



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 04:51 AM BST

PDB ID : 1XLT
Title : Crystal structure of Transhydrogenase [(domain I)2:domain III] heterotrimer complex
Authors : Sundaresan, V.; Chartron, J.; Yamaguchi, M.; Stout, C.D.
Deposited on : 2004-09-30
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

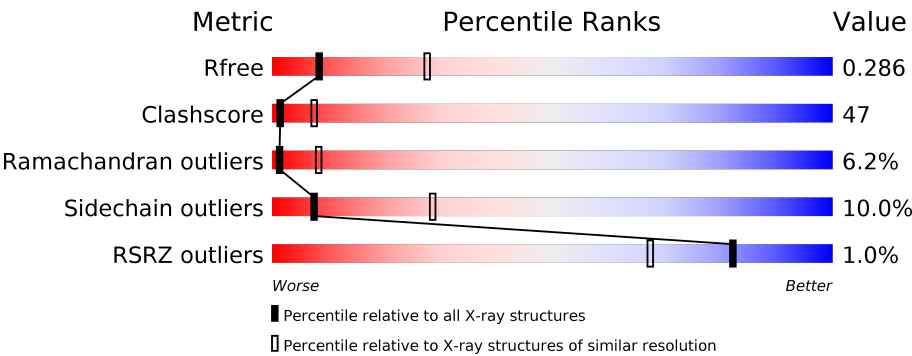
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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




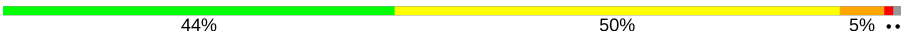
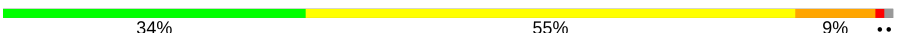
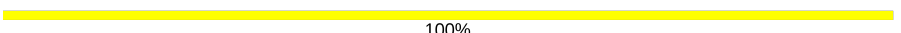

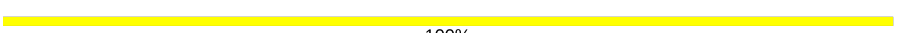
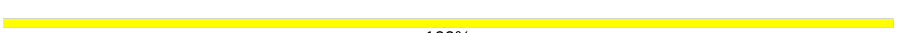


| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 1094 (3.10-3.10) |
| Clashscore | 141614 | 1184 (3.10-3.10) |
| Ramachandran outliers | 138981 | 1141 (3.10-3.10) |
| Sidechain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

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 384 | |
| 1 | B | 384 | |
| 1 | D | 384 | |
| 1 | E | 384 | |
| 1 | G | 384 | |
| 1 | H | 384 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 2 | C | 174 |  |
| 2 | F | 174 |  |
| 2 | I | 174 |  |
| 3 | J | 2 |  |
| 3 | K | 2 |  |
| 3 | L | 2 |  |
| 3 | M | 2 |  |
| 3 | N | 2 |  |
| 3 | O | 2 |  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3 | GLC | N | 1 | - | - | - | X |

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 20480 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 NAD(P) transhydrogenase subunit alpha part 1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 363 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2670 | 1688 | 462 | 504 | 16 | | | |
| 1 | B | 359 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2643 | 1673 | 458 | 496 | 16 | | | |
| 1 | D | 378 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2779 | 1753 | 479 | 529 | 18 | | | |
| 1 | E | 359 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2644 | 1673 | 458 | 497 | 16 | | | |
| 1 | G | 364 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2675 | 1691 | 463 | 505 | 16 | | | |
| 1 | H | 357 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2632 | 1665 | 456 | 495 | 16 | | | |

- Molecule 2 is a protein called NAD(P) transhydrogenase subunit beta.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 2 | C | 174 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1318 | 833 | 221 | 252 | 12 | | | |
| 2 | F | 173 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1307 | 827 | 217 | 251 | 12 | | | |
| 2 | I | 173 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1307 | 827 | 217 | 251 | 12 | | | |

There are 9 discrepancies between the modelled and reference sequences:

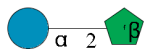
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------------|------------|
| C | 291 | ARG | - | cloning artifact | UNP Q59765 |
| C | 292 | HIS | - | cloning artifact | UNP Q59765 |
| C | 293 | MET | - | cloning artifact | UNP Q59765 |
| F | 291 | ARG | - | cloning artifact | UNP Q59765 |
| F | 292 | HIS | - | cloning artifact | UNP Q59765 |
| F | 293 | MET | - | cloning artifact | UNP Q59765 |

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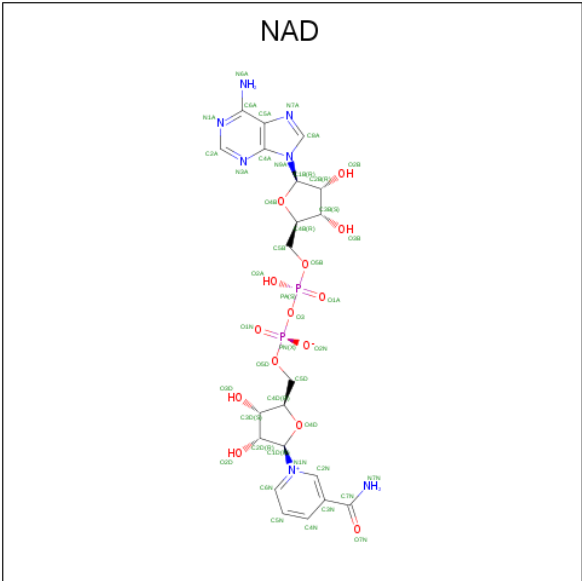
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------------|------------|
| I | 291 | ARG | - | cloning artifact | UNP Q59765 |
| I | 292 | HIS | - | cloning artifact | UNP Q59765 |
| I | 293 | MET | - | cloning artifact | UNP Q59765 |

- Molecule 3 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|---------|---------|-------|
| 3 | J | 2 | Total | C | O | 0 | 0 | 0 |
| | | | 23 | 12 | 11 | | | |
| 3 | K | 2 | Total | C | O | 0 | 0 | 0 |
| | | | 23 | 12 | 11 | | | |
| 3 | L | 2 | Total | C | O | 0 | 0 | 0 |
| | | | 23 | 12 | 11 | | | |
| 3 | M | 2 | Total | C | O | 0 | 0 | 0 |
| | | | 23 | 12 | 11 | | | |
| 3 | N | 2 | Total | C | O | 0 | 0 | 0 |
| | | | 23 | 12 | 11 | | | |
| 3 | O | 2 | Total | C | O | 0 | 0 | 0 |
| | | | 23 | 12 | 11 | | | |

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).

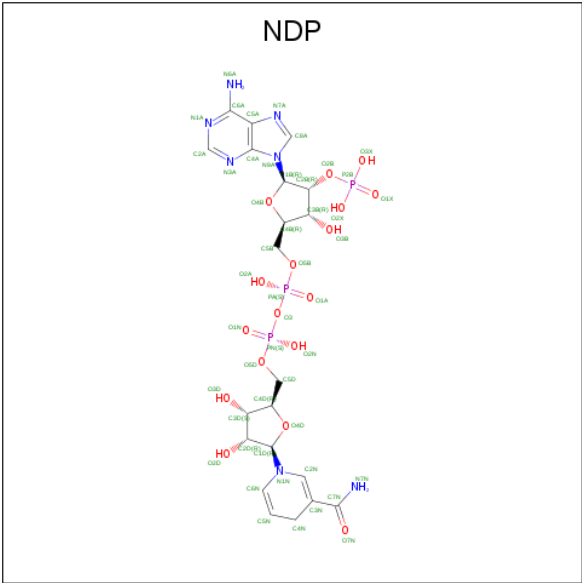


| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 4 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 44 | 21 | 7 | 14 | 2 | | |
| 4 | B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 44 | 21 | 7 | 14 | 2 | | |
| 4 | D | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 44 | 21 | 7 | 14 | 2 | | |
| 4 | G | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 44 | 21 | 7 | 14 | 2 | | |
| 4 | H | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 44 | 21 | 7 | 14 | 2 | | |

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5 | G | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 5 | A | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 5 | D | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 6 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 6 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 48 | 21 | 7 | 17 | 3 | | |

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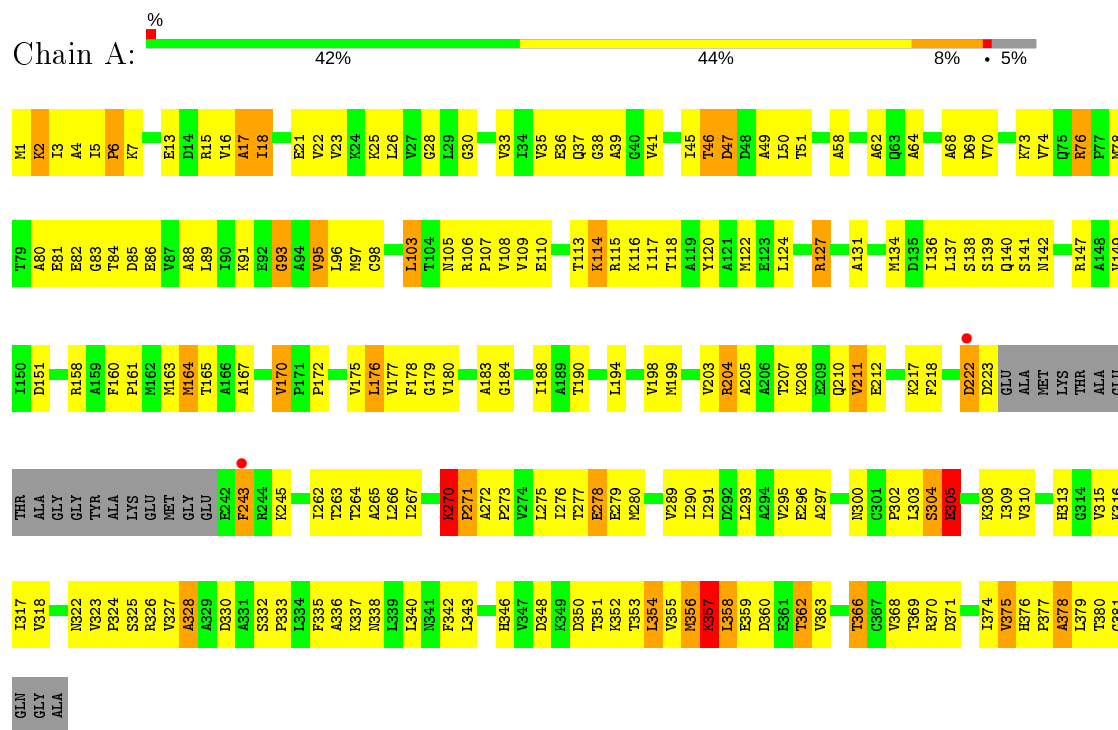
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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 6 | F | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 48 | 21 | 7 | 17 | 3 | | |
| 6 | I | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 48 | 21 | 7 | 17 | 3 | | |

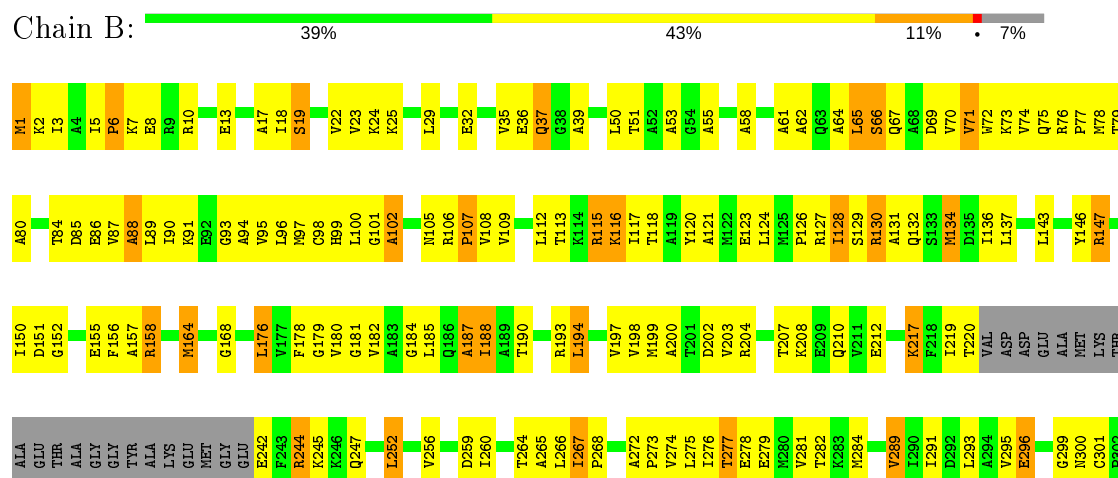
3 Residue-property plots

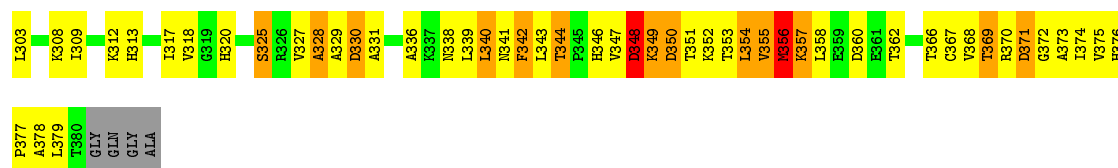
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: NAD(P) transhydrogenase subunit alpha part 1

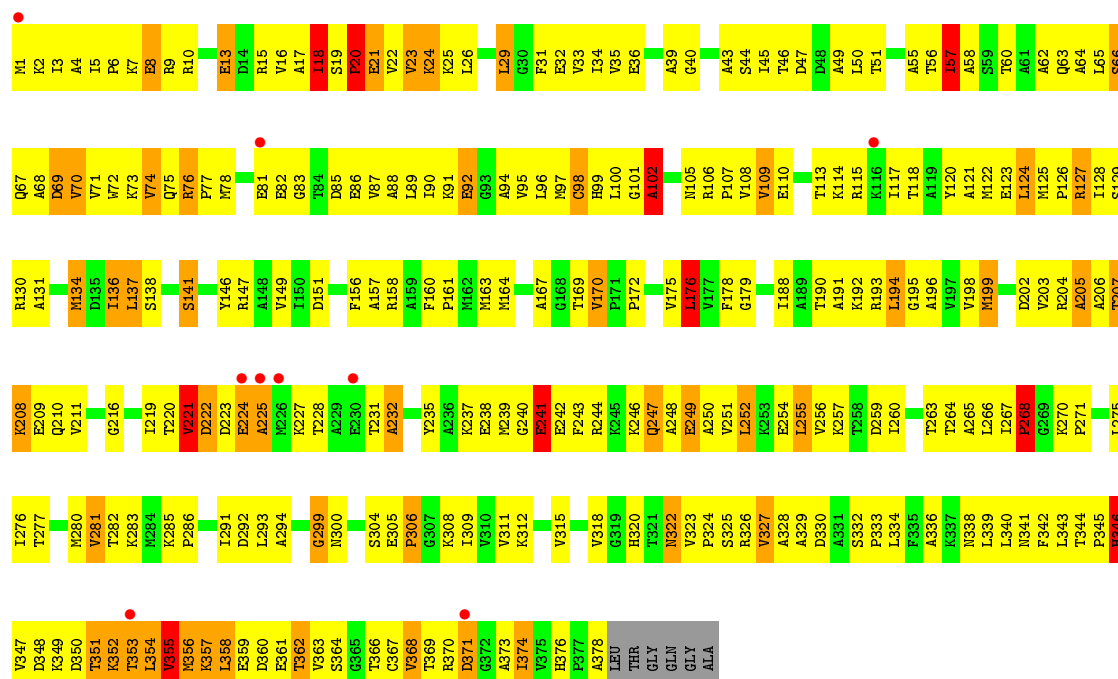


- Molecule 1: NAD(P) transhydrogenase subunit alpha part 1

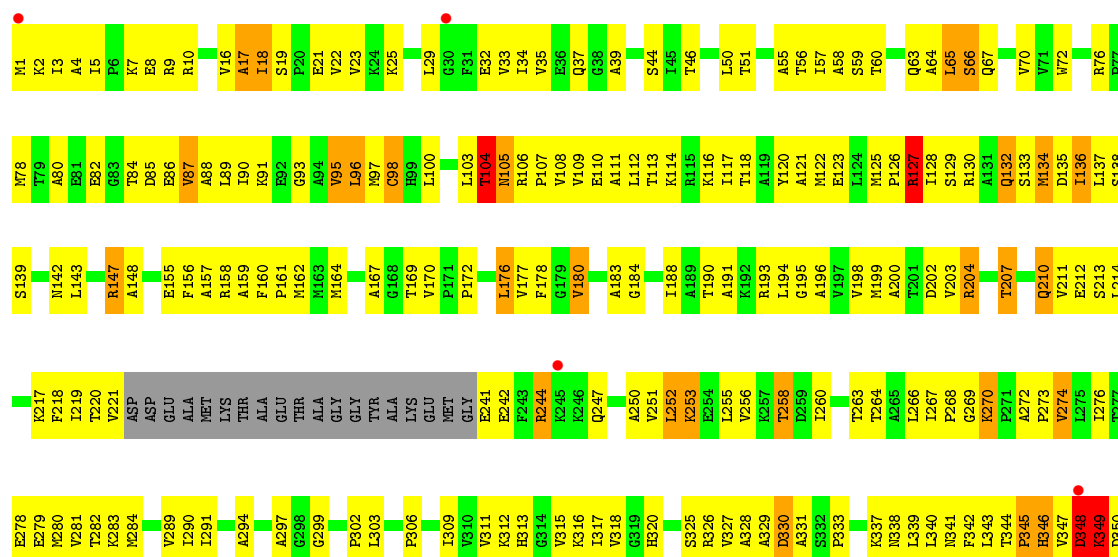


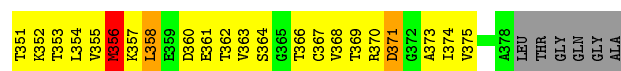


• Molecule 1: NAD(P) transhydrogenase subunit alpha part 1

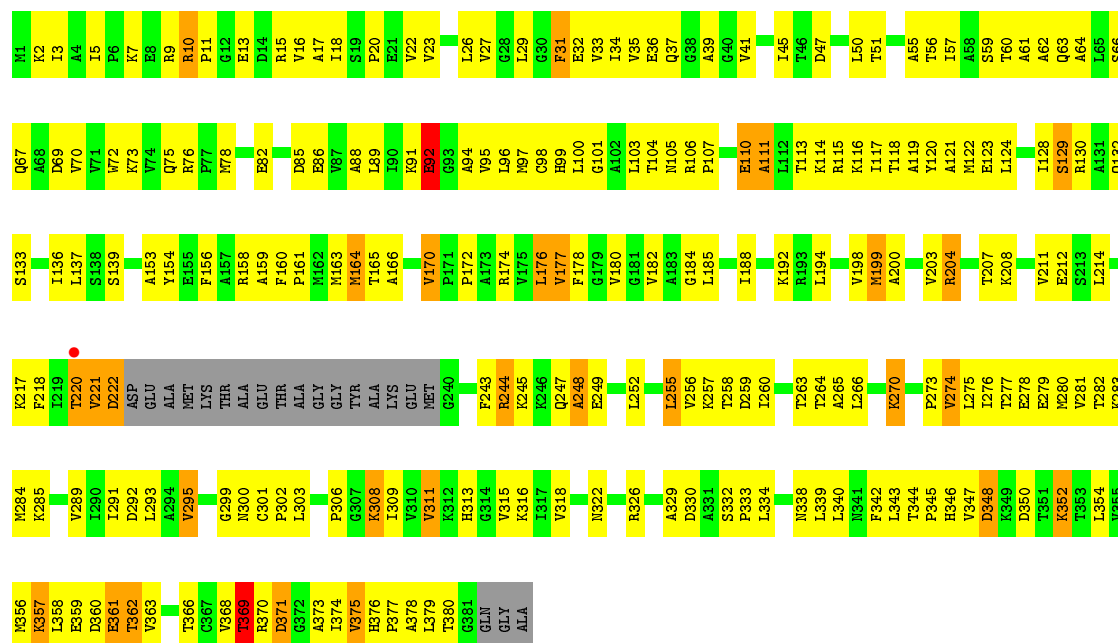
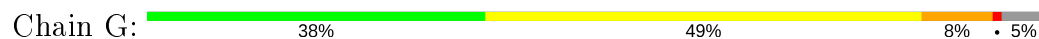


• Molecule 1: NAD(P) transhydrogenase subunit alpha part 1

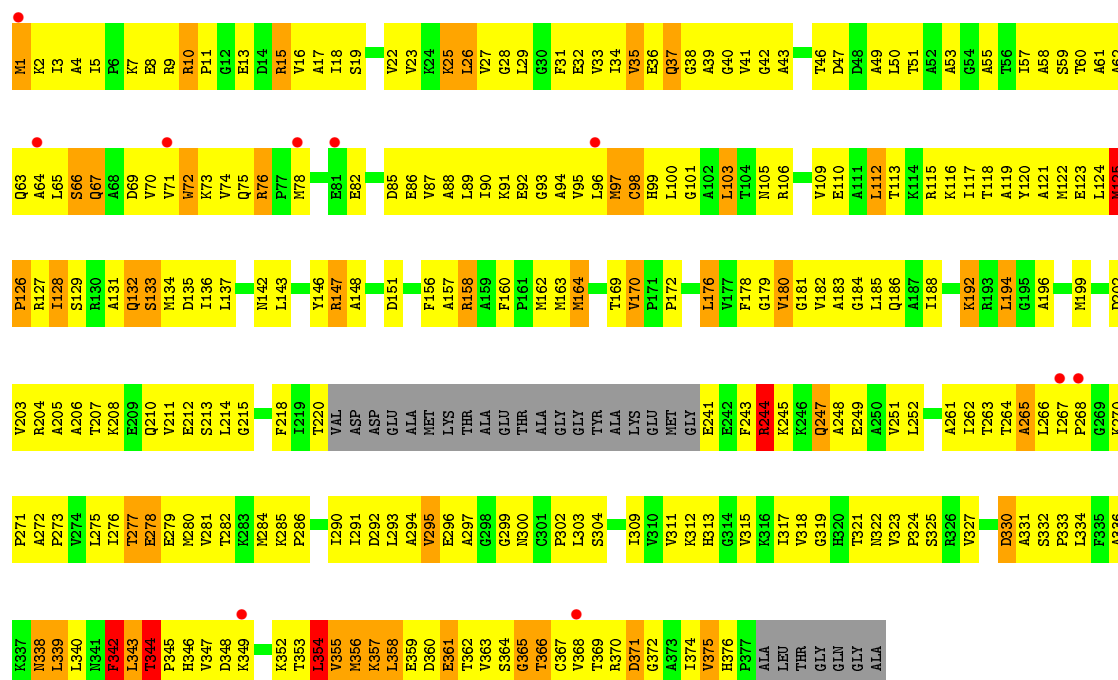




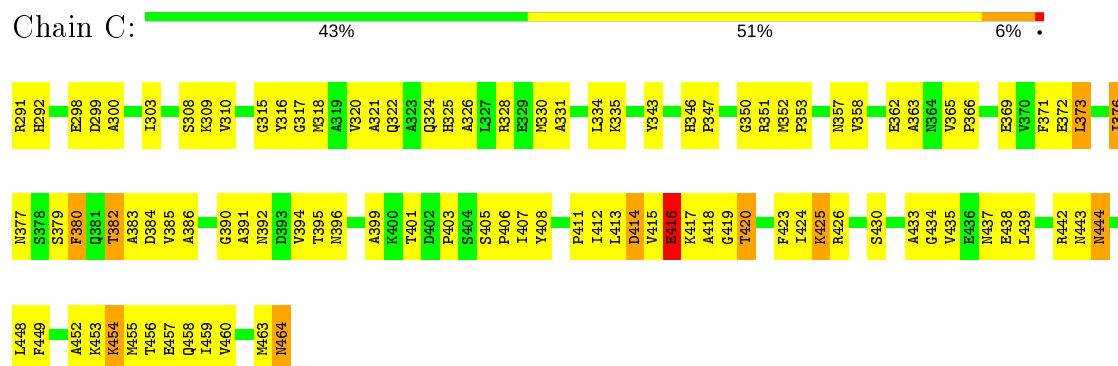
- Molecule 1: NAD(P) transhydrogenase subunit alpha part 1



- Molecule 1: NAD(P) transhydrogenase subunit alpha part 1



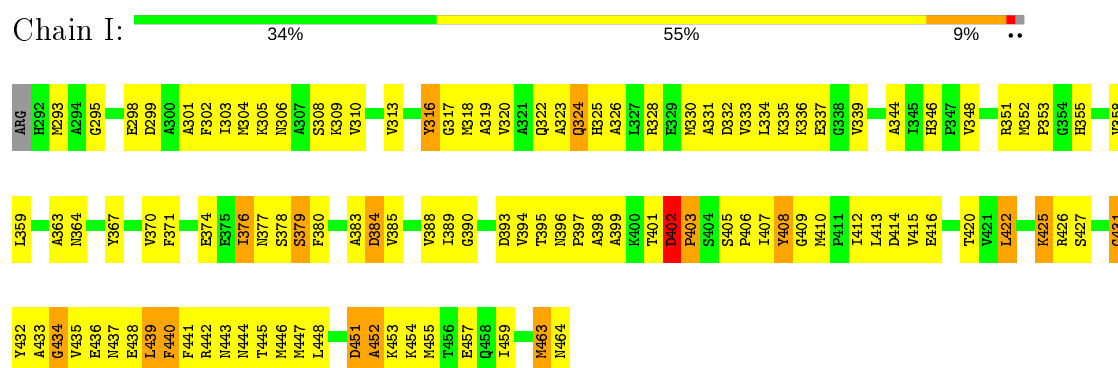
- Molecule 2: NAD(P) transhydrogenase subunit beta



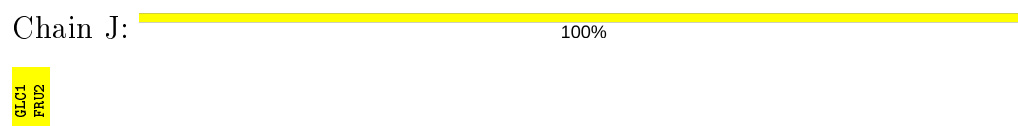
- Molecule 2: NAD(P) transhydrogenase subunit beta



- Molecule 2: NAD(P) transhydrogenase subunit beta



- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose





- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain L:  100%



- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain M:  100%



- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain N:  100%



- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain O:  50% 50%



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 95.37Å 171.08Å 203.18Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 43.68 – 3.10 43.68 – 3.00 | Depositor EDS |
| % Data completeness (in resolution range) | 96.5 (43.68-3.10) 95.9 (43.68-3.00) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | 0.12 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.66 (at 3.01Å) | Xtriage |
| Refinement program | CNS 1.1 | Depositor |
| R, R_{free} | 0.232 , 0.310 0.220 , 0.286 | Depositor DCC |
| R_{free} test set | 2977 reflections (4.61%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 78.5 | Xtriage |
| Anisotropy | 0.114 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.29 , 47.2 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.93 | EDS |
| Total number of atoms | 20480 | wwPDB-VP |
| Average B, all atoms (Å ²) | 60.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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, GLC, FRU, NAD, NA

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 | 0.52 | 1/2705 (0.0%) | 0.82 | 4/3668 (0.1%) |
| 1 | B | 0.48 | 0/2678 | 0.79 | 2/3631 (0.1%) |
| 1 | D | 0.54 | 0/2816 | 1.02 | 10/3816 (0.3%) |
| 1 | E | 0.50 | 1/2679 (0.0%) | 0.87 | 7/3632 (0.2%) |
| 1 | G | 0.46 | 0/2710 | 0.81 | 5/3674 (0.1%) |
| 1 | H | 0.54 | 1/2667 (0.0%) | 0.99 | 14/3615 (0.4%) |
| 2 | C | 0.46 | 0/1342 | 0.66 | 0/1813 |
| 2 | F | 0.46 | 0/1331 | 0.65 | 0/1799 |
| 2 | I | 0.51 | 0/1331 | 0.85 | 3/1799 (0.2%) |
| All | All | 0.50 | 3/20259 (0.0%) | 0.86 | 45/27447 (0.2%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 1 |
| 1 | B | 0 | 1 |
| 1 | D | 0 | 5 |
| 1 | E | 0 | 1 |
| 1 | H | 1 | 2 |
| 2 | I | 0 | 1 |
| All | All | 1 | 11 |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | A | 204 | ARG | N-CA | -8.40 | 1.29 | 1.46 |
| 1 | H | 343 | LEU | C-N | -6.48 | 1.19 | 1.34 |
| 1 | E | 349 | LYS | C-O | 6.47 | 1.35 | 1.23 |

All (45) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | H | 125 | MET | C-N-CD | 9.48 | 148.30 | 128.40 |
| 1 | D | 371 | ASP | CB-CG-OD2 | 8.76 | 126.18 | 118.30 |
| 1 | A | 47 | ASP | CB-CG-OD1 | 8.75 | 126.18 | 118.30 |
| 1 | D | 221 | VAL | O-C-N | 8.62 | 136.49 | 122.70 |
| 1 | G | 350 | ASP | CB-CG-OD2 | 8.56 | 126.01 | 118.30 |
| 1 | H | 371 | ASP | CB-CG-OD2 | 8.45 | 125.91 | 118.30 |
| 2 | I | 403 | PRO | CA-N-CD | -8.24 | 99.97 | 111.50 |
| 1 | H | 375 | VAL | N-CA-C | 8.14 | 132.97 | 111.00 |
| 1 | E | 348 | ASP | C-N-CA | -8.07 | 101.53 | 121.70 |
| 1 | E | 348 | ASP | CB-CG-OD2 | -7.77 | 111.31 | 118.30 |
| 2 | I | 402 | ASP | CB-CG-OD1 | 7.72 | 125.25 | 118.30 |
| 1 | H | 126 | PRO | CA-N-CD | -7.67 | 100.77 | 111.50 |
| 1 | D | 67 | GLN | O-C-N | -7.58 | 110.58 | 122.70 |
| 1 | H | 345 | PRO | CA-N-CD | -7.38 | 101.17 | 111.50 |
| 1 | H | 342 | PHE | CB-CG-CD2 | 6.95 | 125.67 | 120.80 |
| 1 | G | 357 | LYS | O-C-N | -6.89 | 111.68 | 122.70 |
| 1 | H | 344 | THR | C-N-CD | 6.72 | 142.51 | 128.40 |
| 1 | G | 357 | LYS | C-N-CA | 6.51 | 137.99 | 121.70 |
| 1 | B | 330 | ASP | CB-CG-OD1 | 6.45 | 124.10 | 118.30 |
| 1 | D | 346 | HIS | CA-CB-CG | 6.43 | 124.53 | 113.60 |
| 1 | E | 349 | LYS | CA-C-N | 6.37 | 131.22 | 117.20 |
| 2 | I | 402 | ASP | CA-C-O | 6.22 | 133.16 | 120.10 |
| 1 | E | 356 | MET | CA-CB-CG | 5.97 | 123.45 | 113.30 |
| 1 | E | 317 | ILE | O-C-N | -5.96 | 113.17 | 122.70 |
| 1 | H | 343 | LEU | C-N-CA | 5.92 | 136.51 | 121.70 |
| 1 | D | 374 | ILE | CA-C-O | 5.89 | 132.47 | 120.10 |
| 1 | H | 133 | SER | O-C-N | -5.86 | 113.33 | 122.70 |
| 1 | D | 220 | THR | O-C-N | -5.57 | 113.78 | 122.70 |
| 1 | H | 365 | GLY | C-N-CA | 5.56 | 135.60 | 121.70 |
| 1 | A | 356 | MET | C-N-CA | 5.52 | 135.51 | 121.70 |
| 1 | H | 127 | ARG | NE-CZ-NH2 | -5.49 | 117.56 | 120.30 |
| 1 | H | 344 | THR | N-CA-C | 5.43 | 125.67 | 111.00 |
| 1 | D | 225 | ALA | CB-CA-C | 5.34 | 118.11 | 110.10 |
| 1 | D | 225 | ALA | N-CA-CB | 5.34 | 117.57 | 110.10 |
| 1 | E | 349 | LYS | CB-CA-C | 5.29 | 120.98 | 110.40 |
| 1 | H | 366 | THR | CA-CB-CG2 | 5.28 | 119.79 | 112.40 |
| 1 | E | 297 | ALA | CB-CA-C | 5.23 | 117.94 | 110.10 |
| 1 | A | 17 | ALA | CB-CA-C | 5.22 | 117.93 | 110.10 |
| 1 | H | 126 | PRO | N-CD-CG | 5.21 | 111.02 | 103.20 |
| 1 | A | 357 | LYS | C-N-CA | 5.16 | 134.59 | 121.70 |
| 1 | B | 356 | MET | O-C-N | -5.14 | 114.48 | 122.70 |
| 1 | G | 352 | LYS | CA-C-O | 5.11 | 130.82 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^{\circ}$) | Ideal($^{\circ}$) |
|-----|-------|-----|------|-----------|------|------------------------|---------------------|
| 1 | D | 57 | ILE | C-N-CA | 5.10 | 134.46 | 121.70 |
| 1 | G | 357 | LYS | CA-C-N | 5.07 | 128.34 | 117.20 |
| 1 | D | 69 | ASP | CB-CG-OD2 | 5.06 | 122.85 | 118.30 |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1 | H | 366 | THR | CA |

All (11) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 18 | ILE | Mainchain |
| 1 | B | 356 | MET | Mainchain |
| 1 | D | 102 | ALA | Mainchain |
| 1 | D | 247 | GLN | Mainchain |
| 1 | D | 346 | HIS | Sidechain |
| 1 | D | 353 | THR | Mainchain |
| 1 | D | 57 | ILE | Mainchain |
| 1 | E | 356 | MET | Mainchain |
| 1 | H | 132 | GLN | Mainchain |
| 1 | H | 343 | LEU | Mainchain |
| 2 | I | 398 | ALA | Mainchain |

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 | 2670 | 0 | 2804 | 200 | 0 |
| 1 | B | 2643 | 0 | 2784 | 248 | 0 |
| 1 | D | 2779 | 0 | 2904 | 367 | 0 |
| 1 | E | 2644 | 0 | 2781 | 268 | 0 |
| 1 | G | 2675 | 0 | 2808 | 241 | 0 |
| 1 | H | 2632 | 0 | 2766 | 391 | 0 |
| 2 | C | 1318 | 0 | 1305 | 109 | 0 |
| 2 | F | 1307 | 0 | 1292 | 92 | 0 |
| 2 | I | 1307 | 0 | 1292 | 123 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3 | J | 23 | 0 | 21 | 0 | 0 |
| 3 | K | 23 | 0 | 21 | 1 | 0 |
| 3 | L | 23 | 0 | 21 | 0 | 0 |
| 3 | M | 23 | 0 | 21 | 0 | 0 |
| 3 | N | 23 | 0 | 21 | 0 | 0 |
| 3 | O | 23 | 0 | 21 | 1 | 0 |
| 4 | A | 44 | 0 | 26 | 2 | 0 |
| 4 | B | 44 | 0 | 25 | 9 | 0 |
| 4 | D | 44 | 0 | 24 | 3 | 0 |
| 4 | G | 44 | 0 | 24 | 6 | 0 |
| 4 | H | 44 | 0 | 26 | 8 | 0 |
| 5 | A | 1 | 0 | 0 | 0 | 0 |
| 5 | D | 1 | 0 | 0 | 0 | 0 |
| 5 | G | 1 | 0 | 0 | 0 | 0 |
| 6 | C | 48 | 0 | 26 | 4 | 0 |
| 6 | F | 48 | 0 | 26 | 10 | 0 |
| 6 | I | 48 | 0 | 26 | 3 | 0 |
| All | All | 20480 | 0 | 21065 | 1966 | 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 47.

All (1966) 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:H:120:TYR:CD2 | 1:H:366:THR:HG22 | 1.64 | 1.31 |
| 1:H:120:TYR:HD2 | 1:H:366:THR:CG2 | 1.47 | 1.27 |
| 2:I:401:THR:O | 2:I:403:PRO:HD3 | 1.32 | 1.25 |
| 1:B:70:VAL:HG23 | 1:B:95:VAL:HB | 1.21 | 1.17 |
| 1:H:120:TYR:CD2 | 1:H:366:THR:CG2 | 2.26 | 1.15 |
| 1:D:62:ALA:HA | 1:D:89:LEU:HD21 | 1.16 | 1.11 |
| 1:H:18:ILE:HD11 | 1:H:23:VAL:HG22 | 1.23 | 1.10 |
| 1:H:120:TYR:HD2 | 1:H:366:THR:HG22 | 0.94 | 1.09 |
| 1:B:264:THR:HG22 | 1:B:293:LEU:HD12 | 1.33 | 1.08 |
| 1:B:29:LEU:HD23 | 1:B:347:VAL:HG11 | 1.35 | 1.08 |
| 1:B:86:GLU:HA | 1:B:89:LEU:HD12 | 1.37 | 1.07 |
| 1:A:270:LYS:HB2 | 1:A:271:PRO:HD3 | 1.37 | 1.06 |
| 1:H:47:ASP:HB3 | 1:H:57:ILE:HD13 | 1.34 | 1.05 |
| 1:H:72:TRP:HB3 | 1:H:97:MET:HB2 | 1.34 | 1.04 |
| 1:H:47:ASP:HB3 | 1:H:57:ILE:CD1 | 1.87 | 1.04 |
| 1:H:370:ARG:CG | 1:H:375:VAL:HG21 | 1.88 | 1.04 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:68:ALA:O | 1:D:91:LYS:HD3 | 1.58 | 1.04 |
| 1:H:129:SER:HA | 1:H:132:GLN:HG3 | 1.39 | 1.04 |
| 1:D:69:ASP:O | 1:D:94:ALA:HB1 | 1.59 | 1.01 |
| 1:H:370:ARG:HG2 | 1:H:375:VAL:CG2 | 1.88 | 1.01 |
| 1:H:47:ASP:CB | 1:H:57:ILE:HD13 | 1.91 | 1.01 |
| 1:A:354:LEU:HD21 | 1:A:356:MET:HE2 | 1.39 | 1.00 |
| 1:H:186:GLN:HA | 2:I:352:MET:HE1 | 1.39 | 1.00 |
| 1:D:361:GLU:HA | 1:D:364:SER:HB3 | 1.43 | 0.99 |
| 1:B:128:ILE:CD1 | 1:B:130:ARG:HD3 | 1.92 | 0.99 |
| 1:H:370:ARG:HG2 | 1:H:375:VAL:HG21 | 1.00 | 0.99 |
| 1:H:362:THR:HG23 | 1:H:363:VAL:H | 1.26 | 0.99 |
| 1:A:46:THR:HG23 | 1:A:49:ALA:HB2 | 1.44 | 0.98 |
| 1:D:73:LYS:O | 1:D:98:CYS:HB2 | 1.65 | 0.97 |
| 1:H:121:ALA:HB1 | 1:H:123:GLU:OE1 | 1.63 | 0.97 |
| 1:A:270:LYS:HB2 | 1:A:271:PRO:CD | 1.95 | 0.96 |
| 1:A:76:ARG:HH21 | 1:A:76:ARG:HG2 | 1.26 | 0.96 |
| 1:E:217:LYS:HD2 | 1:E:217:LYS:H | 1.27 | 0.96 |
| 1:H:8:GLU:HG2 | 1:H:74:VAL:HG22 | 1.46 | 0.96 |
| 2:C:399:ALA:HB2 | 2:C:407:ILE:HG13 | 1.46 | 0.96 |
| 1:E:176:LEU:HB2 | 1:E:258:THR:HG21 | 1.45 | 0.95 |
| 1:H:74:VAL:HG23 | 1:H:75:GLN:H | 1.29 | 0.95 |
| 1:E:199:MET:HG3 | 1:E:219:ILE:HD11 | 1.48 | 0.95 |
| 1:B:61:ALA:O | 1:B:65:LEU:HD13 | 1.68 | 0.94 |
| 2:F:399:ALA:HA | 2:F:408:TYR:HA | 1.46 | 0.94 |
| 1:G:35:VAL:HG21 | 1:G:50:LEU:HD13 | 1.49 | 0.93 |
| 1:H:129:SER:CA | 1:H:132:GLN:HG3 | 1.98 | 0.93 |
| 2:F:432:TYR:CD2 | 6:F:500:NDP:H1D | 2.03 | 0.93 |
| 1:H:357:LYS:HB3 | 1:H:360:ASP:HB2 | 1.49 | 0.93 |
| 2:I:437:ASN:HB3 | 2:I:440:PHE:CE1 | 2.04 | 0.93 |
| 1:E:184:GLY:O | 1:E:188:ILE:HG12 | 1.69 | 0.93 |
| 1:D:358:LEU:HD13 | 1:D:370:ARG:HH22 | 1.34 | 0.93 |
| 1:G:85:ASP:OD2 | 1:G:88:ALA:HB2 | 1.68 | 0.93 |
| 1:D:342:PHE:CZ | 1:D:362:THR:O | 2.22 | 0.93 |
| 1:H:354:LEU:H | 1:H:354:LEU:HD23 | 1.32 | 0.93 |
| 1:B:128:ILE:HD12 | 1:B:130:ARG:HD3 | 1.47 | 0.92 |
| 1:E:188:ILE:HG23 | 1:E:198:VAL:HG11 | 1.52 | 0.92 |
| 1:G:120:TYR:HB3 | 1:G:366:THR:HG22 | 1.52 | 0.92 |
| 1:B:349:LYS:HG3 | 1:B:350:ASP:H | 1.33 | 0.92 |
| 1:G:329:ALA:HB3 | 1:H:158:ARG:HG2 | 1.52 | 0.92 |
| 1:G:78:MET:HB2 | 1:G:86:GLU:HG3 | 1.52 | 0.92 |
| 1:D:275:LEU:HD12 | 1:D:300:ASN:HD22 | 1.31 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:401:THR:O | 2:F:403:PRO:HD3 | 1.69 | 0.92 |
| 1:H:35:VAL:HG21 | 1:H:50:LEU:HD23 | 1.52 | 0.92 |
| 1:H:78:MET:HB2 | 1:H:86:GLU:HB2 | 1.49 | 0.91 |
| 1:D:247:GLN:HE22 | 4:D:400:NAD:H61A | 1.19 | 0.91 |
| 2:I:399:ALA:HA | 2:I:408:TYR:HA | 1.53 | 0.91 |
| 1:H:72:TRP:CZ3 | 1:H:339:LEU:HB3 | 2.06 | 0.91 |
| 1:D:163:MET:HE1 | 1:E:142:ASN:HD21 | 1.34 | 0.91 |
| 1:A:264:THR:HG22 | 1:A:293:LEU:HD12 | 1.54 | 0.90 |
| 1:A:354:LEU:HD21 | 1:A:356:MET:CE | 2.01 | 0.90 |
| 1:E:125:MET:SD | 1:E:126:PRO:HD2 | 2.12 | 0.89 |
| 1:D:87:VAL:O | 1:D:115:ARG:HD3 | 1.73 | 0.88 |
| 1:H:261:ALA:HB3 | 1:H:290:ILE:HG13 | 1.53 | 0.88 |
| 2:C:464:ASN:HD22 | 2:C:464:ASN:C | 1.77 | 0.88 |
| 1:D:322:ASN:HD22 | 1:D:325:SER:HB2 | 1.35 | 0.88 |
| 1:B:106:ARG:O | 1:B:109:VAL:HG12 | 1.74 | 0.88 |
| 1:H:122:MET:H | 1:H:122:MET:HE2 | 1.38 | 0.88 |
| 1:H:47:ASP:CB | 1:H:57:ILE:CD1 | 2.51 | 0.88 |
| 1:E:95:VAL:HG12 | 1:E:118:THR:HB | 1.55 | 0.87 |
| 2:F:324:GLN:NE2 | 2:F:359:LEU:HD22 | 1.90 | 0.86 |
| 1:H:119:ALA:O | 1:H:367:CYS:HA | 1.74 | 0.86 |
| 1:D:270:LYS:HE2 | 1:D:270:LYS:HA | 1.57 | 0.86 |
| 1:D:342:PHE:O | 1:D:345:PRO:HD2 | 1.75 | 0.86 |
| 1:D:88:ALA:HA | 1:D:115:ARG:HD2 | 1.57 | 0.86 |
| 1:H:129:SER:HA | 1:H:132:GLN:CG | 2.05 | 0.86 |
| 1:E:278:GLU:O | 1:E:281:VAL:HG12 | 1.75 | 0.86 |
| 1:H:120:TYR:HA | 1:H:366:THR:HG23 | 1.56 | 0.86 |
| 2:I:399:ALA:HB2 | 2:I:407:ILE:HG13 | 1.57 | 0.86 |
| 1:A:289:VAL:HG22 | 1:A:316:LYS:HB2 | 1.56 | 0.86 |
| 1:G:72:TRP:HE1 | 1:G:97:MET:HE1 | 1.36 | 0.86 |
| 1:H:18:ILE:HD11 | 1:H:23:VAL:CG2 | 2.05 | 0.85 |
| 1:D:329:ALA:HB3 | 1:E:158:ARG:HG3 | 1.59 | 0.85 |
| 1:H:10:ARG:HH21 | 1:H:78:MET:HA | 1.38 | 0.85 |
| 1:D:21:GLU:CD | 2:I:308:SER:HB2 | 1.97 | 0.85 |
| 1:H:243:PHE:O | 1:H:247:GLN:HB3 | 1.75 | 0.85 |
| 2:C:392:ASN:O | 2:C:395:THR:HG22 | 1.76 | 0.85 |
| 1:H:10:ARG:NH2 | 1:H:78:MET:HA | 1.92 | 0.85 |
| 1:A:105:ASN:O | 1:A:108:VAL:HG12 | 1.76 | 0.84 |
| 1:D:70:VAL:HG12 | 1:D:95:VAL:HB | 1.58 | 0.84 |
| 1:A:265:ALA:HB3 | 1:A:300:ASN:ND2 | 1.93 | 0.84 |
| 1:D:175:VAL:HG12 | 1:D:176:LEU:H | 1.43 | 0.83 |
| 1:D:246:LYS:O | 1:D:249:GLU:HB3 | 1.78 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:367:CYS:SG | 1:H:370:ARG:HD3 | 2.18 | 0.83 |
| 1:A:277:THR:H | 1:A:280:MET:CE | 1.91 | 0.83 |
| 1:G:376:HIS:O | 1:G:380:THR:HG22 | 1.78 | 0.83 |
| 1:H:136:ILE:HG13 | 1:H:137:LEU:N | 1.93 | 0.83 |
| 1:D:270:LYS:HB3 | 1:D:271:PRO:HD2 | 1.60 | 0.83 |
| 1:D:68:ALA:O | 1:D:91:LYS:CD | 2.27 | 0.83 |
| 1:E:253:LYS:O | 1:E:253:LYS:HE3 | 1.78 | 0.83 |
| 1:E:349:LYS:HG3 | 1:E:349:LYS:O | 1.77 | 0.82 |
| 1:E:90:ILE:HD13 | 1:E:117:ILE:HD13 | 1.61 | 0.82 |
| 2:F:432:TYR:CE2 | 6:F:500:NDP:H6N | 2.14 | 0.82 |
| 1:G:158:ARG:HB2 | 1:H:330:ASP:OD2 | 1.80 | 0.82 |
| 1:H:93:GLY:HA2 | 1:H:116:LYS:HB2 | 1.61 | 0.82 |
| 1:B:340:LEU:O | 1:B:344:THR:HG23 | 1.79 | 0.82 |
| 1:G:256:VAL:HG12 | 1:G:283:LYS:O | 1.79 | 0.82 |
| 1:E:358:LEU:HD12 | 1:E:358:LEU:H | 1.43 | 0.81 |
| 1:E:87:VAL:HG23 | 1:E:112:LEU:HG | 1.62 | 0.81 |
| 1:A:291:ILE:HD13 | 1:A:318:VAL:HB | 1.61 | 0.81 |
| 1:H:61:ALA:HB1 | 1:H:89:LEU:HD13 | 1.61 | 0.81 |
| 1:D:239:MET:HB2 | 1:D:244:ARG:HE | 1.44 | 0.81 |
| 1:G:115:ARG:NH2 | 1:G:115:ARG:HB3 | 1.96 | 0.81 |
| 1:D:160:PHE:O | 1:D:172:PRO:HA | 1.81 | 0.81 |
| 2:I:403:PRO:HA | 2:I:408:TYR:CG | 2.16 | 0.81 |
| 1:D:354:LEU:HD21 | 1:D:356:MET:SD | 2.20 | 0.81 |
| 1:H:136:ILE:HA | 1:H:338:ASN:OD1 | 1.80 | 0.81 |
| 1:H:67:GLN:H | 1:H:67:GLN:NE2 | 1.78 | 0.81 |
| 1:A:58:ALA:HB3 | 1:A:64:ALA:HB2 | 1.62 | 0.81 |
| 1:D:294:ALA:HB3 | 1:D:300:ASN:OD1 | 1.81 | 0.80 |
| 1:D:5:ILE:HG23 | 1:D:72:TRP:O | 1.81 | 0.80 |
| 1:H:93:GLY:HA2 | 1:H:116:LYS:CB | 2.12 | 0.80 |
| 1:G:10:ARG:HH12 | 1:G:76:ARG:NH2 | 1.80 | 0.80 |
| 1:B:8:GLU:CD | 1:B:74:VAL:HG22 | 2.01 | 0.80 |
| 1:G:163:MET:HB2 | 1:G:170:VAL:CG1 | 2.11 | 0.80 |
| 1:H:106:ARG:O | 1:H:109:VAL:HG12 | 1.82 | 0.80 |
| 1:D:92:GLU:HB2 | 1:D:115:ARG:O | 1.81 | 0.79 |
| 2:I:451:ASP:OD1 | 2:I:453:LYS:HB3 | 1.82 | 0.79 |
| 1:G:221:VAL:HG11 | 1:G:243:PHE:CZ | 2.17 | 0.79 |
| 1:H:67:GLN:HA | 1:H:91:LYS:HE3 | 1.62 | 0.79 |
| 2:C:454:LYS:HE2 | 2:C:454:LYS:HA | 1.65 | 0.79 |
| 1:E:255:LEU:HA | 1:E:258:THR:OG1 | 1.82 | 0.79 |
| 2:I:305:LYS:HE2 | 2:I:337:GLU:OE1 | 1.82 | 0.79 |
| 1:D:90:ILE:HD13 | 1:D:117:ILE:HD13 | 1.63 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:163:MET:HB2 | 1:D:170:VAL:CG1 | 2.13 | 0.78 |
| 1:D:175:VAL:HG21 | 1:D:191:ALA:HB1 | 1.63 | 0.78 |
| 1:D:346:HIS:HB3 | 1:D:355:VAL:O | 1.83 | 0.78 |
| 1:H:278:GLU:O | 1:H:281:VAL:HG22 | 1.84 | 0.78 |
| 2:I:336:LYS:HG3 | 2:I:337:GLU:N | 1.97 | 0.78 |
| 1:B:25:LYS:O | 1:B:29:LEU:HD13 | 1.82 | 0.78 |
| 2:I:422:LEU:HG | 2:I:448:LEU:HD11 | 1.66 | 0.77 |
| 1:G:260:ILE:HG12 | 1:G:289:VAL:HG12 | 1.66 | 0.77 |
| 1:G:29:LEU:HD11 | 1:G:344:THR:HG22 | 1.66 | 0.77 |
| 1:H:362:THR:HG23 | 1:H:363:VAL:N | 2.00 | 0.77 |
| 1:E:278:GLU:HB2 | 1:E:303:LEU:HD11 | 1.64 | 0.77 |
| 1:H:340:LEU:HD12 | 1:H:344:THR:HG23 | 1.66 | 0.77 |
| 1:B:134:MET:HG2 | 1:B:342:PHE:N | 2.00 | 0.77 |
| 1:H:15:ARG:HG2 | 1:H:15:ARG:HH21 | 1.48 | 0.77 |
| 1:B:120:TYR:OH | 1:B:356:MET:HG3 | 1.84 | 0.77 |
| 1:E:177:VAL:HG21 | 1:E:188:ILE:HD13 | 1.67 | 0.77 |
| 1:B:123:GLU:HA | 1:B:137:LEU:HD11 | 1.65 | 0.77 |
| 1:G:203:VAL:HG23 | 1:G:204:ARG:N | 2.00 | 0.77 |
| 2:I:451:ASP:HB3 | 2:I:454:LYS:HG2 | 1.66 | 0.77 |
| 1:A:163:MET:HB2 | 1:A:170:VAL:HG13 | 1.66 | 0.76 |
| 1:H:65:LEU:HD23 | 1:H:90:ILE:HG23 | 1.65 | 0.76 |
| 1:B:274:VAL:HG11 | 1:B:277:THR:HG23 | 1.67 | 0.76 |
| 2:C:399:ALA:HB2 | 2:C:407:ILE:CG1 | 2.15 | 0.76 |
| 1:E:86:GLU:HA | 1:E:89:LEU:HD13 | 1.67 | 0.76 |
| 2:I:401:THR:O | 2:I:403:PRO:CD | 2.24 | 0.76 |
| 1:D:91:LYS:O | 1:D:92:GLU:O | 2.03 | 0.76 |
| 1:G:115:ARG:HH21 | 1:G:115:ARG:HB3 | 1.50 | 0.76 |
| 1:A:332:SER:HB2 | 1:A:333:PRO:HD3 | 1.67 | 0.76 |
| 2:C:330:MET:HG3 | 2:C:463:MET:HE1 | 1.66 | 0.76 |
| 2:F:324:GLN:HE21 | 2:F:359:LEU:HD22 | 1.49 | 0.76 |
| 1:H:120:TYR:HD2 | 1:H:366:THR:HG21 | 1.47 | 0.76 |
| 2:I:316:TYR:O | 2:I:320:VAL:HG23 | 1.86 | 0.76 |
| 1:G:118:THR:HA | 1:G:369:THR:O | 1.85 | 0.76 |
| 1:E:125:MET:HE2 | 1:E:134:MET:HB2 | 1.67 | 0.76 |
| 1:H:112:LEU:HB3 | 1:H:117:ILE:HG13 | 1.66 | 0.76 |
| 1:H:100:LEU:HB2 | 1:H:121:ALA:HB2 | 1.65 | 0.76 |
| 1:A:376:HIS:HD2 | 1:A:378:ALA:HB2 | 1.50 | 0.75 |
| 1:G:170:VAL:HG23 | 1:H:330:ASP:OD1 | 1.85 | 0.75 |
| 1:H:113:THR:HG21 | 1:H:374:ILE:HG13 | 1.66 | 0.75 |
| 1:D:47:ASP:HA | 1:D:50:LEU:HD13 | 1.69 | 0.75 |
| 1:G:203:VAL:HG23 | 1:G:204:ARG:H | 1.51 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:264:THR:HG22 | 1:G:293:LEU:HD12 | 1.68 | 0.75 |
| 1:D:368:VAL:HA | 1:D:376:HIS:HB2 | 1.69 | 0.75 |
| 1:D:291:ILE:N | 1:D:291:ILE:HD12 | 2.02 | 0.75 |
| 2:I:437:ASN:HB3 | 2:I:440:PHE:HE1 | 1.49 | 0.75 |
| 1:A:106:ARG:N | 1:A:107:PRO:HD2 | 2.01 | 0.75 |
| 1:D:203:VAL:HG12 | 1:D:243:PHE:HE2 | 1.51 | 0.75 |
| 1:D:369:THR:HA | 1:D:373:ALA:O | 1.87 | 0.75 |
| 1:E:60:THR:CG2 | 1:E:63:GLN:HG3 | 2.16 | 0.75 |
| 2:F:354:GLY:O | 2:F:358:VAL:HG23 | 1.86 | 0.75 |
| 1:G:120:TYR:HB3 | 1:G:366:THR:CG2 | 2.15 | 0.75 |
| 1:D:3:ILE:O | 1:D:33:VAL:HA | 1.87 | 0.74 |
| 1:H:142:ASN:HD22 | 2:I:353:PRO:HD2 | 1.50 | 0.74 |
| 1:B:369:THR:HB | 1:B:374:ILE:HA | 1.68 | 0.74 |
| 1:A:165:THR:HG22 | 2:C:353:PRO:HB3 | 1.70 | 0.74 |
| 1:A:368:VAL:HA | 1:A:376:HIS:HB2 | 1.69 | 0.74 |
| 1:D:276:ILE:HA | 1:D:280:MET:HE3 | 1.69 | 0.74 |
| 2:F:348:VAL:HG21 | 2:F:410:MET:HE1 | 1.69 | 0.74 |
| 2:I:425:LYS:HD3 | 2:I:427:SER:O | 1.88 | 0.74 |
| 2:I:295:GLY:HA3 | 2:I:446:MET:HE2 | 1.70 | 0.73 |
| 2:F:328:ARG:HD3 | 2:F:363:ALA:O | 1.88 | 0.73 |
| 1:D:10:ARG:HH21 | 1:D:10:ARG:HG3 | 1.52 | 0.73 |
| 2:F:432:TYR:CZ | 6:F:500:NDP:H6N | 2.23 | 0.73 |
| 1:H:184:GLY:O | 1:H:188:ILE:HG13 | 1.88 | 0.73 |
| 1:H:74:VAL:HG23 | 1:H:75:GLN:N | 2.03 | 0.73 |
| 1:D:157:ALA:O | 1:E:329:ALA:HB3 | 1.89 | 0.73 |
| 1:E:86:GLU:HA | 1:E:89:LEU:CD1 | 2.19 | 0.73 |
| 1:H:118:THR:HA | 1:H:369:THR:O | 1.89 | 0.73 |
| 1:E:217:LYS:N | 1:E:217:LYS:HD2 | 2.04 | 0.73 |
| 1:E:66:SER:O | 1:E:91:LYS:HB2 | 1.89 | 0.73 |
| 1:D:308:LYS:HG2 | 1:D:309:ILE:H | 1.51 | 0.73 |
| 1:B:113:THR:HG23 | 1:B:373:ALA:HA | 1.70 | 0.72 |
| 1:B:368:VAL:HA | 1:B:376:HIS:HB2 | 1.70 | 0.72 |
| 1:G:2:LYS:HA | 1:G:32:GLU:HB2 | 1.70 | 0.72 |
| 1:H:116:LYS:HA | 1:H:372:GLY:N | 2.04 | 0.72 |
| 1:D:163:MET:HB2 | 1:D:170:VAL:HG13 | 1.71 | 0.72 |
| 1:G:62:ALA:HB2 | 1:G:89:LEU:HD23 | 1.71 | 0.72 |
| 1:A:376:HIS:CD2 | 1:A:378:ALA:HB2 | 2.24 | 0.72 |
| 1:D:164:MET:HG2 | 2:F:357:ASN:HD21 | 1.54 | 0.72 |
| 1:E:244:ARG:CB | 1:E:244:ARG:HH21 | 2.02 | 0.72 |
| 1:H:367:CYS:SG | 1:H:370:ARG:CD | 2.77 | 0.72 |
| 1:E:341:ASN:O | 1:E:345:PRO:HD3 | 1.90 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:61:ALA:O | 1:H:89:LEU:HB3 | 1.90 | 0.72 |
| 2:C:454:LYS:O | 2:C:458:GLN:HG3 | 1.90 | 0.72 |
| 1:H:93:GLY:CA | 1:H:116:LYS:HB2 | 2.20 | 0.72 |
| 1:B:118:THR:HA | 1:B:369:THR:O | 1.89 | 0.72 |
| 1:D:264:THR:HG22 | 1:D:293:LEU:HD12 | 1.72 | 0.72 |
| 1:G:347:VAL:HG12 | 1:G:348:ASP:O | 1.89 | 0.72 |
| 1:H:186:GLN:HA | 2:I:352:MET:CE | 2.16 | 0.72 |
| 1:D:23:VAL:HG11 | 1:D:55:ALA:HB2 | 1.71 | 0.71 |
| 1:A:276:ILE:HA | 1:A:280:MET:CE | 2.21 | 0.71 |
| 1:B:128:ILE:HD11 | 1:B:130:ARG:HD3 | 1.70 | 0.71 |
| 1:E:90:ILE:CD1 | 1:E:117:ILE:HD13 | 2.19 | 0.71 |
| 1:G:166:ALA:HB1 | 1:H:133:SER:HA | 1.71 | 0.71 |
| 1:A:278:GLU:HB2 | 1:A:303:LEU:HD11 | 1.72 | 0.71 |
| 1:E:312:LYS:HE3 | 1:E:313:HIS:NE2 | 2.05 | 0.71 |
| 1:H:180:VAL:HG11 | 1:H:207:THR:HG23 | 1.71 | 0.71 |
| 1:B:147:ARG:HD2 | 1:B:151:ASP:OD2 | 1.91 | 0.71 |
| 1:D:285:LYS:HD3 | 1:D:286:PRO:N | 2.04 | 0.71 |
| 1:D:293:LEU:CD2 | 1:D:323:VAL:HG21 | 2.21 | 0.71 |
| 1:H:32:GLU:HA | 1:H:32:GLU:OE2 | 1.90 | 0.71 |
| 1:H:63:GLN:HA | 1:H:63:GLN:HE21 | 1.56 | 0.71 |
| 2:C:322:GLN:NE2 | 2:C:324:GLN:HE22 | 1.89 | 0.71 |
| 1:H:368:VAL:O | 1:H:375:VAL:N | 2.21 | 0.71 |
| 1:E:244:ARG:HB3 | 1:E:244:ARG:HH21 | 1.56 | 0.71 |
| 1:H:93:GLY:HA2 | 1:H:116:LYS:O | 1.90 | 0.70 |
| 1:G:106:ARG:N | 1:G:107:PRO:HD2 | 2.05 | 0.70 |
| 1:G:275:LEU:HB2 | 1:G:300:ASN:HB3 | 1.72 | 0.70 |
| 1:H:202:ASP:HA | 4:H:400:NAD:H8A | 1.71 | 0.70 |
| 1:A:76:ARG:NH2 | 1:A:76:ARG:HG2 | 1.97 | 0.70 |
| 1:H:120:TYR:CD2 | 1:H:366:THR:HG21 | 2.23 | 0.70 |
| 1:D:207:THR:HA | 1:D:210:GLN:HE21 | 1.56 | 0.70 |
| 1:H:120:TYR:CA | 1:H:366:THR:HG23 | 2.21 | 0.70 |
| 1:B:346:HIS:O | 1:B:355:VAL:HG12 | 1.91 | 0.70 |
| 1:D:120:TYR:HD1 | 1:D:366:THR:O | 1.75 | 0.70 |
| 1:E:25:LYS:O | 1:E:29:LEU:HD13 | 1.92 | 0.70 |
| 1:D:357:LYS:O | 1:D:359:GLU:HG3 | 1.90 | 0.70 |
| 1:B:94:ALA:O | 1:B:117:ILE:HG23 | 1.91 | 0.70 |
| 1:E:93:GLY:HA2 | 1:E:116:LYS:HD2 | 1.74 | 0.70 |
| 1:E:125:MET:HE3 | 1:E:342:PHE:HD2 | 1.57 | 0.70 |
| 1:E:5:ILE:HD13 | 1:E:35:VAL:HG22 | 1.73 | 0.70 |
| 1:D:265:ALA:O | 1:D:266:LEU:HD23 | 1.90 | 0.70 |
| 1:B:3:ILE:HG13 | 1:B:70:VAL:HG13 | 1.74 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:208:LYS:HD2 | 1:D:208:LYS:C | 2.12 | 0.70 |
| 1:G:330:ASP:OD1 | 1:H:158:ARG:HD2 | 1.91 | 0.69 |
| 1:B:164:MET:CE | 1:B:164:MET:HA | 2.22 | 0.69 |
| 1:E:118:THR:HA | 1:E:369:THR:O | 1.93 | 0.69 |
| 1:G:243:PHE:C | 1:G:245:LYS:H | 1.96 | 0.69 |
| 1:D:120:TYR:HB3 | 1:D:366:THR:HG22 | 1.73 | 0.69 |
| 1:H:3:ILE:HA | 1:H:70:VAL:O | 1.92 | 0.69 |
| 1:A:46:THR:O | 1:A:49:ALA:HB3 | 1.92 | 0.69 |
| 1:E:93:GLY:CA | 1:E:116:LYS:HD2 | 2.22 | 0.69 |
| 1:H:8:GLU:HG2 | 1:H:74:VAL:CG2 | 2.20 | 0.69 |
| 1:B:70:VAL:HG23 | 1:B:95:VAL:CB | 2.11 | 0.69 |
| 1:D:326:ARG:HG2 | 1:D:326:ARG:HH11 | 1.57 | 0.69 |
| 1:D:358:LEU:HD13 | 1:D:370:ARG:NH2 | 2.06 | 0.69 |
| 1:H:103:LEU:H | 1:H:103:LEU:HD12 | 1.57 | 0.69 |
| 1:A:120:TYR:HE2 | 1:A:363:VAL:HG13 | 1.57 | 0.69 |
| 1:B:99:HIS:HD2 | 1:B:101:GLY:H | 1.39 | 0.69 |
| 1:B:164:MET:HE2 | 1:B:164:MET:HA | 1.74 | 0.69 |
| 1:D:136:ILE:HG22 | 1:D:338:ASN:HB3 | 1.73 | 0.69 |
| 1:H:126:PRO:O | 1:H:128:ILE:HG12 | 1.92 | 0.69 |
| 2:I:399:ALA:HB2 | 2:I:407:ILE:CG1 | 2.22 | 0.69 |
| 2:F:299:ASP:O | 2:F:303:ILE:HG13 | 1.92 | 0.69 |
| 1:H:1:MET:HG2 | 1:H:31:PHE:HA | 1.75 | 0.69 |
| 2:I:403:PRO:HG3 | 2:I:408:TYR:CE1 | 2.28 | 0.69 |
| 1:D:332:SER:HB2 | 1:D:333:PRO:HD3 | 1.75 | 0.69 |
| 1:D:163:MET:CE | 1:E:142:ASN:HD21 | 2.05 | 0.69 |
| 2:F:403:PRO:HA | 2:F:408:TYR:CG | 2.27 | 0.69 |
| 1:E:278:GLU:O | 1:E:282:THR:HG23 | 1.93 | 0.69 |
| 1:B:199:MET:HG3 | 1:B:217:LYS:O | 1.93 | 0.69 |
| 2:C:325:HIS:CE1 | 2:C:363:ALA:HA | 2.27 | 0.69 |
| 1:E:121:ALA:HB1 | 1:E:123:GLU:OE1 | 1.93 | 0.69 |
| 1:E:362:THR:HG23 | 1:E:363:VAL:N | 2.06 | 0.69 |
| 1:G:247:GLN:HG2 | 1:G:248:ALA:N | 2.08 | 0.68 |
| 1:H:348:ASP:HB2 | 1:H:355:VAL:HB | 1.75 | 0.68 |
| 1:E:120:TYR:HD1 | 1:E:366:THR:O | 1.75 | 0.68 |
| 1:D:188:ILE:HG12 | 1:D:198:VAL:HG11 | 1.75 | 0.68 |
| 1:D:113:THR:HA | 1:D:369:THR:HG21 | 1.76 | 0.68 |
| 1:E:128:ILE:CD1 | 1:E:130:ARG:HH21 | 2.07 | 0.68 |
| 1:H:291:ILE:HD12 | 1:H:291:ILE:N | 2.08 | 0.68 |
| 1:E:320:HIS:ND1 | 1:E:326:ARG:CZ | 2.56 | 0.68 |
| 1:G:72:TRP:HE1 | 1:G:97:MET:CE | 2.07 | 0.68 |
| 1:B:6:PRO:HD2 | 1:B:72:TRP:O | 1.93 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:323:VAL:HA | 1:D:326:ARG:HD3 | 1.76 | 0.68 |
| 1:D:367:CYS:O | 1:D:376:HIS:HB2 | 1.93 | 0.68 |
| 1:E:361:GLU:HA | 1:E:364:SER:HB3 | 1.74 | 0.68 |
| 1:H:178:PHE:HE1 | 1:H:276:ILE:HD11 | 1.59 | 0.68 |
| 1:H:210:GLN:O | 1:H:213:SER:HB3 | 1.93 | 0.68 |
| 1:A:7:LYS:HB2 | 1:A:39:ALA:HA | 1.75 | 0.68 |
| 1:B:308:LYS:HG3 | 1:B:309:ILE:H | 1.58 | 0.68 |
| 1:G:121:ALA:HB3 | 1:G:124:LEU:HD12 | 1.74 | 0.68 |
| 1:G:368:VAL:HG23 | 1:G:369:THR:HG22 | 1.76 | 0.68 |
| 1:D:90:ILE:CD1 | 1:D:117:ILE:HD13 | 2.23 | 0.68 |
| 1:G:265:ALA:CB | 1:G:275:LEU:HD11 | 2.24 | 0.68 |
| 1:B:208:LYS:O | 1:B:212:GLU:HG3 | 1.94 | 0.67 |
| 2:I:318:MET:HE3 | 2:I:324:GLN:H | 1.59 | 0.67 |
| 1:D:225:ALA:C | 1:D:227:LYS:H | 1.97 | 0.67 |
| 1:G:105:ASN:C | 1:G:107:PRO:HD2 | 2.14 | 0.67 |
| 1:G:376:HIS:HD2 | 1:G:378:ALA:HB2 | 1.59 | 0.67 |
| 1:H:3:ILE:HG13 | 1:H:70:VAL:O | 1.94 | 0.67 |
| 1:H:8:GLU:CG | 1:H:74:VAL:HG22 | 2.23 | 0.67 |
| 1:B:354:LEU:HD21 | 1:B:356:MET:HG2 | 1.76 | 0.67 |
| 2:C:299:ASP:O | 2:C:303:ILE:HG13 | 1.94 | 0.67 |
| 1:D:248:ALA:HA | 1:D:251:VAL:HG22 | 1.76 | 0.67 |
| 1:D:285:LYS:NZ | 1:D:286:PRO:HG2 | 2.10 | 0.67 |
| 1:H:129:SER:HA | 1:H:132:GLN:CD | 2.14 | 0.67 |
| 1:E:112:LEU:HD12 | 1:E:112:LEU:H | 1.60 | 0.67 |
| 1:G:160:PHE:O | 1:G:172:PRO:HA | 1.95 | 0.67 |
| 1:B:370:ARG:HG2 | 1:B:375:VAL:HG21 | 1.76 | 0.67 |
| 2:F:312:ILE:HG21 | 2:F:327:LEU:HD21 | 1.77 | 0.67 |
| 1:H:158:ARG:HB3 | 1:H:158:ARG:HH11 | 1.60 | 0.67 |
| 1:A:265:ALA:HB3 | 1:A:300:ASN:HD21 | 1.58 | 0.67 |
| 2:C:396:ASN:O | 2:C:412:ILE:HD13 | 1.94 | 0.67 |
| 1:D:342:PHE:HZ | 1:D:362:THR:O | 1.73 | 0.67 |
| 1:D:78:MET:HA | 1:D:82:GLU:OE1 | 1.94 | 0.67 |
| 1:H:266:LEU:O | 1:H:267:ILE:HG13 | 1.95 | 0.67 |
| 1:A:164:MET:HE3 | 2:C:357:ASN:OD1 | 1.95 | 0.67 |
| 1:B:244:ARG:HD3 | 1:B:244:ARG:H | 1.60 | 0.67 |
| 1:D:354:LEU:HD23 | 1:D:355:VAL:N | 2.10 | 0.67 |
| 1:E:97:MET:O | 1:E:98:CYS:HB3 | 1.95 | 0.67 |
| 1:G:265:ALA:HB3 | 1:G:275:LEU:HD11 | 1.77 | 0.67 |
| 1:B:217:LYS:HE3 | 1:B:217:LYS:HA | 1.75 | 0.67 |
| 1:E:113:THR:HG23 | 1:E:373:ALA:HA | 1.75 | 0.67 |
| 1:G:278:GLU:O | 1:G:282:THR:HG23 | 1.95 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:247:GLN:HE21 | 1:H:248:ALA:N | 1.93 | 0.67 |
| 2:F:381:GLN:HG2 | 2:F:417:LYS:HE2 | 1.76 | 0.66 |
| 1:B:108:VAL:O | 1:B:112:LEU:HD13 | 1.94 | 0.66 |
| 1:G:263:THR:OG1 | 1:G:292:ASP:HA | 1.95 | 0.66 |
| 1:G:78:MET:H | 1:G:86:GLU:HB2 | 1.59 | 0.66 |
| 1:H:69:ASP:O | 1:H:95:VAL:HG23 | 1.95 | 0.66 |
| 1:H:218:PHE:HD2 | 1:H:220:THR:HG23 | 1.59 | 0.66 |
| 1:H:110:GLU:HA | 1:H:374:ILE:HD11 | 1.77 | 0.66 |
| 2:C:310:VAL:HG22 | 2:C:385:VAL:HB | 1.77 | 0.66 |
| 1:B:349:LYS:HG3 | 1:B:350:ASP:N | 2.07 | 0.66 |
| 1:E:204:ARG:O | 1:E:207:THR:HB | 1.96 | 0.66 |
| 1:H:182:VAL:HG13 | 1:H:183:ALA:N | 2.11 | 0.66 |
| 1:H:284:MET:SD | 1:H:290:ILE:HD11 | 2.36 | 0.66 |
| 2:C:309:LYS:NZ | 2:C:382:THR:HB | 2.11 | 0.66 |
| 1:G:362:THR:CG2 | 1:G:363:VAL:N | 2.59 | 0.66 |
| 2:I:318:MET:HG3 | 2:I:319:ALA:N | 2.11 | 0.66 |
| 1:A:277:THR:H | 1:A:280:MET:HE2 | 1.60 | 0.66 |
| 1:G:359:GLU:CD | 1:G:359:GLU:H | 1.99 | 0.66 |
| 1:H:264:THR:HG22 | 1:H:293:LEU:HD12 | 1.78 | 0.66 |
| 1:A:93:GLY:HA2 | 1:A:116:LYS:O | 1.95 | 0.66 |
| 1:D:20:PRO:HD3 | 1:D:45:ILE:HG21 | 1.78 | 0.66 |
| 1:E:284:MET:HE1 | 1:E:315:VAL:HG11 | 1.77 | 0.66 |
| 2:F:446:MET:HE3 | 2:F:448:LEU:HD21 | 1.78 | 0.66 |
| 1:H:346:HIS:HB3 | 1:H:356:MET:HB3 | 1.78 | 0.66 |
| 2:F:388:VAL:HG13 | 2:F:391:ALA:HB3 | 1.78 | 0.66 |
| 1:D:167:ALA:O | 1:E:337:LYS:HD2 | 1.96 | 0.66 |
| 1:D:70:VAL:HA | 1:D:95:VAL:O | 1.96 | 0.66 |
| 1:D:96:LEU:HD23 | 1:D:96:LEU:O | 1.96 | 0.65 |
| 1:E:60:THR:HG22 | 1:E:63:GLN:HG3 | 1.76 | 0.65 |
| 1:G:362:THR:HG22 | 1:G:363:VAL:N | 2.11 | 0.65 |
| 1:H:178:PHE:CE1 | 1:H:276:ILE:HD11 | 2.30 | 0.65 |
| 1:B:267:ILE:CD1 | 4:B:400:NAD:N1A | 2.59 | 0.65 |
| 1:D:87:VAL:O | 1:D:115:ARG:CD | 2.44 | 0.65 |
| 2:C:433:ALA:O | 2:C:435:VAL:HG23 | 1.96 | 0.65 |
| 1:D:354:LEU:C | 1:D:355:VAL:HG22 | 2.16 | 0.65 |
| 1:G:113:THR:HG23 | 1:G:373:ALA:HA | 1.78 | 0.65 |
| 1:B:136:ILE:HA | 1:B:338:ASN:OD1 | 1.97 | 0.65 |
| 1:H:355:VAL:O | 1:H:355:VAL:HG13 | 1.95 | 0.65 |
| 1:D:277:THR:H | 1:D:280:MET:HE3 | 1.62 | 0.65 |
| 1:D:50:LEU:H | 1:D:50:LEU:HD12 | 1.61 | 0.65 |
| 1:H:136:ILE:HG13 | 1:H:137:LEU:H | 1.61 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:401:THR:C | 2:I:403:PRO:HD3 | 2.15 | 0.65 |
| 1:D:322:ASN:ND2 | 1:D:325:SER:HB2 | 2.11 | 0.65 |
| 1:H:5:ILE:HB | 1:H:35:VAL:HG12 | 1.79 | 0.65 |
| 1:G:120:TYR:OH | 1:G:356:MET:HG3 | 1.97 | 0.65 |
| 1:H:7:LYS:HB2 | 1:H:39:ALA:HA | 1.79 | 0.65 |
| 1:B:136:ILE:HG13 | 1:B:137:LEU:HD12 | 1.77 | 0.65 |
| 1:A:167:ALA:HB2 | 1:B:338:ASN:HD21 | 1.62 | 0.65 |
| 1:G:362:THR:HG22 | 1:G:363:VAL:H | 1.61 | 0.65 |
| 1:G:89:LEU:H | 1:G:89:LEU:HD12 | 1.60 | 0.65 |
| 1:A:136:ILE:HG13 | 1:A:137:LEU:N | 2.12 | 0.65 |
| 1:D:97:MET:HB2 | 1:D:122:MET:CE | 2.27 | 0.65 |
| 1:G:5:ILE:HB | 1:G:35:VAL:HG12 | 1.79 | 0.65 |
| 2:F:304:MET:HG2 | 2:F:385:VAL:HG11 | 1.79 | 0.64 |
| 2:I:432:TYR:C | 2:I:434:GLY:H | 1.98 | 0.64 |
| 2:F:454:LYS:HA | 2:F:457:GLU:OE1 | 1.96 | 0.64 |
| 1:H:295:VAL:HG23 | 1:H:304:SER:HB2 | 1.79 | 0.64 |
| 2:I:437:ASN:HB3 | 2:I:440:PHE:CD1 | 2.32 | 0.64 |
| 2:C:420:THR:HB | 1:H:162:MET:CE | 2.28 | 0.64 |
| 1:D:57:ILE:HD12 | 1:D:58:ALA:H | 1.61 | 0.64 |
| 1:G:103:LEU:HD13 | 1:G:124:LEU:HD21 | 1.78 | 0.64 |
| 1:H:281:VAL:HG11 | 1:H:303:LEU:HD12 | 1.79 | 0.64 |
| 1:D:88:ALA:HA | 1:D:115:ARG:CD | 2.27 | 0.64 |
| 1:H:247:GLN:NE2 | 1:H:248:ALA:N | 2.45 | 0.64 |
| 1:H:5:ILE:HG13 | 1:H:72:TRP:CD1 | 2.33 | 0.64 |
| 1:B:143:LEU:HD12 | 1:B:331:ALA:HB2 | 1.78 | 0.64 |
| 1:E:128:ILE:HD11 | 1:E:130:ARG:HH21 | 1.63 | 0.64 |
| 1:H:208:LYS:NZ | 1:H:220:THR:HG21 | 2.12 | 0.64 |
| 1:H:241:GLU:O | 1:H:245:LYS:HG2 | 1.97 | 0.64 |
| 1:B:10:ARG:HH11 | 1:B:10:ARG:HG3 | 1.62 | 0.64 |
| 1:B:29:LEU:CD2 | 1:B:347:VAL:HG11 | 2.21 | 0.64 |
| 1:G:67:GLN:HA | 1:G:91:LYS:HD3 | 1.80 | 0.64 |
| 1:H:162:MET:HB2 | 1:H:172:PRO:HD3 | 1.80 | 0.64 |
| 1:A:304:SER:O | 1:A:305:GLU:C | 2.36 | 0.64 |
| 1:G:66:SER:O | 1:G:91:LYS:HB3 | 1.98 | 0.64 |
| 1:A:207:THR:HG22 | 1:A:218:PHE:HE1 | 1.63 | 0.64 |
| 1:D:329:ALA:HB3 | 1:E:157:ALA:O | 1.98 | 0.64 |
| 1:G:94:ALA:O | 1:G:117:ILE:HG23 | 1.98 | 0.64 |
| 1:B:180:VAL:HG23 | 1:B:202:ASP:HB2 | 1.79 | 0.64 |
| 2:F:366:PRO:HB2 | 2:F:369:GLU:HG3 | 1.80 | 0.63 |
| 1:G:273:PRO:HG3 | 4:G:400:NAD:H2A | 1.80 | 0.63 |
| 1:A:6:PRO:HA | 1:A:36:GLU:HG2 | 1.81 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:264:THR:CG2 | 1:B:293:LEU:HD12 | 2.20 | 0.63 |
| 1:B:126:PRO:HG2 | 1:B:362:THR:HA | 1.80 | 0.63 |
| 1:D:246:LYS:O | 1:D:249:GLU:CB | 2.46 | 0.63 |
| 1:D:346:HIS:CD2 | 1:D:356:MET:HA | 2.34 | 0.63 |
| 1:B:376:HIS:HB3 | 1:B:379:LEU:HD13 | 1.80 | 0.63 |
| 1:D:106:ARG:O | 1:D:109:VAL:HG22 | 1.98 | 0.63 |
| 1:E:136:ILE:CD1 | 1:E:137:LEU:HD12 | 2.28 | 0.63 |
| 1:A:375:VAL:O | 1:A:375:VAL:HG22 | 1.98 | 0.63 |
| 1:B:19:SER:HB3 | 1:B:22:VAL:HG23 | 1.80 | 0.63 |
| 1:D:263:THR:OG1 | 1:D:292:ASP:HA | 1.97 | 0.63 |
| 1:A:180:VAL:HG11 | 1:A:207:THR:HG23 | 1.80 | 0.63 |
| 1:G:120:TYR:CE2 | 1:G:363:VAL:HG13 | 2.33 | 0.63 |
| 1:B:86:GLU:O | 1:B:89:LEU:HB2 | 1.98 | 0.63 |
| 2:C:430:SER:OG | 2:C:434:GLY:HA2 | 1.99 | 0.63 |
| 1:E:374:ILE:H | 1:E:374:ILE:HD12 | 1.63 | 0.63 |
| 1:G:282:THR:HG22 | 1:G:313:HIS:HD2 | 1.64 | 0.63 |
| 1:E:362:THR:CG2 | 1:E:363:VAL:N | 2.60 | 0.63 |
| 1:H:122:MET:CE | 1:H:122:MET:H | 2.12 | 0.63 |
| 2:I:410:MET:O | 2:I:410:MET:HG3 | 1.99 | 0.63 |
| 1:A:276:ILE:HA | 1:A:280:MET:HE3 | 1.81 | 0.63 |
| 1:A:376:HIS:HD2 | 1:A:378:ALA:CB | 2.12 | 0.63 |
| 2:C:424:ILE:O | 2:C:424:ILE:HG22 | 1.99 | 0.63 |
| 1:D:3:ILE:HB | 1:D:70:VAL:HG23 | 1.81 | 0.63 |
| 1:E:89:LEU:H | 1:E:89:LEU:HD12 | 1.64 | 0.63 |
| 1:B:5:ILE:N | 1:B:5:ILE:HD12 | 2.14 | 0.62 |
| 1:E:34:ILE:CD1 | 1:E:56:THR:HB | 2.28 | 0.62 |
| 1:H:120:TYR:HB3 | 1:H:366:THR:HG21 | 1.80 | 0.62 |
| 1:A:120:TYR:CE2 | 1:A:363:VAL:HG13 | 2.34 | 0.62 |
| 1:D:121:ALA:O | 1:D:124:LEU:HB2 | 1.99 | 0.62 |
| 1:B:147:ARG:CD | 1:B:151:ASP:OD2 | 2.47 | 0.62 |
| 1:D:277:THR:H | 1:D:280:MET:CE | 2.12 | 0.62 |
| 1:D:2:LYS:HD2 | 1:D:32:GLU:HB3 | 1.81 | 0.62 |
| 1:E:86:GLU:C | 1:E:88:ALA:H | 2.03 | 0.62 |
| 1:G:5:ILE:N | 1:G:5:ILE:HD12 | 2.14 | 0.62 |
| 2:F:344:ALA:HB2 | 2:F:376:ILE:HD13 | 1.82 | 0.62 |
| 1:H:272:ALA:HB1 | 1:H:273:PRO:HD2 | 1.80 | 0.62 |
| 1:D:163:MET:HE1 | 1:E:142:ASN:ND2 | 2.11 | 0.62 |
| 1:H:362:THR:CG2 | 1:H:363:VAL:H | 2.07 | 0.62 |
| 2:I:377:ASN:O | 2:I:379:SER:N | 2.31 | 0.62 |
| 1:H:276:ILE:O | 1:H:302:PRO:HD2 | 1.99 | 0.62 |
| 1:D:178:PHE:CE2 | 1:D:276:ILE:HD11 | 2.35 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:252:LEU:O | 1:B:256:VAL:HG23 | 2.00 | 0.61 |
| 1:A:342:PHE:CE1 | 1:A:362:THR:HG23 | 2.34 | 0.61 |
| 1:D:194:LEU:HD21 | 1:E:194:LEU:HD13 | 1.82 | 0.61 |
| 1:E:348:ASP:CG | 1:E:351:THR:HB | 2.20 | 0.61 |
| 1:E:60:THR:HG22 | 1:E:63:GLN:CG | 2.29 | 0.61 |
| 2:I:323:ALA:O | 2:I:325:HIS:N | 2.34 | 0.61 |
| 2:C:395:THR:HG23 | 2:C:437:ASN:HD21 | 1.64 | 0.61 |
| 1:H:60:THR:HG23 | 1:H:63:GLN:H | 1.63 | 0.61 |
| 2:I:330:MET:HG3 | 2:I:463:MET:HE3 | 1.82 | 0.61 |
| 1:A:163:MET:HB2 | 1:A:170:VAL:CG1 | 2.29 | 0.61 |
| 1:A:322:ASN:ND2 | 1:A:325:SER:HB2 | 2.14 | 0.61 |
| 1:B:274:VAL:CG1 | 1:B:277:THR:HG23 | 2.31 | 0.61 |
| 2:C:316:TYR:O | 2:C:320:VAL:HG23 | 2.00 | 0.61 |
| 2:C:403:PRO:HA | 2:C:408:TYR:CG | 2.34 | 0.61 |
| 2:C:464:ASN:ND2 | 2:C:464:ASN:C | 2.48 | 0.61 |
| 1:D:3:ILE:HG13 | 1:D:70:VAL:O | 2.01 | 0.61 |
| 1:G:243:PHE:O | 1:G:247:GLN:HB3 | 2.00 | 0.61 |
| 1:G:257:LYS:HA | 1:G:285:LYS:HE3 | 1.82 | 0.61 |
| 1:B:96:LEU:HD23 | 1:B:112:LEU:HD21 | 1.82 | 0.61 |
| 1:E:16:VAL:HG22 | 1:E:18:ILE:HG22 | 1.82 | 0.61 |
| 1:G:326:ARG:HH21 | 1:G:326:ARG:HG2 | 1.66 | 0.61 |
| 1:G:376:HIS:HD2 | 1:G:378:ALA:CB | 2.13 | 0.61 |
| 1:H:34:ILE:HG23 | 1:H:58:ALA:HB2 | 1.82 | 0.61 |
| 2:I:437:ASN:CB | 2:I:440:PHE:HE1 | 2.13 | 0.61 |
| 1:D:120:TYR:CD1 | 1:D:366:THR:O | 2.54 | 0.61 |
| 1:D:136:ILE:HD13 | 1:D:137:LEU:N | 2.16 | 0.61 |
| 1:D:366:THR:HG22 | 1:D:366:THR:O | 1.99 | 0.61 |
| 1:D:92:GLU:H | 1:D:115:ARG:HH21 | 1.47 | 0.61 |
| 1:E:93:GLY:N | 1:E:116:LYS:O | 2.32 | 0.61 |
| 2:F:451:ASP:H | 2:F:454:LYS:HE3 | 1.65 | 0.61 |
| 1:H:321:THR:O | 1:H:322:ASN:HB2 | 2.00 | 0.61 |
| 1:B:1:MET:CE | 1:B:353:THR:HA | 2.30 | 0.61 |
| 1:D:5:ILE:HG12 | 1:D:18:ILE:HB | 1.82 | 0.61 |
| 1:G:36:GLU:OE1 | 1:G:61:ALA:HB2 | 2.01 | 0.61 |
| 1:A:45:ILE:HG22 | 1:A:50:LEU:HD21 | 1.81 | 0.61 |
| 1:B:190:THR:O | 1:B:193:ARG:HG2 | 2.00 | 0.61 |
| 1:G:139:SER:HB2 | 1:G:334:LEU:HD23 | 1.82 | 0.61 |
| 1:G:374:ILE:HD12 | 1:G:374:ILE:H | 1.66 | 0.61 |
| 1:H:2:LYS:HD3 | 1:H:32:GLU:HB2 | 1.82 | 0.61 |
| 2:I:308:SER:HB3 | 2:I:384:ASP:OD2 | 2.00 | 0.61 |
| 2:F:310:VAL:HG22 | 2:F:385:VAL:HB | 1.83 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:64:ALA:C | 1:H:65:LEU:HD12 | 2.21 | 0.61 |
| 1:B:19:SER:O | 1:B:23:VAL:HG23 | 1.99 | 0.61 |
| 1:B:22:VAL:HG21 | 1:B:336:ALA:HB1 | 1.83 | 0.61 |
| 1:D:285:LYS:C | 1:D:285:LYS:HD3 | 2.22 | 0.61 |
| 1:H:120:TYR:CB | 1:H:366:THR:CG2 | 2.79 | 0.61 |
| 1:H:208:LYS:HZ2 | 1:H:220:THR:HG21 | 1.66 | 0.61 |
| 1:E:342:PHE:CD1 | 1:E:342:PHE:O | 2.54 | 0.60 |
| 2:I:403:PRO:HA | 2:I:408:TYR:CD2 | 2.35 | 0.60 |
| 2:C:424:ILE:HD12 | 2:C:424:ILE:N | 2.16 | 0.60 |
| 1:E:169:THR:HG22 | 1:E:170:VAL:N | 2.16 | 0.60 |
| 1:B:312:LYS:HG2 | 1:B:313:HIS:CD2 | 2.36 | 0.60 |
| 2:C:403:PRO:HA | 2:C:408:TYR:CD1 | 2.36 | 0.60 |
| 1:E:34:ILE:HD13 | 1:E:56:THR:HB | 1.81 | 0.60 |
| 1:D:131:ALA:HB1 | 1:D:134:MET:HG3 | 1.83 | 0.60 |
| 1:D:76:ARG:HG2 | 1:D:100:LEU:HA | 1.83 | 0.60 |
| 1:D:97:MET:HB2 | 1:D:122:MET:HE1 | 1.84 | 0.60 |
| 1:E:125:MET:HE3 | 1:E:134:MET:SD | 2.42 | 0.60 |
| 1:E:360:ASP:CG | 1:E:362:THR:HG22 | 2.21 | 0.60 |
| 1:G:221:VAL:HG12 | 1:G:222:ASP:N | 2.16 | 0.60 |
| 1:G:9:ARG:NH2 | 1:G:36:GLU:OE2 | 2.34 | 0.60 |
| 1:H:112:LEU:HD12 | 1:H:112:LEU:N | 2.15 | 0.60 |
| 1:H:163:MET:HB2 | 1:H:170:VAL:HG23 | 1.83 | 0.60 |
| 1:H:47:ASP:HB2 | 1:H:57:ILE:CD1 | 2.32 | 0.60 |
| 1:H:70:VAL:HA | 1:H:95:VAL:HB | 1.83 | 0.60 |
| 1:A:141:SER:O | 1:A:183:ALA:HB2 | 2.01 | 0.60 |
| 1:B:120:TYR:CE1 | 1:B:367:CYS:HB2 | 2.36 | 0.60 |
| 2:C:303:ILE:HG12 | 1:H:169:THR:CG2 | 2.31 | 0.60 |
| 1:D:50:LEU:O | 1:D:55:ALA:HB3 | 2.02 | 0.60 |
| 1:E:284:MET:CE | 1:E:290:ILE:HD11 | 2.32 | 0.60 |
| 1:A:376:HIS:CD2 | 1:A:378:ALA:H | 2.19 | 0.60 |
| 2:C:373:LEU:HD23 | 2:C:373:LEU:C | 2.22 | 0.60 |
| 1:D:158:ARG:HG3 | 1:E:329:ALA:HB3 | 1.84 | 0.60 |
| 1:B:118:THR:HG23 | 1:B:370:ARG:HB3 | 1.83 | 0.60 |
| 1:D:265:ALA:HB3 | 1:D:300:ASN:HD21 | 1.67 | 0.60 |
| 1:D:91:LYS:O | 1:D:92:GLU:C | 2.40 | 0.60 |
| 2:I:453:LYS:O | 2:I:457:GLU:HG3 | 2.01 | 0.60 |
| 1:D:68:ALA:H | 1:D:91:LYS:HD2 | 1.67 | 0.60 |
| 1:G:104:THR:HG22 | 1:G:104:THR:O | 2.02 | 0.60 |
| 2:C:321:ALA:CB | 2:C:452:ALA:HB3 | 2.31 | 0.59 |
| 1:D:342:PHE:CE1 | 1:D:362:THR:HG23 | 2.37 | 0.59 |
| 1:E:138:SER:OG | 1:E:139:SER:N | 2.35 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:115:ARG:HH21 | 1:G:115:ARG:CB | 2.13 | 0.59 |
| 1:G:311:VAL:HG13 | 1:G:316:LYS:HG2 | 1.83 | 0.59 |
| 1:G:10:ARG:HG2 | 1:G:75:GLN:HG2 | 1.83 | 0.59 |
| 1:H:87:VAL:HG21 | 1:H:112:LEU:HA | 1.83 | 0.59 |
| 1:A:277:THR:H | 1:A:280:MET:HE3 | 1.65 | 0.59 |
| 1:B:146:TYR:CE2 | 1:B:150:ILE:HG13 | 2.37 | 0.59 |
| 1:H:278:GLU:O | 1:H:282:THR:HG23 | 2.02 | 0.59 |
| 1:H:28:GLY:C | 1:H:29:LEU:HD12 | 2.22 | 0.59 |
| 1:H:5:ILE:HG13 | 1:H:72:TRP:HD1 | 1.68 | 0.59 |
| 1:A:13:GLU:OE2 | 1:A:15:ARG:HB2 | 2.02 | 0.59 |
| 1:B:99:HIS:CD2 | 1:B:101:GLY:H | 2.19 | 0.59 |
| 1:G:374:ILE:HD12 | 1:G:374:ILE:N | 2.17 | 0.59 |
| 1:G:2:LYS:O | 1:G:69:ASP:HB2 | 2.03 | 0.59 |
| 1:H:147:ARG:NH1 | 1:H:151:ASP:OD1 | 2.35 | 0.59 |
| 1:H:142:ASN:ND2 | 2:I:353:PRO:HB2 | 2.17 | 0.59 |
| 1:A:106:ARG:HH12 | 1:A:379:LEU:HG | 1.65 | 0.59 |
| 1:D:280:MET:C | 1:D:282:THR:H | 2.05 | 0.59 |
| 1:G:128:ILE:HD12 | 1:G:129:SER:H | 1.67 | 0.59 |
| 1:H:131:ALA:HA | 1:H:134:MET:CE | 2.32 | 0.59 |
| 1:H:162:MET:HE2 | 1:H:164:MET:SD | 2.42 | 0.59 |
| 1:D:221:VAL:HG11 | 1:D:250:ALA:HB3 | 1.82 | 0.59 |
| 1:D:13:GLU:OE1 | 1:D:322:ASN:ND2 | 2.36 | 0.59 |
| 1:H:4:ALA:O | 1:H:71:VAL:HG23 | 2.03 | 0.59 |
| 1:E:219:ILE:HG22 | 1:E:219:ILE:O | 2.02 | 0.59 |
| 1:G:34:ILE:HD13 | 1:G:56:THR:HB | 1.83 | 0.59 |
| 1:G:37:GLN:NE2 | 1:G:59:SER:HA | 2.17 | 0.59 |
| 1:G:78:MET:HA | 1:G:82:GLU:OE1 | 2.02 | 0.59 |
| 1:H:18:ILE:CD1 | 1:H:23:VAL:HG22 | 2.16 | 0.59 |
| 1:H:47:ASP:HB2 | 1:H:57:ILE:HD13 | 1.80 | 0.59 |
| 1:D:5:ILE:N | 1:D:5:ILE:HD12 | 2.18 | 0.59 |
| 1:H:347:VAL:C | 1:H:355:VAL:HG12 | 2.23 | 0.59 |
| 1:H:72:TRP:HA | 1:H:97:MET:O | 2.02 | 0.59 |
| 1:B:7:LYS:HG3 | 1:B:39:ALA:HA | 1.85 | 0.59 |
| 2:F:407:ILE:HG13 | 2:F:408:TYR:N | 2.18 | 0.59 |
| 1:H:15:ARG:HB2 | 1:H:332:SER:OG | 2.02 | 0.59 |
| 1:G:5:ILE:HG12 | 1:G:18:ILE:HB | 1.85 | 0.59 |
| 1:H:7:LYS:HB2 | 1:H:39:ALA:CB | 2.33 | 0.59 |
| 1:A:58:ALA:CB | 1:A:64:ALA:HB2 | 2.33 | 0.59 |
| 1:E:60:THR:HG23 | 1:E:63:GLN:H | 1.67 | 0.59 |
| 2:F:437:ASN:C | 2:F:439:LEU:H | 2.06 | 0.59 |
| 2:I:346:HIS:CD2 | 2:I:394:VAL:HB | 2.38 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:131:ALA:HA | 1:A:134:MET:HE2 | 1.83 | 0.58 |
| 1:H:67:GLN:HA | 1:H:91:LYS:CE | 2.32 | 0.58 |
| 2:C:346:HIS:HD2 | 2:C:373:LEU:HD12 | 1.69 | 0.58 |
| 1:D:252:LEU:O | 1:D:256:VAL:HG13 | 2.03 | 0.58 |
| 1:D:360:ASP:OD2 | 1:D:362:THR:HB | 2.04 | 0.58 |
| 1:D:73:LYS:O | 1:D:98:CYS:CB | 2.45 | 0.58 |
| 1:E:76:ARG:HD2 | 1:E:108:VAL:HG21 | 1.85 | 0.58 |
| 1:G:120:TYR:HE2 | 1:G:363:VAL:HG13 | 1.67 | 0.58 |
| 1:G:374:ILE:H | 1:G:374:ILE:CD1 | 2.17 | 0.58 |
| 1:B:73:LYS:HZ1 | 1:B:77:PRO:HD3 | 1.66 | 0.58 |
| 1:H:163:MET:HB2 | 1:H:170:VAL:CG2 | 2.34 | 0.58 |
| 1:H:7:LYS:HD2 | 1:H:38:GLY:O | 2.03 | 0.58 |
| 1:A:131:ALA:HA | 1:A:134:MET:CE | 2.33 | 0.58 |
| 1:D:125:MET:HE3 | 1:D:134:MET:HB2 | 1.85 | 0.58 |
| 1:E:89:LEU:N | 1:E:89:LEU:HD12 | 2.18 | 0.58 |
| 1:G:309:ILE:HG23 | 1:G:318:VAL:HG22 | 1.84 | 0.58 |
| 1:H:63:GLN:HA | 1:H:63:GLN:NE2 | 2.19 | 0.58 |
| 1:D:106:ARG:HB2 | 1:D:107:PRO:HD3 | 1.84 | 0.58 |
| 1:D:237:LYS:HA | 1:D:267:ILE:HG23 | 1.86 | 0.58 |
| 1:D:25:LYS:HB3 | 1:D:340:LEU:HD11 | 1.84 | 0.58 |
| 1:H:60:THR:O | 1:H:64:ALA:HB3 | 2.04 | 0.58 |
| 1:D:106:ARG:H | 1:D:106:ARG:HD2 | 1.67 | 0.58 |
| 1:D:308:LYS:HD2 | 1:D:309:ILE:O | 2.04 | 0.58 |
| 1:H:125:MET:HA | 1:H:125:MET:CE | 2.34 | 0.58 |
| 1:B:66:SER:HB2 | 1:B:67:GLN:OE1 | 2.04 | 0.58 |
| 1:H:113:THR:O | 1:H:372:GLY:HA2 | 2.03 | 0.58 |
| 1:B:188:ILE:HG23 | 1:B:198:VAL:HG11 | 1.86 | 0.58 |
| 1:D:99:HIS:CE1 | 1:D:123:GLU:HB3 | 2.39 | 0.58 |
| 1:E:176:LEU:HD23 | 1:E:199:MET:O | 2.02 | 0.58 |
| 2:F:446:MET:CE | 2:F:448:LEU:HD21 | 2.32 | 0.58 |
| 1:H:120:TYR:CG | 1:H:366:THR:CG2 | 2.86 | 0.58 |
| 1:E:202:ASP:OD2 | 1:E:203:VAL:N | 2.36 | 0.57 |
| 1:G:10:ARG:NH1 | 1:G:76:ARG:CZ | 2.67 | 0.57 |
| 1:E:374:ILE:N | 1:E:374:ILE:HD12 | 2.19 | 0.57 |
| 1:E:86:GLU:O | 1:E:88:ALA:N | 2.37 | 0.57 |
| 1:H:142:ASN:ND2 | 2:I:353:PRO:HD2 | 2.18 | 0.57 |
| 2:I:325:HIS:CE1 | 2:I:363:ALA:HA | 2.39 | 0.57 |
| 2:C:371:PHE:HB2 | 2:C:376:ILE:HG12 | 1.85 | 0.57 |
| 1:D:293:LEU:HD21 | 1:D:323:VAL:HG21 | 1.86 | 0.57 |
| 1:E:106:ARG:HB3 | 1:E:107:PRO:HD3 | 1.86 | 0.57 |
| 1:E:183:ALA:HB3 | 1:E:264:THR:CG2 | 2.34 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:313:VAL:HB | 2:I:388:VAL:HG22 | 1.86 | 0.57 |
| 1:B:100:LEU:C | 1:B:102:ALA:N | 2.55 | 0.57 |
| 1:D:357:LYS:O | 1:D:359:GLU:N | 2.37 | 0.57 |
| 1:G:180:VAL:HG21 | 1:G:211:VAL:HG21 | 1.86 | 0.57 |
| 1:H:124:LEU:HD13 | 1:H:365:GLY:O | 2.04 | 0.57 |
| 1:H:67:GLN:H | 1:H:67:GLN:CD | 2.07 | 0.57 |
| 1:D:179:GLY:HA2 | 4:D:400:NAD:H8A | 1.85 | 0.57 |
| 1:E:183:ALA:HB3 | 1:E:264:THR:HG21 | 1.85 | 0.57 |
| 1:G:160:PHE:N | 1:G:161:PRO:HD2 | 2.19 | 0.57 |
| 1:G:34:ILE:CD1 | 1:G:56:THR:HB | 2.34 | 0.57 |
| 1:G:10:ARG:NH1 | 1:G:76:ARG:NH2 | 2.51 | 0.57 |
| 1:B:136:ILE:HG13 | 1:B:137:LEU:N | 2.18 | 0.57 |
| 1:D:60:THR:OG1 | 1:D:63:GLN:HG2 | 2.05 | 0.57 |
| 1:D:329:ALA:CB | 1:E:158:ARG:HG3 | 2.33 | 0.57 |
| 1:E:16:VAL:O | 1:E:18:ILE:N | 2.38 | 0.57 |
| 1:H:16:VAL:HG22 | 1:H:17:ALA:H | 1.69 | 0.57 |
| 1:H:309:ILE:HG12 | 1:H:318:VAL:HG13 | 1.85 | 0.57 |
| 1:B:67:GLN:O | 1:B:67:GLN:HG2 | 2.05 | 0.57 |
| 1:D:151:ASP:CG | 1:D:326:ARG:HH21 | 2.08 | 0.57 |
| 1:G:273:PRO:HG3 | 4:G:400:NAD:C2A | 2.34 | 0.57 |
| 1:A:97:MET:HE3 | 1:A:343:LEU:HD12 | 1.85 | 0.57 |
| 1:D:4:ALA:HB1 | 1:D:34:ILE:O | 2.04 | 0.57 |
| 1:E:127:ARG:NH2 | 1:E:132:GLN:HG3 | 2.20 | 0.57 |
| 1:E:370:ARG:HH21 | 1:E:375:VAL:HG11 | 1.70 | 0.57 |
| 2:F:373:LEU:HD23 | 2:F:373:LEU:C | 2.24 | 0.57 |
| 1:G:282:THR:HG22 | 1:G:313:HIS:CD2 | 2.39 | 0.57 |
| 1:B:242:GLU:O | 1:B:245:LYS:HB3 | 2.05 | 0.57 |
| 1:D:326:ARG:HG2 | 1:D:326:ARG:NH1 | 2.20 | 0.57 |
| 1:H:346:HIS:NE2 | 1:H:362:THR:HG21 | 2.20 | 0.57 |
| 1:A:69:ASP:O | 1:A:95:VAL:HG23 | 2.05 | 0.57 |
| 1:B:18:ILE:HG12 | 1:B:19:SER:N | 2.19 | 0.57 |
| 1:B:62:ALA:HA | 1:B:89:LEU:HD22 | 1.87 | 0.57 |
| 2:C:414:ASP:HB3 | 2:C:417:LYS:HE3 | 1.87 | 0.57 |
| 1:D:221:VAL:CG1 | 1:D:250:ALA:HB3 | 2.34 | 0.57 |
| 2:F:437:ASN:HB3 | 2:F:440:PHE:CE2 | 2.40 | 0.57 |
| 1:H:202:ASP:CG | 4:H:400:NAD:H8A | 2.25 | 0.57 |
| 1:E:136:ILE:HD12 | 1:E:137:LEU:HD12 | 1.87 | 0.56 |
| 1:E:199:MET:CG | 1:E:219:ILE:HD11 | 2.28 | 0.56 |
| 1:H:282:THR:HG22 | 1:H:313:HIS:CD2 | 2.39 | 0.56 |
| 1:B:266:LEU:H | 4:B:400:NAD:H52A | 1.70 | 0.56 |
| 1:B:5:ILE:HG13 | 1:B:72:TRP:HB2 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:222:ASP:HB2 | 1:D:227:LYS:HE2 | 1.86 | 0.56 |
| 1:G:200:ALA:HB3 | 1:G:211:VAL:HG11 | 1.88 | 0.56 |
| 1:G:243:PHE:O | 1:G:245:LYS:N | 2.38 | 0.56 |
| 1:H:2:LYS:O | 1:H:69:ASP:HB2 | 2.04 | 0.56 |
| 2:I:310:VAL:HG22 | 2:I:385:VAL:HB | 1.86 | 0.56 |
| 1:A:276:ILE:HA | 1:A:280:MET:HE1 | 1.87 | 0.56 |
| 2:F:450:GLY:HA3 | 2:F:455:MET:CE | 2.35 | 0.56 |
| 1:A:178:PHE:HB3 | 1:A:275:LEU:HD13 | 1.87 | 0.56 |
| 1:D:175:VAL:HG12 | 1:D:176:LEU:N | 2.17 | 0.56 |
| 1:E:125:MET:CE | 1:E:134:MET:HB2 | 2.34 | 0.56 |
| 1:H:243:PHE:C | 1:H:245:LYS:H | 2.08 | 0.56 |
| 1:H:312:LYS:HG3 | 1:H:313:HIS:CD2 | 2.40 | 0.56 |
| 1:H:70:VAL:HG23 | 1:H:95:VAL:HB | 1.87 | 0.56 |
| 2:I:302:PHE:O | 2:I:306:ASN:HB2 | 2.06 | 0.56 |
| 2:I:380:PHE:HZ | 2:I:413:LEU:HD22 | 1.70 | 0.56 |
| 2:I:440:PHE:HD2 | 2:I:447:MET:SD | 2.28 | 0.56 |
| 2:I:439:LEU:C | 2:I:441:PHE:H | 2.08 | 0.56 |
| 1:A:80:ALA:HA | 1:A:85:ASP:HB2 | 1.87 | 0.56 |
| 1:B:96:LEU:HD23 | 1:B:112:LEU:CD2 | 2.36 | 0.56 |
| 1:D:50:LEU:C | 1:D:55:ALA:HB3 | 2.25 | 0.56 |
| 1:E:143:LEU:HD12 | 1:E:331:ALA:HB2 | 1.86 | 0.56 |
| 1:E:250:ALA:O | 1:E:253:LYS:HB3 | 2.05 | 0.56 |
| 1:H:73:LYS:HD2 | 1:H:75:GLN:O | 2.05 | 0.56 |
| 2:I:304:MET:C | 2:I:306:ASN:H | 2.05 | 0.56 |
| 1:B:137:LEU:H | 1:B:137:LEU:HD12 | 1.71 | 0.56 |
| 1:B:190:THR:HA | 1:B:193:ARG:HD2 | 1.87 | 0.56 |
| 1:D:208:LYS:HD2 | 1:D:209:GLU:N | 2.20 | 0.56 |
| 1:D:281:VAL:O | 1:D:281:VAL:HG12 | 2.04 | 0.56 |
| 1:E:264:THR:O | 1:E:264:THR:HG22 | 2.04 | 0.56 |
| 1:E:362:THR:CG2 | 1:E:363:VAL:H | 2.18 | 0.56 |
| 1:G:118:THR:CB | 1:G:370:ARG:HA | 2.35 | 0.56 |
| 1:H:124:LEU:O | 1:H:125:MET:C | 2.44 | 0.56 |
| 1:D:351:THR:O | 1:D:353:THR:HG22 | 2.06 | 0.56 |
| 1:D:35:VAL:HG21 | 1:D:50:LEU:HD23 | 1.87 | 0.56 |
| 1:E:128:ILE:HG13 | 1:E:128:ILE:O | 2.04 | 0.56 |
| 1:G:199:MET:CE | 1:G:217:LYS:HB2 | 2.35 | 0.56 |
| 1:H:116:LYS:HA | 1:H:372:GLY:H | 1.69 | 0.56 |
| 1:H:265:ALA:HB3 | 1:H:300:ASN:OD1 | 2.04 | 0.56 |
| 1:B:73:LYS:HZ1 | 1:B:77:PRO:CD | 2.18 | 0.56 |
| 1:D:342:PHE:CE1 | 1:D:362:THR:O | 2.58 | 0.56 |
| 1:E:160:PHE:CZ | 1:E:260:ILE:HD12 | 2.40 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:7:LYS:HB2 | 1:E:39:ALA:CB | 2.36 | 0.56 |
| 1:G:342:PHE:HE1 | 1:G:362:THR:HG23 | 1.71 | 0.56 |
| 2:C:303:ILE:HG12 | 1:H:169:THR:HG21 | 1.87 | 0.56 |
| 1:H:179:GLY:O | 1:H:181:GLY:N | 2.39 | 0.56 |
| 1:H:182:VAL:HG13 | 1:H:183:ALA:H | 1.70 | 0.56 |
| 1:B:354:LEU:HD11 | 1:B:356:MET:SD | 2.46 | 0.56 |
| 1:D:68:ALA:O | 1:D:91:LYS:CG | 2.54 | 0.56 |
| 1:G:274:VAL:HG13 | 1:G:302:PRO:HD3 | 1.88 | 0.56 |
| 1:H:202:ASP:HA | 4:H:400:NAD:C8A | 2.35 | 0.56 |
| 2:I:393:ASP:OD1 | 2:I:431:GLY:HA3 | 2.05 | 0.56 |
| 1:D:285:LYS:HZ1 | 1:E:44:SER:HB3 | 1.70 | 0.56 |
| 1:G:281:VAL:O | 1:G:281:VAL:HG12 | 2.06 | 0.56 |
| 2:I:452:ALA:H | 6:I:500:NDP:C2A | 2.19 | 0.56 |
| 1:B:87:VAL:HG13 | 1:B:88:ALA:N | 2.21 | 0.56 |
| 1:B:66:SER:O | 1:B:91:LYS:HB2 | 2.06 | 0.56 |
| 1:D:221:VAL:HG21 | 1:D:247:GLN:HA | 1.88 | 0.56 |
| 2:F:410:MET:HG3 | 2:F:411:PRO:HD2 | 1.88 | 0.56 |
| 1:H:72:TRP:CE3 | 1:H:339:LEU:HB3 | 2.40 | 0.56 |
| 1:A:270:LYS:CB | 1:A:271:PRO:CD | 2.78 | 0.55 |
| 1:B:291:ILE:HD13 | 1:B:318:VAL:HB | 1.88 | 0.55 |
| 1:D:2:LYS:HD2 | 1:D:32:GLU:CB | 2.35 | 0.55 |
| 1:G:180:VAL:HG12 | 1:G:185:LEU:HG | 1.89 | 0.55 |
| 1:G:255:LEU:HD21 | 1:G:276:ILE:HD11 | 1.87 | 0.55 |
| 1:H:18:ILE:HG12 | 1:H:19:SER:N | 2.21 | 0.55 |
| 2:I:451:ASP:O | 2:I:452:ALA:C | 2.44 | 0.55 |
| 2:C:346:HIS:CD2 | 2:C:373:LEU:HD12 | 2.41 | 0.55 |
| 1:G:164:MET:HE1 | 2:I:370:VAL:HG12 | 1.88 | 0.55 |
| 2:I:298:GLU:N | 2:I:298:GLU:OE2 | 2.37 | 0.55 |
| 1:G:164:MET:CE | 2:I:370:VAL:HG12 | 2.36 | 0.55 |
| 1:A:2:LYS:HB3 | 1:A:68:ALA:HA | 1.88 | 0.55 |
| 1:D:24:LYS:NZ | 1:D:24:LYS:HB3 | 2.21 | 0.55 |
| 1:G:344:THR:OG1 | 1:G:345:PRO:HD3 | 2.06 | 0.55 |
| 1:H:74:VAL:CG2 | 1:H:75:GLN:H | 2.12 | 0.55 |
| 1:G:376:HIS:CD2 | 1:G:378:ALA:HB2 | 2.40 | 0.55 |
| 1:H:295:VAL:O | 1:H:295:VAL:HG22 | 2.06 | 0.55 |
| 1:H:47:ASP:CB | 1:H:57:ILE:HD11 | 2.35 | 0.55 |
| 1:A:149:VAL:HG11 | 1:A:190:THR:HG22 | 1.89 | 0.55 |
| 1:B:76:ARG:HB3 | 1:B:100:LEU:HA | 1.88 | 0.55 |
| 1:H:92:GLU:HB2 | 1:H:116:LYS:NZ | 2.21 | 0.55 |
| 1:B:120:TYR:HB3 | 1:B:366:THR:HG21 | 1.88 | 0.55 |
| 1:H:181:GLY:O | 1:H:185:LEU:HD12 | 2.06 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:33:VAL:O | 1:H:34:ILE:HD12 | 2.06 | 0.55 |
| 2:F:455:MET:O | 2:F:459:ILE:HG13 | 2.06 | 0.55 |
| 1:D:223:ASP:HB3 | 1:D:228:THR:HG21 | 1.89 | 0.55 |
| 1:E:2:LYS:HD3 | 1:E:32:GLU:CB | 2.36 | 0.55 |
| 1:G:326:ARG:NH2 | 1:G:326:ARG:HG2 | 2.22 | 0.55 |
| 1:H:156:PHE:CE2 | 1:H:158:ARG:HB2 | 2.41 | 0.55 |
| 1:G:326:ARG:O | 3:O:2:FRU:O4 | 2.25 | 0.55 |
| 1:A:194:LEU:HD21 | 1:B:194:LEU:HG | 1.88 | 0.55 |
| 1:D:34:ILE:HG23 | 1:D:56:THR:O | 2.07 | 0.55 |
| 1:D:26:LEU:HD11 | 1:D:72:TRP:CZ3 | 2.42 | 0.55 |
| 1:G:106:ARG:N | 1:G:107:PRO:CD | 2.69 | 0.55 |
| 1:G:111:ALA:HA | 1:G:114:LYS:HG3 | 1.88 | 0.55 |
| 1:H:8:GLU:H | 1:H:8:GLU:CD | 2.09 | 0.55 |
| 1:E:108:VAL:O | 1:E:112:LEU:HD12 | 2.07 | 0.55 |
| 1:G:280:MET:C | 1:G:282:THR:H | 2.10 | 0.55 |
| 1:E:284:MET:HE2 | 1:E:290:ILE:HD11 | 1.89 | 0.54 |
| 1:G:23:VAL:HG11 | 1:G:55:ALA:HB2 | 1.89 | 0.54 |
| 2:C:315:GLY:HA3 | 2:C:391:ALA:HB2 | 1.89 | 0.54 |
| 1:D:18:ILE:C | 1:D:18:ILE:HD13 | 2.28 | 0.54 |
| 1:D:29:LEU:HD22 | 1:D:347:VAL:HG11 | 1.90 | 0.54 |
| 1:D:344:THR:HA | 1:D:347:VAL:HG23 | 1.88 | 0.54 |
| 1:D:357:LYS:C | 1:D:359:GLU:H | 2.10 | 0.54 |
| 1:E:9:ARG:O | 1:E:10:ARG:C | 2.45 | 0.54 |
| 2:I:305:LYS:HB2 | 2:I:337:GLU:OE1 | 2.06 | 0.54 |
| 2:I:323:ALA:O | 2:I:326:ALA:N | 2.35 | 0.54 |
| 2:I:371:PHE:HB2 | 2:I:376:ILE:HB | 1.89 | 0.54 |
| 2:I:403:PRO:HG3 | 2:I:408:TYR:CZ | 2.42 | 0.54 |
| 1:A:375:VAL:CG2 | 1:A:375:VAL:O | 2.55 | 0.54 |
| 2:C:324:GLN:HB2 | 2:C:363:ALA:HB2 | 1.89 | 0.54 |
| 1:D:32:GLU:O | 1:D:34:ILE:HD12 | 2.07 | 0.54 |
| 1:E:1:MET:CG | 1:E:352:LYS:O | 2.55 | 0.54 |
| 1:G:180:VAL:HG21 | 1:G:211:VAL:CG2 | 2.36 | 0.54 |
| 1:G:182:VAL:HG12 | 4:G:400:NAD:O1N | 2.07 | 0.54 |
| 1:H:25:LYS:CE | 1:H:25:LYS:HA | 2.37 | 0.54 |
| 1:H:277:THR:OG1 | 1:H:280:MET:HG3 | 2.08 | 0.54 |
| 1:H:8:GLU:HG3 | 1:H:73:LYS:HE2 | 1.89 | 0.54 |
| 2:I:422:LEU:HD12 | 2:I:446:MET:HB3 | 1.88 | 0.54 |
| 2:C:399:ALA:HA | 2:C:408:TYR:HA | 1.90 | 0.54 |
| 1:H:15:ARG:CG | 1:H:15:ARG:HH21 | 2.19 | 0.54 |
| 1:H:300:ASN:N | 1:H:300:ASN:HD22 | 2.06 | 0.54 |
| 2:I:330:MET:HG3 | 2:I:463:MET:CE | 2.36 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:180:VAL:HG21 | 1:A:207:THR:HG21 | 1.88 | 0.54 |
| 1:A:277:THR:O | 1:A:279:GLU:N | 2.41 | 0.54 |
| 1:A:380:THR:HG22 | 1:A:380:THR:O | 2.08 | 0.54 |
| 1:B:118:THR:HA | 1:B:370:ARG:HA | 1.90 | 0.54 |
| 1:D:164:MET:HG3 | 2:F:345:ILE:HG21 | 1.89 | 0.54 |
| 1:D:205:ALA:C | 1:D:207:THR:H | 2.11 | 0.54 |
| 1:D:2:LYS:NZ | 1:D:32:GLU:HG2 | 2.23 | 0.54 |
| 1:E:303:LEU:H | 1:E:303:LEU:HD12 | 1.73 | 0.54 |
| 1:H:202:ASP:CB | 1:H:207:THR:HG21 | 2.38 | 0.54 |
| 2:I:422:LEU:HG | 2:I:448:LEU:CD1 | 2.35 | 0.54 |
| 1:A:147:ARG:HG3 | 1:A:151:ASP:OD2 | 2.07 | 0.54 |
| 1:B:370:ARG:HH12 | 1:B:375:VAL:HG11 | 1.72 | 0.54 |
| 1:D:10:ARG:HG3 | 1:D:10:ARG:NH2 | 2.21 | 0.54 |
| 1:E:121:ALA:HB1 | 1:E:123:GLU:CD | 2.28 | 0.54 |
| 1:D:164:MET:HG2 | 2:F:357:ASN:ND2 | 2.22 | 0.54 |
| 1:A:21:GLU:CD | 1:A:21:GLU:H | 2.10 | 0.54 |
| 1:D:294:ALA:O | 1:D:299:GLY:N | 2.41 | 0.54 |
| 1:D:4:ALA:HB2 | 1:D:34:ILE:HB | 1.90 | 0.54 |
| 1:A:97:MET:CE | 1:A:343:LEU:HD12 | 2.38 | 0.54 |
| 2:C:330:MET:HG2 | 2:C:334:LEU:CD2 | 2.38 | 0.54 |
| 1:D:193:ARG:HB3 | 1:E:193:ARG:O | 2.07 | 0.54 |
| 2:I:309:LYS:O | 2:I:384:ASP:HB2 | 2.08 | 0.54 |
| 1:E:177:VAL:CG2 | 1:E:188:ILE:HD13 | 2.38 | 0.54 |
| 1:H:291:ILE:HD12 | 1:H:291:ILE:H | 1.73 | 0.54 |
| 1:A:360:ASP:OD2 | 1:A:362:THR:HB | 2.08 | 0.54 |
| 1:B:204:ARG:HH21 | 1:B:207:THR:HG22 | 1.73 | 0.54 |
| 1:B:379:LEU:N | 1:B:379:LEU:HD12 | 2.23 | 0.54 |
| 1:B:5:ILE:HG23 | 1:B:17:ALA:HB3 | 1.89 | 0.54 |
| 2:C:321:ALA:O | 2:C:322:GLN:HB2 | 2.08 | 0.54 |
| 1:D:270:LYS:HB3 | 1:D:271:PRO:CD | 2.36 | 0.54 |
| 1:E:369:THR:O | 1:E:369:THR:HG23 | 2.06 | 0.54 |
| 1:E:78:MET:HG3 | 1:E:86:GLU:OE1 | 2.08 | 0.54 |
| 2:F:348:VAL:HG21 | 2:F:410:MET:CE | 2.37 | 0.54 |
| 1:A:354:LEU:HD11 | 1:A:356:MET:HE1 | 1.90 | 0.53 |
| 1:A:80:ALA:CA | 1:A:85:ASP:HB2 | 2.38 | 0.53 |
| 1:B:128:ILE:HG12 | 1:B:131:ALA:CB | 2.37 | 0.53 |
| 1:B:244:ARG:HA | 1:B:247:GLN:HB3 | 1.90 | 0.53 |
| 1:G:62:ALA:HB2 | 1:G:89:LEU:CD2 | 2.37 | 0.53 |
| 1:H:203:VAL:HG12 | 1:H:243:PHE:CZ | 2.44 | 0.53 |
| 1:B:199:MET:HE2 | 1:B:217:LYS:HB3 | 1.89 | 0.53 |
| 1:E:108:VAL:O | 1:E:111:ALA:HB3 | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:86:GLU:C | 1:E:88:ALA:N | 2.61 | 0.53 |
| 1:H:7:LYS:HB2 | 1:H:39:ALA:CA | 2.38 | 0.53 |
| 2:I:395:THR:HB | 2:I:415:VAL:HG21 | 1.89 | 0.53 |
| 1:A:140:GLN:C | 1:A:142:ASN:H | 2.11 | 0.53 |
| 1:B:106:ARG:HB3 | 1:B:107:PRO:HD3 | 1.90 | 0.53 |
| 2:C:379:SER:O | 2:C:382:THR:N | 2.41 | 0.53 |
| 1:E:58:ALA:CB | 1:E:64:ALA:HA | 2.38 | 0.53 |
| 1:D:164:MET:CG | 2:F:357:ASN:HD21 | 2.21 | 0.53 |
| 1:H:214:LEU:HD11 | 2:I:352:MET:SD | 2.49 | 0.53 |
| 1:B:100:LEU:O | 1:B:102:ALA:N | 2.42 | 0.53 |
| 2:C:321:ALA:HB3 | 2:C:452:ALA:HB3 | 1.90 | 0.53 |
| 1:A:4:ALA:HB1 | 1:A:64:ALA:O | 2.08 | 0.53 |
| 1:B:120:TYR:HB3 | 1:B:366:THR:CG2 | 2.39 | 0.53 |
| 1:B:137:LEU:N | 1:B:137:LEU:HD12 | 2.24 | 0.53 |
| 1:D:293:LEU:HD23 | 1:D:323:VAL:HG21 | 1.91 | 0.53 |
| 1:G:284:MET:HG3 | 1:G:315:VAL:HG21 | 1.90 | 0.53 |
| 1:A:265:ALA:CB | 1:A:275:LEU:HD11 | 2.39 | 0.53 |
| 1:D:6:PRO:HD2 | 1:D:72:TRP:O | 2.08 | 0.53 |
| 1:E:5:ILE:HD12 | 1:E:5:ILE:N | 2.24 | 0.53 |
| 1:G:62:ALA:CA | 1:G:89:LEU:HD23 | 2.38 | 0.53 |
| 1:H:112:LEU:CD1 | 1:H:112:LEU:N | 2.71 | 0.53 |
| 1:H:7:LYS:O | 1:H:9:ARG:HD2 | 2.09 | 0.53 |
| 1:A:113:THR:HG22 | 1:A:114:LYS:N | 2.24 | 0.53 |
| 1:A:327:VAL:HG12 | 1:A:327:VAL:O | 2.08 | 0.53 |
| 1:B:190:THR:HA | 1:B:193:ARG:CD | 2.39 | 0.53 |
| 1:D:8:GLU:HB3 | 1:D:13:GLU:HB3 | 1.91 | 0.53 |
| 1:E:344:THR:O | 1:E:347:VAL:HG12 | 2.08 | 0.53 |
| 2:F:346:HIS:HB3 | 2:F:349:ALA:HB2 | 1.90 | 0.53 |
| 1:G:203:VAL:CG2 | 1:G:204:ARG:H | 2.18 | 0.53 |
| 1:G:95:VAL:HG22 | 1:G:118:THR:HG23 | 1.90 | 0.53 |
| 1:H:263:THR:OG1 | 1:H:292:ASP:HA | 2.08 | 0.53 |
| 1:H:295:VAL:CG2 | 1:H:304:SER:HB2 | 2.39 | 0.53 |
| 1:H:38:GLY:H | 1:H:47:ASP:CG | 2.12 | 0.53 |
| 1:H:203:VAL:H | 4:H:400:NAD:C8A | 2.21 | 0.53 |
| 2:I:463:MET:O | 2:I:464:ASN:HB2 | 2.09 | 0.53 |
| 1:A:327:VAL:HG12 | 1:A:330:ASP:HB2 | 1.91 | 0.53 |
| 2:C:420:THR:HB | 1:H:162:MET:HE1 | 1.91 | 0.53 |
| 1:D:202:ASP:OD1 | 1:D:203:VAL:N | 2.41 | 0.53 |
| 1:E:214:LEU:HD21 | 2:F:355:HIS:CD2 | 2.44 | 0.53 |
| 2:F:374:GLU:H | 2:F:374:GLU:CD | 2.11 | 0.53 |
| 1:G:128:ILE:HD12 | 1:G:129:SER:N | 2.23 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:62:ALA:CB | 1:G:89:LEU:HD23 | 2.37 | 0.53 |
| 1:D:123:GLU:HG2 | 1:D:124:LEU:HD13 | 1.89 | 0.53 |
| 2:F:445:THR:HG22 | 2:F:446:MET:N | 2.24 | 0.53 |
| 1:G:22:VAL:HG13 | 1:G:340:LEU:HD12 | 1.91 | 0.53 |
| 2:I:331:ALA:O | 2:I:335:LYS:HD3 | 2.09 | 0.53 |
| 1:B:100:LEU:C | 1:B:102:ALA:H | 2.13 | 0.53 |
| 1:B:272:ALA:HB1 | 1:B:300:ASN:HD21 | 1.74 | 0.53 |
| 1:B:71:VAL:HG12 | 1:B:96:LEU:HA | 1.90 | 0.53 |
| 2:C:392:ASN:HB3 | 6:C:500:NDP:O1A | 2.09 | 0.53 |
| 1:D:122:MET:C | 1:D:124:LEU:H | 2.11 | 0.53 |
| 1:D:244:ARG:N | 1:D:244:ARG:HD3 | 2.24 | 0.53 |
| 1:D:8:GLU:OE1 | 1:D:75:GLN:N | 2.40 | 0.53 |
| 1:E:80:ALA:HA | 1:E:85:ASP:HB2 | 1.91 | 0.53 |
| 1:G:194:LEU:HD11 | 1:H:194:LEU:HG | 1.91 | 0.53 |
| 1:H:176:LEU:HA | 1:H:199:MET:O | 2.09 | 0.53 |
| 2:I:451:ASP:H | 2:I:454:LYS:HE2 | 1.73 | 0.53 |
| 1:A:277:THR:N | 1:A:280:MET:HE3 | 2.24 | 0.52 |
| 1:B:265:ALA:HB3 | 1:B:275:LEU:HD11 | 1.90 | 0.52 |
| 1:B:5:ILE:HD13 | 1:B:18:ILE:HD12 | 1.91 | 0.52 |
| 1:D:267:ILE:O | 1:D:268:PRO:O | 2.27 | 0.52 |
| 1:E:3:ILE:O | 1:E:3:ILE:HG23 | 2.08 | 0.52 |
| 2:F:416:GLU:HG3 | 2:F:439:LEU:HD11 | 1.91 | 0.52 |
| 1:G:153:ALA:HA | 1:G:160:PHE:CE1 | 2.44 | 0.52 |
| 1:B:1:MET:HE2 | 1:B:353:THR:HA | 1.91 | 0.52 |
| 1:E:2:LYS:HD3 | 1:E:32:GLU:HB2 | 1.90 | 0.52 |
| 1:E:312:LYS:O | 1:E:313:HIS:HB2 | 2.09 | 0.52 |
| 1:G:78:MET:N | 1:G:86:GLU:HB2 | 2.23 | 0.52 |
| 2:C:455:MET:O | 2:C:459:ILE:HG13 | 2.10 | 0.52 |
| 1:D:105:ASN:O | 1:D:108:VAL:HG12 | 2.09 | 0.52 |
| 1:E:178:PHE:CE1 | 1:E:276:ILE:HD11 | 2.44 | 0.52 |
| 1:G:177:VAL:HG11 | 1:G:188:ILE:HG12 | 1.91 | 0.52 |
| 1:H:103:LEU:HD12 | 1:H:103:LEU:N | 2.23 | 0.52 |
| 1:H:330:ASP:C | 1:H:333:PRO:HD2 | 2.29 | 0.52 |
| 1:H:85:ASP:OD2 | 1:H:88:ALA:HB3 | 2.09 | 0.52 |
| 1:B:273:PRO:HG3 | 4:B:400:NAD:N6A | 2.24 | 0.52 |
| 1:D:265:ALA:HB3 | 1:D:300:ASN:ND2 | 2.24 | 0.52 |
| 1:D:327:VAL:O | 1:D:329:ALA:N | 2.43 | 0.52 |
| 1:D:342:PHE:C | 1:D:345:PRO:HD2 | 2.29 | 0.52 |
| 1:D:3:ILE:HG22 | 1:D:31:PHE:HB3 | 1.90 | 0.52 |
| 1:H:294:ALA:C | 1:H:296:GLU:H | 2.12 | 0.52 |
| 1:B:73:LYS:HZ1 | 1:B:77:PRO:N | 2.07 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:308:LYS:HG2 | 1:D:309:ILE:N | 2.23 | 0.52 |
| 1:E:136:ILE:C | 1:E:136:ILE:HD12 | 2.30 | 0.52 |
| 1:E:252:LEU:O | 1:E:256:VAL:HG22 | 2.10 | 0.52 |
| 2:F:374:GLU:OE1 | 2:F:374:GLU:N | 2.42 | 0.52 |
| 1:H:122:MET:C | 1:H:124:LEU:H | 2.13 | 0.52 |
| 1:B:278:GLU:O | 1:B:281:VAL:HG22 | 2.10 | 0.52 |
| 1:E:180:VAL:O | 1:E:180:VAL:HG12 | 2.09 | 0.52 |
| 1:E:291:ILE:HD13 | 1:E:318:VAL:HB | 1.91 | 0.52 |
| 1:E:58:ALA:HB3 | 1:E:64:ALA:HB2 | 1.90 | 0.52 |
| 2:F:450:GLY:HA3 | 2:F:455:MET:HE3 | 1.92 | 0.52 |
| 1:G:370:ARG:O | 1:G:371:ASP:C | 2.46 | 0.52 |
| 1:A:46:THR:HG23 | 1:A:49:ALA:CB | 2.30 | 0.52 |
| 1:A:85:ASP:OD2 | 1:A:88:ALA:HB2 | 2.09 | 0.52 |
| 2:C:456:THR:O | 2:C:460:VAL:HG23 | 2.10 | 0.52 |
| 1:E:264:THR:CG2 | 1:E:264:THR:O | 2.57 | 0.52 |
| 1:H:277:THR:O | 1:H:281:VAL:HG13 | 2.10 | 0.52 |
| 1:H:340:LEU:CD1 | 1:H:344:THR:HG23 | 2.38 | 0.52 |
| 2:I:319:ALA:HA | 2:I:359:LEU:HD13 | 1.92 | 0.52 |
| 2:I:333:VAL:O | 2:I:336:LYS:HG2 | 2.09 | 0.52 |
| 1:A:207:THR:HG22 | 1:A:218:PHE:CE1 | 2.42 | 0.52 |
| 1:A:355:VAL:HG13 | 1:A:355:VAL:O | 2.10 | 0.52 |
| 1:B:368:VAL:CG1 | 1:B:379:LEU:HD22 | 2.40 | 0.52 |
| 1:B:78:MET:HG3 | 1:B:86:GLU:OE1 | 2.10 | 0.52 |
| 1:E:260:ILE:HG12 | 1:E:289:VAL:CG1 | 2.40 | 0.52 |
| 2:F:459:ILE:O | 2:F:463:MET:HG3 | 2.10 | 0.52 |
| 1:G:7:LYS:HG3 | 1:G:39:ALA:HA | 1.92 | 0.52 |
| 1:H:98:CYS:N | 1:H:122:MET:HE1 | 2.25 | 0.52 |
| 2:I:324:GLN:HG2 | 2:I:325:HIS:H | 1.75 | 0.52 |
| 1:A:275:LEU:O | 1:A:280:MET:HE1 | 2.10 | 0.52 |
| 1:A:370:ARG:HD2 | 1:A:375:VAL:HG11 | 1.92 | 0.52 |
| 2:C:346:HIS:CD2 | 2:C:347:PRO:HD2 | 2.45 | 0.52 |
| 1:D:203:VAL:HG23 | 1:D:204:ARG:HG3 | 1.90 | 0.52 |
| 1:D:18:ILE:HD12 | 1:D:50:LEU:HD23 | 1.90 | 0.52 |
| 1:E:22:VAL:HG13 | 1:E:340:LEU:HD22 | 1.92 | 0.52 |
| 1:E:72:TRP:NE1 | 1:E:97:MET:CE | 2.73 | 0.52 |
| 1:H:147:ARG:HG3 | 1:H:327:VAL:HG22 | 1.92 | 0.52 |
| 1:H:203:VAL:HG23 | 1:H:204:ARG:H | 1.75 | 0.52 |
| 1:H:203:VAL:HG23 | 1:H:204:ARG:N | 2.24 | 0.52 |
| 1:B:184:GLY:O | 1:B:187:ALA:HB3 | 2.10 | 0.52 |
| 1:B:242:GLU:HA | 1:B:242:GLU:OE2 | 2.10 | 0.52 |
| 2:C:309:LYS:HZ1 | 2:C:382:THR:HB | 1.74 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:323:VAL:HB | 1:D:324:PRO:HD3 | 1.92 | 0.52 |
| 1:E:207:THR:HG22 | 1:E:218:PHE:CE2 | 2.44 | 0.52 |
| 1:G:132:GLN:HG2 | 4:G:400:NAD:O7N | 2.10 | 0.52 |
| 2:I:336:LYS:HG3 | 2:I:337:GLU:H | 1.75 | 0.52 |
| 2:I:453:LYS:HE2 | 2:I:457:GLU:CD | 2.31 | 0.52 |
| 1:A:115:ARG:O | 1:A:116:LYS:HB2 | 2.10 | 0.51 |
| 1:A:277:THR:C | 1:A:279:GLU:N | 2.64 | 0.51 |
| 1:A:262:ILE:HD13 | 1:A:291:ILE:HB | 1.91 | 0.51 |
| 1:A:305:GLU:HB3 | 1:A:308:LYS:HD2 | 1.92 | 0.51 |
| 1:A:374:ILE:HB | 1:A:380:THR:HG21 | 1.92 | 0.51 |
| 1:B:370:ARG:NH1 | 1:B:375:VAL:HG11 | 2.24 | 0.51 |
| 1:E:120:TYR:OH | 1:E:356:MET:HG3 | 2.10 | 0.51 |
| 2:F:424:ILE:O | 2:F:424:ILE:HG22 | 2.09 | 0.51 |
| 1:H:180:VAL:O | 1:H:180:VAL:HG12 | 2.10 | 0.51 |
| 1:H:37:GLN:HA | 1:H:57:ILE:CG2 | 2.40 | 0.51 |
| 2:I:317:GLY:HA3 | 2:I:390:GLY:HA3 | 1.92 | 0.51 |
| 1:D:282:THR:O | 1:D:282:THR:HG22 | 2.11 | 0.51 |
| 1:E:320:HIS:CE1 | 1:E:326:ARG:NH2 | 2.79 | 0.51 |
| 1:G:203:VAL:CG2 | 1:G:204:ARG:N | 2.69 | 0.51 |
| 1:A:222:ASP:OD2 | 1:A:222:ASP:N | 2.44 | 0.51 |
| 1:A:80:ALA:HB2 | 1:A:85:ASP:HB2 | 1.91 | 0.51 |
| 1:B:339:LEU:O | 1:B:341:ASN:N | 2.44 | 0.51 |
| 1:D:68:ALA:N | 1:D:91:LYS:HD2 | 2.25 | 0.51 |
| 1:E:252:LEU:HG | 1:E:252:LEU:O | 2.08 | 0.51 |
| 2:F:407:ILE:O | 2:F:408:TYR:C | 2.49 | 0.51 |
| 1:G:208:LYS:O | 1:G:212:GLU:HG3 | 2.09 | 0.51 |
| 1:H:103:LEU:HD11 | 1:H:124:LEU:HD21 | 1.91 | 0.51 |
| 1:H:125:MET:HA | 1:H:125:MET:HE2 | 1.92 | 0.51 |
| 1:H:128:ILE:O | 1:H:132:GLN:CG | 2.58 | 0.51 |
| 1:H:96:LEU:HD23 | 1:H:96:LEU:C | 2.30 | 0.51 |
| 2:I:304:MET:C | 2:I:306:ASN:N | 2.63 | 0.51 |
| 2:I:380:PHE:CZ | 2:I:413:LEU:HD22 | 2.44 | 0.51 |
| 2:I:432:TYR:C | 2:I:434:GLY:N | 2.64 | 0.51 |
| 1:D:285:LYS:NZ | 1:E:44:SER:HB3 | 2.26 | 0.51 |
| 1:D:3:ILE:CB | 1:D:70:VAL:HG23 | 2.41 | 0.51 |
| 1:D:7:LYS:O | 1:D:9:ARG:HG3 | 2.11 | 0.51 |
| 1:E:125:MET:CE | 1:E:342:PHE:HD2 | 2.20 | 0.51 |
| 1:E:19:SER:O | 1:E:23:VAL:HG23 | 2.09 | 0.51 |
| 1:B:244:ARG:CD | 1:B:244:ARG:H | 2.24 | 0.51 |
| 1:E:266:LEU:HD13 | 1:E:294:ALA:HA | 1.92 | 0.51 |
| 1:G:176:LEU:HD23 | 1:G:199:MET:O | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:211:VAL:HG12 | 1:A:212:GLU:N | 2.25 | 0.51 |
| 1:D:248:ALA:HA | 1:D:251:VAL:CG2 | 2.40 | 0.51 |
| 1:D:267:ILE:HD11 | 4:D:400:NAD:H2A | 1.93 | 0.51 |
| 1:D:89:LEU:HD23 | 1:D:89:LEU:O | 2.11 | 0.51 |
| 2:F:432:TYR:CD2 | 6:F:500:NDP:C1D | 2.84 | 0.51 |
| 1:H:266:LEU:HD12 | 1:H:272:ALA:HB2 | 1.92 | 0.51 |
| 1:H:368:VAL:HG13 | 1:H:376:HIS:HB3 | 1.93 | 0.51 |
| 1:H:202:ASP:CA | 4:H:400:NAD:H8A | 2.39 | 0.51 |
| 2:I:445:THR:HG22 | 2:I:447:MET:HE2 | 1.93 | 0.51 |
| 1:B:275:LEU:HG | 1:B:300:ASN:HB3 | 1.93 | 0.51 |
| 1:B:73:LYS:NZ | 1:B:75:GLN:O | 2.38 | 0.51 |
| 1:D:91:LYS:HG3 | 1:D:91:LYS:O | 2.11 | 0.51 |
| 1:D:160:PHE:N | 1:D:161:PRO:HD2 | 2.26 | 0.51 |
| 1:D:275:LEU:CD1 | 1:D:300:ASN:HD22 | 2.13 | 0.51 |
| 1:E:136:ILE:HA | 1:E:338:ASN:OD1 | 2.10 | 0.51 |
| 1:E:60:THR:HG22 | 1:E:63:GLN:HB2 | 1.93 | 0.51 |
| 1:G:113:THR:CG2 | 1:G:373:ALA:HA | 2.41 | 0.51 |
| 1:G:13:GLU:OE2 | 1:G:15:ARG:HB2 | 2.11 | 0.51 |
| 1:G:133:SER:O | 1:G:338:ASN:HA | 2.11 | 0.51 |
| 1:H:120:TYR:HB3 | 1:H:366:THR:CG2 | 2.40 | 0.51 |
| 1:H:128:ILE:HG12 | 1:H:131:ALA:HB3 | 1.93 | 0.51 |
| 1:A:160:PHE:O | 1:A:172:PRO:HA | 2.11 | 0.51 |
| 2:C:309:LYS:HZ3 | 2:C:382:THR:HB | 1.76 | 0.51 |
| 1:D:136:ILE:HG22 | 1:D:338:ASN:CB | 2.39 | 0.51 |
| 1:D:304:SER:O | 1:D:305:GLU:HG2 | 2.11 | 0.51 |
| 2:F:412:ILE:HD12 | 2:F:412:ILE:O | 2.11 | 0.51 |
| 1:G:154:TYR:O | 1:H:147:ARG:NH2 | 2.36 | 0.51 |
| 1:G:23:VAL:HG13 | 1:G:33:VAL:HG11 | 1.93 | 0.51 |
| 1:G:23:VAL:CG1 | 1:G:55:ALA:HB2 | 2.40 | 0.51 |
| 1:H:182:VAL:CG1 | 1:H:183:ALA:N | 2.74 | 0.51 |
| 1:H:266:LEU:HD13 | 1:H:294:ALA:HB2 | 1.92 | 0.51 |
| 2:I:336:LYS:CG | 2:I:337:GLU:N | 2.72 | 0.51 |
| 1:A:17:ALA:HB2 | 1:A:74:VAL:HG22 | 1.92 | 0.51 |
| 1:E:7:LYS:HB2 | 1:E:39:ALA:HA | 1.92 | 0.51 |
| 1:H:112:LEU:O | 1:H:115:ARG:HB2 | 2.11 | 0.51 |
| 1:H:61:ALA:O | 1:H:65:LEU:HD22 | 2.11 | 0.51 |
| 2:I:389:ILE:HG23 | 2:I:389:ILE:O | 2.10 | 0.51 |
| 1:B:188:ILE:HA | 1:B:198:VAL:HG11 | 1.93 | 0.50 |
| 1:B:281:VAL:HA | 1:B:284:MET:HE3 | 1.93 | 0.50 |
| 1:B:22:VAL:HG21 | 1:B:336:ALA:CB | 2.41 | 0.50 |
| 1:B:74:VAL:HG23 | 1:B:75:GLN:N | 2.26 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:C:413:LEU:O | 2:C:415:VAL:N | 2.43 | 0.50 |
| 1:D:267:ILE:O | 1:D:267:ILE:HG22 | 2.10 | 0.50 |
| 1:E:270:LYS:N | 1:E:270:LYS:HE3 | 2.26 | 0.50 |
| 2:F:432:TYR:HD2 | 6:F:500:NDP:H1D | 1.68 | 0.50 |
| 1:G:128:ILE:O | 1:G:130:ARG:N | 2.44 | 0.50 |
| 1:H:129:SER:C | 1:H:132:GLN:HG3 | 2.31 | 0.50 |
| 1:H:29:LEU:CD2 | 1:H:344:THR:HG22 | 2.41 | 0.50 |
| 1:H:357:LYS:HB3 | 1:H:360:ASP:CB | 2.34 | 0.50 |
| 2:I:433:ALA:C | 2:I:435:VAL:H | 2.14 | 0.50 |
| 1:A:273:PRO:O | 1:A:300:ASN:HA | 2.10 | 0.50 |
| 1:B:98:CYS:SG | 1:B:100:LEU:HG | 2.52 | 0.50 |
| 1:B:3:ILE:HG13 | 1:B:70:VAL:CG1 | 2.41 | 0.50 |
| 1:E:212:GLU:C | 1:E:214:LEU:N | 2.63 | 0.50 |
| 1:E:279:GLU:O | 1:E:282:THR:OG1 | 2.20 | 0.50 |
| 1:H:65:LEU:N | 1:H:65:LEU:HD12 | 2.26 | 0.50 |
| 2:I:324:GLN:HG2 | 2:I:325:HIS:N | 2.26 | 0.50 |
| 1:A:313:HIS:O | 1:A:315:VAL:HG23 | 2.11 | 0.50 |
| 1:D:16:VAL:HG11 | 1:D:40:GLY:HA3 | 1.91 | 0.50 |
| 1:D:252:LEU:C | 1:D:254:GLU:H | 2.13 | 0.50 |
| 1:D:5:ILE:N | 1:D:34:ILE:O | 2.41 | 0.50 |
| 1:D:7:LYS:HB2 | 1:D:39:ALA:HA | 1.92 | 0.50 |
| 1:G:158:ARG:HD3 | 1:H:330:ASP:OD2 | 2.10 | 0.50 |
| 1:G:22:VAL:HG13 | 1:G:340:LEU:CD1 | 2.41 | 0.50 |
| 1:G:89:LEU:N | 1:G:89:LEU:HD12 | 2.26 | 0.50 |
| 1:H:179:GLY:HA3 | 1:H:264:THR:OG1 | 2.12 | 0.50 |
| 1:H:3:ILE:CG2 | 1:H:33:VAL:HG22 | 2.41 | 0.50 |
| 2:I:328:ARG:HD2 | 2:I:328:ARG:O | 2.11 | 0.50 |
| 1:D:23:VAL:O | 1:D:26:LEU:N | 2.42 | 0.50 |
| 1:D:291:ILE:CD1 | 1:D:291:ILE:N | 2.74 | 0.50 |
| 1:D:5:ILE:O | 1:D:35:VAL:HA | 2.11 | 0.50 |
| 1:D:97:MET:HB2 | 1:D:122:MET:HE2 | 1.94 | 0.50 |
| 1:E:176:LEU:HA | 1:E:199:MET:O | 2.12 | 0.50 |
| 1:B:5:ILE:HB | 1:B:35:VAL:HG12 | 1.94 | 0.50 |
| 1:D:343:LEU:HG | 1:D:354:LEU:HD12 | 1.93 | 0.50 |
| 1:D:74:VAL:HG12 | 1:D:75:GLN:N | 2.26 | 0.50 |
| 1:B:134:MET:HG2 | 1:B:342:PHE:H | 1.75 | 0.50 |
| 1:B:176:LEU:HA | 1:B:199:MET:O | 2.12 | 0.50 |
| 1:D:23:VAL:CG1 | 1:D:55:ALA:HB2 | 2.39 | 0.50 |
| 1:D:285:LYS:HD3 | 1:D:286:PRO:CD | 2.42 | 0.50 |
| 1:D:68:ALA:C | 1:D:91:LYS:HD3 | 2.29 | 0.50 |
| 1:E:266:LEU:CD1 | 1:E:294:ALA:HA | 2.42 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:374:ILE:H | 1:E:374:ILE:CD1 | 2.24 | 0.50 |
| 1:G:199:MET:HE1 | 1:G:217:LYS:HB2 | 1.93 | 0.50 |
| 1:G:208:LYS:NZ | 1:G:220:THR:HG23 | 2.27 | 0.50 |
| 1:G:299:GLY:C | 1:G:301:CYS:H | 2.15 | 0.50 |
| 1:G:86:GLU:HA | 1:G:89:LEU:HD13 | 1.92 | 0.50 |
| 1:H:180:VAL:HG21 | 1:H:211:VAL:CG2 | 2.41 | 0.50 |
| 1:D:252:LEU:HD23 | 1:D:252:LEU:C | 2.32 | 0.50 |
| 1:D:294:ALA:CB | 1:D:300:ASN:OD1 | 2.58 | 0.50 |
| 1:D:376:HIS:CD2 | 1:D:378:ALA:HB2 | 2.46 | 0.50 |
| 1:E:105:ASN:O | 1:E:109:VAL:HG23 | 2.12 | 0.50 |
| 1:G:78:MET:H | 1:G:86:GLU:CB | 2.24 | 0.50 |
| 1:G:97:MET:HE1 | 1:G:343:LEU:HD13 | 1.93 | 0.50 |
| 1:H:103:LEU:CD1 | 1:H:103:LEU:H | 2.23 | 0.50 |
| 1:H:182:VAL:CG1 | 1:H:183:ALA:H | 2.25 | 0.50 |
| 1:H:297:ALA:C | 1:H:299:GLY:H | 2.15 | 0.50 |
| 1:B:29:LEU:HD21 | 1:B:344:THR:HB | 1.93 | 0.50 |
| 1:D:191:ALA:O | 1:D:196:ALA:HB3 | 2.12 | 0.50 |
| 1:E:120:TYR:CD1 | 1:E:366:THR:O | 2.61 | 0.50 |
| 1:H:243:PHE:O | 1:H:245:LYS:N | 2.40 | 0.50 |
| 1:E:282:THR:HG22 | 1:E:313:HIS:CE1 | 2.47 | 0.50 |
| 1:H:311:VAL:HG23 | 1:H:315:VAL:O | 2.12 | 0.50 |
| 1:H:360:ASP:O | 1:H:362:THR:N | 2.45 | 0.50 |
| 1:H:113:THR:HG23 | 1:H:369:THR:OG1 | 2.12 | 0.50 |
| 1:A:74:VAL:HA | 1:A:335:PHE:CE2 | 2.47 | 0.49 |
| 1:D:78:MET:HB2 | 1:D:86:GLU:HG3 | 1.92 | 0.49 |
| 2:F:437:ASN:HB3 | 2:F:440:PHE:CZ | 2.47 | 0.49 |
| 1:G:380:THR:HG23 | 1:G:380:THR:O | 2.12 | 0.49 |
| 1:E:172:PRO:HG3 | 2:I:443:ASN:O | 2.12 | 0.49 |
| 1:B:156:PHE:CZ | 1:B:259:ASP:HB3 | 2.47 | 0.49 |
| 1:D:46:THR:O | 1:D:50:LEU:HD12 | 2.12 | 0.49 |
| 1:E:360:ASP:OD1 | 1:E:362:THR:HG22 | 2.12 | 0.49 |
| 1:G:160:PHE:CZ | 1:G:260:ILE:HD12 | 2.47 | 0.49 |
| 1:G:291:ILE:HG22 | 1:G:291:ILE:O | 2.10 | 0.49 |
| 1:H:58:ALA:CB | 1:H:64:ALA:HA | 2.42 | 0.49 |
| 1:D:360:ASP:CG | 1:D:362:THR:HB | 2.33 | 0.49 |
| 1:E:366:THR:O | 1:E:366:THR:HG22 | 2.11 | 0.49 |
| 1:G:360:ASP:OD1 | 1:G:362:THR:HB | 2.12 | 0.49 |
| 1:H:244:ARG:HE | 1:H:247:GLN:HE22 | 1.59 | 0.49 |
| 1:G:158:ARG:HB2 | 1:H:330:ASP:HB2 | 1.95 | 0.49 |
| 1:H:113:THR:HG22 | 1:H:372:GLY:O | 2.13 | 0.49 |
| 1:A:223:ASP:OD2 | 1:A:243:PHE:HZ | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:1:MET:SD | 1:D:353:THR:HA | 2.52 | 0.49 |
| 1:E:180:VAL:HG11 | 1:E:211:VAL:HG22 | 1.95 | 0.49 |
| 1:E:272:ALA:CB | 1:E:299:GLY:H | 2.25 | 0.49 |
| 2:I:337:GLU:O | 2:I:337:GLU:HG3 | 2.13 | 0.49 |
| 1:B:18:ILE:HG12 | 1:B:19:SER:H | 1.77 | 0.49 |
| 1:E:128:ILE:HD11 | 1:E:130:ARG:NH2 | 2.26 | 0.49 |
| 1:E:200:ALA:O | 1:E:219:ILE:HG12 | 2.12 | 0.49 |
| 1:E:370:ARG:HB2 | 1:E:375:VAL:HG21 | 1.94 | 0.49 |
| 1:H:266:LEU:HD12 | 1:H:272:ALA:CB | 2.42 | 0.49 |
| 1:H:292:ASP:HB3 | 1:H:295:VAL:HB | 1.94 | 0.49 |
| 1:B:344:THR:HA | 1:B:347:VAL:HG12 | 1.95 | 0.49 |
| 1:D:199:MET:CG | 1:D:219:ILE:HD11 | 2.43 | 0.49 |
| 1:D:334:LEU:HD22 | 1:E:167:ALA:CB | 2.43 | 0.49 |
| 1:G:57:ILE:HG22 | 1:G:57:ILE:O | 2.11 | 0.49 |
| 1:H:135:ASP:OD2 | 1:H:135:ASP:C | 2.50 | 0.49 |
| 1:H:51:THR:HG23 | 1:H:55:ALA:O | 2.13 | 0.49 |
| 1:H:61:ALA:C | 1:H:65:LEU:HD13 | 2.32 | 0.49 |
| 1:A:163:MET:HE3 | 1:A:170:VAL:HG11 | 1.95 | 0.49 |
| 1:A:184:GLY:O | 1:A:188:ILE:HG13 | 2.13 | 0.49 |
| 1:A:295:VAL:HG13 | 1:A:296:GLU:N | 2.28 | 0.49 |
| 1:A:22:VAL:HG13 | 1:A:340:LEU:HD22 | 1.94 | 0.49 |
| 1:A:354:LEU:HG | 1:A:355:VAL:N | 2.28 | 0.49 |
| 1:B:178:PHE:HB3 | 1:B:275:LEU:HD13 | 1.95 | 0.49 |
| 1:B:343:LEU:HD23 | 1:B:344:THR:N | 2.28 | 0.49 |
| 2:F:401:THR:O | 2:F:403:PRO:CD | 2.52 | 0.49 |
| 1:G:248:ALA:HB1 | 1:G:280:MET:CE | 2.42 | 0.49 |
| 1:B:100:LEU:HD12 | 1:B:121:ALA:HA | 1.95 | 0.49 |
| 1:B:181:GLY:HA3 | 4:B:400:NAD:O1N | 2.13 | 0.49 |
| 2:C:350:GLY:C | 6:C:500:NDP:H71N | 2.16 | 0.49 |
| 1:D:95:VAL:HG22 | 1:D:118:THR:HB | 1.93 | 0.49 |
| 1:D:224:GLU:H | 1:D:227:LYS:HG2 | 1.78 | 0.49 |
| 1:D:330:ASP:CG | 1:E:158:ARG:HG2 | 2.33 | 0.49 |
| 1:D:344:THR:HA | 1:D:347:VAL:CG2 | 2.43 | 0.49 |
| 1:D:118:THR:HG23 | 1:D:370:ARG:HG3 | 1.95 | 0.49 |
| 1:E:164:MET:SD | 2:I:446:MET:HE1 | 2.53 | 0.49 |
| 1:G:10:ARG:NH2 | 1:G:78:MET:HG3 | 2.27 | 0.49 |
| 1:H:115:ARG:O | 1:H:116:LYS:HB2 | 2.13 | 0.49 |
| 1:H:348:ASP:N | 1:H:353:THR:O | 2.43 | 0.49 |
| 1:H:357:LYS:C | 1:H:359:GLU:H | 2.16 | 0.49 |
| 1:B:339:LEU:O | 1:B:340:LEU:C | 2.50 | 0.49 |
| 1:D:343:LEU:HD23 | 1:D:343:LEU:C | 2.33 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:26:LEU:O | 1:G:31:PHE:HB2 | 2.12 | 0.49 |
| 1:G:73:LYS:HE3 | 1:G:75:GLN:O | 2.13 | 0.49 |
| 1:G:72:TRP:NE1 | 1:G:97:MET:HE1 | 2.17 | 0.49 |
| 2:I:451:ASP:O | 2:I:454:LYS:N | 2.45 | 0.49 |
| 1:A:103:LEU:HD21 | 1:A:124:LEU:HD11 | 1.94 | 0.49 |
| 1:A:265:ALA:HB2 | 1:A:275:LEU:HD11 | 1.95 | 0.49 |
| 1:B:19:SER:HB3 | 1:B:22:VAL:CG2 | 2.42 | 0.49 |
| 1:G:244:ARG:HG2 | 1:G:244:ARG:O | 2.13 | 0.49 |
| 1:H:119:ALA:H | 1:H:369:THR:CG2 | 2.26 | 0.49 |
| 1:H:25:LYS:HA | 1:H:25:LYS:HE3 | 1.94 | 0.49 |
| 2:I:402:ASP:O | 2:I:408:TYR:HB2 | 2.13 | 0.49 |
| 1:B:128:ILE:HG12 | 1:B:131:ALA:HB3 | 1.95 | 0.48 |
| 1:E:122:MET:CE | 1:E:339:LEU:HG | 2.43 | 0.48 |
| 2:F:305:LYS:HZ2 | 2:F:337:GLU:HG3 | 1.77 | 0.48 |
| 1:G:279:GLU:O | 1:G:283:LYS:HG2 | 2.13 | 0.48 |
| 1:H:178:PHE:CD2 | 1:H:275:LEU:HD13 | 2.48 | 0.48 |
| 1:H:97:MET:SD | 1:H:342:PHE:HE1 | 2.36 | 0.48 |
| 1:A:305:GLU:HB2 | 1:A:310:VAL:HG21 | 1.96 | 0.48 |
| 1:A:363:VAL:O | 1:A:363:VAL:HG12 | 2.13 | 0.48 |
| 1:A:17:ALA:HB2 | 1:A:74:VAL:CG2 | 2.43 | 0.48 |
| 1:B:113:THR:HG23 | 1:B:372:GLY:O | 2.14 | 0.48 |
| 1:D:105:ASN:O | 1:D:109:VAL:HG13 | 2.13 | 0.48 |
| 1:D:108:VAL:HG13 | 1:D:109:VAL:N | 2.27 | 0.48 |
| 1:D:97:MET:O | 1:D:98:CYS:HB3 | 2.13 | 0.48 |
| 1:G:130:ARG:NH1 | 1:G:360:ASP:OD1 | 2.45 | 0.48 |
| 2:I:435:VAL:HG22 | 2:I:436:GLU:N | 2.28 | 0.48 |
| 1:A:163:MET:CE | 1:A:170:VAL:HG11 | 2.43 | 0.48 |
| 1:A:362:THR:HG22 | 1:A:363:VAL:N | 2.28 | 0.48 |
| 1:A:80:ALA:CB | 1:A:85:ASP:HB2 | 2.42 | 0.48 |
| 1:B:341:ASN:O | 1:B:343:LEU:N | 2.45 | 0.48 |
| 2:C:392:ASN:O | 2:C:395:THR:CG2 | 2.57 | 0.48 |
| 2:C:395:THR:HG21 | 2:C:423:PHE:HE2 | 1.78 | 0.48 |
| 1:D:311:VAL:HA | 1:D:315:VAL:O | 2.13 | 0.48 |
| 1:D:354:LEU:C | 1:D:354:LEU:HD23 | 2.32 | 0.48 |
| 1:E:10:ARG:NH2 | 1:E:76:ARG:HG3 | 2.27 | 0.48 |
| 2:F:407:ILE:O | 2:F:408:TYR:O | 2.31 | 0.48 |
| 1:H:27:VAL:HA | 1:H:31:PHE:O | 2.14 | 0.48 |
| 1:H:276:ILE:HA | 1:H:280:MET:SD | 2.53 | 0.48 |
| 1:E:169:THR:OG1 | 2:I:303:ILE:HG12 | 2.12 | 0.48 |
| 1:A:138:SER:C | 1:A:140:GLN:H | 2.16 | 0.48 |
| 1:D:134:MET:CE | 1:D:341:ASN:O | 2.61 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:239:MET:H | 1:D:244:ARG:HH11 | 1.59 | 0.48 |
| 1:D:343:LEU:HD23 | 1:D:347:VAL:CG2 | 2.43 | 0.48 |
| 1:D:85:ASP:OD2 | 1:D:88:ALA:HB3 | 2.14 | 0.48 |
| 1:H:10:ARG:HH11 | 1:H:76:ARG:HE | 1.62 | 0.48 |
| 2:I:316:TYR:CD1 | 2:I:351:ARG:HG2 | 2.49 | 0.48 |
| 2:I:435:VAL:HG22 | 2:I:436:GLU:O | 2.14 | 0.48 |
| 2:I:437:ASN:C | 2:I:439:LEU:H | 2.17 | 0.48 |
| 1:B:267:ILE:HD11 | 4:B:400:NAD:N1A | 2.29 | 0.48 |
| 1:B:85:ASP:OD1 | 1:B:88:ALA:HB3 | 2.13 | 0.48 |
| 1:B:90:ILE:O | 1:B:91:LYS:C | 2.50 | 0.48 |
| 2:C:308:SER:HB2 | 2:C:384:ASP:OD2 | 2.14 | 0.48 |
| 2:C:425:LYS:CB | 2:C:425:LYS:HZ3 | 2.27 | 0.48 |
| 1:D:223:ASP:HA | 1:D:227:LYS:HG2 | 1.95 | 0.48 |
| 1:D:239:MET:HB2 | 1:D:244:ARG:NE | 2.19 | 0.48 |
| 1:G:96:LEU:HB3 | 1:G:119:ALA:HB2 | 1.95 | 0.48 |
| 1:G:332:SER:HB2 | 1:G:333:PRO:HD3 | 1.95 | 0.48 |
| 2:I:439:LEU:O | 2:I:441:PHE:N | 2.47 | 0.48 |
| 2:C:420:THR:HB | 1:H:162:MET:HE3 | 1.96 | 0.48 |
| 1:D:247:GLN:O | 1:D:249:GLU:N | 2.46 | 0.48 |
| 1:G:342:PHE:CE1 | 1:G:362:THR:HG23 | 2.48 | 0.48 |
| 1:H:98:CYS:O | 1:H:121:ALA:HA | 2.13 | 0.48 |
| 1:H:121:ALA:HB1 | 1:H:123:GLU:CD | 2.32 | 0.48 |
| 1:H:245:LYS:C | 1:H:247:GLN:H | 2.16 | 0.48 |
| 1:H:368:VAL:HG13 | 1:H:376:HIS:CB | 2.43 | 0.48 |
| 1:H:367:CYS:SG | 1:H:370:ARG:HD2 | 2.52 | 0.48 |
| 1:H:13:GLU:HG2 | 1:H:74:VAL:HG21 | 1.96 | 0.48 |
| 1:A:140:GLN:C | 1:A:142:ASN:N | 2.67 | 0.48 |
| 1:A:120:TYR:HB3 | 1:A:366:THR:HG23 | 1.96 | 0.48 |
| 1:D:158:ARG:HG3 | 1:E:329:ALA:CB | 2.43 | 0.48 |
| 1:D:340:LEU:C | 1:D:340:LEU:HD23 | 2.33 | 0.48 |
| 1:D:36:GLU:HB3 | 1:D:39:ALA:HB2 | 1.96 | 0.48 |
| 1:D:7:LYS:HB2 | 1:D:39:ALA:CB | 2.43 | 0.48 |
| 1:D:68:ALA:H | 1:D:91:LYS:CD | 2.27 | 0.48 |
| 1:A:138:SER:OG | 4:A:400:NAD:H5N | 2.12 | 0.48 |
| 1:B:93:GLY:HA2 | 1:B:116:LYS:O | 2.14 | 0.48 |
| 2:C:371:PHE:HB2 | 2:C:376:ILE:CG1 | 2.43 | 0.48 |
| 1:E:135:ASP:O | 1:E:137:LEU:N | 2.47 | 0.48 |
| 1:E:156:PHE:CE2 | 1:E:158:ARG:HB2 | 2.49 | 0.48 |
| 2:F:377:ASN:OD1 | 2:F:413:LEU:HA | 2.13 | 0.48 |
| 1:G:354:LEU:C | 1:G:354:LEU:HD23 | 2.34 | 0.48 |
| 1:H:147:ARG:CG | 1:H:327:VAL:HG22 | 2.44 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:3:ILE:HG23 | 1:H:33:VAL:HG22 | 1.95 | 0.48 |
| 1:A:180:VAL:HG12 | 1:A:180:VAL:O | 2.14 | 0.48 |
| 1:B:207:THR:HA | 1:B:210:GLN:HG3 | 1.96 | 0.48 |
| 1:B:50:LEU:O | 1:B:53:ALA:N | 2.46 | 0.48 |
| 1:D:343:LEU:O | 1:D:347:VAL:HG23 | 2.14 | 0.48 |
| 1:E:161:PRO:HB3 | 1:E:195:GLY:HA3 | 1.96 | 0.48 |
| 1:E:37:GLN:HG2 | 1:E:59:SER:HA | 1.95 | 0.48 |
| 1:E:78:MET:HA | 1:E:82:GLU:OE2 | 2.14 | 0.48 |
| 1:G:97:MET:CE | 1:G:343:LEU:HD13 | 2.43 | 0.48 |
| 1:H:203:VAL:HG13 | 4:H:400:NAD:N7A | 2.28 | 0.48 |
| 1:H:361:GLU:HA | 1:H:364:SER:OG | 2.13 | 0.48 |
| 1:B:13:GLU:OE1 | 1:B:75:GLN:NE2 | 2.37 | 0.48 |
| 1:D:354:LEU:O | 1:D:355:VAL:HG22 | 2.14 | 0.48 |
| 1:E:3:ILE:HA | 1:E:70:VAL:O | 2.14 | 0.48 |
| 1:H:91:LYS:O | 1:H:94:ALA:HB2 | 2.14 | 0.48 |
| 1:A:21:GLU:N | 1:A:21:GLU:CD | 2.68 | 0.47 |
| 1:A:7:LYS:H | 1:A:36:GLU:CG | 2.27 | 0.47 |
| 1:B:265:ALA:CB | 1:B:275:LEU:HD11 | 2.43 | 0.47 |
| 1:B:295:VAL:HG13 | 1:B:296:GLU:N | 2.28 | 0.47 |
| 2:C:444:ASN:HD22 | 2:C:444:ASN:C | 2.17 | 0.47 |
| 1:D:125:MET:CE | 1:D:134:MET:HB2 | 2.44 | 0.47 |
| 1:D:126:PRO:O | 1:D:128:ILE:N | 2.43 | 0.47 |
| 1:D:275:LEU:O | 1:D:280:MET:HE1 | 2.14 | 0.47 |
| 1:D:46:THR:O | 1:D:49:ALA:N | 2.46 | 0.47 |
| 1:D:57:ILE:HD12 | 1:D:58:ALA:O | 2.14 | 0.47 |
| 1:E:120:TYR:HB3 | 1:E:366:THR:HG22 | 1.96 | 0.47 |
| 1:G:332:SER:O | 1:G:333:PRO:C | 2.53 | 0.47 |
| 1:H:98:CYS:H | 1:H:122:MET:HE1 | 1.79 | 0.47 |
| 1:B:1:MET:HE1 | 1:B:353:THR:HA | 1.96 | 0.47 |
| 1:B:113:THR:CG2 | 1:B:373:ALA:HA | 2.40 | 0.47 |
| 1:E:302:PRO:HG2 | 1:E:303:LEU:HD12 | 1.97 | 0.47 |
| 1:H:330:ASP:O | 1:H:333:PRO:HD2 | 2.14 | 0.47 |
| 1:H:47:ASP:HB3 | 1:H:57:ILE:CG1 | 2.43 | 0.47 |
| 2:C:425:LYS:HZ3 | 2:C:425:LYS:HB3 | 1.78 | 0.47 |
| 1:D:202:ASP:HB3 | 1:D:207:THR:HG21 | 1.96 | 0.47 |
| 1:D:47:ASP:OD2 | 1:D:57:ILE:HD13 | 2.14 | 0.47 |
| 1:E:123:GLU:HA | 1:E:137:LEU:HD11 | 1.95 | 0.47 |
| 1:E:220:THR:O | 1:E:221:VAL:C | 2.52 | 0.47 |
| 1:A:158:ARG:HG3 | 1:B:329:ALA:HB3 | 1.95 | 0.47 |
| 1:A:177:VAL:O | 1:A:177:VAL:HG13 | 2.14 | 0.47 |
| 1:B:325:SER:O | 1:B:328:ALA:HB2 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:322:ASN:HD22 | 1:D:325:SER:CB | 2.16 | 0.47 |
| 1:D:354:LEU:C | 1:D:355:VAL:CG2 | 2.83 | 0.47 |
| 2:F:393:ASP:O | 2:F:395:THR:N | 2.47 | 0.47 |
| 2:I:295:GLY:HA3 | 2:I:446:MET:CE | 2.44 | 0.47 |
| 1:A:5:ILE:HG21 | 1:A:18:ILE:HG22 | 1.97 | 0.47 |
| 1:B:72:TRP:CD2 | 1:B:339:LEU:HD23 | 2.49 | 0.47 |
| 1:B:120:TYR:HE1 | 1:B:367:CYS:HB2 | 1.79 | 0.47 |
| 1:B:96:LEU:HD12 | 1:B:97:MET:N | 2.29 | 0.47 |
| 1:D:199:MET:HG2 | 1:D:219:ILE:HD11 | 1.97 | 0.47 |
| 1:E:155:GLU:HG3 | 1:E:318:VAL:HG21 | 1.96 | 0.47 |
| 1:E:46:THR:O | 1:E:50:LEU:HB2 | 2.13 | 0.47 |
| 2:F:405:SER:C | 2:F:407:ILE:H | 2.18 | 0.47 |
| 1:G:174:ARG:HB2 | 1:G:258:THR:HA | 1.97 | 0.47 |
| 1:G:5:ILE:HG23 | 1:G:17:ALA:HB3 | 1.96 | 0.47 |
| 1:H:128:ILE:O | 1:H:132:GLN:HG2 | 2.14 | 0.47 |
| 1:H:129:SER:HA | 1:H:132:GLN:NE2 | 2.29 | 0.47 |
| 1:H:3:ILE:CG1 | 1:H:70:VAL:HG13 | 2.45 | 0.47 |
| 2:I:363:ALA:O | 2:I:364:ASN:HB2 | 2.14 | 0.47 |
| 1:B:105:ASN:HB3 | 1:B:108:VAL:HG12 | 1.97 | 0.47 |
| 2:C:330:MET:HB2 | 2:C:460:VAL:HG22 | 1.97 | 0.47 |
| 1:D:130:ARG:NH1 | 1:D:360:ASP:OD2 | 2.48 | 0.47 |
| 1:E:210:GLN:H | 1:E:210:GLN:HG2 | 1.37 | 0.47 |
| 1:E:72:TRP:HE1 | 1:E:97:MET:HE2 | 1.79 | 0.47 |
| 2:F:334:LEU:HB3 | 2:F:339:VAL:HB | 1.96 | 0.47 |
| 1:G:188:ILE:CG2 | 1:G:214:LEU:HD13 | 2.44 | 0.47 |
| 1:G:248:ALA:HB1 | 1:G:280:MET:HE1 | 1.95 | 0.47 |
| 1:G:346:HIS:CE1 | 1:G:363:VAL:CG2 | 2.98 | 0.47 |
| 1:A:1:MET:CE | 1:A:1:MET:HA | 2.44 | 0.47 |
| 1:A:207:THR:O | 1:A:210:GLN:HB2 | 2.15 | 0.47 |
| 1:A:266:LEU:O | 1:A:267:ILE:HG13 | 2.15 | 0.47 |
| 2:I:397:PRO:HB3 | 2:I:416:GLU:OE2 | 2.15 | 0.47 |
| 2:I:439:LEU:C | 2:I:441:PHE:N | 2.68 | 0.47 |
| 2:I:426:ARG:NH2 | 6:I:500:NDP:O3X | 2.45 | 0.47 |
| 1:A:28:GLY:C | 1:A:30:GLY:H | 2.17 | 0.47 |
| 1:B:312:LYS:HE2 | 1:B:313:HIS:NE2 | 2.30 | 0.47 |
| 2:C:416:GLU:HG3 | 2:C:442:ARG:HH12 | 1.79 | 0.47 |
| 1:D:221:VAL:CG2 | 1:D:247:GLN:HA | 2.45 | 0.47 |
| 1:D:248:ALA:HB1 | 1:D:280:MET:SD | 2.55 | 0.47 |
| 1:D:320:HIS:CD2 | 1:D:326:ARG:CZ | 2.98 | 0.47 |
| 1:E:244:ARG:CB | 1:E:244:ARG:NH2 | 2.75 | 0.47 |
| 1:E:1:MET:HG2 | 1:E:352:LYS:O | 2.13 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:347:VAL:HG13 | 1:H:347:VAL:O | 2.14 | 0.47 |
| 1:A:15:ARG:NH1 | 1:A:324:PRO:HB2 | 2.30 | 0.47 |
| 1:B:2:LYS:N | 1:B:69:ASP:OD1 | 2.41 | 0.47 |
| 1:D:68:ALA:O | 1:D:91:LYS:HG2 | 2.14 | 0.47 |
| 1:E:127:ARG:HH22 | 1:E:132:GLN:HG3 | 1.78 | 0.47 |
| 1:H:25:LYS:HG2 | 1:H:340:LEU:HD21 | 1.97 | 0.47 |
| 1:A:106:ARG:O | 1:A:109:VAL:N | 2.47 | 0.47 |
| 1:A:377:PRO:HA | 1:A:381:GLY:HA3 | 1.96 | 0.47 |
| 1:E:362:THR:HG23 | 1:E:363:VAL:HG23 | 1.97 | 0.47 |
| 1:E:65:LEU:O | 1:E:67:GLN:N | 2.48 | 0.47 |
| 2:F:326:ALA:O | 2:F:329:GLU:HB2 | 2.15 | 0.47 |
| 2:F:414:ASP:HB3 | 2:F:417:LYS:HG3 | 1.96 | 0.47 |
| 1:G:208:LYS:HZ2 | 1:G:220:THR:HG23 | 1.80 | 0.47 |
| 1:G:256:VAL:HG23 | 1:G:257:LYS:HG3 | 1.97 | 0.47 |
| 1:H:112:LEU:CD1 | 1:H:112:LEU:H | 2.28 | 0.47 |
| 2:I:416:GLU:OE1 | 2:I:442:ARG:NH1 | 2.48 | 0.47 |
| 2:I:433:ALA:O | 2:I:435:VAL:N | 2.47 | 0.47 |
| 1:B:267:ILE:HG12 | 4:B:400:NAD:C2A | 2.45 | 0.47 |
| 2:C:343:TYR:N | 2:C:343:TYR:CD1 | 2.83 | 0.47 |
| 1:D:358:LEU:CD1 | 1:D:370:ARG:HH22 | 2.18 | 0.47 |
| 1:D:94:ALA:O | 1:D:117:ILE:HG23 | 2.15 | 0.47 |
| 1:E:169:THR:CG2 | 1:E:170:VAL:N | 2.77 | 0.47 |
| 1:H:92:GLU:HB2 | 1:H:116:LYS:HZ3 | 1.78 | 0.47 |
| 1:H:9:ARG:NH2 | 1:H:36:GLU:OE1 | 2.48 | 0.47 |
| 1:B:8:GLU:OE1 | 1:B:74:VAL:HG22 | 2.15 | 0.46 |
| 1:E:136:ILE:HD12 | 1:E:137:LEU:N | 2.30 | 0.46 |
| 1:E:23:VAL:HG11 | 1:E:55:ALA:HB2 | 1.97 | 0.46 |
| 2:F:403:PRO:HA | 2:F:408:TYR:CD1 | 2.49 | 0.46 |
| 1:H:101:GLY:N | 1:H:123:GLU:OE2 | 2.41 | 0.46 |
| 1:H:18:ILE:CD1 | 1:H:23:VAL:CG2 | 2.87 | 0.46 |
| 1:H:241:GLU:HG2 | 1:H:244:ARG:HB2 | 1.97 | 0.46 |
| 1:H:35:VAL:HG21 | 1:H:50:LEU:CD2 | 2.36 | 0.46 |
| 1:A:272:ALA:HB2 | 1:A:297:ALA:HB3 | 1.98 | 0.46 |
| 1:B:260:ILE:HD13 | 1:B:289:VAL:HG13 | 1.97 | 0.46 |
| 2:C:395:THR:OG1 | 2:C:415:VAL:HG21 | 2.15 | 0.46 |
| 2:C:423:PHE:C | 2:C:424:ILE:HD12 | 2.35 | 0.46 |
| 1:D:351:THR:O | 1:D:352:LYS:C | 2.53 | 0.46 |
| 1:G:114:LYS:C | 1:G:116:LYS:H | 2.18 | 0.46 |
| 1:H:5:ILE:CG1 | 1:H:72:TRP:CD1 | 2.97 | 0.46 |
| 1:B:219:ILE:O | 1:B:220:THR:HG23 | 2.15 | 0.46 |
| 1:B:369:THR:HA | 1:B:375:VAL:HG23 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:300:ALA:HB2 | 2:C:448:LEU:HD11 | 1.98 | 0.46 |
| 1:A:164:MET:CE | 2:C:357:ASN:HD21 | 2.29 | 0.46 |
| 2:C:444:ASN:ND2 | 2:C:444:ASN:C | 2.69 | 0.46 |
| 1:G:255:LEU:HD21 | 1:G:276:ILE:CD1 | 2.45 | 0.46 |
| 1:H:330:ASP:O | 1:H:333:PRO:HG2 | 2.14 | 0.46 |
| 2:I:396:ASN:O | 2:I:412:ILE:HD13 | 2.15 | 0.46 |
| 1:A:23:VAL:HG22 | 1:A:33:VAL:HG11 | 1.97 | 0.46 |
| 1:D:311:VAL:O | 1:D:312:LYS:HG2 | 2.16 | 0.46 |
| 1:D:4:ALA:CB | 1:D:34:ILE:HB | 2.45 | 0.46 |
| 1:E:136:ILE:HD11 | 1:E:137:LEU:HD12 | 1.96 | 0.46 |
| 1:E:178:PHE:HB2 | 1:E:263:THR:HA | 1.96 | 0.46 |
| 1:E:25:LYS:HG2 | 1:E:340:LEU:HD21 | 1.96 | 0.46 |
| 1:G:163:MET:HB2 | 1:G:170:VAL:HG13 | 1.94 | 0.46 |
| 1:B:128:ILE:HD12 | 1:B:130:ARG:CD | 2.32 | 0.46 |
| 1:B:366:THR:HG22 | 1:B:367:CYS:N | 2.30 | 0.46 |
| 1:B:5:ILE:O | 1:B:35:VAL:HA | 2.15 | 0.46 |
| 2:C:403:PRO:HG3 | 2:C:408:TYR:CZ | 2.51 | 0.46 |
| 2:C:425:LYS:CB | 2:C:425:LYS:NZ | 2.79 | 0.46 |
| 1:D:280:MET:C | 1:D:282:THR:N | 2.69 | 0.46 |
| 1:E:110:GLU:O | 1:E:113:THR:HB | 2.15 | 0.46 |
| 1:E:17:ALA:O | 1:E:18:ILE:HB | 2.15 | 0.46 |
| 2:F:452:ALA:H | 6:F:500:NDP:C2A | 2.28 | 0.46 |
| 2:I:453:LYS:HE2 | 2:I:457:GLU:OE2 | 2.16 | 0.46 |
| 1:B:50:LEU:HB3 | 1:B:55:ALA:HB3 | 1.97 | 0.46 |
| 2:C:322:GLN:HE22 | 2:C:324:GLN:HE22 | 1.60 | 0.46 |
| 1:D:19:SER:OG | 1:D:22:VAL:HG23 | 2.15 | 0.46 |
| 1:D:318:VAL:HG13 | 1:D:320:HIS:CE1 | 2.51 | 0.46 |
| 1:E:341:ASN:O | 1:E:345:PRO:CD | 2.63 | 0.46 |
| 1:G:373:ALA:O | 1:G:375:VAL:HG13 | 2.16 | 0.46 |
| 1:H:264:THR:O | 1:H:265:ALA:C | 2.53 | 0.46 |
| 1:H:281:VAL:HG21 | 1:H:303:LEU:HD11 | 1.98 | 0.46 |
| 1:H:354:LEU:H | 1:H:354:LEU:CD2 | 2.09 | 0.46 |
| 1:A:351:THR:HB | 1:A:353:THR:HG22 | 1.98 | 0.46 |
| 1:B:207:THR:O | 1:B:210:GLN:N | 2.49 | 0.46 |
| 1:A:165:THR:CG2 | 2:C:353:PRO:HB3 | 2.42 | 0.46 |
| 2:C:317:GLY:HA3 | 2:C:390:GLY:CA | 2.46 | 0.46 |
| 1:D:16:VAL:HG22 | 1:D:18:ILE:HG22 | 1.97 | 0.46 |
| 1:D:91:LYS:C | 1:D:92:GLU:O | 2.52 | 0.46 |
| 1:E:344:THR:N | 1:E:345:PRO:CD | 2.79 | 0.46 |
| 2:F:328:ARG:HB3 | 2:F:328:ARG:CZ | 2.45 | 0.46 |
| 1:H:5:ILE:HD11 | 1:H:72:TRP:HE1 | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:108:VAL:O | 1:B:112:LEU:CD1 | 2.61 | 0.46 |
| 1:B:188:ILE:HD11 | 1:B:200:ALA:HB2 | 1.98 | 0.46 |
| 1:D:344:THR:N | 1:D:345:PRO:CD | 2.78 | 0.46 |
| 1:D:113:THR:CA | 1:D:369:THR:HG21 | 2.46 | 0.46 |
| 1:D:146:TYR:CE2 | 1:E:159:ALA:HA | 2.51 | 0.46 |
| 1:G:47:ASP:HB3 | 1:G:57:ILE:HG12 | 1.98 | 0.46 |
| 1:H:295:VAL:HG11 | 1:H:319:GLY:CA | 2.46 | 0.46 |
| 1:H:348:ASP:N | 1:H:355:VAL:HG12 | 2.31 | 0.46 |
| 1:H:40:GLY:O | 1:H:43:ALA:N | 2.47 | 0.46 |
| 1:A:120:TYR:HD2 | 1:A:366:THR:HG22 | 1.81 | 0.46 |
| 2:C:330:MET:HG3 | 2:C:463:MET:CE | 2.42 | 0.46 |
| 1:D:120:TYR:CE1 | 1:D:363:VAL:HG13 | 2.50 | 0.46 |
| 1:E:112:LEU:HB3 | 1:E:117:ILE:HB | 1.98 | 0.46 |
| 1:E:136:ILE:HG22 | 1:E:338:ASN:CB | 2.45 | 0.46 |
| 1:H:218:PHE:HD2 | 1:H:220:THR:CG2 | 2.25 | 0.46 |
| 1:H:3:ILE:HG13 | 1:H:70:VAL:HG13 | 1.97 | 0.46 |
| 2:I:399:ALA:CA | 2:I:408:TYR:HA | 2.34 | 0.46 |
| 1:D:13:GLU:HA | 1:D:13:GLU:OE1 | 2.16 | 0.46 |
| 1:D:360:ASP:C | 1:D:362:THR:H | 2.18 | 0.46 |
| 1:D:113:THR:HA | 1:D:369:THR:CG2 | 2.44 | 0.46 |
| 1:E:19:SER:OG | 1:E:22:VAL:HG23 | 2.16 | 0.46 |
| 1:E:327:VAL:HG12 | 1:E:327:VAL:O | 2.16 | 0.46 |
| 2:F:453:LYS:HE2 | 2:F:457:GLU:OE2 | 2.16 | 0.46 |
| 1:H:210:GLN:HA | 1:H:213:SER:HB3 | 1.97 | 0.46 |
| 1:A:38:GLY:N | 1:A:47:ASP:OD1 | 2.48 | 0.45 |
| 1:B:10:ARG:CG | 1:B:10:ARG:HH11 | 2.29 | 0.45 |
| 1:B:10:ARG:NH1 | 1:B:76:ARG:O | 2.49 | 0.45 |
| 1:B:190:THR:HA | 1:B:193:ARG:HG2 | 1.98 | 0.45 |
| 1:B:346:HIS:HD1 | 1:B:356:MET:CE | 2.29 | 0.45 |
| 2:C:416:GLU:HB3 | 2:C:439:LEU:HD21 | 1.98 | 0.45 |
| 1:E:162:MET:HE1 | 2:I:420:THR:HG23 | 1.99 | 0.45 |
| 1:E:25:LYS:CG | 1:E:340:LEU:HD21 | 2.45 | 0.45 |
| 1:H:192:LYS:HE2 | 1:H:215:GLY:HA3 | 1.98 | 0.45 |
| 1:H:7:LYS:HB2 | 1:H:39:ALA:HB2 | 1.96 | 0.45 |
| 2:I:313:VAL:HG22 | 2:I:344:ALA:HB3 | 1.98 | 0.45 |
| 2:I:317:GLY:HA3 | 2:I:390:GLY:CA | 2.46 | 0.45 |
| 1:B:295:VAL:HG11 | 1:B:320:HIS:O | 2.16 | 0.45 |
| 2:C:366:PRO:HB2 | 2:C:369:GLU:HG3 | 1.98 | 0.45 |
| 1:D:198:VAL:HG12 | 1:D:199:MET:N | 2.32 | 0.45 |
| 1:E:130:ARG:HG2 | 1:E:130:ARG:O | 2.16 | 0.45 |
| 1:E:147:ARG:O | 1:E:148:ALA:C | 2.55 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:368:VAL:HG12 | 1:E:368:VAL:O | 2.16 | 0.45 |
| 1:E:97:MET:O | 1:E:98:CYS:CB | 2.61 | 0.45 |
| 1:H:131:ALA:HA | 1:H:134:MET:HE3 | 1.97 | 0.45 |
| 1:H:204:ARG:C | 1:H:206:ALA:H | 2.20 | 0.45 |
| 1:H:41:VAL:HG13 | 1:H:42:GLY:N | 2.32 | 0.45 |
| 2:I:455:MET:O | 2:I:459:ILE:HG13 | 2.16 | 0.45 |
| 1:B:185:LEU:HD13 | 2:C:352:MET:HB3 | 1.97 | 0.45 |
| 2:C:330:MET:HG2 | 2:C:334:LEU:HD21 | 1.98 | 0.45 |
| 1:D:255:LEU:C | 1:D:257:LYS:H | 2.19 | 0.45 |
| 1:D:85:ASP:OD2 | 1:D:88:ALA:CB | 2.63 | 0.45 |
| 2:F:437:ASN:C | 2:F:439:LEU:N | 2.68 | 0.45 |
| 1:G:266:LEU:H | 4:G:400:NAD:H51A | 1.81 | 0.45 |
| 1:H:100:LEU:CB | 1:H:121:ALA:HB2 | 2.42 | 0.45 |
| 1:H:208:LYS:HZ2 | 1:H:220:THR:CG2 | 2.29 | 0.45 |
| 1:H:181:GLY:HA2 | 4:H:400:NAD:H52N | 1.98 | 0.45 |
| 1:A:188:ILE:HG23 | 1:A:198:VAL:HG11 | 1.98 | 0.45 |
| 1:B:73:LYS:HB3 | 1:B:73:LYS:NZ | 2.32 | 0.45 |
| 2:C:459:ILE:O | 2:C:463:MET:HG3 | 2.16 | 0.45 |
| 1:D:22:VAL:HG21 | 1:D:336:ALA:HB1 | 1.97 | 0.45 |
| 1:D:29:LEU:CD2 | 1:D:347:VAL:HG11 | 2.46 | 0.45 |
| 2:F:318:MET:CE | 2:F:324:GLN:HG2 | 2.47 | 0.45 |
| 1:E:130:ARG:HD3 | 2:F:409:GLY:HA3 | 1.99 | 0.45 |
| 1:G:265:ALA:HB2 | 1:G:275:LEU:HD11 | 1.99 | 0.45 |
| 1:H:65:LEU:O | 1:H:66:SER:C | 2.53 | 0.45 |
| 2:I:437:ASN:OD1 | 2:I:439:LEU:HB2 | 2.16 | 0.45 |
| 1:A:16:VAL:HG22 | 1:A:18:ILE:HG22 | 1.97 | 0.45 |
| 1:B:354:LEU:C | 1:B:354:LEU:HD23 | 2.36 | 0.45 |
| 1:B:62:ALA:C | 1:B:64:ALA:H | 2.19 | 0.45 |
| 2:C:379:SER:O | 2:C:380:PHE:C | 2.54 | 0.45 |
| 1:D:16:VAL:HG13 | 1:D:16:VAL:O | 2.17 | 0.45 |
| 1:E:207:THR:O | 1:E:211:VAL:HG23 | 2.17 | 0.45 |
| 1:G:34:ILE:HG22 | 1:G:64:ALA:HB1 | 1.97 | 0.45 |
| 1:H:244:ARG:NH2 | 1:H:275:LEU:HD21 | 2.32 | 0.45 |
| 1:A:106:ARG:N | 1:A:107:PRO:CD | 2.75 | 0.45 |
| 2:C:362:GLU:O | 2:C:362:GLU:HG2 | 2.15 | 0.45 |
| 1:D:240:GLY:O | 1:D:242:GLU:N | 2.49 | 0.45 |
| 1:D:97:MET:CE | 1:D:343:LEU:HD12 | 2.47 | 0.45 |
| 1:E:342:PHE:CD1 | 1:E:342:PHE:C | 2.89 | 0.45 |
| 2:F:376:ILE:HG12 | 2:F:376:ILE:O | 2.15 | 0.45 |
| 2:F:401:THR:OG1 | 2:F:402:ASP:N | 2.48 | 0.45 |
| 1:G:16:VAL:HG22 | 1:G:17:ALA:H | 1.82 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:25:LYS:O | 1:H:29:LEU:HD13 | 2.17 | 0.45 |
| 1:H:62:ALA:O | 1:H:66:SER:N | 2.50 | 0.45 |
| 2:I:440:PHE:HD2 | 2:I:447:MET:CE | 2.29 | 0.45 |
| 1:B:281:VAL:HG23 | 1:B:313:HIS:HD2 | 1.81 | 0.45 |
| 1:B:346:HIS:O | 1:B:348:ASP:N | 2.49 | 0.45 |
| 1:E:369:THR:CG2 | 1:E:369:THR:O | 2.64 | 0.45 |
| 1:G:221:VAL:HG12 | 1:G:222:ASP:H | 1.80 | 0.45 |
| 1:G:92:GLU:HG2 | 1:G:92:GLU:H | 1.52 | 0.45 |
| 1:H:3:ILE:O | 1:H:33:VAL:HA | 2.15 | 0.45 |
| 2:I:332:ASP:O | 2:I:333:VAL:C | 2.54 | 0.45 |
| 1:B:79:THR:O | 1:B:84:THR:O | 2.35 | 0.45 |
| 2:C:418:ALA:O | 2:C:419:GLY:C | 2.55 | 0.45 |
| 1:D:164:MET:HE2 | 1:D:169:THR:HG23 | 1.99 | 0.45 |
| 1:D:252:LEU:HD11 | 1:D:283:LYS:HD3 | 1.99 | 0.45 |
| 1:E:267:ILE:HG12 | 1:E:273:PRO:HD3 | 1.98 | 0.45 |
| 2:F:300:ALA:O | 2:F:304:MET:HE2 | 2.17 | 0.45 |
| 1:H:245:LYS:C | 1:H:247:GLN:N | 2.70 | 0.45 |
| 1:B:272:ALA:HB1 | 1:B:300:ASN:ND2 | 2.32 | 0.45 |
| 2:C:453:LYS:O | 2:C:457:GLU:HG3 | 2.17 | 0.45 |
| 1:D:23:VAL:O | 1:D:26:LEU:HB2 | 2.17 | 0.45 |
| 1:D:332:SER:CB | 1:D:333:PRO:HD3 | 2.45 | 0.45 |
| 2:F:445:THR:CG2 | 2:F:446:MET:N | 2.80 | 0.45 |
| 1:G:63:GLN:OE1 | 1:G:63:GLN:HA | 2.16 | 0.45 |
| 1:A:3:ILE:HG13 | 1:A:70:VAL:HG13 | 1.99 | 0.45 |
| 1:B:276:ILE:O | 1:B:301:CYS:HA | 2.17 | 0.45 |
| 1:B:87:VAL:C | 1:B:89:LEU:H | 2.20 | 0.45 |
| 2:C:309:LYS:HE2 | 2:C:382:THR:O | 2.17 | 0.45 |
| 1:D:160:PHE:CZ | 1:D:260:ILE:HD12 | 2.51 | 0.45 |
| 1:G:270:LYS:N | 1:G:270:LYS:HD2 | 2.31 | 0.45 |
| 1:H:63:GLN:CA | 1:H:63:GLN:HE21 | 2.21 | 0.45 |
| 2:I:299:ASP:O | 2:I:303:ILE:HG13 | 2.17 | 0.45 |
| 1:B:105:ASN:O | 1:B:108:VAL:HG12 | 2.17 | 0.44 |
| 2:C:385:VAL:HG12 | 2:C:386:ALA:N | 2.32 | 0.44 |
| 1:D:3:ILE:HB | 1:D:70:VAL:CG2 | 2.47 | 0.44 |
| 1:D:57:ILE:HD12 | 1:D:58:ALA:N | 2.30 | 0.44 |
| 1:D:65:LEU:HD22 | 1:D:71:VAL:HG13 | 1.99 | 0.44 |
| 1:E:272:ALA:HB3 | 1:E:299:GLY:H | 1.82 | 0.44 |
| 1:G:101:GLY:N | 1:G:123:GLU:OE2 | 2.50 | 0.44 |
| 1:H:120:TYR:CB | 1:H:366:THR:HG23 | 2.47 | 0.44 |
| 1:H:99:HIS:CE1 | 1:H:123:GLU:HB3 | 2.52 | 0.44 |
| 1:H:325:SER:C | 1:H:327:VAL:H | 2.20 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:356:MET:O | 1:H:358:LEU:N | 2.50 | 0.44 |
| 1:H:66:SER:HB3 | 1:H:67:GLN:NE2 | 2.32 | 0.44 |
| 1:A:18:ILE:N | 1:A:336:ALA:HB2 | 2.32 | 0.44 |
| 1:B:244:ARG:N | 1:B:244:ARG:HD3 | 2.28 | 0.44 |
| 2:C:420:THR:HG21 | 1:H:169:THR:OG1 | 2.18 | 0.44 |
| 1:E:284:MET:HE3 | 1:E:315:VAL:HG21 | 1.99 | 0.44 |
| 1:E:143:LEU:HD13 | 1:E:327:VAL:HG11 | 2.00 | 0.44 |
| 1:G:121:ALA:HB1 | 1:G:123:GLU:OE1 | 2.16 | 0.44 |
| 1:H:125:MET:HG3 | 1:H:131:ALA:HB1 | 1.97 | 0.44 |
| 1:A:167:ALA:HB2 | 1:B:338:ASN:ND2 | 2.31 | 0.44 |
| 1:B:147:ARG:HH11 | 1:B:151:ASP:CG | 2.19 | 0.44 |
| 1:D:205:ALA:C | 1:D:207:THR:N | 2.71 | 0.44 |
| 1:D:277:THR:O | 1:D:280:MET:N | 2.46 | 0.44 |
| 1:D:362:THR:O | 1:D:362:THR:CG2 | 2.65 | 0.44 |
| 1:E:132:GLN:O | 1:E:133:SER:C | 2.56 | 0.44 |
| 1:E:273:PRO:O | 1:E:274:VAL:C | 2.55 | 0.44 |
| 1:H:113:THR:HG21 | 1:H:374:ILE:CG1 | 2.43 | 0.44 |
| 2:I:396:ASN:HA | 2:I:397:PRO:HD2 | 1.85 | 0.44 |
| 1:A:277:THR:C | 1:A:279:GLU:H | 2.20 | 0.44 |
| 1:A:161:PRO:CB | 1:B:193:ARG:HH12 | 2.29 | 0.44 |
| 1:D:149:VAL:HG11 | 1:D:190:THR:HG22 | 1.99 | 0.44 |
| 1:D:43:ALA:O | 1:D:44:SER:HB2 | 2.18 | 0.44 |
| 2:F:442:ARG:HH11 | 2:F:442:ARG:HG3 | 1.82 | 0.44 |
| 1:G:200:ALA:HB3 | 1:G:211:VAL:CG1 | 2.47 | 0.44 |
| 1:H:72:TRP:CA | 1:H:97:MET:O | 2.64 | 0.44 |
| 1:B:3:ILE:O | 1:B:3:ILE:HG23 | 2.17 | 0.44 |
| 2:C:401:THR:O | 2:C:408:TYR:CE2 | 2.71 | 0.44 |
| 2:C:373:LEU:HD11 | 2:C:411:PRO:HB2 | 1.99 | 0.44 |
| 1:E:160:PHE:CE1 | 1:E:260:ILE:HD12 | 2.52 | 0.44 |
| 1:E:7:LYS:HE3 | 1:E:8:GLU:O | 2.18 | 0.44 |
| 2:F:305:LYS:NZ | 2:F:337:GLU:HG3 | 2.33 | 0.44 |
| 2:F:347:PRO:HD3 | 2:F:373:LEU:HB2 | 1.98 | 0.44 |
| 1:G:121:ALA:HB3 | 1:G:124:LEU:CD1 | 2.45 | 0.44 |
| 1:H:75:GLN:O | 1:H:76:ARG:C | 2.55 | 0.44 |
| 1:A:161:PRO:HB3 | 1:B:193:ARG:NH1 | 2.32 | 0.44 |
| 2:C:373:LEU:HG | 2:C:377:ASN:HD21 | 1.81 | 0.44 |
| 1:D:294:ALA:O | 1:D:299:GLY:HA2 | 2.17 | 0.44 |
| 1:D:334:LEU:HD22 | 1:E:167:ALA:HB1 | 1.99 | 0.44 |
| 1:D:9:ARG:CB | 1:D:9:ARG:HH11 | 2.31 | 0.44 |
| 1:E:338:ASN:HD22 | 1:E:338:ASN:HA | 1.64 | 0.44 |
| 1:G:163:MET:HB2 | 1:G:170:VAL:HG12 | 1.96 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:66:SER:O | 1:H:91:LYS:HB2 | 2.17 | 0.44 |
| 1:A:105:ASN:C | 1:A:107:PRO:HD2 | 2.38 | 0.44 |
| 1:A:176:LEU:HD13 | 1:A:178:PHE:CZ | 2.53 | 0.44 |
| 1:A:359:GLU:H | 1:A:359:GLU:CD | 2.21 | 0.44 |
| 1:A:118:THR:HA | 1:A:369:THR:O | 2.18 | 0.44 |
| 1:D:362:THR:O | 1:D:362:THR:HG23 | 2.17 | 0.44 |
| 1:E:122:MET:HE2 | 1:E:339:LEU:HG | 1.99 | 0.44 |
| 1:G:165:THR:CG2 | 2:I:353:PRO:HB3 | 2.47 | 0.44 |
| 1:G:16:VAL:HG22 | 1:G:17:ALA:N | 2.33 | 0.44 |
| 1:G:247:GLN:C | 1:G:249:GLU:H | 2.21 | 0.44 |
| 1:G:278:GLU:HG3 | 1:G:303:LEU:CD1 | 2.48 | 0.44 |
| 1:G:10:ARG:CG | 1:G:75:GLN:HG2 | 2.46 | 0.44 |
| 1:H:119:ALA:H | 1:H:369:THR:HG23 | 1.83 | 0.44 |
| 1:H:122:MET:SD | 1:H:122:MET:N | 2.91 | 0.44 |
| 1:A:337:LYS:HZ2 | 1:B:168:GLY:HA3 | 1.82 | 0.44 |
| 1:B:71:VAL:CG1 | 1:B:96:LEU:HD13 | 2.48 | 0.44 |
| 2:C:292:HIS:CD2 | 2:C:292:HIS:O | 2.71 | 0.44 |
| 1:E:51:THR:CG2 | 1:E:57:ILE:HG23 | 2.48 | 0.44 |
| 1:G:184:GLY:O | 1:G:188:ILE:HG13 | 2.17 | 0.44 |
| 1:H:284:MET:CE | 1:H:290:ILE:HD11 | 2.48 | 0.44 |
| 1:H:33:VAL:HB | 1:H:55:ALA:HB2 | 1.99 | 0.44 |
| 1:B:121:ALA:HB3 | 1:B:124:LEU:HD12 | 1.98 | 0.44 |
| 2:C:438:GLU:O | 2:C:438:GLU:HG2 | 2.17 | 0.44 |
| 1:D:203:VAL:O | 1:D:228:THR:HB | 2.17 | 0.44 |
| 1:G:37:GLN:HE21 | 1:G:59:SER:HA | 1.82 | 0.44 |
| 1:H:19:SER:HB3 | 1:H:22:VAL:HB | 2.00 | 0.44 |
| 1:H:10:ARG:HH22 | 1:H:82:GLU:CD | 2.21 | 0.44 |
| 1:A:175:VAL:HG12 | 1:A:176:LEU:N | 2.33 | 0.43 |
| 1:A:351:THR:O | 1:A:352:LYS:C | 2.56 | 0.43 |
| 1:A:354:LEU:HD21 | 1:A:356:MET:HE1 | 1.93 | 0.43 |
| 1:B:100:LEU:O | 1:B:101:GLY:C | 2.56 | 0.43 |
| 1:D:109:VAL:CG2 | 1:D:110:GLU:N | 2.81 | 0.43 |
| 1:D:24:LYS:C | 1:D:26:LEU:H | 2.21 | 0.43 |
| 1:G:110:GLU:O | 1:G:114:LYS:HG2 | 2.18 | 0.43 |
| 1:A:139:SER:OG | 1:A:338:ASN:ND2 | 2.42 | 0.43 |
| 1:A:120:TYR:CZ | 1:A:356:MET:HG2 | 2.53 | 0.43 |
| 1:B:129:SER:O | 1:B:132:GLN:HG3 | 2.17 | 0.43 |
| 1:E:117:ILE:O | 1:E:369:THR:HG23 | 2.18 | 0.43 |
| 1:E:100:LEU:HD12 | 1:E:121:ALA:HB2 | 2.00 | 0.43 |
| 1:E:7:LYS:HB2 | 1:E:39:ALA:CA | 2.48 | 0.43 |
| 1:G:10:ARG:HG3 | 1:G:11:PRO:HD2 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:208:LYS:HZ2 | 1:G:218:PHE:HD2 | 1.66 | 0.43 |
| 1:G:214:LEU:HA | 1:G:214:LEU:HD23 | 1.85 | 0.43 |
| 1:H:346:HIS:HB3 | 1:H:356:MET:HA | 1.99 | 0.43 |
| 1:H:347:VAL:CA | 1:H:355:VAL:HG12 | 2.47 | 0.43 |
| 1:H:368:VAL:HG22 | 1:H:376:HIS:HB2 | 2.00 | 0.43 |
| 1:H:67:GLN:N | 1:H:67:GLN:NE2 | 2.56 | 0.43 |
| 2:C:330:MET:HB2 | 2:C:460:VAL:CG2 | 2.48 | 0.43 |
| 1:D:241:GLU:O | 1:D:241:GLU:OE2 | 2.36 | 0.43 |
| 1:D:2:LYS:HZ3 | 1:D:32:GLU:HG2 | 1.83 | 0.43 |
| 1:D:194:LEU:CD2 | 1:E:194:LEU:HD13 | 2.47 | 0.43 |
| 1:E:247:GLN:O | 1:E:251:VAL:HG23 | 2.18 | 0.43 |
| 1:E:346:HIS:HB3 | 1:E:356:MET:HA | 1.99 | 0.43 |
| 2:F:298:GLU:CD | 2:F:298:GLU:H | 2.22 | 0.43 |
| 1:G:156:PHE:CZ | 1:G:259:ASP:HB3 | 2.54 | 0.43 |
| 1:G:200:ALA:O | 1:G:218:PHE:HA | 2.19 | 0.43 |
| 1:G:329:ALA:HB3 | 1:H:157:ALA:O | 2.18 | 0.43 |
| 1:A:357:LYS:O | 1:A:359:GLU:OE2 | 2.36 | 0.43 |
| 2:C:326:ALA:HB1 | 2:C:456:THR:HB | 2.01 | 0.43 |
| 2:C:405:SER:HA | 2:C:406:PRO:HD3 | 1.73 | 0.43 |
| 1:D:348:ASP:OD2 | 1:D:353:THR:N | 2.46 | 0.43 |
| 1:G:199:MET:HE3 | 1:G:217:LYS:HB2 | 2.00 | 0.43 |
| 1:G:244:ARG:O | 1:G:244:ARG:CG | 2.65 | 0.43 |
| 1:H:120:TYR:CB | 1:H:366:THR:HG21 | 2.45 | 0.43 |
| 1:A:326:ARG:HG2 | 1:A:326:ARG:HH11 | 1.82 | 0.43 |
| 1:B:36:GLU:O | 1:B:39:ALA:HB2 | 2.18 | 0.43 |
| 1:B:62:ALA:C | 1:B:64:ALA:N | 2.72 | 0.43 |
| 1:D:100:LEU:O | 1:D:102:ALA:N | 2.51 | 0.43 |
| 1:D:255:LEU:C | 1:D:257:LYS:N | 2.71 | 0.43 |
| 1:D:9:ARG:NH1 | 1:D:9:ARG:HB3 | 2.33 | 0.43 |
| 1:E:220:THR:HG23 | 1:E:221:VAL:N | 2.34 | 0.43 |
| 1:E:23:VAL:CG1 | 1:E:55:ALA:HB2 | 2.49 | 0.43 |
| 1:H:128:ILE:HD11 | 1:H:131:ALA:H | 1.84 | 0.43 |
| 1:H:213:SER:OG | 2:I:355:HIS:CE1 | 2.71 | 0.43 |
| 1:H:73:LYS:CD | 1:H:75:GLN:O | 2.66 | 0.43 |
| 1:A:62:ALA:HA | 1:A:89:LEU:HD22 | 2.00 | 0.43 |
| 1:B:85:ASP:OD1 | 1:B:88:ALA:CB | 2.66 | 0.43 |
| 1:B:99:HIS:C | 1:B:99:HIS:CD2 | 2.92 | 0.43 |
| 1:D:5:ILE:HD13 | 1:D:18:ILE:HG13 | 2.01 | 0.43 |
| 1:D:193:ARG:C | 1:D:195:GLY:H | 2.22 | 0.43 |
| 1:D:264:THR:CG2 | 1:D:293:LEU:HD12 | 2.44 | 0.43 |
| 1:E:190:THR:O | 1:E:191:ALA:C | 2.56 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:280:MET:O | 1:E:283:LYS:N | 2.45 | 0.43 |
| 1:E:370:ARG:O | 1:E:371:ASP:C | 2.57 | 0.43 |
| 1:G:207:THR:O | 1:G:208:LYS:C | 2.57 | 0.43 |
| 1:G:26:LEU:O | 1:G:29:LEU:HB2 | 2.18 | 0.43 |
| 1:H:18:ILE:HG12 | 1:H:19:SER:H | 1.83 | 0.43 |
| 1:H:66:SER:CB | 1:H:67:GLN:NE2 | 2.81 | 0.43 |
| 1:B:2:LYS:HE3 | 1:B:32:GLU:OE1 | 2.18 | 0.43 |
| 1:B:134:MET:HE1 | 1:B:362:THR:HG21 | 2.00 | 0.43 |
| 2:C:377:ASN:OD1 | 2:C:413:LEU:HA | 2.19 | 0.43 |
| 1:D:175:VAL:HG23 | 1:D:196:ALA:HB1 | 2.01 | 0.43 |
| 2:F:416:GLU:HG3 | 2:F:439:LEU:CD1 | 2.48 | 0.43 |
| 1:A:205:ALA:C | 1:A:207:THR:N | 2.72 | 0.43 |
| 1:D:211:VAL:HG12 | 1:D:216:GLY:O | 2.19 | 0.43 |
| 1:D:356:MET:HB3 | 1:D:363:VAL:HG11 | 2.00 | 0.43 |
| 1:G:247:GLN:O | 1:G:249:GLU:N | 2.52 | 0.43 |
| 1:H:113:THR:C | 1:H:115:ARG:H | 2.20 | 0.43 |
| 1:H:128:ILE:HD11 | 1:H:131:ALA:CB | 2.48 | 0.43 |
| 1:H:185:LEU:O | 1:H:214:LEU:CD1 | 2.67 | 0.43 |
| 1:H:282:THR:HG22 | 1:H:313:HIS:NE2 | 2.34 | 0.43 |
| 1:H:29:LEU:HD21 | 1:H:344:THR:HG22 | 2.01 | 0.43 |
| 1:H:346:HIS:CB | 1:H:356:MET:HA | 2.48 | 0.43 |
| 1:A:291:ILE:CD1 | 1:A:318:VAL:HB | 2.40 | 0.43 |
| 1:B:202:ASP:OD1 | 1:B:203:VAL:N | 2.51 | 0.43 |
| 1:B:152:GLY:HA2 | 1:B:291:ILE:HD11 | 2.01 | 0.43 |
| 1:B:308:LYS:CG | 1:B:309:ILE:H | 2.26 | 0.43 |
| 1:B:357:LYS:O | 1:B:360:ASP:HB3 | 2.19 | 0.43 |
| 1:D:175:VAL:HA | 1:D:260:ILE:O | 2.19 | 0.43 |
| 1:D:292:ASP:OD2 | 1:D:300:ASN:N | 2.52 | 0.43 |
| 1:D:147:ARG:HG2 | 1:D:323:VAL:HG13 | 2.01 | 0.43 |
| 1:D:361:GLU:CA | 1:D:364:SER:HB3 | 2.31 | 0.43 |
| 1:D:78:MET:CE | 1:D:82:GLU:HG2 | 2.49 | 0.43 |
| 1:E:120:TYR:HA | 1:E:367:CYS:HA | 2.00 | 0.43 |
| 2:F:316:TYR:HB2 | 2:F:350:GLY:HA2 | 2.00 | 0.43 |
| 2:F:437:ASN:O | 2:F:439:LEU:N | 2.52 | 0.43 |
| 2:F:460:VAL:HG12 | 2:F:460:VAL:O | 2.19 | 0.43 |
| 2:F:352:MET:N | 6:F:500:NDP:N7N | 2.66 | 0.43 |
| 1:H:202:ASP:O | 1:H:218:PHE:HZ | 2.01 | 0.43 |
| 1:H:278:GLU:OE1 | 1:H:312:LYS:HE2 | 2.19 | 0.43 |
| 1:B:210:GLN:HE22 | 2:C:351:ARG:HD2 | 1.84 | 0.43 |
| 1:G:95:VAL:HA | 1:G:118:THR:O | 2.18 | 0.43 |
| 1:H:285:LYS:HA | 1:H:286:PRO:HD3 | 1.80 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:355:VAL:CG1 | 1:H:355:VAL:O | 2.65 | 0.43 |
| 1:A:245:LYS:HA | 1:A:245:LYS:HD2 | 1.86 | 0.42 |
| 1:A:343:LEU:HD23 | 1:A:343:LEU:C | 2.39 | 0.42 |
| 1:A:78:MET:HG3 | 1:A:86:GLU:OE1 | 2.19 | 0.42 |
| 1:B:130:ARG:HG3 | 1:B:130:ARG:H | 1.44 | 0.42 |
| 1:B:87:VAL:HG13 | 1:B:88:ALA:H | 1.81 | 0.42 |
| 1:E:4:ALA:HA | 1:E:34:ILE:O | 2.19 | 0.42 |
| 2:F:430:SER:OG | 2:F:434:GLY:HA2 | 2.19 | 0.42 |
| 1:H:65:LEU:HB3 | 1:H:90:ILE:HA | 2.01 | 0.42 |
| 1:D:121:ALA:HB1 | 1:D:124:LEU:HD22 | 2.01 | 0.42 |
| 1:E:65:LEU:HD12 | 1:E:89:LEU:HB2 | 2.01 | 0.42 |
| 2:F:442:ARG:HA | 2:F:442:ARG:HD3 | 1.57 | 0.42 |
| 1:G:380:THR:CG2 | 1:G:380:THR:O | 2.68 | 0.42 |
| 1:H:148:ALA:HB1 | 1:H:262:ILE:HG21 | 2.00 | 0.42 |
| 1:H:323:VAL:N | 1:H:324:PRO:CD | 2.82 | 0.42 |
| 1:A:136:ILE:HA | 1:A:338:ASN:ND2 | 2.34 | 0.42 |
| 1:B:88:ALA:HA | 1:B:115:ARG:HD2 | 2.01 | 0.42 |
| 1:D:163:MET:HE2 | 1:D:163:MET:HB2 | 1.84 | 0.42 |
| 1:D:127:ARG:NE | 1:D:235:TYR:CE2 | 2.87 | 0.42 |
| 1:D:68:ALA:N | 1:D:91:LYS:CD | 2.83 | 0.42 |
| 1:E:309:ILE:HG23 | 1:E:318:VAL:HG22 | 2.00 | 0.42 |
| 1:E:97:MET:HE2 | 1:E:343:LEU:HD12 | 2.00 | 0.42 |
| 2:F:292:HIS:O | 2:F:293:MET:CB | 2.68 | 0.42 |
| 1:G:97:MET:O | 1:G:98:CYS:HB3 | 2.18 | 0.42 |
| 1:H:72:TRP:CB | 1:H:97:MET:HB2 | 2.25 | 0.42 |
| 1:A:343:LEU:HD23 | 1:A:343:LEU:O | 2.19 | 0.42 |
| 2:C:365:VAL:HA | 2:C:366:PRO:HD3 | 1.75 | 0.42 |
| 2:C:317:GLY:HA3 | 2:C:390:GLY:HA3 | 2.02 | 0.42 |
| 1:D:26:LEU:HD23 | 1:D:26:LEU:HA | 1.89 | 0.42 |
| 1:D:18:ILE:CD1 | 1:D:50:LEU:HD23 | 2.50 | 0.42 |
| 1:E:23:VAL:HG21 | 1:E:50:LEU:CD1 | 2.49 | 0.42 |
| 1:H:71:VAL:O | 1:H:96:LEU:HA | 2.20 | 0.42 |
| 1:A:118:THR:HA | 1:A:370:ARG:HA | 2.01 | 0.42 |
| 1:A:73:LYS:HB3 | 1:A:73:LYS:HE3 | 1.76 | 0.42 |
| 1:B:348:ASP:CG | 1:B:351:THR:HB | 2.40 | 0.42 |
| 1:D:231:THR:O | 1:D:232:ALA:C | 2.58 | 0.42 |
| 1:D:263:THR:HB | 1:D:300:ASN:HB2 | 2.02 | 0.42 |
| 1:D:343:LEU:HD23 | 1:D:347:VAL:HG22 | 2.02 | 0.42 |
| 1:E:112:LEU:HD12 | 1:E:112:LEU:N | 2.32 | 0.42 |
| 1:E:362:THR:CG2 | 1:E:363:VAL:HG23 | 2.50 | 0.42 |
| 2:F:296:SER:OG | 2:F:298:GLU:HG2 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:172:PRO:HB3 | 2:I:367:TYR:HE2 | 1.84 | 0.42 |
| 1:G:243:PHE:C | 1:G:245:LYS:N | 2.64 | 0.42 |
| 1:G:118:THR:HB | 1:G:370:ARG:HA | 2.02 | 0.42 |
| 2:I:380:PHE:O | 2:I:383:ALA:HB3 | 2.20 | 0.42 |
| 1:A:5:ILE:O | 1:A:35:VAL:HA | 2.19 | 0.42 |
| 1:B:197:VAL:HG12 | 1:B:197:VAL:O | 2.19 | 0.42 |
| 1:B:303:LEU:HB2 | 1:B:317:ILE:HD13 | 2.01 | 0.42 |
| 1:B:78:MET:N | 1:B:86:GLU:OE1 | 2.47 | 0.42 |
| 1:D:120:TYR:CZ | 1:D:356:MET:HG2 | 2.54 | 0.42 |
| 1:E:106:ARG:N | 1:E:107:PRO:CD | 2.82 | 0.42 |
| 1:E:268:PRO:O | 1:E:270:LYS:N | 2.53 | 0.42 |
| 2:I:454:LYS:HG3 | 2:I:455:MET:N | 2.35 | 0.42 |
| 1:D:247:GLN:C | 1:D:249:GLU:H | 2.23 | 0.42 |
| 1:E:121:ALA:C | 1:E:366:THR:HG23 | 2.40 | 0.42 |
| 1:G:295:VAL:HG21 | 1:G:306:PRO:HA | 2.01 | 0.42 |
| 1:G:76:ARG:HD3 | 1:G:100:LEU:O | 2.19 | 0.42 |
| 1:A:177:VAL:HA | 1:A:262:ILE:O | 2.19 | 0.42 |
| 1:A:290:ILE:HD12 | 1:A:317:ILE:CD1 | 2.49 | 0.42 |
| 1:A:327:VAL:O | 1:A:328:ALA:C | 2.58 | 0.42 |
| 1:A:362:THR:HG22 | 1:A:363:VAL:HG23 | 2.01 | 0.42 |
| 1:B:281:VAL:HG23 | 1:B:313:HIS:CD2 | 2.54 | 0.42 |
| 1:D:204:ARG:O | 1:D:206:ALA:N | 2.53 | 0.42 |
| 1:D:320:HIS:CD2 | 1:D:326:ARG:NH2 | 2.88 | 0.42 |
| 1:D:72:TRP:CE2 | 1:D:339:LEU:HB3 | 2.54 | 0.42 |
| 1:G:128:ILE:C | 1:G:130:ARG:H | 2.23 | 0.42 |
| 1:H:370:ARG:O | 1:H:371:ASP:C | 2.57 | 0.42 |
| 2:I:393:ASP:OD2 | 6:I:500:NDP:O3D | 2.35 | 0.42 |
| 1:A:302:PRO:HG2 | 1:A:303:LEU:HD12 | 2.02 | 0.42 |
| 1:B:187:ALA:O | 1:B:188:ILE:C | 2.57 | 0.42 |
| 1:B:58:ALA:HB3 | 1:B:64:ALA:HB2 | 2.01 | 0.42 |
| 2:C:399:ALA:HB2 | 2:C:407:ILE:CD1 | 2.49 | 0.42 |
| 1:D:51:THR:OG1 | 1:D:57:ILE:HG22 | 2.20 | 0.42 |
| 1:E:138:SER:O | 1:E:139:SER:C | 2.58 | 0.42 |
| 2:F:292:HIS:O | 2:F:293:MET:HB2 | 2.20 | 0.42 |
| 1:G:379:LEU:HD22 | 1:G:379:LEU:N | 2.35 | 0.42 |
| 1:H:22:VAL:HG21 | 1:H:336:ALA:HB1 | 2.02 | 0.42 |
| 1:H:281:VAL:CG2 | 1:H:282:THR:N | 2.83 | 0.42 |
| 2:I:318:MET:O | 2:I:322:GLN:N | 2.52 | 0.42 |
| 2:I:405:SER:OG | 2:I:406:PRO:HD2 | 2.20 | 0.42 |
| 1:A:264:THR:CG2 | 1:A:293:LEU:HD12 | 2.37 | 0.42 |
| 1:A:293:LEU:HD22 | 1:A:323:VAL:HG21 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:3:ILE:HD13 | 1:A:26:LEU:HD13 | 2.02 | 0.42 |
| 1:B:67:GLN:OE1 | 1:B:67:GLN:N | 2.44 | 0.42 |
| 1:B:80:ALA:HB2 | 1:B:85:ASP:OD2 | 2.20 | 0.42 |
| 2:C:415:VAL:C | 2:C:417:LYS:H | 2.23 | 0.42 |
| 2:C:394:VAL:HG22 | 6:C:500:NDP:O1N | 2.20 | 0.42 |
| 1:D:356:MET:SD | 1:D:356:MET:N | 2.93 | 0.42 |
| 1:E:143:LEU:HD13 | 1:E:327:VAL:CG1 | 2.50 | 0.42 |
| 1:E:325:SER:C | 1:E:327:VAL:H | 2.23 | 0.42 |
| 2:F:429:ALA:HB3 | 6:F:500:NDP:O1X | 2.18 | 0.42 |
| 2:F:439:LEU:C | 2:F:441:PHE:H | 2.24 | 0.42 |
| 1:H:46:THR:OG1 | 1:H:49:ALA:CB | 2.68 | 0.42 |
| 1:A:179:GLY:O | 1:A:184:GLY:HA3 | 2.20 | 0.41 |
| 1:A:368:VAL:O | 1:A:368:VAL:HG12 | 2.20 | 0.41 |
| 1:B:352:LYS:HG2 | 1:B:352:LYS:O | 2.20 | 0.41 |
| 2:C:416:GLU:HB3 | 2:C:439:LEU:CD2 | 2.50 | 0.41 |
| 1:D:17:ALA:O | 1:D:18:ILE:HB | 2.19 | 0.41 |
| 1:E:60:THR:HG22 | 1:E:63:GLN:CB | 2.50 | 0.41 |
| 1:G:375:VAL:O | 1:G:375:VAL:HG23 | 2.20 | 0.41 |
| 1:H:340:LEU:CD1 | 1:H:344:THR:CG2 | 2.98 | 0.41 |
| 1:A:115:ARG:HB2 | 1:A:117:ILE:HG12 | 2.01 | 0.41 |
| 1:A:207:THR:CG2 | 1:A:218:PHE:HE1 | 2.29 | 0.41 |
| 1:A:326:ARG:HG2 | 1:A:326:ARG:NH1 | 2.35 | 0.41 |
| 1:A:342:PHE:CD2 | 1:A:342:PHE:C | 2.93 | 0.41 |
| 1:B:58:ALA:CB | 1:B:64:ALA:HA | 2.51 | 0.41 |
| 2:C:426:ARG:O | 2:C:449:PHE:HD1 | 2.02 | 0.41 |
| 1:D:294:ALA:C | 1:D:299:GLY:HA2 | 2.40 | 0.41 |
| 1:D:344:THR:CA | 1:D:347:VAL:HG23 | 2.50 | 0.41 |
| 1:D:346:HIS:HD2 | 1:D:357:LYS:H | 1.67 | 0.41 |
| 1:E:95:VAL:CG1 | 1:E:118:THR:HB | 2.39 | 0.41 |
| 1:H:208:LYS:O | 1:H:212:GLU:HB2 | 2.20 | 0.41 |
| 1:A:330:ASP:O | 1:A:333:PRO:HD2 | 2.19 | 0.41 |
| 1:D:156:PHE:CZ | 1:D:259:ASP:HB3 | 2.55 | 0.41 |
| 1:D:356:MET:HB3 | 1:D:363:VAL:HG21 | 2.02 | 0.41 |
| 1:E:3:ILE:CG2 | 1:E:33:VAL:HG22 | 2.50 | 0.41 |
| 2:F:365:VAL:O | 2:F:366:PRO:C | 2.59 | 0.41 |
| 1:G:20:PRO:HD3 | 1:G:45:ILE:HD13 | 2.03 | 0.41 |
| 1:H:143:LEU:HA | 1:H:143:LEU:HD23 | 1.81 | 0.41 |
| 1:H:362:THR:HG23 | 1:H:363:VAL:HG23 | 2.02 | 0.41 |
| 1:A:118:THR:HG23 | 1:A:370:ARG:HB3 | 2.03 | 0.41 |
| 1:B:36:GLU:O | 1:B:37:GLN:C | 2.58 | 0.41 |
| 1:B:106:ARG:HH12 | 1:B:374:ILE:CD1 | 2.34 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:16:VAL:HG13 | 1:E:16:VAL:O | 2.20 | 0.41 |
| 1:G:153:ALA:HA | 1:G:160:PHE:HE1 | 1.82 | 0.41 |
| 1:G:176:LEU:HD13 | 1:G:178:PHE:HE2 | 1.86 | 0.41 |
| 1:G:265:ALA:HA | 4:G:400:NAD:O4B | 2.19 | 0.41 |
| 1:G:361:GLU:H | 1:G:361:GLU:HG2 | 1.48 | 0.41 |
| 1:H:241:GLU:CG | 1:H:244:ARG:HB2 | 2.49 | 0.41 |
| 1:A:97:MET:O | 1:A:98:CYS:HB3 | 2.19 | 0.41 |
| 1:B:181:GLY:O | 1:B:182:VAL:C | 2.59 | 0.41 |
| 1:B:242:GLU:O | 1:B:245:LYS:CB | 2.67 | 0.41 |
| 1:D:100:LEU:C | 1:D:102:ALA:N | 2.74 | 0.41 |
| 1:D:164:MET:CE | 1:D:169:THR:HG23 | 2.50 | 0.41 |
| 1:D:224:GLU:N | 1:D:227:LYS:HG2 | 2.35 | 0.41 |
| 1:G:346:HIS:ND1 | 1:G:356:MET:CE | 2.84 | 0.41 |
| 1:G:9:ARG:O | 1:G:10:ARG:C | 2.59 | 0.41 |
| 1:H:249:GLU:C | 1:H:251:VAL:H | 2.23 | 0.41 |
| 1:H:29:LEU:N | 1:H:29:LEU:HD12 | 2.35 | 0.41 |
| 1:H:368:VAL:HG12 | 1:H:374:ILE:HG23 | 2.03 | 0.41 |
| 1:H:73:LYS:HG3 | 1:H:98:CYS:SG | 2.61 | 0.41 |
| 2:I:402:ASP:OD1 | 2:I:405:SER:HB2 | 2.19 | 0.41 |
| 1:A:205:ALA:C | 1:A:207:THR:H | 2.24 | 0.41 |
| 1:D:204:ARG:C | 1:D:206:ALA:N | 2.73 | 0.41 |
| 1:D:222:ASP:O | 1:D:227:LYS:HE3 | 2.21 | 0.41 |
| 1:E:212:GLU:C | 1:E:214:LEU:H | 2.23 | 0.41 |
| 1:E:289:VAL:HA | 1:E:316:LYS:O | 2.20 | 0.41 |
| 1:E:330:ASP:O | 1:E:333:PRO:HD2 | 2.20 | 0.41 |
| 1:E:348:ASP:OD1 | 1:E:352:LYS:N | 2.53 | 0.41 |
| 1:G:122:MET:HG3 | 1:G:339:LEU:HD21 | 2.02 | 0.41 |
| 1:H:348:ASP:HB3 | 1:H:353:THR:HG22 | 2.02 | 0.41 |
| 1:A:138:SER:OG | 4:A:400:NAD:C5N | 2.68 | 0.41 |
| 1:B:10:ARG:HH12 | 1:B:76:ARG:HG2 | 1.85 | 0.41 |
| 1:B:299:GLY:C | 1:B:301:CYS:H | 2.23 | 0.41 |
| 1:B:73:LYS:HZ2 | 1:B:73:LYS:CB | 2.33 | 0.41 |
| 2:C:331:ALA:O | 2:C:335:LYS:HG3 | 2.20 | 0.41 |
| 1:D:122:MET:C | 1:D:124:LEU:N | 2.74 | 0.41 |
| 1:E:353:THR:HG22 | 1:E:354:LEU:O | 2.20 | 0.41 |
| 2:F:454:LYS:CG | 2:F:455:MET:N | 2.83 | 0.41 |
| 1:G:346:HIS:HE1 | 1:G:363:VAL:CG2 | 2.34 | 0.41 |
| 1:G:3:ILE:HG13 | 1:G:70:VAL:HG13 | 2.03 | 0.41 |
| 1:H:180:VAL:HB | 1:H:202:ASP:OD2 | 2.20 | 0.41 |
| 2:I:407:ILE:O | 2:I:409:GLY:N | 2.53 | 0.41 |
| 1:A:158:ARG:HG2 | 1:A:158:ARG:HH11 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:128:ILE:HG12 | 1:B:131:ALA:HB2 | 2.02 | 0.41 |
| 1:B:134:MET:HG2 | 1:B:342:PHE:CA | 2.51 | 0.41 |
| 1:B:208:LYS:NZ | 1:B:212:GLU:OE2 | 2.45 | 0.41 |
| 2:C:424:ILE:N | 2:C:424:ILE:CD1 | 2.82 | 0.41 |
| 1:D:244:ARG:H | 1:D:244:ARG:HD3 | 1.85 | 0.41 |
| 1:D:349:LYS:N | 1:D:349:LYS:HD2 | 2.35 | 0.41 |
| 1:E:284:MET:HE1 | 1:E:290:ILE:HD11 | 2.02 | 0.41 |
| 1:E:343:LEU:HD23 | 1:E:343:LEU:C | 2.41 | 0.41 |
| 1:E:358:LEU:CD1 | 1:E:358:LEU:H | 2.15 | 0.41 |
| 1:G:96:LEU:HB3 | 1:G:119:ALA:CB | 2.51 | 0.41 |
| 1:G:249:GLU:HA | 1:G:249:GLU:OE1 | 2.21 | 0.41 |
| 1:G:280:MET:C | 1:G:282:THR:N | 2.72 | 0.41 |
| 1:H:25:LYS:CA | 1:H:25:LYS:HE3 | 2.51 | 0.41 |
| 1:H:277:THR:O | 1:H:278:GLU:C | 2.58 | 0.41 |
| 1:A:340:LEU:HA | 1:A:340:LEU:HD12 | 1.77 | 0.41 |
| 1:D:175:VAL:CG1 | 1:D:176:LEU:H | 2.24 | 0.41 |
| 1:E:103:LEU:O | 1:E:104:THR:HG23 | 2.20 | 0.41 |
| 1:E:311:VAL:HG13 | 1:E:311:VAL:O | 2.20 | 0.41 |
| 1:E:7:LYS:HB2 | 1:E:39:ALA:HB2 | 2.01 | 0.41 |
| 1:G:176:LEU:HG | 1:G:199:MET:HB3 | 2.03 | 0.41 |
| 1:G:277:THR:C | 1:G:279:GLU:N | 2.74 | 0.41 |
| 1:H:317:ILE:N | 1:H:317:ILE:HD12 | 2.36 | 0.41 |
| 2:I:425:LYS:HE2 | 2:I:425:LYS:HB3 | 1.75 | 0.41 |
| 2:C:328:ARG:C | 2:C:328:ARG:HD2 | 2.40 | 0.41 |
| 2:C:414:ASP:HB3 | 2:C:417:LYS:HG3 | 2.02 | 0.41 |
| 1:D:138:SER:HA | 1:D:141:SER:HB3 | 2.03 | 0.41 |
| 1:D:35:VAL:HG21 | 1:D:50:LEU:CD2 | 2.49 | 0.41 |
| 1:D:65:LEU:HD23 | 1:D:65:LEU:N | 2.36 | 0.41 |
| 1:D:62:ALA:O | 1:D:66:SER:HB3 | 2.20 | 0.41 |
| 2:F:425:LYS:HB2 | 6:F:500:NDP:O2X | 2.21 | 0.41 |
| 1:H:15:ARG:CG | 1:H:15:ARG:NH2 | 2.83 | 0.41 |
| 1:H:50:LEU:HD12 | 1:H:50:LEU:HA | 1.93 | 0.41 |
| 1:A:158:ARG:HB3 | 1:B:330:ASP:OD2 | 2.21 | 0.41 |
| 1:A:178:PHE:HB2 | 1:A:263:THR:HG22 | 2.01 | 0.41 |
| 1:A:45:ILE:HG22 | 1:A:50:LEU:CD2 | 2.49 | 0.41 |
| 1:B:155:GLU:HA | 3:K:2:FRU:H61 | 2.02 | 0.41 |
| 2:C:399:ALA:CB | 2:C:407:ILE:HG13 | 2.33 | 0.41 |
| 1:D:193:ARG:O | 1:D:195:GLY:N | 2.54 | 0.41 |
| 1:D:223:ASP:HB2 | 1:D:228:THR:OG1 | 2.21 | 0.41 |
| 1:D:305:GLU:HA | 1:D:306:PRO:HD2 | 1.89 | 0.41 |
| 1:D:15:ARG:NH1 | 1:D:324:PRO:HB2 | 2.36 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:110:GLU:O | 1:E:114:LYS:HG3 | 2.20 | 0.41 |
| 1:E:84:THR:O | 1:E:84:THR:HG23 | 2.20 | 0.41 |
| 2:F:321:ALA:O | 2:F:322:GLN:HB2 | 2.21 | 0.41 |
| 1:E:213:SER:O | 2:F:322:GLN:NE2 | 2.54 | 0.41 |
| 1:G:128:ILE:HG13 | 1:G:130:ARG:H | 1.86 | 0.41 |
| 1:H:143:LEU:HD12 | 1:H:331:ALA:HA | 2.03 | 0.41 |
| 1:H:2:LYS:O | 1:H:70:VAL:HG12 | 2.21 | 0.41 |
| 1:H:61:ALA:O | 1:H:65:LEU:HD13 | 2.20 | 0.41 |
| 1:A:362:THR:CG2 | 1:A:363:VAL:N | 2.83 | 0.40 |
| 1:B:5:ILE:CG2 | 1:B:17:ALA:HB3 | 2.51 | 0.40 |
| 1:B:267:ILE:HG12 | 4:B:400:NAD:N1A | 2.36 | 0.40 |
| 2:C:425:LYS:NZ | 6:C:500:NDP:O2B | 2.54 | 0.40 |
| 2:C:454:LYS:CE | 2:C:454:LYS:HA | 2.43 | 0.40 |
| 1:D:125:MET:SD | 1:D:126:PRO:HD2 | 2.61 | 0.40 |
| 1:E:72:TRP:CZ2 | 1:E:339:LEU:HB3 | 2.56 | 0.40 |
| 1:E:87:VAL:HG22 | 1:E:87:VAL:O | 2.20 | 0.40 |
| 1:H:346:HIS:NE2 | 1:H:362:THR:CG2 | 2.83 | 0.40 |
| 1:H:91:LYS:HB2 | 1:H:91:LYS:HE3 | 1.87 | 0.40 |
| 1:B:158:ARG:HE | 1:B:158:ARG:HB3 | 1.70 | 0.40 |
| 1:B:24:LYS:HG3 | 1:B:24:LYS:H | 1.68 | 0.40 |
| 1:G:308:LYS:HD3 | 1:G:308:LYS:N | 2.36 | 0.40 |
| 1:H:178:PHE:HD1 | 1:H:263:THR:HG22 | 1.87 | 0.40 |
| 1:A:122:MET:C | 1:A:124:LEU:H | 2.24 | 0.40 |
| 1:A:208:LYS:O | 1:A:212:GLU:HG3 | 2.21 | 0.40 |
| 1:A:28:GLY:C | 1:A:30:GLY:N | 2.74 | 0.40 |
| 1:A:309:ILE:HG13 | 1:A:318:VAL:HG13 | 2.03 | 0.40 |
| 1:B:282:THR:HG22 | 1:B:313:HIS:CG | 2.56 | 0.40 |
| 1:B:336:ALA:O | 1:B:339:LEU:HB2 | 2.20 | 0.40 |
| 1:B:360:ASP:OD2 | 1:B:360:ASP:C | 2.58 | 0.40 |
| 1:B:267:ILE:HD13 | 4:B:400:NAD:N1A | 2.37 | 0.40 |
| 1:B:2:LYS:HB2 | 1:B:69:ASP:OD1 | 2.21 | 0.40 |
| 1:D:100:LEU:O | 1:D:101:GLY:C | 2.60 | 0.40 |
| 1:D:71:VAL:HB | 1:D:96:LEU:HD12 | 2.03 | 0.40 |
| 2:F:345:ILE:CG1 | 2:F:370:VAL:HG13 | 2.51 | 0.40 |
| 2:F:432:TYR:CD2 | 6:F:500:NDP:H6N | 2.55 | 0.40 |
| 1:G:47:ASP:O | 1:G:51:THR:HG23 | 2.21 | 0.40 |
| 1:G:159:ALA:HA | 1:H:146:TYR:CE2 | 2.55 | 0.40 |
| 2:C:443:ASN:ND2 | 1:H:196:ALA:O | 2.54 | 0.40 |
| 1:H:267:ILE:HA | 1:H:268:PRO:HD2 | 1.86 | 0.40 |
| 1:H:349:LYS:HG2 | 1:H:349:LYS:H | 1.58 | 0.40 |
| 1:H:51:THR:C | 1:H:53:ALA:H | 2.25 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:301:ALA:O | 2:I:305:LYS:HG2 | 2.21 | 0.40 |
| 2:I:318:MET:HB2 | 2:I:323:ALA:HB3 | 2.03 | 0.40 |
| 1:A:18:ILE:HD11 | 1:A:23:VAL:HG23 | 2.04 | 0.40 |
| 1:A:204:ARG:O | 1:A:207:THR:HB | 2.22 | 0.40 |
| 1:A:22:VAL:O | 1:A:25:LYS:N | 2.55 | 0.40 |
| 1:A:368:VAL:O | 1:A:374:ILE:HG23 | 2.22 | 0.40 |
| 1:B:147:ARG:HD3 | 1:B:151:ASP:OD2 | 2.20 | 0.40 |
| 1:B:327:VAL:O | 1:B:329:ALA:N | 2.55 | 0.40 |
| 4:B:400:NAD:O3B | 4:B:400:NAD:O1N | 2.25 | 0.40 |
| 1:E:96:LEU:HD22 | 1:E:112:LEU:CD2 | 2.51 | 0.40 |
| 1:G:136:ILE:HG13 | 1:G:137:LEU:N | 2.36 | 0.40 |
| 1:H:147:ARG:HG3 | 1:H:327:VAL:CG2 | 2.50 | 0.40 |
| 1:H:26:LEU:HD21 | 1:H:72:TRP:HZ2 | 1.85 | 0.40 |
| 2:I:318:MET:HE1 | 2:I:324:GLN:HB3 | 2.04 | 0.40 |
| 2:C:309:LYS:HE3 | 2:C:383:ALA:HB2 | 2.02 | 0.40 |
| 1:D:17:ALA:HB1 | 1:D:339:LEU:CD1 | 2.52 | 0.40 |
| 1:D:223:ASP:HA | 1:D:227:LYS:CG | 2.51 | 0.40 |
| 1:E:143:LEU:CD1 | 1:E:331:ALA:HB2 | 2.51 | 0.40 |
| 1:G:7:LYS:CG | 1:G:39:ALA:HA | 2.51 | 0.40 |
| 1:G:69:ASP:O | 1:G:94:ALA:HB1 | 2.22 | 0.40 |
| 1:G:99:HIS:HB2 | 1:G:136:ILE:CD1 | 2.51 | 0.40 |
| 1:H:270:LYS:HB2 | 1:H:271:PRO:CD | 2.51 | 0.40 |
| 1:H:203:VAL:HG22 | 4:H:400:NAD:C8A | 2.51 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 1 | A | 359/384 (94%) | 289 (80%) | 51 (14%) | 19 (5%) | 2 | 12 |
| 1 | B | 355/384 (92%) | 273 (77%) | 57 (16%) | 25 (7%) | 1 | 7 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1 | D | 376/384 (98%) | 277 (74%) | 66 (18%) | 33 (9%) | 1 | 4 |
| 1 | E | 355/384 (92%) | 265 (75%) | 66 (19%) | 24 (7%) | 1 | 7 |
| 1 | G | 360/384 (94%) | 292 (81%) | 50 (14%) | 18 (5%) | 2 | 13 |
| 1 | H | 353/384 (92%) | 258 (73%) | 77 (22%) | 18 (5%) | 2 | 13 |
| 2 | C | 172/174 (99%) | 133 (77%) | 35 (20%) | 4 (2%) | 6 | 28 |
| 2 | F | 171/174 (98%) | 141 (82%) | 21 (12%) | 9 (5%) | 2 | 12 |
| 2 | I | 171/174 (98%) | 125 (73%) | 29 (17%) | 17 (10%) | 0 | 3 |
| All | All | 2672/2826 (95%) | 2053 (77%) | 452 (17%) | 167 (6%) | 1 | 8 |

All (167) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 270 | LYS |
| 1 | A | 357 | LYS |
| 1 | A | 358 | LEU |
| 1 | A | 378 | ALA |
| 1 | B | 371 | ASP |
| 1 | D | 18 | ILE |
| 1 | D | 66 | SER |
| 1 | D | 92 | GLU |
| 1 | D | 127 | ARG |
| 1 | D | 222 | ASP |
| 1 | D | 224 | GLU |
| 1 | D | 241 | GLU |
| 1 | D | 268 | PRO |
| 1 | D | 328 | ALA |
| 1 | E | 66 | SER |
| 1 | E | 98 | CYS |
| 1 | E | 328 | ALA |
| 1 | E | 348 | ASP |
| 1 | E | 356 | MET |
| 2 | F | 402 | ASP |
| 2 | F | 408 | TYR |
| 1 | G | 129 | SER |
| 1 | G | 248 | ALA |
| 1 | G | 274 | VAL |
| 1 | G | 357 | LYS |
| 2 | I | 324 | GLN |
| 2 | I | 378 | SER |
| 2 | I | 402 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | I | 463 | MET |
| 1 | A | 37 | GLN |
| 1 | A | 93 | GLY |
| 1 | A | 328 | ALA |
| 1 | B | 51 | THR |
| 1 | B | 66 | SER |
| 1 | B | 102 | ALA |
| 1 | B | 328 | ALA |
| 1 | B | 342 | PHE |
| 1 | B | 348 | ASP |
| 1 | B | 355 | VAL |
| 1 | B | 357 | LYS |
| 2 | C | 414 | ASP |
| 1 | D | 194 | LEU |
| 1 | D | 352 | LYS |
| 1 | D | 355 | VAL |
| 1 | D | 374 | ILE |
| 1 | E | 17 | ALA |
| 1 | E | 127 | ARG |
| 1 | E | 136 | ILE |
| 1 | E | 371 | ASP |
| 2 | F | 394 | VAL |
| 2 | F | 438 | GLU |
| 1 | G | 204 | ARG |
| 1 | G | 221 | VAL |
| 1 | G | 244 | ARG |
| 1 | G | 358 | LEU |
| 1 | H | 180 | VAL |
| 1 | H | 295 | VAL |
| 1 | H | 357 | LYS |
| 1 | H | 361 | GLU |
| 2 | I | 374 | GLU |
| 2 | I | 379 | SER |
| 2 | I | 408 | TYR |
| 1 | A | 82 | GLU |
| 1 | A | 127 | ARG |
| 1 | A | 278 | GLU |
| 1 | A | 304 | SER |
| 1 | A | 346 | HIS |
| 1 | A | 371 | ASP |
| 1 | B | 37 | GLN |
| 1 | B | 88 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 127 | ARG |
| 1 | B | 157 | ALA |
| 1 | B | 268 | PRO |
| 1 | B | 340 | LEU |
| 1 | B | 378 | ALA |
| 2 | C | 373 | LEU |
| 2 | C | 380 | PHE |
| 2 | C | 416 | GLU |
| 1 | D | 64 | ALA |
| 1 | D | 102 | ALA |
| 1 | D | 232 | ALA |
| 1 | D | 357 | LYS |
| 1 | E | 87 | VAL |
| 1 | E | 104 | THR |
| 1 | E | 196 | ALA |
| 1 | E | 204 | ARG |
| 1 | E | 274 | VAL |
| 1 | E | 357 | LYS |
| 2 | F | 293 | MET |
| 1 | G | 92 | GLU |
| 1 | G | 111 | ALA |
| 1 | G | 348 | ASP |
| 1 | G | 371 | ASP |
| 1 | H | 66 | SER |
| 1 | H | 128 | ILE |
| 1 | H | 244 | ARG |
| 1 | H | 265 | ALA |
| 1 | H | 338 | ASN |
| 1 | H | 344 | THR |
| 1 | H | 354 | LEU |
| 2 | I | 414 | ASP |
| 2 | I | 431 | GLY |
| 2 | I | 434 | GLY |
| 2 | I | 438 | GLU |
| 2 | I | 440 | PHE |
| 1 | A | 114 | LYS |
| 1 | B | 116 | LYS |
| 1 | B | 158 | ARG |
| 1 | B | 187 | ALA |
| 1 | B | 188 | ILE |
| 1 | B | 349 | LYS |
| 1 | D | 74 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 76 | ARG |
| 1 | D | 83 | GLY |
| 1 | D | 176 | LEU |
| 1 | D | 205 | ALA |
| 1 | D | 238 | GLU |
| 1 | E | 358 | LEU |
| 2 | F | 324 | GLN |
| 2 | F | 347 | PRO |
| 2 | F | 373 | LEU |
| 1 | H | 11 | PRO |
| 1 | H | 98 | CYS |
| 2 | I | 293 | MET |
| 2 | I | 452 | ALA |
| 1 | A | 103 | LEU |
| 1 | B | 6 | PRO |
| 1 | D | 98 | CYS |
| 1 | D | 141 | SER |
| 1 | D | 358 | LEU |
| 1 | E | 65 | LEU |
| 1 | E | 129 | SER |
| 1 | G | 322 | ASN |
| 1 | G | 369 | THR |
| 2 | I | 444 | ASN |
| 1 | D | 77 | PRO |
| 1 | D | 281 | VAL |
| 1 | E | 269 | GLY |
| 1 | G | 110 | GLU |
| 1 | G | 295 | VAL |
| 1 | H | 103 | LEU |
| 1 | H | 125 | MET |
| 1 | H | 205 | ALA |
| 1 | H | 358 | LEU |
| 2 | I | 316 | TYR |
| 2 | I | 339 | VAL |
| 1 | A | 305 | GLU |
| 1 | D | 20 | PRO |
| 1 | E | 355 | VAL |
| 1 | H | 355 | VAL |
| 1 | B | 128 | ILE |
| 1 | D | 306 | PRO |
| 1 | G | 375 | VAL |
| 1 | G | 377 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 377 | PRO |
| 1 | D | 299 | GLY |
| 1 | E | 18 | ILE |
| 1 | E | 306 | PRO |
| 2 | F | 376 | ILE |
| 1 | B | 179 | GLY |
| 1 | D | 23 | VAL |
| 1 | D | 327 | VAL |
| 1 | E | 180 | VAL |
| 1 | A | 6 | PRO |
| 1 | A | 83 | GLY |
| 1 | A | 375 | VAL |
| 1 | E | 345 | 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 | 284/296 (96%) | 254 (89%) | 30 (11%) | 6 | 26 |
| 1 | B | 281/296 (95%) | 253 (90%) | 28 (10%) | 7 | 28 |
| 1 | D | 293/296 (99%) | 255 (87%) | 38 (13%) | 4 | 18 |
| 1 | E | 281/296 (95%) | 257 (92%) | 24 (8%) | 10 | 37 |
| 1 | G | 284/296 (96%) | 260 (92%) | 24 (8%) | 10 | 37 |
| 1 | H | 280/296 (95%) | 243 (87%) | 37 (13%) | 4 | 17 |
| 2 | C | 138/138 (100%) | 125 (91%) | 13 (9%) | 8 | 32 |
| 2 | F | 137/138 (99%) | 128 (93%) | 9 (7%) | 16 | 47 |
| 2 | I | 137/138 (99%) | 128 (93%) | 9 (7%) | 16 | 47 |
| All | All | 2115/2190 (97%) | 1903 (90%) | 212 (10%) | 7 | 28 |

All (212) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 2 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 41 | VAL |
| 1 | A | 46 | THR |
| 1 | A | 51 | THR |
| 1 | A | 76 | ARG |
| 1 | A | 81 | GLU |
| 1 | A | 84 | THR |
| 1 | A | 91 | LYS |
| 1 | A | 95 | VAL |
| 1 | A | 96 | LEU |
| 1 | A | 110 | GLU |
| 1 | A | 127 | ARG |
| 1 | A | 164 | MET |
| 1 | A | 170 | VAL |
| 1 | A | 176 | LEU |
| 1 | A | 199 | MET |
| 1 | A | 203 | VAL |
| 1 | A | 211 | VAL |
| 1 | A | 217 | LYS |
| 1 | A | 222 | ASP |
| 1 | A | 243 | PHE |
| 1 | A | 270 | LYS |
| 1 | A | 271 | PRO |
| 1 | A | 305 | GLU |
| 1 | A | 348 | ASP |
| 1 | A | 350 | ASP |
| 1 | A | 354 | LEU |
| 1 | A | 358 | LEU |
| 1 | A | 362 | THR |
| 1 | A | 366 | THR |
| 1 | B | 1 | MET |
| 1 | B | 19 | SER |
| 1 | B | 65 | LEU |
| 1 | B | 71 | VAL |
| 1 | B | 107 | PRO |
| 1 | B | 115 | ARG |
| 1 | B | 130 | ARG |
| 1 | B | 134 | MET |
| 1 | B | 147 | ARG |
| 1 | B | 164 | MET |
| 1 | B | 176 | LEU |
| 1 | B | 194 | LEU |
| 1 | B | 217 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 244 | ARG |
| 1 | B | 252 | LEU |
| 1 | B | 267 | ILE |
| 1 | B | 277 | THR |
| 1 | B | 279 | GLU |
| 1 | B | 289 | VAL |
| 1 | B | 296 | GLU |
| 1 | B | 325 | SER |
| 1 | B | 344 | THR |
| 1 | B | 348 | ASP |
| 1 | B | 350 | ASP |
| 1 | B | 354 | LEU |
| 1 | B | 358 | LEU |
| 1 | B | 369 | THR |
| 1 | B | 371 | ASP |
| 2 | C | 291 | ARG |
| 2 | C | 298 | GLU |
| 2 | C | 318 | MET |
| 2 | C | 358 | VAL |
| 2 | C | 372 | GLU |
| 2 | C | 376 | ILE |
| 2 | C | 382 | THR |
| 2 | C | 416 | GLU |
| 2 | C | 420 | THR |
| 2 | C | 425 | LYS |
| 2 | C | 444 | ASN |
| 2 | C | 454 | LYS |
| 2 | C | 464 | ASN |
| 1 | D | 8 | GLU |
| 1 | D | 13 | GLU |
| 1 | D | 18 | ILE |
| 1 | D | 20 | PRO |
| 1 | D | 21 | GLU |
| 1 | D | 24 | LYS |
| 1 | D | 29 | LEU |
| 1 | D | 70 | VAL |
| 1 | D | 81 | GLU |
| 1 | D | 109 | VAL |
| 1 | D | 114 | LYS |
| 1 | D | 124 | LEU |
| 1 | D | 129 | SER |
| 1 | D | 134 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 136 | ILE |
| 1 | D | 137 | LEU |
| 1 | D | 170 | VAL |
| 1 | D | 176 | LEU |
| 1 | D | 192 | LYS |
| 1 | D | 199 | MET |
| 1 | D | 207 | THR |
| 1 | D | 208 | LYS |
| 1 | D | 221 | VAL |
| 1 | D | 241 | GLU |
| 1 | D | 249 | GLU |
| 1 | D | 252 | LEU |
| 1 | D | 255 | LEU |
| 1 | D | 268 | PRO |
| 1 | D | 322 | ASN |
| 1 | D | 346 | HIS |
| 1 | D | 350 | ASP |
| 1 | D | 351 | THR |
| 1 | D | 354 | LEU |
| 1 | D | 355 | VAL |
| 1 | D | 356 | MET |
| 1 | D | 362 | THR |
| 1 | D | 368 | VAL |
| 1 | D | 371 | ASP |
| 1 | E | 21 | GLU |
| 1 | E | 95 | VAL |
| 1 | E | 96 | LEU |
| 1 | E | 104 | THR |
| 1 | E | 105 | ASN |
| 1 | E | 127 | ARG |
| 1 | E | 132 | GLN |
| 1 | E | 134 | MET |
| 1 | E | 147 | ARG |
| 1 | E | 176 | LEU |
| 1 | E | 207 | THR |
| 1 | E | 210 | GLN |
| 1 | E | 241 | GLU |
| 1 | E | 242 | GLU |
| 1 | E | 244 | ARG |
| 1 | E | 252 | LEU |
| 1 | E | 253 | LYS |
| 1 | E | 258 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 270 | LYS |
| 1 | E | 330 | ASP |
| 1 | E | 346 | HIS |
| 1 | E | 348 | ASP |
| 1 | E | 349 | LYS |
| 1 | E | 350 | ASP |
| 2 | F | 298 | GLU |
| 2 | F | 318 | MET |
| 2 | F | 324 | GLN |
| 2 | F | 342 | SER |
| 2 | F | 364 | ASN |
| 2 | F | 367 | TYR |
| 2 | F | 374 | GLU |
| 2 | F | 384 | ASP |
| 2 | F | 420 | THR |
| 1 | G | 10 | ARG |
| 1 | G | 27 | VAL |
| 1 | G | 31 | PHE |
| 1 | G | 41 | VAL |
| 1 | G | 60 | THR |
| 1 | G | 92 | GLU |
| 1 | G | 164 | MET |
| 1 | G | 170 | VAL |
| 1 | G | 176 | LEU |
| 1 | G | 177 | VAL |
| 1 | G | 192 | LYS |
| 1 | G | 198 | VAL |
| 1 | G | 199 | MET |
| 1 | G | 220 | THR |
| 1 | G | 222 | ASP |
| 1 | G | 252 | LEU |
| 1 | G | 255 | LEU |
| 1 | G | 270 | LYS |
| 1 | G | 308 | LYS |
| 1 | G | 311 | VAL |
| 1 | G | 352 | LYS |
| 1 | G | 361 | GLU |
| 1 | G | 362 | THR |
| 1 | G | 369 | THR |
| 1 | H | 1 | MET |
| 1 | H | 10 | ARG |
| 1 | H | 15 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | H | 25 | LYS |
| 1 | H | 26 | LEU |
| 1 | H | 35 | VAL |
| 1 | H | 37 | GLN |
| 1 | H | 59 | SER |
| 1 | H | 67 | GLN |
| 1 | H | 72 | TRP |
| 1 | H | 76 | ARG |
| 1 | H | 97 | MET |
| 1 | H | 105 | ASN |
| 1 | H | 112 | LEU |
| 1 | H | 125 | MET |
| 1 | H | 147 | ARG |
| 1 | H | 158 | ARG |
| 1 | H | 160 | PHE |
| 1 | H | 164 | MET |
| 1 | H | 170 | VAL |
| 1 | H | 176 | LEU |
| 1 | H | 192 | LYS |
| 1 | H | 194 | LEU |
| 1 | H | 244 | ARG |
| 1 | H | 247 | GLN |
| 1 | H | 252 | LEU |
| 1 | H | 277 | THR |
| 1 | H | 278 | GLU |
| 1 | H | 279 | GLU |
| 1 | H | 330 | ASP |
| 1 | H | 334 | LEU |
| 1 | H | 339 | LEU |
| 1 | H | 342 | PHE |
| 1 | H | 344 | THR |
| 1 | H | 352 | LYS |
| 1 | H | 354 | LEU |
| 1 | H | 356 | MET |
| 2 | I | 334 | LEU |
| 2 | I | 348 | VAL |
| 2 | I | 358 | VAL |
| 2 | I | 376 | ILE |
| 2 | I | 384 | ASP |
| 2 | I | 422 | LEU |
| 2 | I | 425 | LYS |
| 2 | I | 439 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | I | 451 | ASP |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 186 | GLN |
| 1 | A | 247 | GLN |
| 1 | A | 322 | ASN |
| 1 | A | 376 | HIS |
| 1 | B | 99 | HIS |
| 1 | B | 105 | ASN |
| 1 | B | 142 | ASN |
| 1 | B | 186 | GLN |
| 1 | B | 210 | GLN |
| 1 | B | 247 | GLN |
| 1 | B | 320 | HIS |
| 1 | B | 376 | HIS |
| 2 | C | 322 | GLN |
| 2 | C | 325 | HIS |
| 2 | C | 364 | ASN |
| 2 | C | 443 | ASN |
| 2 | C | 444 | ASN |
| 2 | C | 458 | GLN |
| 2 | C | 464 | ASN |
| 1 | D | 75 | GLN |
| 1 | D | 99 | HIS |
| 1 | D | 105 | ASN |
| 1 | D | 186 | GLN |
| 1 | D | 210 | GLN |
| 1 | D | 247 | GLN |
| 1 | D | 300 | ASN |
| 1 | D | 320 | HIS |
| 1 | D | 322 | ASN |
| 1 | D | 338 | ASN |
| 1 | D | 346 | HIS |
| 1 | D | 376 | HIS |
| 1 | E | 63 | GLN |
| 1 | E | 132 | GLN |
| 1 | E | 142 | ASN |
| 1 | E | 186 | GLN |
| 1 | E | 341 | ASN |
| 2 | F | 324 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | F | 458 | GLN |
| 1 | G | 37 | GLN |
| 1 | G | 142 | ASN |
| 1 | G | 186 | GLN |
| 1 | G | 338 | ASN |
| 1 | G | 341 | ASN |
| 1 | G | 376 | HIS |
| 1 | H | 63 | GLN |
| 1 | H | 67 | GLN |
| 1 | H | 105 | ASN |
| 1 | H | 142 | ASN |
| 1 | H | 247 | GLN |
| 1 | H | 300 | ASN |
| 1 | H | 322 | ASN |
| 1 | H | 341 | ASN |
| 1 | H | 376 | HIS |
| 2 | I | 325 | HIS |
| 2 | I | 357 | ASN |
| 2 | I | 443 | ASN |
| 2 | I | 461 | GLN |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

12 monosaccharides 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 | GLC | J | 1 | 3 | 11,11,12 | 1.25 | 1 (9%) | 15,15,17 | 0.77 | 1 (6%) |
| 3 | FRU | J | 2 | 3 | 11,12,12 | 1.46 | 2 (18%) | 10,18,18 | 0.59 | 0 |
| 3 | GLC | K | 1 | 3 | 11,11,12 | 1.17 | 1 (9%) | 15,15,17 | 0.91 | 1 (6%) |
| 3 | FRU | K | 2 | 3 | 11,12,12 | 1.53 | 2 (18%) | 10,18,18 | 0.65 | 0 |
| 3 | GLC | L | 1 | 3 | 11,11,12 | 1.29 | 1 (9%) | 15,15,17 | 0.85 | 1 (6%) |
| 3 | FRU | L | 2 | 3 | 11,12,12 | 1.53 | 2 (18%) | 10,18,18 | 0.64 | 0 |
| 3 | GLC | M | 1 | 3 | 11,11,12 | 1.03 | 1 (9%) | 15,15,17 | 0.84 | 1 (6%) |
| 3 | FRU | M | 2 | 3 | 11,12,12 | 1.63 | 2 (18%) | 10,18,18 | 0.71 | 0 |
| 3 | GLC | N | 1 | 3 | 11,11,12 | 1.37 | 1 (9%) | 15,15,17 | 0.92 | 1 (6%) |
| 3 | FRU | N | 2 | 3 | 11,12,12 | 1.67 | 3 (27%) | 10,18,18 | 0.62 | 0 |
| 3 | GLC | O | 1 | 3 | 11,11,12 | 1.34 | 1 (9%) | 15,15,17 | 0.84 | 1 (6%) |
| 3 | FRU | O | 2 | 3 | 11,12,12 | 1.54 | 2 (18%) | 10,18,18 | 0.68 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 3 | GLC | J | 1 | 3 | - | 2/2/19/22 | 0/1/1/1 |
| 3 | FRU | J | 2 | 3 | - | 0/5/24/24 | 0/1/1/1 |
| 3 | GLC | K | 1 | 3 | - | 1/2/19/22 | 0/1/1/1 |
| 3 | FRU | K | 2 | 3 | - | 2/5/24/24 | 0/1/1/1 |
| 3 | GLC | L | 1 | 3 | - | 2/2/19/22 | 0/1/1/1 |
| 3 | FRU | L | 2 | 3 | - | 0/5/24/24 | 0/1/1/1 |
| 3 | GLC | M | 1 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | FRU | M | 2 | 3 | - | 0/5/24/24 | 0/1/1/1 |
| 3 | GLC | N | 1 | 3 | - | 2/2/19/22 | 0/1/1/1 |
| 3 | FRU | N | 2 | 3 | - | 2/5/24/24 | 0/1/1/1 |
| 3 | GLC | O | 1 | 3 | - | 2/2/19/22 | 0/1/1/1 |
| 3 | FRU | O | 2 | 3 | - | 2/5/24/24 | 0/1/1/1 |

All (19) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3 | M | 2 | FRU | C4-C5 | -4.13 | 1.42 | 1.53 |
| 3 | J | 2 | FRU | C4-C5 | -3.91 | 1.43 | 1.53 |
| 3 | L | 2 | FRU | C4-C5 | -3.83 | 1.43 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3 | N | 2 | FRU | O2-C2 | 3.62 | 1.46 | 1.40 |
| 3 | O | 2 | FRU | C4-C5 | -3.54 | 1.44 | 1.53 |
| 3 | N | 1 | GLC | O5-C1 | 3.52 | 1.49 | 1.43 |
| 3 | K | 2 | FRU | O2-C2 | 3.48 | 1.46 | 1.40 |
| 3 | N | 2 | FRU | C4-C5 | -3.39 | 1.44 | 1.53 |
| 3 | K | 2 | FRU | C4-C5 | -3.38 | 1.44 | 1.53 |
| 3 | O | 1 | GLC | O5-C1 | 3.26 | 1.48 | 1.43 |
| 3 | L | 1 | GLC | O5-C1 | 3.17 | 1.48 | 1.43 |
| 3 | O | 2 | FRU | O2-C2 | 3.15 | 1.46 | 1.40 |
| 3 | K | 1 | GLC | O5-C1 | 3.12 | 1.48 | 1.43 |
| 3 | J | 1 | GLC | O5-C1 | 3.09 | 1.48 | 1.43 |
| 3 | M | 2 | FRU | O2-C2 | 3.00 | 1.45 | 1.40 |
| 3 | L | 2 | FRU | O2-C2 | 2.98 | 1.45 | 1.40 |
| 3 | M | 1 | GLC | O5-C1 | 2.78 | 1.48 | 1.43 |
| 3 | J | 2 | FRU | O2-C2 | 2.56 | 1.45 | 1.40 |
| 3 | N | 2 | FRU | C1-C2 | 2.12 | 1.55 | 1.52 |

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3 | M | 1 | GLC | C2-C3-C4 | -2.46 | 106.64 | 110.89 |
| 3 | O | 1 | GLC | C2-C3-C4 | -2.39 | 106.76 | 110.89 |
| 3 | L | 1 | GLC | C2-C3-C4 | -2.39 | 106.76 | 110.89 |
| 3 | N | 1 | GLC | C2-C3-C4 | -2.38 | 106.77 | 110.89 |
| 3 | J | 1 | GLC | C2-C3-C4 | -2.37 | 106.80 | 110.89 |
| 3 | K | 1 | GLC | C2-C3-C4 | -2.24 | 107.02 | 110.89 |

There are no chirality outliers.

All (15) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 3 | K | 2 | FRU | C4-C5-C6-O6 |
| 3 | K | 2 | FRU | O5-C5-C6-O6 |
| 3 | N | 1 | GLC | O5-C5-C6-O6 |
| 3 | N | 2 | FRU | C4-C5-C6-O6 |
| 3 | N | 2 | FRU | O5-C5-C6-O6 |
| 3 | N | 1 | GLC | C4-C5-C6-O6 |
| 3 | O | 1 | GLC | C4-C5-C6-O6 |
| 3 | O | 2 | FRU | O5-C5-C6-O6 |
| 3 | J | 1 | GLC | C4-C5-C6-O6 |
| 3 | L | 1 | GLC | C4-C5-C6-O6 |
| 3 | O | 2 | FRU | C4-C5-C6-O6 |

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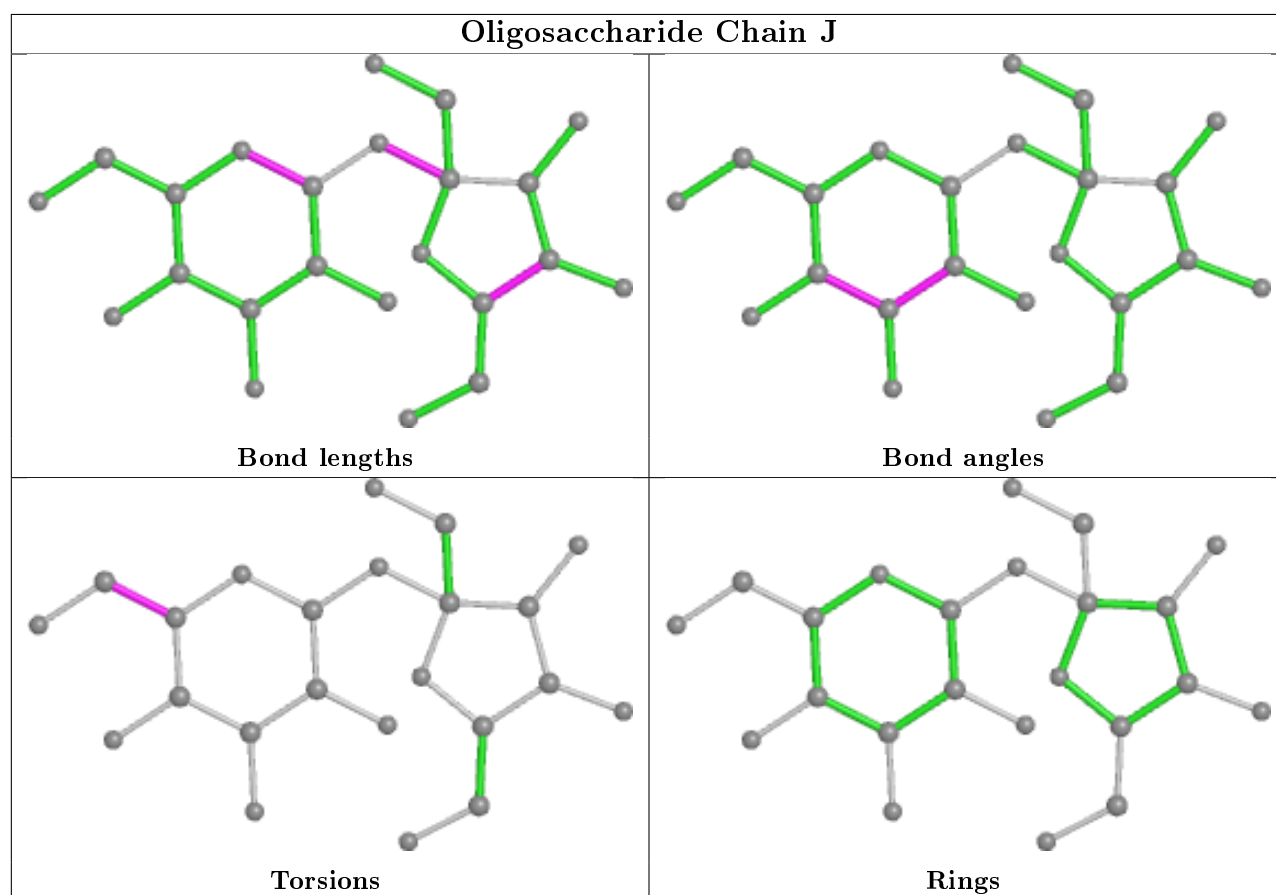
| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 3 | O | 1 | GLC | O5-C5-C6-O6 |
| 3 | J | 1 | GLC | O5-C5-C6-O6 |
| 3 | K | 1 | GLC | C4-C5-C6-O6 |
| 3 | L | 1 | GLC | O5-C5-C6-O6 |

There are no ring outliers.

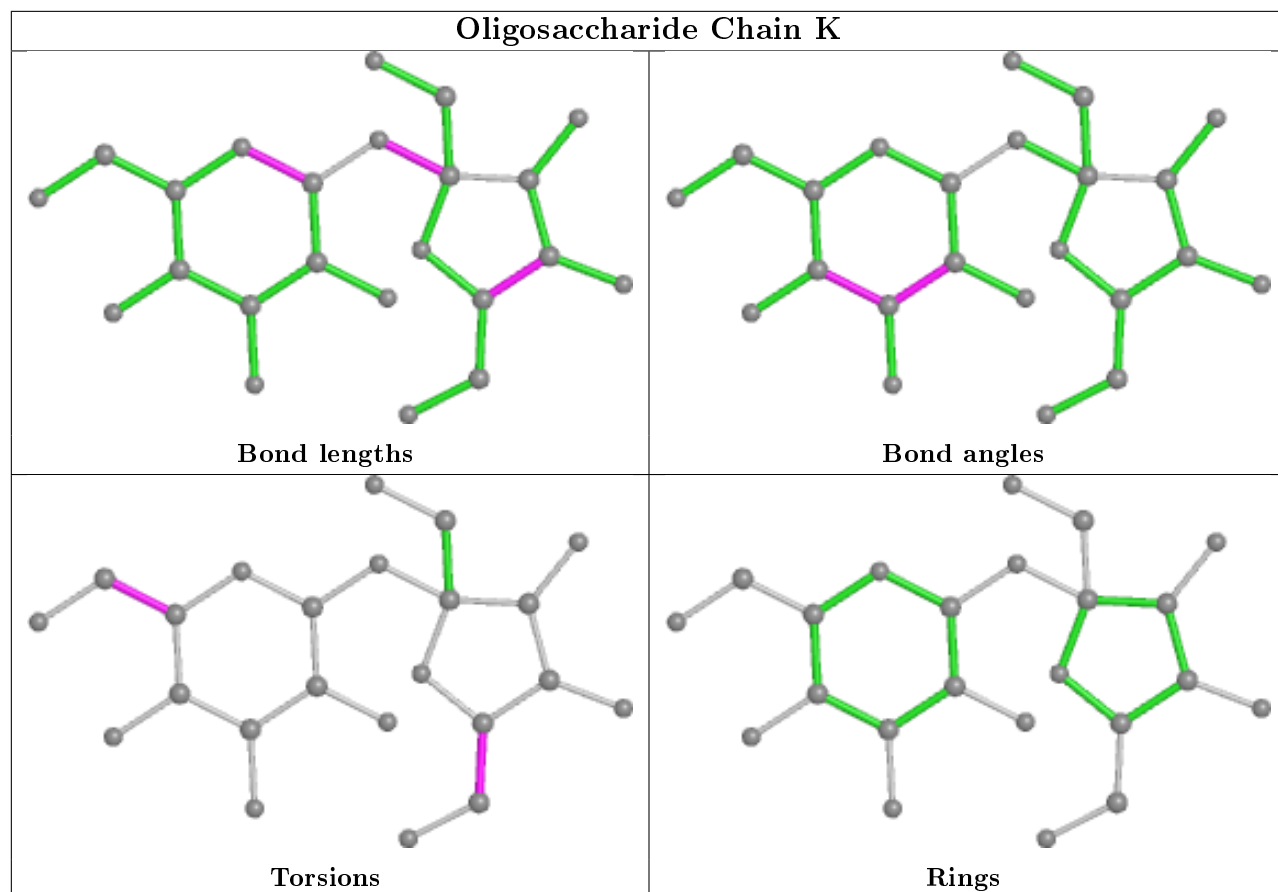
2 monomers are involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3 | O | 2 | FRU | 1 | 0 |
| 3 | K | 2 | FRU | 1 | 0 |

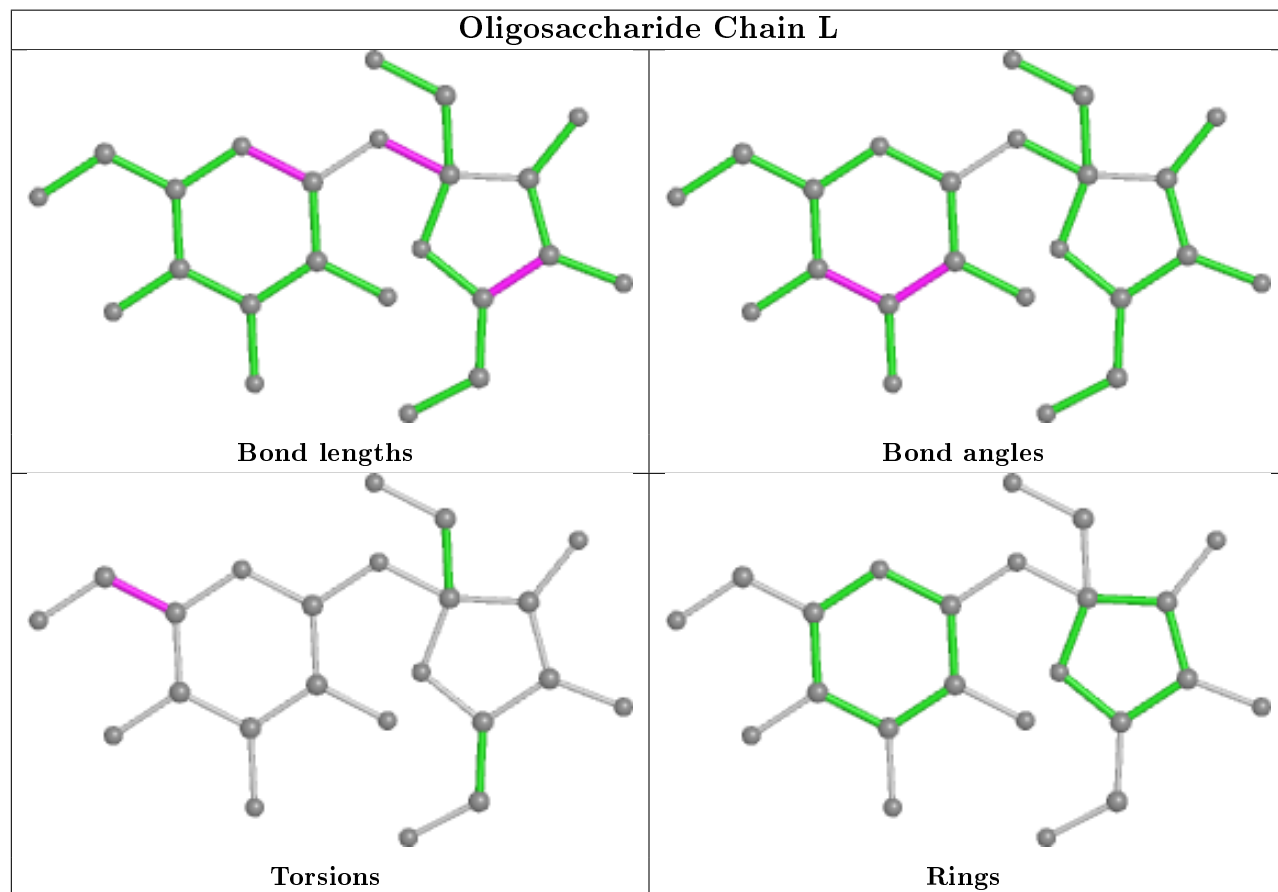
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



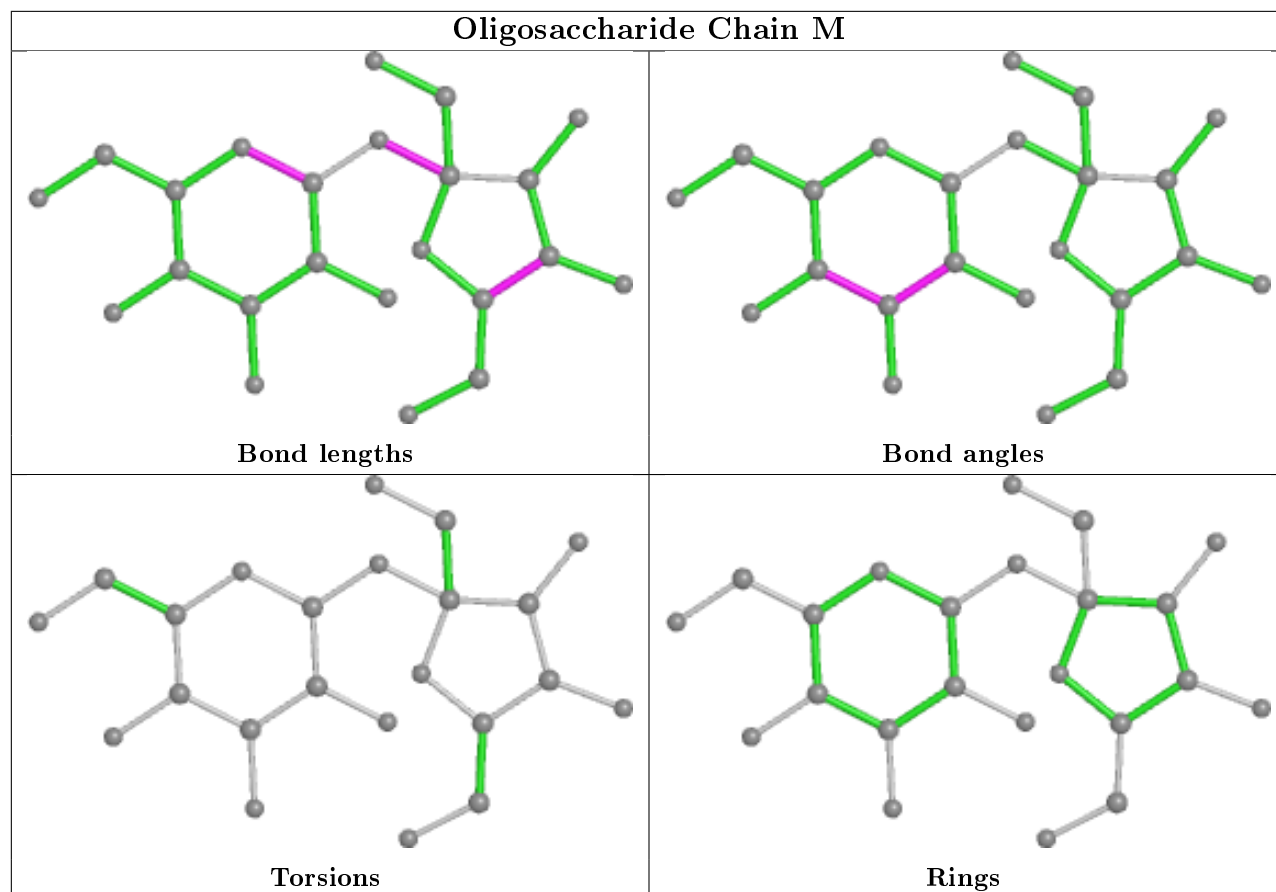
Oligosaccharide Chain K



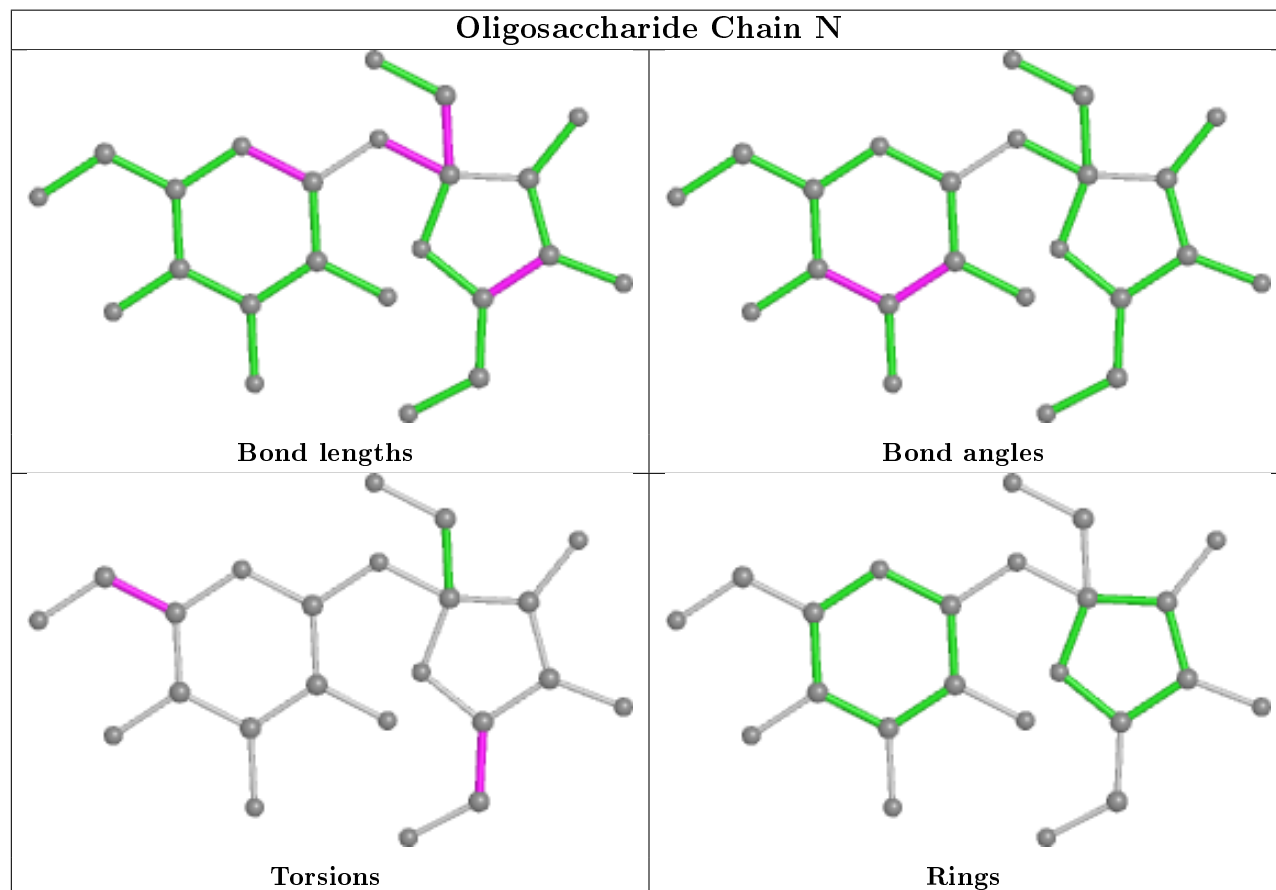
Oligosaccharide Chain L

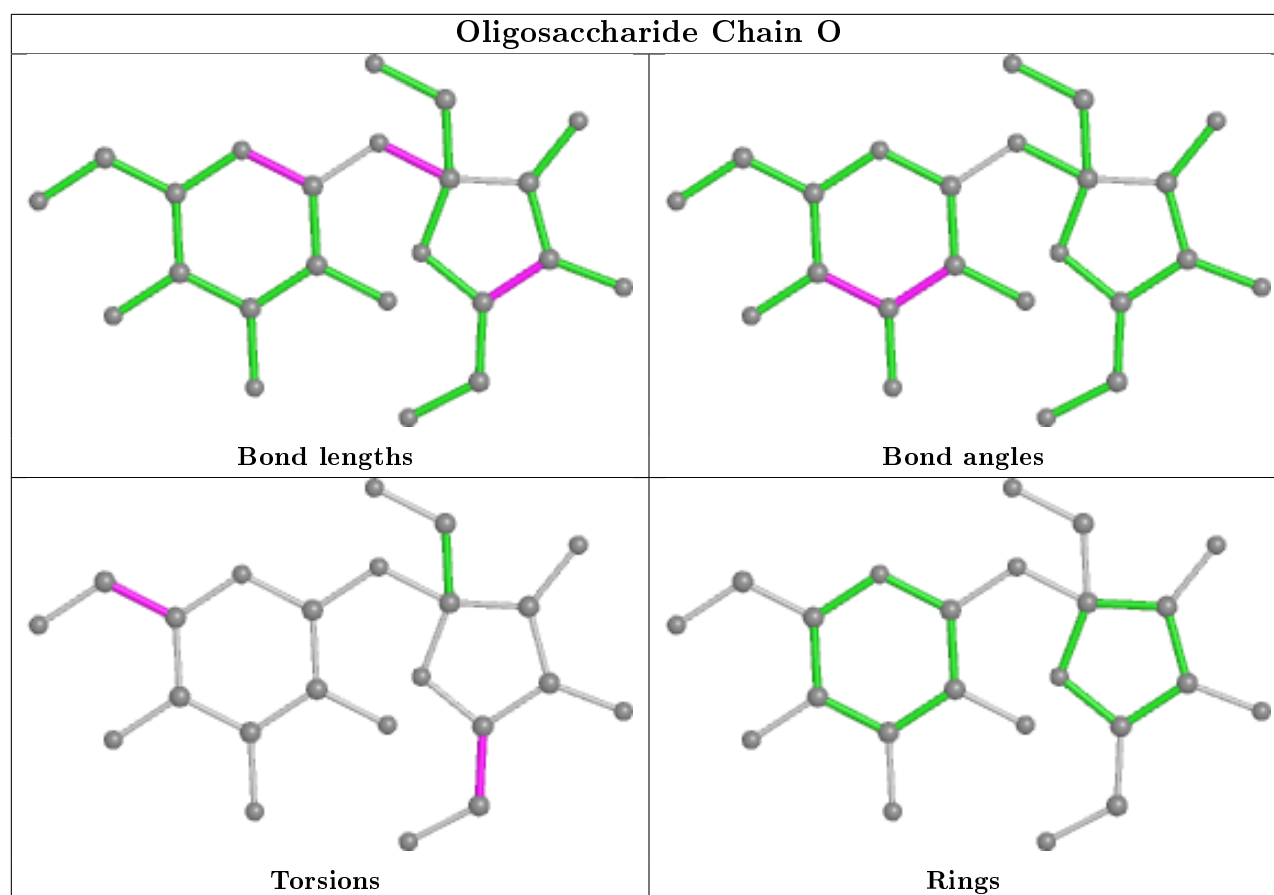


Oligosaccharide Chain M



Oligosaccharide Chain N





5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 4 | NAD | H | 400 | - | 42,48,48 | 2.47 | 15 (35%) | 50,73,73 | 2.27 | 17 (34%) |
| 6 | NDP | I | 500 | - | 45,52,52 | 2.39 | 16 (35%) | 53,80,80 | 2.04 | 18 (33%) |
| 4 | NAD | A | 400 | - | 42,48,48 | 2.58 | 18 (42%) | 50,73,73 | 2.49 | 21 (42%) |
| 4 | NAD | B | 400 | - | 42,48,48 | 2.75 | 19 (45%) | 50,73,73 | 2.64 | 17 (34%) |
| 4 | NAD | G | 400 | - | 42,48,48 | 2.55 | 14 (33%) | 50,73,73 | 2.82 | 21 (42%) |
| 6 | NDP | F | 500 | - | 45,52,52 | 2.05 | 13 (28%) | 53,80,80 | 1.95 | 17 (32%) |
| 6 | NDP | C | 500 | - | 45,52,52 | 2.02 | 15 (33%) | 53,80,80 | 2.02 | 20 (37%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 4 | NAD | D | 400 | - | 42,48,48 | 2.47 | 14 (33%) | 50,73,73 | 2.26 | 20 (40%) |

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 |
|-----|------|-------|-----|------|---------|-------------|---------|
| 4 | NAD | H | 400 | - | - | 11/26/62/62 | 0/5/5/5 |
| 6 | NDP | I | 500 | - | - | 13/30/77/77 | 0/5/5/5 |
| 4 | NAD | A | 400 | - | - | 15/26/62/62 | 0/5/5/5 |
| 4 | NAD | B | 400 | - | - | 16/26/62/62 | 0/5/5/5 |
| 4 | NAD | G | 400 | - | - | 8/26/62/62 | 0/5/5/5 |
| 6 | NDP | F | 500 | - | - | 14/30/77/77 | 0/5/5/5 |
| 6 | NDP | C | 500 | - | - | 12/30/77/77 | 0/5/5/5 |
| 4 | NAD | D | 400 | - | - | 9/26/62/62 | 0/5/5/5 |

All (124) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6 | I | 500 | NDP | O4D-C1D | 8.19 | 1.61 | 1.42 |
| 4 | B | 400 | NAD | O4B-C1B | 7.74 | 1.51 | 1.41 |
| 4 | H | 400 | NAD | O4B-C1B | 7.44 | 1.51 | 1.41 |
| 4 | A | 400 | NAD | O4B-C1B | 7.32 | 1.51 | 1.41 |
| 4 | D | 400 | NAD | O4B-C1B | 7.20 | 1.51 | 1.41 |
| 4 | B | 400 | NAD | C2N-N1N | 7.14 | 1.43 | 1.35 |
| 4 | G | 400 | NAD | C2N-N1N | 7.02 | 1.43 | 1.35 |
| 4 | G | 400 | NAD | O4B-C1B | 6.81 | 1.50 | 1.41 |
| 4 | A | 400 | NAD | C2N-N1N | 6.50 | 1.42 | 1.35 |
| 6 | I | 500 | NDP | O4B-C1B | 6.29 | 1.49 | 1.41 |
| 6 | C | 500 | NDP | O4B-C1B | 6.19 | 1.49 | 1.41 |
| 6 | F | 500 | NDP | O4B-C1B | 5.85 | 1.49 | 1.41 |
| 4 | D | 400 | NAD | C2N-N1N | 5.54 | 1.41 | 1.35 |
| 4 | H | 400 | NAD | C2N-N1N | 5.52 | 1.41 | 1.35 |
| 4 | G | 400 | NAD | C2B-C1B | -5.31 | 1.45 | 1.53 |
| 4 | A | 400 | NAD | O4D-C1D | 5.15 | 1.48 | 1.41 |
| 4 | H | 400 | NAD | C2B-C1B | -5.10 | 1.46 | 1.53 |
| 4 | B | 400 | NAD | C6N-N1N | 4.83 | 1.47 | 1.35 |
| 4 | G | 400 | NAD | C6N-N1N | 4.78 | 1.47 | 1.35 |
| 4 | B | 400 | NAD | C2B-C1B | -4.71 | 1.46 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | D | 400 | NAD | C5A-C4A | 4.57 | 1.53 | 1.40 |
| 4 | A | 400 | NAD | C2B-C1B | -4.57 | 1.46 | 1.53 |
| 4 | G | 400 | NAD | C2N-C3N | 4.56 | 1.46 | 1.39 |
| 4 | H | 400 | NAD | C6N-N1N | 4.48 | 1.46 | 1.35 |
| 4 | B | 400 | NAD | C2N-C3N | 4.38 | 1.45 | 1.39 |
| 4 | D | 400 | NAD | C6N-N1N | 4.35 | 1.46 | 1.35 |
| 4 | H | 400 | NAD | PN-O5D | -4.33 | 1.41 | 1.59 |
| 4 | H | 400 | NAD | C5A-C4A | 4.27 | 1.52 | 1.40 |
| 4 | B | 400 | NAD | O4D-C1D | 4.26 | 1.47 | 1.41 |
| 4 | G | 400 | NAD | C5A-C4A | 4.26 | 1.52 | 1.40 |
| 4 | B | 400 | NAD | C5A-C4A | 4.25 | 1.52 | 1.40 |
| 6 | I | 500 | NDP | C5A-C4A | 4.24 | 1.52 | 1.40 |
| 6 | F | 500 | NDP | C5A-C4A | 4.10 | 1.51 | 1.40 |
| 4 | D | 400 | NAD | C2B-C1B | -4.07 | 1.47 | 1.53 |
| 4 | D | 400 | NAD | O4D-C1D | 4.03 | 1.46 | 1.41 |
| 6 | F | 500 | NDP | C4N-C5N | -4.03 | 1.38 | 1.48 |
| 4 | A | 400 | NAD | C6N-N1N | 4.02 | 1.45 | 1.35 |
| 4 | A | 400 | NAD | C5A-C4A | 3.99 | 1.51 | 1.40 |
| 4 | A | 400 | NAD | C2N-C3N | 3.87 | 1.45 | 1.39 |
| 6 | I | 500 | NDP | C4N-C5N | -3.82 | 1.38 | 1.48 |
| 6 | I | 500 | NDP | C2N-C3N | 3.71 | 1.45 | 1.34 |
| 4 | D | 400 | NAD | C2N-C3N | 3.67 | 1.44 | 1.39 |
| 4 | D | 400 | NAD | C4N-C3N | 3.63 | 1.45 | 1.39 |
| 6 | F | 500 | NDP | C2N-C3N | 3.60 | 1.45 | 1.34 |
| 6 | C | 500 | NDP | C4N-C5N | -3.58 | 1.39 | 1.48 |
| 4 | B | 400 | NAD | C2D-C1D | 3.56 | 1.59 | 1.53 |
| 6 | F | 500 | NDP | C4N-C3N | -3.47 | 1.43 | 1.49 |
| 4 | H | 400 | NAD | C2N-C3N | 3.47 | 1.44 | 1.39 |
| 6 | C | 500 | NDP | C5A-C4A | 3.37 | 1.49 | 1.40 |
| 6 | F | 500 | NDP | C2D-C1D | 3.34 | 1.64 | 1.53 |
| 4 | D | 400 | NAD | C2A-N1A | 3.29 | 1.40 | 1.33 |
| 6 | I | 500 | NDP | C4N-C3N | -3.21 | 1.43 | 1.49 |
| 4 | G | 400 | NAD | C4N-C3N | 3.18 | 1.44 | 1.39 |
| 4 | H | 400 | NAD | C4N-C3N | 3.18 | 1.44 | 1.39 |
| 4 | B | 400 | NAD | C4N-C3N | 3.18 | 1.44 | 1.39 |
| 4 | B | 400 | NAD | PN-O2N | 3.17 | 1.70 | 1.55 |
| 6 | C | 500 | NDP | C6N-N1N | 3.13 | 1.45 | 1.37 |
| 6 | F | 500 | NDP | C3B-C4B | -3.12 | 1.45 | 1.53 |
| 6 | I | 500 | NDP | C6N-C5N | 3.12 | 1.38 | 1.33 |
| 6 | C | 500 | NDP | C4N-C3N | -3.11 | 1.43 | 1.49 |
| 6 | C | 500 | NDP | C6N-C5N | 3.06 | 1.38 | 1.33 |
| 6 | C | 500 | NDP | C2N-C3N | 3.06 | 1.43 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6 | C | 500 | NDP | C3B-C2B | -3.05 | 1.46 | 1.52 |
| 6 | I | 500 | NDP | C6N-N1N | 3.05 | 1.44 | 1.37 |
| 4 | G | 400 | NAD | C2D-C1D | -3.03 | 1.49 | 1.53 |
| 6 | I | 500 | NDP | C3B-C2B | -2.99 | 1.46 | 1.52 |
| 4 | G | 400 | NAD | C2A-N1A | 2.95 | 1.39 | 1.33 |
| 6 | C | 500 | NDP | P2B-O3X | -2.92 | 1.43 | 1.54 |
| 4 | D | 400 | NAD | C3B-C4B | -2.87 | 1.45 | 1.53 |
| 4 | H | 400 | NAD | C2A-N1A | 2.86 | 1.39 | 1.33 |
| 6 | F | 500 | NDP | C6N-N1N | 2.83 | 1.44 | 1.37 |
| 6 | I | 500 | NDP | C2A-N1A | 2.81 | 1.39 | 1.33 |
| 4 | G | 400 | NAD | O2B-C2B | -2.73 | 1.36 | 1.43 |
| 6 | C | 500 | NDP | O4D-C1D | 2.73 | 1.48 | 1.42 |
| 4 | B | 400 | NAD | C2D-C3D | 2.71 | 1.60 | 1.53 |
| 4 | D | 400 | NAD | O2B-C2B | -2.70 | 1.36 | 1.43 |
| 4 | B | 400 | NAD | C2A-N1A | 2.70 | 1.38 | 1.33 |
| 4 | A | 400 | NAD | C2D-C3D | 2.69 | 1.60 | 1.53 |
| 4 | A | 400 | NAD | PN-O5D | -2.65 | 1.48 | 1.59 |
| 6 | F | 500 | NDP | C6N-C5N | 2.65 | 1.38 | 1.33 |
| 6 | I | 500 | NDP | C2A-N3A | 2.64 | 1.36 | 1.32 |
| 4 | A | 400 | NAD | C2A-N1A | 2.61 | 1.38 | 1.33 |
| 4 | D | 400 | NAD | C2A-N3A | 2.61 | 1.36 | 1.32 |
| 4 | A | 400 | NAD | C2D-C1D | 2.61 | 1.57 | 1.53 |
| 4 | G | 400 | NAD | C2A-N3A | 2.60 | 1.36 | 1.32 |
| 6 | C | 500 | NDP | C3B-C4B | -2.60 | 1.46 | 1.53 |
| 4 | H | 400 | NAD | C2A-N3A | 2.58 | 1.36 | 1.32 |
| 4 | G | 400 | NAD | C3B-C4B | -2.57 | 1.46 | 1.53 |
| 6 | I | 500 | NDP | P2B-O3X | -2.54 | 1.45 | 1.54 |
| 6 | F | 500 | NDP | C3B-C2B | -2.53 | 1.47 | 1.52 |
| 4 | A | 400 | NAD | C4N-C3N | 2.50 | 1.43 | 1.39 |
| 6 | F | 500 | NDP | C2A-N1A | 2.49 | 1.38 | 1.33 |
| 4 | B | 400 | NAD | O2B-C2B | -2.49 | 1.37 | 1.43 |
| 6 | F | 500 | NDP | P2B-O3X | -2.48 | 1.45 | 1.54 |
| 4 | B | 400 | NAD | O5B-C5B | -2.46 | 1.35 | 1.44 |
| 4 | A | 400 | NAD | PN-O2N | -2.44 | 1.43 | 1.55 |
| 4 | H | 400 | NAD | O2B-C2B | -2.43 | 1.37 | 1.43 |
| 6 | C | 500 | NDP | C1D-N1N | 2.42 | 1.53 | 1.46 |
| 6 | I | 500 | NDP | C3B-C4B | -2.42 | 1.46 | 1.53 |
| 4 | G | 400 | NAD | C2D-C3D | 2.40 | 1.59 | 1.53 |
| 4 | A | 400 | NAD | O2B-C2B | -2.40 | 1.37 | 1.43 |
| 4 | D | 400 | NAD | C2B-C3B | -2.39 | 1.46 | 1.53 |
| 4 | A | 400 | NAD | C2A-N3A | 2.36 | 1.35 | 1.32 |
| 4 | G | 400 | NAD | C2B-C3B | -2.36 | 1.46 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | B | 400 | NAD | C2B-C3B | -2.36 | 1.46 | 1.53 |
| 6 | I | 500 | NDP | P2B-O2X | -2.34 | 1.45 | 1.54 |
| 6 | I | 500 | NDP | O2B-C2B | -2.27 | 1.35 | 1.44 |
| 4 | D | 400 | NAD | C2D-C1D | 2.26 | 1.57 | 1.53 |
| 6 | C | 500 | NDP | C2A-N1A | 2.24 | 1.38 | 1.33 |
| 4 | H | 400 | NAD | C2B-C3B | -2.24 | 1.47 | 1.53 |
| 4 | A | 400 | NAD | O3B-C3B | 2.23 | 1.48 | 1.43 |
| 4 | H | 400 | NAD | O3D-C3D | 2.23 | 1.48 | 1.43 |
| 4 | A | 400 | NAD | PN-O1N | -2.21 | 1.43 | 1.50 |
| 4 | H | 400 | NAD | C3B-C4B | -2.19 | 1.47 | 1.53 |
| 4 | B | 400 | NAD | C2A-N3A | 2.18 | 1.35 | 1.32 |
| 6 | C | 500 | NDP | O3B-C3B | 2.17 | 1.48 | 1.43 |
| 6 | F | 500 | NDP | P2B-O2X | -2.14 | 1.46 | 1.54 |
| 6 | C | 500 | NDP | O2B-C2B | -2.13 | 1.36 | 1.44 |
| 4 | A | 400 | NAD | O3D-C3D | 2.11 | 1.47 | 1.43 |
| 4 | B | 400 | NAD | C3B-C4B | -2.10 | 1.47 | 1.53 |
| 4 | B | 400 | NAD | C5B-C4B | -2.08 | 1.45 | 1.51 |
| 4 | B | 400 | NAD | C5D-C4D | -2.04 | 1.45 | 1.51 |
| 4 | H | 400 | NAD | C2D-C3D | 2.02 | 1.58 | 1.53 |
| 6 | I | 500 | NDP | O2D-C2D | -2.01 | 1.38 | 1.43 |

All (151) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4 | G | 400 | NAD | O5D-C5D-C4D | 9.82 | 142.78 | 108.99 |
| 4 | B | 400 | NAD | O4B-C4B-C5B | 8.58 | 137.60 | 109.37 |
| 4 | B | 400 | NAD | C6N-N1N-C2N | -8.28 | 114.42 | 121.97 |
| 4 | G | 400 | NAD | C6N-N1N-C2N | -7.62 | 115.02 | 121.97 |
| 4 | A | 400 | NAD | C6N-N1N-C2N | -7.47 | 115.17 | 121.97 |
| 4 | H | 400 | NAD | C6N-N1N-C2N | -6.90 | 115.68 | 121.97 |
| 4 | D | 400 | NAD | C6N-N1N-C2N | -6.85 | 115.73 | 121.97 |
| 4 | B | 400 | NAD | O5D-C5D-C4D | 5.91 | 129.33 | 108.99 |
| 4 | G | 400 | NAD | O4D-C1D-C2D | 5.59 | 115.10 | 106.93 |
| 4 | H | 400 | NAD | O4D-C4D-C3D | 5.23 | 115.47 | 105.11 |
| 4 | A | 400 | NAD | O4D-C4D-C3D | 4.83 | 114.68 | 105.11 |
| 4 | A | 400 | NAD | O2B-C2B-C3B | 4.77 | 127.26 | 111.82 |
| 4 | D | 400 | NAD | O4D-C4D-C3D | 4.72 | 114.46 | 105.11 |
| 4 | B | 400 | NAD | C2B-C3B-C4B | 4.68 | 111.74 | 102.64 |
| 4 | H | 400 | NAD | O2B-C2B-C3B | 4.59 | 126.68 | 111.82 |
| 4 | G | 400 | NAD | O4D-C4D-C3D | 4.55 | 114.12 | 105.11 |
| 6 | C | 500 | NDP | O5B-C5B-C4B | 4.55 | 124.65 | 108.99 |
| 4 | B | 400 | NAD | O2B-C2B-C3B | 4.50 | 126.39 | 111.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6 | I | 500 | NDP | C2D-C1D-N1N | 4.48 | 124.53 | 113.30 |
| 6 | I | 500 | NDP | O5B-C5B-C4B | 4.46 | 124.34 | 108.99 |
| 4 | A | 400 | NAD | O5D-C5D-C4D | 4.44 | 124.28 | 108.99 |
| 6 | F | 500 | NDP | C2B-C3B-C4B | 4.40 | 111.55 | 101.99 |
| 6 | F | 500 | NDP | O5D-C5D-C4D | 4.37 | 124.04 | 108.99 |
| 6 | I | 500 | NDP | O4D-C4D-C3D | 4.35 | 113.72 | 105.11 |
| 6 | F | 500 | NDP | O5B-C5B-C4B | 4.32 | 123.87 | 108.99 |
| 6 | C | 500 | NDP | O5D-C5D-C4D | 4.32 | 123.87 | 108.99 |
| 4 | A | 400 | NAD | PN-O5D-C5D | 4.31 | 146.98 | 121.68 |
| 6 | C | 500 | NDP | O4D-C1D-N1N | -4.31 | 99.63 | 108.06 |
| 4 | D | 400 | NAD | O5D-C5D-C4D | 4.28 | 123.72 | 108.99 |
| 4 | H | 400 | NAD | O5B-C5B-C4B | 4.23 | 123.56 | 108.99 |
| 6 | F | 500 | NDP | O4D-C4D-C3D | 4.23 | 113.48 | 105.11 |
| 4 | A | 400 | NAD | C3N-C7N-N7N | -4.23 | 112.68 | 117.75 |
| 4 | G | 400 | NAD | C3N-C7N-N7N | -4.18 | 112.74 | 117.75 |
| 4 | H | 400 | NAD | C2B-C3B-C4B | 4.16 | 110.73 | 102.64 |
| 4 | G | 400 | NAD | O2B-C2B-C3B | 4.14 | 125.21 | 111.82 |
| 4 | G | 400 | NAD | C2B-C3B-C4B | 4.13 | 110.67 | 102.64 |
| 4 | A | 400 | NAD | O5B-C5B-C4B | 4.06 | 122.98 | 108.99 |
| 6 | F | 500 | NDP | O2B-C2B-C3B | 4.02 | 126.24 | 111.68 |
| 4 | A | 400 | NAD | C2B-C3B-C4B | 4.01 | 110.44 | 102.64 |
| 4 | H | 400 | NAD | C3N-C7N-N7N | -3.99 | 112.96 | 117.75 |
| 4 | G | 400 | NAD | O5B-C5B-C4B | 3.98 | 122.68 | 108.99 |
| 6 | C | 500 | NDP | C2B-C3B-C4B | 3.86 | 110.39 | 101.99 |
| 6 | I | 500 | NDP | C4D-O4D-C1D | -3.79 | 101.11 | 109.47 |
| 4 | D | 400 | NAD | O2B-C2B-C3B | 3.77 | 124.01 | 111.82 |
| 4 | D | 400 | NAD | C2B-C3B-C4B | 3.76 | 109.94 | 102.64 |
| 4 | D | 400 | NAD | O5B-C5B-C4B | 3.74 | 121.86 | 108.99 |
| 4 | B | 400 | NAD | C3N-C7N-N7N | -3.71 | 113.30 | 117.75 |
| 4 | H | 400 | NAD | O4D-C1D-C2D | 3.64 | 112.24 | 106.93 |
| 6 | I | 500 | NDP | O2B-C2B-C3B | 3.56 | 124.59 | 111.68 |
| 4 | D | 400 | NAD | O4B-C4B-C5B | 3.55 | 121.04 | 109.37 |
| 4 | A | 400 | NAD | N3A-C2A-N1A | -3.54 | 123.14 | 128.68 |
| 6 | I | 500 | NDP | C2B-C3B-C4B | 3.54 | 109.68 | 101.99 |
| 6 | C | 500 | NDP | O4D-C4D-C3D | 3.52 | 112.09 | 105.11 |
| 4 | B | 400 | NAD | O4D-C4D-C3D | 3.52 | 112.08 | 105.11 |
| 4 | B | 400 | NAD | N3A-C2A-N1A | -3.50 | 123.21 | 128.68 |
| 4 | G | 400 | NAD | PN-O5D-C5D | 3.50 | 142.19 | 121.68 |
| 6 | I | 500 | NDP | PN-O5D-C5D | -3.45 | 101.46 | 121.68 |
| 4 | H | 400 | NAD | N3A-C2A-N1A | -3.41 | 123.36 | 128.68 |
| 6 | F | 500 | NDP | O4D-C1D-N1N | -3.39 | 101.43 | 108.06 |
| 6 | C | 500 | NDP | N3A-C2A-N1A | -3.37 | 123.41 | 128.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6 | C | 500 | NDP | O2B-C2B-C3B | 3.37 | 123.89 | 111.68 |
| 6 | I | 500 | NDP | C2D-C3D-C4D | -3.34 | 96.15 | 102.64 |
| 6 | C | 500 | NDP | C2D-C3D-C4D | -3.34 | 96.16 | 102.64 |
| 4 | G | 400 | NAD | N3A-C2A-N1A | -3.30 | 123.51 | 128.68 |
| 4 | D | 400 | NAD | O3D-C3D-C4D | 3.19 | 120.29 | 111.05 |
| 4 | G | 400 | NAD | C5N-C6N-N1N | 3.19 | 124.97 | 120.40 |
| 4 | B | 400 | NAD | C5N-C6N-N1N | 3.17 | 124.95 | 120.40 |
| 4 | A | 400 | NAD | C5N-C6N-N1N | 3.16 | 124.94 | 120.40 |
| 4 | H | 400 | NAD | O3D-C3D-C4D | 3.14 | 120.14 | 111.05 |
| 4 | D | 400 | NAD | C3N-C7N-N7N | -3.13 | 114.00 | 117.75 |
| 6 | I | 500 | NDP | N3A-C2A-N1A | -3.09 | 123.84 | 128.68 |
| 6 | I | 500 | NDP | C3N-C7N-N7N | -3.05 | 112.25 | 117.67 |
| 6 | F | 500 | NDP | N3A-C2A-N1A | -3.02 | 123.96 | 128.68 |
| 6 | F | 500 | NDP | O3D-C3D-C4D | 3.00 | 119.73 | 111.05 |
| 4 | H | 400 | NAD | O4B-C4B-C5B | 2.96 | 119.12 | 109.37 |
| 4 | A | 400 | NAD | C2D-C3D-C4D | -2.93 | 96.94 | 102.64 |
| 6 | I | 500 | NDP | O4B-C4B-C5B | 2.93 | 119.00 | 109.37 |
| 4 | A | 400 | NAD | O3D-C3D-C4D | 2.93 | 119.51 | 111.05 |
| 4 | G | 400 | NAD | O4B-C4B-C5B | 2.90 | 118.91 | 109.37 |
| 4 | D | 400 | NAD | C5N-C6N-N1N | 2.87 | 124.52 | 120.40 |
| 4 | G | 400 | NAD | O3D-C3D-C4D | 2.86 | 119.31 | 111.05 |
| 4 | G | 400 | NAD | PN-O3-PA | -2.85 | 123.04 | 132.83 |
| 4 | H | 400 | NAD | C5N-C6N-N1N | 2.84 | 124.48 | 120.40 |
| 6 | C | 500 | NDP | C2D-C1D-N1N | 2.84 | 120.41 | 113.30 |
| 4 | B | 400 | NAD | C3B-C2B-C1B | 2.82 | 105.22 | 100.98 |
| 6 | C | 500 | NDP | O4B-C4B-C5B | 2.81 | 118.63 | 109.37 |
| 4 | D | 400 | NAD | N3A-C2A-N1A | -2.81 | 124.29 | 128.68 |
| 4 | G | 400 | NAD | C5D-C4D-C3D | -2.72 | 104.98 | 115.18 |
| 4 | A | 400 | NAD | C2N-C3N-C4N | 2.70 | 121.32 | 118.26 |
| 4 | B | 400 | NAD | O3D-C3D-C4D | 2.69 | 118.84 | 111.05 |
| 6 | I | 500 | NDP | O3D-C3D-C4D | 2.69 | 118.83 | 111.05 |
| 6 | C | 500 | NDP | O5D-PN-O1N | 2.65 | 119.42 | 109.07 |
| 6 | C | 500 | NDP | C4D-O4D-C1D | -2.63 | 103.66 | 109.47 |
| 6 | F | 500 | NDP | O4B-C4B-C5B | 2.57 | 117.83 | 109.37 |
| 6 | F | 500 | NDP | O5D-PN-O1N | 2.55 | 119.02 | 109.07 |
| 6 | C | 500 | NDP | O4D-C4D-C5D | 2.54 | 117.74 | 109.37 |
| 6 | F | 500 | NDP | C4D-O4D-C1D | -2.53 | 103.89 | 109.47 |
| 4 | A | 400 | NAD | O4B-C4B-C5B | 2.52 | 117.68 | 109.37 |
| 4 | H | 400 | NAD | C2N-C3N-C4N | 2.46 | 121.04 | 118.26 |
| 6 | C | 500 | NDP | O3D-C3D-C4D | 2.46 | 118.15 | 111.05 |
| 6 | F | 500 | NDP | C3N-C7N-N7N | -2.45 | 113.31 | 117.67 |
| 4 | B | 400 | NAD | O5D-PN-O1N | 2.43 | 118.58 | 109.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4 | A | 400 | NAD | O7N-C7N-N7N | 2.43 | 126.03 | 122.58 |
| 4 | A | 400 | NAD | PN-O3-PA | -2.41 | 124.56 | 132.83 |
| 4 | A | 400 | NAD | O2D-C2D-C3D | 2.41 | 119.61 | 111.82 |
| 4 | A | 400 | NAD | PA-O5B-C5B | 2.40 | 135.73 | 121.68 |
| 6 | F | 500 | NDP | C3N-C2N-N1N | -2.38 | 119.70 | 123.10 |
| 4 | D | 400 | NAD | C3D-C2D-C1D | 2.37 | 104.55 | 100.98 |
| 4 | D | 400 | NAD | O4B-C1B-C2B | -2.36 | 103.47 | 106.93 |
| 4 | B | 400 | NAD | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 6 | I | 500 | NDP | PN-O3-PA | -2.33 | 124.83 | 132.83 |
| 4 | H | 400 | NAD | O7N-C7N-N7N | 2.32 | 125.87 | 122.58 |
| 6 | F | 500 | NDP | C2D-C3D-C4D | -2.28 | 98.21 | 102.64 |
| 4 | A | 400 | NAD | O4B-C4B-C3B | -2.28 | 100.61 | 105.11 |
| 4 | G | 400 | NAD | O4D-C4D-C5D | -2.26 | 101.93 | 109.37 |
| 6 | I | 500 | NDP | O2D-C2D-C3D | 2.25 | 119.09 | 111.82 |
| 4 | B | 400 | NAD | PN-O5D-C5D | 2.24 | 134.82 | 121.68 |
| 4 | H | 400 | NAD | PA-O5B-C5B | 2.24 | 134.79 | 121.68 |
| 4 | D | 400 | NAD | O5D-PN-O1N | 2.24 | 117.80 | 109.07 |
| 6 | C | 500 | NDP | PN-O3-PA | -2.23 | 125.16 | 132.83 |
| 6 | C | 500 | NDP | C2A-N1A-C6A | 2.23 | 122.57 | 118.75 |
| 4 | H | 400 | NAD | O5D-C5D-C4D | 2.23 | 116.67 | 108.99 |
| 4 | G | 400 | NAD | O4B-C4B-C3B | -2.23 | 100.70 | 105.11 |
| 6 | I | 500 | NDP | C3D-C2D-C1D | 2.23 | 105.66 | 101.43 |
| 4 | D | 400 | NAD | O4B-C4B-C3B | -2.23 | 100.71 | 105.11 |
| 4 | A | 400 | NAD | O4D-C4D-C5D | 2.23 | 116.70 | 109.37 |
| 6 | C | 500 | NDP | PN-O5D-C5D | 2.22 | 134.68 | 121.68 |
| 4 | B | 400 | NAD | C2A-N1A-C6A | 2.22 | 122.55 | 118.75 |
| 4 | D | 400 | NAD | O4D-C1D-C2D | 2.21 | 110.15 | 106.93 |
| 4 | G | 400 | NAD | C2N-C3N-C4N | 2.21 | 120.76 | 118.26 |
| 4 | H | 400 | NAD | C2A-N1A-C6A | 2.20 | 122.51 | 118.75 |
| 4 | D | 400 | NAD | C2D-C3D-C4D | -2.19 | 98.39 | 102.64 |
| 4 | D | 400 | NAD | O4D-C4D-C5D | 2.18 | 116.54 | 109.37 |
| 6 | I | 500 | NDP | O4B-C4B-C3B | -2.17 | 100.82 | 105.11 |
| 4 | H | 400 | NAD | O4B-C4B-C3B | -2.14 | 100.88 | 105.11 |
| 6 | I | 500 | NDP | O4D-C1D-N1N | -2.14 | 103.87 | 108.06 |
| 6 | F | 500 | NDP | PN-O5D-C5D | 2.12 | 134.14 | 121.68 |
| 6 | F | 500 | NDP | O4D-C4D-C5D | 2.12 | 116.36 | 109.37 |
| 4 | A | 400 | NAD | C2A-N1A-C6A | 2.11 | 122.37 | 118.75 |
| 4 | B | 400 | NAD | C2D-C3D-C4D | -2.11 | 98.55 | 102.64 |
| 6 | F | 500 | NDP | C2A-N1A-C6A | 2.10 | 122.35 | 118.75 |
| 6 | C | 500 | NDP | O2D-C2D-C3D | 2.09 | 118.59 | 111.82 |
| 6 | C | 500 | NDP | O4B-C4B-C3B | -2.09 | 100.98 | 105.11 |
| 4 | D | 400 | NAD | C2N-C3N-C4N | 2.09 | 120.62 | 118.26 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4 | G | 400 | NAD | O2D-C2D-C3D | 2.07 | 118.51 | 111.82 |
| 4 | B | 400 | NAD | C3D-C2D-C1D | 2.05 | 104.06 | 100.98 |
| 6 | I | 500 | NDP | C3N-C2N-N1N | -2.04 | 120.19 | 123.10 |
| 4 | G | 400 | NAD | C2A-N1A-C6A | 2.03 | 122.22 | 118.75 |
| 6 | C | 500 | NDP | O2A-PA-O1A | 2.02 | 122.24 | 112.24 |
| 4 | G | 400 | NAD | PA-O5B-C5B | 2.02 | 133.54 | 121.68 |
| 4 | D | 400 | NAD | PN-O5D-C5D | 2.00 | 133.43 | 121.68 |

There are no chirality outliers.

All (98) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 4 | H | 400 | NAD | C5B-O5B-PA-O1A |
| 4 | H | 400 | NAD | C5B-O5B-PA-O2A |
| 4 | H | 400 | NAD | C5D-O5D-PN-O3 |
| 4 | H | 400 | NAD | C5D-O5D-PN-O1N |
| 4 | H | 400 | NAD | O4D-C1D-N1N-C2N |
| 4 | H | 400 | NAD | O4D-C1D-N1N-C6N |
| 6 | I | 500 | NDP | C5B-O5B-PA-O3 |
| 6 | I | 500 | NDP | C2N-C3N-C7N-N7N |
| 4 | A | 400 | NAD | PN-O3-PA-O5B |
| 4 | A | 400 | NAD | O4B-C4B-C5B-O5B |
| 4 | A | 400 | NAD | C5D-O5D-PN-O1N |
| 4 | A | 400 | NAD | O4D-C1D-N1N-C2N |
| 4 | A | 400 | NAD | O4D-C1D-N1N-C6N |
| 4 | A | 400 | NAD | C2D-C1D-N1N-C2N |
| 4 | A | 400 | NAD | C2D-C1D-N1N-C6N |
| 4 | B | 400 | NAD | C5B-O5B-PA-O1A |
| 4 | B | 400 | NAD | O4D-C4D-C5D-O5D |
| 4 | B | 400 | NAD | C2D-C1D-N1N-C2N |
| 4 | B | 400 | NAD | C2D-C1D-N1N-C6N |
| 4 | B | 400 | NAD | C2N-C3N-C7N-O7N |
| 4 | B | 400 | NAD | C2N-C3N-C7N-N7N |
| 4 | G | 400 | NAD | C5B-O5B-PA-O1A |
| 4 | G | 400 | NAD | C5B-O5B-PA-O2A |
| 6 | F | 500 | NDP | C5B-O5B-PA-O1A |
| 6 | F | 500 | NDP | C5D-O5D-PN-O2N |
| 6 | F | 500 | NDP | O4D-C4D-C5D-O5D |
| 6 | F | 500 | NDP | C2N-C3N-C7N-N7N |
| 6 | C | 500 | NDP | C1B-C2B-O2B-P2B |
| 6 | C | 500 | NDP | C5D-O5D-PN-O2N |
| 6 | C | 500 | NDP | O4D-C4D-C5D-O5D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 6 | C | 500 | NDP | C2N-C3N-C7N-N7N |
| 4 | D | 400 | NAD | C5B-O5B-PA-O1A |
| 4 | D | 400 | NAD | C5B-O5B-PA-O3 |
| 4 | D | 400 | NAD | PN-O3-PA-O5B |
| 4 | D | 400 | NAD | C5D-O5D-PN-O1N |
| 4 | D | 400 | NAD | O4D-C1D-N1N-C6N |
| 4 | B | 400 | NAD | C4N-C3N-C7N-O7N |
| 4 | B | 400 | NAD | C4N-C3N-C7N-N7N |
| 4 | H | 400 | NAD | O4D-C4D-C5D-O5D |
| 4 | H | 400 | NAD | C3D-C4D-C5D-O5D |
| 6 | I | 500 | NDP | O4B-C4B-C5B-O5B |
| 4 | A | 400 | NAD | C3B-C4B-C5B-O5B |
| 4 | B | 400 | NAD | O4B-C4B-C5B-O5B |
| 6 | F | 500 | NDP | O4B-C4B-C5B-O5B |
| 4 | D | 400 | NAD | C3D-C4D-C5D-O5D |
| 6 | I | 500 | NDP | C1B-C2B-O2B-P2B |
| 4 | A | 400 | NAD | C2N-C3N-C7N-O7N |
| 6 | F | 500 | NDP | C1B-C2B-O2B-P2B |
| 6 | F | 500 | NDP | C2D-C1D-N1N-C6N |
| 6 | C | 500 | NDP | C2D-C1D-N1N-C6N |
| 4 | A | 400 | NAD | C2N-C3N-C7N-N7N |
| 4 | B | 400 | NAD | C3D-C4D-C5D-O5D |
| 6 | F | 500 | NDP | C3B-C4B-C5B-O5B |
| 4 | D | 400 | NAD | O4D-C4D-C5D-O5D |
| 6 | I | 500 | NDP | C3B-C2B-O2B-P2B |
| 6 | F | 500 | NDP | C3B-C2B-O2B-P2B |
| 6 | C | 500 | NDP | C3B-C2B-O2B-P2B |
| 4 | A | 400 | NAD | C4N-C3N-C7N-O7N |
| 6 | F | 500 | NDP | C2D-C1D-N1N-C2N |
| 6 | C | 500 | NDP | C2D-C1D-N1N-C2N |
| 6 | I | 500 | NDP | C3B-C4B-C5B-O5B |
| 6 | C | 500 | NDP | O4B-C4B-C5B-O5B |
| 4 | A | 400 | NAD | C4N-C3N-C7N-N7N |
| 4 | H | 400 | NAD | C4B-C5B-O5B-PA |
| 4 | A | 400 | NAD | C4D-C5D-O5D-PN |
| 4 | H | 400 | NAD | O4B-C4B-C5B-O5B |
| 6 | C | 500 | NDP | C3B-C4B-C5B-O5B |
| 4 | G | 400 | NAD | C4D-C5D-O5D-PN |
| 4 | B | 400 | NAD | C4D-C5D-O5D-PN |
| 4 | G | 400 | NAD | C4B-C5B-O5B-PA |
| 4 | B | 400 | NAD | PN-O3-PA-O5B |
| 6 | C | 500 | NDP | O4D-C1D-N1N-C6N |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 6 | F | 500 | NDP | C2B-O2B-P2B-O1X |
| 6 | C | 500 | NDP | O4D-C1D-N1N-C2N |
| 4 | A | 400 | NAD | C5D-O5D-PN-O3 |
| 4 | B | 400 | NAD | C5D-O5D-PN-O3 |
| 4 | D | 400 | NAD | C5D-O5D-PN-O3 |
| 6 | F | 500 | NDP | O4D-C1D-N1N-C6N |
| 6 | I | 500 | NDP | C5B-O5B-PA-O1A |
| 6 | I | 500 | NDP | C5B-O5B-PA-O2A |
| 4 | G | 400 | NAD | O4D-C4D-C5D-O5D |
| 4 | D | 400 | NAD | O4B-C4B-C5B-O5B |
| 6 | F | 500 | NDP | O4D-C1D-N1N-C2N |
| 6 | I | 500 | NDP | O4D-C1D-N1N-C6N |
| 6 | I | 500 | NDP | C2D-C1D-N1N-C6N |
| 4 | B | 400 | NAD | PN-O3-PA-O1A |
| 4 | A | 400 | NAD | O4D-C4D-C5D-O5D |
| 4 | G | 400 | NAD | C3D-C4D-C5D-O5D |
| 6 | C | 500 | NDP | C3D-C4D-C5D-O5D |
| 4 | H | 400 | NAD | C5B-O5B-PA-O3 |
| 4 | B | 400 | NAD | C5B-O5B-PA-O3 |
| 4 | G | 400 | NAD | C5B-O5B-PA-O3 |
| 6 | F | 500 | NDP | C5B-O5B-PA-O3 |
| 4 | B | 400 | NAD | PA-O3-PN-O1N |
| 6 | I | 500 | NDP | O4D-C4D-C5D-O5D |
| 4 | G | 400 | NAD | O4B-C4B-C5B-O5B |
| 6 | I | 500 | NDP | O4D-C1D-N1N-C2N |
| 6 | I | 500 | NDP | C2D-C1D-N1N-C2N |

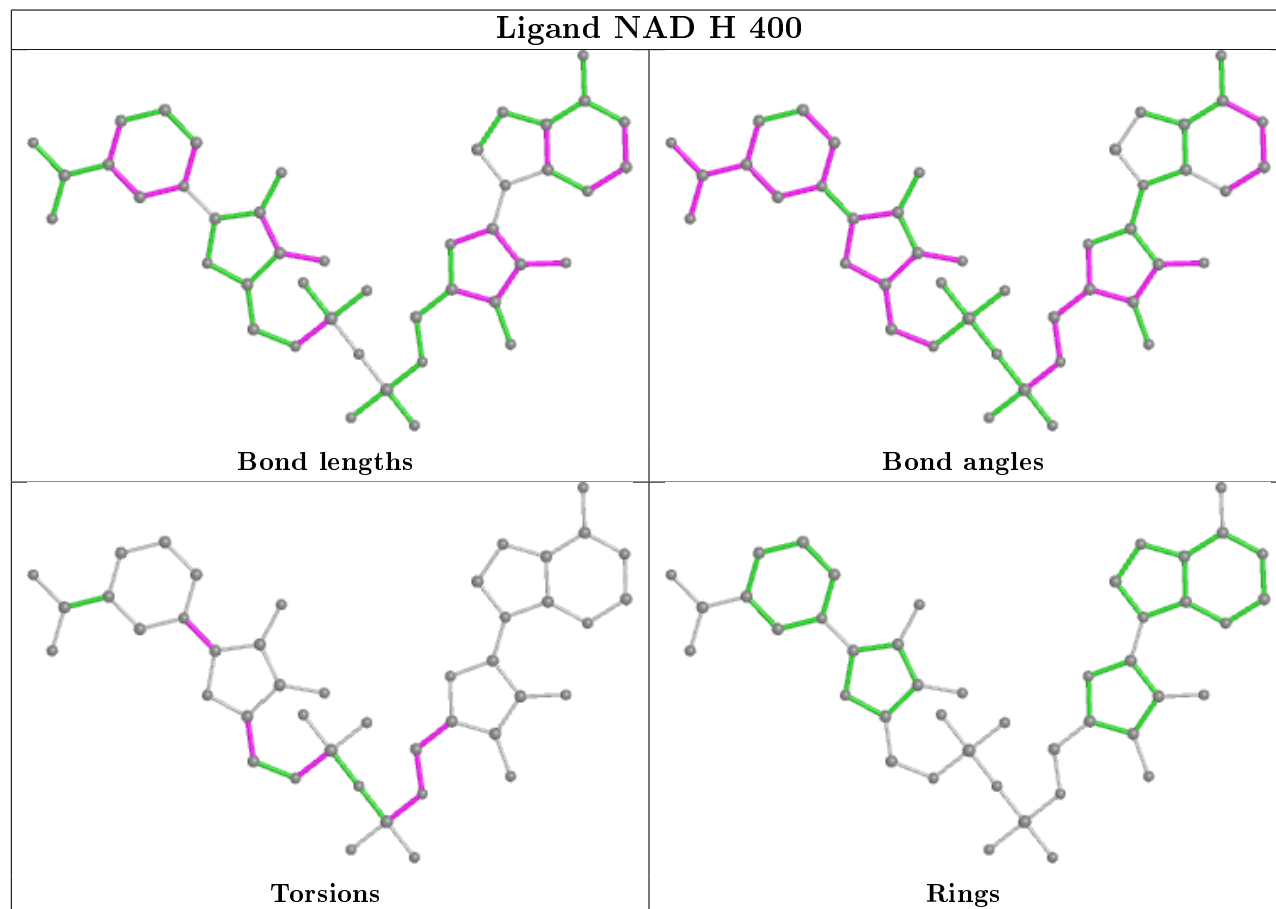
There are no ring outliers.

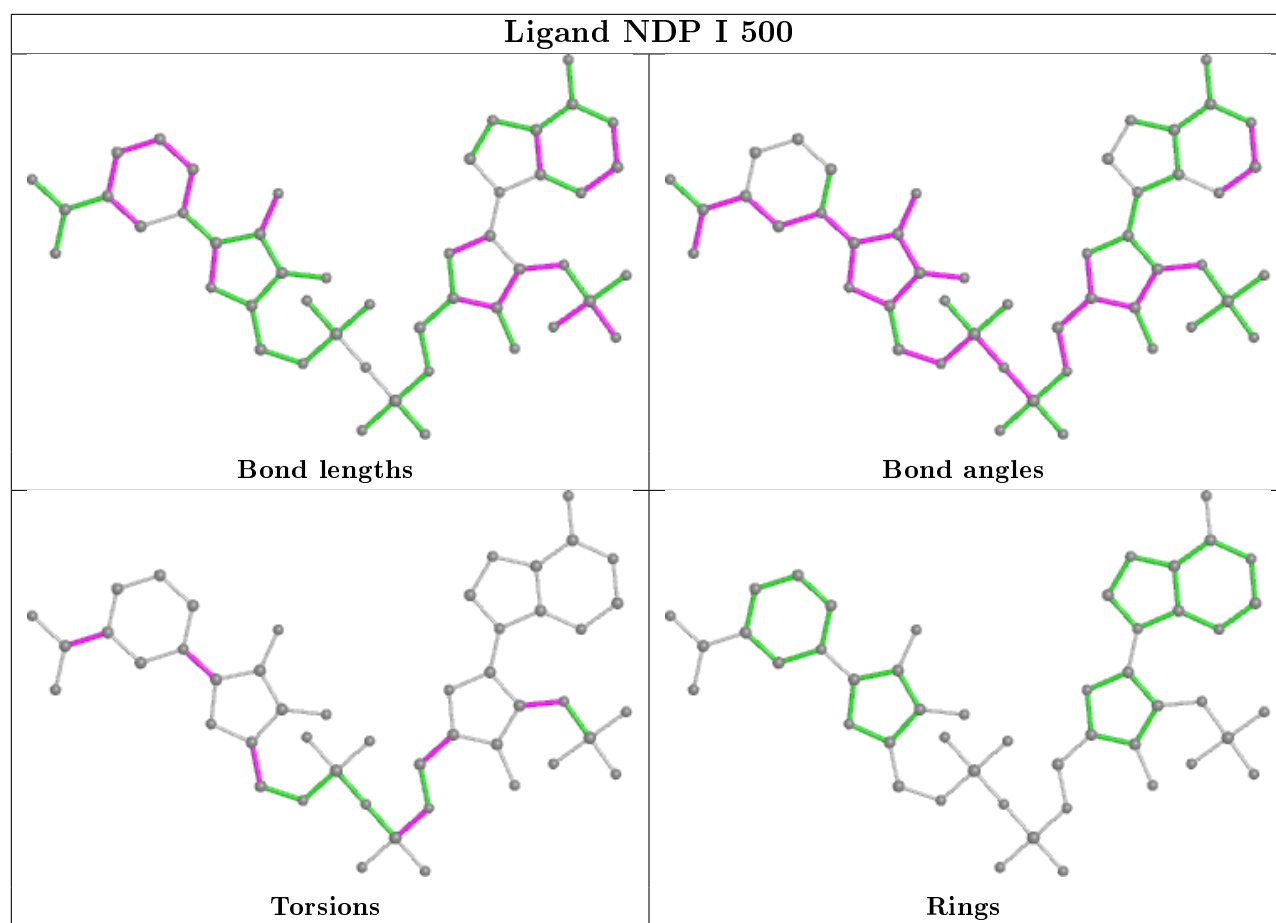
8 monomers are involved in 45 short contacts:

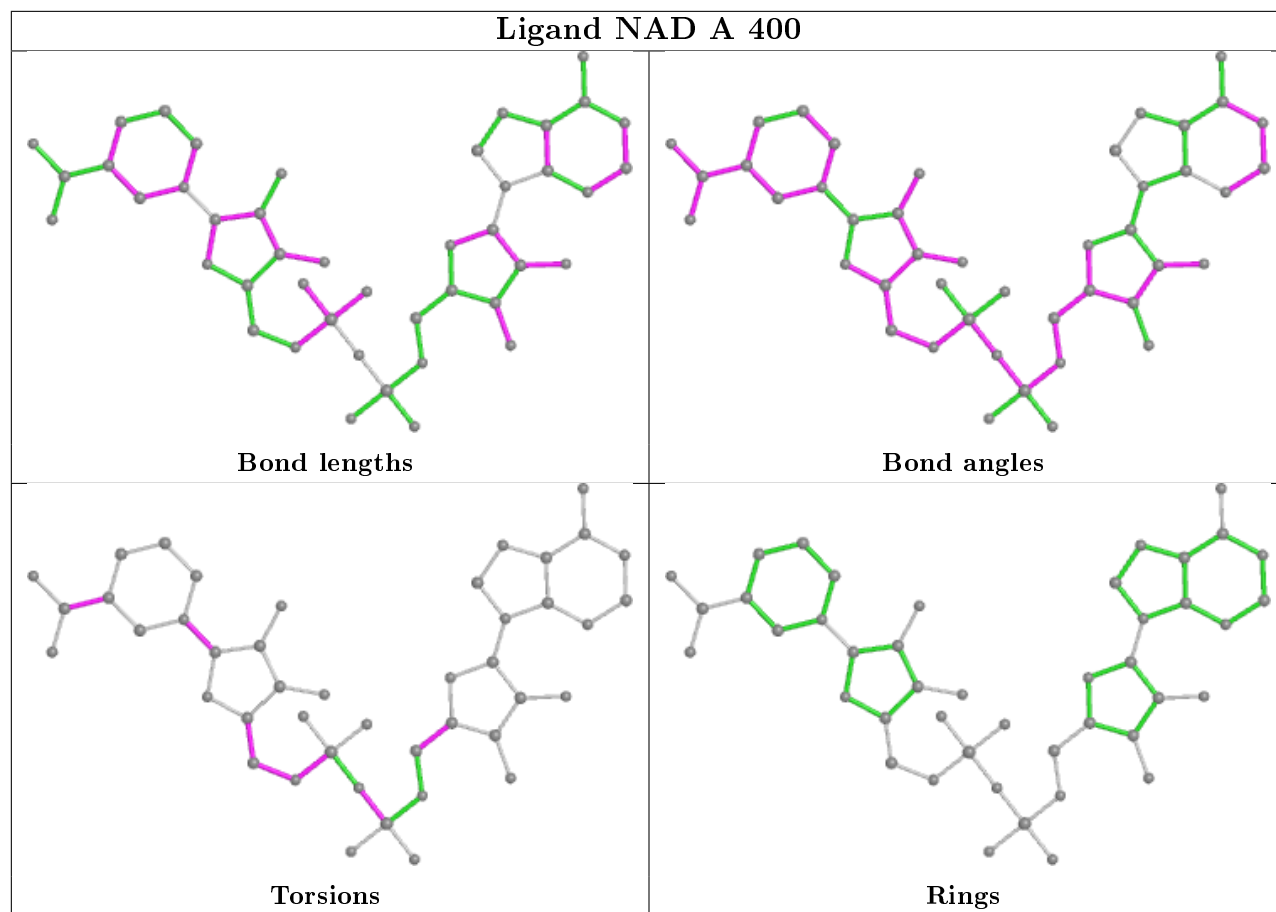
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4 | H | 400 | NAD | 8 | 0 |
| 6 | I | 500 | NDP | 3 | 0 |
| 4 | A | 400 | NAD | 2 | 0 |
| 4 | B | 400 | NAD | 9 | 0 |
| 4 | G | 400 | NAD | 6 | 0 |
| 6 | F | 500 | NDP | 10 | 0 |
| 6 | C | 500 | NDP | 4 | 0 |
| 4 | D | 400 | NAD | 3 | 0 |

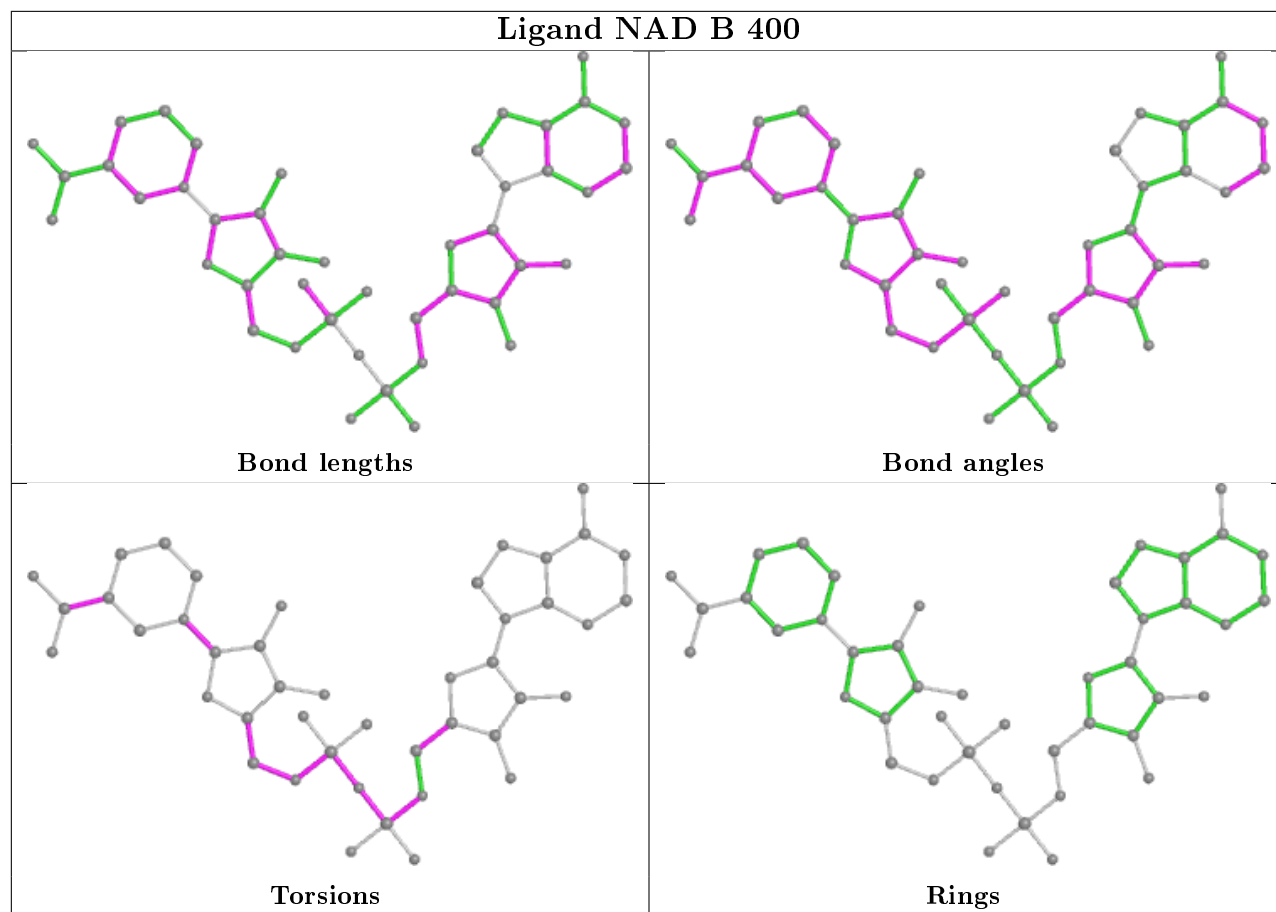
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

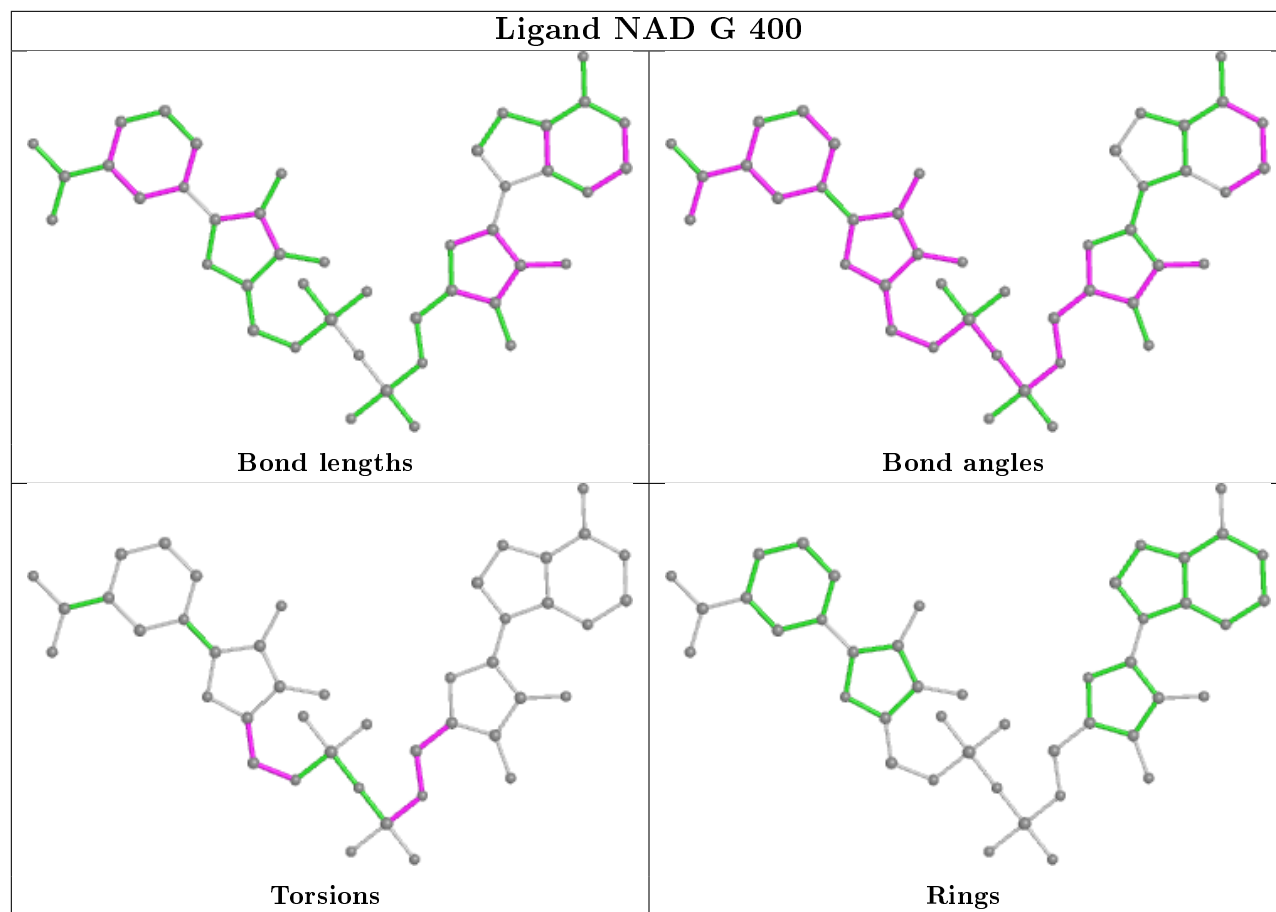
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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

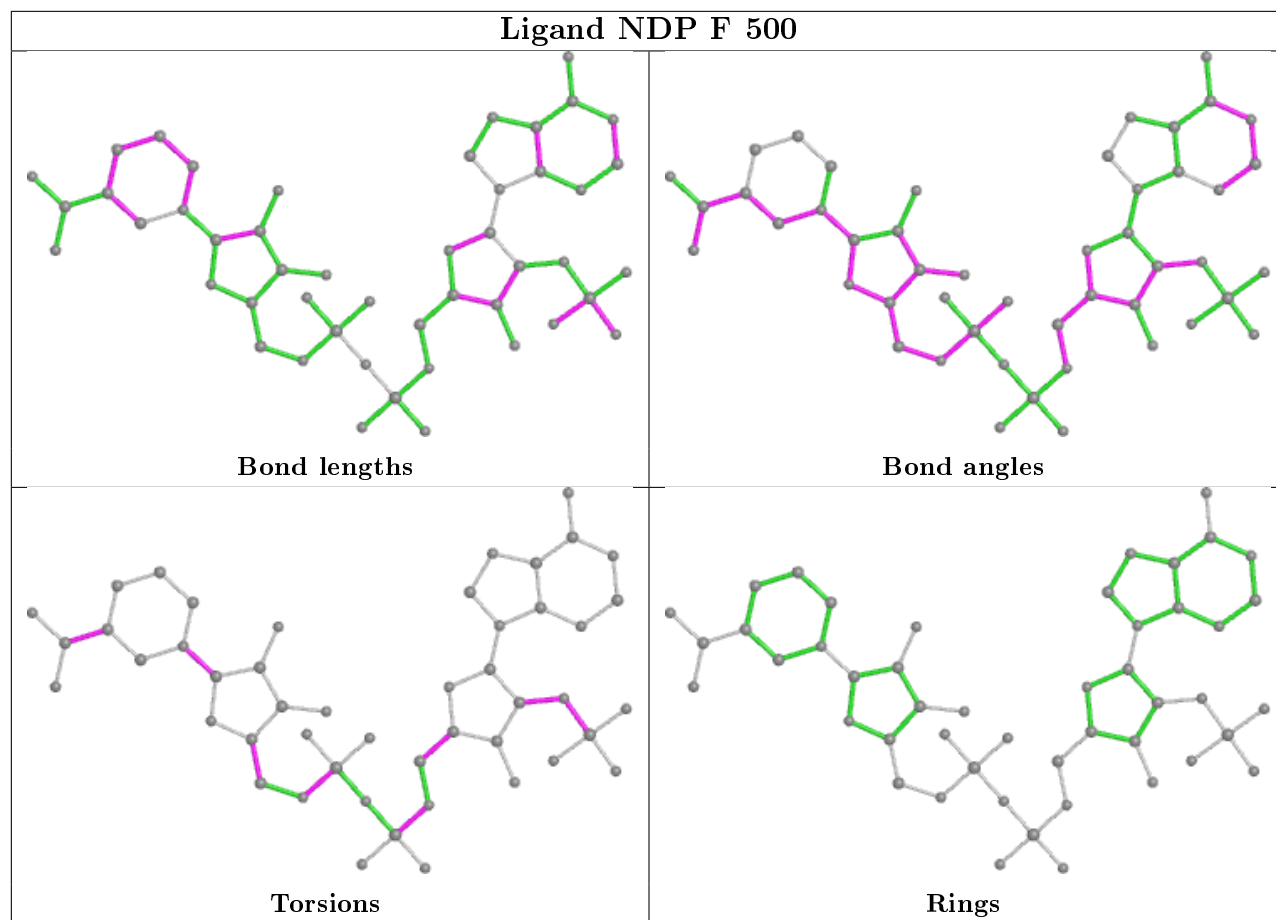


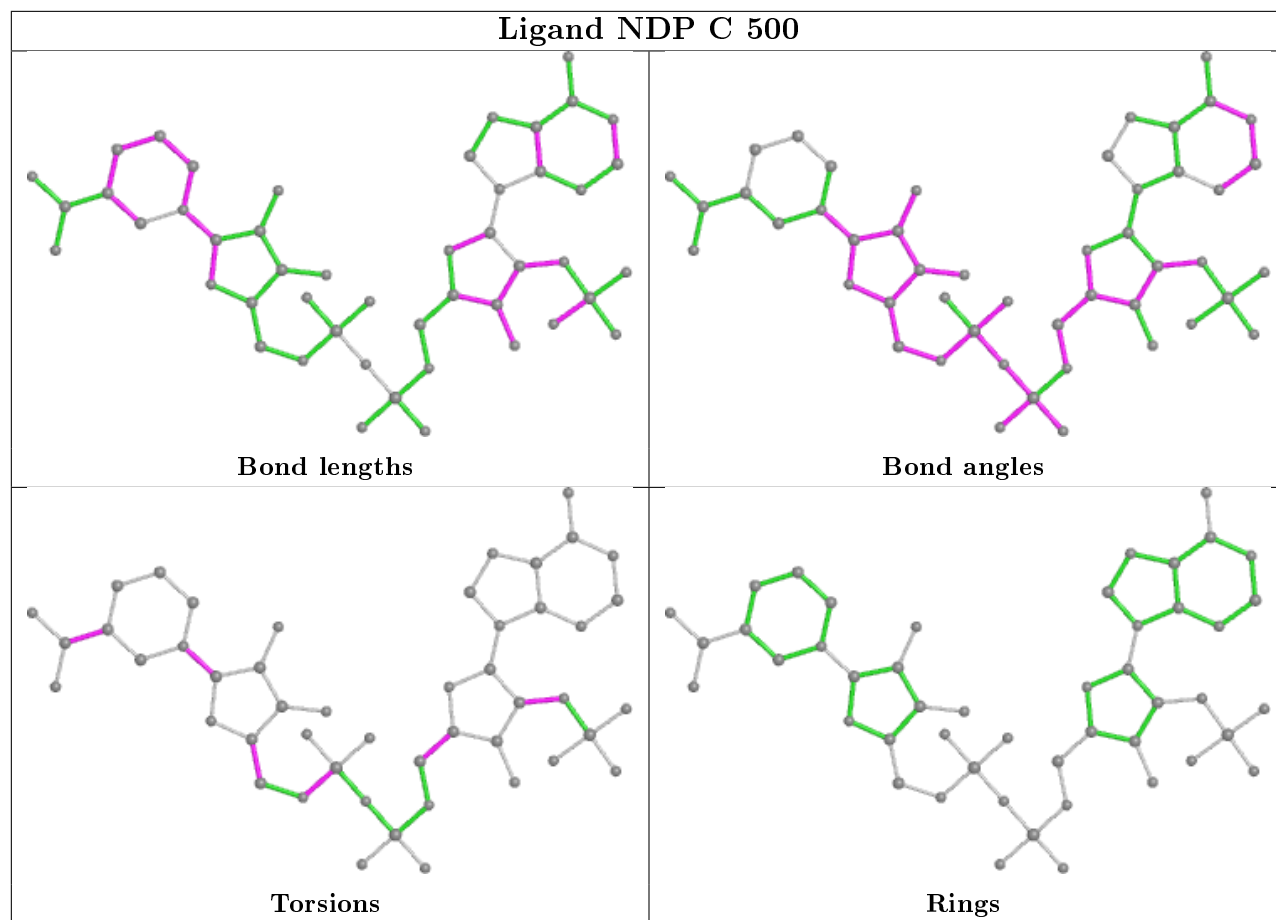


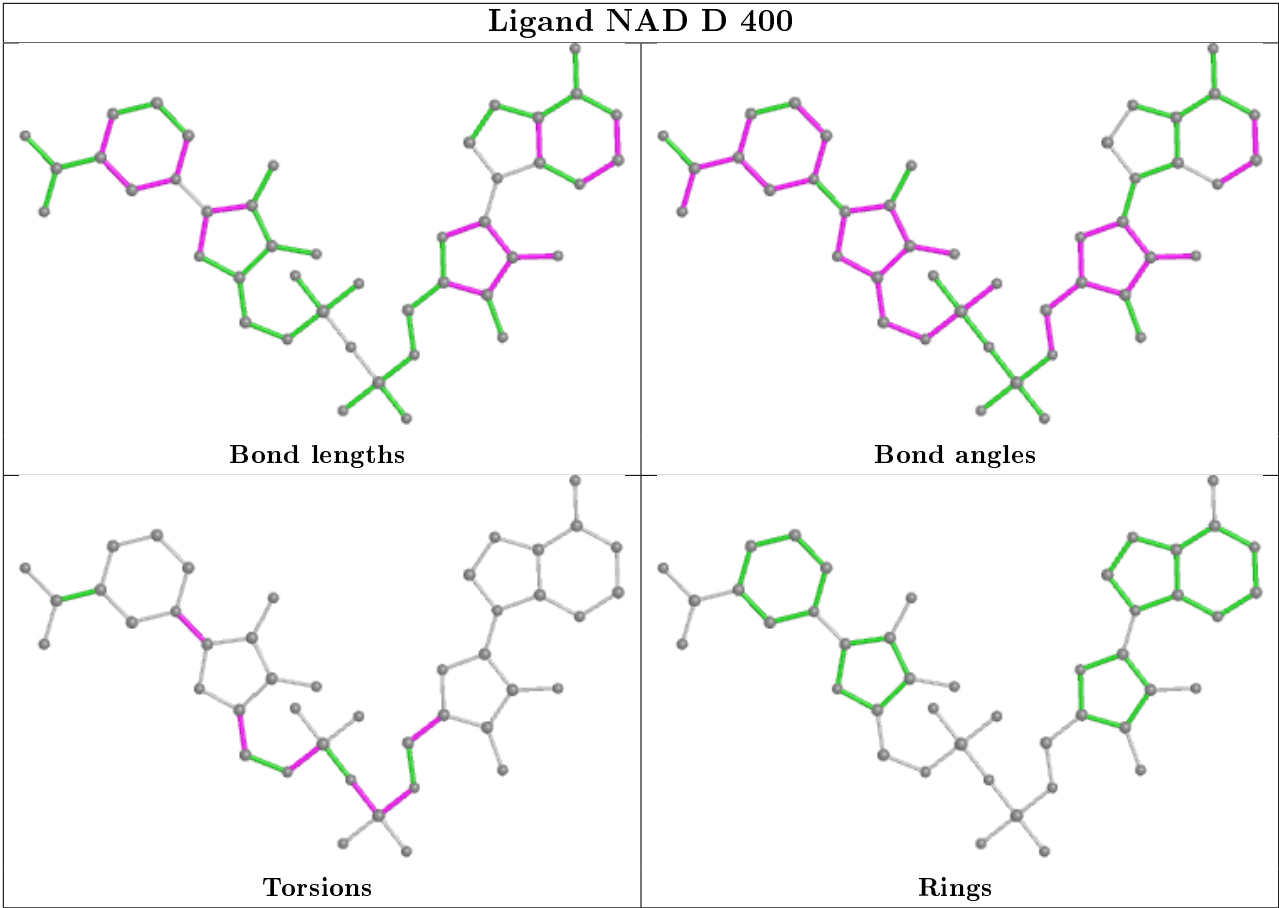












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1 | H | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | H | 343:LEU | C | 344:THR | N | 1.19 |

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 | 363/384 (94%) | -0.20 | 2 (0%) 89 78 | 30, 51, 77, 102 | 0 |
| 1 | B | 359/384 (93%) | -0.23 | 0 100 100 | 28, 52, 72, 98 | 0 |
| 1 | D | 378/384 (98%) | 0.01 | 9 (2%) 59 37 | 36, 68, 94, 104 | 0 |
| 1 | E | 359/384 (93%) | -0.18 | 4 (1%) 80 64 | 33, 60, 79, 91 | 0 |
| 1 | G | 364/384 (94%) | -0.21 | 1 (0%) 94 88 | 35, 59, 84, 102 | 0 |
| 1 | H | 357/384 (92%) | 0.06 | 10 (2%) 53 30 | 39, 72, 96, 104 | 0 |
| 2 | C | 174/174 (100%) | -0.39 | 0 100 100 | 32, 47, 61, 68 | 0 |
| 2 | F | 173/174 (99%) | -0.36 | 0 100 100 | 40, 52, 63, 75 | 0 |
| 2 | I | 173/174 (99%) | -0.27 | 0 100 100 | 42, 58, 73, 79 | 0 |
| All | All | 2700/2826 (95%) | -0.17 | 26 (0%) 82 67 | 28, 57, 90, 104 | 0 |

All (26) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | D | 1 | MET | 3.8 |
| 1 | H | 96 | LEU | 3.3 |
| 1 | D | 225 | ALA | 3.3 |
| 1 | H | 64 | ALA | 3.2 |
| 1 | D | 371 | ASP | 3.0 |
| 1 | D | 224 | GLU | 3.0 |
| 1 | D | 226 | MET | 3.0 |
| 1 | E | 30 | GLY | 2.9 |
| 1 | H | 81 | GLU | 2.5 |
| 1 | D | 116 | LYS | 2.5 |
| 1 | H | 1 | MET | 2.5 |
| 1 | H | 268 | PRO | 2.4 |
| 1 | E | 1 | MET | 2.4 |
| 1 | D | 230 | GLU | 2.4 |
| 1 | E | 245 | LYS | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | H | 71 | VAL | 2.2 |
| 1 | H | 78 | MET | 2.2 |
| 1 | H | 368 | VAL | 2.2 |
| 1 | D | 81 | GLU | 2.2 |
| 1 | H | 267 | ILE | 2.2 |
| 1 | G | 220 | THR | 2.1 |
| 1 | D | 353 | THR | 2.1 |
| 1 | H | 349 | LYS | 2.0 |
| 1 | A | 243 | PHE | 2.0 |
| 1 | A | 222 | ASP | 2.0 |
| 1 | E | 348 | ASP | 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 ⓘ

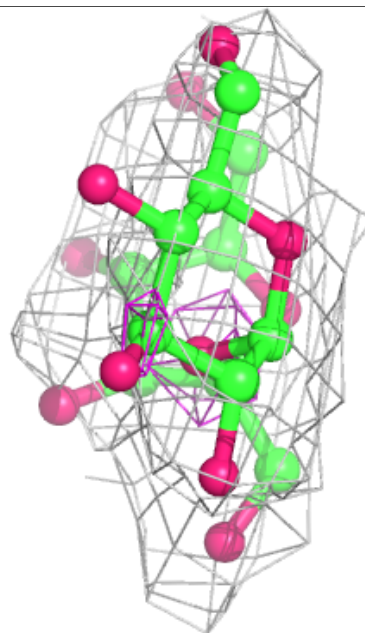
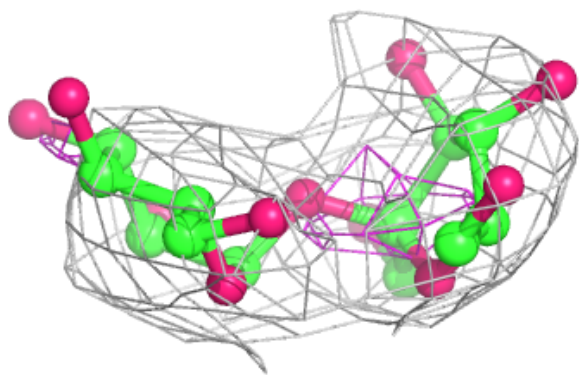
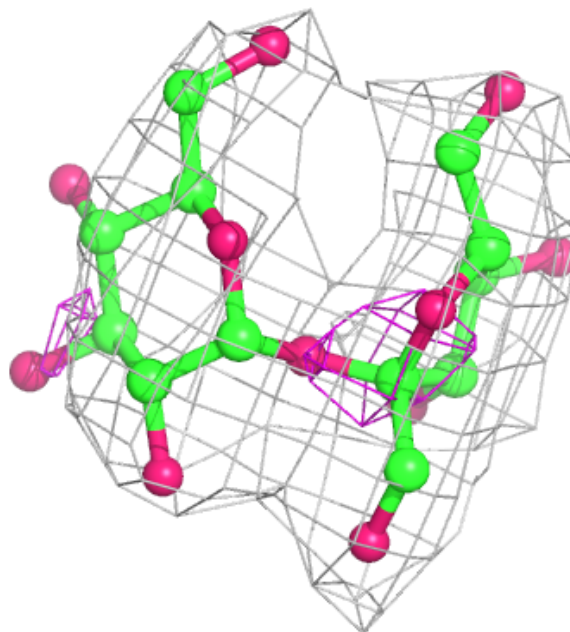
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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 | GLC | N | 1 | 11/12 | 0.71 | 0.47 | 97,99,99,99 | 0 |
| 3 | FRU | K | 2 | 12/12 | 0.71 | 0.32 | 84,88,89,89 | 0 |
| 3 | FRU | N | 2 | 12/12 | 0.79 | 0.36 | 98,99,99,99 | 0 |
| 3 | GLC | O | 1 | 11/12 | 0.83 | 0.36 | 82,83,83,84 | 0 |
| 3 | FRU | L | 2 | 12/12 | 0.85 | 0.26 | 81,82,83,83 | 0 |
| 3 | FRU | M | 2 | 12/12 | 0.87 | 0.27 | 70,74,75,76 | 0 |
| 3 | GLC | M | 1 | 11/12 | 0.88 | 0.21 | 76,76,77,77 | 0 |
| 3 | GLC | J | 1 | 11/12 | 0.88 | 0.23 | 76,77,79,79 | 0 |
| 3 | FRU | O | 2 | 12/12 | 0.89 | 0.40 | 84,85,85,87 | 0 |
| 3 | GLC | K | 1 | 11/12 | 0.89 | 0.26 | 86,88,88,88 | 0 |
| 3 | FRU | J | 2 | 12/12 | 0.90 | 0.20 | 70,73,75,76 | 0 |
| 3 | GLC | L | 1 | 11/12 | 0.90 | 0.29 | 79,82,82,83 | 0 |

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

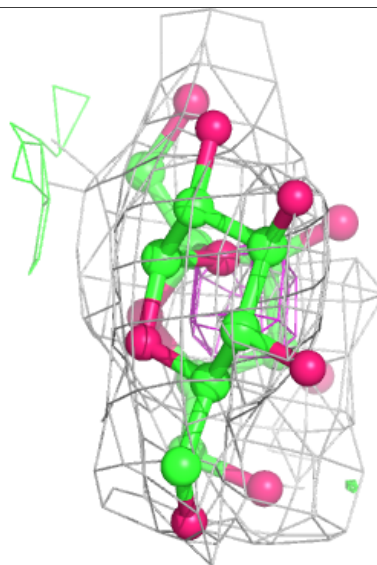
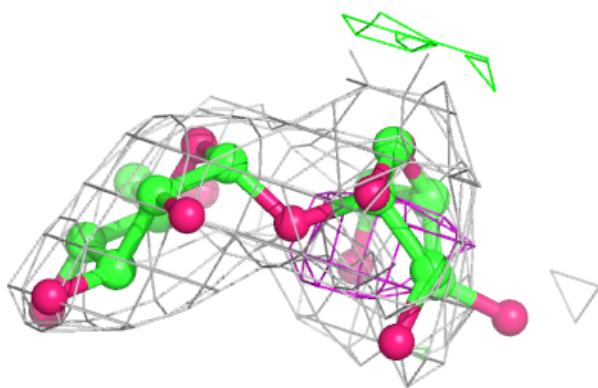
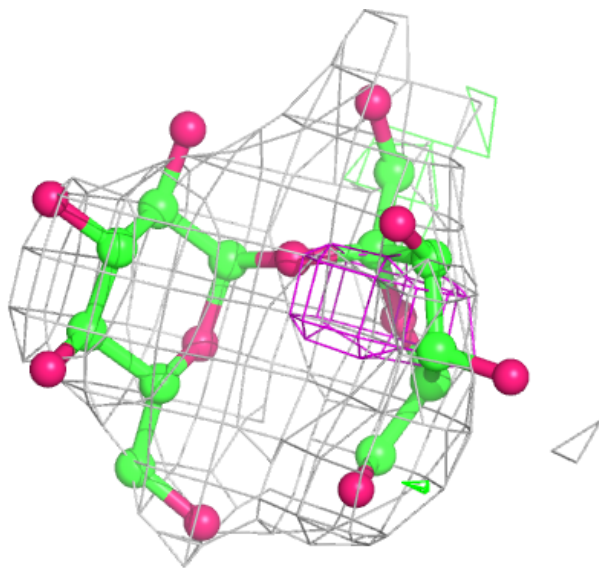
Electron density around Chain J:

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



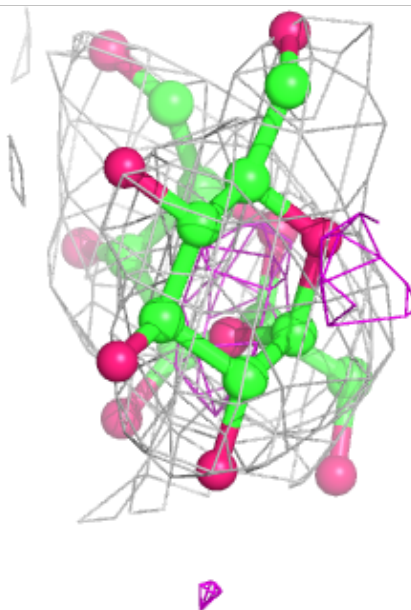
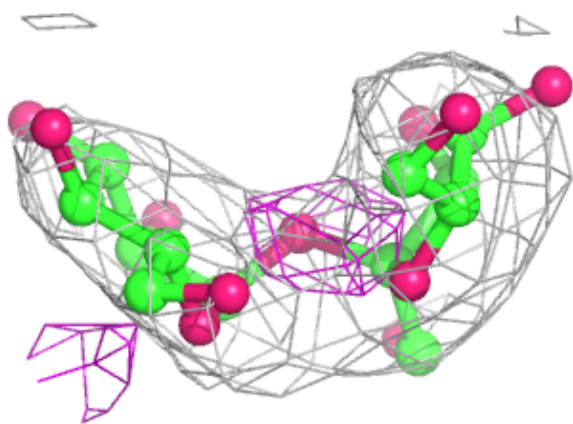
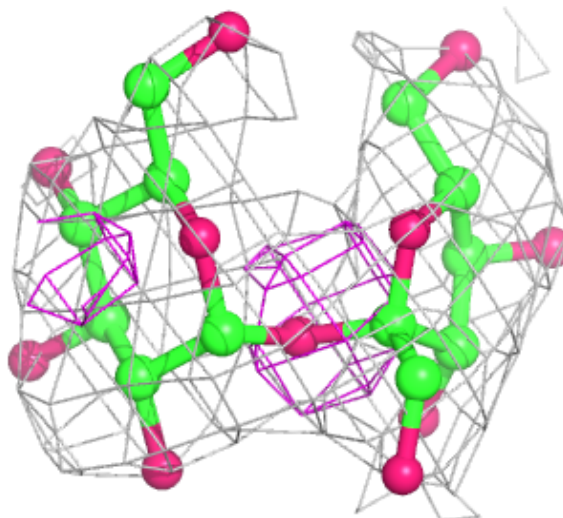
Electron density around Chain K:

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



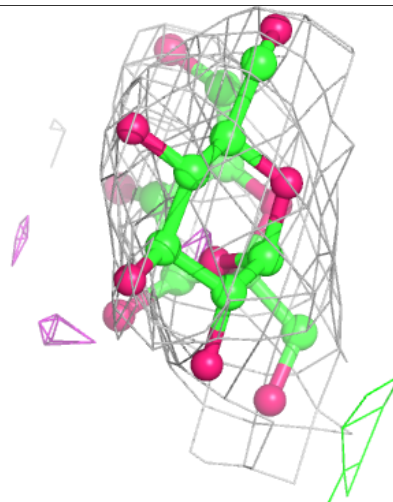
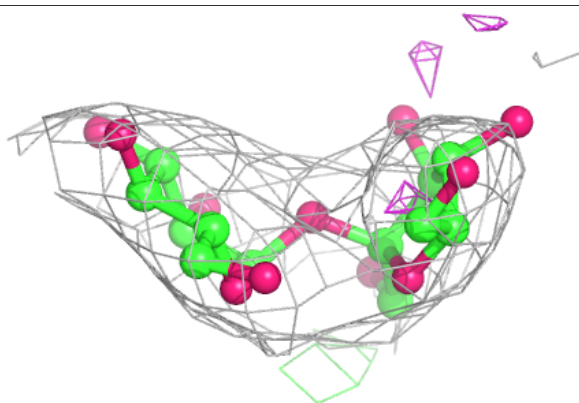
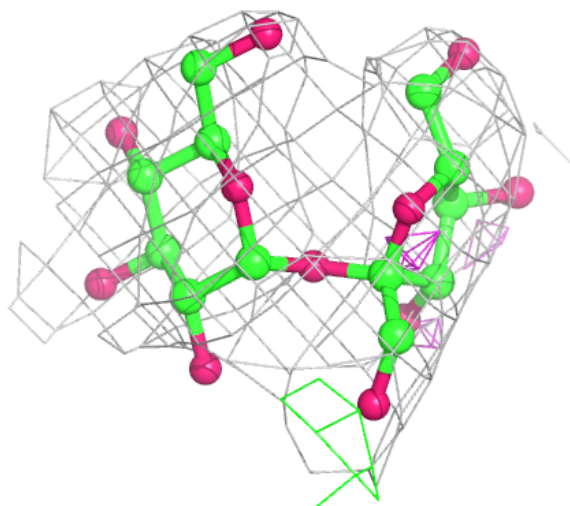
Electron density around Chain L:

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



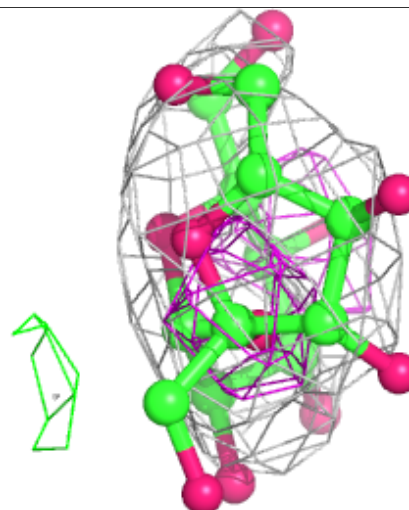
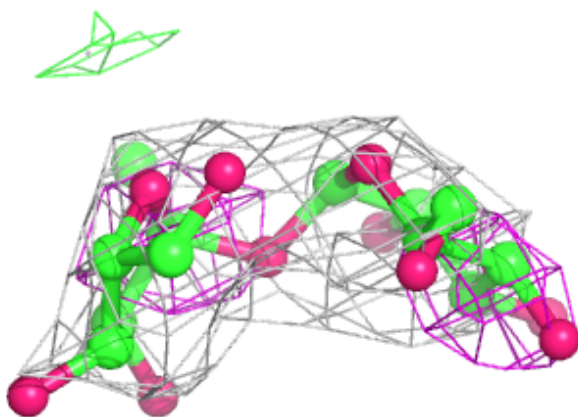
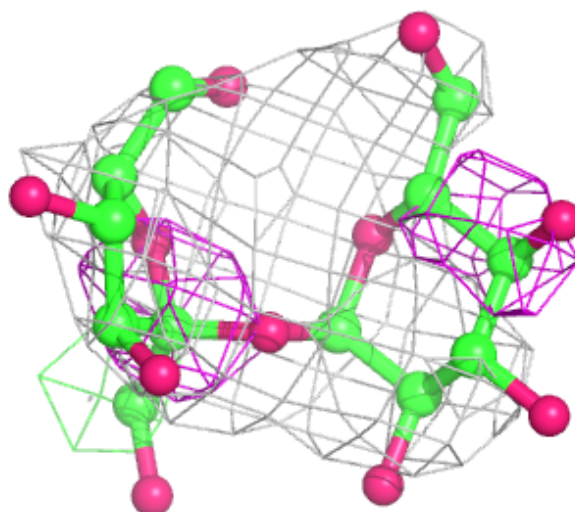
Electron density around Chain M:

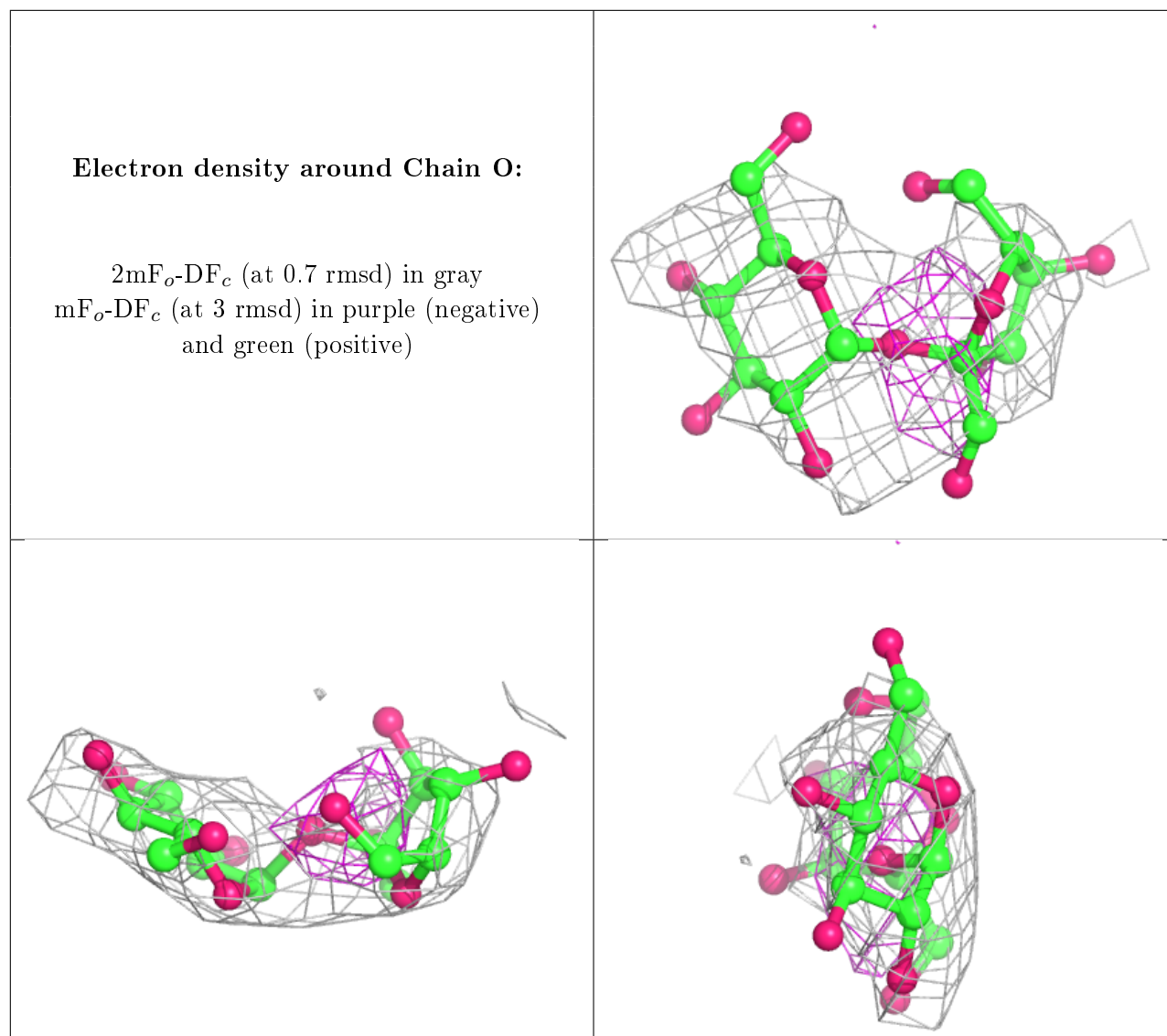
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain N:

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





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.

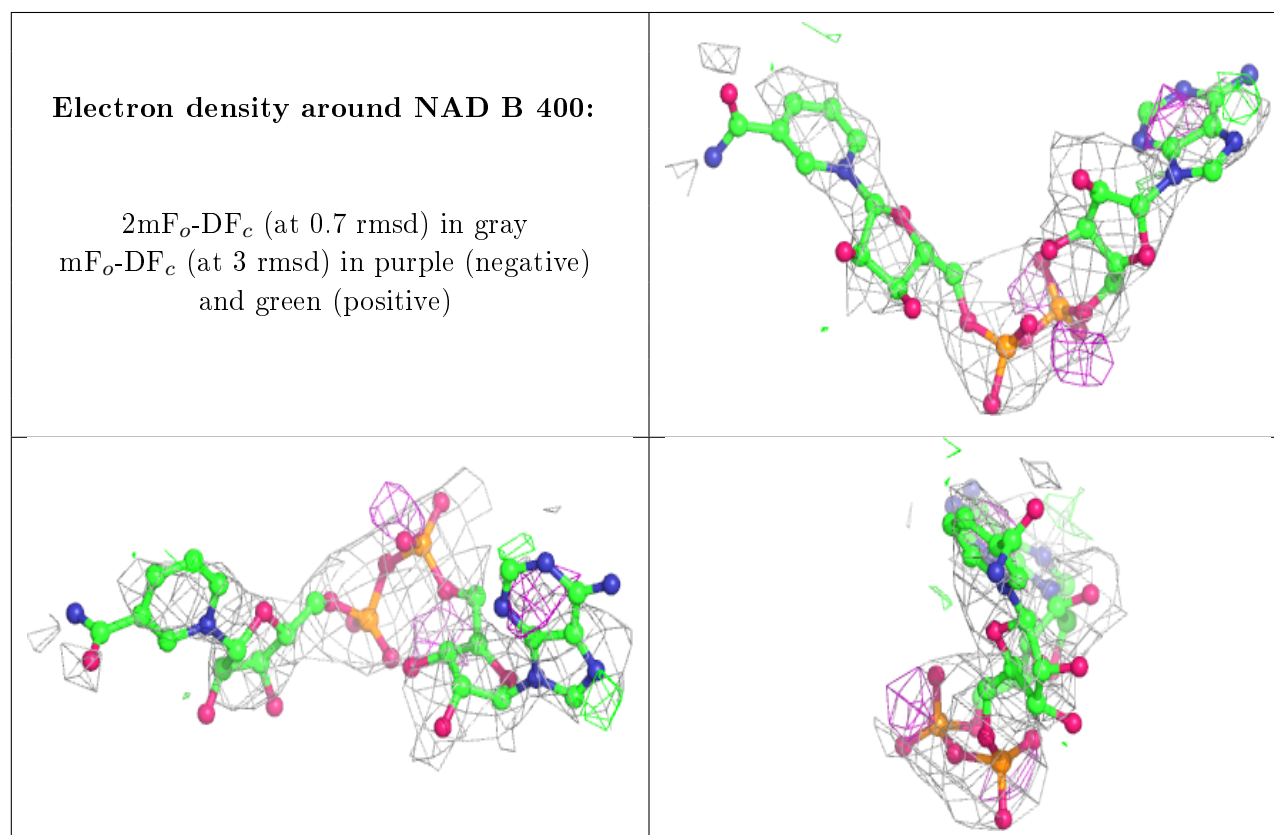
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 4 | NAD | B | 400 | 44/44 | 0.75 | 0.36 | 104,104,105,105 | 0 |
| 4 | NAD | H | 400 | 44/44 | 0.85 | 0.28 | 88,90,99,101 | 0 |
| 5 | NA | A | 601 | 1/1 | 0.87 | 0.24 | 50,50,50,50 | 0 |
| 4 | NAD | G | 400 | 44/44 | 0.90 | 0.24 | 65,72,87,87 | 0 |
| 4 | NAD | A | 400 | 44/44 | 0.91 | 0.21 | 65,71,75,75 | 0 |
| 6 | NDP | I | 500 | 48/48 | 0.92 | 0.17 | 56,58,64,64 | 0 |
| 5 | NA | D | 602 | 1/1 | 0.92 | 0.18 | 69,69,69,69 | 0 |

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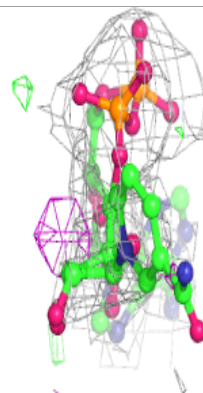
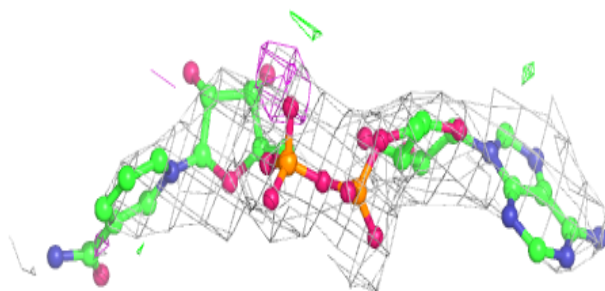
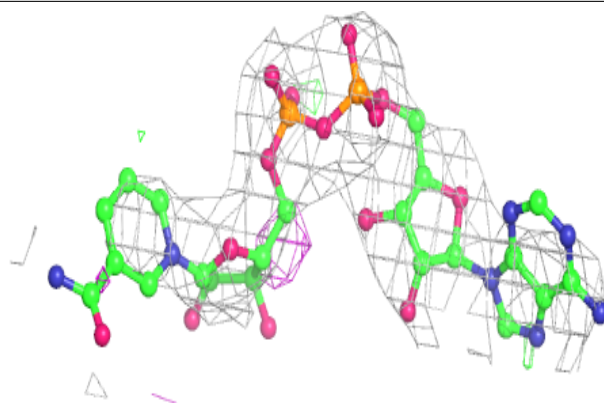
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 4 | NAD | D | 400 | 44/44 | 0.93 | 0.20 | 54,60,64,65 | 0 |
| 6 | NDP | F | 500 | 48/48 | 0.94 | 0.18 | 48,52,56,58 | 0 |
| 5 | NA | G | 603 | 1/1 | 0.95 | 0.10 | 48,48,48,48 | 0 |
| 6 | NDP | C | 500 | 48/48 | 0.95 | 0.17 | 38,40,44,46 | 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.

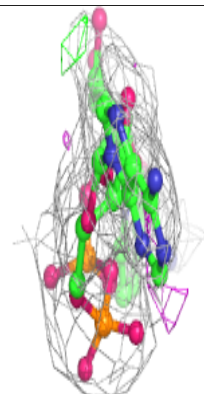
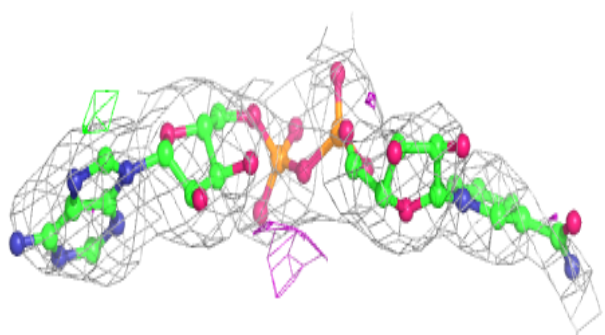
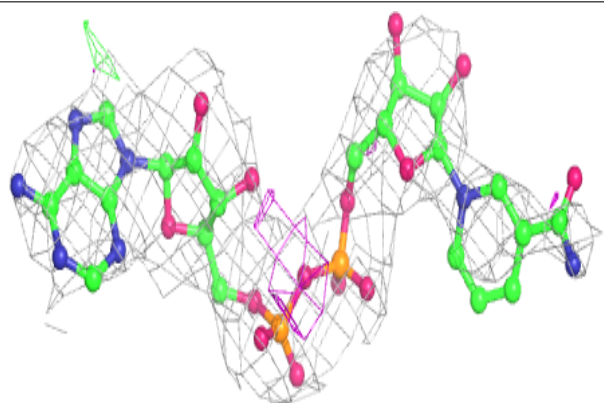


Electron density around NAD H 400:

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

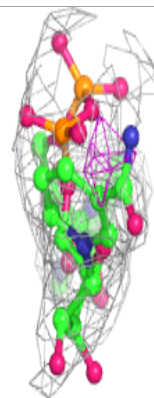
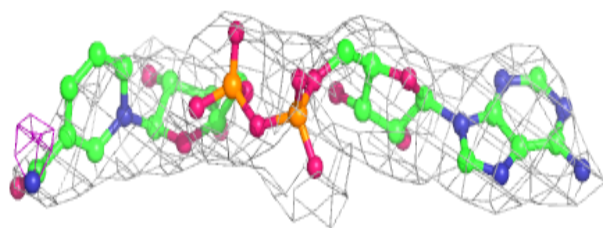
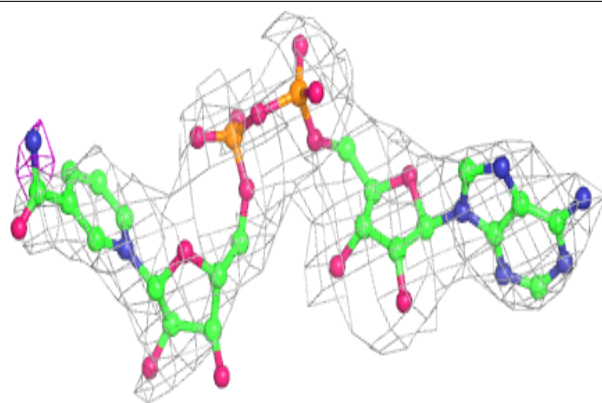
**Electron density around NAD G 400:**

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

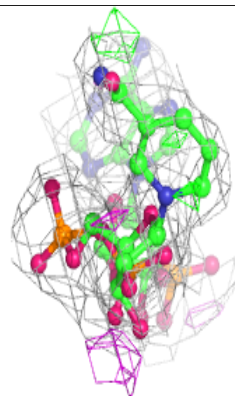
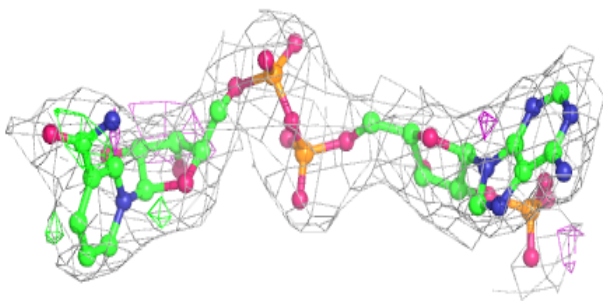
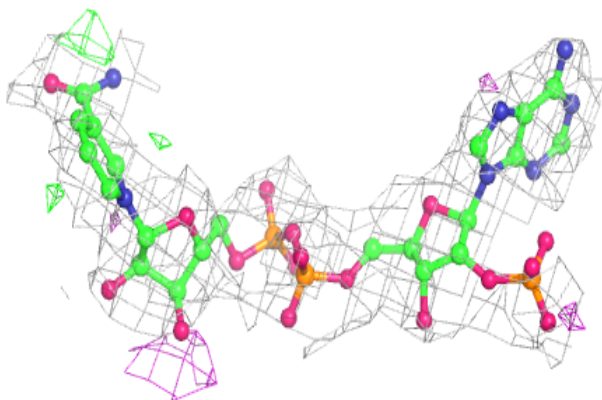


Electron density around NAD A 400:

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

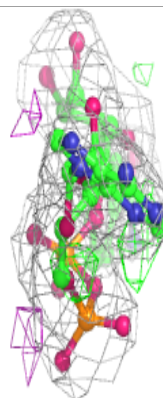
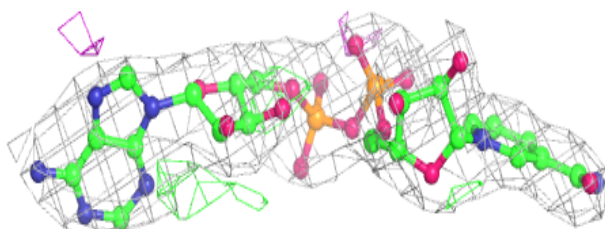
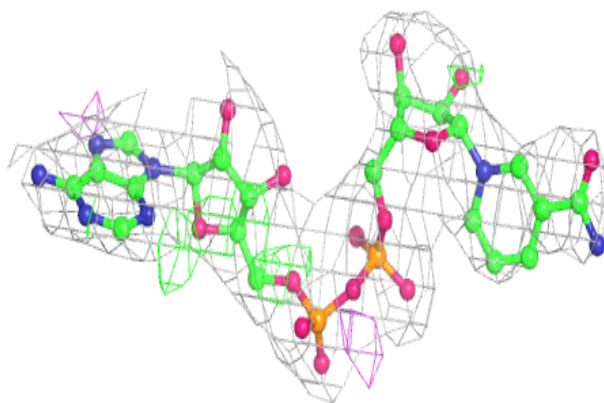
**Electron density around NDP I 500:**

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

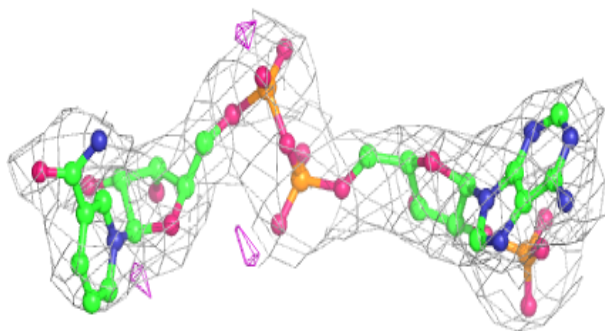
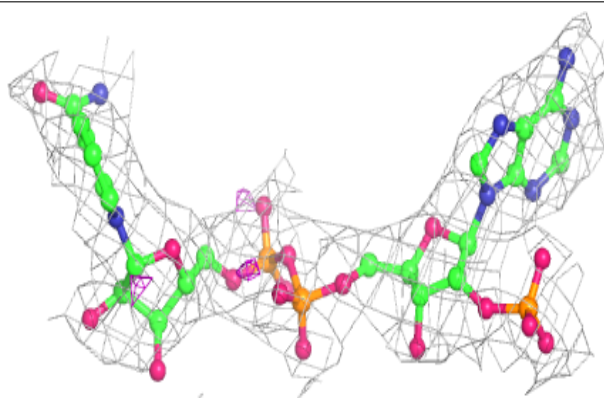


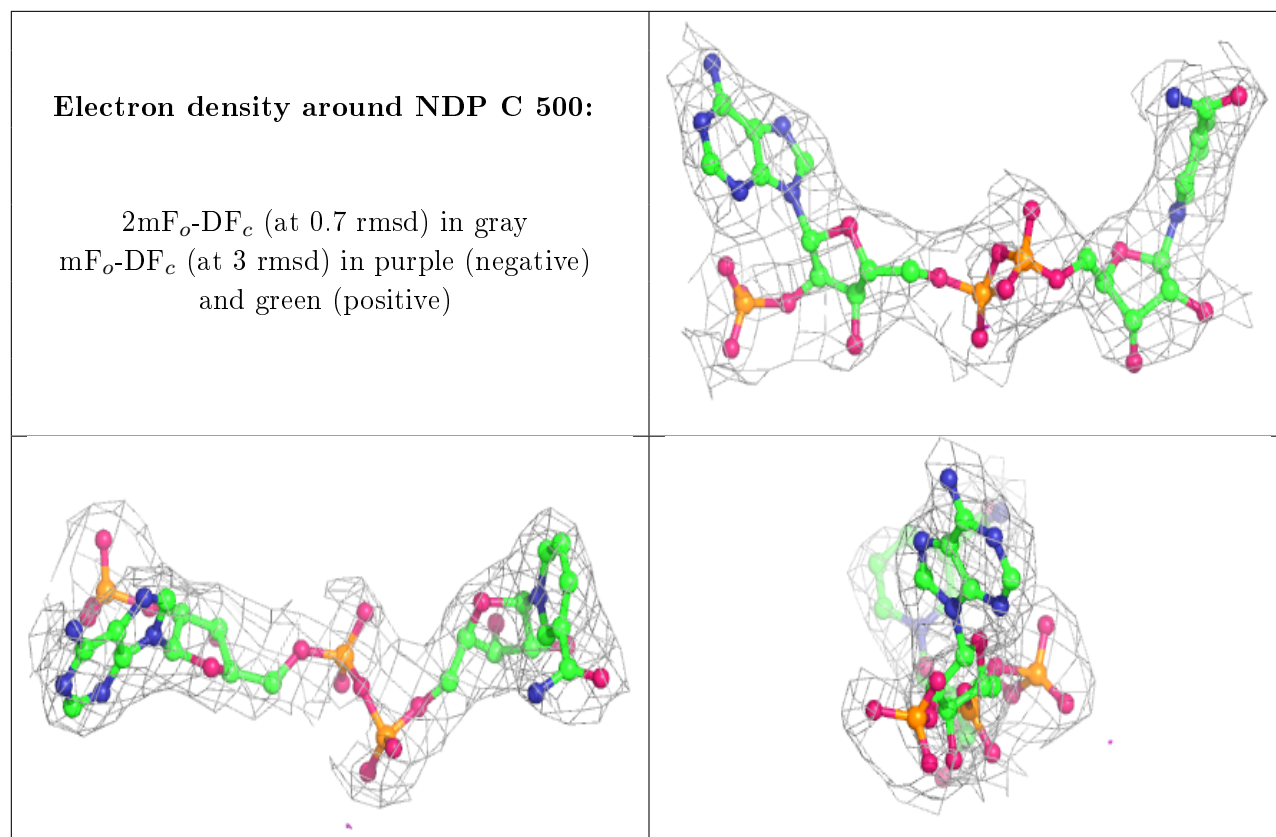
Electron density around NAD D 400:

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

**Electron density around NDP F 500:**

$2mF_o-DF_c$ (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.