | 2.06 | 0.54 |
| 1:F:221:ARG:NH1 | 3:F:601:NDP:O3X | 2.41 | 0.54 |
| 1:A:12:ASP:HB2 | 1:A:153:SER:O | 2.08 | 0.54 |
| 1:B:123:LYS:O | 1:B:124:LYS:HB2 | 2.07 | 0.54 |
| 1:C:193:THR:OG1 | 1:C:194:LEU:N | 2.39 | 0.54 |
| 1:E:305:VAL:O | 1:E:305:VAL:HG12 | 2.08 | 0.54 |
| 1:E:232:MET:CE | 1:E:441:LEU:HB2 | 2.34 | 0.54 |
| 1:C:286:THR:HG22 | 1:C:286:THR:O | 2.07 | 0.54 |
| 1:C:370:VAL:O | 1:C:370:VAL:HG23 | 2.07 | 0.54 |
| 1:D:236:ILE:CG1 | 1:D:441:LEU:HD11 | 2.38 | 0.54 |
| 1:D:343:THR:CB | 1:D:344:PRO:CD | 2.84 | 0.54 |
| 1:D:426:ILE:C | 1:D:426:ILE:HD12 | 2.29 | 0.54 |
| 1:E:383:CYS:SG | 1:E:456:LEU:HD12 | 2.48 | 0.54 |
| 1:A:98:TRP:HE1 | 1:A:102:THR:HG21 | 1.70 | 0.54 |
| 1:D:418:ASN:ND2 | 1:D:419:ASN:N | 2.56 | 0.54 |
| 1:E:426:ILE:O | 1:E:426:ILE:HG13 | 2.07 | 0.54 |
| 1:A:177:CYS:SG | 1:A:256:ILE:HD12 | 2.47 | 0.53 |
| 1:B:332:ILE:HG12 | 1:B:333:GLY:N | 2.23 | 0.53 |
| 1:A:90:LEU:CD2 | 1:B:90:LEU:HD21 | 2.36 | 0.53 |
| 1:D:78:GLN:NE2 | 1:D:82:ASP:OD1 | 2.41 | 0.53 |
| 1:F:192:LYS:N | 1:F:285:ASN:ND2 | 2.44 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:191:GLY:O | 1:A:193:THR:CG2 | 2.56 | 0.53 |
| 1:A:313:THR:O | 1:A:315:LYS:N | 2.42 | 0.53 |
| 1:B:172:GLY:HA2 | 1:B:175:GLU:CG | 2.37 | 0.53 |
| 1:B:222:SER:OG | 3:B:601:NDP:O3X | 2.24 | 0.53 |
| 1:C:376:THR:HB | 1:C:377:PRO:CD | 2.39 | 0.53 |
| 1:E:141:MET:HE1 | 1:E:149:GLU:OE2 | 2.09 | 0.53 |
| 1:B:472:HIS:ND1 | 1:B:473:PRO:HA | 2.23 | 0.53 |
| 1:D:478:ILE:N | 1:D:478:ILE:HD12 | 2.24 | 0.53 |
| 1:D:98:TRP:CE2 | 1:D:102:THR:HG21 | 2.43 | 0.53 |
| 1:F:470:GLY:HA2 | 1:F:480:THR:HG21 | 1.89 | 0.53 |
| 1:B:131:TYR:CE2 | 2:B:600:FAD:N6A | 2.77 | 0.53 |
| 1:C:432:ASN:O | 1:C:433:GLU:HB2 | 2.08 | 0.53 |
| 1:D:144:ASN:HD22 | 1:D:146:LYS:N | 1.99 | 0.53 |
| 1:E:323:GLN:HB2 | 1:E:330:TYR:HE1 | 1.74 | 0.53 |
| 1:A:240:MET:HE2 | 1:A:247:PHE:CZ | 2.43 | 0.53 |
| 1:A:478:ILE:H | 1:A:478:ILE:CD1 | 2.04 | 0.53 |
| 1:C:34:PHE:CD1 | 1:C:34:PHE:N | 2.75 | 0.53 |
| 1:D:66:PRO:HG3 | 1:D:109:ILE:HD11 | 1.91 | 0.53 |
| 1:A:99:GLU:CG | 1:D:146:LYS:HD3 | 2.35 | 0.53 |
| 1:D:263:THR:CB | 1:D:264:PRO:HD3 | 2.39 | 0.53 |
| 1:C:447:GLU:CD | 1:D:474:VAL:HG13 | 2.29 | 0.53 |
| 1:D:221:ARG:HH12 | 3:D:601:NDP:P2B | 2.31 | 0.53 |
| 1:E:431:ASP:OD1 | 1:E:431:ASP:O | 2.25 | 0.53 |
| 1:F:318:VAL:HG23 | 1:F:323:GLN:O | 2.09 | 0.53 |
| 1:B:281:GLU:O | 1:B:282:ASP:O | 2.26 | 0.53 |
| 1:C:103:GLU:O | 1:C:107:ASN:HB2 | 2.08 | 0.53 |
| 1:D:272:LYS:CG | 1:D:273:SER:N | 2.70 | 0.53 |
| 1:F:438:PHE:CE1 | 1:F:479:PHE:CE1 | 2.96 | 0.53 |
| 1:A:249:ARG:HB3 | 1:A:250:GLN:HE22 | 1.73 | 0.53 |
| 1:C:58:THR:HB | 2:C:600:FAD:O2A | 2.09 | 0.53 |
| 1:C:376:THR:HB | 1:C:377:PRO:HD2 | 1.90 | 0.53 |
| 1:F:194:LEU:HB2 | 1:F:284:PHE:CE2 | 2.44 | 0.53 |
| 1:A:163:GLU:HB3 | 1:A:295:SER:HA | 1.91 | 0.53 |
| 1:C:310:ASN:HD22 | 1:C:310:ASN:C | 2.12 | 0.53 |
| 1:C:421:CYS:HA | 1:C:441:LEU:O | 2.09 | 0.53 |
| 1:E:336:LEU:HB3 | 1:E:339:LYS:HG2 | 1.91 | 0.53 |
| 1:E:414:PRO:O | 1:E:415:SER:HB2 | 2.09 | 0.53 |
| 1:B:263:THR:OG1 | 1:B:264:PRO:CD | 2.57 | 0.52 |
| 1:C:283:GLU:CD | 1:C:283:GLU:H | 2.12 | 0.52 |
| 1:C:404:SER:HA | 1:C:492:ILE:HG21 | 1.89 | 0.52 |
| 1:F:224:LEU:HD21 | 1:F:249:ARG:NH1 | 2.24 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:22:SER:CB | 1:F:343:THR:HG23 | 2.39 | 0.52 |
| 1:B:371:PRO:CG | 1:B:453:ALA:HB1 | 2.37 | 0.52 |
| 1:A:471:ILE:CG2 | 1:B:373:THR:HG23 | 2.39 | 0.52 |
| 1:C:356:ARG:HG2 | 1:C:361:SER:O | 2.07 | 0.52 |
| 1:D:144:ASN:HB2 | 1:D:148:LYS:O | 2.09 | 0.52 |
| 1:E:321:GLU:O | 1:E:356:ARG:NH1 | 2.40 | 0.52 |
| 1:F:263:THR:O | 1:F:265:GLY:N | 2.42 | 0.52 |
| 1:A:98:TRP:NE1 | 1:A:102:THR:CG2 | 2.63 | 0.52 |
| 1:C:221:ARG:O | 1:C:250:GLN:HA | 2.09 | 0.52 |
| 1:C:178:ILE:HD11 | 1:C:286:THR:HG22 | 1.90 | 0.52 |
| 1:D:13:PHE:O | 1:D:154:ALA:HA | 2.09 | 0.52 |
| 1:F:267:LEU:O | 1:F:283:GLU:HA | 2.10 | 0.52 |
| 1:A:220:VAL:O | 1:A:220:VAL:HG23 | 2.08 | 0.52 |
| 1:A:273:SER:OG | 1:A:275:ASN:HB3 | 2.09 | 0.52 |
| 1:A:411:TRP:O | 1:A:414:PRO:HD2 | 2.09 | 0.52 |
| 1:B:29:LYS:HG2 | 1:B:30:GLU:N | 2.24 | 0.52 |
| 1:C:291:VAL:HG13 | 3:C:601:NDP:C4A | 2.39 | 0.52 |
| 1:A:321:GLU:O | 1:A:322:GLU:HB2 | 2.09 | 0.52 |
| 1:A:424:LYS:HG2 | 1:A:439:HIS:HB2 | 1.91 | 0.52 |
| 1:C:60:VAL:O | 1:C:109:ILE:HD13 | 2.08 | 0.52 |
| 1:E:205:CYS:HA | 1:E:208:PHE:CE2 | 2.44 | 0.52 |
| 1:F:110:GLY:HA2 | 1:F:113:ASN:ND2 | 2.22 | 0.52 |
| 1:F:258:GLN:NE2 | 1:F:261:ALA:N | 2.58 | 0.52 |
| 1:A:200:TYR:O | 1:A:204:GLU:HG3 | 2.09 | 0.52 |
| 3:A:601:NDP:O2N | 3:A:601:NDP:O5B | 2.27 | 0.52 |
| 1:A:450:GLN:HE22 | 1:B:471:ILE:H | 1.58 | 0.52 |
| 1:C:114:TRP:CE3 | 1:C:117:ARG:HD2 | 2.45 | 0.52 |
| 1:D:272:LYS:NZ | 1:D:276:SER:HA | 2.25 | 0.52 |
| 1:E:186:LEU:CD2 | 1:E:188:TYR:CZ | 2.93 | 0.52 |
| 1:E:273:SER:CB | 1:E:275:ASN:OD1 | 2.58 | 0.52 |
| 1:B:55:LEU:HD13 | 1:B:116:TYR:CB | 2.40 | 0.52 |
| 1:B:277:GLU:HG2 | 1:B:278:GLU:N | 2.25 | 0.52 |
| 1:C:71:HIS:O | 1:C:74:ALA:HB3 | 2.10 | 0.52 |
| 1:D:250:GLN:O | 1:D:273:SER:HB3 | 2.07 | 0.52 |
| 1:F:167:TYR:CE2 | 1:F:174:LYS:HA | 2.45 | 0.52 |
| 1:B:319:THR:CG2 | 1:B:323:GLN:HB3 | 2.39 | 0.52 |
| 1:B:488:SER:OG | 1:B:489:GLY:N | 2.43 | 0.52 |
| 1:C:116:TYR:O | 1:C:119:ALA:HB3 | 2.10 | 0.52 |
| 1:C:224:LEU:HD11 | 1:C:249:ARG:HH12 | 1.75 | 0.52 |
| 1:C:366:ASP:C | 1:C:366:ASP:OD1 | 2.48 | 0.52 |
| 1:D:343:THR:HB | 1:D:344:PRO:HD3 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:193:THR:HB | 1:A:286:THR:O | 2.10 | 0.52 |
| 1:A:67:LYS:HD2 | 1:A:68:LYS:N | 2.24 | 0.52 |
| 1:E:373:THR:HB | 1:E:381:GLY:HA2 | 1.91 | 0.52 |
| 1:F:141:MET:CE | 1:F:143:THR:OG1 | 2.58 | 0.52 |
| 1:F:336:LEU:HB3 | 1:F:339:LYS:HG2 | 1.92 | 0.52 |
| 1:A:82:ASP:OD2 | 1:A:416:ARG:NH1 | 2.40 | 0.52 |
| 1:B:91:GLU:OE1 | 1:B:91:GLU:C | 2.48 | 0.52 |
| 1:C:114:TRP:O | 1:C:118:VAL:HG23 | 2.10 | 0.52 |
| 1:D:317:PRO:C | 1:D:318:VAL:HG13 | 2.31 | 0.52 |
| 1:D:336:LEU:HB3 | 1:D:339:LYS:CG | 2.40 | 0.52 |
| 1:E:172:GLY:HA2 | 1:E:175:GLU:HG2 | 1.92 | 0.52 |
| 1:B:380:TYR:OH | 1:B:439:HIS:HD2 | 1.93 | 0.51 |
| 1:C:308:LYS:H | 1:C:325:ASN:HD21 | 1.58 | 0.51 |
| 1:C:348:GLN:O | 1:C:352:LEU:HB2 | 2.10 | 0.51 |
| 1:D:407:TRP:CD2 | 1:D:418:ASN:CG | 2.83 | 0.51 |
| 1:A:310:ASN:HD22 | 1:A:312:LYS:H | 1.58 | 0.51 |
| 1:B:61:ASN:HA | 1:B:109:ILE:HD13 | 1.91 | 0.51 |
| 1:C:138:HIS:HD2 | 1:C:328:TYR:CE2 | 2.29 | 0.51 |
| 1:D:336:LEU:HB3 | 1:D:339:LYS:HG2 | 1.93 | 0.51 |
| 1:E:108:HIS:NE2 | 1:F:412:THR:HG21 | 2.25 | 0.51 |
| 1:E:203:LEU:HD22 | 1:E:240:MET:SD | 2.50 | 0.51 |
| 1:A:29:LYS:HG3 | 1:A:30:GLU:N | 2.24 | 0.51 |
| 1:A:440:VAL:HB | 1:A:479:PHE:CZ | 2.45 | 0.51 |
| 1:B:440:VAL:O | 1:B:440:VAL:HG13 | 2.09 | 0.51 |
| 1:C:168:LEU:HB3 | 1:C:170:ILE:HG23 | 1.92 | 0.51 |
| 1:C:403:HIS:CE1 | 1:C:492:ILE:CD1 | 2.87 | 0.51 |
| 1:E:343:THR:HB | 1:E:344:PRO:CD | 2.35 | 0.51 |
| 1:F:469:ILE:N | 1:F:469:ILE:CD1 | 2.67 | 0.51 |
| 1:E:450:GLN:NE2 | 1:F:470:GLY:HA2 | 2.23 | 0.51 |
| 1:C:285:ASN:ND2 | 1:C:285:ASN:N | 2.54 | 0.51 |
| 1:C:161:THR:HG23 | 1:C:335:ILE:HD13 | 1.92 | 0.51 |
| 1:D:272:LYS:CE | 1:D:276:SER:HA | 2.41 | 0.51 |
| 1:D:402:TYR:CD2 | 1:D:462:LYS:HE2 | 2.45 | 0.51 |
| 1:E:343:THR:CB | 1:E:344:PRO:CD | 2.89 | 0.51 |
| 1:A:474:VAL:HG13 | 1:B:447:GLU:CD | 2.31 | 0.51 |
| 1:C:212:ILE:O | 1:C:212:ILE:CG2 | 2.58 | 0.51 |
| 1:C:20:GLY:HA2 | 1:C:25:LEU:HD21 | 1.92 | 0.51 |
| 1:E:161:THR:HB | 2:E:600:FAD:C8A | 2.41 | 0.51 |
| 1:E:208:PHE:CE1 | 1:E:209:LEU:HD13 | 2.46 | 0.51 |
| 1:F:332:ILE:HG23 | 1:F:333:GLY:N | 2.25 | 0.51 |
| 1:A:402:TYR:CD2 | 1:A:485:THR:HG22 | 2.45 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:98:TRP:O | 1:C:102:THR:OG1 | 2.28 | 0.51 |
| 1:C:361:SER:OG | 1:C:363:VAL:HG22 | 2.11 | 0.51 |
| 1:C:478:ILE:HD12 | 1:C:479:PHE:H | 1.76 | 0.51 |
| 1:D:405:PHE:CD1 | 1:D:492:ILE:HD12 | 2.45 | 0.51 |
| 1:A:131:TYR:CE1 | 2:A:600:FAD:N6A | 2.79 | 0.51 |
| 1:A:310:ASN:C | 1:A:310:ASN:ND2 | 2.64 | 0.51 |
| 1:A:345:VAL:HG22 | 1:B:469:ILE:HD13 | 1.91 | 0.51 |
| 1:B:305:VAL:CG1 | 1:B:328:TYR:OH | 2.59 | 0.51 |
| 1:B:409:LEU:O | 1:B:412:THR:HG23 | 2.10 | 0.51 |
| 1:C:260:GLU:HB2 | 1:C:266:ARG:HB3 | 1.93 | 0.51 |
| 1:C:251:PHE:HE2 | 1:C:279:THR:HG1 | 1.59 | 0.51 |
| 1:A:380:TYR:OH | 1:A:439:HIS:HD2 | 1.93 | 0.51 |
| 1:C:405:PHE:H | 1:C:492:ILE:CG2 | 2.22 | 0.51 |
| 1:C:412:THR:O | 1:C:415:SER:N | 2.40 | 0.51 |
| 1:C:86:TYR:O | 1:D:101:MET:HB2 | 2.10 | 0.51 |
| 1:D:291:VAL:HG22 | 3:D:601:NDP:C4A | 2.41 | 0.51 |
| 1:F:434:ARG:HG2 | 1:F:434:ARG:NH1 | 2.20 | 0.51 |
| 1:A:229:ASP:OD1 | 1:A:229:ASP:C | 2.49 | 0.51 |
| 1:A:318:VAL:HG13 | 1:A:322:GLU:HA | 1.89 | 0.51 |
| 1:A:308:LYS:N | 1:A:325:ASN:HD21 | 2.03 | 0.51 |
| 1:B:328:TYR:HD1 | 1:B:328:TYR:H | 1.59 | 0.51 |
| 1:D:376:THR:HB | 1:D:377:PRO:CD | 2.41 | 0.51 |
| 1:E:68:LYS:O | 1:E:71:HIS:HB3 | 2.11 | 0.51 |
| 1:F:281:GLU:OE1 | 1:F:281:GLU:HA | 2.10 | 0.51 |
| 1:A:236:ILE:HD11 | 1:A:380:TYR:CD2 | 2.45 | 0.51 |
| 1:A:428:ASN:ND2 | 1:A:431:ASP:CB | 2.74 | 0.51 |
| 1:A:96:HIS:CD2 | 1:A:212:ILE:HG23 | 2.46 | 0.51 |
| 1:B:281:GLU:C | 1:B:282:ASP:O | 2.49 | 0.51 |
| 1:B:67:LYS:HE2 | 1:B:204:GLU:OE2 | 2.10 | 0.51 |
| 1:C:67:LYS:HE2 | 2:C:600:FAD:H6 | 1.92 | 0.51 |
| 1:C:448:VAL:HG12 | 1:D:447:GLU:HB3 | 1.92 | 0.51 |
| 1:E:438:PHE:CZ | 1:E:452:PHE:CD2 | 2.98 | 0.51 |
| 1:F:275:ASN:OD1 | 1:F:277:GLU:HG2 | 2.11 | 0.51 |
| 1:A:480:THR:HG23 | 1:A:481:THR:HG23 | 1.93 | 0.50 |
| 1:B:70:MET:SD | 1:B:101:MET:HE3 | 2.51 | 0.50 |
| 1:B:68:LYS:HE2 | 1:B:375:PHE:CE2 | 2.46 | 0.50 |
| 1:B:402:TYR:HB3 | 1:B:482:LEU:HB3 | 1.93 | 0.50 |
| 1:D:478:ILE:HD12 | 1:D:479:PHE:N | 2.26 | 0.50 |
| 1:E:140:ILE:HG23 | 1:E:140:ILE:O | 2.10 | 0.50 |
| 1:E:426:ILE:HG12 | 1:E:437:GLY:CA | 2.38 | 0.50 |
| 1:F:58:THR:HG22 | 1:F:62:VAL:CG2 | 2.41 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:258:GLN:NE2 | 1:B:261:ALA:HB2 | 2.26 | 0.50 |
| 1:B:326:VAL:CG1 | 1:B:328:TYR:CE1 | 2.95 | 0.50 |
| 1:B:67:LYS:NZ | 2:B:600:FAD:O4 | 2.44 | 0.50 |
| 1:C:106:GLN:HA | 1:C:109:ILE:HG13 | 1.93 | 0.50 |
| 1:C:220:VAL:HG21 | 1:C:249:ARG:CD | 2.40 | 0.50 |
| 1:C:250:GLN:O | 1:C:273:SER:HB2 | 2.11 | 0.50 |
| 1:C:449:THR:O | 1:C:450:GLN:C | 2.49 | 0.50 |
| 1:D:317:PRO:O | 1:D:318:VAL:HG12 | 2.11 | 0.50 |
| 1:F:309:ILE:HG13 | 1:F:309:ILE:O | 2.10 | 0.50 |
| 1:A:320:ASP:OD1 | 1:A:320:ASP:C | 2.50 | 0.50 |
| 1:A:357:LEU:C | 1:A:358:TYR:CD1 | 2.85 | 0.50 |
| 2:A:600:FAD:O2A | 2:A:600:FAD:O5' | 2.27 | 0.50 |
| 1:C:223:ILE:HD12 | 1:C:230:GLN:NE2 | 2.26 | 0.50 |
| 1:C:55:LEU:HD22 | 1:C:56:GLY:N | 2.26 | 0.50 |
| 1:F:273:SER:OG | 1:F:275:ASN:HB3 | 2.12 | 0.50 |
| 1:C:66:PRO:O | 1:C:70:MET:HB2 | 2.12 | 0.50 |
| 1:D:411:TRP:CE2 | 1:D:416:ARG:NH2 | 2.80 | 0.50 |
| 1:E:487:ARG:HG3 | 1:E:487:ARG:O | 2.11 | 0.50 |
| 1:F:348:GLN:HG2 | 1:F:351:ARG:NH1 | 2.27 | 0.50 |
| 1:F:58:THR:OG1 | 2:F:600:FAD:O1A | 2.29 | 0.50 |
| 1:A:268:LYS:HE2 | 1:A:280:ILE:HD12 | 1.93 | 0.50 |
| 1:B:168:LEU:HD13 | 1:B:168:LEU:N | 2.27 | 0.50 |
| 1:B:256:ILE:HG13 | 1:B:256:ILE:O | 2.12 | 0.50 |
| 1:C:266:ARG:HG3 | 1:C:283:GLU:HB3 | 1.94 | 0.50 |
| 2:C:600:FAD:O1A | 2:C:600:FAD:H5'1 | 2.12 | 0.50 |
| 1:C:58:THR:OG1 | 2:C:600:FAD:O2A | 2.30 | 0.50 |
| 1:C:80:LEU:O | 1:C:81:LYS:C | 2.50 | 0.50 |
| 1:A:387:GLU:OE2 | 1:A:486:LYS:NZ | 2.42 | 0.50 |
| 1:A:438:PHE:CE2 | 1:A:452:PHE:CG | 3.00 | 0.50 |
| 1:C:252:VAL:CG1 | 1:C:253:PRO:HD2 | 2.42 | 0.50 |
| 1:C:133:LYS:HA | 1:C:301:GLY:H | 1.77 | 0.50 |
| 1:C:387:GLU:HA | 1:C:426:ILE:HD13 | 1.93 | 0.50 |
| 1:C:75:LEU:O | 1:C:78:GLN:N | 2.43 | 0.50 |
| 1:D:193:THR:HG23 | 1:D:286:THR:O | 2.12 | 0.50 |
| 1:E:170:ILE:CD1 | 1:E:253:PRO:HB2 | 2.41 | 0.50 |
| 1:E:34:PHE:CE2 | 1:E:359:GLY:HA2 | 2.46 | 0.50 |
| 1:E:71:HIS:CD2 | 1:E:375:PHE:HB3 | 2.46 | 0.50 |
| 1:A:204:GLU:OE2 | 1:A:375:PHE:N | 2.40 | 0.50 |
| 1:A:62:VAL:O | 1:A:62:VAL:HG23 | 2.11 | 0.50 |
| 1:A:91:GLU:O | 1:A:93:THR:N | 2.45 | 0.50 |
| 1:C:189:CYS:C | 1:C:191:GLY:H | 2.15 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:228:PHE:O | 1:C:229:ASP:C | 2.48 | 0.50 |
| 1:C:220:VAL:CG2 | 1:C:249:ARG:HD2 | 2.41 | 0.50 |
| 1:C:365:CYS:SG | 1:C:367:TYR:CZ | 3.05 | 0.50 |
| 1:C:75:LEU:O | 1:C:76:LEU:C | 2.49 | 0.50 |
| 1:D:170:ILE:O | 1:D:170:ILE:HG13 | 2.12 | 0.50 |
| 1:B:168:LEU:O | 1:B:173:ASP:OD2 | 2.30 | 0.50 |
| 1:B:318:VAL:HG22 | 1:B:323:GLN:O | 2.11 | 0.50 |
| 1:D:167:TYR:CE2 | 1:D:174:LYS:HA | 2.46 | 0.50 |
| 1:E:195:VAL:HG21 | 1:E:206:ALA:HB2 | 1.93 | 0.50 |
| 1:F:34:PHE:HZ | 1:F:355:GLN:HE22 | 1.58 | 0.50 |
| 1:B:172:GLY:O | 1:B:175:GLU:HG2 | 2.12 | 0.50 |
| 1:C:164:ARG:HB3 | 1:C:165:PRO:CD | 2.36 | 0.50 |
| 1:F:172:GLY:HA2 | 1:F:175:GLU:CG | 2.41 | 0.50 |
| 1:F:209:LEU:HG | 1:F:214:LEU:HD12 | 1.94 | 0.50 |
| 1:F:434:ARG:CG | 1:F:434:ARG:HH11 | 2.18 | 0.50 |
| 1:B:216:VAL:HG12 | 1:B:217:THR:N | 2.26 | 0.49 |
| 1:B:472:HIS:HD1 | 1:B:473:PRO:HA | 1.77 | 0.49 |
| 1:D:267:LEU:N | 1:D:267:LEU:HD13 | 2.27 | 0.49 |
| 1:D:407:TRP:CB | 1:D:418:ASN:HD21 | 2.22 | 0.49 |
| 1:E:162:GLY:O | 1:E:335:ILE:HD11 | 2.12 | 0.49 |
| 1:C:163:GLU:O | 1:C:164:ARG:HG2 | 2.12 | 0.49 |
| 1:C:209:LEU:HD12 | 1:C:214:LEU:HD12 | 1.94 | 0.49 |
| 1:E:413:VAL:N | 1:E:414:PRO:CD | 2.75 | 0.49 |
| 1:E:460:LEU:HA | 1:F:458:CYS:SG | 2.53 | 0.49 |
| 1:F:371:PRO:O | 1:F:371:PRO:HG2 | 2.12 | 0.49 |
| 1:F:380:TYR:CD1 | 1:F:381:GLY:N | 2.80 | 0.49 |
| 1:B:319:THR:HG21 | 1:B:323:GLN:HB3 | 1.93 | 0.49 |
| 1:C:225:LEU:N | 1:C:225:LEU:HD12 | 2.27 | 0.49 |
| 1:C:232:MET:O | 1:C:233:ALA:C | 2.48 | 0.49 |
| 1:C:43:PHE:HD1 | 1:C:44:VAL:O | 1.95 | 0.49 |
| 1:D:249:ARG:HB3 | 1:D:250:GLN:NE2 | 2.27 | 0.49 |
| 1:E:119:ALA:O | 1:E:123:LYS:HG3 | 2.12 | 0.49 |
| 1:F:270:THR:HG22 | 1:F:280:ILE:HG22 | 1.94 | 0.49 |
| 1:F:395:GLY:O | 1:F:396:GLU:C | 2.51 | 0.49 |
| 1:A:295:SER:HB3 | 1:A:335:ILE:CD1 | 2.39 | 0.49 |
| 1:C:205:CYS:C | 1:C:207:GLY:N | 2.66 | 0.49 |
| 1:C:239:HIS:CE1 | 1:C:378:LEU:HG | 2.48 | 0.49 |
| 1:D:409:LEU:HD12 | 1:D:409:LEU:O | 2.12 | 0.49 |
| 1:E:404:SER:CB | 1:E:478:ILE:HD11 | 2.40 | 0.49 |
| 1:F:180:SER:O | 1:F:181:ASP:C | 2.51 | 0.49 |
| 1:A:387:GLU:HA | 1:A:426:ILE:HD13 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:225:LEU:HD12 | 1:C:225:LEU:H | 1.78 | 0.49 |
| 1:C:342:LEU:HB2 | 1:C:345:VAL:HG21 | 1.93 | 0.49 |
| 1:D:270:THR:CG2 | 1:D:280:ILE:HG22 | 2.43 | 0.49 |
| 1:D:317:PRO:O | 1:D:318:VAL:CG1 | 2.61 | 0.49 |
| 1:E:470:GLY:O | 1:F:344:PRO:HG2 | 2.13 | 0.49 |
| 1:B:141:MET:HE3 | 1:B:149:GLU:HG2 | 1.94 | 0.49 |
| 1:C:188:TYR:HD2 | 1:C:263:THR:HG22 | 1.75 | 0.49 |
| 1:C:401:VAL:HG22 | 1:C:486:LYS:HB2 | 1.93 | 0.49 |
| 1:D:454:ALA:O | 1:D:457:LYS:HB2 | 2.13 | 0.49 |
| 1:E:406:PHE:CE2 | 1:E:421:CYS:HB3 | 2.45 | 0.49 |
| 1:E:418:ASN:ND2 | 1:E:419:ASN:N | 2.60 | 0.49 |
| 1:A:55:LEU:HD13 | 1:A:116:TYR:HB3 | 1.93 | 0.49 |
| 1:A:78:GLN:HE21 | 1:A:416:ARG:HH11 | 1.53 | 0.49 |
| 1:B:163:GLU:OE2 | 1:B:334:ASP:HB3 | 2.13 | 0.49 |
| 1:C:30:GLU:HA | 1:C:33:LYS:HD3 | 1.95 | 0.49 |
| 1:D:380:TYR:OH | 1:D:439:HIS:HD2 | 1.95 | 0.49 |
| 1:D:13:PHE:CE2 | 1:D:39:MET:HB2 | 2.47 | 0.49 |
| 1:F:472:HIS:ND1 | 1:F:473:PRO:CA | 2.76 | 0.49 |
| 1:A:451:GLY:HA2 | 1:B:452:PHE:CE1 | 2.48 | 0.49 |
| 1:C:328:TYR:C | 1:C:328:TYR:CD1 | 2.85 | 0.49 |
| 1:C:494:GLN:O | 1:C:495:SER:O | 2.30 | 0.49 |
| 1:D:317:PRO:C | 1:D:318:VAL:CG1 | 2.80 | 0.49 |
| 1:E:361:SER:OG | 1:E:363:VAL:HG23 | 2.13 | 0.49 |
| 1:A:428:ASN:ND2 | 1:A:431:ASP:HB3 | 2.28 | 0.49 |
| 1:B:150:LYS:HG2 | 1:B:152:TYR:CZ | 2.48 | 0.49 |
| 1:B:268:LYS:NZ | 1:B:280:ILE:HD12 | 2.28 | 0.49 |
| 1:A:68:LYS:NZ | 1:B:473:PRO:O | 2.41 | 0.49 |
| 1:E:376:THR:O | 1:E:377:PRO:C | 2.50 | 0.49 |
| 1:E:418:ASN:HD21 | 1:E:495:SER:HB3 | 1.77 | 0.49 |
| 1:E:499:GLY:HA3 | 1:F:29:LYS:HZ3 | 1.78 | 0.49 |
| 1:F:438:PHE:CE2 | 1:F:449:THR:HG23 | 2.48 | 0.49 |
| 1:A:134:PHE:HB2 | 1:A:301:GLY:O | 2.13 | 0.49 |
| 1:A:217:THR:HA | 1:A:246:LYS:O | 2.12 | 0.49 |
| 1:B:168:LEU:HD11 | 1:B:291:VAL:HG11 | 1.94 | 0.49 |
| 1:D:173:ASP:HB2 | 1:D:289:LEU:HD11 | 1.94 | 0.49 |
| 1:D:291:VAL:O | 1:D:291:VAL:CG1 | 2.59 | 0.49 |
| 1:D:411:TRP:O | 1:D:414:PRO:HD2 | 2.12 | 0.49 |
| 1:E:163:GLU:OE2 | 1:E:334:ASP:HB3 | 2.13 | 0.49 |
| 1:A:472:HIS:O | 2:B:600:FAD:N3 | 2.46 | 0.48 |
| 1:C:153:SER:CB | 4:C:2002:HOH:O | 2.57 | 0.48 |
| 1:D:67:LYS:CD | 1:D:204:GLU:OE1 | 2.61 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:195:VAL:HG22 | 1:F:288:LEU:HB3 | 1.94 | 0.48 |
| 1:A:13:PHE:O | 1:A:154:ALA:HA | 2.12 | 0.48 |
| 1:A:443:PRO:O | 1:A:444:ASN:HB2 | 2.12 | 0.48 |
| 1:B:303:GLU:OE1 | 1:B:304:THR:HG23 | 2.13 | 0.48 |
| 1:B:434:ARG:HG2 | 1:B:434:ARG:HH11 | 1.79 | 0.48 |
| 1:C:192:LYS:HE2 | 1:C:215:ASP:CG | 2.32 | 0.48 |
| 1:C:305:VAL:HG11 | 1:C:329:ILE:HD11 | 1.95 | 0.48 |
| 1:C:328:TYR:C | 1:C:328:TYR:HD1 | 2.17 | 0.48 |
| 1:D:229:ASP:C | 1:D:229:ASP:OD1 | 2.52 | 0.48 |
| 1:A:97:ASP:C | 1:A:97:ASP:OD1 | 2.51 | 0.48 |
| 1:B:263:THR:CB | 1:B:264:PRO:HD3 | 2.42 | 0.48 |
| 1:B:65:ILE:HB | 1:B:66:PRO:HD2 | 1.95 | 0.48 |
| 1:B:91:GLU:O | 1:B:92:ASP:C | 2.51 | 0.48 |
| 1:C:172:GLY:HA3 | 1:C:256:ILE:CG2 | 2.42 | 0.48 |
| 1:C:316:ILE:CG2 | 1:C:324:THR:CG2 | 2.91 | 0.48 |
| 1:C:474:VAL:HG12 | 1:D:447:GLU:OE1 | 2.13 | 0.48 |
| 1:D:275:ASN:ND2 | 1:D:277:GLU:HB3 | 2.28 | 0.48 |
| 1:E:425:VAL:HG13 | 1:E:435:VAL:HG13 | 1.95 | 0.48 |
| 1:F:412:THR:O | 1:F:415:SER:N | 2.46 | 0.48 |
| 1:A:212:ILE:HD12 | 1:A:212:ILE:HA | 1.28 | 0.48 |
| 1:A:64:CYS:O | 1:A:65:ILE:C | 2.50 | 0.48 |
| 1:B:390:ALA:HB2 | 1:B:426:ILE:HD12 | 1.96 | 0.48 |
| 1:B:401:VAL:O | 1:B:401:VAL:HG12 | 2.13 | 0.48 |
| 1:C:114:TRP:CZ3 | 1:C:117:ARG:HD2 | 2.48 | 0.48 |
| 1:C:43:PHE:HB2 | 1:C:130:ALA:C | 2.33 | 0.48 |
| 1:C:411:TRP:O | 1:C:414:PRO:HD2 | 2.12 | 0.48 |
| 1:C:438:PHE:CE2 | 1:C:452:PHE:CB | 2.96 | 0.48 |
| 1:C:83:SER:HB3 | 1:C:88:TRP:HB2 | 1.96 | 0.48 |
| 1:E:447:GLU:CD | 1:F:474:VAL:HG13 | 2.33 | 0.48 |
| 1:F:478:ILE:HD13 | 1:F:479:PHE:N | 2.28 | 0.48 |
| 1:A:263:THR:HG1 | 1:A:264:PRO:HD3 | 1.76 | 0.48 |
| 1:B:374:VAL:CG1 | 1:B:380:TYR:HB3 | 2.43 | 0.48 |
| 1:C:72:GLN:OE1 | 1:C:72:GLN:HA | 2.14 | 0.48 |
| 1:D:426:ILE:HG13 | 1:D:426:ILE:O | 2.13 | 0.48 |
| 1:F:208:PHE:CE1 | 1:F:209:LEU:HD13 | 2.49 | 0.48 |
| 1:B:70:MET:SD | 1:B:101:MET:HE1 | 2.53 | 0.48 |
| 1:B:259:ILE:HD11 | 1:B:268:LYS:HB2 | 1.95 | 0.48 |
| 1:C:166:ARG:HD3 | 1:C:294:ASP:OD1 | 2.13 | 0.48 |
| 1:C:233:ALA:O | 1:C:236:ILE:HB | 2.14 | 0.48 |
| 1:D:78:GLN:HE21 | 1:D:416:ARG:NH1 | 2.12 | 0.48 |
| 1:D:209:LEU:O | 1:D:212:ILE:HG22 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:272:LYS:NZ | 1:D:276:SER:OG | 2.41 | 0.48 |
| 1:E:233:ALA:HA | 1:E:236:ILE:HD12 | 1.96 | 0.48 |
| 1:E:323:GLN:HB2 | 1:E:330:TYR:CE1 | 2.49 | 0.48 |
| 1:E:325:ASN:ND2 | 1:E:325:ASN:H | 2.10 | 0.48 |
| 1:F:486:LYS:O | 1:F:488:SER:N | 2.46 | 0.48 |
| 1:F:491:ASP:OD2 | 1:F:493:LEU:HB2 | 2.13 | 0.48 |
| 1:C:255:LYS:HZ2 | 1:C:270:THR:HG21 | 1.79 | 0.48 |
| 1:C:477:GLU:O | 1:C:478:ILE:C | 2.47 | 0.48 |
| 1:D:191:GLY:HA3 | 1:D:285:ASN:HD22 | 1.78 | 0.48 |
| 1:D:267:LEU:CD1 | 1:D:267:LEU:N | 2.75 | 0.48 |
| 1:D:272:LYS:HG2 | 1:D:273:SER:N | 2.28 | 0.48 |
| 1:D:407:TRP:CZ3 | 1:D:412:THR:HG22 | 2.49 | 0.48 |
| 1:E:267:LEU:O | 1:E:283:GLU:HA | 2.13 | 0.48 |
| 1:E:418:ASN:HD22 | 1:E:419:ASN:H | 1.62 | 0.48 |
| 1:E:499:GLY:HA3 | 1:F:29:LYS:NZ | 2.29 | 0.48 |
| 1:F:340:LEU:HG | 1:F:370:VAL:HG21 | 1.95 | 0.48 |
| 1:A:267:LEU:CD2 | 1:A:267:LEU:N | 2.74 | 0.48 |
| 1:B:448:VAL:HG22 | 1:B:476:ALA:HB2 | 1.94 | 0.48 |
| 1:C:178:ILE:HB | 1:C:182:ASP:CB | 2.43 | 0.48 |
| 1:C:258:GLN:NE2 | 1:C:260:GLU:O | 2.47 | 0.48 |
| 1:E:173:ASP:C | 1:E:173:ASP:OD1 | 2.52 | 0.48 |
| 1:E:308:LYS:N | 1:E:325:ASN:HD21 | 1.99 | 0.48 |
| 1:F:368:ASP:O | 1:F:457:LYS:NZ | 2.46 | 0.48 |
| 1:D:402:TYR:HB3 | 1:D:482:LEU:HB3 | 1.95 | 0.48 |
| 1:D:402:TYR:CD1 | 1:D:402:TYR:N | 2.82 | 0.48 |
| 1:D:407:TRP:CB | 1:D:418:ASN:ND2 | 2.77 | 0.48 |
| 1:F:221:ARG:HH12 | 3:F:601:NDP:P2B | 2.36 | 0.48 |
| 1:B:284:PHE:N | 1:B:284:PHE:CD1 | 2.82 | 0.47 |
| 1:B:374:VAL:O | 1:B:374:VAL:CG1 | 2.62 | 0.47 |
| 1:E:426:ILE:CG1 | 1:E:437:GLY:CA | 2.88 | 0.47 |
| 1:E:473:PRO:O | 1:E:473:PRO:CG | 2.56 | 0.47 |
| 1:F:263:THR:OG1 | 1:F:264:PRO:CD | 2.62 | 0.47 |
| 1:F:406:PHE:CE1 | 1:F:421:CYS:CB | 2.94 | 0.47 |
| 1:A:331:ALA:O | 1:A:332:ILE:HG12 | 2.14 | 0.47 |
| 1:C:134:PHE:HB2 | 1:C:301:GLY:O | 2.13 | 0.47 |
| 1:C:205:CYS:O | 1:C:207:GLY:N | 2.47 | 0.47 |
| 1:C:229:ASP:OD1 | 1:C:229:ASP:C | 2.53 | 0.47 |
| 1:E:273:SER:HB2 | 1:E:275:ASN:OD1 | 2.14 | 0.47 |
| 1:B:205:CYS:HA | 1:B:208:PHE:CE2 | 2.49 | 0.47 |
| 1:B:273:SER:OG | 1:B:275:ASN:HB3 | 2.14 | 0.47 |
| 1:A:470:GLY:CA | 1:B:450:GLN:HE22 | 2.25 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:427:CYS:HA | 1:C:434:ARG:O | 2.14 | 0.47 |
| 1:D:378:LEU:HD11 | 1:D:442:GLY:HA2 | 1.96 | 0.47 |
| 1:E:178:ILE:HB | 1:E:182:ASP:HB2 | 1.96 | 0.47 |
| 1:E:223:ILE:CD1 | 1:E:230:GLN:NE2 | 2.77 | 0.47 |
| 1:F:194:LEU:HD22 | 1:F:284:PHE:CE1 | 2.49 | 0.47 |
| 1:F:221:ARG:HH11 | 1:F:221:ARG:CB | 2.27 | 0.47 |
| 1:A:348:GLN:HE22 | 1:A:351:ARG:HH12 | 1.57 | 0.47 |
| 1:B:383:CYS:SG | 1:B:456:LEU:HD12 | 2.54 | 0.47 |
| 1:C:395:GLY:O | 1:C:396:GLU:C | 2.52 | 0.47 |
| 1:D:150:LYS:HG2 | 1:D:152:TYR:CZ | 2.48 | 0.47 |
| 1:D:394:PHE:CE2 | 1:D:428:ASN:ND2 | 2.82 | 0.47 |
| 1:F:223:ILE:HG12 | 1:F:230:GLN:NE2 | 2.28 | 0.47 |
| 1:F:196:VAL:O | 1:F:291:VAL:HG23 | 2.13 | 0.47 |
| 1:A:353:LEU:HA | 1:A:356:ARG:HH21 | 1.78 | 0.47 |
| 1:C:167:TYR:HD2 | 1:C:173:ASP:O | 1.98 | 0.47 |
| 1:C:321:GLU:O | 1:C:322:GLU:HB2 | 2.13 | 0.47 |
| 1:C:403:HIS:CD2 | 1:C:492:ILE:HD11 | 2.48 | 0.47 |
| 1:F:303:GLU:N | 1:F:303:GLU:OE1 | 2.48 | 0.47 |
| 1:F:34:PHE:CZ | 1:F:355:GLN:NE2 | 2.83 | 0.47 |
| 1:B:395:GLY:O | 1:B:396:GLU:C | 2.52 | 0.47 |
| 1:C:220:VAL:HG23 | 1:C:250:GLN:H | 1.79 | 0.47 |
| 1:D:133:LYS:O | 1:D:140:ILE:HG13 | 2.15 | 0.47 |
| 1:E:16:ILE:HB | 1:E:157:PHE:CE1 | 2.50 | 0.47 |
| 1:E:263:THR:O | 1:E:265:GLY:N | 2.47 | 0.47 |
| 1:E:305:VAL:HG11 | 1:E:329:ILE:HD11 | 1.97 | 0.47 |
| 1:C:127:TYR:CD1 | 1:C:128:GLU:N | 2.82 | 0.47 |
| 1:C:67:LYS:NZ | 1:C:204:GLU:OE2 | 2.47 | 0.47 |
| 1:C:320:ASP:O | 1:C:364:LYS:CG | 2.49 | 0.47 |
| 1:D:352:LEU:O | 1:D:355:GLN:HB2 | 2.15 | 0.47 |
| 1:E:263:THR:CB | 1:E:264:PRO:HD3 | 2.18 | 0.47 |
| 1:E:30:GLU:OE1 | 1:E:355:GLN:NE2 | 2.45 | 0.47 |
| 1:F:203:LEU:HD22 | 1:F:240:MET:CE | 2.44 | 0.47 |
| 1:A:273:SER:OG | 1:A:275:ASN:N | 2.46 | 0.47 |
| 1:A:47:THR:HG23 | 1:A:51:THR:O | 2.15 | 0.47 |
| 1:A:83:SER:HB2 | 1:A:88:TRP:HB2 | 1.97 | 0.47 |
| 1:E:212:ILE:HA | 1:E:212:ILE:HD12 | 1.55 | 0.47 |
| 1:A:11:TYR:CE2 | 1:A:155:GLU:HG3 | 2.50 | 0.47 |
| 1:A:395:GLY:O | 1:A:396:GLU:C | 2.53 | 0.47 |
| 1:B:236:ILE:HG21 | 1:B:376:THR:HG21 | 1.96 | 0.47 |
| 1:C:371:PRO:HB3 | 1:C:453:ALA:HB2 | 1.97 | 0.47 |
| 1:D:343:THR:CB | 1:D:344:PRO:HD3 | 2.45 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:387:GLU:O | 1:F:391:VAL:HG13 | 2.14 | 0.47 |
| 1:A:163:GLU:OE2 | 1:A:334:ASP:HB3 | 2.15 | 0.47 |
| 1:A:191:GLY:O | 1:A:193:THR:HG22 | 2.15 | 0.47 |
| 1:A:475:CYS:O | 1:A:478:ILE:HD11 | 2.15 | 0.47 |
| 1:A:471:ILE:HG13 | 1:B:371:PRO:HB2 | 1.97 | 0.47 |
| 1:C:18:ILE:HD11 | 1:C:159:ILE:CG2 | 2.45 | 0.47 |
| 1:C:70:MET:HB3 | 1:C:208:PHE:CE2 | 2.50 | 0.47 |
| 1:C:398:ASN:O | 1:C:429:LEU:HB2 | 2.15 | 0.47 |
| 1:C:431:ASP:O | 1:C:432:ASN:HB2 | 2.14 | 0.47 |
| 1:C:477:GLU:CA | 1:D:450:GLN:HE21 | 2.24 | 0.47 |
| 1:F:273:SER:HB2 | 1:F:274:THR:H | 1.51 | 0.47 |
| 1:F:469:ILE:H | 1:F:469:ILE:HD12 | 1.79 | 0.47 |
| 1:F:65:ILE:HD13 | 1:F:65:ILE:HA | 1.71 | 0.47 |
| 1:A:348:GLN:HE22 | 1:A:351:ARG:CZ | 2.24 | 0.47 |
| 1:B:9:LYS:O | 1:B:9:LYS:HD2 | 2.14 | 0.47 |
| 1:C:198:ALA:HB1 | 1:C:224:LEU:HA | 1.97 | 0.47 |
| 1:C:221:ARG:NH1 | 3:C:601:NDP:O2X | 2.48 | 0.47 |
| 1:C:36:LYS:HE3 | 1:C:358:TYR:CD2 | 2.48 | 0.47 |
| 1:D:220:VAL:CG2 | 1:D:249:ARG:HE | 2.28 | 0.47 |
| 1:D:388:GLU:O | 1:D:391:VAL:HG22 | 2.15 | 0.47 |
| 1:F:223:ILE:HG12 | 1:F:224:LEU:N | 2.29 | 0.47 |
| 1:B:98:TRP:HB3 | 1:B:189:CYS:HB2 | 1.97 | 0.46 |
| 1:B:30:GLU:O | 1:B:31:ALA:C | 2.53 | 0.46 |
| 1:C:316:ILE:CG2 | 1:C:324:THR:HG21 | 2.45 | 0.46 |
| 1:C:319:THR:OG1 | 1:C:323:GLN:O | 2.33 | 0.46 |
| 1:C:474:VAL:HG12 | 1:C:475:CYS:N | 2.29 | 0.46 |
| 1:D:440:VAL:O | 1:D:440:VAL:HG13 | 2.14 | 0.46 |
| 1:D:47:THR:HB | 1:D:48:PRO:HD2 | 1.96 | 0.46 |
| 1:E:186:LEU:HD22 | 1:E:188:TYR:CE2 | 2.50 | 0.46 |
| 1:E:378:LEU:HD11 | 1:E:442:GLY:HA2 | 1.96 | 0.46 |
| 1:F:418:ASN:O | 1:F:420:LYS:HG2 | 2.15 | 0.46 |
| 1:A:292:GLY:O | 1:A:293:ARG:HG2 | 2.15 | 0.46 |
| 1:A:491:ASP:OD2 | 1:A:493:LEU:HB2 | 2.15 | 0.46 |
| 1:D:114:TRP:O | 1:D:114:TRP:CE3 | 2.68 | 0.46 |
| 1:F:413:VAL:N | 1:F:414:PRO:CD | 2.77 | 0.46 |
| 1:F:91:GLU:O | 1:F:91:GLU:HG2 | 2.14 | 0.46 |
| 1:B:229:ASP:HB2 | 1:B:386:SER:HB2 | 1.98 | 0.46 |
| 1:B:220:VAL:HG21 | 1:B:249:ARG:NE | 2.31 | 0.46 |
| 1:B:426:ILE:CG1 | 1:B:437:GLY:CA | 2.89 | 0.46 |
| 1:C:21:GLY:HA3 | 2:C:600:FAD:O3P | 2.16 | 0.46 |
| 1:D:376:THR:HB | 1:D:377:PRO:HD2 | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:380:TYR:CE1 | 1:E:382:CYS:HB3 | 2.50 | 0.46 |
| 1:A:158:LEU:HD11 | 1:A:332:ILE:HG12 | 1.95 | 0.46 |
| 1:A:307:VAL:HG13 | 1:A:324:THR:HG21 | 1.97 | 0.46 |
| 1:A:425:VAL:HG13 | 1:A:435:VAL:HG13 | 1.96 | 0.46 |
| 1:B:229:ASP:OD1 | 1:B:231:ASP:N | 2.48 | 0.46 |
| 1:B:254:THR:HG23 | 1:B:271:ALA:HA | 1.97 | 0.46 |
| 1:B:482:LEU:HD23 | 1:B:482:LEU:HA | 1.40 | 0.46 |
| 1:C:32:ALA:HB2 | 1:C:125:VAL:CG2 | 2.46 | 0.46 |
| 1:C:386:SER:OG | 1:C:388:GLU:HG2 | 2.15 | 0.46 |
| 1:D:316:ILE:HG13 | 1:D:335:ILE:CG2 | 2.45 | 0.46 |
| 1:D:230:GLN:HB2 | 1:D:388:GLU:OE2 | 2.15 | 0.46 |
| 1:D:407:TRP:CD1 | 1:D:418:ASN:ND2 | 2.82 | 0.46 |
| 1:E:203:LEU:HD23 | 1:E:203:LEU:HA | 1.56 | 0.46 |
| 1:F:229:ASP:OD2 | 1:F:232:MET:HG2 | 2.15 | 0.46 |
| 1:A:263:THR:O | 1:A:264:PRO:C | 2.50 | 0.46 |
| 1:A:30:GLU:OE1 | 1:A:33:LYS:HD2 | 2.15 | 0.46 |
| 1:A:47:THR:HG1 | 1:A:51:THR:H | 1.63 | 0.46 |
| 1:B:47:THR:HB | 1:B:48:PRO:CD | 2.46 | 0.46 |
| 1:C:307:VAL:HG21 | 1:C:329:ILE:HG21 | 1.97 | 0.46 |
| 1:C:412:THR:HB | 1:D:108:HIS:CD2 | 2.50 | 0.46 |
| 1:D:98:TRP:NE1 | 1:D:102:THR:CG2 | 2.72 | 0.46 |
| 1:A:134:PHE:CE1 | 1:A:157:PHE:CD2 | 3.04 | 0.46 |
| 1:A:348:GLN:NE2 | 1:A:351:ARG:CZ | 2.79 | 0.46 |
| 1:B:356:ARG:HG2 | 1:B:361:SER:O | 2.15 | 0.46 |
| 1:C:55:LEU:HD13 | 1:C:116:TYR:CB | 2.44 | 0.46 |
| 1:D:270:THR:HG21 | 1:D:280:ILE:HG22 | 1.97 | 0.46 |
| 1:D:96:HIS:NE2 | 1:D:212:ILE:HG13 | 2.30 | 0.46 |
| 1:E:134:PHE:HE1 | 1:E:157:PHE:CD2 | 2.34 | 0.46 |
| 1:A:469:ILE:HD13 | 1:A:469:ILE:N | 2.31 | 0.46 |
| 1:B:172:GLY:HA2 | 1:B:175:GLU:HG2 | 1.96 | 0.46 |
| 1:B:23:GLY:HA3 | 1:B:332:ILE:HD13 | 1.98 | 0.46 |
| 1:B:374:VAL:HG12 | 1:B:380:TYR:HB3 | 1.97 | 0.46 |
| 1:C:158:LEU:HD11 | 1:C:332:ILE:HB | 1.97 | 0.46 |
| 1:C:309:ILE:CG2 | 1:C:316:ILE:HG12 | 2.43 | 0.46 |
| 1:C:433:GLU:O | 1:C:434:ARG:C | 2.54 | 0.46 |
| 1:A:262:GLY:C | 1:A:263:THR:O | 2.54 | 0.46 |
| 1:B:164:ARG:NH2 | 1:B:181:ASP:OD2 | 2.45 | 0.46 |
| 1:C:194:LEU:HD22 | 1:C:287:VAL:HG13 | 1.98 | 0.46 |
| 1:D:469:ILE:CG2 | 1:D:470:GLY:N | 2.79 | 0.46 |
| 1:D:90:LEU:CD2 | 1:D:90:LEU:N | 2.78 | 0.46 |
| 1:E:38:VAL:HG22 | 1:E:125:VAL:HG13 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:470:GLY:CA | 1:F:480:THR:HG21 | 2.46 | 0.46 |
| 1:A:284:PHE:N | 1:A:284:PHE:CD1 | 2.84 | 0.46 |
| 1:C:55:LEU:HD11 | 1:C:116:TYR:HB3 | 1.97 | 0.46 |
| 1:C:220:VAL:CG2 | 1:C:249:ARG:NE | 2.70 | 0.46 |
| 1:C:393:LYS:HG2 | 1:C:394:PHE:CE1 | 2.51 | 0.46 |
| 1:C:201:VAL:HG22 | 2:C:600:FAD:HM73 | 1.97 | 0.46 |
| 1:C:293:ARG:NH1 | 2:C:600:FAD:HM81 | 2.31 | 0.46 |
| 1:D:258:GLN:HE22 | 1:D:261:ALA:HB2 | 1.79 | 0.46 |
| 1:D:263:THR:O | 1:D:265:GLY:N | 2.49 | 0.46 |
| 1:D:407:TRP:HB2 | 1:D:418:ASN:ND2 | 2.24 | 0.46 |
| 1:E:138:HIS:CD2 | 1:E:154:ALA:O | 2.65 | 0.46 |
| 1:A:14:ASP:OD2 | 1:A:37:LYS:N | 2.47 | 0.46 |
| 1:A:471:ILE:H | 1:B:450:GLN:HE22 | 1.64 | 0.46 |
| 1:A:471:ILE:HG21 | 1:B:373:THR:CG2 | 2.42 | 0.46 |
| 1:B:120:LEU:HD22 | 1:B:125:VAL:CG1 | 2.45 | 0.46 |
| 1:B:49:LEU:HA | 1:B:49:LEU:HD13 | 1.65 | 0.46 |
| 1:C:63:GLY:O | 1:C:64:CYS:C | 2.53 | 0.46 |
| 1:E:281:GLU:HA | 1:E:281:GLU:OE1 | 2.14 | 0.46 |
| 1:E:49:LEU:CD2 | 1:E:49:LEU:N | 2.78 | 0.46 |
| 1:F:162:GLY:O | 1:F:335:ILE:HD11 | 2.16 | 0.46 |
| 1:A:269:VAL:HG12 | 1:A:281:GLU:OE1 | 2.17 | 0.45 |
| 1:B:348:GLN:NE2 | 1:B:351:ARG:HH12 | 2.13 | 0.45 |
| 1:B:418:ASN:OD1 | 1:B:419:ASN:N | 2.47 | 0.45 |
| 1:B:461:THR:H | 1:B:464:GLN:HG3 | 1.80 | 0.45 |
| 1:D:140:ILE:CG1 | 1:D:141:MET:N | 2.79 | 0.45 |
| 1:D:225:LEU:O | 1:D:226:ARG:C | 2.55 | 0.45 |
| 1:D:282:ASP:N | 1:D:282:ASP:OD1 | 2.48 | 0.45 |
| 1:D:90:LEU:CD2 | 1:D:90:LEU:H | 2.29 | 0.45 |
| 1:D:91:GLU:HA | 1:D:91:GLU:OE1 | 2.12 | 0.45 |
| 1:F:498:CYS:SG | 1:F:499:GLY:N | 2.89 | 0.45 |
| 1:C:225:LEU:O | 1:C:228:PHE:HB2 | 2.16 | 0.45 |
| 1:C:438:PHE:C | 1:C:439:HIS:ND1 | 2.69 | 0.45 |
| 1:D:287:VAL:O | 1:D:287:VAL:HG12 | 2.16 | 0.45 |
| 1:C:477:GLU:CA | 1:D:450:GLN:NE2 | 2.73 | 0.45 |
| 1:F:109:ILE:HA | 1:F:112:LEU:HD12 | 1.99 | 0.45 |
| 1:F:168:LEU:O | 1:F:173:ASP:OD2 | 2.33 | 0.45 |
| 1:F:396:GLU:O | 1:F:396:GLU:OE2 | 2.33 | 0.45 |
| 1:F:428:ASN:ND2 | 1:F:431:ASP:CB | 2.73 | 0.45 |
| 1:C:181:ASP:OD1 | 1:C:181:ASP:N | 2.48 | 0.45 |
| 1:C:255:LYS:HZ3 | 1:C:270:THR:HG23 | 1.80 | 0.45 |
| 1:C:473:PRO:O | 1:C:473:PRO:CG | 2.60 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:90:LEU:HG | 1:C:91:GLU:N | 2.32 | 0.45 |
| 1:D:301:GLY:C | 1:D:303:GLU:OE1 | 2.54 | 0.45 |
| 2:D:600:FAD:O5' | 2:D:600:FAD:O2A | 2.35 | 0.45 |
| 1:E:164:ARG:HA | 1:E:164:ARG:HD2 | 1.73 | 0.45 |
| 1:B:305:VAL:HG12 | 1:B:328:TYR:OH | 2.16 | 0.45 |
| 1:A:450:GLN:NE2 | 1:B:471:ILE:H | 2.14 | 0.45 |
| 1:E:36:LYS:HA | 1:E:36:LYS:HD3 | 1.76 | 0.45 |
| 1:F:250:GLN:O | 1:F:251:PHE:CD1 | 2.69 | 0.45 |
| 1:F:406:PHE:HE2 | 1:F:423:ALA:HB2 | 1.82 | 0.45 |
| 1:F:478:ILE:HD13 | 1:F:479:PHE:H | 1.81 | 0.45 |
| 1:A:114:TRP:HB3 | 1:D:114:TRP:CE2 | 2.50 | 0.45 |
| 1:A:220:VAL:O | 1:A:220:VAL:CG2 | 2.65 | 0.45 |
| 1:A:435:VAL:HG23 | 1:A:460:LEU:O | 2.17 | 0.45 |
| 1:E:219:MET:HB2 | 1:E:219:MET:HE2 | 1.69 | 0.45 |
| 1:E:86:TYR:O | 1:F:96:HIS:CE1 | 2.60 | 0.45 |
| 1:F:55:LEU:HD22 | 1:F:56:GLY:N | 2.31 | 0.45 |
| 1:B:262:GLY:C | 1:B:263:THR:O | 2.55 | 0.45 |
| 1:B:21:GLY:HA3 | 2:B:600:FAD:O5B | 2.17 | 0.45 |
| 1:C:134:PHE:HB3 | 1:C:305:VAL:CG2 | 2.46 | 0.45 |
| 1:C:229:ASP:HB2 | 1:C:386:SER:HB2 | 1.99 | 0.45 |
| 1:C:98:TRP:HD1 | 1:C:189:CYS:CA | 2.19 | 0.45 |
| 1:D:138:HIS:HD2 | 1:D:154:ALA:O | 1.99 | 0.45 |
| 1:D:69:LEU:O | 1:D:72:GLN:HB3 | 2.16 | 0.45 |
| 1:F:292:GLY:O | 1:F:293:ARG:HG2 | 2.16 | 0.45 |
| 1:A:167:TYR:HB3 | 1:A:173:ASP:OD2 | 2.17 | 0.45 |
| 1:A:412:THR:O | 1:A:415:SER:N | 2.48 | 0.45 |
| 1:B:426:ILE:O | 1:B:426:ILE:HG13 | 2.16 | 0.45 |
| 1:C:291:VAL:CG1 | 3:C:601:NDP:C8A | 2.95 | 0.45 |
| 1:C:342:LEU:O | 1:C:345:VAL:HB | 2.15 | 0.45 |
| 1:C:76:LEU:O | 1:C:79:ALA:HB3 | 2.17 | 0.45 |
| 2:E:600:FAD:H9 | 2:E:600:FAD:H1'1 | 1.42 | 0.45 |
| 1:F:318:VAL:HG23 | 1:F:323:GLN:C | 2.37 | 0.45 |
| 1:A:357:LEU:HB3 | 1:A:358:TYR:CD1 | 2.51 | 0.45 |
| 1:A:55:LEU:HA | 1:A:55:LEU:HD23 | 1.54 | 0.45 |
| 1:B:17:ILE:HG12 | 1:B:158:LEU:HD23 | 1.98 | 0.45 |
| 1:B:469:ILE:CG2 | 1:B:470:GLY:N | 2.80 | 0.45 |
| 1:B:65:ILE:CG2 | 1:B:66:PRO:CD | 2.91 | 0.45 |
| 1:C:100:LYS:O | 1:C:100:LYS:HD3 | 2.16 | 0.45 |
| 1:C:365:CYS:SG | 1:C:367:TYR:CE2 | 3.10 | 0.45 |
| 1:A:134:PHE:HE1 | 1:A:157:PHE:CD2 | 2.34 | 0.45 |
| 1:A:403:HIS:CE1 | 1:A:486:LYS:HG3 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:335:ILE:HA | 1:B:335:ILE:HD12 | 1.73 | 0.45 |
| 1:C:167:TYR:CD2 | 1:C:173:ASP:O | 2.70 | 0.45 |
| 1:C:30:GLU:O | 1:C:33:LYS:HB2 | 2.17 | 0.45 |
| 1:D:114:TRP:CE3 | 1:D:118:VAL:HG23 | 2.51 | 0.45 |
| 1:D:138:HIS:O | 1:D:153:SER:HA | 2.17 | 0.45 |
| 1:D:72:GLN:HA | 1:D:72:GLN:HE21 | 1.81 | 0.45 |
| 1:D:84:ARG:HE | 1:D:84:ARG:HB2 | 1.52 | 0.45 |
| 1:E:108:HIS:CE1 | 1:E:112:LEU:HD11 | 2.52 | 0.45 |
| 1:E:273:SER:OG | 1:E:275:ASN:OD1 | 2.23 | 0.45 |
| 1:E:480:THR:HG22 | 1:E:481:THR:HG23 | 1.98 | 0.45 |
| 1:A:195:VAL:HG22 | 1:A:288:LEU:HB3 | 1.98 | 0.45 |
| 1:A:176:TYR:HB3 | 1:A:267:LEU:CD1 | 2.47 | 0.45 |
| 1:B:216:VAL:CG1 | 1:B:217:THR:N | 2.80 | 0.45 |
| 1:B:230:GLN:HA | 1:B:230:GLN:NE2 | 2.32 | 0.45 |
| 1:C:109:ILE:O | 1:C:112:LEU:N | 2.50 | 0.45 |
| 1:C:172:GLY:HA3 | 1:C:256:ILE:HG22 | 1.99 | 0.45 |
| 1:C:409:LEU:O | 1:C:409:LEU:HD12 | 2.17 | 0.45 |
| 1:E:228:PHE:N | 1:E:228:PHE:CD1 | 2.85 | 0.45 |
| 1:E:408:PRO:HG2 | 1:E:411:TRP:CD2 | 2.51 | 0.45 |
| 1:F:150:LYS:HD3 | 1:F:152:TYR:CZ | 2.51 | 0.45 |
| 1:C:415:SER:O | 1:C:415:SER:OG | 2.29 | 0.44 |
| 1:C:451:GLY:O | 1:C:454:ALA:HB3 | 2.17 | 0.44 |
| 1:E:317:PRO:C | 1:E:318:VAL:CG2 | 2.86 | 0.44 |
| 1:E:318:VAL:HG12 | 1:E:323:GLN:O | 2.16 | 0.44 |
| 1:F:194:LEU:HB2 | 1:F:284:PHE:CZ | 2.52 | 0.44 |
| 1:F:318:VAL:HG21 | 1:F:322:GLU:HA | 1.99 | 0.44 |
| 1:F:472:HIS:CE1 | 1:F:473:PRO:HB3 | 2.51 | 0.44 |
| 1:A:471:ILE:CG1 | 1:B:371:PRO:HB2 | 2.47 | 0.44 |
| 1:A:496:GLY:C | 1:A:497:CYS:SG | 2.95 | 0.44 |
| 1:B:151:VAL:HG12 | 1:B:152:TYR:N | 2.31 | 0.44 |
| 1:B:98:TRP:CB | 1:B:189:CYS:HB2 | 2.48 | 0.44 |
| 1:B:55:LEU:CD1 | 1:B:116:TYR:HB3 | 2.46 | 0.44 |
| 1:C:130:ALA:HB1 | 1:C:143:THR:O | 2.17 | 0.44 |
| 1:C:186:LEU:HA | 1:C:187:PRO:HD2 | 1.78 | 0.44 |
| 1:C:58:THR:HG1 | 2:C:600:FAD:PA | 2.40 | 0.44 |
| 1:D:309:ILE:HG21 | 1:D:309:ILE:HD13 | 1.64 | 0.44 |
| 1:E:266:ARG:NH1 | 1:E:283:GLU:OE1 | 2.48 | 0.44 |
| 1:A:117:ARG:NH2 | 1:D:107:ASN:ND2 | 2.65 | 0.44 |
| 1:A:413:VAL:N | 1:A:414:PRO:CD | 2.81 | 0.44 |
| 1:A:487:ARG:HE | 1:A:487:ARG:HB2 | 1.60 | 0.44 |
| 1:B:399:ILE:HA | 1:B:399:ILE:HD12 | 1.47 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:49:LEU:HD13 | 1:C:49:LEU:HA | 1.84 | 0.44 |
| 1:C:162:GLY:HA3 | 2:C:600:FAD:O1A | 2.18 | 0.44 |
| 1:F:221:ARG:NH1 | 1:F:221:ARG:HG2 | 2.32 | 0.44 |
| 1:F:343:THR:N | 1:F:344:PRO:CD | 2.80 | 0.44 |
| 1:A:192:LYS:N | 1:A:285:ASN:HD22 | 2.13 | 0.44 |
| 1:A:303:GLU:OE1 | 1:A:304:THR:HG23 | 2.17 | 0.44 |
| 1:B:376:THR:O | 1:B:377:PRO:C | 2.56 | 0.44 |
| 1:C:208:PHE:CD1 | 1:C:208:PHE:C | 2.90 | 0.44 |
| 1:C:20:GLY:HA3 | 1:C:42:ASP:CB | 2.47 | 0.44 |
| 1:D:86:TYR:CZ | 1:D:413:VAL:HB | 2.51 | 0.44 |
| 1:E:410:GLU:HG3 | 1:F:72:GLN:NE2 | 2.31 | 0.44 |
| 1:A:188:TYR:C | 1:A:188:TYR:CD1 | 2.90 | 0.44 |
| 1:A:216:VAL:CG1 | 1:A:217:THR:N | 2.80 | 0.44 |
| 1:A:29:LYS:CG | 1:A:30:GLU:N | 2.79 | 0.44 |
| 1:A:351:ARG:NH2 | 1:A:352:LEU:HD21 | 2.33 | 0.44 |
| 1:B:180:SER:O | 1:B:181:ASP:C | 2.53 | 0.44 |
| 1:E:269:VAL:O | 1:E:281:GLU:HB2 | 2.17 | 0.44 |
| 1:E:272:LYS:HG2 | 1:E:273:SER:H | 1.82 | 0.44 |
| 1:F:49:LEU:CD2 | 1:F:49:LEU:N | 2.78 | 0.44 |
| 1:A:449:THR:O | 1:A:450:GLN:C | 2.56 | 0.44 |
| 1:C:209:LEU:HA | 1:C:209:LEU:HD13 | 1.67 | 0.44 |
| 1:C:401:VAL:O | 1:C:401:VAL:HG23 | 2.18 | 0.44 |
| 1:C:472:HIS:CD2 | 1:C:477:GLU:OE2 | 2.59 | 0.44 |
| 1:C:98:TRP:CE3 | 1:C:102:THR:OG1 | 2.57 | 0.44 |
| 1:D:343:THR:HG22 | 1:D:344:PRO:HD3 | 2.00 | 0.44 |
| 1:E:316:ILE:HA | 1:E:317:PRO:HD3 | 1.88 | 0.44 |
| 1:E:412:THR:O | 1:E:415:SER:N | 2.48 | 0.44 |
| 1:F:418:ASN:OD1 | 1:F:419:ASN:N | 2.50 | 0.44 |
| 1:F:42:ASP:HA | 2:F:600:FAD:N3A | 2.33 | 0.44 |
| 1:A:275:ASN:CG | 1:A:275:ASN:O | 2.56 | 0.44 |
| 1:A:408:PRO:O | 1:A:409:LEU:C | 2.54 | 0.44 |
| 1:A:428:ASN:ND2 | 1:A:431:ASP:HB2 | 2.32 | 0.44 |
| 1:C:332:ILE:CG2 | 1:C:333:GLY:N | 2.80 | 0.44 |
| 1:C:427:CYS:HB3 | 1:C:433:GLU:C | 2.38 | 0.44 |
| 1:D:30:GLU:O | 1:D:31:ALA:C | 2.54 | 0.44 |
| 1:D:76:LEU:HD23 | 1:D:76:LEU:HA | 1.77 | 0.44 |
| 1:E:469:ILE:CG2 | 1:E:470:GLY:N | 2.79 | 0.44 |
| 1:A:161:THR:HB | 2:A:600:FAD:C8A | 2.48 | 0.44 |
| 1:B:292:GLY:C | 1:B:293:ARG:HG2 | 2.38 | 0.44 |
| 1:C:256:ILE:HG12 | 1:C:257:GLU:N | 2.32 | 0.44 |
| 1:C:425:VAL:CG1 | 1:C:435:VAL:HG13 | 2.44 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:477:GLU:O | 1:C:480:THR:HG23 | 2.17 | 0.44 |
| 1:D:186:LEU:HA | 1:D:187:PRO:HD3 | 1.67 | 0.44 |
| 1:D:281:GLU:OE1 | 1:D:281:GLU:HA | 2.17 | 0.44 |
| 1:E:462:LYS:NZ | 1:E:482:LEU:O | 2.41 | 0.44 |
| 1:F:82:ASP:OD2 | 1:F:416:ARG:NH1 | 2.51 | 0.44 |
| 1:A:335:ILE:HD12 | 1:A:335:ILE:HA | 1.79 | 0.44 |
| 1:A:482:LEU:HD23 | 1:A:482:LEU:HA | 1.78 | 0.44 |
| 1:C:194:LEU:HD23 | 1:C:195:VAL:N | 2.33 | 0.44 |
| 1:C:188:TYR:CD1 | 1:C:263:THR:O | 2.71 | 0.44 |
| 1:C:239:HIS:CE1 | 1:C:378:LEU:HB2 | 2.53 | 0.44 |
| 1:C:461:THR:HG1 | 1:C:464:GLN:HG3 | 1.77 | 0.44 |
| 1:C:65:ILE:HG22 | 1:C:66:PRO:CD | 2.48 | 0.44 |
| 1:D:395:GLY:O | 1:D:396:GLU:C | 2.56 | 0.44 |
| 1:E:200:TYR:O | 1:E:201:VAL:C | 2.56 | 0.44 |
| 1:E:233:ALA:O | 1:E:236:ILE:HB | 2.18 | 0.44 |
| 1:E:196:VAL:O | 1:E:291:VAL:HG13 | 2.17 | 0.44 |
| 1:E:91:GLU:C | 1:E:93:THR:H | 2.22 | 0.44 |
| 1:A:331:ALA:C | 1:A:332:ILE:HG12 | 2.39 | 0.43 |
| 1:A:422:TYR:HE2 | 1:A:424:LYS:HE2 | 1.82 | 0.43 |
| 1:B:68:LYS:O | 1:B:71:HIS:HB3 | 2.18 | 0.43 |
| 1:B:83:SER:HB2 | 1:B:88:TRP:CD1 | 2.53 | 0.43 |
| 1:C:196:VAL:O | 1:C:291:VAL:HG22 | 2.14 | 0.43 |
| 1:C:208:PHE:HD1 | 1:C:209:LEU:N | 2.13 | 0.43 |
| 1:C:376:THR:CB | 1:C:377:PRO:CD | 2.94 | 0.43 |
| 1:D:389:LYS:HD2 | 1:D:389:LYS:HA | 1.83 | 0.43 |
| 1:F:378:LEU:HD11 | 1:F:442:GLY:HA2 | 2.00 | 0.43 |
| 1:B:220:VAL:HG21 | 1:B:249:ARG:HE | 1.83 | 0.43 |
| 1:B:305:VAL:HG11 | 1:B:329:ILE:HD11 | 2.00 | 0.43 |
| 1:C:137:PRO:O | 1:C:138:HIS:CB | 2.66 | 0.43 |
| 1:C:30:GLU:O | 1:C:31:ALA:C | 2.56 | 0.43 |
| 1:C:428:ASN:OD1 | 1:C:428:ASN:C | 2.56 | 0.43 |
| 1:D:403:HIS:C | 1:D:403:HIS:CD2 | 2.91 | 0.43 |
| 1:E:106:GLN:OE1 | 1:E:185:SER:HB3 | 2.18 | 0.43 |
| 1:E:373:THR:CG2 | 1:F:471:ILE:CG2 | 2.92 | 0.43 |
| 1:E:469:ILE:HG23 | 1:E:470:GLY:N | 2.32 | 0.43 |
| 1:A:493:LEU:O | 1:A:494:GLN:CG | 2.57 | 0.43 |
| 1:A:91:GLU:O | 1:A:92:ASP:C | 2.57 | 0.43 |
| 1:B:186:LEU:HD12 | 1:B:190:PRO:HG3 | 2.00 | 0.43 |
| 1:E:209:LEU:O | 1:E:212:ILE:HG22 | 2.18 | 0.43 |
| 1:E:438:PHE:C | 1:E:439:HIS:ND1 | 2.71 | 0.43 |
| 1:B:16:ILE:HB | 1:B:157:PHE:CD1 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:336:LEU:HB3 | 1:B:339:LYS:HG2 | 2.00 | 0.43 |
| 1:C:307:VAL:HG13 | 1:C:325:ASN:HD21 | 1.84 | 0.43 |
| 1:C:158:LEU:HA | 1:C:330:TYR:O | 2.18 | 0.43 |
| 1:D:263:THR:CB | 1:D:264:PRO:CD | 2.96 | 0.43 |
| 1:D:316:ILE:O | 1:D:318:VAL:HG13 | 2.18 | 0.43 |
| 1:D:488:SER:OG | 1:D:489:GLY:N | 2.51 | 0.43 |
| 1:A:189:CYS:HA | 1:A:190:PRO:HD3 | 1.85 | 0.43 |
| 1:A:307:VAL:HA | 1:A:325:ASN:HD21 | 1.83 | 0.43 |
| 1:B:248:ILE:CD1 | 1:B:281:GLU:OE2 | 2.67 | 0.43 |
| 1:B:256:ILE:HD11 | 1:B:267:LEU:HB3 | 2.00 | 0.43 |
| 1:B:387:GLU:O | 1:B:391:VAL:HG13 | 2.19 | 0.43 |
| 1:B:387:GLU:HG3 | 1:B:401:VAL:HG21 | 2.01 | 0.43 |
| 1:B:443:PRO:O | 1:B:444:ASN:C | 2.55 | 0.43 |
| 1:C:212:ILE:HD12 | 1:C:212:ILE:HA | 1.78 | 0.43 |
| 1:C:25:LEU:HD11 | 1:C:55:LEU:HD22 | 2.00 | 0.43 |
| 1:C:41:LEU:CD1 | 1:C:130:ALA:HB3 | 2.48 | 0.43 |
| 1:D:331:ALA:O | 1:D:332:ILE:HD13 | 2.19 | 0.43 |
| 1:D:80:LEU:HD23 | 1:D:80:LEU:HA | 1.74 | 0.43 |
| 1:E:475:CYS:HB2 | 1:F:447:GLU:OE1 | 2.19 | 0.43 |
| 1:F:235:LYS:HE2 | 1:F:422:TYR:CD2 | 2.53 | 0.43 |
| 1:F:90:LEU:HA | 1:F:90:LEU:HD23 | 1.55 | 0.43 |
| 1:E:88:TRP:HE3 | 1:F:94:VAL:HG12 | 1.83 | 0.43 |
| 1:B:411:TRP:N | 1:B:411:TRP:CD1 | 2.85 | 0.43 |
| 1:C:98:TRP:NE1 | 1:C:190:PRO:CD | 2.49 | 0.43 |
| 1:D:212:ILE:HA | 1:D:212:ILE:HD12 | 1.57 | 0.43 |
| 1:A:112:LEU:HD23 | 1:A:112:LEU:HA | 1.55 | 0.43 |
| 1:A:122:GLU:OE1 | 1:A:122:GLU:HA | 2.18 | 0.43 |
| 1:A:13:PHE:HE2 | 1:A:152:TYR:CD2 | 2.37 | 0.43 |
| 1:B:318:VAL:HG22 | 1:B:323:GLN:C | 2.39 | 0.43 |
| 1:B:319:THR:C | 1:B:321:GLU:H | 2.21 | 0.43 |
| 1:B:454:ALA:O | 1:B:457:LYS:HB2 | 2.18 | 0.43 |
| 1:B:45:THR:HA | 1:B:46:PRO:HD3 | 1.73 | 0.43 |
| 3:B:601:NDP:H8A | 3:B:601:NDP:H51A | 2.00 | 0.43 |
| 1:D:396:GLU:C | 1:D:396:GLU:CD | 2.77 | 0.43 |
| 1:F:225:LEU:HD12 | 1:F:228:PHE:CD2 | 2.53 | 0.43 |
| 1:A:18:ILE:HD13 | 1:A:18:ILE:HG21 | 1.72 | 0.43 |
| 1:B:478:ILE:H | 1:B:478:ILE:HG13 | 1.35 | 0.43 |
| 1:B:465:LEU:HD21 | 1:B:479:PHE:O | 2.19 | 0.43 |
| 1:C:166:ARG:HB2 | 1:C:294:ASP:OD1 | 2.19 | 0.43 |
| 1:C:161:THR:N | 1:C:335:ILE:HD11 | 2.33 | 0.43 |
| 1:C:413:VAL:N | 1:C:414:PRO:CD | 2.82 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:413:VAL:N | 1:D:414:PRO:HD3 | 2.34 | 0.43 |
| 1:E:375:PHE:CD1 | 1:E:375:PHE:N | 2.87 | 0.43 |
| 1:F:141:MET:HE3 | 1:F:143:THR:OG1 | 2.19 | 0.43 |
| 1:F:209:LEU:HA | 1:F:209:LEU:HD12 | 1.63 | 0.43 |
| 1:F:325:ASN:N | 1:F:325:ASN:ND2 | 2.51 | 0.43 |
| 1:A:280:ILE:HG13 | 1:A:280:ILE:O | 2.19 | 0.43 |
| 1:A:292:GLY:C | 1:A:293:ARG:HG2 | 2.39 | 0.43 |
| 1:B:209:LEU:HB3 | 1:B:216:VAL:HG21 | 1.99 | 0.43 |
| 1:C:313:THR:OG1 | 1:C:314:GLY:N | 2.52 | 0.43 |
| 1:D:195:VAL:HG22 | 1:D:288:LEU:HB2 | 2.00 | 0.43 |
| 1:E:140:ILE:CG2 | 1:E:140:ILE:O | 2.67 | 0.43 |
| 1:E:228:PHE:O | 1:E:230:GLN:N | 2.50 | 0.43 |
| 1:E:90:LEU:HD23 | 1:E:90:LEU:HA | 1.74 | 0.43 |
| 1:F:185:SER:O | 1:F:186:LEU:C | 2.55 | 0.43 |
| 1:F:318:VAL:CG2 | 1:F:323:GLN:O | 2.67 | 0.43 |
| 1:F:422:TYR:CE1 | 1:F:424:LYS:HB3 | 2.48 | 0.43 |
| 1:A:144:ASN:OD1 | 1:A:146:LYS:N | 2.51 | 0.43 |
| 1:C:343:THR:N | 1:C:344:PRO:CD | 2.82 | 0.43 |
| 1:D:185:SER:O | 1:D:186:LEU:C | 2.57 | 0.43 |
| 1:D:232:MET:CE | 1:D:441:LEU:HB2 | 2.49 | 0.43 |
| 1:E:192:LYS:HG3 | 1:E:215:ASP:OD1 | 2.19 | 0.43 |
| 1:E:373:THR:HG21 | 1:E:446:GLY:CA | 2.47 | 0.43 |
| 1:F:217:THR:HA | 1:F:246:LYS:O | 2.19 | 0.43 |
| 1:A:273:SER:OG | 1:A:274:THR:N | 2.49 | 0.42 |
| 1:A:475:CYS:O | 1:A:478:ILE:CD1 | 2.66 | 0.42 |
| 1:A:487:ARG:O | 1:A:487:ARG:HG3 | 2.17 | 0.42 |
| 1:C:237:GLY:O | 1:C:238:GLU:C | 2.54 | 0.42 |
| 2:D:600:FAD:H1' | 2:D:600:FAD:H9 | 1.81 | 0.42 |
| 1:D:80:LEU:O | 1:D:83:SER:OG | 2.36 | 0.42 |
| 1:E:257:GLU:H | 1:E:257:GLU:HG2 | 1.72 | 0.42 |
| 1:E:335:ILE:HD12 | 1:E:335:ILE:HA | 1.76 | 0.42 |
| 1:F:438:PHE:CE1 | 1:F:479:PHE:CZ | 3.07 | 0.42 |
| 1:F:47:THR:HB | 1:F:48:PRO:HD2 | 2.00 | 0.42 |
| 2:F:600:FAD:O2A | 2:F:600:FAD:O5' | 2.37 | 0.42 |
| 1:A:282:ASP:O | 1:A:284:PHE:CE1 | 2.72 | 0.42 |
| 1:A:325:ASN:O | 1:A:327:PRO:HD3 | 2.19 | 0.42 |
| 1:B:74:ALA:HA | 1:B:212:ILE:CD1 | 2.50 | 0.42 |
| 1:B:403:HIS:CD2 | 1:B:492:ILE:CD1 | 3.01 | 0.42 |
| 1:E:17:ILE:HG12 | 1:E:158:LEU:HD23 | 2.00 | 0.42 |
| 1:E:168:LEU:N | 1:E:168:LEU:CD1 | 2.81 | 0.42 |
| 1:E:310:ASN:ND2 | 1:E:313:THR:HG23 | 2.34 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:323:GLN:CA | 1:F:330:TYR:CD1 | 2.98 | 0.42 |
| 1:B:60:VAL:HG13 | 1:B:112:LEU:CD1 | 2.49 | 0.42 |
| 1:A:371:PRO:HB2 | 1:B:471:ILE:HD11 | 2.01 | 0.42 |
| 2:B:600:FAD:H1'1 | 2:B:600:FAD:H9 | 1.65 | 0.42 |
| 1:C:189:CYS:C | 1:C:191:GLY:N | 2.72 | 0.42 |
| 1:C:18:ILE:HG21 | 1:C:18:ILE:HD13 | 1.73 | 0.42 |
| 1:D:411:TRP:CZ2 | 1:D:443:PRO:HG3 | 2.54 | 0.42 |
| 1:E:488:SER:O | 1:E:489:GLY:C | 2.55 | 0.42 |
| 1:F:223:ILE:HD11 | 1:F:230:GLN:CG | 2.49 | 0.42 |
| 1:C:70:MET:HG3 | 1:C:101:MET:HE1 | 2.01 | 0.42 |
| 1:C:278:GLU:CD | 1:C:278:GLU:C | 2.78 | 0.42 |
| 1:C:34:PHE:HZ | 1:C:355:GLN:HE22 | 1.68 | 0.42 |
| 1:D:114:TRP:CE3 | 1:D:118:VAL:CG2 | 3.01 | 0.42 |
| 1:D:158:LEU:HA | 1:D:330:TYR:O | 2.20 | 0.42 |
| 1:E:203:LEU:HD22 | 1:E:240:MET:HE1 | 2.00 | 0.42 |
| 1:E:21:GLY:HA2 | 1:E:57:GLY:HA3 | 2.02 | 0.42 |
| 1:E:380:TYR:OH | 1:E:439:HIS:HD2 | 2.02 | 0.42 |
| 1:F:217:THR:HG23 | 1:F:246:LYS:CB | 2.48 | 0.42 |
| 1:A:106:GLN:O | 1:A:107:ASN:C | 2.56 | 0.42 |
| 1:A:334:ASP:OD2 | 2:A:600:FAD:H5'1 | 2.20 | 0.42 |
| 1:B:168:LEU:CD1 | 1:B:168:LEU:N | 2.81 | 0.42 |
| 1:B:292:GLY:O | 1:B:293:ARG:HG2 | 2.19 | 0.42 |
| 1:C:183:LEU:C | 1:C:185:SER:N | 2.70 | 0.42 |
| 1:C:212:ILE:O | 1:C:212:ILE:HG23 | 2.18 | 0.42 |
| 1:C:224:LEU:H | 1:C:224:LEU:CD1 | 2.01 | 0.42 |
| 1:C:134:PHE:CG | 1:C:305:VAL:HG21 | 2.54 | 0.42 |
| 1:D:114:TRP:HE3 | 1:D:118:VAL:HG23 | 1.84 | 0.42 |
| 1:D:223:ILE:HG12 | 1:D:226:ARG:NH2 | 2.34 | 0.42 |
| 1:F:163:GLU:HB3 | 1:F:294:ASP:C | 2.40 | 0.42 |
| 1:F:221:ARG:CG | 1:F:221:ARG:NH1 | 2.80 | 0.42 |
| 1:A:163:GLU:HB3 | 1:A:294:ASP:C | 2.40 | 0.42 |
| 1:B:106:GLN:O | 1:B:107:ASN:C | 2.57 | 0.42 |
| 1:B:403:HIS:HD2 | 1:B:403:HIS:O | 2.03 | 0.42 |
| 1:C:274:THR:O | 1:C:274:THR:OG1 | 2.34 | 0.42 |
| 1:C:336:LEU:HD23 | 1:C:336:LEU:HA | 1.79 | 0.42 |
| 1:C:348:GLN:NE2 | 1:C:352:LEU:HD22 | 2.34 | 0.42 |
| 1:C:40:VAL:HG12 | 1:C:126:VAL:O | 2.18 | 0.42 |
| 1:C:291:VAL:HG13 | 3:C:601:NDP:C8A | 2.49 | 0.42 |
| 1:D:43:PHE:HD2 | 1:D:130:ALA:HA | 1.85 | 0.42 |
| 1:D:186:LEU:HA | 1:D:186:LEU:HD23 | 1.71 | 0.42 |
| 1:D:194:LEU:HD22 | 1:D:284:PHE:CZ | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:303:GLU:N | 1:D:303:GLU:CD | 2.56 | 0.42 |
| 1:D:334:ASP:OD1 | 2:D:600:FAD:H5'2 | 2.20 | 0.42 |
| 1:F:351:ARG:NH2 | 1:F:352:LEU:HD21 | 2.35 | 0.42 |
| 1:A:112:LEU:O | 1:A:113:ASN:C | 2.57 | 0.42 |
| 1:A:316:ILE:HA | 1:A:317:PRO:HD3 | 1.88 | 0.42 |
| 1:B:161:THR:HB | 2:B:600:FAD:C8A | 2.49 | 0.42 |
| 1:B:272:LYS:HG2 | 1:B:273:SER:N | 2.35 | 0.42 |
| 1:B:22:SER:HG | 1:B:343:THR:HG23 | 1.83 | 0.42 |
| 1:C:365:CYS:SG | 1:C:365:CYS:O | 2.77 | 0.42 |
| 1:C:429:LEU:HA | 1:C:429:LEU:HD12 | 1.70 | 0.42 |
| 1:D:400:GLU:HG2 | 1:D:429:LEU:CD1 | 2.44 | 0.42 |
| 1:D:41:LEU:HD23 | 1:D:41:LEU:N | 2.35 | 0.42 |
| 1:C:473:PRO:HG2 | 1:D:68:LYS:HD3 | 2.01 | 0.42 |
| 1:E:173:ASP:CG | 1:E:174:LYS:N | 2.71 | 0.42 |
| 1:E:96:HIS:CD2 | 1:E:212:ILE:HG13 | 2.55 | 0.42 |
| 1:F:186:LEU:HD22 | 1:F:186:LEU:HA | 1.71 | 0.42 |
| 1:F:208:PHE:O | 1:F:209:LEU:C | 2.57 | 0.42 |
| 1:F:426:ILE:CD1 | 1:F:436:VAL:CG2 | 2.92 | 0.42 |
| 1:A:45:THR:HA | 1:A:46:PRO:HD3 | 1.81 | 0.42 |
| 1:B:144:ASN:CG | 1:B:145:ASN:N | 2.72 | 0.42 |
| 1:C:192:LYS:O | 1:C:192:LYS:HG2 | 2.18 | 0.42 |
| 1:C:373:THR:OG1 | 1:D:471:ILE:HG21 | 2.19 | 0.42 |
| 1:D:86:TYR:HE1 | 1:D:414:PRO:HG3 | 1.84 | 0.42 |
| 1:D:494:GLN:HB2 | 1:D:494:GLN:HE21 | 1.72 | 0.42 |
| 1:F:60:VAL:CG1 | 1:F:112:LEU:HD13 | 2.49 | 0.42 |
| 1:F:131:TYR:C | 1:F:131:TYR:CD1 | 2.92 | 0.42 |
| 1:A:267:LEU:O | 1:A:283:GLU:CB | 2.68 | 0.42 |
| 1:A:323:GLN:NE2 | 1:A:327:PRO:HA | 2.35 | 0.42 |
| 1:A:58:THR:O | 1:A:63:GLY:N | 2.53 | 0.42 |
| 1:A:67:LYS:NZ | 1:A:204:GLU:CD | 2.73 | 0.42 |
| 1:A:85:ASN:HB2 | 1:A:413:VAL:HG12 | 2.02 | 0.42 |
| 1:B:16:ILE:HD13 | 1:B:16:ILE:HG21 | 1.77 | 0.42 |
| 1:B:168:LEU:CD1 | 1:B:291:VAL:HG11 | 2.49 | 0.42 |
| 1:B:432:ASN:O | 1:B:433:GLU:HB2 | 2.20 | 0.42 |
| 1:C:164:ARG:HH11 | 1:C:165:PRO:HD2 | 1.85 | 0.42 |
| 1:C:422:TYR:CE1 | 1:C:424:LYS:HB3 | 2.55 | 0.42 |
| 1:D:200:TYR:O | 1:D:201:VAL:C | 2.58 | 0.42 |
| 1:D:233:ALA:O | 1:D:236:ILE:HB | 2.20 | 0.42 |
| 1:D:221:ARG:HB2 | 1:D:252:VAL:HG22 | 2.01 | 0.42 |
| 1:D:407:TRP:CE3 | 1:D:412:THR:HG22 | 2.54 | 0.42 |
| 1:E:112:LEU:O | 1:E:113:ASN:C | 2.59 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:67:LYS:HE2 | 1:E:67:LYS:HB3 | 1.80 | 0.42 |
| 1:F:12:ASP:HB2 | 1:F:153:SER:O | 2.20 | 0.42 |
| 1:F:195:VAL:HG22 | 1:F:288:LEU:CB | 2.50 | 0.42 |
| 1:F:321:GLU:HG2 | 1:F:356:ARG:NH1 | 2.35 | 0.42 |
| 1:A:263:THR:CB | 1:A:264:PRO:CD | 2.97 | 0.42 |
| 1:A:429:LEU:HD23 | 1:A:433:GLU:HG2 | 2.02 | 0.42 |
| 1:B:47:THR:HG21 | 1:B:182:ASP:OD1 | 2.20 | 0.42 |
| 1:C:34:PHE:HZ | 1:C:355:GLN:NE2 | 2.18 | 0.42 |
| 1:C:85:ASN:OD1 | 1:C:85:ASN:N | 2.52 | 0.42 |
| 1:C:98:TRP:HE1 | 1:C:190:PRO:CD | 2.23 | 0.42 |
| 1:D:343:THR:HB | 1:D:344:PRO:HD2 | 1.99 | 0.42 |
| 1:D:478:ILE:HD12 | 1:D:479:PHE:H | 1.84 | 0.42 |
| 3:D:601:NDP:O2A | 3:D:601:NDP:O2N | 2.38 | 0.42 |
| 1:E:302:LEU:HA | 1:E:302:LEU:HD23 | 1.75 | 0.42 |
| 1:E:313:THR:C | 1:E:315:LYS:H | 2.20 | 0.42 |
| 1:E:371:PRO:HB2 | 1:F:471:ILE:CD1 | 2.44 | 0.42 |
| 1:E:426:ILE:CD1 | 1:E:436:VAL:HG23 | 2.49 | 0.42 |
| 1:E:55:LEU:HD13 | 1:E:116:TYR:HB3 | 2.02 | 0.42 |
| 1:F:189:CYS:HA | 1:F:190:PRO:HD3 | 1.96 | 0.42 |
| 1:F:72:GLN:HG3 | 1:F:76:LEU:HD22 | 2.01 | 0.42 |
| 1:C:191:GLY:O | 1:C:193:THR:N | 2.53 | 0.41 |
| 1:C:325:ASN:ND2 | 1:C:325:ASN:N | 2.68 | 0.41 |
| 1:D:343:THR:CG2 | 1:D:344:PRO:HD3 | 2.50 | 0.41 |
| 1:F:178:ILE:HB | 1:F:182:ASP:HB2 | 2.02 | 0.41 |
| 1:F:221:ARG:NH1 | 3:F:601:NDP:P2B | 2.93 | 0.41 |
| 1:A:383:CYS:SG | 1:A:456:LEU:HD12 | 2.60 | 0.41 |
| 1:B:221:ARG:NH1 | 3:B:601:NDP:C4A | 2.83 | 0.41 |
| 1:C:67:LYS:NZ | 1:C:204:GLU:CD | 2.73 | 0.41 |
| 1:C:21:GLY:HA2 | 1:C:57:GLY:CA | 2.50 | 0.41 |
| 1:C:401:VAL:CG2 | 1:C:486:LYS:HB2 | 2.50 | 0.41 |
| 1:C:53:TRP:HB2 | 1:C:61:ASN:OD1 | 2.20 | 0.41 |
| 1:D:195:VAL:HG22 | 1:D:288:LEU:CB | 2.50 | 0.41 |
| 1:E:431:ASP:OD1 | 1:E:431:ASP:C | 2.58 | 0.41 |
| 1:E:474:VAL:O | 1:E:475:CYS:C | 2.58 | 0.41 |
| 1:E:497:CYS:SG | 1:F:112:LEU:CD2 | 3.08 | 0.41 |
| 1:F:158:LEU:HD22 | 1:F:353:LEU:HD23 | 2.02 | 0.41 |
| 1:F:168:LEU:HD21 | 1:F:253:PRO:HG2 | 2.02 | 0.41 |
| 1:E:471:ILE:HD12 | 1:F:450:GLN:HB2 | 2.02 | 0.41 |
| 1:A:176:TYR:HB3 | 1:A:267:LEU:HD12 | 2.02 | 0.41 |
| 1:A:191:GLY:O | 1:A:193:THR:HG23 | 2.19 | 0.41 |
| 1:A:225:LEU:HA | 1:A:225:LEU:HD23 | 1.79 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:491:ASP:OD1 | 1:B:493:LEU:HG | 2.19 | 0.41 |
| 1:B:58:THR:HG23 | 1:B:62:VAL:HG23 | 2.02 | 0.41 |
| 1:C:326:VAL:HA | 1:C:327:PRO:HD2 | 1.92 | 0.41 |
| 1:C:43:PHE:CD1 | 1:C:44:VAL:O | 2.73 | 0.41 |
| 2:C:600:FAD:H1'1 | 2:C:600:FAD:H9 | 1.79 | 0.41 |
| 1:C:88:TRP:CZ3 | 1:D:96:HIS:HB2 | 2.55 | 0.41 |
| 1:E:370:VAL:CG2 | 1:E:370:VAL:O | 2.67 | 0.41 |
| 1:F:221:ARG:HB3 | 1:F:221:ARG:HH11 | 1.85 | 0.41 |
| 1:F:291:VAL:O | 3:F:601:NDP:H52A | 2.19 | 0.41 |
| 1:F:318:VAL:HG22 | 1:F:319:THR:H | 1.85 | 0.41 |
| 1:F:318:VAL:HG22 | 1:F:319:THR:N | 2.34 | 0.41 |
| 1:F:493:LEU:O | 1:F:494:GLN:CG | 2.64 | 0.41 |
| 1:A:403:HIS:ND1 | 1:A:422:TYR:OH | 2.39 | 0.41 |
| 1:A:471:ILE:H | 1:B:450:GLN:NE2 | 2.19 | 0.41 |
| 1:A:91:GLU:HG3 | 1:A:93:THR:H | 1.85 | 0.41 |
| 1:B:464:GLN:O | 1:B:467:SER:OG | 2.25 | 0.41 |
| 1:C:179:SER:N | 1:C:182:ASP:HB2 | 2.27 | 0.41 |
| 1:C:272:LYS:HG3 | 1:C:273:SER:H | 1.85 | 0.41 |
| 1:C:277:GLU:OE1 | 1:C:277:GLU:HA | 2.20 | 0.41 |
| 1:C:69:LEU:HA | 1:C:69:LEU:HD23 | 1.85 | 0.41 |
| 1:D:176:TYR:CE1 | 1:D:258:GLN:OE1 | 2.74 | 0.41 |
| 1:E:269:VAL:HG12 | 1:E:270:THR:N | 2.35 | 0.41 |
| 1:E:332:ILE:HD11 | 1:E:349:ALA:HB1 | 2.01 | 0.41 |
| 1:E:388:GLU:HG2 | 1:E:389:LYS:N | 2.34 | 0.41 |
| 1:E:395:GLY:O | 1:E:396:GLU:C | 2.59 | 0.41 |
| 1:E:440:VAL:HG13 | 1:E:440:VAL:O | 2.19 | 0.41 |
| 1:F:72:GLN:HG3 | 1:F:72:GLN:O | 2.20 | 0.41 |
| 1:A:318:VAL:HG13 | 1:A:322:GLU:CA | 2.49 | 0.41 |
| 1:A:84:ARG:HH11 | 1:A:84:ARG:CG | 2.26 | 0.41 |
| 1:B:175:GLU:CD | 1:B:175:GLU:H | 2.24 | 0.41 |
| 1:B:308:LYS:N | 1:B:325:ASN:HD21 | 2.14 | 0.41 |
| 1:C:183:LEU:HD21 | 1:C:209:LEU:HD21 | 2.02 | 0.41 |
| 1:C:267:LEU:HD23 | 1:C:267:LEU:N | 2.35 | 0.41 |
| 1:C:297:THR:HG21 | 1:C:316:ILE:HD11 | 2.01 | 0.41 |
| 1:E:440:VAL:HG22 | 1:E:441:LEU:N | 2.35 | 0.41 |
| 1:F:288:LEU:HD22 | 1:F:290:ALA:H | 1.86 | 0.41 |
| 1:F:438:PHE:HE2 | 1:F:449:THR:HG23 | 1.84 | 0.41 |
| 1:B:185:SER:O | 1:B:186:LEU:C | 2.58 | 0.41 |
| 1:B:86:TYR:CE2 | 1:B:414:PRO:HD3 | 2.54 | 0.41 |
| 1:C:452:PHE:O | 1:C:455:ALA:N | 2.53 | 0.41 |
| 1:C:478:ILE:N | 1:C:478:ILE:HD12 | 2.36 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:401:VAL:HG22 | 1:D:426:ILE:HB | 2.03 | 0.41 |
| 1:E:305:VAL:HG11 | 1:E:329:ILE:CD1 | 2.49 | 0.41 |
| 1:F:137:PRO:O | 1:F:139:LYS:N | 2.53 | 0.41 |
| 1:F:313:THR:C | 1:F:315:LYS:H | 2.15 | 0.41 |
| 1:A:450:GLN:HE22 | 1:B:470:GLY:CA | 2.32 | 0.41 |
| 1:B:336:LEU:HB3 | 1:B:339:LYS:CG | 2.51 | 0.41 |
| 1:B:402:TYR:CD1 | 1:B:402:TYR:N | 2.89 | 0.41 |
| 1:C:27:ALA:O | 1:C:28:ALA:C | 2.59 | 0.41 |
| 1:C:422:TYR:CD1 | 1:C:422:TYR:C | 2.94 | 0.41 |
| 1:C:72:GLN:O | 1:C:73:ALA:C | 2.57 | 0.41 |
| 1:D:21:GLY:HA3 | 2:D:600:FAD:O5B | 2.20 | 0.41 |
| 1:E:158:LEU:HA | 1:E:330:TYR:O | 2.21 | 0.41 |
| 1:F:109:ILE:HG22 | 1:F:113:ASN:HD21 | 1.86 | 0.41 |
| 1:F:212:ILE:HD12 | 1:F:212:ILE:HA | 1.67 | 0.41 |
| 1:F:319:THR:C | 1:F:321:GLU:H | 2.23 | 0.41 |
| 1:F:406:PHE:CZ | 1:F:421:CYS:HB3 | 2.56 | 0.41 |
| 1:C:168:LEU:HD12 | 1:C:168:LEU:HA | 1.66 | 0.41 |
| 1:C:188:TYR:O | 1:C:190:PRO:CD | 2.66 | 0.41 |
| 1:D:232:MET:HE1 | 1:D:441:LEU:HB2 | 2.03 | 0.41 |
| 1:D:460:LEU:HD21 | 1:D:465:LEU:HD13 | 2.03 | 0.41 |
| 1:E:45:THR:HA | 1:E:46:PRO:HD3 | 1.78 | 0.41 |
| 1:E:497:CYS:SG | 1:F:112:LEU:HD22 | 2.61 | 0.41 |
| 2:F:600:FAD:H8A | 2:F:600:FAD:H2B | 1.79 | 0.41 |
| 1:F:91:GLU:O | 1:F:92:ASP:C | 2.58 | 0.41 |
| 1:A:209:LEU:HA | 1:A:209:LEU:HD12 | 1.78 | 0.41 |
| 1:A:34:PHE:CE2 | 1:A:359:GLY:CA | 3.03 | 0.41 |
| 1:A:386:SER:HB3 | 1:A:389:LYS:HB2 | 2.03 | 0.41 |
| 1:B:194:LEU:HB2 | 1:B:284:PHE:CE2 | 2.56 | 0.41 |
| 1:B:403:HIS:C | 1:B:403:HIS:CD2 | 2.94 | 0.41 |
| 1:C:170:ILE:O | 1:C:173:ASP:OD1 | 2.39 | 0.41 |
| 1:C:260:GLU:CB | 1:C:266:ARG:HB3 | 2.51 | 0.41 |
| 1:C:42:ASP:HA | 2:C:600:FAD:N3A | 2.36 | 0.41 |
| 1:D:367:TYR:CD1 | 1:D:367:TYR:N | 2.88 | 0.41 |
| 1:D:91:GLU:O | 1:D:92:ASP:C | 2.59 | 0.41 |
| 1:E:361:SER:OG | 1:E:362:THR:N | 2.54 | 0.41 |
| 1:F:489:GLY:O | 1:F:490:GLY:O | 2.37 | 0.41 |
| 1:A:136:GLY:O | 1:A:137:PRO:C | 2.59 | 0.41 |
| 1:A:21:GLY:HA2 | 1:A:57:GLY:HA3 | 2.02 | 0.41 |
| 1:A:170:ILE:HB | 1:A:254:THR:O | 2.21 | 0.41 |
| 1:A:274:THR:HG23 | 1:A:274:THR:H | 1.48 | 0.41 |
| 1:A:371:PRO:HB3 | 1:A:453:ALA:HB2 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:322:GLU:O | 1:C:330:TYR:HD2 | 2.03 | 0.41 |
| 1:C:440:VAL:HG13 | 1:C:440:VAL:O | 2.20 | 0.41 |
| 1:C:65:ILE:C | 1:C:67:LYS:N | 2.73 | 0.41 |
| 1:D:278:GLU:OE2 | 1:D:280:ILE:HG23 | 2.21 | 0.41 |
| 1:D:397:GLU:HG2 | 1:D:397:GLU:H | 1.54 | 0.41 |
| 1:E:255:LYS:HE3 | 1:E:270:THR:HG21 | 2.03 | 0.41 |
| 1:F:475:CYS:O | 1:F:477:GLU:N | 2.54 | 0.41 |
| 1:A:343:THR:O | 1:A:347:ILE:HG23 | 2.21 | 0.41 |
| 1:A:382:CYS:HA | 1:A:438:PHE:O | 2.21 | 0.41 |
| 1:A:344:PRO:HG3 | 1:B:472:HIS:HB2 | 2.02 | 0.41 |
| 1:B:64:CYS:O | 1:B:65:ILE:C | 2.59 | 0.41 |
| 1:C:58:THR:HG21 | 1:C:293:ARG:HH22 | 1.86 | 0.41 |
| 1:D:288:LEU:HD23 | 1:D:288:LEU:HA | 1.78 | 0.41 |
| 1:D:386:SER:OG | 1:D:389:LYS:HB2 | 2.21 | 0.41 |
| 1:D:472:HIS:HA | 1:D:473:PRO:HA | 1.82 | 0.41 |
| 1:E:163:GLU:HB3 | 1:E:295:SER:HA | 2.03 | 0.41 |
| 1:F:101:MET:O | 1:F:105:VAL:HG23 | 2.21 | 0.41 |
| 1:F:475:CYS:O | 1:F:476:ALA:C | 2.59 | 0.41 |
| 1:C:20:GLY:CA | 1:C:42:ASP:HB2 | 2.51 | 0.40 |
| 1:C:337:GLU:O | 1:C:339:LYS:HG2 | 2.21 | 0.40 |
| 1:D:163:GLU:HB3 | 1:D:295:SER:CA | 2.46 | 0.40 |
| 1:D:366:ASP:OD1 | 1:D:366:ASP:C | 2.59 | 0.40 |
| 1:D:411:TRP:NE1 | 1:D:416:ARG:NH2 | 2.69 | 0.40 |
| 1:E:342:LEU:O | 1:E:345:VAL:HB | 2.20 | 0.40 |
| 1:F:39:MET:SD | 1:F:41:LEU:HD21 | 2.61 | 0.40 |
| 1:F:65:ILE:HB | 1:F:66:PRO:HD3 | 2.02 | 0.40 |
| 1:B:221:ARG:HD3 | 3:B:601:NDP:C2A | 2.51 | 0.40 |
| 1:C:170:ILE:HD12 | 1:C:254:THR:C | 2.42 | 0.40 |
| 1:C:70:MET:HB3 | 1:C:208:PHE:CD2 | 2.57 | 0.40 |
| 1:D:430:LYS:HB2 | 1:D:430:LYS:HE3 | 1.52 | 0.40 |
| 1:C:474:VAL:CG1 | 1:D:447:GLU:CD | 2.89 | 0.40 |
| 1:D:67:LYS:HB3 | 1:D:67:LYS:HE2 | 1.84 | 0.40 |
| 1:E:386:SER:O | 1:E:387:GLU:C | 2.56 | 0.40 |
| 1:A:402:TYR:CD1 | 1:A:462:LYS:HE2 | 2.56 | 0.40 |
| 1:B:228:PHE:O | 1:B:229:ASP:C | 2.60 | 0.40 |
| 1:D:292:GLY:HA2 | 3:D:601:NDP:O2N | 2.21 | 0.40 |
| 1:D:382:CYS:HA | 1:D:438:PHE:O | 2.20 | 0.40 |
| 1:E:136:GLY:O | 1:E:137:PRO:C | 2.59 | 0.40 |
| 1:E:86:TYR:O | 1:F:101:MET:HB2 | 2.22 | 0.40 |
| 1:F:166:ARG:HG3 | 1:F:294:ASP:OD2 | 2.21 | 0.40 |
| 1:F:221:ARG:HH11 | 1:F:221:ARG:HG2 | 1.85 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:302:LEU:HD23 | 1:F:302:LEU:HA | 1.76 | 0.40 |
| 1:F:413:VAL:HB | 1:F:414:PRO:HD3 | 2.04 | 0.40 |
| 1:A:185:SER:O | 1:A:186:LEU:C | 2.59 | 0.40 |
| 1:A:195:VAL:HB | 1:A:218:VAL:HG22 | 2.03 | 0.40 |
| 1:A:42:ASP:OD1 | 2:A:600:FAD:H1B | 2.22 | 0.40 |
| 1:A:497:CYS:SG | 1:B:112:LEU:HD22 | 2.61 | 0.40 |
| 1:B:267:LEU:O | 1:B:283:GLU:HA | 2.21 | 0.40 |
| 1:B:371:PRO:HD3 | 1:B:383:CYS:SG | 2.61 | 0.40 |
| 1:C:461:THR:HG23 | 1:C:464:GLN:OE1 | 2.21 | 0.40 |
| 1:D:21:GLY:HA2 | 1:D:57:GLY:HA3 | 2.03 | 0.40 |
| 1:D:324:THR:HB | 1:D:325:ASN:HD22 | 1.84 | 0.40 |
| 1:D:332:ILE:HA | 1:D:332:ILE:HD12 | 1.53 | 0.40 |
| 1:D:61:ASN:C | 1:D:62:VAL:CG1 | 2.89 | 0.40 |
| 1:E:309:ILE:HG21 | 1:E:309:ILE:HD13 | 1.58 | 0.40 |
| 1:F:123:LYS:O | 1:F:124:LYS:HB2 | 2.21 | 0.40 |
| 1:A:154:ALA:HB3 | 1:A:157:PHE:CE1 | 2.56 | 0.40 |
| 1:A:309:ILE:HA | 1:A:317:PRO:HD3 | 2.04 | 0.40 |
| 1:A:318:VAL:CG1 | 1:A:322:GLU:CA | 2.89 | 0.40 |
| 1:C:31:ALA:C | 1:C:33:LYS:N | 2.69 | 0.40 |
| 1:D:9:LYS:HB3 | 1:D:11:TYR:CE1 | 2.57 | 0.40 |
| 1:D:193:THR:HG22 | 1:D:194:LEU:N | 2.37 | 0.40 |
| 1:D:209:LEU:HD12 | 1:D:209:LEU:HA | 1.75 | 0.40 |
| 1:D:332:ILE:HD11 | 1:D:349:ALA:HB1 | 2.03 | 0.40 |
| 1:E:232:MET:HE2 | 1:E:232:MET:HB3 | 1.95 | 0.40 |
| 1:E:258:GLN:HA | 1:E:267:LEU:HD12 | 2.04 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|----|
| 1 | A | 488/499 (98%) | 445 (91%) | 36 (7%) | 7 (1%) | 11 | 43 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1 | B | 485/499 (97%) | 436 (90%) | 40 (8%) | 9 (2%) | 8 | 36 |
| 1 | C | 480/499 (96%) | 395 (82%) | 70 (15%) | 15 (3%) | 4 | 23 |
| 1 | D | 485/499 (97%) | 439 (90%) | 37 (8%) | 9 (2%) | 8 | 36 |
| 1 | E | 489/499 (98%) | 441 (90%) | 39 (8%) | 9 (2%) | 8 | 37 |
| 1 | F | 488/499 (98%) | 438 (90%) | 40 (8%) | 10 (2%) | 7 | 34 |
| All | All | 2915/2994 (97%) | 2594 (89%) | 262 (9%) | 59 (2%) | 7 | 34 |

All (59) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 263 | THR |
| 1 | A | 489 | GLY |
| 1 | B | 92 | ASP |
| 1 | B | 263 | THR |
| 1 | B | 314 | GLY |
| 1 | B | 489 | GLY |
| 1 | C | 32 | ALA |
| 1 | C | 184 | PHE |
| 1 | C | 190 | PRO |
| 1 | C | 191 | GLY |
| 1 | C | 192 | LYS |
| 1 | C | 489 | GLY |
| 1 | D | 92 | ASP |
| 1 | D | 263 | THR |
| 1 | D | 314 | GLY |
| 1 | D | 489 | GLY |
| 1 | E | 263 | THR |
| 1 | E | 314 | GLY |
| 1 | E | 489 | GLY |
| 1 | F | 263 | THR |
| 1 | F | 314 | GLY |
| 1 | A | 314 | GLY |
| 1 | C | 287 | VAL |
| 1 | E | 92 | ASP |
| 1 | E | 283 | GLU |
| 1 | F | 92 | ASP |
| 1 | F | 283 | GLU |
| 1 | F | 487 | ARG |
| 1 | F | 490 | GLY |
| 1 | A | 92 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 206 | ALA |
| 1 | C | 327 | PRO |
| 1 | C | 396 | GLU |
| 1 | D | 144 | ASN |
| 1 | D | 494 | GLN |
| 1 | E | 229 | ASP |
| 1 | F | 144 | ASN |
| 1 | F | 229 | ASP |
| 1 | A | 229 | ASP |
| 1 | A | 291 | VAL |
| 1 | C | 44 | VAL |
| 1 | C | 113 | ASN |
| 1 | D | 35 | ASP |
| 1 | D | 229 | ASP |
| 1 | E | 35 | ASP |
| 1 | A | 35 | ASP |
| 1 | B | 144 | ASN |
| 1 | B | 282 | ASP |
| 1 | B | 229 | ASP |
| 1 | B | 291 | VAL |
| 1 | C | 62 | VAL |
| 1 | E | 291 | VAL |
| 1 | F | 488 | SER |
| 1 | F | 291 | VAL |
| 1 | D | 291 | VAL |
| 1 | E | 62 | VAL |
| 1 | C | 264 | PRO |
| 1 | B | 62 | VAL |
| 1 | C | 473 | PRO |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1 | A | 406/414 (98%) | 352 (87%) | 54 (13%) | 4 | 17 |
| 1 | B | 405/414 (98%) | 344 (85%) | 61 (15%) | 3 | 14 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1 | C | 400/414 (97%) | 325 (81%) | 75 (19%) | 1 | 8 |
| 1 | D | 405/414 (98%) | 342 (84%) | 63 (16%) | 2 | 13 |
| 1 | E | 407/414 (98%) | 354 (87%) | 53 (13%) | 4 | 19 |
| 1 | F | 406/414 (98%) | 349 (86%) | 57 (14%) | 3 | 16 |
| All | All | 2429/2484 (98%) | 2066 (85%) | 363 (15%) | 3 | 14 |

All (363) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 14 | ASP |
| 1 | A | 38 | VAL |
| 1 | A | 40 | VAL |
| 1 | A | 55 | LEU |
| 1 | A | 64 | CYS |
| 1 | A | 76 | LEU |
| 1 | A | 85 | ASN |
| 1 | A | 94 | VAL |
| 1 | A | 99 | GLU |
| 1 | A | 102 | THR |
| 1 | A | 107 | ASN |
| 1 | A | 144 | ASN |
| 1 | A | 163 | GLU |
| 1 | A | 166 | ARG |
| 1 | A | 168 | LEU |
| 1 | A | 179 | SER |
| 1 | A | 185 | SER |
| 1 | A | 193 | THR |
| 1 | A | 209 | LEU |
| 1 | A | 212 | ILE |
| 1 | A | 221 | ARG |
| 1 | A | 245 | ILE |
| 1 | A | 246 | LYS |
| 1 | A | 257 | GLU |
| 1 | A | 259 | ILE |
| 1 | A | 267 | LEU |
| 1 | A | 270 | THR |
| 1 | A | 282 | ASP |
| 1 | A | 283 | GLU |
| 1 | A | 303 | GLU |
| 1 | A | 305 | VAL |
| 1 | A | 309 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 310 | ASN |
| 1 | A | 324 | THR |
| 1 | A | 335 | ILE |
| 1 | A | 347 | ILE |
| 1 | A | 356 | ARG |
| 1 | A | 358 | TYR |
| 1 | A | 361 | SER |
| 1 | A | 363 | VAL |
| 1 | A | 364 | LYS |
| 1 | A | 365 | CYS |
| 1 | A | 372 | THR |
| 1 | A | 373 | THR |
| 1 | A | 399 | ILE |
| 1 | A | 403 | HIS |
| 1 | A | 416 | ARG |
| 1 | A | 426 | ILE |
| 1 | A | 434 | ARG |
| 1 | A | 461 | THR |
| 1 | A | 469 | ILE |
| 1 | A | 473 | PRO |
| 1 | A | 478 | ILE |
| 1 | A | 487 | ARG |
| 1 | B | 9 | LYS |
| 1 | B | 22 | SER |
| 1 | B | 39 | MET |
| 1 | B | 40 | VAL |
| 1 | B | 51 | THR |
| 1 | B | 55 | LEU |
| 1 | B | 64 | CYS |
| 1 | B | 67 | LYS |
| 1 | B | 76 | LEU |
| 1 | B | 84 | ARG |
| 1 | B | 89 | LYS |
| 1 | B | 91 | GLU |
| 1 | B | 92 | ASP |
| 1 | B | 99 | GLU |
| 1 | B | 107 | ASN |
| 1 | B | 111 | SER |
| 1 | B | 129 | ASN |
| 1 | B | 150 | LYS |
| 1 | B | 163 | GLU |
| 1 | B | 168 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 185 | SER |
| 1 | B | 186 | LEU |
| 1 | B | 209 | LEU |
| 1 | B | 212 | ILE |
| 1 | B | 220 | VAL |
| 1 | B | 221 | ARG |
| 1 | B | 223 | ILE |
| 1 | B | 256 | ILE |
| 1 | B | 257 | GLU |
| 1 | B | 263 | THR |
| 1 | B | 268 | LYS |
| 1 | B | 272 | LYS |
| 1 | B | 276 | SER |
| 1 | B | 278 | GLU |
| 1 | B | 280 | ILE |
| 1 | B | 282 | ASP |
| 1 | B | 288 | LEU |
| 1 | B | 293 | ARG |
| 1 | B | 297 | THR |
| 1 | B | 303 | GLU |
| 1 | B | 305 | VAL |
| 1 | B | 310 | ASN |
| 1 | B | 318 | VAL |
| 1 | B | 325 | ASN |
| 1 | B | 335 | ILE |
| 1 | B | 336 | LEU |
| 1 | B | 340 | LEU |
| 1 | B | 344 | PRO |
| 1 | B | 347 | ILE |
| 1 | B | 348 | GLN |
| 1 | B | 373 | THR |
| 1 | B | 391 | VAL |
| 1 | B | 397 | GLU |
| 1 | B | 399 | ILE |
| 1 | B | 403 | HIS |
| 1 | B | 416 | ARG |
| 1 | B | 464 | GLN |
| 1 | B | 469 | ILE |
| 1 | B | 478 | ILE |
| 1 | B | 487 | ARG |
| 1 | B | 494 | GLN |
| 1 | C | 33 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 37 | LYS |
| 1 | C | 45 | THR |
| 1 | C | 52 | ASN |
| 1 | C | 55 | LEU |
| 1 | C | 64 | CYS |
| 1 | C | 98 | TRP |
| 1 | C | 100 | LYS |
| 1 | C | 102 | THR |
| 1 | C | 104 | SER |
| 1 | C | 129 | ASN |
| 1 | C | 135 | ILE |
| 1 | C | 138 | HIS |
| 1 | C | 139 | LYS |
| 1 | C | 141 | MET |
| 1 | C | 143 | THR |
| 1 | C | 152 | TYR |
| 1 | C | 153 | SER |
| 1 | C | 159 | ILE |
| 1 | C | 161 | THR |
| 1 | C | 163 | GLU |
| 1 | C | 168 | LEU |
| 1 | C | 175 | GLU |
| 1 | C | 178 | ILE |
| 1 | C | 180 | SER |
| 1 | C | 181 | ASP |
| 1 | C | 193 | THR |
| 1 | C | 209 | LEU |
| 1 | C | 212 | ILE |
| 1 | C | 220 | VAL |
| 1 | C | 224 | LEU |
| 1 | C | 234 | ASN |
| 1 | C | 255 | LYS |
| 1 | C | 258 | GLN |
| 1 | C | 259 | ILE |
| 1 | C | 260 | GLU |
| 1 | C | 263 | THR |
| 1 | C | 267 | LEU |
| 1 | C | 269 | VAL |
| 1 | C | 273 | SER |
| 1 | C | 274 | THR |
| 1 | C | 276 | SER |
| 1 | C | 278 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 283 | GLU |
| 1 | C | 285 | ASN |
| 1 | C | 288 | LEU |
| 1 | C | 289 | LEU |
| 1 | C | 294 | ASP |
| 1 | C | 297 | THR |
| 1 | C | 310 | ASN |
| 1 | C | 312 | LYS |
| 1 | C | 318 | VAL |
| 1 | C | 319 | THR |
| 1 | C | 324 | THR |
| 1 | C | 325 | ASN |
| 1 | C | 327 | PRO |
| 1 | C | 328 | TYR |
| 1 | C | 347 | ILE |
| 1 | C | 352 | LEU |
| 1 | C | 363 | VAL |
| 1 | C | 365 | CYS |
| 1 | C | 372 | THR |
| 1 | C | 376 | THR |
| 1 | C | 378 | LEU |
| 1 | C | 385 | LEU |
| 1 | C | 389 | LYS |
| 1 | C | 397 | GLU |
| 1 | C | 399 | ILE |
| 1 | C | 403 | HIS |
| 1 | C | 404 | SER |
| 1 | C | 429 | LEU |
| 1 | C | 441 | LEU |
| 1 | C | 469 | ILE |
| 1 | C | 478 | ILE |
| 1 | C | 488 | SER |
| 1 | D | 52 | ASN |
| 1 | D | 55 | LEU |
| 1 | D | 64 | CYS |
| 1 | D | 78 | GLN |
| 1 | D | 84 | ARG |
| 1 | D | 85 | ASN |
| 1 | D | 89 | LYS |
| 1 | D | 90 | LEU |
| 1 | D | 91 | GLU |
| 1 | D | 92 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 102 | THR |
| 1 | D | 123 | LYS |
| 1 | D | 139 | LYS |
| 1 | D | 168 | LEU |
| 1 | D | 185 | SER |
| 1 | D | 186 | LEU |
| 1 | D | 209 | LEU |
| 1 | D | 212 | ILE |
| 1 | D | 220 | VAL |
| 1 | D | 221 | ARG |
| 1 | D | 250 | GLN |
| 1 | D | 251 | PHE |
| 1 | D | 256 | ILE |
| 1 | D | 263 | THR |
| 1 | D | 266 | ARG |
| 1 | D | 267 | LEU |
| 1 | D | 268 | LYS |
| 1 | D | 272 | LYS |
| 1 | D | 276 | SER |
| 1 | D | 277 | GLU |
| 1 | D | 278 | GLU |
| 1 | D | 282 | ASP |
| 1 | D | 283 | GLU |
| 1 | D | 284 | PHE |
| 1 | D | 288 | LEU |
| 1 | D | 291 | VAL |
| 1 | D | 303 | GLU |
| 1 | D | 305 | VAL |
| 1 | D | 325 | ASN |
| 1 | D | 332 | ILE |
| 1 | D | 347 | ILE |
| 1 | D | 364 | LYS |
| 1 | D | 365 | CYS |
| 1 | D | 370 | VAL |
| 1 | D | 372 | THR |
| 1 | D | 373 | THR |
| 1 | D | 376 | THR |
| 1 | D | 382 | CYS |
| 1 | D | 396 | GLU |
| 1 | D | 403 | HIS |
| 1 | D | 409 | LEU |
| 1 | D | 410 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 416 | ARG |
| 1 | D | 418 | ASN |
| 1 | D | 426 | ILE |
| 1 | D | 430 | LYS |
| 1 | D | 436 | VAL |
| 1 | D | 473 | PRO |
| 1 | D | 478 | ILE |
| 1 | D | 485 | THR |
| 1 | D | 492 | ILE |
| 1 | D | 493 | LEU |
| 1 | D | 494 | GLN |
| 1 | E | 22 | SER |
| 1 | E | 29 | LYS |
| 1 | E | 38 | VAL |
| 1 | E | 40 | VAL |
| 1 | E | 52 | ASN |
| 1 | E | 55 | LEU |
| 1 | E | 64 | CYS |
| 1 | E | 72 | GLN |
| 1 | E | 76 | LEU |
| 1 | E | 104 | SER |
| 1 | E | 107 | ASN |
| 1 | E | 133 | LYS |
| 1 | E | 163 | GLU |
| 1 | E | 168 | LEU |
| 1 | E | 173 | ASP |
| 1 | E | 185 | SER |
| 1 | E | 193 | THR |
| 1 | E | 200 | TYR |
| 1 | E | 209 | LEU |
| 1 | E | 212 | ILE |
| 1 | E | 215 | ASP |
| 1 | E | 219 | MET |
| 1 | E | 221 | ARG |
| 1 | E | 228 | PHE |
| 1 | E | 266 | ARG |
| 1 | E | 267 | LEU |
| 1 | E | 275 | ASN |
| 1 | E | 276 | SER |
| 1 | E | 277 | GLU |
| 1 | E | 288 | LEU |
| 1 | E | 291 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 297 | THR |
| 1 | E | 303 | GLU |
| 1 | E | 308 | LYS |
| 1 | E | 309 | ILE |
| 1 | E | 318 | VAL |
| 1 | E | 335 | ILE |
| 1 | E | 336 | LEU |
| 1 | E | 347 | ILE |
| 1 | E | 362 | THR |
| 1 | E | 370 | VAL |
| 1 | E | 373 | THR |
| 1 | E | 391 | VAL |
| 1 | E | 403 | HIS |
| 1 | E | 415 | SER |
| 1 | E | 416 | ARG |
| 1 | E | 434 | ARG |
| 1 | E | 450 | GLN |
| 1 | E | 473 | PRO |
| 1 | E | 478 | ILE |
| 1 | E | 480 | THR |
| 1 | E | 491 | ASP |
| 1 | E | 498 | CYS |
| 1 | F | 29 | LYS |
| 1 | F | 40 | VAL |
| 1 | F | 55 | LEU |
| 1 | F | 58 | THR |
| 1 | F | 64 | CYS |
| 1 | F | 67 | LYS |
| 1 | F | 76 | LEU |
| 1 | F | 81 | LYS |
| 1 | F | 89 | LYS |
| 1 | F | 91 | GLU |
| 1 | F | 92 | ASP |
| 1 | F | 99 | GLU |
| 1 | F | 102 | THR |
| 1 | F | 104 | SER |
| 1 | F | 107 | ASN |
| 1 | F | 139 | LYS |
| 1 | F | 163 | GLU |
| 1 | F | 168 | LEU |
| 1 | F | 170 | ILE |
| 1 | F | 175 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 185 | SER |
| 1 | F | 186 | LEU |
| 1 | F | 193 | THR |
| 1 | F | 209 | LEU |
| 1 | F | 212 | ILE |
| 1 | F | 220 | VAL |
| 1 | F | 221 | ARG |
| 1 | F | 223 | ILE |
| 1 | F | 225 | LEU |
| 1 | F | 250 | GLN |
| 1 | F | 254 | THR |
| 1 | F | 256 | ILE |
| 1 | F | 257 | GLU |
| 1 | F | 267 | LEU |
| 1 | F | 275 | ASN |
| 1 | F | 276 | SER |
| 1 | F | 277 | GLU |
| 1 | F | 282 | ASP |
| 1 | F | 288 | LEU |
| 1 | F | 303 | GLU |
| 1 | F | 308 | LYS |
| 1 | F | 325 | ASN |
| 1 | F | 332 | ILE |
| 1 | F | 347 | ILE |
| 1 | F | 364 | LYS |
| 1 | F | 365 | CYS |
| 1 | F | 391 | VAL |
| 1 | F | 396 | GLU |
| 1 | F | 403 | HIS |
| 1 | F | 404 | SER |
| 1 | F | 416 | ARG |
| 1 | F | 422 | TYR |
| 1 | F | 426 | ILE |
| 1 | F | 434 | ARG |
| 1 | F | 463 | GLN |
| 1 | F | 478 | ILE |
| 1 | F | 497 | CYS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 72 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 78 | GLN |
| 1 | A | 96 | HIS |
| 1 | A | 113 | ASN |
| 1 | A | 138 | HIS |
| 1 | A | 250 | GLN |
| 1 | A | 285 | ASN |
| 1 | A | 310 | ASN |
| 1 | A | 325 | ASN |
| 1 | A | 348 | GLN |
| 1 | A | 418 | ASN |
| 1 | A | 439 | HIS |
| 1 | A | 450 | GLN |
| 1 | B | 96 | HIS |
| 1 | B | 106 | GLN |
| 1 | B | 107 | ASN |
| 1 | B | 113 | ASN |
| 1 | B | 129 | ASN |
| 1 | B | 138 | HIS |
| 1 | B | 239 | HIS |
| 1 | B | 285 | ASN |
| 1 | B | 310 | ASN |
| 1 | B | 325 | ASN |
| 1 | B | 439 | HIS |
| 1 | B | 450 | GLN |
| 1 | C | 72 | GLN |
| 1 | C | 96 | HIS |
| 1 | C | 129 | ASN |
| 1 | C | 138 | HIS |
| 1 | C | 230 | GLN |
| 1 | C | 234 | ASN |
| 1 | C | 250 | GLN |
| 1 | C | 258 | GLN |
| 1 | C | 285 | ASN |
| 1 | C | 310 | ASN |
| 1 | C | 325 | ASN |
| 1 | C | 348 | GLN |
| 1 | C | 355 | GLN |
| 1 | C | 418 | ASN |
| 1 | C | 439 | HIS |
| 1 | C | 444 | ASN |
| 1 | C | 472 | HIS |
| 1 | D | 52 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 61 | ASN |
| 1 | D | 72 | GLN |
| 1 | D | 78 | GLN |
| 1 | D | 106 | GLN |
| 1 | D | 107 | ASN |
| 1 | D | 108 | HIS |
| 1 | D | 138 | HIS |
| 1 | D | 144 | ASN |
| 1 | D | 250 | GLN |
| 1 | D | 275 | ASN |
| 1 | D | 285 | ASN |
| 1 | D | 325 | ASN |
| 1 | D | 403 | HIS |
| 1 | D | 418 | ASN |
| 1 | D | 439 | HIS |
| 1 | D | 472 | HIS |
| 1 | D | 494 | GLN |
| 1 | E | 72 | GLN |
| 1 | E | 113 | ASN |
| 1 | E | 138 | HIS |
| 1 | E | 285 | ASN |
| 1 | E | 323 | GLN |
| 1 | E | 325 | ASN |
| 1 | E | 418 | ASN |
| 1 | E | 419 | ASN |
| 1 | E | 439 | HIS |
| 1 | E | 450 | GLN |
| 1 | F | 71 | HIS |
| 1 | F | 72 | GLN |
| 1 | F | 78 | GLN |
| 1 | F | 96 | HIS |
| 1 | F | 107 | ASN |
| 1 | F | 113 | ASN |
| 1 | F | 138 | HIS |
| 1 | F | 230 | GLN |
| 1 | F | 234 | ASN |
| 1 | F | 250 | GLN |
| 1 | F | 258 | GLN |
| 1 | F | 285 | ASN |
| 1 | F | 325 | ASN |
| 1 | F | 355 | GLN |
| 1 | F | 428 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 439 | HIS |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

12 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$ |
| 3 | NDP | E | 601 | - | 36,42,52 | 1.48 | 6 (16%) | 43,65,80 | 1.33 | 4 (9%) |
| 2 | FAD | B | 600 | - | 51,58,58 | 1.46 | 10 (19%) | 60,89,89 | 1.82 | 13 (21%) |
| 3 | NDP | C | 601 | - | 36,42,52 | 1.56 | 8 (22%) | 43,65,80 | 1.72 | 10 (23%) |
| 2 | FAD | D | 600 | - | 51,58,58 | 1.59 | 10 (19%) | 60,89,89 | 1.91 | 13 (21%) |
| 3 | NDP | A | 601 | - | 36,42,52 | 1.49 | 5 (13%) | 43,65,80 | 1.57 | 7 (16%) |
| 2 | FAD | F | 600 | - | 51,58,58 | 1.31 | 6 (11%) | 60,89,89 | 1.78 | 11 (18%) |
| 2 | FAD | A | 600 | - | 51,58,58 | 1.39 | 5 (9%) | 60,89,89 | 2.00 | 14 (23%) |
| 2 | FAD | C | 600 | - | 51,58,58 | 1.49 | 8 (15%) | 60,89,89 | 2.10 | 18 (30%) |
| 2 | FAD | E | 600 | - | 51,58,58 | 1.55 | 8 (15%) | 60,89,89 | 2.39 | 15 (25%) |
| 3 | NDP | F | 601 | - | 36,42,52 | 1.55 | 7 (19%) | 43,65,80 | 1.43 | 8 (18%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 3 | NDP | D | 601 | - | 36,42,52 | 1.45 | 5 (13%) | 43,65,80 | 1.67 | 9 (20%) |
| 3 | NDP | B | 601 | - | 36,42,52 | 1.77 | 9 (25%) | 43,65,80 | 1.52 | 9 (20%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-------------|---------|
| 3 | NDP | E | 601 | - | - | 5/23/56/77 | 0/4/4/5 |
| 2 | FAD | B | 600 | - | - | 4/30/50/50 | 0/6/6/6 |
| 3 | NDP | C | 601 | - | - | 5/23/56/77 | 0/4/4/5 |
| 2 | FAD | D | 600 | - | - | 5/30/50/50 | 0/6/6/6 |
| 3 | NDP | A | 601 | - | - | 13/23/56/77 | 0/4/4/5 |
| 2 | FAD | F | 600 | - | - | 10/30/50/50 | 0/6/6/6 |
| 2 | FAD | A | 600 | - | - | 9/30/50/50 | 0/6/6/6 |
| 2 | FAD | C | 600 | - | - | 10/30/50/50 | 0/6/6/6 |
| 2 | FAD | E | 600 | - | - | 10/30/50/50 | 0/6/6/6 |
| 3 | NDP | F | 601 | - | - | 6/23/56/77 | 0/4/4/5 |
| 3 | NDP | D | 601 | - | - | 12/23/56/77 | 0/4/4/5 |
| 3 | NDP | B | 601 | - | - | 9/23/56/77 | 0/4/4/5 |

All (87) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | A | 600 | FAD | C2A-N3A | 4.49 | 1.39 | 1.32 |
| 2 | E | 600 | FAD | C2A-N3A | 4.48 | 1.39 | 1.32 |
| 2 | B | 600 | FAD | C2A-N3A | 4.41 | 1.39 | 1.32 |
| 2 | D | 600 | FAD | C2A-N3A | 4.29 | 1.39 | 1.32 |
| 3 | C | 601 | NDP | P2B-O3X | 4.17 | 1.70 | 1.54 |
| 3 | B | 601 | NDP | P2B-O3X | 4.11 | 1.70 | 1.54 |
| 3 | B | 601 | NDP | C2A-N1A | 4.05 | 1.41 | 1.33 |
| 3 | A | 601 | NDP | P2B-O2X | 4.03 | 1.70 | 1.54 |
| 2 | C | 600 | FAD | C2A-N3A | 4.00 | 1.38 | 1.32 |
| 3 | B | 601 | NDP | P2B-O2X | 3.87 | 1.69 | 1.54 |
| 3 | E | 601 | NDP | P2B-O2X | 3.84 | 1.69 | 1.54 |
| 2 | C | 600 | FAD | C4X-N5 | 3.80 | 1.38 | 1.33 |
| 2 | C | 600 | FAD | C10-N1 | 3.78 | 1.38 | 1.33 |
| 3 | E | 601 | NDP | P2B-O3X | 3.76 | 1.69 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3 | F | 601 | NDP | P2B-O3X | 3.76 | 1.69 | 1.54 |
| 3 | F | 601 | NDP | P2B-O2X | 3.70 | 1.69 | 1.54 |
| 2 | F | 600 | FAD | C10-N1 | 3.69 | 1.38 | 1.33 |
| 3 | D | 601 | NDP | P2B-O3X | 3.68 | 1.69 | 1.54 |
| 2 | F | 600 | FAD | C2A-N3A | 3.67 | 1.38 | 1.32 |
| 2 | A | 600 | FAD | C1'-N10 | 3.66 | 1.52 | 1.48 |
| 3 | C | 601 | NDP | P2B-O2X | 3.62 | 1.68 | 1.54 |
| 2 | D | 600 | FAD | C2B-C1B | -3.59 | 1.48 | 1.53 |
| 3 | D | 601 | NDP | P2B-O2X | 3.58 | 1.68 | 1.54 |
| 3 | A | 601 | NDP | PN-O2N | 3.57 | 1.72 | 1.55 |
| 2 | D | 600 | FAD | C2A-N1A | 3.55 | 1.40 | 1.33 |
| 3 | B | 601 | NDP | C5A-C4A | 3.51 | 1.50 | 1.40 |
| 2 | E | 600 | FAD | C4X-N5 | 3.49 | 1.38 | 1.33 |
| 3 | E | 601 | NDP | PA-O2A | 3.48 | 1.71 | 1.55 |
| 2 | C | 600 | FAD | C1'-N10 | 3.45 | 1.51 | 1.48 |
| 2 | F | 600 | FAD | C4X-N5 | 3.41 | 1.38 | 1.33 |
| 2 | E | 600 | FAD | C1'-N10 | 3.40 | 1.51 | 1.48 |
| 3 | A | 601 | NDP | P2B-O3X | 3.38 | 1.67 | 1.54 |
| 2 | E | 600 | FAD | C10-N1 | 3.27 | 1.37 | 1.33 |
| 3 | A | 601 | NDP | PA-O2A | 3.27 | 1.70 | 1.55 |
| 2 | D | 600 | FAD | C5'-C4' | 3.23 | 1.56 | 1.51 |
| 3 | D | 601 | NDP | PN-O2N | 3.23 | 1.70 | 1.55 |
| 2 | B | 600 | FAD | C1'-N10 | 3.20 | 1.51 | 1.48 |
| 3 | D | 601 | NDP | C5A-C4A | 3.19 | 1.49 | 1.40 |
| 3 | E | 601 | NDP | PN-O2N | 3.18 | 1.70 | 1.55 |
| 3 | D | 601 | NDP | PA-O2A | 3.18 | 1.70 | 1.55 |
| 3 | C | 601 | NDP | PN-O2N | 3.17 | 1.70 | 1.55 |
| 3 | F | 601 | NDP | PN-O2N | 3.16 | 1.70 | 1.55 |
| 3 | C | 601 | NDP | PA-O2A | 3.16 | 1.70 | 1.55 |
| 3 | F | 601 | NDP | PA-O2A | 3.14 | 1.70 | 1.55 |
| 2 | A | 600 | FAD | C4X-N5 | 3.11 | 1.37 | 1.33 |
| 3 | B | 601 | NDP | PA-O2A | 3.09 | 1.69 | 1.55 |
| 2 | B | 600 | FAD | C2A-N1A | 3.06 | 1.39 | 1.33 |
| 3 | A | 601 | NDP | C5A-C4A | 2.99 | 1.48 | 1.40 |
| 3 | B | 601 | NDP | C2A-N3A | 2.97 | 1.36 | 1.32 |
| 2 | B | 600 | FAD | C4X-C10 | -2.91 | 1.35 | 1.38 |
| 2 | F | 600 | FAD | C2A-N1A | 2.83 | 1.39 | 1.33 |
| 3 | B | 601 | NDP | PN-O2N | 2.82 | 1.68 | 1.55 |
| 3 | F | 601 | NDP | C5A-C4A | 2.82 | 1.48 | 1.40 |
| 2 | A | 600 | FAD | C2A-N1A | 2.68 | 1.38 | 1.33 |
| 2 | B | 600 | FAD | C4X-N5 | 2.62 | 1.37 | 1.33 |
| 2 | E | 600 | FAD | C2B-C1B | -2.60 | 1.49 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | C | 600 | FAD | C5'-C4' | 2.57 | 1.55 | 1.51 |
| 3 | E | 601 | NDP | C5A-C4A | 2.57 | 1.47 | 1.40 |
| 3 | C | 601 | NDP | C5A-C4A | 2.53 | 1.47 | 1.40 |
| 2 | C | 600 | FAD | C2A-N1A | 2.49 | 1.38 | 1.33 |
| 2 | A | 600 | FAD | C9A-C5X | -2.45 | 1.37 | 1.42 |
| 3 | F | 601 | NDP | O4B-C1B | 2.44 | 1.44 | 1.41 |
| 3 | C | 601 | NDP | C2A-N3A | 2.44 | 1.36 | 1.32 |
| 3 | B | 601 | NDP | C6A-C5A | 2.43 | 1.52 | 1.43 |
| 2 | D | 600 | FAD | C5X-N5 | 2.36 | 1.39 | 1.35 |
| 3 | C | 601 | NDP | P2B-O2B | 2.35 | 1.63 | 1.59 |
| 2 | D | 600 | FAD | C4-C4X | -2.35 | 1.37 | 1.41 |
| 2 | C | 600 | FAD | C4-N3 | 2.31 | 1.37 | 1.33 |
| 2 | D | 600 | FAD | O4B-C1B | 2.27 | 1.44 | 1.41 |
| 2 | E | 600 | FAD | C2A-N1A | 2.26 | 1.38 | 1.33 |
| 2 | C | 600 | FAD | C5X-N5 | 2.23 | 1.39 | 1.35 |
| 2 | B | 600 | FAD | C4-C4X | -2.20 | 1.37 | 1.41 |
| 3 | B | 601 | NDP | C6A-N6A | 2.19 | 1.42 | 1.34 |
| 3 | E | 601 | NDP | C4A-N3A | -2.18 | 1.32 | 1.35 |
| 2 | D | 600 | FAD | C9A-C5X | -2.17 | 1.38 | 1.42 |
| 3 | C | 601 | NDP | O4B-C1B | 2.12 | 1.44 | 1.41 |
| 2 | F | 600 | FAD | C5X-N5 | 2.11 | 1.38 | 1.35 |
| 2 | F | 600 | FAD | C2B-C1B | -2.11 | 1.50 | 1.53 |
| 2 | D | 600 | FAD | C4X-N5 | 2.10 | 1.36 | 1.33 |
| 2 | B | 600 | FAD | C5'-C4' | 2.09 | 1.54 | 1.51 |
| 2 | B | 600 | FAD | O4B-C4B | -2.08 | 1.40 | 1.45 |
| 3 | F | 601 | NDP | C6A-C5A | 2.07 | 1.51 | 1.43 |
| 2 | E | 600 | FAD | C4-C4X | -2.04 | 1.37 | 1.41 |
| 2 | D | 600 | FAD | C1'-N10 | 2.03 | 1.50 | 1.48 |
| 2 | E | 600 | FAD | C5X-N5 | 2.02 | 1.38 | 1.35 |
| 2 | B | 600 | FAD | C2B-C1B | -2.01 | 1.50 | 1.53 |
| 2 | B | 600 | FAD | C4-N3 | 2.00 | 1.36 | 1.33 |

All (131) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | E | 600 | FAD | C1'-N10-C10 | 9.86 | 127.24 | 118.41 |
| 2 | E | 600 | FAD | C5X-C9A-N10 | 8.13 | 123.61 | 117.72 |
| 2 | A | 600 | FAD | P-O3P-PA | -6.71 | 109.79 | 132.83 |
| 2 | D | 600 | FAD | P-O3P-PA | -6.11 | 111.86 | 132.83 |
| 2 | F | 600 | FAD | C4-N3-C2 | 5.78 | 120.02 | 115.14 |
| 2 | B | 600 | FAD | N3A-C2A-N1A | -5.76 | 119.68 | 128.68 |
| 2 | C | 600 | FAD | N3A-C2A-N1A | -5.64 | 119.87 | 128.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | A | 600 | FAD | C4-N3-C2 | 5.64 | 119.90 | 115.14 |
| 2 | F | 600 | FAD | N3A-C2A-N1A | -5.56 | 119.99 | 128.68 |
| 2 | C | 600 | FAD | C4-N3-C2 | 5.37 | 119.68 | 115.14 |
| 2 | D | 600 | FAD | N3A-C2A-N1A | -5.35 | 120.32 | 128.68 |
| 2 | C | 600 | FAD | P-O3P-PA | -5.23 | 114.88 | 132.83 |
| 3 | A | 601 | NDP | PN-O3-PA | -5.13 | 115.23 | 132.83 |
| 2 | A | 600 | FAD | N3A-C2A-N1A | -5.03 | 120.81 | 128.68 |
| 2 | B | 600 | FAD | P-O3P-PA | -4.90 | 116.01 | 132.83 |
| 2 | B | 600 | FAD | C1'-N10-C10 | 4.77 | 122.68 | 118.41 |
| 2 | C | 600 | FAD | C1'-N10-C10 | 4.73 | 122.65 | 118.41 |
| 3 | D | 601 | NDP | PN-O3-PA | -4.69 | 116.73 | 132.83 |
| 3 | C | 601 | NDP | O3B-C3B-C4B | -4.69 | 97.50 | 111.05 |
| 2 | B | 600 | FAD | O3B-C3B-C4B | -4.59 | 97.78 | 111.05 |
| 2 | E | 600 | FAD | N3A-C2A-N1A | -4.44 | 121.74 | 128.68 |
| 2 | F | 600 | FAD | P-O3P-PA | -4.36 | 117.86 | 132.83 |
| 2 | F | 600 | FAD | C1'-N10-C9A | 4.33 | 121.70 | 118.29 |
| 2 | C | 600 | FAD | C2B-C3B-C4B | -4.32 | 94.25 | 102.64 |
| 2 | D | 600 | FAD | C4-N3-C2 | 4.16 | 118.66 | 115.14 |
| 2 | D | 600 | FAD | C1'-N10-C9A | 4.15 | 121.56 | 118.29 |
| 2 | E | 600 | FAD | C4-N3-C2 | 4.11 | 118.61 | 115.14 |
| 3 | D | 601 | NDP | N3A-C2A-N1A | -4.02 | 122.39 | 128.68 |
| 3 | E | 601 | NDP | C1B-N9A-C4A | -3.98 | 119.64 | 126.64 |
| 2 | E | 600 | FAD | C1'-N10-C9A | -3.95 | 115.18 | 118.29 |
| 2 | D | 600 | FAD | C5X-C9A-N10 | 3.88 | 120.53 | 117.72 |
| 2 | A | 600 | FAD | C5X-C9A-N10 | 3.84 | 120.50 | 117.72 |
| 3 | B | 601 | NDP | PN-O3-PA | -3.81 | 119.77 | 132.83 |
| 3 | F | 601 | NDP | N3A-C2A-N1A | -3.79 | 122.75 | 128.68 |
| 2 | D | 600 | FAD | O4B-C1B-C2B | -3.77 | 101.41 | 106.93 |
| 2 | E | 600 | FAD | P-O3P-PA | -3.75 | 119.95 | 132.83 |
| 3 | C | 601 | NDP | C3B-C2B-C1B | -3.68 | 95.97 | 102.89 |
| 3 | D | 601 | NDP | C2A-N1A-C6A | 3.67 | 125.02 | 118.75 |
| 2 | C | 600 | FAD | C5X-C9A-N10 | 3.65 | 120.36 | 117.72 |
| 2 | B | 600 | FAD | C5X-C9A-N10 | 3.64 | 120.35 | 117.72 |
| 3 | E | 601 | NDP | N3A-C2A-N1A | -3.61 | 123.04 | 128.68 |
| 2 | A | 600 | FAD | C4X-N5-C5X | 3.51 | 120.28 | 116.77 |
| 2 | C | 600 | FAD | C4X-N5-C5X | 3.49 | 120.26 | 116.77 |
| 2 | E | 600 | FAD | C6-C5X-N5 | 3.48 | 122.89 | 119.05 |
| 2 | F | 600 | FAD | O4B-C1B-C2B | -3.45 | 101.88 | 106.93 |
| 2 | C | 600 | FAD | O4B-C1B-C2B | -3.40 | 101.96 | 106.93 |
| 2 | E | 600 | FAD | C9A-N10-C10 | -3.39 | 117.47 | 121.91 |
| 3 | C | 601 | NDP | N3A-C2A-N1A | -3.38 | 123.40 | 128.68 |
| 2 | D | 600 | FAD | C10-C4X-N5 | -3.34 | 118.95 | 121.26 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | D | 601 | NDP | O5B-C5B-C4B | 3.32 | 120.40 | 108.99 |
| 3 | C | 601 | NDP | PN-O3-PA | -3.25 | 121.66 | 132.83 |
| 2 | A | 600 | FAD | O5B-C5B-C4B | -3.23 | 97.89 | 108.99 |
| 2 | B | 600 | FAD | C4X-N5-C5X | 3.22 | 119.99 | 116.77 |
| 3 | C | 601 | NDP | C2B-C3B-C4B | 3.21 | 108.96 | 101.99 |
| 3 | A | 601 | NDP | N3A-C2A-N1A | -3.17 | 123.73 | 128.68 |
| 2 | B | 600 | FAD | O3'-C3'-C2' | -3.15 | 101.20 | 108.81 |
| 2 | A | 600 | FAD | O3B-C3B-C4B | -3.13 | 102.01 | 111.05 |
| 3 | F | 601 | NDP | C4A-C5A-N7A | -3.09 | 106.17 | 109.40 |
| 2 | A | 600 | FAD | O4'-C4'-C5' | -3.07 | 103.01 | 109.92 |
| 2 | C | 600 | FAD | C5A-C6A-N6A | -3.06 | 115.70 | 120.35 |
| 2 | A | 600 | FAD | C4X-C4-N3 | -3.02 | 119.30 | 123.43 |
| 3 | B | 601 | NDP | O4D-C4D-C3D | 3.02 | 107.38 | 104.70 |
| 2 | E | 600 | FAD | C4A-C5A-N7A | -3.00 | 106.27 | 109.40 |
| 3 | B | 601 | NDP | C5A-C6A-N1A | -2.88 | 113.81 | 120.35 |
| 2 | E | 600 | FAD | C4X-N5-C5X | 2.84 | 119.61 | 116.77 |
| 3 | E | 601 | NDP | C2A-N1A-C6A | 2.80 | 123.53 | 118.75 |
| 3 | F | 601 | NDP | C2A-N1A-C6A | 2.79 | 123.53 | 118.75 |
| 3 | E | 601 | NDP | C1D-C2D-C3D | 2.78 | 105.86 | 101.63 |
| 3 | C | 601 | NDP | O4D-C4D-C3D | 2.77 | 107.16 | 104.70 |
| 2 | D | 600 | FAD | C3B-C2B-C1B | -2.76 | 96.82 | 100.98 |
| 2 | D | 600 | FAD | C9A-N10-C10 | -2.76 | 118.30 | 121.91 |
| 2 | A | 600 | FAD | C10-C4X-N5 | -2.75 | 119.36 | 121.26 |
| 3 | A | 601 | NDP | O3B-C3B-C2B | -2.73 | 103.42 | 111.17 |
| 2 | D | 600 | FAD | C4X-C10-N10 | 2.72 | 123.10 | 120.30 |
| 2 | C | 600 | FAD | O5B-PA-O1A | 2.71 | 119.66 | 109.07 |
| 2 | C | 600 | FAD | C10-C4X-N5 | -2.70 | 119.39 | 121.26 |
| 3 | B | 601 | NDP | C1D-C2D-C3D | 2.68 | 105.71 | 101.63 |
| 2 | C | 600 | FAD | O4B-C4B-C3B | -2.66 | 99.85 | 105.11 |
| 2 | E | 600 | FAD | C3B-C2B-C1B | -2.66 | 96.98 | 100.98 |
| 3 | A | 601 | NDP | O5B-C5B-C4B | 2.66 | 118.13 | 108.99 |
| 2 | F | 600 | FAD | C4X-N5-C5X | 2.65 | 119.42 | 116.77 |
| 2 | E | 600 | FAD | C9A-C5X-N5 | -2.64 | 118.22 | 122.36 |
| 3 | B | 601 | NDP | O5B-C5B-C4B | 2.64 | 118.09 | 108.99 |
| 2 | F | 600 | FAD | C5X-C9A-N10 | 2.61 | 119.61 | 117.72 |
| 3 | B | 601 | NDP | O2B-C2B-C3B | 2.58 | 121.04 | 111.68 |
| 3 | D | 601 | NDP | O2X-P2B-O2B | 2.56 | 117.46 | 105.99 |
| 3 | C | 601 | NDP | C1D-C2D-C3D | 2.55 | 105.52 | 101.63 |
| 2 | B | 600 | FAD | C4-C4X-C10 | 2.52 | 121.62 | 119.95 |
| 2 | E | 600 | FAD | O2'-C2'-C3' | 2.51 | 115.21 | 109.10 |
| 3 | A | 601 | NDP | C1D-C2D-C3D | 2.51 | 105.45 | 101.63 |
| 3 | F | 601 | NDP | C1D-C2D-C3D | 2.47 | 105.40 | 101.63 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | C | 600 | FAD | C4X-C4-N3 | -2.45 | 120.08 | 123.43 |
| 3 | C | 601 | NDP | O3B-C3B-C2B | -2.45 | 104.21 | 111.17 |
| 3 | D | 601 | NDP | C1D-C2D-C3D | 2.41 | 105.30 | 101.63 |
| 2 | D | 600 | FAD | C4X-N5-C5X | 2.40 | 119.17 | 116.77 |
| 2 | A | 600 | FAD | C1'-N10-C9A | 2.39 | 120.17 | 118.29 |
| 2 | D | 600 | FAD | C4-C4X-N5 | 2.38 | 121.32 | 118.60 |
| 3 | F | 601 | NDP | O5B-C5B-C4B | 2.38 | 117.18 | 108.99 |
| 2 | F | 600 | FAD | C10-C4X-N5 | -2.37 | 119.62 | 121.26 |
| 3 | F | 601 | NDP | O3B-C3B-C4B | -2.36 | 104.22 | 111.05 |
| 2 | F | 600 | FAD | C4-C4X-N5 | 2.36 | 121.30 | 118.60 |
| 2 | B | 600 | FAD | C6-C5X-C9A | 2.34 | 122.12 | 119.05 |
| 3 | D | 601 | NDP | N6A-C6A-N1A | 2.34 | 123.42 | 118.57 |
| 3 | D | 601 | NDP | C5A-C6A-N1A | -2.33 | 115.08 | 120.35 |
| 3 | A | 601 | NDP | C2A-N1A-C6A | 2.32 | 122.73 | 118.75 |
| 2 | E | 600 | FAD | O3B-C3B-C4B | -2.32 | 104.34 | 111.05 |
| 3 | B | 601 | NDP | C4A-C5A-N7A | -2.32 | 106.99 | 109.40 |
| 2 | C | 600 | FAD | C9A-N10-C10 | -2.31 | 118.88 | 121.91 |
| 2 | C | 600 | FAD | PA-O5B-C5B | 2.29 | 135.10 | 121.68 |
| 2 | C | 600 | FAD | O2B-C2B-C3B | -2.26 | 104.52 | 111.82 |
| 2 | C | 600 | FAD | O2B-C2B-C1B | -2.21 | 102.71 | 110.85 |
| 2 | A | 600 | FAD | O4'-C4'-C3' | 2.20 | 114.45 | 109.10 |
| 3 | F | 601 | NDP | C5A-C6A-N1A | -2.19 | 115.40 | 120.35 |
| 2 | A | 600 | FAD | C1'-C2'-C3' | 2.18 | 115.88 | 109.79 |
| 3 | C | 601 | NDP | N6A-C6A-N1A | 2.17 | 123.08 | 118.57 |
| 2 | B | 600 | FAD | C3B-C2B-C1B | -2.14 | 97.76 | 100.98 |
| 2 | E | 600 | FAD | N6A-C6A-N1A | -2.13 | 114.14 | 118.57 |
| 3 | D | 601 | NDP | O5B-PA-O1A | 2.13 | 117.39 | 109.07 |
| 2 | D | 600 | FAD | O2B-C2B-C1B | -2.12 | 103.01 | 110.85 |
| 2 | A | 600 | FAD | C9A-N10-C10 | -2.12 | 119.13 | 121.91 |
| 2 | B | 600 | FAD | C9A-C5X-N5 | -2.12 | 119.05 | 122.36 |
| 3 | C | 601 | NDP | O4B-C1B-C2B | -2.10 | 102.94 | 106.59 |
| 3 | F | 601 | NDP | N6A-C6A-N1A | 2.08 | 122.90 | 118.57 |
| 2 | C | 600 | FAD | C5B-C4B-C3B | 2.08 | 122.98 | 115.18 |
| 2 | B | 600 | FAD | O2'-C2'-C3' | 2.07 | 114.13 | 109.10 |
| 2 | F | 600 | FAD | C4X-C4-N3 | -2.05 | 120.63 | 123.43 |
| 2 | B | 600 | FAD | N6A-C6A-N1A | -2.04 | 114.35 | 118.57 |
| 3 | B | 601 | NDP | C5A-C6A-N6A | 2.03 | 123.44 | 120.35 |
| 3 | A | 601 | NDP | O4B-C4B-C5B | -2.03 | 102.71 | 109.37 |
| 2 | F | 600 | FAD | O4'-C4'-C3' | 2.01 | 113.98 | 109.10 |
| 3 | B | 601 | NDP | N6A-C6A-N1A | 2.00 | 122.73 | 118.57 |

There are no chirality outliers.

All (98) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | B | 600 | FAD | C2'-C1'-N10-C9A |
| 3 | C | 601 | NDP | O4B-C4B-C5B-O5B |
| 3 | C | 601 | NDP | PA-O3-PN-O5D |
| 2 | D | 600 | FAD | O4B-C4B-C5B-O5B |
| 2 | D | 600 | FAD | PA-O3P-P-O5' |
| 3 | A | 601 | NDP | C5D-O5D-PN-O3 |
| 3 | A | 601 | NDP | C5D-O5D-PN-O1N |
| 3 | A | 601 | NDP | C5D-O5D-PN-O2N |
| 3 | A | 601 | NDP | O4D-C4D-C5D-O5D |
| 3 | A | 601 | NDP | C3D-C4D-C5D-O5D |
| 2 | F | 600 | FAD | O4B-C4B-C5B-O5B |
| 2 | F | 600 | FAD | C2'-C3'-C4'-O4' |
| 2 | F | 600 | FAD | O3'-C3'-C4'-O4' |
| 2 | F | 600 | FAD | O3'-C3'-C4'-C5' |
| 2 | F | 600 | FAD | PA-O3P-P-O5' |
| 2 | A | 600 | FAD | O4'-C4'-C5'-O5' |
| 2 | A | 600 | FAD | C5'-O5'-P-O2P |
| 2 | C | 600 | FAD | C3B-C4B-C5B-O5B |
| 2 | C | 600 | FAD | N10-C1'-C2'-O2' |
| 2 | C | 600 | FAD | N10-C1'-C2'-C3' |
| 2 | C | 600 | FAD | C2'-C3'-C4'-O4' |
| 2 | C | 600 | FAD | C2'-C3'-C4'-C5' |
| 2 | C | 600 | FAD | O3'-C3'-C4'-O4' |
| 2 | E | 600 | FAD | O4B-C4B-C5B-O5B |
| 2 | E | 600 | FAD | C2'-C1'-N10-C9A |
| 2 | E | 600 | FAD | C5'-O5'-P-O2P |
| 3 | F | 601 | NDP | C5D-O5D-PN-O1N |
| 3 | F | 601 | NDP | C5D-O5D-PN-O2N |
| 3 | D | 601 | NDP | C5B-O5B-PA-O3 |
| 3 | D | 601 | NDP | C5D-O5D-PN-O3 |
| 3 | D | 601 | NDP | C5D-O5D-PN-O2N |
| 3 | E | 601 | NDP | O4B-C4B-C5B-O5B |
| 3 | E | 601 | NDP | C3B-C4B-C5B-O5B |
| 3 | E | 601 | NDP | O4D-C4D-C5D-O5D |
| 3 | E | 601 | NDP | C3D-C4D-C5D-O5D |
| 2 | B | 600 | FAD | O4B-C4B-C5B-O5B |
| 2 | B | 600 | FAD | C3B-C4B-C5B-O5B |
| 3 | C | 601 | NDP | C3B-C4B-C5B-O5B |
| 2 | D | 600 | FAD | C3B-C4B-C5B-O5B |
| 2 | F | 600 | FAD | C3B-C4B-C5B-O5B |
| 2 | A | 600 | FAD | O4B-C4B-C5B-O5B |
| 3 | B | 601 | NDP | O4D-C4D-C5D-O5D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 3 | B | 601 | NDP | C3D-C4D-C5D-O5D |
| 3 | E | 601 | NDP | C4D-C5D-O5D-PN |
| 2 | C | 600 | FAD | O3'-C3'-C4'-C5' |
| 2 | F | 600 | FAD | C2'-C3'-C4'-C5' |
| 2 | A | 600 | FAD | C3B-C4B-C5B-O5B |
| 2 | E | 600 | FAD | C3B-C4B-C5B-O5B |
| 3 | D | 601 | NDP | O4B-C4B-C5B-O5B |
| 3 | D | 601 | NDP | C3B-C4B-C5B-O5B |
| 2 | C | 600 | FAD | O4B-C4B-C5B-O5B |
| 3 | D | 601 | NDP | C4B-C5B-O5B-PA |
| 3 | A | 601 | NDP | PN-O3-PA-O5B |
| 2 | A | 600 | FAD | PA-O3P-P-O5' |
| 2 | E | 600 | FAD | PA-O3P-P-O5' |
| 3 | F | 601 | NDP | PA-O3-PN-O5D |
| 3 | F | 601 | NDP | C2B-O2B-P2B-O1X |
| 3 | B | 601 | NDP | C4D-C5D-O5D-PN |
| 2 | F | 600 | FAD | C5'-O5'-P-O3P |
| 2 | A | 600 | FAD | C5'-O5'-P-O3P |
| 2 | C | 600 | FAD | C5B-O5B-PA-O3P |
| 2 | E | 600 | FAD | P-O3P-PA-O2A |
| 3 | D | 601 | NDP | PN-O3-PA-O2A |
| 3 | B | 601 | NDP | PA-O3-PN-O1N |
| 3 | C | 601 | NDP | C4B-C5B-O5B-PA |
| 2 | F | 600 | FAD | C5'-O5'-P-O1P |
| 2 | F | 600 | FAD | C5'-O5'-P-O2P |
| 2 | A | 600 | FAD | C5'-O5'-P-O1P |
| 2 | C | 600 | FAD | C5B-O5B-PA-O2A |
| 2 | E | 600 | FAD | C5'-O5'-P-O1P |
| 3 | D | 601 | NDP | C5B-O5B-PA-O1A |
| 3 | D | 601 | NDP | C5D-O5D-PN-O1N |
| 2 | D | 600 | FAD | P-O3P-PA-O2A |
| 2 | A | 600 | FAD | P-O3P-PA-O2A |
| 3 | B | 601 | NDP | C4B-C5B-O5B-PA |
| 3 | A | 601 | NDP | C4B-C5B-O5B-PA |
| 3 | A | 601 | NDP | PA-O3-PN-O1N |
| 3 | B | 601 | NDP | PA-O3-PN-O2N |
| 3 | A | 601 | NDP | C3B-C4B-C5B-O5B |
| 3 | A | 601 | NDP | C2B-O2B-P2B-O1X |
| 2 | B | 600 | FAD | C5B-O5B-PA-O3P |
| 3 | C | 601 | NDP | C5D-O5D-PN-O3 |
| 3 | A | 601 | NDP | C2B-O2B-P2B-O3X |
| 3 | F | 601 | NDP | C5D-O5D-PN-O3 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 3 | D | 601 | NDP | C2B-O2B-P2B-O3X |
| 3 | B | 601 | NDP | C2B-O2B-P2B-O3X |
| 3 | A | 601 | NDP | O4B-C4B-C5B-O5B |
| 3 | D | 601 | NDP | O4D-C4D-C5D-O5D |
| 2 | D | 600 | FAD | P-O3P-PA-O1A |
| 2 | A | 600 | FAD | P-O3P-PA-O1A |
| 2 | E | 600 | FAD | P-O3P-PA-O1A |
| 2 | E | 600 | FAD | PA-O3P-P-O2P |
| 3 | D | 601 | NDP | PN-O3-PA-O1A |
| 3 | A | 601 | NDP | C5B-O5B-PA-O1A |
| 3 | B | 601 | NDP | C5B-O5B-PA-O1A |
| 3 | F | 601 | NDP | O4B-C4B-C5B-O5B |
| 3 | B | 601 | NDP | O4B-C4B-C5B-O5B |
| 2 | E | 600 | FAD | O4'-C4'-C5'-O5' |

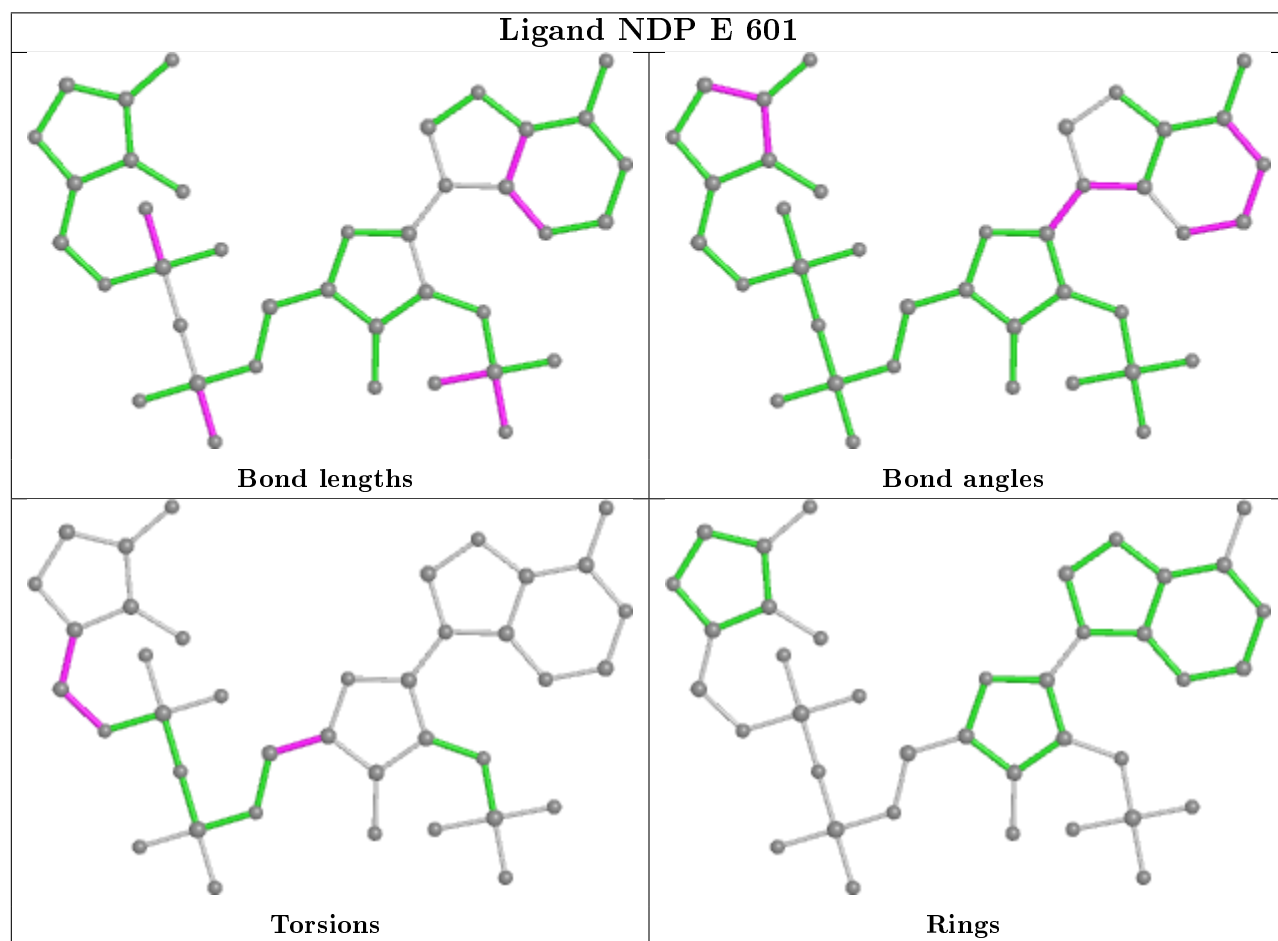
There are no ring outliers.

12 monomers are involved in 71 short contacts:

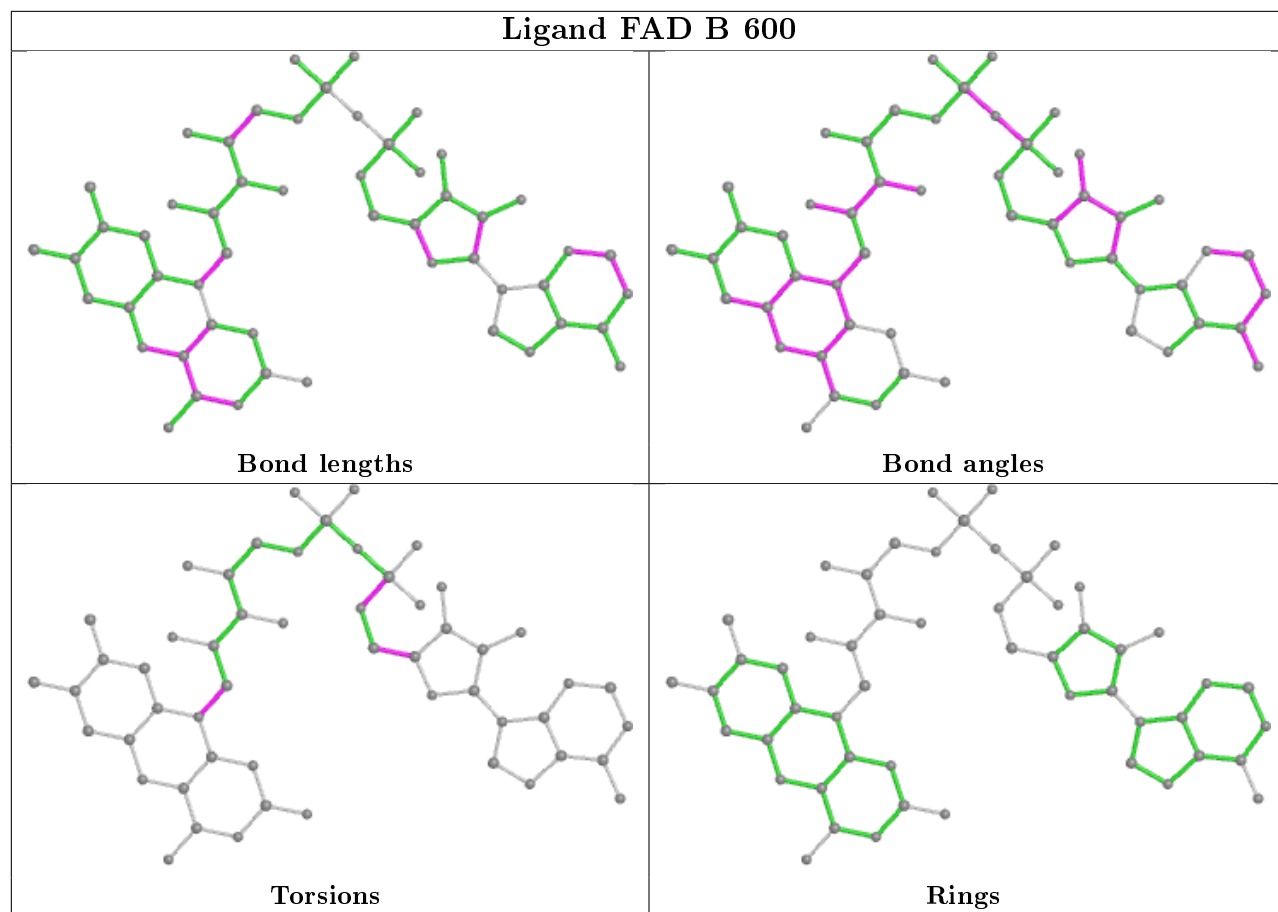
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3 | E | 601 | NDP | 1 | 0 |
| 2 | B | 600 | FAD | 10 | 0 |
| 3 | C | 601 | NDP | 6 | 0 |
| 2 | D | 600 | FAD | 4 | 0 |
| 3 | A | 601 | NDP | 2 | 0 |
| 2 | F | 600 | FAD | 5 | 0 |
| 2 | A | 600 | FAD | 5 | 0 |
| 2 | C | 600 | FAD | 17 | 0 |
| 2 | E | 600 | FAD | 3 | 0 |
| 3 | F | 601 | NDP | 4 | 0 |
| 3 | D | 601 | NDP | 6 | 0 |
| 3 | B | 601 | NDP | 8 | 0 |

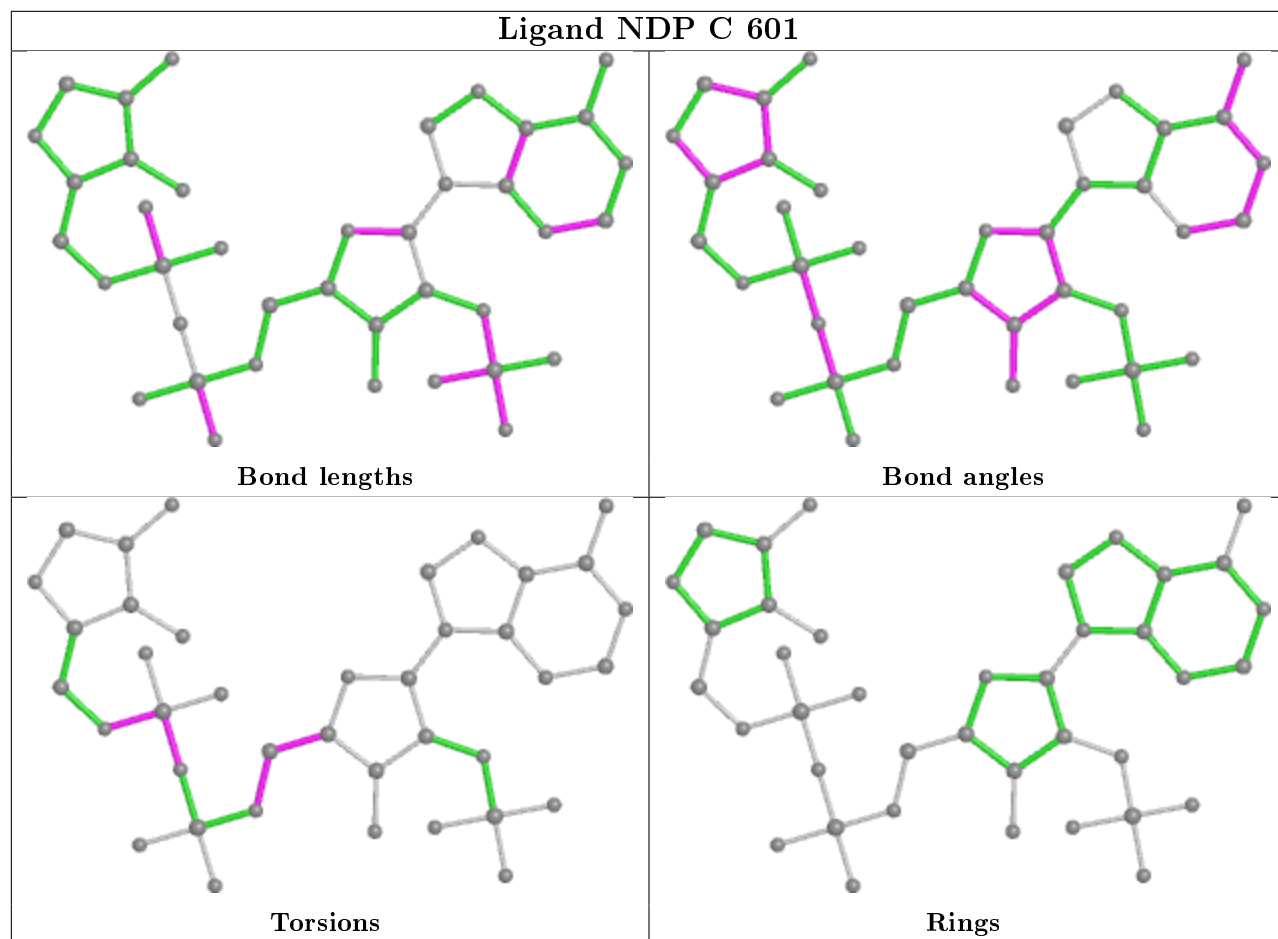
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

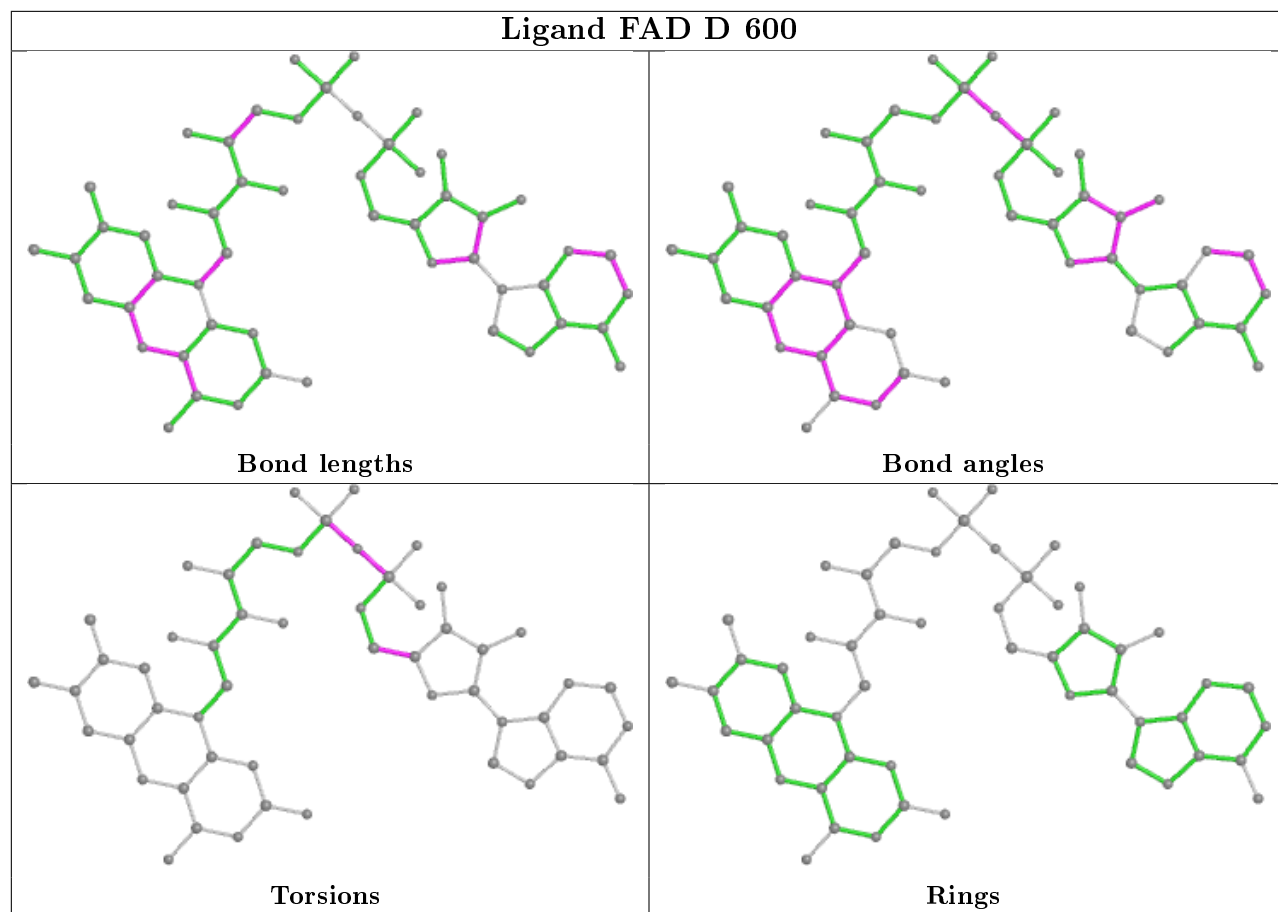
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

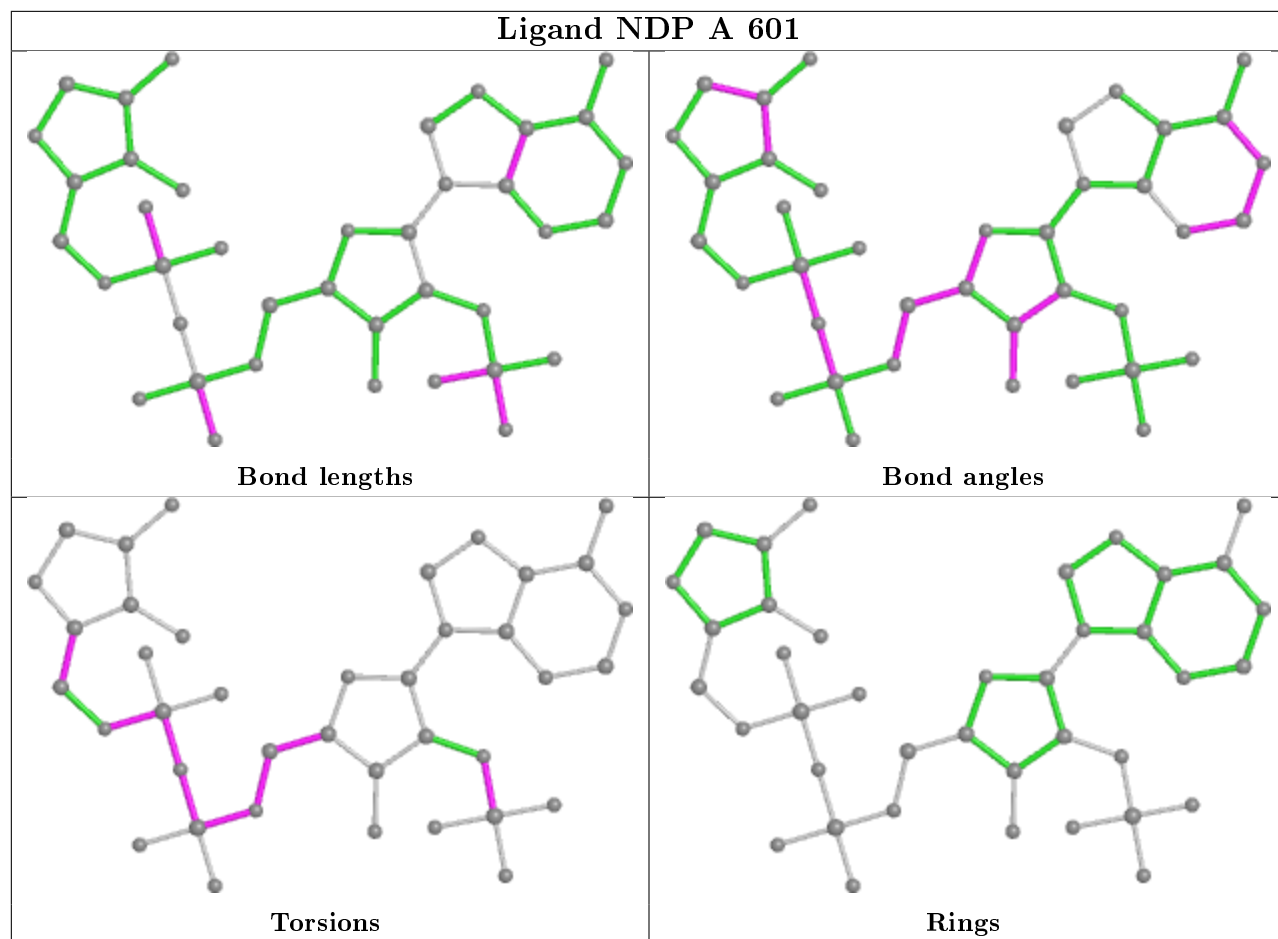


Ligand FAD B 600

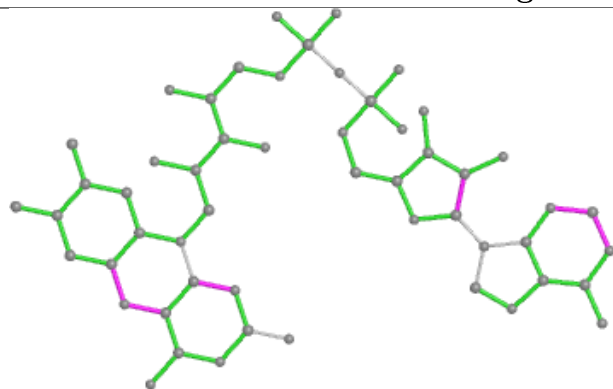




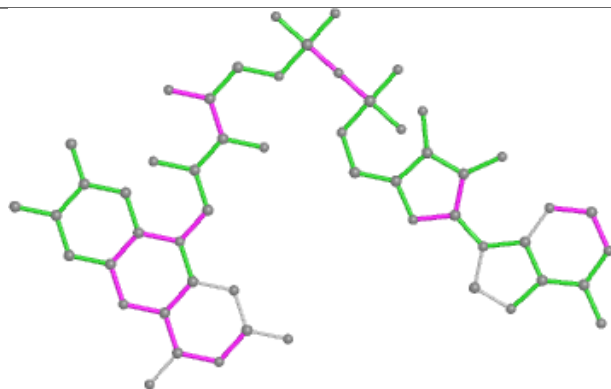




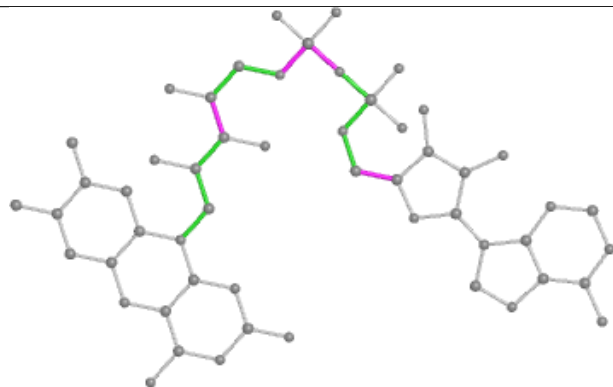
Ligand FAD F 600



Bond lengths



Bond angles

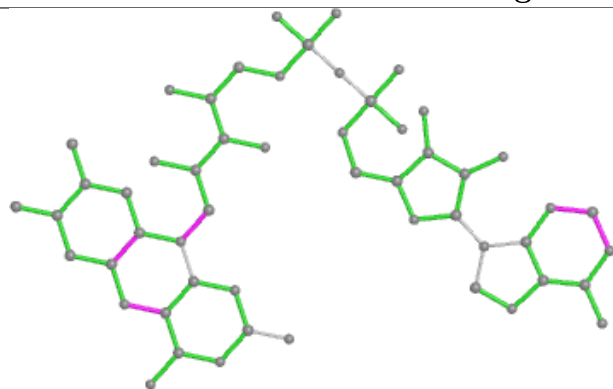


Torsions

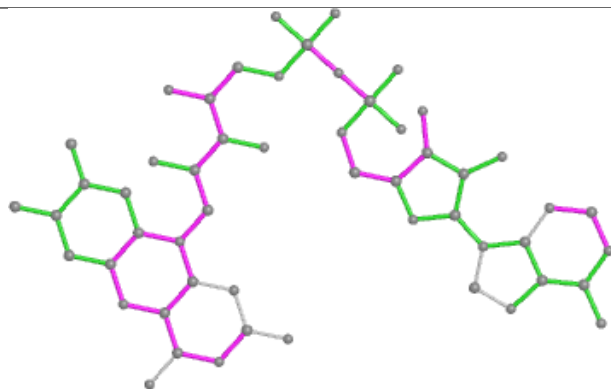


Rings

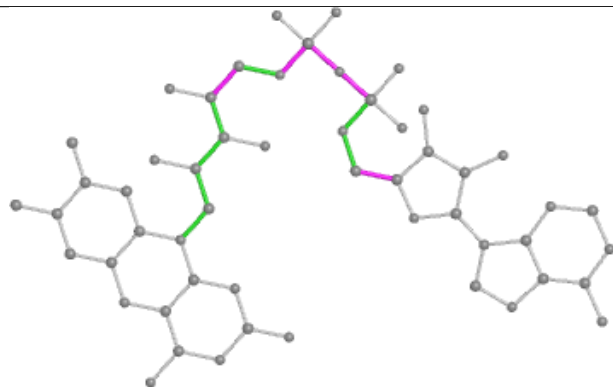
Ligand FAD A 600



Bond lengths



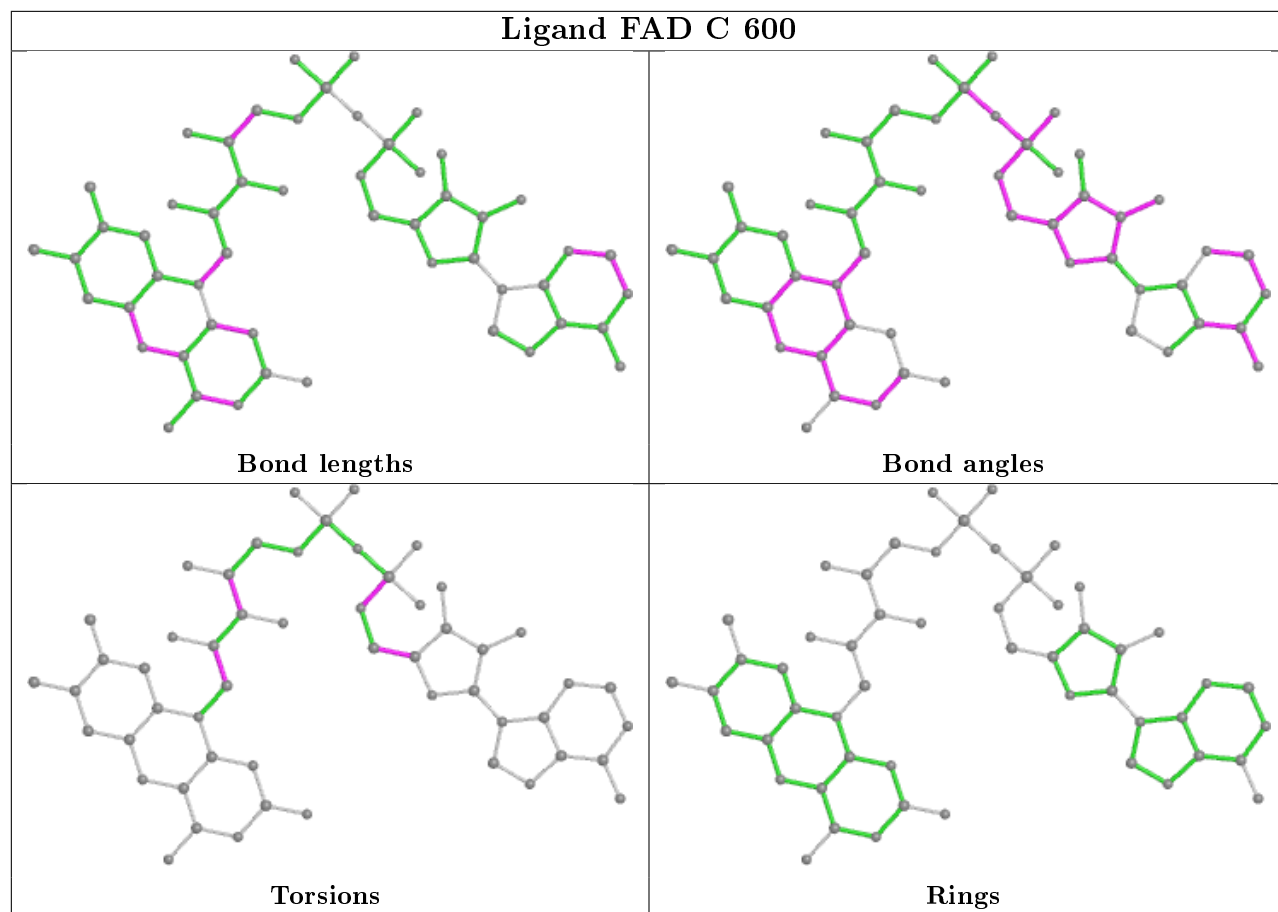
Bond angles



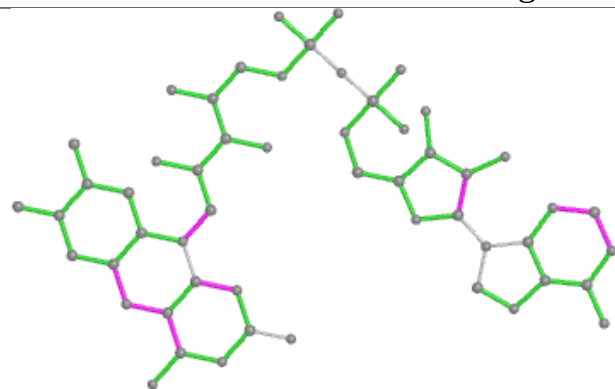
Torsions



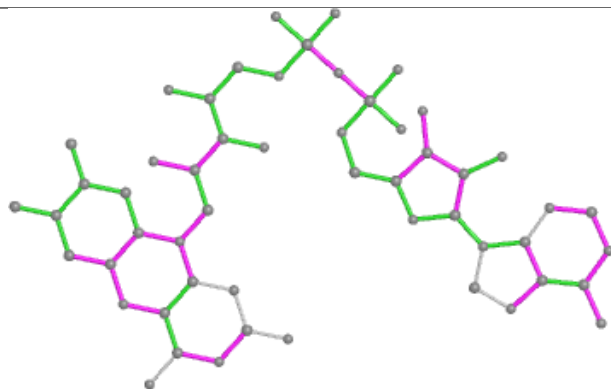
Rings



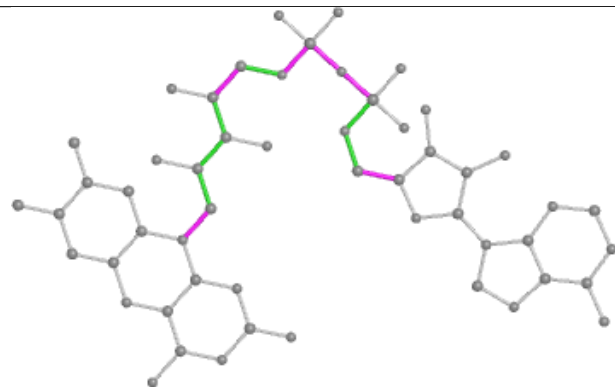
Ligand FAD E 600



Bond lengths



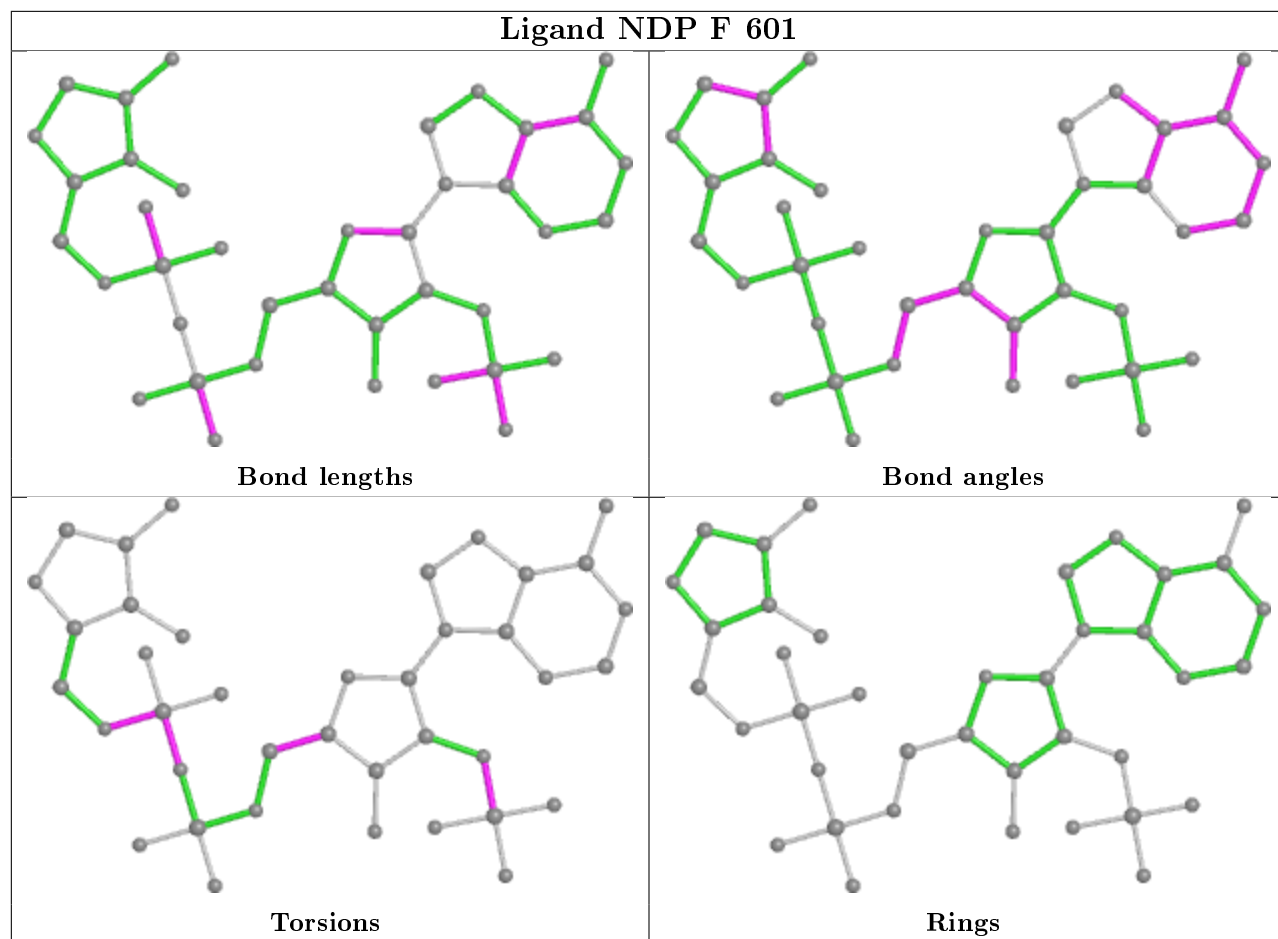
Bond angles

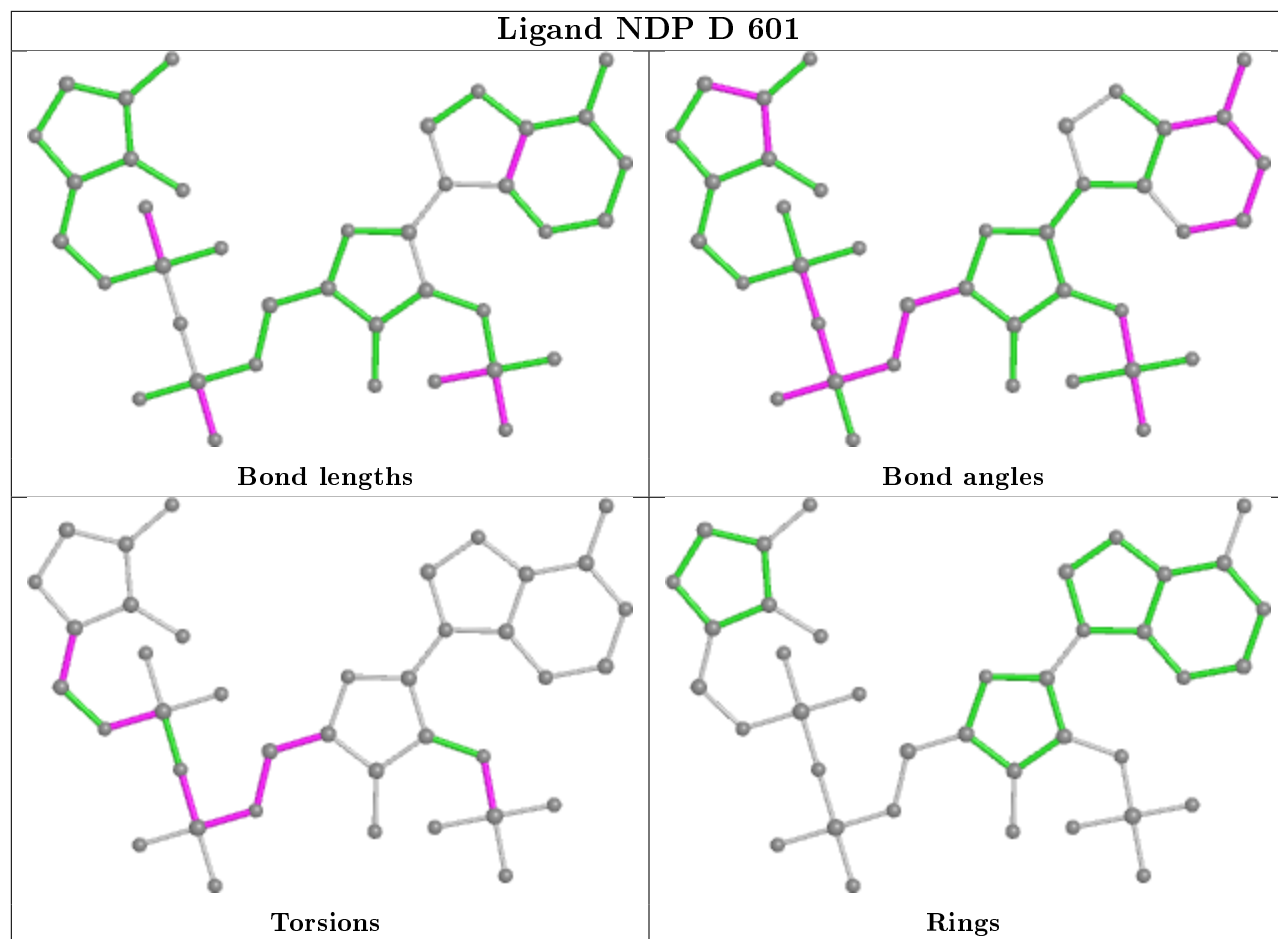


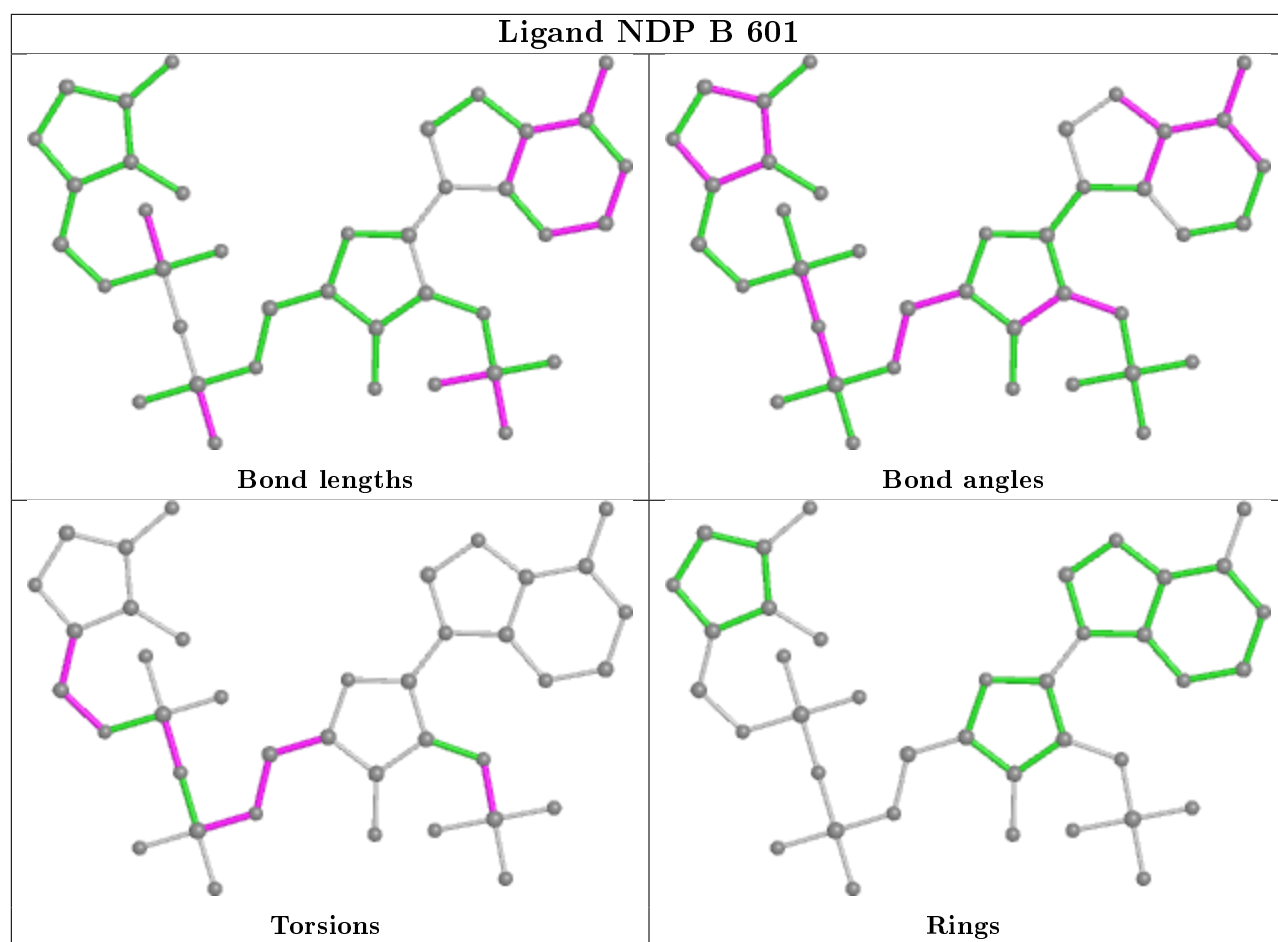
Torsions



Rings







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 | 490/499 (98%) | -0.38 | 2 (0%) 92 79 | 7, 13, 20, 49 | 0 |
| 1 | B | 487/499 (97%) | -0.48 | 1 (0%) 95 87 | 6, 13, 20, 39 | 0 |
| 1 | C | 482/499 (96%) | 0.11 | 16 (3%) 46 20 | 6, 13, 19, 44 | 0 |
| 1 | D | 487/499 (97%) | -0.33 | 4 (0%) 86 65 | 6, 12, 19, 38 | 0 |
| 1 | E | 491/499 (98%) | -0.39 | 4 (0%) 86 65 | 7, 13, 20, 48 | 0 |
| 1 | F | 490/499 (98%) | -0.24 | 6 (1%) 79 54 | 6, 13, 20, 48 | 0 |
| All | All | 2927/2994 (97%) | -0.29 | 33 (1%) 80 56 | 6, 13, 20, 49 | 0 |

All (33) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | E | 497 | CYS | 6.9 |
| 1 | E | 495 | SER | 5.5 |
| 1 | C | 297 | THR | 5.1 |
| 1 | F | 495 | SER | 5.1 |
| 1 | A | 498 | CYS | 3.6 |
| 1 | C | 306 | GLY | 3.6 |
| 1 | D | 494 | GLN | 3.3 |
| 1 | A | 497 | CYS | 3.1 |
| 1 | F | 498 | CYS | 3.1 |
| 1 | E | 498 | CYS | 3.0 |
| 1 | C | 35 | ASP | 2.9 |
| 1 | D | 495 | SER | 2.8 |
| 1 | C | 296 | CYS | 2.8 |
| 1 | E | 496 | GLY | 2.8 |
| 1 | C | 256 | ILE | 2.6 |
| 1 | C | 135 | ILE | 2.6 |
| 1 | C | 275 | ASN | 2.6 |
| 1 | F | 494 | GLN | 2.5 |
| 1 | C | 335 | ILE | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | C | 134 | PHE | 2.3 |
| 1 | C | 361 | SER | 2.3 |
| 1 | F | 297 | THR | 2.2 |
| 1 | C | 182 | ASP | 2.2 |
| 1 | F | 496 | GLY | 2.2 |
| 1 | D | 394 | PHE | 2.2 |
| 1 | C | 250 | GLN | 2.2 |
| 1 | C | 257 | GLU | 2.2 |
| 1 | B | 494 | GLN | 2.2 |
| 1 | F | 499 | GLY | 2.1 |
| 1 | D | 114 | TRP | 2.1 |
| 1 | C | 298 | ARG | 2.0 |
| 1 | C | 281 | GLU | 2.0 |
| 1 | C | 168 | LEU | 2.0 |

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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.

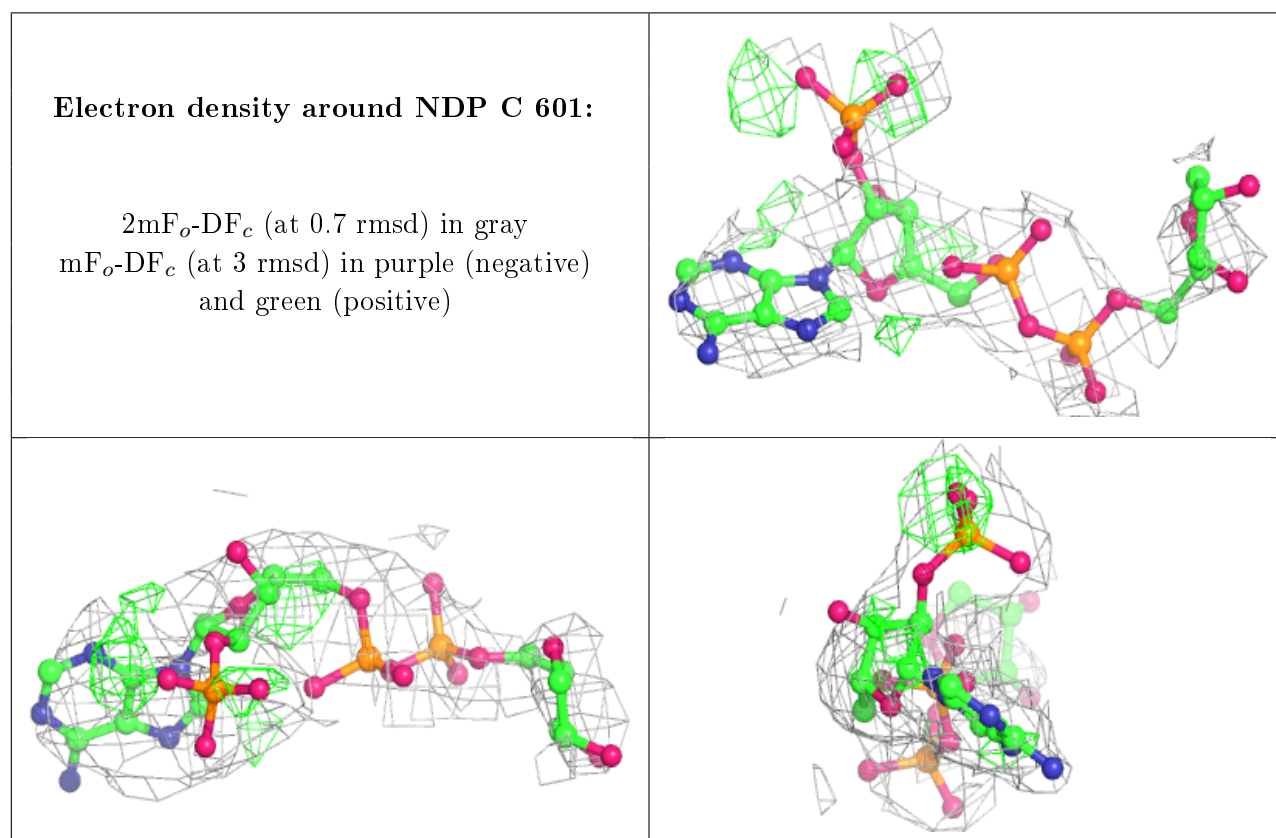
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 3 | NDP | C | 601 | 39/48 | 0.77 | 0.26 | 82,92,100,101 | 0 |
| 3 | NDP | F | 601 | 39/48 | 0.78 | 0.29 | 72,95,112,112 | 0 |
| 3 | NDP | A | 601 | 39/48 | 0.85 | 0.22 | 41,49,78,78 | 0 |
| 3 | NDP | D | 601 | 39/48 | 0.85 | 0.20 | 44,55,77,77 | 0 |
| 2 | FAD | C | 600 | 53/53 | 0.86 | 0.28 | 34,45,49,51 | 0 |
| 3 | NDP | B | 601 | 39/48 | 0.89 | 0.22 | 31,50,69,71 | 0 |
| 3 | NDP | E | 601 | 39/48 | 0.91 | 0.21 | 45,52,76,79 | 0 |
| 2 | FAD | F | 600 | 53/53 | 0.92 | 0.26 | 27,33,53,55 | 0 |
| 2 | FAD | E | 600 | 53/53 | 0.94 | 0.28 | 10,17,54,56 | 0 |

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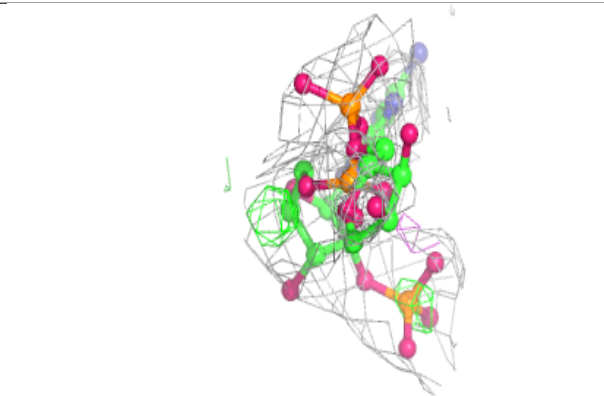
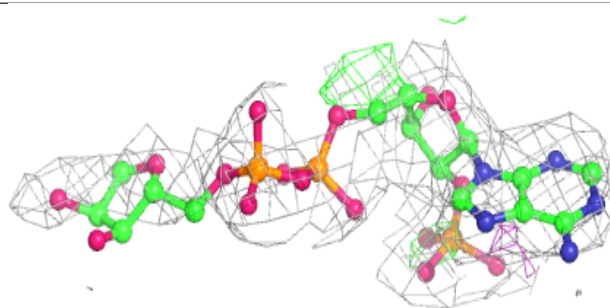
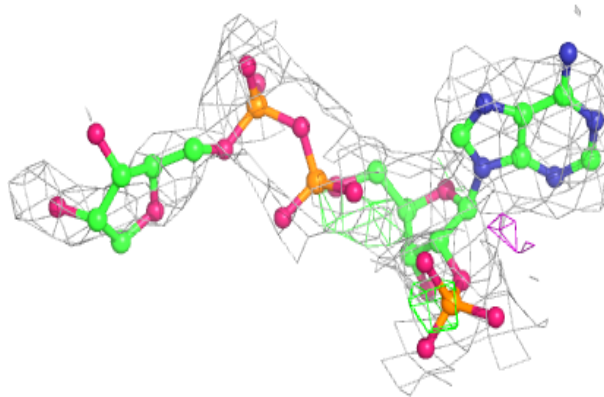
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2 | FAD | A | 600 | 53/53 | 0.94 | 0.22 | 14,24,36,36 | 0 |
| 2 | FAD | B | 600 | 53/53 | 0.95 | 0.25 | 18,26,42,46 | 0 |
| 2 | FAD | D | 600 | 53/53 | 0.95 | 0.29 | 20,29,40,47 | 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.

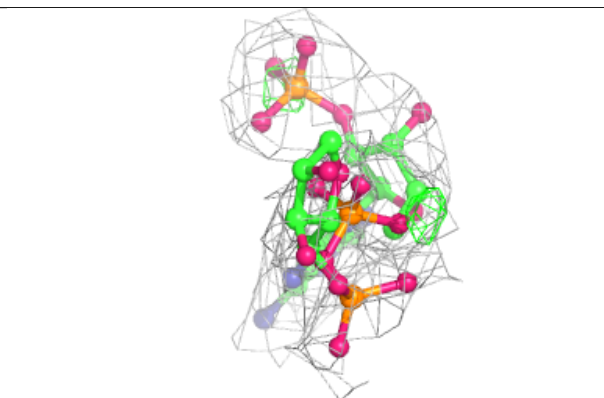
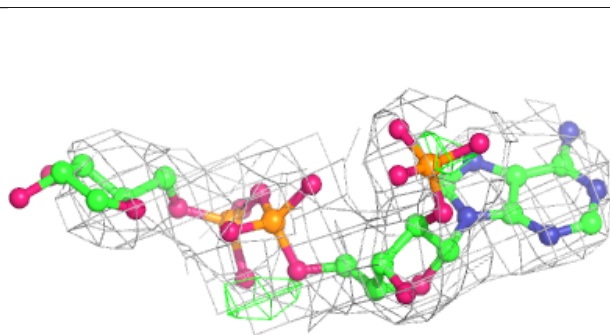
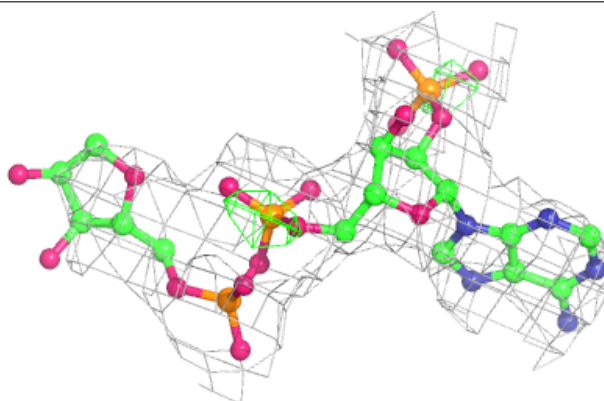


Electron density around NDP F 601:

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

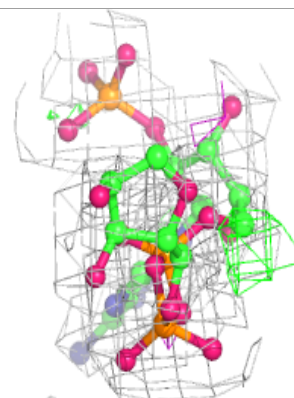
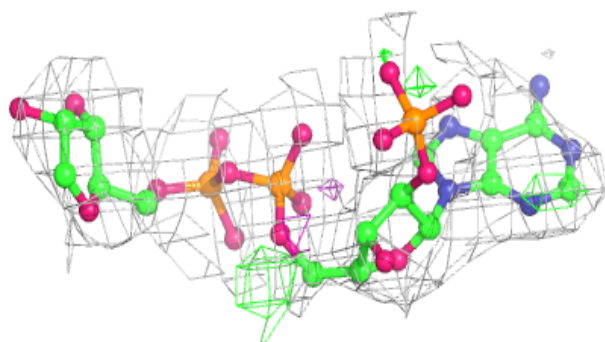
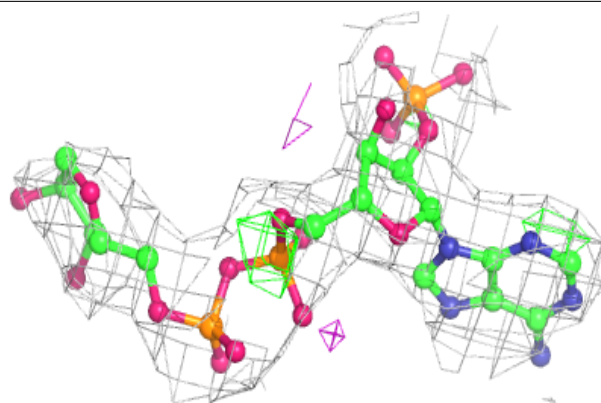
**Electron density around NDP A 601:**

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

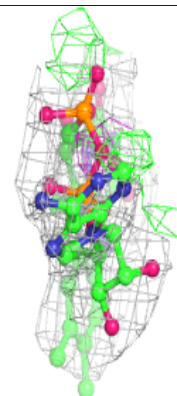
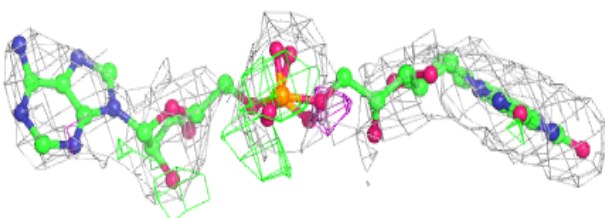
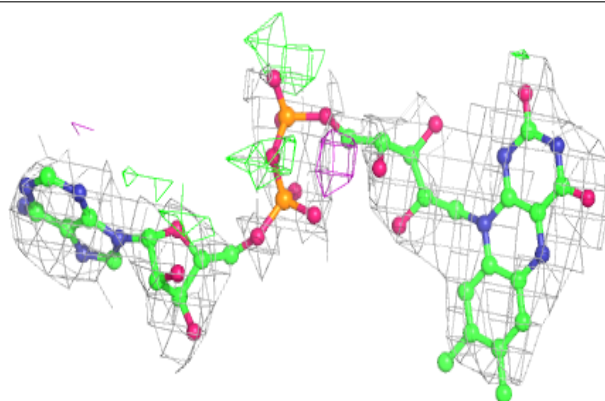


Electron density around NDP D 601:

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

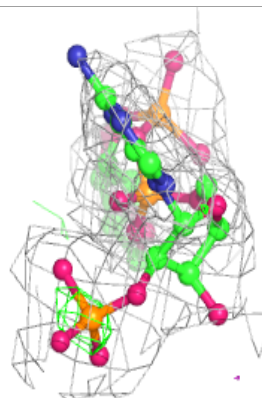
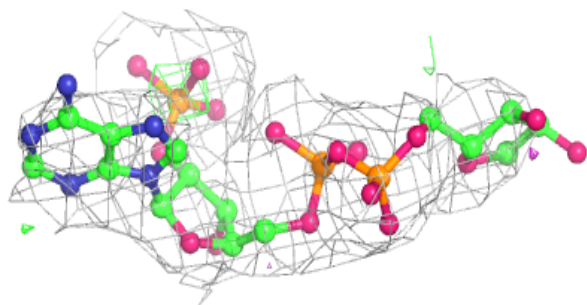
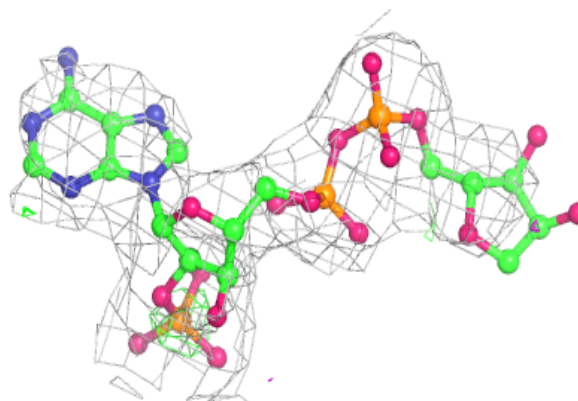
**Electron density around FAD C 600:**

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

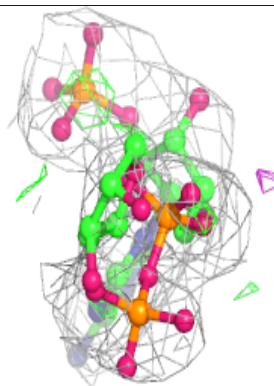
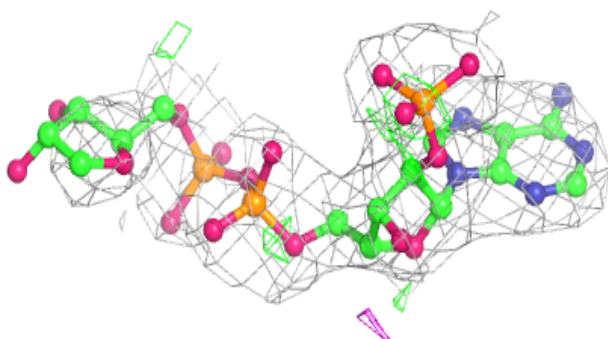
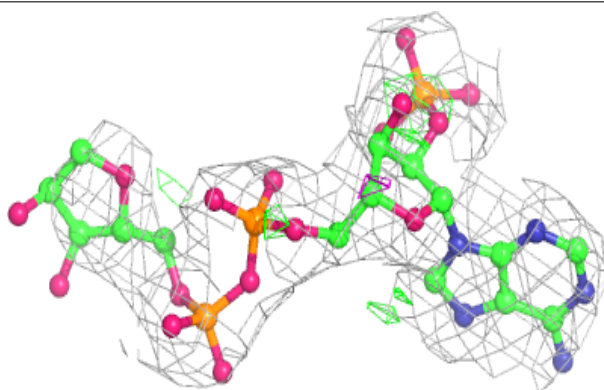


Electron density around NDP B 601:

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

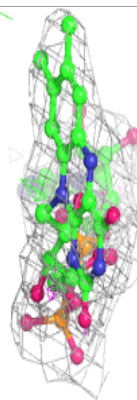
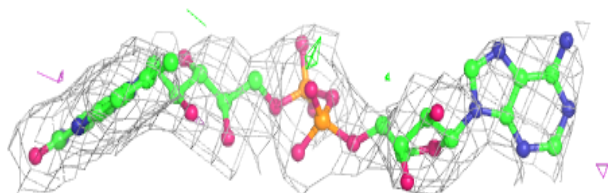
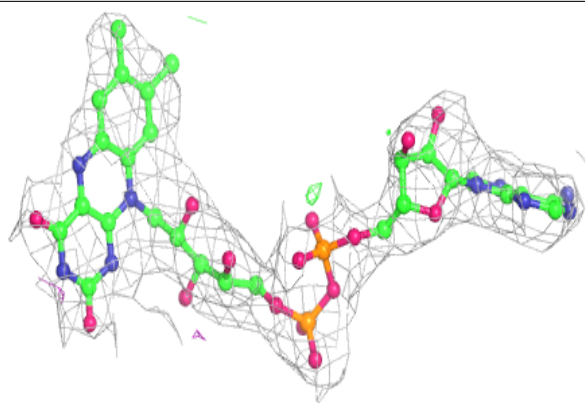
**Electron density around NDP E 601:**

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

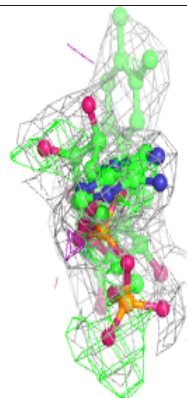
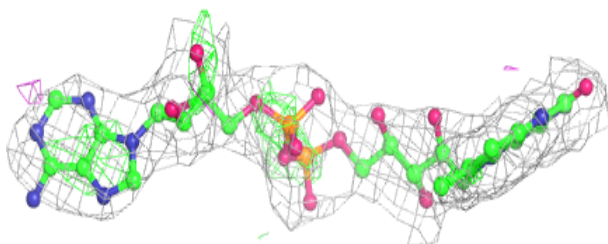
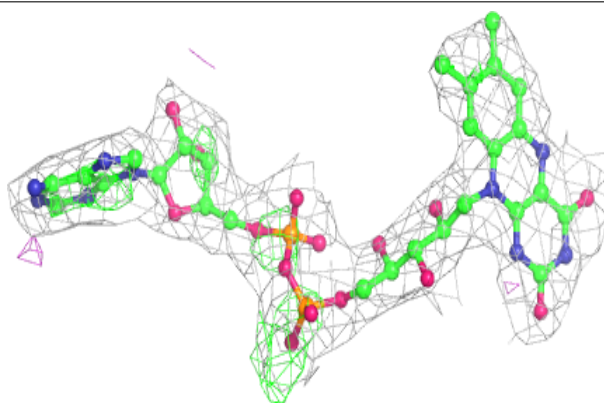


Electron density around FAD F 600:

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

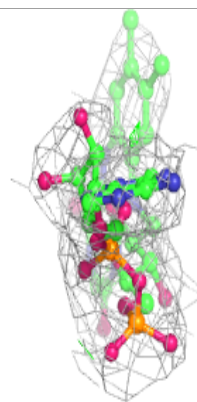
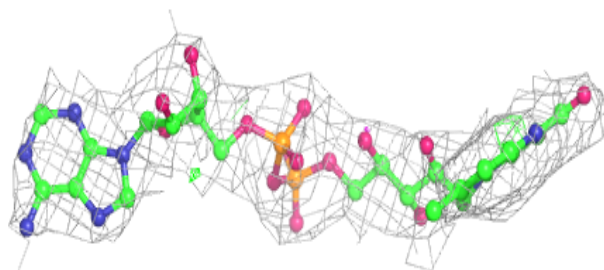
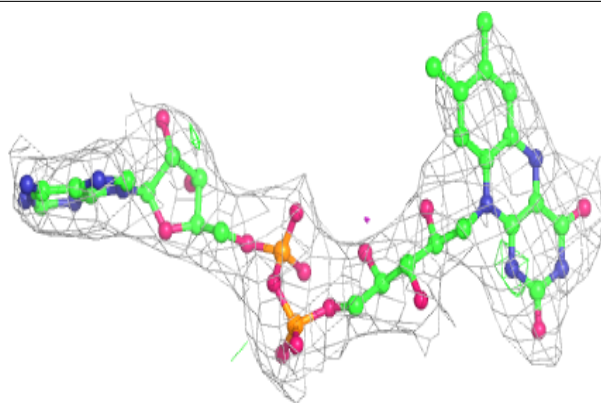
**Electron density around FAD E 600:**

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

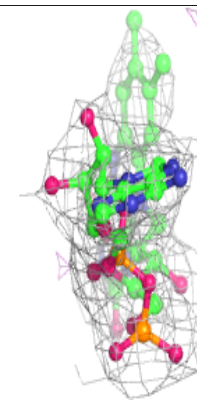
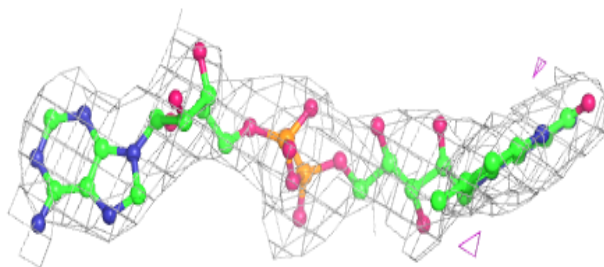
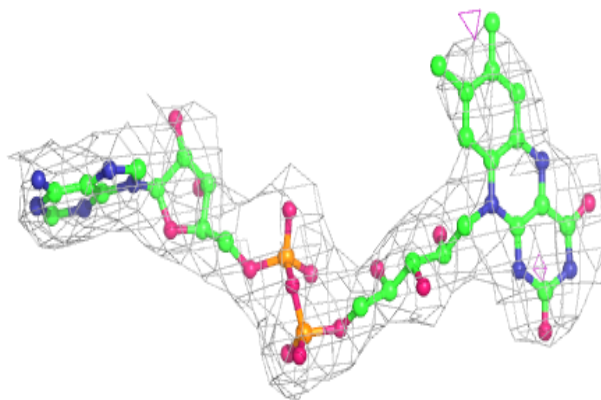


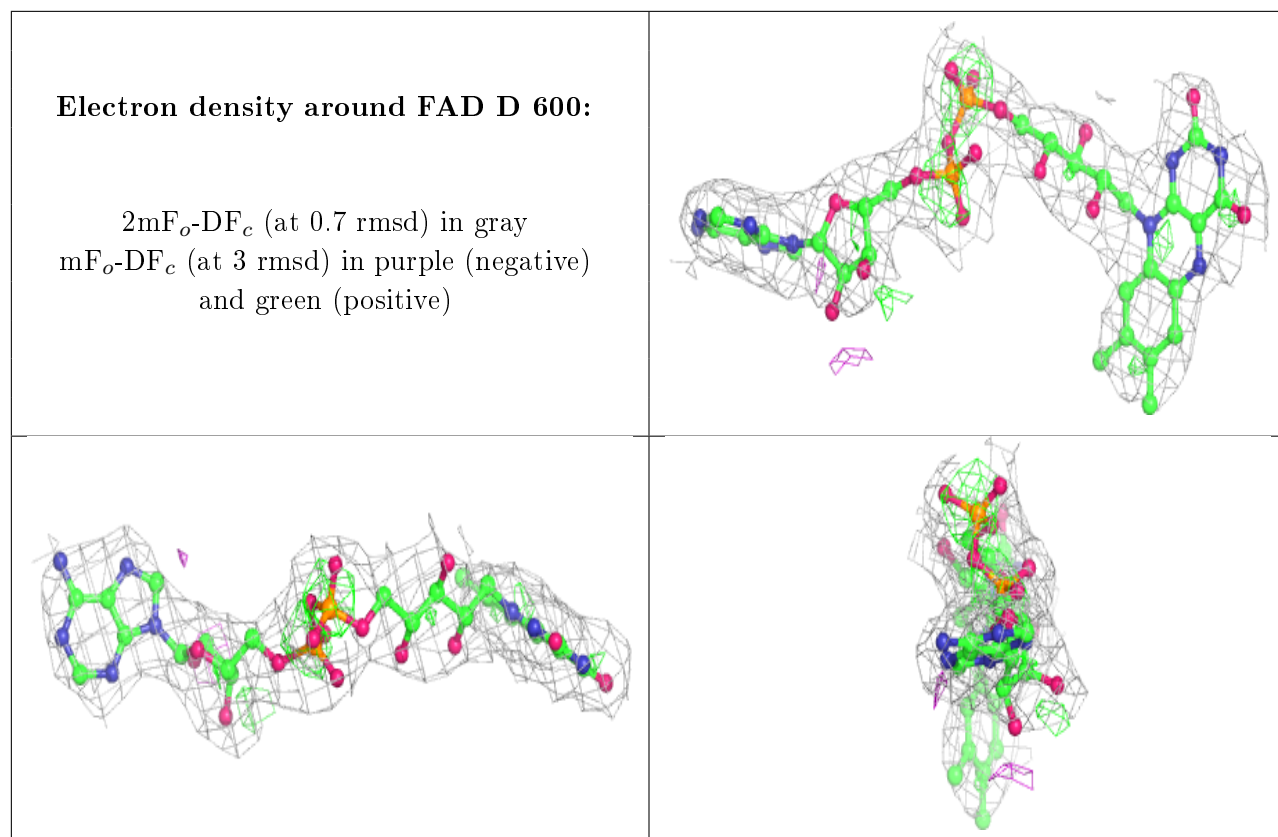
Electron density around FAD A 600:

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

**Electron density around FAD B 600:**

$2mF_o-DF_c$ (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.