



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:32 PM GMT

PDB ID : 1U1I
Title : Myo-inositol phosphate synthase mIPS from *A. fulgidus*
Authors : Stieglitz, K.A.; Yang, H.; Roberts, M.F.; Stec, B.
Deposited on : 2004-07-15
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

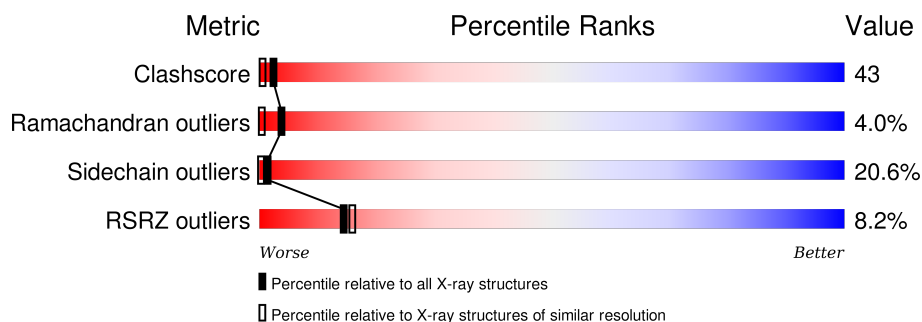
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore | 102246 | 5398 (1.90-1.90) |
| Ramachandran outliers | 100387 | 5338 (1.90-1.90) |
| Sidechain outliers | 100360 | 5339 (1.90-1.90) |
| RSRZ outliers | 91569 | 4766 (1.90-1.90) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 392 | <div> <div>7%</div> <div>32%</div> <div>51%</div> <div>16%</div> <div>.</div> </div> |
| 1 | B | 392 | <div> <div>11%</div> <div>31%</div> <div>57%</div> <div>12%</div> </div> |
| 1 | C | 392 | <div> <div>6%</div> <div>34%</div> <div>54%</div> <div>11%</div> <div>.</div> </div> |
| 1 | D | 392 | <div> <div>9%</div> <div>28%</div> <div>56%</div> <div>15%</div> <div>.</div> </div> |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 2 | PO4 | C | 1195 | - | - | X | X |
| 2 | PO4 | D | 1595 | - | - | X | - |

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13553 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 myo-inositol-1-phosphate synthase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 392 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3084 | 1996 | 499 | 576 | 13 | | | |
| 1 | B | 392 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3084 | 1996 | 499 | 576 | 13 | | | |
| 1 | C | 392 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3084 | 1996 | 499 | 576 | 13 | | | |
| 1 | D | 392 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3084 | 1996 | 499 | 576 | 13 | | | |

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2 | A | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |

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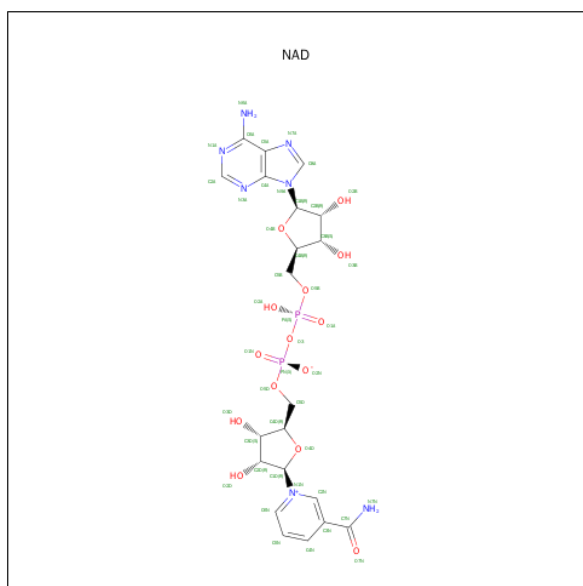
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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2 | C | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | D | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 3 | B | 1 | Total | K | 0 | 0 |
| | | | 1 | 1 | | |
| 3 | C | 1 | Total | K | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



| 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 | C | 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 | | |

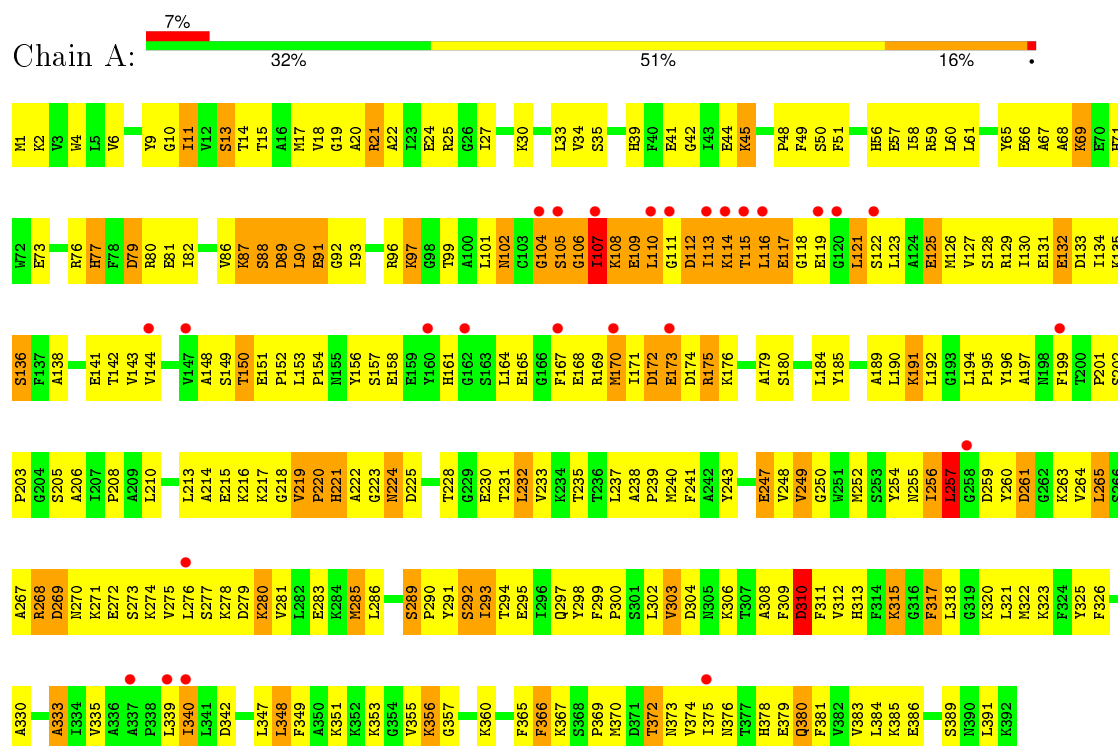
- Molecule 5 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 5 | A | 245 | Total 245 | O 245 | 0 | 0 |
| 5 | B | 249 | Total 249 | O 249 | 0 | 0 |
| 5 | C | 293 | Total 293 | O 293 | 0 | 0 |
| 5 | D | 232 | Total 232 | O 232 | 0 | 0 |

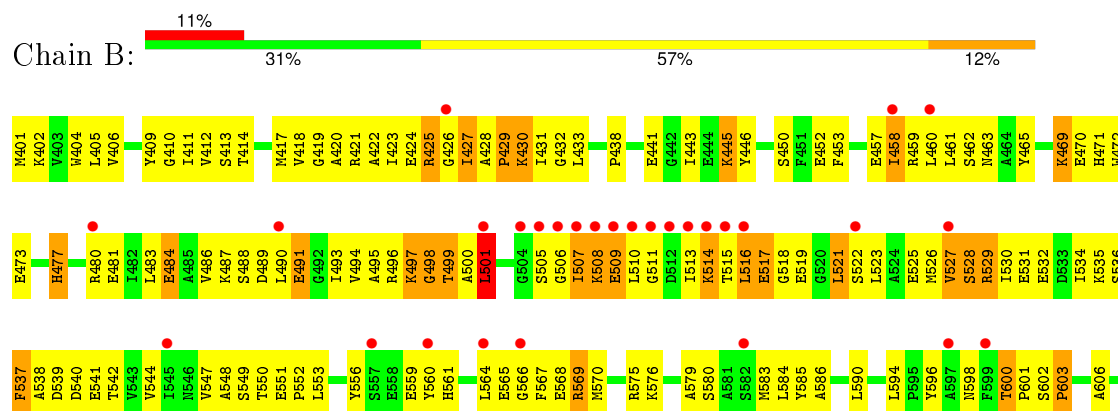
3 Residue-property plots

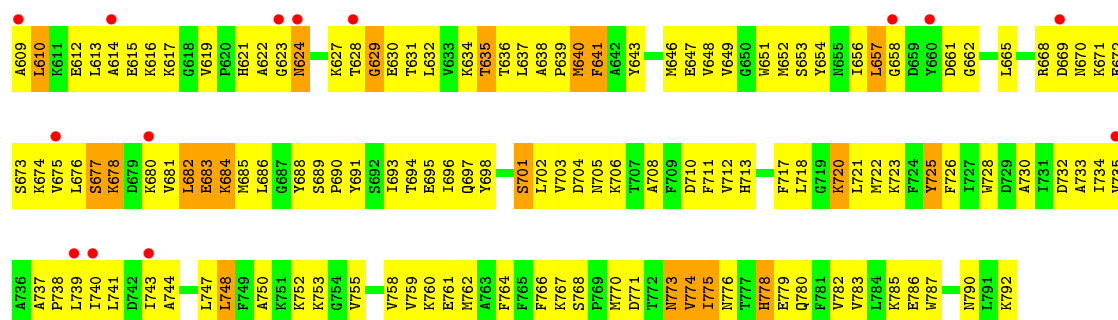
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: myo-inositol-1-phosphate synthase

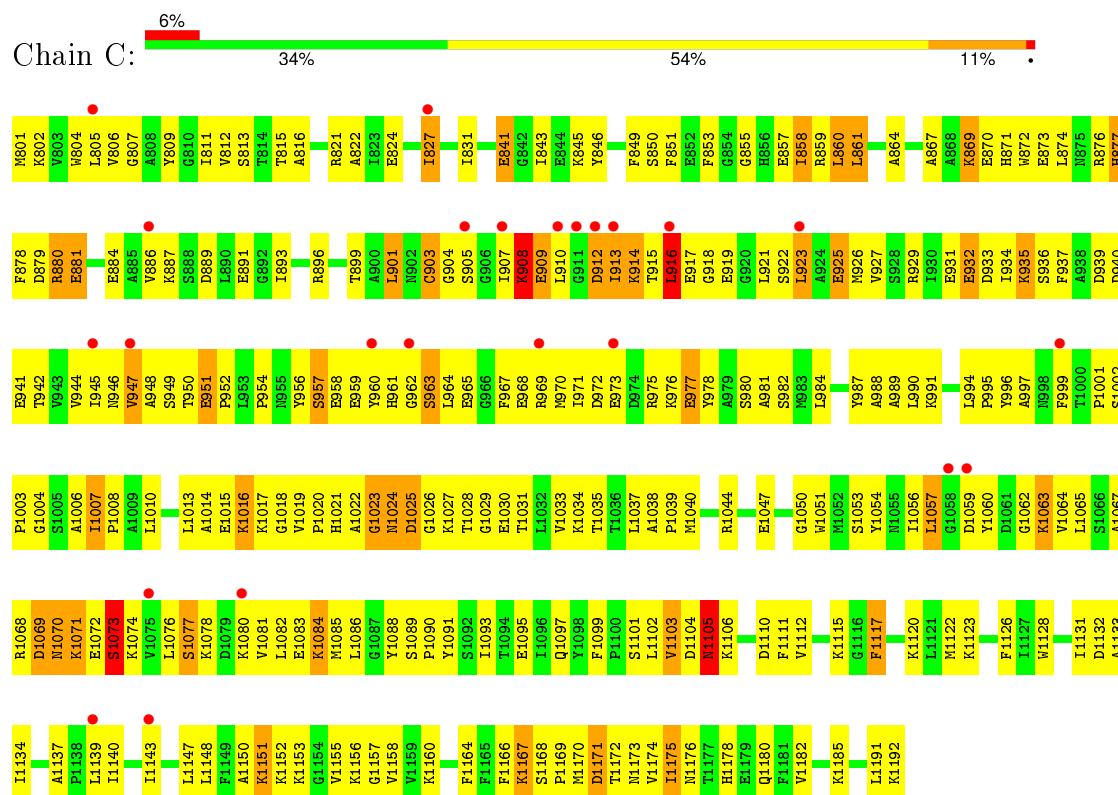


• Molecule 1: myo-inositol-1-phosphate synthase

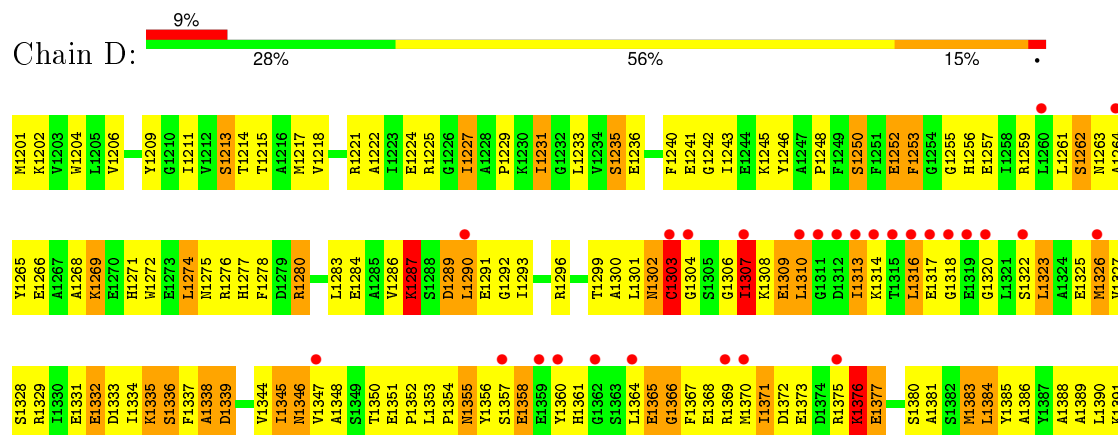




• Molecule 1: myo-inositol-1-phosphate synthase



• Molecule 1: myo-inositol-1-phosphate synthase





4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 62.77Å 83.94Å 91.79Å 65.79° 72.43° 74.98° | Depositor |
| Resolution (Å) | 37.60 – 1.90 37.65 – 1.90 | Depositor EDS |
| % Data completeness (in resolution range) | 100.0 (37.60-1.90) 67.2 (37.65-1.90) | Depositor EDS |
| R_{merge} | 0.05 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.52 (at 1.89Å) | Xtriage |
| Refinement program | SHELXL-97 | Depositor |
| R, R_{free} | 0.211 , 0.284 0.217 , (Not available) | Depositor DCC |
| R_{free} test set | No test flags present. | DCC |
| Wilson B-factor (Å ²) | 26.5 | Xtriage |
| Anisotropy | 0.222 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.36 , 248.2 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$ | Xtriage |
| Outliers | 0 of 92872 reflections | Xtriage |
| F_o, F_c correlation | 0.94 | EDS |
| Total number of atoms | 13553 | wwPDB-VP |
| Average B, all atoms (Å ²) | 45.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K, PO4, NAD

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | A | 0.31 | 0/3155 | 0.83 | 3/4257 (0.1%) |
| 1 | B | 0.31 | 0/3155 | 0.82 | 1/4257 (0.0%) |
| 1 | C | 0.31 | 0/3155 | 0.84 | 2/4257 (0.0%) |
| 1 | D | 0.30 | 0/3155 | 0.82 | 0/4257 |
| All | All | 0.31 | 0/12620 | 0.83 | 6/17028 (0.0%) |

There are no bond length outliers.

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 222 | ALA | C-N-CA | 7.75 | 138.58 | 122.30 |
| 1 | C | 1023 | GLY | C-N-CA | 7.32 | 139.99 | 121.70 |
| 1 | A | 257 | LEU | CA-CB-CG | 6.04 | 129.20 | 115.30 |
| 1 | B | 643 | TYR | CB-CG-CD2 | 5.81 | 124.49 | 121.00 |
| 1 | A | 310 | ASP | CB-CG-OD2 | -5.28 | 113.55 | 118.30 |
| 1 | C | 1128 | TRP | C-N-CA | 5.06 | 134.35 | 121.70 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 3084 | 0 | 3084 | 264 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | B | 3084 | 0 | 3081 | 281 | 0 |
| 1 | C | 3084 | 0 | 3081 | 270 | 0 |
| 1 | D | 3084 | 0 | 3081 | 300 | 0 |
| 2 | A | 5 | 0 | 0 | 1 | 0 |
| 2 | B | 5 | 0 | 0 | 1 | 0 |
| 2 | C | 5 | 0 | 0 | 2 | 0 |
| 2 | D | 5 | 0 | 0 | 2 | 0 |
| 3 | B | 1 | 0 | 0 | 0 | 0 |
| 3 | C | 1 | 0 | 0 | 0 | 0 |
| 4 | A | 44 | 0 | 26 | 6 | 0 |
| 4 | B | 44 | 0 | 26 | 5 | 0 |
| 4 | C | 44 | 0 | 26 | 8 | 0 |
| 4 | D | 44 | 0 | 25 | 9 | 0 |
| 5 | A | 245 | 0 | 0 | 17 | 0 |
| 5 | B | 249 | 0 | 0 | 16 | 0 |
| 5 | C | 293 | 0 | 0 | 6 | 0 |
| 5 | D | 232 | 0 | 0 | 9 | 0 |
| All | All | 13553 | 0 | 12430 | 1067 | 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 43.

All (1067) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:916:LEU:HD11 | 1:C:926:MET:CG | 1.46 | 1.45 |
| 1:C:916:LEU:HD12 | 1:C:926:MET:SD | 1.52 | 1.45 |
| 1:C:916:LEU:CD1 | 1:C:926:MET:HG2 | 1.51 | 1.38 |
| 1:C:916:LEU:CD1 | 1:C:926:MET:CG | 2.03 | 1.36 |
| 1:C:916:LEU:CD1 | 1:C:926:MET:SD | 2.19 | 1.28 |
| 1:C:916:LEU:HD11 | 1:C:926:MET:HG2 | 1.04 | 1.01 |
| 1:D:1398:ASN:HD22 | 1:D:1424:ASN:HA | 1.23 | 1.01 |
| 1:B:411:ILE:HD12 | 1:B:471:HIS:HB3 | 1.42 | 1.00 |
| 1:D:1280:ARG:HD2 | 1:D:1283:LEU:HD23 | 1.46 | 0.98 |
| 1:C:916:LEU:HD11 | 1:C:926:MET:CB | 1.95 | 0.96 |
| 1:D:1351:GLU:HG2 | 1:D:1402:SER:HB2 | 1.46 | 0.96 |
| 1:A:170:MET:HG3 | 1:A:175:ARG:HB2 | 1.45 | 0.96 |
| 1:D:1428:THR:HG21 | 4:D:1596:NAD:H71N | 1.32 | 0.93 |
| 1:C:1084:LYS:HB3 | 1:C:1173:ASN:HD21 | 1.34 | 0.93 |
| 1:B:523:LEU:HD13 | 1:B:576:LYS:HG2 | 1.51 | 0.92 |
| 1:B:776:ASN:HB3 | 1:B:779:GLU:HB2 | 1.51 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:58:ILE:HD12 | 1:A:110:LEU:HD11 | 1.51 | 0.91 |
| 1:C:859:ARG:HG3 | 1:C:910:LEU:HD11 | 1.51 | 0.91 |
| 1:A:11:ILE:HG13 | 1:A:71:HIS:HB3 | 1.52 | 0.90 |
| 1:D:1316:LEU:HD21 | 1:D:1326:MET:HG2 | 1.55 | 0.89 |
| 1:A:97:LYS:HE3 | 1:A:113:ILE:HD11 | 1.53 | 0.89 |
| 1:C:1131:ILE:HB | 1:D:1520:LYS:HE2 | 1.53 | 0.89 |
| 1:C:1134:ILE:HG12 | 1:D:1520:LYS:HD3 | 1.55 | 0.86 |
| 1:A:257:LEU:HG | 1:A:306:LYS:HG3 | 1.56 | 0.85 |
| 1:A:90:LEU:HA | 1:A:93:ILE:HD12 | 1.58 | 0.84 |
| 1:C:916:LEU:HD12 | 1:C:926:MET:CG | 1.89 | 0.84 |
| 1:C:1065:LEU:HD22 | 1:C:1071:LYS:HA | 1.60 | 0.83 |
| 1:A:173:GLU:HB3 | 1:A:175:ARG:HD3 | 1.60 | 0.83 |
| 1:D:1364:LEU:HD11 | 1:D:1412:GLU:HB3 | 1.62 | 0.82 |
| 1:B:695:GLU:HG2 | 1:B:697:GLN:HE21 | 1.45 | 0.81 |
| 1:B:510:LEU:HA | 1:B:513:ILE:HD12 | 1.63 | 0.81 |
| 1:A:97:LYS:HG2 | 1:A:115:THR:HB | 1.62 | 0.81 |
| 1:B:606:ALA:HB2 | 1:B:624:ASN:HD21 | 1.45 | 0.81 |
| 1:D:1567:LYS:HE2 | 2:D:1595:PO4:O4 | 1.81 | 0.81 |
| 1:C:923:LEU:HD23 | 1:C:971:ILE:HA | 1.62 | 0.80 |
| 1:B:523:LEU:HD21 | 1:B:579:ALA:HB2 | 1.62 | 0.80 |
| 1:C:877:HIS:HB2 | 1:C:1134:ILE:HD11 | 1.64 | 0.79 |
| 1:B:576:LYS:HB3 | 5:B:2404:HOH:O | 1.83 | 0.79 |
| 1:B:553:LEU:HD13 | 1:B:672:GLU:OE2 | 1.83 | 0.79 |
| 1:D:1354:PRO:HB3 | 1:D:1403:PRO:HG3 | 1.64 | 0.79 |
| 1:A:61:LEU:HD12 | 1:A:67:ALA:HB2 | 1.65 | 0.78 |
| 1:C:909:GLU:O | 1:C:910:LEU:HD13 | 1.83 | 0.78 |
| 1:B:522:SER:O | 1:B:526:MET:HG3 | 1.83 | 0.78 |
| 1:B:598:ASN:OD1 | 1:B:600:THR:HG23 | 1.84 | 0.78 |
| 1:B:661:ASP:O | 1:B:665:LEU:HG | 1.84 | 0.78 |
| 1:A:272:GLU:O | 1:A:276:LEU:HG | 1.84 | 0.78 |
| 1:D:1284:GLU:O | 1:D:1287:LYS:HB2 | 1.83 | 0.78 |
| 1:C:1028:THR:OG1 | 4:C:1196:NAD:H4N | 1.84 | 0.78 |
| 1:B:678:LYS:HB3 | 1:B:694:THR:HG21 | 1.66 | 0.78 |
| 1:A:114:LYS:HG2 | 1:A:119:GLU:HA | 1.66 | 0.77 |
| 1:B:782:VAL:HA | 1:B:785:LYS:HD3 | 1.64 | 0.77 |
| 1:D:1476:LEU:HD22 | 1:D:1480:LYS:HZ2 | 1.50 | 0.77 |
| 1:D:1532:ASP:HB3 | 4:D:1596:NAD:H72N | 1.48 | 0.77 |
| 1:C:1069:ASP:O | 1:C:1072:GLU:HB3 | 1.85 | 0.77 |
| 1:C:904:GLY:O | 1:C:907:ILE:HG13 | 1.84 | 0.77 |
| 1:C:1031:THR:O | 1:C:1035:THR:HG23 | 1.85 | 0.77 |
| 1:D:1421:HIS:O | 1:D:1558:VAL:HA | 1.85 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:409:TYR:HE2 | 1:B:461:LEU:H | 1.34 | 0.76 |
| 1:D:1214:THR:O | 1:D:1218:VAL:HG23 | 1.85 | 0.76 |
| 1:A:131:GLU:O | 1:A:135:LYS:HB2 | 1.86 | 0.75 |
| 1:C:990:LEU:HD22 | 1:C:1014:ALA:HB2 | 1.67 | 0.75 |
| 1:D:1277:HIS:O | 1:D:1534:ILE:HD11 | 1.86 | 0.75 |
| 1:C:1077:SER:O | 1:C:1081:VAL:HG23 | 1.87 | 0.75 |
| 1:B:637:LEU:O | 1:B:640:MET:HB3 | 1.86 | 0.75 |
| 1:A:11:ILE:HD13 | 1:A:333:ALA:HB2 | 1.68 | 0.75 |
| 1:B:460:LEU:HD21 | 1:B:495:ALA:O | 1.87 | 0.75 |
| 1:C:1014:ALA:HB1 | 1:C:1019:VAL:O | 1.85 | 0.75 |
| 1:A:367:LYS:HE2 | 2:A:395:PO4:O4 | 1.87 | 0.74 |
| 1:D:1424:ASN:O | 1:D:1566:PHE:HB3 | 1.88 | 0.74 |
| 1:A:376:ASN:HB3 | 1:A:379:GLU:HB2 | 1.67 | 0.74 |
| 1:B:490:LEU:HA | 1:B:493:ILE:HG13 | 1.69 | 0.74 |
| 1:B:547:VAL:HG22 | 4:B:796:NAD:H51N | 1.68 | 0.74 |
| 1:D:1299:THR:HG21 | 1:D:1384:LEU:HD12 | 1.69 | 0.74 |
| 1:D:1468:ARG:HH22 | 1:D:1472:GLU:HG3 | 1.53 | 0.74 |
| 1:A:260:TYR:HA | 1:A:263:LYS:HG3 | 1.69 | 0.74 |
| 1:A:154:PRO:HG3 | 1:A:203:PRO:HG3 | 1.69 | 0.74 |
| 1:D:1448:VAL:O | 1:D:1490:PRO:HB3 | 1.85 | 0.74 |
| 1:D:1253:PHE:O | 1:D:1293:ILE:HD12 | 1.88 | 0.74 |
| 1:D:1515:LYS:HE3 | 1:D:1519:GLY:HA2 | 1.70 | 0.74 |
| 1:A:254:TYR:OH | 1:A:297:GLN:HG3 | 1.88 | 0.74 |
| 1:B:613:LEU:O | 1:B:617:LYS:HB2 | 1.88 | 0.73 |
| 1:C:1160:LYS:HG2 | 1:C:1171:ASP:HB2 | 1.69 | 0.73 |
| 1:A:269:ASP:HB2 | 1:A:270:ASN:OD1 | 1.88 | 0.73 |
| 1:B:671:LYS:HE2 | 1:B:675:VAL:HG21 | 1.69 | 0.73 |
| 1:C:922:SER:OG | 1:C:925:GLU:HG3 | 1.88 | 0.73 |
| 1:B:522:SER:OG | 1:B:525:GLU:HB2 | 1.89 | 0.73 |
| 1:B:430:LYS:HE3 | 5:B:2422:HOH:O | 1.87 | 0.73 |
| 1:D:1327:VAL:HG21 | 1:D:1371:ILE:HD11 | 1.71 | 0.73 |
| 1:D:1398:ASN:ND2 | 1:D:1424:ASN:HA | 2.03 | 0.72 |
| 1:B:564:LEU:HB3 | 5:B:1792:HOH:O | 1.89 | 0.72 |
| 1:C:884:GLU:O | 1:C:887:LYS:HB3 | 1.89 | 0.72 |
| 1:C:1026:GLY:O | 4:C:1196:NAD:H5N | 1.89 | 0.72 |
| 1:D:1364:LEU:HD12 | 1:D:1364:LEU:H | 1.53 | 0.72 |
| 1:D:1259:ARG:HG2 | 1:D:1310:LEU:HG | 1.71 | 0.72 |
| 1:B:559:GLU:HB2 | 1:B:569:ARG:HH12 | 1.53 | 0.72 |
| 1:A:102:ASN:HB3 | 5:A:1976:HOH:O | 1.88 | 0.72 |
| 1:D:1428:THR:HG21 | 4:D:1596:NAD:N7N | 2.05 | 0.72 |
| 1:A:96:ARG:HD3 | 1:A:133:ASP:HB3 | 1.71 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:1151:LYS:HE2 | 5:C:2191:HOH:O | 1.89 | 0.72 |
| 1:C:922:SER:O | 1:C:926:MET:HG3 | 1.90 | 0.72 |
| 1:D:1393:GLY:HA2 | 1:D:1419:VAL:HG21 | 1.72 | 0.72 |
| 1:C:921:LEU:HD21 | 1:C:929:ARG:NH1 | 2.04 | 0.71 |
| 1:D:1331:GLU:HG3 | 1:D:1388:ALA:HB1 | 1.70 | 0.71 |
| 1:D:1242:GLY:O | 1:D:1245:LYS:HG2 | 1.89 | 0.71 |
| 1:D:1357:SER:H | 1:D:1361:HIS:HD2 | 1.37 | 0.71 |
| 1:C:923:LEU:O | 1:C:927:VAL:HG23 | 1.90 | 0.71 |
| 1:C:919:GLU:HB2 | 1:C:921:LEU:HD13 | 1.73 | 0.71 |
| 1:C:1117:PHE:HA | 1:D:1231:ILE:O | 1.90 | 0.71 |
| 1:C:964:LEU:HD21 | 1:C:1013:LEU:HD13 | 1.70 | 0.71 |
| 1:A:240:MET:HB2 | 1:B:636:THR:HG21 | 1.72 | 0.71 |
| 1:D:1242:GLY:O | 1:D:1245:LYS:HE2 | 1.90 | 0.71 |
| 1:D:1474:LYS:HE2 | 1:D:1567:LYS:HZ1 | 1.54 | 0.71 |
| 1:D:1364:LEU:O | 1:D:1368:GLU:HB2 | 1.91 | 0.71 |
| 1:C:1037:LEU:O | 1:C:1040:MET:HB3 | 1.91 | 0.70 |
| 1:C:1153:LYS:HB3 | 1:C:1191:LEU:HD22 | 1.74 | 0.70 |
| 1:C:1178:HIS:O | 1:C:1182:VAL:HG23 | 1.92 | 0.70 |
| 1:A:318:LEU:HD21 | 1:B:419:GLY:HA2 | 1.73 | 0.70 |
| 1:B:411:ILE:HG12 | 1:B:733:ALA:HB2 | 1.74 | 0.70 |
| 1:C:811:ILE:HD12 | 1:C:871:HIS:HB3 | 1.72 | 0.70 |
| 1:A:249:VAL:HG23 | 1:A:313:HIS:O | 1.92 | 0.70 |
| 1:B:774:VAL:HG13 | 1:B:779:GLU:OE2 | 1.91 | 0.70 |
| 1:D:1397:ALA:HB2 | 1:D:1547:LEU:HD11 | 1.74 | 0.69 |
| 1:B:641:PHE:HB3 | 1:B:646:MET:HB2 | 1.74 | 0.69 |
| 1:D:1587:TRP:O | 1:D:1591:LEU:HG | 1.91 | 0.69 |
| 1:B:776:ASN:O | 1:B:780:GLN:HG3 | 1.92 | 0.69 |
| 1:A:6:VAL:HG12 | 1:A:148:ALA:HB2 | 1.75 | 0.69 |
| 1:C:821:ARG:HD2 | 1:C:889:ASP:OD1 | 1.92 | 0.69 |
| 1:A:127:VAL:HG21 | 1:A:171:ILE:HD12 | 1.74 | 0.69 |
| 1:B:677:SER:HB2 | 1:B:767:LYS:HD2 | 1.75 | 0.69 |
| 1:B:497:LYS:HD2 | 1:B:497:LYS:H | 1.56 | 0.69 |
| 1:D:1435:THR:HA | 1:D:1485:MET:HE1 | 1.75 | 0.69 |
| 1:B:417:MET:HE1 | 1:B:453:PHE:HB3 | 1.74 | 0.69 |
| 1:A:127:VAL:HG22 | 1:A:184:LEU:HD22 | 1.74 | 0.69 |
| 1:C:1067:ALA:O | 1:C:1071:LYS:HD2 | 1.92 | 0.68 |
| 1:A:201:PRO:HB3 | 1:A:225:ASP:OD2 | 1.93 | 0.68 |
| 1:A:213:LEU:O | 1:A:217:LYS:HD3 | 1.93 | 0.68 |
| 1:C:899:THR:HB | 1:C:916:LEU:HD23 | 1.75 | 0.68 |
| 1:C:1117:PHE:HB2 | 1:D:1538:PRO:HG3 | 1.76 | 0.68 |
| 1:B:720:LYS:HE2 | 1:B:721:LEU:O | 1.94 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:708:ALA:HB3 | 1:B:728:TRP:HB3 | 1.75 | 0.68 |
| 1:A:223:GLY:O | 1:A:370:MET:HG3 | 1.94 | 0.67 |
| 1:B:484:GLU:O | 1:B:487:LYS:HB3 | 1.94 | 0.67 |
| 1:D:1202:LYS:HD3 | 1:D:1339:ASP:OD2 | 1.95 | 0.67 |
| 1:B:420:ALA:O | 1:B:424:GLU:HG3 | 1.94 | 0.67 |
| 1:B:544:VAL:O | 1:B:596:TYR:HA | 1.94 | 0.67 |
| 1:C:1006:ALA:HA | 1:C:1170:MET:HE3 | 1.77 | 0.67 |
| 1:D:1303:CYS:HB3 | 1:D:1352:PRO:HD2 | 1.77 | 0.67 |
| 1:A:60:LEU:HB2 | 1:A:97:LYS:HZ1 | 1.59 | 0.67 |
| 1:D:1467:ALA:O | 1:D:1471:LYS:HB2 | 1.94 | 0.67 |
| 1:B:480:ARG:HB2 | 5:B:1611:HOH:O | 1.93 | 0.67 |
| 1:B:668:ARG:HA | 1:B:671:LYS:HB3 | 1.77 | 0.67 |
| 1:D:1217:MET:HE3 | 1:D:1253:PHE:HB2 | 1.76 | 0.67 |
| 1:A:205:SER:HA | 1:A:210:LEU:HD12 | 1.77 | 0.67 |
| 1:C:916:LEU:CG | 1:C:926:MET:SD | 2.82 | 0.66 |
| 1:D:1429:GLY:O | 1:D:1433:VAL:HG23 | 1.96 | 0.66 |
| 1:D:1476:LEU:HD22 | 1:D:1480:LYS:NZ | 2.11 | 0.66 |
| 1:C:999:PHE:O | 1:C:1025:ASP:HA | 1.94 | 0.66 |
| 1:C:915:THR:O | 1:C:919:GLU:HG3 | 1.96 | 0.66 |
| 1:C:1020:PRO:HA | 1:C:1157:GLY:O | 1.96 | 0.66 |
| 1:B:421:ARG:O | 1:B:425:ARG:HG3 | 1.95 | 0.66 |
| 1:C:1115:LYS:HG3 | 1:C:1120:LYS:O | 1.95 | 0.66 |
| 1:D:1381:ALA:O | 1:D:1384:LEU:HB2 | 1.95 | 0.66 |
| 1:A:22:ALA:O | 1:A:27:ILE:HG13 | 1.95 | 0.66 |
| 1:B:469:LYS:O | 1:B:473:GLU:HG2 | 1.95 | 0.66 |
| 1:B:501:LEU:HD23 | 1:B:517:GLU:OE1 | 1.96 | 0.66 |
| 1:D:1329:ARG:HA | 1:D:1332:GLU:HB2 | 1.78 | 0.66 |
| 1:B:552:PRO:HD3 | 1:B:670:ASN:OD1 | 1.96 | 0.66 |
| 1:C:1067:ALA:O | 1:C:1071:LYS:HB3 | 1.96 | 0.65 |
| 1:D:1302:ASN:ND2 | 1:D:1377:GLU:HA | 2.11 | 0.65 |
| 1:B:424:GLU:OE1 | 1:B:450:SER:HA | 1.96 | 0.65 |
| 1:A:225:ASP:OD1 | 1:A:367:LYS:HE3 | 1.96 | 0.65 |
| 1:B:550:THR:HG23 | 1:B:601:PRO:HD2 | 1.78 | 0.65 |
| 1:B:556:TYR:HA | 1:B:561:HIS:ND1 | 2.11 | 0.65 |
| 1:C:824:GLU:OE2 | 1:C:850:SER:HA | 1.96 | 0.65 |
| 1:C:1024:ASN:HB2 | 1:C:1168:SER:O | 1.95 | 0.65 |
| 1:B:761:GLU:HG2 | 1:B:787:TRP:HB2 | 1.77 | 0.65 |
| 1:B:559:GLU:HB2 | 1:B:569:ARG:NH1 | 2.11 | 0.65 |
| 1:A:4:TRP:HH2 | 1:A:96:ARG:HD2 | 1.61 | 0.65 |
| 1:C:960:TYR:HB3 | 1:C:970:MET:HB2 | 1.79 | 0.65 |
| 1:C:1176:ASN:O | 1:C:1180:GLN:HG3 | 1.97 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:104:GLY:HA3 | 1:A:152:PRO:HG3 | 1.77 | 0.65 |
| 1:C:1016:LYS:HG3 | 1:C:1016:LYS:O | 1.96 | 0.65 |
| 1:B:549:SER:HB2 | 4:B:796:NAD:H8A | 1.79 | 0.65 |
| 1:B:462:SER:O | 1:B:494:VAL:HG22 | 1.97 | 0.64 |
| 1:D:1213:SER:O | 1:D:1217:MET:HG3 | 1.98 | 0.64 |
| 1:D:1400:THR:OG1 | 1:D:1402:SER:HB3 | 1.97 | 0.64 |
| 1:A:56:HIS:HB2 | 5:A:2000:HOH:O | 1.97 | 0.64 |
| 1:C:1064:VAL:HG13 | 1:C:1070:ASN:HD22 | 1.61 | 0.64 |
| 1:D:1365:GLU:HA | 5:D:1818:HOH:O | 1.97 | 0.64 |
| 1:A:372:THR:HG23 | 1:A:374:VAL:H | 1.63 | 0.64 |
| 1:D:1272:TRP:CH2 | 1:D:1280:ARG:HB2 | 2.33 | 0.64 |
| 1:A:190:LEU:HD13 | 1:A:214:ALA:HB2 | 1.79 | 0.64 |
| 1:D:1265:TYR:N | 1:D:1290:LEU:HB3 | 2.13 | 0.64 |
| 1:D:1475:VAL:O | 1:D:1478:LYS:HG3 | 1.98 | 0.64 |
| 1:A:122:SER:OG | 1:A:125:GLU:HG3 | 1.97 | 0.64 |
| 1:D:1229:PRO:HB2 | 1:D:1231:ILE:HG12 | 1.80 | 0.63 |
| 1:D:1390:LEU:HD12 | 1:D:1410:LEU:HD13 | 1.81 | 0.63 |
| 1:B:509:GLU:HG3 | 1:B:510:LEU:HD13 | 1.80 | 0.63 |
| 1:D:1368:GLU:HB3 | 5:D:1818:HOH:O | 1.98 | 0.63 |
| 1:B:515:THR:HG23 | 1:B:519:GLU:OE1 | 1.98 | 0.63 |
| 1:A:250:GLY:HA2 | 1:A:291:TYR:O | 1.99 | 0.63 |
| 1:B:438:PRO:O | 1:B:441:GLU:HB2 | 1.98 | 0.63 |
| 1:D:1303:CYS:SG | 1:D:1352:PRO:HG2 | 2.39 | 0.63 |
| 1:A:232:LEU:HD13 | 1:B:640:MET:SD | 2.38 | 0.63 |
| 1:A:197:ALA:HB2 | 1:A:347:LEU:HD11 | 1.80 | 0.63 |
| 1:A:148:ALA:O | 4:A:396:NAD:H4D | 1.97 | 0.63 |
| 1:B:519:GLU:HG2 | 5:B:2276:HOH:O | 1.99 | 0.63 |
| 1:A:356:LYS:HG2 | 5:A:1863:HOH:O | 1.98 | 0.63 |
| 1:B:409:TYR:HB2 | 1:B:457:GLU:OE2 | 1.98 | 0.63 |
| 1:A:228:THR:HB | 1:A:335:VAL:HG23 | 1.81 | 0.63 |
| 1:C:1106:LYS:HB3 | 1:C:1132:ASP:OD1 | 1.99 | 0.63 |
| 1:B:426:GLY:HA2 | 5:B:2115:HOH:O | 1.98 | 0.63 |
| 1:A:158:GLU:O | 1:A:158:GLU:HG3 | 1.98 | 0.63 |
| 1:A:230:GLU:OE1 | 1:A:308:ALA:HB1 | 1.99 | 0.63 |
| 1:C:1025:ASP:O | 1:C:1166:PHE:HA | 1.99 | 0.62 |
| 1:B:560:TYR:CD2 | 1:B:570:MET:HB2 | 2.34 | 0.62 |
| 1:D:1272:TRP:CZ3 | 1:D:1280:ARG:HD3 | 2.35 | 0.62 |
| 1:A:220:PRO:HB3 | 1:A:355:VAL:HG12 | 1.82 | 0.62 |
| 1:D:1559:VAL:HB | 1:D:1562:MET:HE2 | 1.81 | 0.62 |
| 1:C:801:MET:HE3 | 1:C:1148:LEU:HD22 | 1.80 | 0.62 |
| 1:A:65:TYR:CE1 | 1:A:87:LYS:HB2 | 2.35 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1476:LEU:HB3 | 1:D:1480:LYS:HZ2 | 1.65 | 0.62 |
| 1:D:1456:ILE:HD12 | 1:D:1502:LEU:HD11 | 1.81 | 0.62 |
| 1:B:741:LEU:O | 1:B:744:ALA:HB3 | 1.99 | 0.61 |
| 1:A:378:HIS:ND1 | 1:B:778:HIS:HB2 | 2.15 | 0.61 |
| 1:D:1369:ARG:O | 1:D:1373:GLU:HG3 | 2.01 | 0.61 |
| 1:B:669:ASP:HB2 | 5:B:1830:HOH:O | 2.01 | 0.61 |
| 1:B:472:TRP:CH2 | 1:B:480:ARG:HG3 | 2.36 | 0.61 |
| 1:A:161:HIS:O | 1:A:208:PRO:HD2 | 2.01 | 0.61 |
| 1:C:956:TYR:OH | 1:C:1008:PRO:HG2 | 2.00 | 0.61 |
| 1:A:235:THR:HA | 1:A:285:MET:SD | 2.40 | 0.61 |
| 1:D:1581:PHE:CE2 | 1:D:1585:LYS:HD2 | 2.36 | 0.61 |
| 1:B:487:LYS:HD3 | 5:B:2073:HOH:O | 2.00 | 0.61 |
| 1:B:517:GLU:HB2 | 1:B:526:MET:SD | 2.40 | 0.61 |
| 1:D:1506:LYS:HD2 | 1:D:1532:ASP:OD2 | 2.00 | 0.61 |
| 1:D:1448:VAL:HG12 | 1:D:1490:PRO:HB3 | 1.83 | 0.61 |
| 1:D:1383:MET:HE1 | 5:D:2579:HOH:O | 1.99 | 0.61 |
| 1:D:1323:LEU:HD22 | 1:D:1376:LYS:HG3 | 1.82 | 0.60 |
| 1:A:311:PHE:CE2 | 1:A:323:LYS:HB3 | 2.35 | 0.60 |
| 1:B:586:ALA:O | 1:B:590:LEU:HG | 2.01 | 0.60 |
| 1:C:1064:VAL:HG13 | 1:C:1070:ASN:ND2 | 2.16 | 0.60 |
| 1:C:804:TRP:CE2 | 1:C:855:GLY:HA2 | 2.36 | 0.60 |
| 1:C:809:TYR:CD2 | 1:C:857:GLU:HG2 | 2.36 | 0.60 |
| 1:A:257:LEU:HB3 | 1:A:306:LYS:HA | 1.83 | 0.60 |
| 1:D:1357:SER:H | 1:D:1361:HIS:CD2 | 2.19 | 0.60 |
| 1:C:948:ALA:O | 4:C:1196:NAD:H4D | 2.02 | 0.60 |
| 1:C:964:LEU:O | 1:C:968:GLU:HG3 | 2.02 | 0.60 |
| 1:A:58:ILE:O | 1:A:110:LEU:HD22 | 2.02 | 0.60 |
| 1:A:97:LYS:O | 1:A:116:LEU:HD23 | 2.02 | 0.60 |
| 1:A:152:PRO:HB3 | 1:A:269:ASP:HB3 | 1.81 | 0.60 |
| 1:D:1552:LYS:O | 1:D:1553:LYS:HD3 | 2.01 | 0.60 |
| 1:D:1532:ASP:HB3 | 4:D:1596:NAD:N7N | 2.17 | 0.60 |
| 1:A:149:SER:H | 4:A:396:NAD:C8A | 2.15 | 0.60 |
| 1:B:602:SER:OG | 1:B:603:PRO:HD2 | 2.02 | 0.59 |
| 1:D:1368:GLU:O | 1:D:1371:ILE:HG22 | 2.02 | 0.59 |
| 1:A:374:VAL:HG13 | 1:A:379:GLU:HB3 | 1.83 | 0.59 |
| 1:C:958:GLU:HG3 | 5:C:1985:HOH:O | 2.02 | 0.59 |
| 1:C:802:LYS:HD2 | 1:C:939:ASP:OD1 | 2.03 | 0.59 |
| 1:B:758:VAL:HG21 | 1:B:771:ASP:OD2 | 2.01 | 0.59 |
| 1:B:409:TYR:CD2 | 1:B:457:GLU:HG2 | 2.37 | 0.59 |
| 1:B:634:LYS:HD3 | 1:B:682:LEU:HD13 | 1.84 | 0.59 |
| 1:C:896:ARG:HD2 | 1:C:933:ASP:OD2 | 2.03 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:758:VAL:HG11 | 1:B:770:MET:HB2 | 1.85 | 0.59 |
| 1:D:1459:ASP:O | 1:D:1463:LYS:HG3 | 2.02 | 0.59 |
| 1:B:470:GLU:O | 1:B:473:GLU:HB2 | 2.03 | 0.59 |
| 1:B:514:LYS:HD2 | 1:B:518:GLY:H | 1.67 | 0.59 |
| 1:A:130:ILE:O | 1:A:134:ILE:HG22 | 2.03 | 0.59 |
| 1:D:1217:MET:HB3 | 1:D:1221:ARG:HH12 | 1.67 | 0.59 |
| 1:D:1329:ARG:O | 1:D:1332:GLU:HB2 | 2.03 | 0.59 |
| 1:A:256:ILE:HD12 | 1:A:302:LEU:HD11 | 1.84 | 0.59 |
| 1:C:910:LEU:HB2 | 1:C:913:ILE:HD13 | 1.84 | 0.59 |
| 1:D:1209:TYR:CE2 | 1:D:1261:LEU:HB2 | 2.38 | 0.59 |
| 1:B:514:LYS:HE2 | 1:B:517:GLU:OE2 | 2.02 | 0.59 |
| 1:A:6:VAL:HG22 | 5:A:2000:HOH:O | 2.02 | 0.59 |
| 1:A:233:VAL:HG22 | 1:B:640:MET:CE | 2.33 | 0.59 |
| 1:A:91:GLU:O | 1:A:91:GLU:HG2 | 2.01 | 0.59 |
| 1:A:237:LEU:O | 1:A:240:MET:HB3 | 2.03 | 0.58 |
| 1:A:123:LEU:O | 1:A:127:VAL:HG23 | 2.03 | 0.58 |
| 1:A:82:ILE:O | 1:A:86:VAL:HG23 | 2.03 | 0.58 |
| 1:B:594:LEU:O | 1:B:619:VAL:HG11 | 2.03 | 0.58 |
| 1:C:1083:GLU:HG2 | 1:C:1089:SER:OG | 2.04 | 0.58 |
| 1:A:322:MET:SD | 1:B:730:ALA:HB1 | 2.44 | 0.58 |
| 1:D:1574:VAL:HG13 | 1:D:1579:GLU:HB3 | 1.86 | 0.58 |
| 1:A:237:LEU:HB2 | 5:A:1803:HOH:O | 2.03 | 0.58 |
| 1:A:220:PRO:HA | 1:A:357:GLY:O | 2.04 | 0.58 |
| 1:B:532:GLU:HA | 1:B:535:LYS:HE2 | 1.84 | 0.58 |
| 1:D:1553:LYS:HE3 | 1:D:1591:LEU:O | 2.04 | 0.58 |
| 1:A:256:ILE:HD12 | 1:A:302:LEU:CD1 | 2.34 | 0.58 |
| 1:C:1021:HIS:CE1 | 1:C:1158:VAL:HG22 | 2.39 | 0.58 |
| 1:B:404:TRP:HB2 | 1:B:537:PHE:CE2 | 2.39 | 0.58 |
| 1:C:1007:ILE:HD11 | 1:C:1010:LEU:HB2 | 1.85 | 0.58 |
| 1:B:652:MET:O | 1:B:710:ASP:HA | 2.04 | 0.58 |
| 1:B:580:SER:O | 1:B:584:LEU:HG | 2.04 | 0.58 |
| 1:B:654:TYR:OH | 1:B:697:GLN:HG3 | 2.04 | 0.57 |
| 1:C:956:TYR:HE2 | 1:C:1008:PRO:HD2 | 1.69 | 0.57 |
| 1:B:706:LYS:HD3 | 1:B:732:ASP:OD2 | 2.04 | 0.57 |
| 1:A:330:ALA:HB1 | 1:B:722:MET:SD | 2.44 | 0.57 |
| 1:D:1287:LYS:O | 1:D:1291:GLU:HG2 | 2.04 | 0.57 |
| 1:B:527:VAL:HG23 | 1:B:528:SER:H | 1.69 | 0.57 |
| 1:A:275:VAL:O | 1:A:278:LYS:HB2 | 2.04 | 0.57 |
| 1:D:1508:ALA:O | 1:D:1527:ILE:HG23 | 2.04 | 0.57 |
| 1:D:1352:PRO:HA | 1:D:1470:ASN:HA | 1.86 | 0.57 |
| 1:C:914:LYS:HD2 | 1:C:918:GLY:O | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1515:LYS:HE3 | 1:D:1519:GLY:CA | 2.34 | 0.57 |
| 1:B:551:GLU:HG3 | 1:B:602:SER:OG | 2.05 | 0.57 |
| 1:D:1280:ARG:O | 1:D:1283:LEU:HB3 | 2.03 | 0.57 |
| 1:B:406:VAL:HG12 | 1:B:548:ALA:HB2 | 1.86 | 0.57 |
| 1:D:1246:TYR:CE1 | 1:D:1553:LYS:HE2 | 2.39 | 0.57 |
| 1:A:275:VAL:HG13 | 1:A:294:THR:CG2 | 2.34 | 0.57 |
| 1:B:564:LEU:O | 1:B:568:GLU:HB2 | 2.05 | 0.57 |
| 1:A:65:TYR:OH | 1:A:69:LYS:HD3 | 2.05 | 0.57 |
| 1:A:381:PHE:CE1 | 1:A:385:LYS:HE2 | 2.39 | 0.57 |
| 1:C:1076:LEU:O | 1:C:1080:LYS:HG3 | 2.05 | 0.57 |
| 1:A:235:THR:HG22 | 1:A:281:VAL:HG11 | 1.86 | 0.57 |
| 1:D:1350:THR:HG23 | 1:D:1401:PRO:HD2 | 1.87 | 0.57 |
| 1:D:1453:SER:HA | 1:D:1510:ASP:OD1 | 2.04 | 0.57 |
| 1:A:77:HIS:H | 1:A:77:HIS:CD2 | 2.23 | 0.57 |
| 1:A:168:GLU:O | 1:A:171:ILE:HB | 2.05 | 0.57 |
| 1:C:1122:MET:SD | 1:D:1530:ALA:HB1 | 2.45 | 0.56 |
| 1:B:469:LYS:HG3 | 1:B:483:LEU:HD21 | 1.86 | 0.56 |
| 1:A:9:TYR:CE2 | 1:A:61:LEU:HB2 | 2.40 | 0.56 |
| 1:B:458:ILE:HD12 | 1:B:510:LEU:HD23 | 1.87 | 0.56 |
| 1:B:616:LYS:HB2 | 5:B:1924:HOH:O | 2.04 | 0.56 |
| 1:D:1353:LEU:HD12 | 1:D:1473:SER:OG | 2.05 | 0.56 |
| 1:D:1354:PRO:CB | 1:D:1403:PRO:HG3 | 2.35 | 0.56 |
| 1:A:10:GLY:HA3 | 5:A:1604:HOH:O | 2.05 | 0.56 |
| 1:D:1423:GLY:O | 1:D:1424:ASN:HB2 | 2.03 | 0.56 |
| 1:D:1425:ASP:OD1 | 1:D:1567:LYS:HE3 | 2.05 | 0.56 |
| 1:B:675:VAL:HG13 | 1:B:694:THR:CG2 | 2.36 | 0.56 |
| 1:C:1033:VAL:HG22 | 1:D:1440:MET:HE1 | 1.88 | 0.56 |
| 1:D:1307:ILE:O | 1:D:1307:ILE:HD13 | 2.06 | 0.56 |
| 1:C:806:VAL:HG12 | 1:C:948:ALA:HB2 | 1.88 | 0.56 |
| 1:D:1323:LEU:HA | 1:D:1326:MET:SD | 2.46 | 0.56 |
| 1:A:101:LEU:HD21 | 1:A:176:LYS:HB3 | 1.87 | 0.56 |
| 1:B:623:GLY:O | 1:B:624:ASN:HB2 | 2.06 | 0.56 |
| 1:B:570:MET:HE3 | 1:B:579:ALA:HB2 | 1.88 | 0.56 |
| 1:A:131:GLU:HG3 | 1:A:192:LEU:HD21 | 1.87 | 0.56 |
| 1:D:1221:ARG:O | 1:D:1225:ARG:HB2 | 2.06 | 0.56 |
| 1:A:104:GLY:CA | 1:A:152:PRO:HG3 | 2.36 | 0.56 |
| 1:D:1224:GLU:OE2 | 1:D:1250:SER:HA | 2.06 | 0.56 |
| 1:D:1355:ASN:HB2 | 5:D:1651:HOH:O | 2.06 | 0.56 |
| 1:C:869:LYS:O | 1:C:873:GLU:HG2 | 2.06 | 0.56 |
| 1:C:1120:LYS:HB2 | 1:D:1534:ILE:HD13 | 1.88 | 0.56 |
| 1:C:861:LEU:HD22 | 1:C:867:ALA:HA | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1563:ALA:HB1 | 1:D:1569:PRO:HB3 | 1.88 | 0.55 |
| 1:A:167:PHE:O | 1:A:170:MET:HB3 | 2.06 | 0.55 |
| 1:A:87:LYS:HG3 | 1:A:88:SER:N | 2.21 | 0.55 |
| 1:C:804:TRP:NE1 | 1:C:934:ILE:HG12 | 2.22 | 0.55 |
| 1:B:675:VAL:HG13 | 1:B:694:THR:HG22 | 1.88 | 0.55 |
| 1:D:1325:GLU:O | 1:D:1328:SER:HB3 | 2.06 | 0.55 |
| 1:B:552:PRO:HA | 1:B:669:ASP:O | 2.06 | 0.55 |
| 1:C:1001:PRO:HG2 | 1:C:1074:LYS:HB2 | 1.88 | 0.55 |
| 1:D:1531:ILE:HD12 | 1:D:1531:ILE:H | 1.72 | 0.55 |
| 1:B:606:ALA:CB | 1:B:624:ASN:HD21 | 2.18 | 0.55 |
| 1:D:1214:THR:HB | 1:D:1268:ALA:HB2 | 1.89 | 0.55 |
| 1:A:79:ASP:HB2 | 1:A:82:ILE:HD12 | 1.87 | 0.55 |
| 1:A:60:LEU:HD13 | 1:A:97:LYS:CD | 2.37 | 0.55 |
| 1:B:457:GLU:O | 1:B:497:LYS:HA | 2.07 | 0.55 |
| 1:D:1221:ARG:HG2 | 1:D:1289:ASP:OD1 | 2.06 | 0.55 |
| 1:D:1456:ILE:O | 1:D:1457:LEU:HB3 | 2.07 | 0.55 |
| 1:C:802:LYS:HB3 | 1:C:937:PHE:CZ | 2.41 | 0.55 |
| 1:B:402:LYS:HG2 | 1:B:452:GLU:HB2 | 1.88 | 0.55 |
| 1:D:1331:GLU:O | 1:D:1335:LYS:HB3 | 2.07 | 0.55 |
| 1:D:1431:THR:OG1 | 1:D:1478:LYS:HB3 | 2.06 | 0.55 |
| 1:C:916:LEU:HD13 | 1:C:921:LEU:HD22 | 1.88 | 0.55 |
| 1:A:225:ASP:O | 1:A:366:PHE:HB3 | 2.06 | 0.55 |
| 1:C:1150:ALA:O | 1:C:1155:VAL:HG23 | 2.07 | 0.55 |
| 1:A:223:GLY:O | 1:A:224:ASN:HB2 | 2.06 | 0.55 |
| 1:D:1217:MET:HB3 | 1:D:1221:ARG:NH1 | 2.22 | 0.55 |
| 1:B:614:ALA:HB1 | 1:B:619:VAL:O | 2.06 | 0.55 |
| 1:D:1271:HIS:HA | 1:D:1274:LEU:HD12 | 1.89 | 0.55 |
| 1:C:1111:PHE:HE2 | 1:C:1123:LYS:HG2 | 1.71 | 0.55 |
| 1:C:1153:LYS:HE3 | 1:C:1191:LEU:O | 2.06 | 0.55 |
| 1:C:813:SER:O | 1:C:816:ALA:HB3 | 2.06 | 0.55 |
| 1:B:432:GLY:O | 1:B:738:PRO:HB2 | 2.06 | 0.55 |
| 1:D:1277:HIS:CD2 | 1:D:1277:HIS:H | 2.23 | 0.54 |
| 1:A:248:VAL:O | 1:A:290:PRO:HB3 | 2.06 | 0.54 |
| 1:A:268:ARG:HH11 | 1:A:268:ARG:HG3 | 1.71 | 0.54 |
| 1:A:173:GLU:HB3 | 1:A:175:ARG:CD | 2.35 | 0.54 |
| 1:B:510:LEU:CA | 1:B:513:ILE:HD12 | 2.33 | 0.54 |
| 1:C:1131:ILE:CB | 1:D:1520:LYS:HE2 | 2.34 | 0.54 |
| 1:B:497:LYS:HE2 | 1:B:515:THR:HB | 1.88 | 0.54 |
| 5:A:1787:HOH:O | 1:B:778:HIS:HB3 | 2.07 | 0.54 |
| 1:A:99:THR:HG22 | 1:A:185:TYR:CE2 | 2.42 | 0.54 |
| 1:D:1567:LYS:CE | 2:D:1595:PO4:O4 | 2.54 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:513:ILE:O | 1:B:514:LYS:HG2 | 2.07 | 0.54 |
| 1:C:932:GLU:HA | 1:C:935:LYS:HD2 | 1.89 | 0.54 |
| 1:C:1070:ASN:O | 1:C:1073:SER:HB2 | 2.08 | 0.54 |
| 1:D:1331:GLU:HG3 | 1:D:1388:ALA:CB | 2.37 | 0.54 |
| 1:D:1561:GLU:HG2 | 1:D:1587:TRP:HB2 | 1.89 | 0.54 |
| 1:C:1153:LYS:CB | 1:C:1191:LEU:HD22 | 2.37 | 0.54 |
| 1:C:853:PHE:HB2 | 1:C:893:ILE:HD13 | 1.89 | 0.54 |
| 1:C:1015:GLU:HG2 | 1:C:1157:GLY:HA2 | 1.89 | 0.54 |
| 1:D:1265:TYR:CA | 1:D:1290:LEU:HB3 | 2.37 | 0.54 |
| 1:C:805:LEU:HD13 | 1:C:813:SER:OG | 2.08 | 0.54 |
| 1:C:1026:GLY:O | 1:C:1167:LYS:HE3 | 2.08 | 0.54 |
| 1:D:1361:HIS:HB3 | 1:D:1407:ILE:HD12 | 1.88 | 0.54 |
| 1:D:1456:ILE:HD12 | 1:D:1502:LEU:CD1 | 2.37 | 0.54 |
| 1:D:1266:GLU:O | 1:D:1269:LYS:HB3 | 2.08 | 0.54 |
| 1:D:1514:PHE:CE2 | 1:D:1522:MET:HE3 | 2.43 | 0.54 |
| 1:D:1407:ILE:CD1 | 1:D:1409:ALA:HB3 | 2.38 | 0.54 |
| 1:C:1007:ILE:CD1 | 1:C:1010:LEU:HB2 | 2.37 | 0.54 |
| 1:B:580:SER:HB3 | 1:B:583:MET:HG3 | 1.90 | 0.54 |
| 1:B:411:ILE:HG12 | 1:B:733:ALA:CB | 2.39 | 0.53 |
| 1:A:233:VAL:HG22 | 1:B:640:MET:HE3 | 1.91 | 0.53 |
| 1:A:353:LYS:HD2 | 1:A:391:LEU:O | 2.09 | 0.53 |
| 1:A:299:PHE:HD2 | 1:C:1093:ILE:HD12 | 1.73 | 0.53 |
| 1:C:1054:TYR:OH | 1:C:1097:GLN:HG3 | 2.09 | 0.53 |
| 1:B:570:MET:HG2 | 1:B:570:MET:O | 2.08 | 0.53 |
| 1:B:695:GLU:HG2 | 1:B:697:GLN:NE2 | 2.18 | 0.53 |
| 1:A:108:LYS:O | 1:A:109:GLU:HG3 | 2.08 | 0.53 |
| 1:D:1344:VAL:HG11 | 1:D:1389:ALA:HB2 | 1.90 | 0.53 |
| 1:C:1120:LYS:CB | 1:D:1534:ILE:HD13 | 2.38 | 0.53 |
| 1:A:365:PHE:HB2 | 1:A:366:PHE:CE1 | 2.43 | 0.53 |
| 1:D:1357:SER:HB3 | 1:D:1360:TYR:HB2 | 1.90 | 0.53 |
| 1:A:298:TYR:CZ | 1:A:300:PRO:HB3 | 2.42 | 0.53 |
| 1:C:944:VAL:HG21 | 1:C:989:ALA:HB2 | 1.89 | 0.53 |
| 1:C:944:VAL:HG12 | 1:C:996:TYR:HD1 | 1.72 | 0.53 |
| 1:A:60:LEU:HB2 | 1:A:97:LYS:NZ | 2.23 | 0.53 |
| 1:A:275:VAL:HG13 | 1:A:294:THR:HG22 | 1.90 | 0.53 |
| 1:B:517:GLU:HB2 | 1:B:526:MET:CE | 2.39 | 0.53 |
| 1:A:213:LEU:O | 1:A:217:LYS:HB2 | 2.09 | 0.53 |
| 1:C:899:THR:HA | 1:C:916:LEU:HB2 | 1.90 | 0.53 |
| 1:B:412:VAL:CG1 | 1:B:547:VAL:HG21 | 2.39 | 0.53 |
| 1:A:376:ASN:O | 1:A:380:GLN:HG3 | 2.08 | 0.53 |
| 1:C:1025:ASP:HB3 | 1:C:1167:LYS:HG3 | 1.90 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1456:ILE:HG13 | 1:D:1507:THR:O | 2.09 | 0.52 |
| 1:C:809:TYR:HB2 | 1:C:857:GLU:OE1 | 2.09 | 0.52 |
| 1:B:570:MET:HG3 | 1:B:575:ARG:HB2 | 1.91 | 0.52 |
| 1:A:374:VAL:HG12 | 1:A:380:GLN:HG2 | 1.91 | 0.52 |
| 1:A:121:LEU:HA | 5:A:2050:HOH:O | 2.09 | 0.52 |
| 1:B:680:LYS:HZ3 | 1:B:683:GLU:HB2 | 1.74 | 0.52 |
| 1:C:1027:LYS:HA | 1:C:1167:LYS:HE3 | 1.92 | 0.52 |
| 1:B:566:GLY:HA2 | 1:B:569:ARG:HD2 | 1.90 | 0.52 |
| 1:B:553:LEU:CD1 | 1:B:672:GLU:HB3 | 2.39 | 0.52 |
| 1:A:276:LEU:O | 1:A:280:LYS:HB2 | 2.10 | 0.52 |
| 1:B:421:ARG:HA | 1:B:421:ARG:NE | 2.24 | 0.52 |
| 1:A:330:ALA:HB2 | 1:B:722:MET:HB3 | 1.92 | 0.52 |
| 1:B:748:LEU:HD13 | 5:B:2108:HOH:O | 2.09 | 0.52 |
| 1:C:916:LEU:HG | 1:C:926:MET:SD | 2.49 | 0.52 |
| 1:D:1423:GLY:HA2 | 1:D:1566:PHE:CE1 | 2.45 | 0.52 |
| 1:C:931:GLU:O | 1:C:935:LYS:HB3 | 2.08 | 0.52 |
| 1:A:122:SER:O | 1:A:126:MET:HB2 | 2.10 | 0.52 |
| 1:A:60:LEU:HD13 | 1:A:97:LYS:CE | 2.40 | 0.52 |
| 1:B:654:TYR:HE1 | 1:B:695:GLU:OE2 | 1.93 | 0.52 |
| 1:A:276:LEU:HA | 1:A:280:LYS:HE2 | 1.92 | 0.52 |
| 1:A:123:LEU:CD1 | 1:A:176:LYS:HG2 | 2.39 | 0.52 |
| 1:C:1057:LEU:HD13 | 1:C:1062:GLY:HA2 | 1.92 | 0.52 |
| 1:B:623:GLY:HA2 | 1:B:766:PHE:CE1 | 2.44 | 0.52 |
| 1:A:153:LEU:HG | 1:A:272:GLU:OE1 | 2.09 | 0.52 |
| 1:D:1420:PRO:HB3 | 1:D:1555:VAL:HG12 | 1.91 | 0.52 |
| 1:C:1139:LEU:O | 1:C:1143:ILE:HG13 | 2.10 | 0.52 |
| 1:A:9:TYR:O | 1:A:71:HIS:HE1 | 1.93 | 0.52 |
| 1:A:228:THR:HG22 | 1:A:339:LEU:CD1 | 2.40 | 0.52 |
| 1:B:567:PHE:O | 1:B:570:MET:HB3 | 2.09 | 0.52 |
| 1:A:56:HIS:CE1 | 1:A:130:ILE:HG23 | 2.45 | 0.52 |
| 1:A:376:ASN:HB3 | 1:A:379:GLU:OE2 | 2.10 | 0.52 |
| 1:A:297:GLN:HG3 | 1:C:1095:GLU:OE1 | 2.10 | 0.52 |
| 1:C:987:TYR:O | 1:C:991:LYS:HB2 | 2.10 | 0.52 |
| 1:D:1435:THR:HA | 1:D:1485:MET:CE | 2.40 | 0.52 |
| 1:C:806:VAL:HB | 1:C:946:ASN:HA | 1.93 | 0.51 |
| 1:B:509:GLU:HG3 | 1:B:510:LEU:CD1 | 2.40 | 0.51 |
| 1:A:115:THR:N | 1:A:119:GLU:HB2 | 2.25 | 0.51 |
| 1:B:678:LYS:HE3 | 2:B:795:PO4:O3 | 2.08 | 0.51 |
| 1:A:127:VAL:HG21 | 1:A:171:ILE:CD1 | 2.39 | 0.51 |
| 1:B:631:THR:O | 1:B:635:THR:HG23 | 2.10 | 0.51 |
| 1:C:967:PHE:O | 1:C:971:ILE:HD12 | 2.09 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1357:SER:CB | 1:D:1360:TYR:HB2 | 2.41 | 0.51 |
| 1:C:1040:MET:HE1 | 1:D:1433:VAL:HA | 1.92 | 0.51 |
| 1:B:764:PHE:HA | 1:B:780:GLN:HB3 | 1.93 | 0.51 |
| 1:B:423:ILE:HG12 | 1:B:429:PRO:O | 2.11 | 0.51 |
| 1:B:514:LYS:HD2 | 1:B:518:GLY:N | 2.25 | 0.51 |
| 1:A:190:LEU:HB3 | 1:A:213:LEU:HD23 | 1.93 | 0.51 |
| 1:C:913:ILE:O | 1:C:913:ILE:HG23 | 2.10 | 0.51 |
| 1:C:947:VAL:O | 1:C:947:VAL:HG13 | 2.10 | 0.51 |
| 1:C:935:LYS:HG2 | 1:C:936:SER:N | 2.25 | 0.51 |
| 1:D:1354:PRO:HG3 | 1:D:1403:PRO:HB3 | 1.92 | 0.51 |
| 1:D:1217:MET:CE | 1:D:1293:ILE:HG21 | 2.41 | 0.51 |
| 1:C:853:PHE:HB2 | 1:C:893:ILE:CD1 | 2.41 | 0.51 |
| 1:C:1057:LEU:HD13 | 1:C:1062:GLY:CA | 2.41 | 0.51 |
| 1:B:406:VAL:HG21 | 1:B:585:TYR:CG | 2.46 | 0.51 |
| 1:B:497:LYS:CG | 1:B:516:LEU:HD23 | 2.40 | 0.51 |
| 1:D:1550:ALA:O | 1:D:1555:VAL:HB | 2.10 | 0.51 |
| 1:A:326:PHE:HA | 1:B:726:PHE:HA | 1.92 | 0.51 |
| 1:D:1470:ASN:ND2 | 1:D:1470:ASN:H | 2.08 | 0.51 |
| 1:B:779:GLU:O | 1:B:783:VAL:HG23 | 2.11 | 0.51 |
| 1:A:298:TYR:OH | 1:A:300:PRO:HB3 | 2.10 | 0.51 |
| 1:A:191:LYS:HE3 | 5:A:2592:HOH:O | 2.11 | 0.51 |
| 1:D:1438:ALA:HB3 | 1:D:1439:PRO:HD3 | 1.92 | 0.51 |
| 1:A:169:ARG:O | 1:A:173:GLU:HB2 | 2.10 | 0.51 |
| 1:B:521:LEU:HD23 | 1:B:525:GLU:HB3 | 1.93 | 0.51 |
| 1:D:1422:ALA:HB2 | 1:D:1559:VAL:H | 1.76 | 0.51 |
| 1:C:1178:HIS:ND1 | 1:D:1578:HIS:HB3 | 2.26 | 0.51 |
| 1:D:1576:ASN:O | 1:D:1580:GLN:HG3 | 2.11 | 0.51 |
| 1:A:173:GLU:OE2 | 1:A:173:GLU:HA | 2.11 | 0.51 |
| 1:A:230:GLU:CD | 1:A:255:ASN:HD21 | 2.15 | 0.51 |
| 1:D:1550:ALA:HB2 | 1:D:1587:TRP:HZ2 | 1.76 | 0.51 |
| 1:C:1006:ALA:HA | 1:C:1170:MET:CE | 2.41 | 0.51 |
| 1:C:1132:ASP:HB3 | 4:C:1196:NAD:C7N | 2.41 | 0.50 |
| 1:D:1448:VAL:O | 1:D:1448:VAL:HG12 | 2.11 | 0.50 |
| 1:B:778:HIS:H | 1:B:778:HIS:CD2 | 2.27 | 0.50 |
| 1:D:1440:MET:O | 1:D:1443:TYR:HB2 | 2.11 | 0.50 |
| 1:C:1111:PHE:CE2 | 1:C:1123:LYS:HG2 | 2.46 | 0.50 |
| 1:B:759:VAL:CG1 | 1:B:762:MET:HG3 | 2.41 | 0.50 |
| 1:B:460:LEU:O | 1:B:461:LEU:HD12 | 2.11 | 0.50 |
| 1:A:127:VAL:CG2 | 1:A:184:LEU:HD22 | 2.41 | 0.50 |
| 1:D:1264:ALA:HB3 | 1:D:1290:LEU:O | 2.11 | 0.50 |
| 1:D:1222:ALA:O | 1:D:1227:ILE:HG13 | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1117:PHE:HB3 | 1:D:1534:ILE:HG23 | 1.92 | 0.50 |
| 1:C:860:LEU:HD13 | 1:C:912:ASP:HB3 | 1.93 | 0.50 |
| 1:C:1106:LYS:HE2 | 2:C:1195:PO4:O1 | 2.11 | 0.50 |
| 1:C:1081:VAL:HG13 | 1:C:1175:ILE:HG21 | 1.93 | 0.50 |
| 1:D:1466:SER:HA | 5:D:2015:HOH:O | 2.11 | 0.50 |
| 1:D:1263:ASN:OD1 | 1:D:1291:GLU:OE1 | 2.30 | 0.50 |
| 1:D:1217:MET:HE2 | 1:D:1253:PHE:CD1 | 2.47 | 0.50 |
| 1:A:176:LYS:HA | 1:A:179:ALA:HB3 | 1.93 | 0.50 |
| 1:B:535:LYS:HG2 | 1:B:536:SER:N | 2.27 | 0.50 |
| 1:B:630:GLU:OE2 | 1:B:710:ASP:OD1 | 2.30 | 0.50 |
| 1:A:99:THR:HG22 | 1:A:185:TYR:CZ | 2.47 | 0.50 |
| 1:D:1563:ALA:CB | 1:D:1569:PRO:HB3 | 2.42 | 0.50 |
| 1:A:97:LYS:HG2 | 1:A:115:THR:CB | 2.38 | 0.50 |
| 1:D:1448:VAL:HG12 | 1:D:1490:PRO:CB | 2.41 | 0.50 |
| 1:A:230:GLU:OE1 | 1:A:310:ASP:OD2 | 2.29 | 0.50 |
| 1:B:635:THR:HA | 1:B:685:MET:HE1 | 1.93 | 0.50 |
| 1:B:422:ALA:HB1 | 1:B:428:ALA:HB2 | 1.94 | 0.50 |
| 1:B:651:TRP:CD2 | 1:B:712:VAL:HG22 | 2.47 | 0.50 |
| 1:C:1023:GLY:HA2 | 1:C:1166:PHE:CE1 | 2.47 | 0.50 |
| 1:C:1023:GLY:HA2 | 1:C:1166:PHE:CZ | 2.47 | 0.50 |
| 1:B:675:VAL:HG23 | 1:B:696:ILE:HD12 | 1.94 | 0.50 |
| 1:C:880:ARG:O | 1:C:884:GLU:OE1 | 2.30 | 0.50 |
| 1:D:1344:VAL:O | 1:D:1344:VAL:HG12 | 2.10 | 0.50 |
| 1:B:401:MET:CE | 1:B:748:LEU:HD22 | 2.42 | 0.50 |
| 1:A:267:ALA:O | 1:A:271:LYS:HB3 | 2.12 | 0.50 |
| 1:D:1351:GLU:HB2 | 1:D:1352:PRO:HD2 | 1.94 | 0.50 |
| 1:C:965:GLU:O | 1:C:965:GLU:HG2 | 2.10 | 0.50 |
| 1:A:21:ARG:O | 1:A:25:ARG:HG3 | 2.11 | 0.50 |
| 1:D:1365:GLU:O | 1:D:1369:ARG:HB2 | 2.12 | 0.49 |
| 1:D:1468:ARG:HA | 1:D:1471:LYS:HB3 | 1.94 | 0.49 |
| 1:D:1591:LEU:O | 1:D:1592:LYS:O | 2.30 | 0.49 |
| 1:B:402:LYS:HB2 | 1:B:542:THR:OG1 | 2.12 | 0.49 |
| 1:A:34:VAL:HB | 1:A:342:ASP:OD1 | 2.12 | 0.49 |
| 1:D:1211:ILE:HG12 | 1:D:1533:ALA:CB | 2.42 | 0.49 |
| 1:C:886:VAL:HG12 | 1:C:886:VAL:O | 2.11 | 0.49 |
| 1:B:547:VAL:O | 1:B:547:VAL:HG13 | 2.12 | 0.49 |
| 1:D:1316:LEU:HD11 | 1:D:1326:MET:HG2 | 1.93 | 0.49 |
| 1:C:957:SER:O | 1:C:961:HIS:HB2 | 2.12 | 0.49 |
| 1:B:516:LEU:HD21 | 1:B:529:ARG:HD2 | 1.93 | 0.49 |
| 1:C:1117:PHE:CG | 1:D:1538:PRO:HG3 | 2.47 | 0.49 |
| 1:D:1328:SER:O | 1:D:1332:GLU:OE1 | 2.30 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:279:ASP:OD2 | 1:A:292:SER:OG | 2.30 | 0.49 |
| 1:D:1474:LYS:HE2 | 1:D:1567:LYS:NZ | 2.25 | 0.49 |
| 1:B:486:VAL:HG12 | 1:B:490:LEU:HG | 1.94 | 0.49 |
| 1:B:515:THR:O | 1:B:519:GLU:OE2 | 2.30 | 0.49 |
| 1:A:105:SER:H | 1:A:269:ASP:CG | 2.15 | 0.49 |
| 1:D:1458:GLY:O | 1:D:1459:ASP:O | 2.30 | 0.49 |
| 1:D:1337:PHE:O | 1:D:1338:ALA:O | 2.30 | 0.49 |
| 1:C:858:ILE:HD13 | 4:C:1196:NAD:C5A | 2.42 | 0.49 |
| 1:C:861:LEU:HD22 | 1:C:867:ALA:CA | 2.43 | 0.49 |
| 1:B:411:ILE:HG22 | 4:B:796:NAD:O2N | 2.13 | 0.49 |
| 1:A:60:LEU:HD13 | 1:A:97:LYS:HD2 | 1.93 | 0.49 |
| 1:B:678:LYS:HB3 | 1:B:694:THR:CG2 | 2.40 | 0.49 |
| 1:B:786:GLU:O | 1:B:790:ASN:OD1 | 2.31 | 0.49 |
| 1:C:1072:GLU:O | 1:C:1076:LEU:HG | 2.12 | 0.49 |
| 1:B:494:VAL:HG12 | 1:B:494:VAL:O | 2.11 | 0.49 |
| 1:C:1083:GLU:OE2 | 1:C:1089:SER:OG | 2.30 | 0.49 |
| 1:C:1056:ILE:HD12 | 1:C:1102:LEU:CD1 | 2.43 | 0.49 |
| 1:A:11:ILE:HG13 | 1:A:71:HIS:CB | 2.35 | 0.49 |
| 1:A:134:ILE:O | 1:A:138:ALA:HB3 | 2.13 | 0.49 |
| 1:B:433:LEU:HD21 | 1:B:741:LEU:HD12 | 1.94 | 0.49 |
| 1:C:1034:LYS:HD3 | 1:C:1082:LEU:HD13 | 1.94 | 0.49 |
| 1:A:92:GLY:HA3 | 5:A:1956:HOH:O | 2.13 | 0.49 |
| 1:A:114:LYS:HG2 | 1:A:119:GLU:CA | 2.40 | 0.49 |
| 1:D:1275:ASN:HB2 | 1:D:1277:HIS:HD2 | 1.76 | 0.49 |
| 1:A:238:ALA:HB3 | 1:A:239:PRO:HD3 | 1.94 | 0.49 |
| 1:A:96:ARG:CD | 1:A:133:ASP:HB3 | 2.40 | 0.49 |
| 1:C:1050:GLY:HA2 | 1:C:1091:TYR:O | 2.13 | 0.49 |
| 1:C:1038:ALA:HB3 | 1:C:1039:PRO:HD3 | 1.95 | 0.49 |
| 1:D:1347:VAL:HG13 | 1:D:1347:VAL:O | 2.12 | 0.49 |
| 1:C:1028:THR:HG22 | 1:C:1139:LEU:HD12 | 1.95 | 0.49 |
| 1:D:1277:HIS:HB2 | 1:D:1534:ILE:HD11 | 1.95 | 0.49 |
| 1:A:88:SER:O | 1:A:91:GLU:OE2 | 2.30 | 0.49 |
| 1:C:805:LEU:O | 1:C:855:GLY:HA3 | 2.11 | 0.49 |
| 1:D:1334:ILE:HG22 | 1:D:1392:LEU:HD12 | 1.95 | 0.49 |
| 1:C:1086:LEU:HB3 | 1:C:1088:TYR:CE1 | 2.48 | 0.49 |
| 1:D:1506:LYS:HD3 | 1:D:1532:ASP:OD1 | 2.13 | 0.48 |
| 1:A:249:VAL:HG21 | 1:A:321:LEU:HD21 | 1.94 | 0.48 |
| 1:C:961:HIS:NE2 | 1:C:978:TYR:HB3 | 2.28 | 0.48 |
| 1:D:1272:TRP:CZ2 | 1:D:1280:ARG:HB2 | 2.48 | 0.48 |
| 1:B:523:LEU:HD21 | 1:B:579:ALA:CB | 2.38 | 0.48 |
| 1:B:711:PHE:CE2 | 1:B:723:LYS:HB3 | 2.48 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1309:GLU:O | 1:D:1309:GLU:OE2 | 2.30 | 0.48 |
| 1:B:459:ARG:HB2 | 1:B:510:LEU:HD11 | 1.94 | 0.48 |
| 1:A:164:LEU:HD11 | 1:A:213:LEU:HD12 | 1.95 | 0.48 |
| 1:A:231:THR:O | 1:A:235:THR:HG23 | 2.13 | 0.48 |
| 1:A:132:GLU:O | 1:A:136:SER:OG | 2.31 | 0.48 |
| 1:B:507:ILE:HD13 | 1:B:508:LYS:N | 2.28 | 0.48 |
| 1:C:1117:PHE:CB | 1:D:1538:PRO:HG3 | 2.42 | 0.48 |
| 1:D:1235:SER:OG | 1:D:1542:ASP:OD2 | 2.30 | 0.48 |
| 1:A:325:TYR:O | 1:B:726:PHE:HB2 | 2.13 | 0.48 |
| 1:A:293:ILE:HD11 | 1:C:1099:PHE:HD2 | 1.78 | 0.48 |
| 1:A:141:GLU:HB3 | 1:A:348:LEU:HD21 | 1.96 | 0.48 |
| 1:C:1020:PRO:HD3 | 1:C:1155:VAL:O | 2.13 | 0.48 |
| 1:A:224:ASN:O | 1:A:366:PHE:HB3 | 2.14 | 0.48 |
| 1:C:1178:HIS:HB3 | 1:D:1578:HIS:ND1 | 2.28 | 0.48 |
| 1:C:811:ILE:CD1 | 1:C:871:HIS:HB3 | 2.42 | 0.48 |
| 1:B:521:LEU:HD23 | 1:B:525:GLU:CG | 2.43 | 0.48 |
| 1:C:877:HIS:H | 1:C:877:HIS:CD2 | 2.31 | 0.48 |
| 1:C:942:THR:HB | 1:C:994:LEU:HD22 | 1.96 | 0.48 |
| 1:A:196:TYR:CE1 | 1:A:205:SER:HB3 | 2.49 | 0.48 |
| 1:A:33:LEU:HD13 | 1:A:49:PHE:HE1 | 1.77 | 0.48 |
| 1:D:1317:GLU:HA | 1:D:1317:GLU:OE2 | 2.13 | 0.48 |
| 1:D:1346:ASN:HD21 | 1:D:1400:THR:HG23 | 1.78 | 0.48 |
| 1:D:1468:ARG:NH2 | 1:D:1472:GLU:HG3 | 2.26 | 0.48 |
| 1:B:515:THR:HG22 | 1:B:515:THR:O | 2.13 | 0.48 |
| 1:A:116:LEU:HD12 | 1:A:126:MET:HG2 | 1.95 | 0.48 |
| 1:A:280:LYS:O | 1:A:283:GLU:OE1 | 2.32 | 0.48 |
| 1:C:903:CYS:HB3 | 1:C:907:ILE:HD11 | 1.95 | 0.48 |
| 1:D:1435:THR:HA | 1:D:1485:MET:SD | 2.53 | 0.48 |
| 1:D:1332:GLU:O | 1:D:1336:SER:OG | 2.30 | 0.48 |
| 1:B:624:ASN:O | 1:B:768:SER:HB3 | 2.14 | 0.48 |
| 1:B:409:TYR:CG | 1:B:457:GLU:HG2 | 2.49 | 0.48 |
| 1:D:1474:LYS:HE3 | 4:D:1596:NAD:C6N | 2.43 | 0.47 |
| 1:C:801:MET:CE | 1:C:1148:LEU:HD22 | 2.44 | 0.47 |
| 1:A:90:LEU:HA | 1:A:93:ILE:CD1 | 2.37 | 0.47 |
| 1:B:480:ARG:HD3 | 1:C:880:ARG:HD2 | 1.97 | 0.47 |
| 1:A:221:HIS:CD2 | 1:A:221:HIS:H | 2.31 | 0.47 |
| 1:D:1396:TYR:CE2 | 1:D:1405:SER:HB3 | 2.49 | 0.47 |
| 1:C:899:THR:HB | 1:C:916:LEU:CD2 | 2.42 | 0.47 |
| 1:A:61:LEU:HD11 | 5:A:1999:HOH:O | 2.14 | 0.47 |
| 1:C:952:PRO:HA | 1:C:1070:ASN:HA | 1.95 | 0.47 |
| 1:C:1040:MET:CE | 1:D:1432:LEU:HG | 2.45 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:164:LEU:HD13 | 1:A:213:LEU:HB2 | 1.96 | 0.47 |
| 1:B:601:PRO:HG2 | 1:B:674:LYS:HD2 | 1.94 | 0.47 |
| 1:C:958:GLU:HG2 | 1:C:962:GLY:HA3 | 1.95 | 0.47 |
| 1:B:737:ALA:HB3 | 1:B:738:PRO:HD3 | 1.96 | 0.47 |
| 1:C:874:LEU:HB3 | 1:C:1103:VAL:HG11 | 1.96 | 0.47 |
| 1:A:280:LYS:HD3 | 1:A:280:LYS:N | 2.29 | 0.47 |
| 1:D:1468:ARG:HG2 | 1:D:1471:LYS:HE2 | 1.96 | 0.47 |
| 1:D:1307:ILE:HG23 | 1:D:1307:ILE:O | 2.14 | 0.47 |
| 1:B:680:LYS:HB2 | 5:B:2394:HOH:O | 2.14 | 0.47 |
| 1:C:957:SER:H | 1:C:961:HIS:HD2 | 1.62 | 0.47 |
| 1:D:1455:ASN:HD22 | 1:D:1506:LYS:NZ | 2.12 | 0.47 |
| 1:B:499:THR:OG1 | 1:B:517:GLU:HB3 | 2.15 | 0.47 |
| 1:B:497:LYS:HG3 | 1:B:516:LEU:HD23 | 1.96 | 0.47 |
| 1:D:1217:MET:O | 1:D:1221:ARG:HD2 | 2.15 | 0.47 |
| 1:B:710:ASP:HB2 | 1:B:726:PHE:CZ | 2.49 | 0.47 |
| 1:D:1453:SER:HB3 | 1:D:1494:THR:HG23 | 1.97 | 0.47 |
| 1:D:1386:ALA:HB2 | 1:D:1396:TYR:CZ | 2.49 | 0.47 |
| 1:A:14:THR:O | 1:A:18:VAL:HG23 | 2.14 | 0.47 |
| 1:B:657:LEU:HD13 | 1:B:662:GLY:CA | 2.44 | 0.47 |
| 1:A:58:ILE:HD13 | 1:A:107:ILE:HD11 | 1.97 | 0.47 |
| 1:A:107:ILE:HG12 | 1:A:107:ILE:O | 2.14 | 0.47 |
| 1:C:864:ALA:HB3 | 1:C:893:ILE:HB | 1.95 | 0.47 |
| 1:D:1582:VAL:O | 1:D:1586:GLU:HG3 | 2.15 | 0.47 |
| 1:B:445:LYS:HB3 | 1:B:446:TYR:CE1 | 2.49 | 0.47 |
| 1:C:1172:THR:OG1 | 1:C:1174:VAL:HG23 | 2.15 | 0.47 |
| 1:D:1460:TYR:HB3 | 4:D:1596:NAD:O1A | 2.15 | 0.47 |
| 1:A:260:TYR:CA | 1:A:263:LYS:HG3 | 2.42 | 0.47 |
| 1:D:1304:GLY:HA3 | 1:D:1307:ILE:HG21 | 1.96 | 0.47 |
| 1:C:1152:LYS:HE2 | 5:C:1801:HOH:O | 2.13 | 0.47 |
| 1:B:470:GLU:HG2 | 1:B:471:HIS:N | 2.29 | 0.47 |
| 1:B:411:ILE:HD11 | 1:B:477:HIS:NE2 | 2.30 | 0.47 |
| 1:B:553:LEU:HD13 | 1:B:672:GLU:HB3 | 1.97 | 0.47 |
| 1:D:1476:LEU:CD2 | 1:D:1480:LYS:HZ2 | 2.25 | 0.47 |
| 1:B:421:ARG:HE | 1:B:421:ARG:HA | 1.80 | 0.47 |
| 1:B:402:LYS:HD3 | 1:B:537:PHE:O | 2.14 | 0.47 |
| 1:C:1038:ALA:HB3 | 1:C:1085:MET:HE1 | 1.96 | 0.47 |
| 1:A:19:GLY:HA2 | 1:B:718:LEU:HD21 | 1.97 | 0.47 |
| 1:A:44:GLU:O | 1:A:48:PRO:HD3 | 2.14 | 0.47 |
| 1:C:1126:PHE:HB2 | 1:D:1525:TYR:O | 2.15 | 0.47 |
| 1:A:114:LYS:O | 1:A:115:THR:OG1 | 2.30 | 0.47 |
| 1:C:1040:MET:CE | 1:D:1433:VAL:HA | 2.45 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:317:PHE:O | 1:A:318:LEU:HB2 | 2.14 | 0.47 |
| 1:C:982:SER:O | 1:C:1004:GLY:HA2 | 2.15 | 0.47 |
| 1:D:1461:ASP:O | 1:D:1465:LEU:HG | 2.15 | 0.47 |
| 1:A:96:ARG:NH1 | 1:A:133:ASP:OD1 | 2.48 | 0.47 |
| 1:D:1306:GLY:C | 1:D:1464:VAL:HG13 | 2.35 | 0.47 |
| 1:B:405:LEU:HD13 | 1:B:413:SER:OG | 2.14 | 0.47 |
| 1:C:859:ARG:NH1 | 1:C:861:LEU:HD11 | 2.30 | 0.46 |
| 1:D:1370:MET:HG2 | 1:D:1371:ILE:N | 2.29 | 0.46 |
| 1:C:1120:LYS:HG2 | 1:D:1534:ILE:HD13 | 1.97 | 0.46 |
| 1:A:254:TYR:HD2 | 1:A:295:GLU:HB2 | 1.80 | 0.46 |
| 1:D:1452:MET:O | 1:D:1510:ASP:HA | 2.14 | 0.46 |
| 1:D:1345:ILE:O | 1:D:1345:ILE:HG22 | 2.15 | 0.46 |
| 1:C:1084:LYS:HG3 | 1:C:1084:LYS:H | 1.47 | 0.46 |
| 1:A:61:LEU:HD12 | 1:A:67:ALA:CB | 2.42 | 0.46 |
| 1:C:932:GLU:HG2 | 1:C:935:LYS:NZ | 2.30 | 0.46 |
| 1:B:782:VAL:O | 1:B:785:LYS:HB2 | 2.14 | 0.46 |
| 1:A:320:LYS:HD2 | 1:A:321:LEU:N | 2.30 | 0.46 |
| 1:D:1586:GLU:O | 1:D:1589:SER:HB2 | 2.15 | 0.46 |
| 1:B:701:SER:HB2 | 1:D:1449:VAL:HG12 | 1.97 | 0.46 |
| 1:C:908:LYS:O | 1:C:909:GLU:HG2 | 2.15 | 0.46 |
| 1:A:219:VAL:HG12 | 1:A:220:PRO:HD2 | 1.97 | 0.46 |
| 1:B:725:TYR:O | 1:B:726:PHE:HB3 | 2.15 | 0.46 |
| 1:B:623:GLY:HA2 | 1:B:766:PHE:CZ | 2.51 | 0.46 |
| 1:C:1018:GLY:HA2 | 1:C:1156:LYS:HB2 | 1.97 | 0.46 |
| 1:A:223:GLY:HA3 | 1:A:366:PHE:CE1 | 2.51 | 0.46 |
| 1:A:374:VAL:CG1 | 1:A:379:GLU:HB3 | 2.45 | 0.46 |
| 1:C:965:GLU:CD | 1:C:969:ARG:HH21 | 2.18 | 0.46 |
| 1:B:628:THR:O | 1:B:629:GLY:O | 2.32 | 0.46 |
| 1:D:1415:GLU:OE1 | 1:D:1415:GLU:HA | 2.15 | 0.46 |
| 1:A:280:LYS:HA | 1:A:283:GLU:OE1 | 2.15 | 0.46 |
| 1:D:1221:ARG:HE | 1:D:1289:ASP:HB3 | 1.81 | 0.46 |
| 1:A:255:ASN:OD1 | 1:A:308:ALA:HB2 | 2.16 | 0.46 |
| 1:C:1040:MET:HE1 | 1:D:1432:LEU:HG | 1.98 | 0.46 |
| 1:D:1206:VAL:HG21 | 1:D:1385:TYR:CG | 2.49 | 0.46 |
| 1:C:947:VAL:O | 4:C:1196:NAD:H51N | 2.15 | 0.46 |
| 1:D:1422:ALA:HB2 | 1:D:1559:VAL:N | 2.30 | 0.46 |
| 1:D:1217:MET:HE3 | 1:D:1293:ILE:HG21 | 1.97 | 0.46 |
| 1:D:1201:MET:O | 1:D:1252:GLU:OE2 | 2.34 | 0.46 |
| 1:A:195:PRO:HD3 | 1:A:351:LYS:HE3 | 1.97 | 0.46 |
| 1:B:463:ASN:ND2 | 1:B:491:GLU:HG3 | 2.31 | 0.46 |
| 1:D:1437:LEU:O | 1:D:1437:LEU:HG | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:463:ASN:OD1 | 1:B:465:TYR:HB3 | 2.16 | 0.46 |
| 1:C:950:THR:HG21 | 1:C:1065:LEU:HD21 | 1.97 | 0.46 |
| 1:B:423:ILE:HG12 | 1:B:428:ALA:O | 2.15 | 0.46 |
| 1:B:551:GLU:HG3 | 1:B:602:SER:CB | 2.46 | 0.45 |
| 1:C:1064:VAL:O | 1:C:1070:ASN:ND2 | 2.49 | 0.45 |
| 1:B:480:ARG:CD | 1:C:880:ARG:HD2 | 2.45 | 0.45 |
| 1:A:247:GLU:HG2 | 1:A:315:LYS:HD3 | 1.98 | 0.45 |
| 1:A:2:LYS:HB2 | 1:A:142:THR:OG1 | 2.16 | 0.45 |
| 1:D:1272:TRP:HE1 | 1:D:1278:PHE:C | 2.19 | 0.45 |
| 1:B:514:LYS:HE2 | 1:B:517:GLU:CG | 2.47 | 0.45 |
| 1:A:114:LYS:HG3 | 1:A:118:GLY:O | 2.17 | 0.45 |
| 1:A:134:ILE:HD11 | 1:A:194:LEU:HD12 | 1.98 | 0.45 |
| 1:C:903:CYS:HA | 1:C:952:PRO:HD2 | 1.98 | 0.45 |
| 1:D:1558:VAL:HG11 | 1:D:1570:MET:HB3 | 1.97 | 0.45 |
| 1:A:196:TYR:O | 1:A:221:HIS:HA | 2.16 | 0.45 |
| 1:C:804:TRP:CE2 | 1:C:934:ILE:HG12 | 2.51 | 0.45 |
| 1:D:1577:THR:HA | 1:D:1580:GLN:HG3 | 1.99 | 0.45 |
| 1:D:1314:LYS:HD3 | 1:D:1318:GLY:HA2 | 1.98 | 0.45 |
| 1:C:1051:TRP:CD2 | 1:C:1112:VAL:HG22 | 2.51 | 0.45 |
| 1:C:809:TYR:O | 1:C:871:HIS:HE1 | 1.99 | 0.45 |
| 1:B:501:LEU:HA | 1:B:517:GLU:OE1 | 2.17 | 0.45 |
| 1:B:560:TYR:CE2 | 1:B:569:ARG:HD3 | 2.51 | 0.45 |
| 1:A:149:SER:H | 4:A:396:NAD:H8A | 1.81 | 0.45 |
| 1:B:628:THR:OG1 | 1:B:629:GLY:N | 2.49 | 0.45 |
| 1:C:822:ALA:O | 1:C:827:ILE:HB | 2.17 | 0.45 |
| 1:C:916:LEU:HD11 | 1:C:926:MET:HB3 | 1.89 | 0.45 |
| 1:D:1398:ASN:ND2 | 1:D:1400:THR:O | 2.50 | 0.45 |
| 1:A:173:GLU:OE1 | 1:A:175:ARG:NH1 | 2.50 | 0.45 |
| 1:D:1368:GLU:OE2 | 1:D:1391:LYS:NZ | 2.50 | 0.45 |
| 1:B:461:LEU:HB3 | 1:B:462:SER:H | 1.65 | 0.45 |
| 1:C:1171:ASP:OD1 | 1:C:1171:ASP:N | 2.50 | 0.45 |
| 1:B:527:VAL:O | 1:B:530:ILE:N | 2.50 | 0.45 |
| 1:C:1091:TYR:HE1 | 1:C:1093:ILE:HD11 | 1.81 | 0.45 |
| 1:D:1542:ASP:O | 1:D:1546:PHE:HD1 | 1.99 | 0.45 |
| 1:C:1044:ARG:NH1 | 1:D:1539:LEU:HD11 | 2.32 | 0.45 |
| 1:B:459:ARG:HG3 | 1:B:510:LEU:HD12 | 1.97 | 0.45 |
| 1:C:1105:ASN:HA | 1:C:1131:ILE:HD13 | 1.97 | 0.45 |
| 1:A:376:ASN:O | 1:A:379:GLU:HB2 | 2.16 | 0.45 |
| 1:C:941:GLU:HB3 | 1:C:1148:LEU:HD21 | 1.97 | 0.45 |
| 1:D:1539:LEU:N | 1:D:1539:LEU:HD23 | 2.31 | 0.45 |
| 1:C:1104:ASP:O | 1:C:1106:LYS:N | 2.50 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:469:LYS:HG3 | 1:B:483:LEU:CD2 | 2.47 | 0.45 |
| 1:A:60:LEU:O | 1:A:61:LEU:HD23 | 2.16 | 0.45 |
| 1:D:1412:GLU:OE2 | 1:D:1412:GLU:N | 2.50 | 0.45 |
| 1:A:243:TYR:OH | 1:A:376:ASN:ND2 | 2.50 | 0.45 |
| 1:D:1269:LYS:NZ | 5:D:2559:HOH:O | 2.50 | 0.45 |
| 1:B:487:LYS:NZ | 1:B:491:GLU:OE2 | 2.50 | 0.45 |
| 1:B:499:THR:N | 1:B:585:TYR:OH | 2.50 | 0.45 |
| 1:A:110:LEU:O | 1:A:112:ASP:N | 2.50 | 0.45 |
| 1:A:115:THR:O | 1:A:129:ARG:NH1 | 2.50 | 0.45 |
| 1:C:1014:ALA:O | 1:C:1018:GLY:N | 2.50 | 0.45 |
| 1:B:417:MET:CE | 1:B:453:PHE:HB3 | 2.45 | 0.45 |
| 1:A:228:THR:HG22 | 1:A:339:LEU:HD12 | 1.99 | 0.45 |
| 1:B:446:TYR:O | 1:B:752:LYS:NZ | 2.50 | 0.45 |
| 1:D:1206:VAL:HG12 | 1:D:1348:ALA:HB2 | 1.99 | 0.45 |
| 1:A:252:MET:HE2 | 1:A:309:PHE:O | 2.16 | 0.45 |
| 1:D:1468:ARG:NH2 | 1:D:1472:GLU:OE1 | 2.50 | 0.45 |
| 1:B:409:TYR:HE2 | 1:B:461:LEU:N | 2.08 | 0.45 |
| 1:B:452:GLU:OE2 | 1:B:452:GLU:N | 2.50 | 0.45 |
| 1:D:1365:GLU:O | 1:D:1369:ARG:N | 2.50 | 0.45 |
| 1:D:1354:PRO:O | 1:D:1356:TYR:N | 2.50 | 0.45 |
| 1:D:1360:TYR:O | 1:D:1367:PHE:N | 2.50 | 0.45 |
| 1:A:235:THR:HG22 | 1:A:281:VAL:CG1 | 2.46 | 0.45 |
| 1:C:959:GLU:N | 1:C:959:GLU:OE2 | 2.50 | 0.45 |
| 1:B:427:ILE:HG23 | 1:B:427:ILE:O | 2.16 | 0.45 |
| 1:B:483:LEU:O | 1:B:487:LYS:N | 2.50 | 0.45 |
| 1:B:539:ASP:OD2 | 1:B:542:THR:OG1 | 2.30 | 0.45 |
| 1:A:153:LEU:HD23 | 1:A:273:SER:OG | 2.17 | 0.44 |
| 1:D:1472:GLU:O | 1:D:1476:LEU:HG | 2.17 | 0.44 |
| 1:D:1277:HIS:HB2 | 1:D:1534:ILE:CD1 | 2.47 | 0.44 |
| 1:B:656:ILE:HD12 | 1:B:702:LEU:CD1 | 2.46 | 0.44 |
| 1:A:110:LEU:HD13 | 1:A:113:ILE:HG21 | 1.98 | 0.44 |
| 1:B:647:GLU:HG3 | 1:B:648:VAL:N | 2.32 | 0.44 |
| 1:C:857:GLU:HG3 | 1:C:859:ARG:H | 1.82 | 0.44 |
| 1:C:921:LEU:HD21 | 1:C:929:ARG:HH12 | 1.78 | 0.44 |
| 1:D:1400:THR:O | 1:D:1425:ASP:N | 2.50 | 0.44 |
| 1:A:105:SER:HB2 | 1:A:269:ASP:OD2 | 2.17 | 0.44 |
| 1:D:1357:SER:OG | 1:D:1360:TYR:N | 2.50 | 0.44 |
| 1:C:968:GLU:OE2 | 1:C:991:LYS:NZ | 2.50 | 0.44 |
| 1:A:199:PHE:HZ | 1:A:339:LEU:HD12 | 1.82 | 0.44 |
| 1:C:1007:ILE:HG12 | 1:C:1010:LEU:H | 1.83 | 0.44 |
| 1:D:1300:ALA:O | 1:D:1301:LEU:HG | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1078:LYS:HB2 | 1:C:1078:LYS:HE3 | 1.76 | 0.44 |
| 1:D:1504:ASP:O | 1:D:1506:LYS:N | 2.50 | 0.44 |
| 1:B:560:TYR:HD2 | 1:B:566:GLY:O | 2.00 | 0.44 |
| 1:B:627:LYS:HD2 | 1:B:632:LEU:HA | 1.99 | 0.44 |
| 1:C:935:LYS:NZ | 5:C:1857:HOH:O | 2.50 | 0.44 |
| 1:A:214:ALA:O | 1:A:218:GLY:N | 2.50 | 0.44 |
| 1:D:1290:LEU:HA | 1:D:1290:LEU:HD12 | 1.71 | 0.44 |
| 1:A:285:MET:HB2 | 1:A:285:MET:HE2 | 1.87 | 0.44 |
| 1:B:539:ASP:OD2 | 1:B:542:THR:N | 2.51 | 0.44 |
| 1:D:1334:ILE:O | 1:D:1337:PHE:N | 2.51 | 0.44 |
| 1:B:506:GLY:N | 5:B:1774:HOH:O | 2.50 | 0.44 |
| 1:A:24:GLU:OE2 | 1:A:51:PHE:N | 2.49 | 0.44 |
| 1:B:497:LYS:HG2 | 1:B:516:LEU:HD23 | 2.00 | 0.44 |
| 1:D:1265:TYR:HA | 1:D:1290:LEU:HB3 | 2.00 | 0.44 |
| 1:B:402:LYS:HB3 | 1:B:542:THR:HG23 | 2.00 | 0.44 |
| 1:C:944:VAL:HG12 | 1:C:996:TYR:CD1 | 2.52 | 0.44 |
| 1:D:1396:TYR:CD2 | 1:D:1405:SER:HB3 | 2.53 | 0.44 |
| 1:C:997:ALA:HB2 | 1:C:1147:LEU:HD11 | 1.98 | 0.44 |
| 1:C:1030:GLU:OE2 | 1:C:1053:SER:HB3 | 2.18 | 0.44 |
| 1:C:807:GLY:HA2 | 4:C:1196:NAD:N3A | 2.31 | 0.44 |
| 1:C:1065:LEU:O | 1:C:1071:LYS:HB2 | 2.16 | 0.44 |
| 1:A:320:LYS:HD2 | 1:A:321:LEU:H | 1.83 | 0.44 |
| 1:A:268:ARG:NH2 | 5:A:1891:HOH:O | 2.50 | 0.44 |
| 1:A:349:PHE:O | 1:A:353:LYS:HG2 | 2.18 | 0.44 |
| 1:C:1152:LYS:HE2 | 5:C:2065:HOH:O | 2.17 | 0.44 |
| 1:C:997:ALA:HA | 1:C:1022:ALA:O | 2.18 | 0.44 |
| 1:C:1169:PRO:HB2 | 1:C:1172:THR:CG2 | 2.48 | 0.44 |
| 1:C:1160:LYS:HE2 | 1:C:1171:ASP:CB | 2.47 | 0.44 |
| 1:A:150:THR:HG22 | 1:A:270:ASN:HB3 | 1.99 | 0.44 |
| 1:A:22:ALA:HB2 | 1:A:82:ILE:HG23 | 1.98 | 0.44 |
| 1:C:802:LYS:HD2 | 1:C:939:ASP:CG | 2.38 | 0.44 |
| 1:C:1056:ILE:HD12 | 1:C:1102:LEU:HD11 | 1.98 | 0.44 |
| 1:C:1085:MET:O | 1:C:1086:LEU:HD23 | 2.17 | 0.44 |
| 1:B:723:LYS:NZ | 1:D:1529:ASP:OD2 | 2.50 | 0.44 |
| 1:C:881:GLU:HG3 | 1:C:881:GLU:H | 1.45 | 0.44 |
| 1:D:1209:TYR:CD2 | 1:D:1257:GLU:HG2 | 2.53 | 0.44 |
| 1:D:1428:THR:CG2 | 4:D:1596:NAD:H4N | 2.48 | 0.44 |
| 1:D:1406:ALA:HA | 1:D:1570:MET:HE1 | 2.00 | 0.44 |
| 1:B:649:VAL:HG21 | 1:B:721:LEU:CD2 | 2.48 | 0.44 |
| 1:D:1418:GLY:C | 1:D:1556:LYS:HB2 | 2.37 | 0.44 |
| 1:B:567:PHE:HB2 | 1:B:609:ALA:HB1 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:144:VAL:HG21 | 1:A:189:ALA:HB2 | 2.00 | 0.44 |
| 1:D:1303:CYS:O | 1:D:1352:PRO:HG3 | 2.17 | 0.43 |
| 1:B:569:ARG:HG2 | 1:B:570:MET:N | 2.32 | 0.43 |
| 1:A:149:SER:OG | 4:A:396:NAD:H8A | 2.18 | 0.43 |
| 1:A:383:VAL:O | 1:A:386:GLU:HB2 | 2.18 | 0.43 |
| 1:D:1289:ASP:O | 1:D:1292:GLY:N | 2.50 | 0.43 |
| 1:A:101:LEU:HD22 | 1:A:179:ALA:O | 2.18 | 0.43 |
| 1:A:311:PHE:CZ | 1:A:323:LYS:HB3 | 2.53 | 0.43 |
| 1:B:680:LYS:NZ | 1:B:684:LYS:HB2 | 2.32 | 0.43 |
| 1:C:815:THR:HB | 1:C:1137:ALA:HB2 | 2.00 | 0.43 |
| 1:B:621:HIS:O | 1:B:622:ALA:HB2 | 2.17 | 0.43 |
| 1:A:289:SER:HB3 | 5:A:2049:HOH:O | 2.17 | 0.43 |
| 1:C:1132:ASP:N | 1:C:1132:ASP:OD1 | 2.50 | 0.43 |
| 1:D:1346:ASN:ND2 | 1:D:1400:THR:HG23 | 2.34 | 0.43 |
| 1:D:1567:LYS:C | 1:D:1569:PRO:HD3 | 2.39 | 0.43 |
| 1:A:203:PRO:O | 1:A:206:ALA:HB3 | 2.18 | 0.43 |
| 1:B:649:VAL:HG23 | 1:B:713:HIS:O | 2.19 | 0.43 |
| 1:D:1233:LEU:HB2 | 1:D:1236:GLU:HB2 | 1.99 | 0.43 |
| 1:A:9:TYR:CD2 | 1:A:57:GLU:HG3 | 2.53 | 0.43 |
| 1:C:995:PRO:HA | 1:C:1019:VAL:CG1 | 2.47 | 0.43 |
| 1:A:260:TYR:O | 1:A:263:LYS:HB2 | 2.19 | 0.43 |
| 1:B:425:ARG:NH2 | 1:B:489:ASP:OD1 | 2.51 | 0.43 |
| 1:D:1248:PRO:O | 1:D:1250:SER:N | 2.50 | 0.43 |
| 1:C:1057:LEU:HD12 | 1:C:1057:LEU:N | 2.33 | 0.43 |
| 1:D:1204:TRP:HE1 | 1:D:1256:HIS:CE1 | 2.36 | 0.43 |
| 1:B:514:LYS:HE2 | 1:B:517:GLU:HG2 | 2.00 | 0.43 |
| 1:B:783:VAL:HG11 | 5:B:1724:HOH:O | 2.18 | 0.43 |
| 1:C:1105:ASN:CA | 1:C:1131:ILE:HD13 | 2.48 | 0.43 |
| 1:C:903:CYS:SG | 1:C:951:GLU:HB2 | 2.58 | 0.43 |
| 1:C:969:ARG:O | 1:C:973:GLU:N | 2.50 | 0.43 |
| 1:D:1211:ILE:O | 1:D:1215:THR:OG1 | 2.30 | 0.43 |
| 1:C:872:TRP:O | 1:C:876:ARG:N | 2.51 | 0.43 |
| 1:B:534:ILE:O | 1:B:538:ALA:HB2 | 2.18 | 0.43 |
| 1:D:1517:PHE:O | 1:D:1518:LEU:HB2 | 2.19 | 0.43 |
| 1:A:172:ASP:OD2 | 1:A:172:ASP:N | 2.50 | 0.43 |
| 1:D:1481:VAL:HG12 | 1:D:1482:LEU:N | 2.33 | 0.43 |
| 1:D:1549:PHE:CZ | 1:D:1591:LEU:HB2 | 2.54 | 0.43 |
| 1:D:1410:LEU:HA | 1:D:1410:LEU:HD22 | 1.83 | 0.43 |
| 1:D:1345:ILE:CD1 | 1:D:1544:ALA:HB2 | 2.49 | 0.43 |
| 1:B:638:ALA:HB3 | 1:B:639:PRO:HD3 | 2.01 | 0.43 |
| 1:A:68:ALA:HA | 5:A:1919:HOH:O | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1185:LYS:NZ | 5:C:2141:HOH:O | 2.52 | 0.43 |
| 1:A:241:PHE:CZ | 1:A:312:VAL:HG11 | 2.53 | 0.43 |
| 1:D:1421:HIS:O | 1:D:1422:ALA:HB2 | 2.19 | 0.43 |
| 1:D:1518:LEU:N | 1:D:1518:LEU:HD23 | 2.33 | 0.43 |
| 1:D:1240:PHE:O | 1:D:1243:ILE:HG22 | 2.19 | 0.43 |
| 1:C:1140:ILE:N | 1:C:1140:ILE:HD13 | 2.32 | 0.43 |
| 1:D:1436:THR:HG22 | 1:D:1436:THR:O | 2.19 | 0.43 |
| 1:B:688:TYR:C | 1:B:690:PRO:HD3 | 2.39 | 0.43 |
| 1:D:1484:LYS:HE2 | 1:D:1573:ASN:OD1 | 2.19 | 0.43 |
| 1:C:1068:ARG:O | 1:C:1072:GLU:HB2 | 2.19 | 0.43 |
| 1:C:1020:PRO:HB3 | 1:C:1155:VAL:HG12 | 2.01 | 0.43 |
| 1:B:759:VAL:HG12 | 1:B:762:MET:HG3 | 2.00 | 0.43 |
| 1:B:701:SER:HB2 | 1:D:1449:VAL:CG1 | 2.48 | 0.43 |
| 1:B:676:LEU:HD23 | 1:B:676:LEU:HA | 1.75 | 0.43 |
| 1:C:841:GLU:HG3 | 1:C:841:GLU:H | 1.59 | 0.43 |
| 1:D:1316:LEU:HD11 | 1:D:1326:MET:CG | 2.47 | 0.43 |
| 1:A:233:VAL:HG22 | 1:B:640:MET:HE1 | 2.00 | 0.43 |
| 1:D:1360:TYR:CZ | 1:D:1375:ARG:HG3 | 2.54 | 0.43 |
| 1:A:265:LEU:HD23 | 1:A:271:LYS:HG3 | 2.01 | 0.43 |
| 1:D:1233:LEU:O | 1:D:1236:GLU:HB2 | 2.18 | 0.43 |
| 1:D:1243:ILE:HD12 | 1:D:1588:TYR:HE1 | 1.84 | 0.43 |
| 1:C:913:ILE:O | 1:C:915:THR:N | 2.50 | 0.43 |
| 1:B:547:VAL:CG2 | 4:B:796:NAD:H51N | 2.44 | 0.43 |
| 1:B:498:GLY:O | 1:B:499:THR:HB | 2.19 | 0.43 |
| 1:C:1068:ARG:HG2 | 1:C:1068:ARG:O | 2.19 | 0.43 |
| 1:A:151:GLU:HG2 | 1:A:152:PRO:HD2 | 2.01 | 0.43 |
| 1:D:1429:GLY:HA3 | 1:D:1528:TRP:CZ2 | 2.54 | 0.43 |
| 1:A:369:PRO:HB2 | 1:A:372:THR:HG22 | 2.00 | 0.42 |
| 1:D:1555:VAL:HG22 | 5:D:2272:HOH:O | 2.18 | 0.42 |
| 1:A:106:GLY:C | 1:A:264:VAL:HG22 | 2.40 | 0.42 |
| 1:C:901:LEU:HD21 | 1:C:976:LYS:HD3 | 2.01 | 0.42 |
| 1:A:89:ASP:OD2 | 1:A:89:ASP:N | 2.50 | 0.42 |
| 1:C:977:GLU:H | 1:C:977:GLU:HG3 | 1.64 | 0.42 |
| 1:B:465:TYR:OH | 1:B:487:LYS:HE2 | 2.19 | 0.42 |
| 1:A:20:ALA:O | 1:A:24:GLU:N | 2.49 | 0.42 |
| 1:D:1491:TYR:HE2 | 1:D:1493:ILE:HD11 | 1.84 | 0.42 |
| 1:A:42:GLY:O | 1:A:45:LYS:HG3 | 2.18 | 0.42 |
| 1:C:1023:GLY:HA2 | 1:C:1166:PHE:CD1 | 2.54 | 0.42 |
| 1:C:1030:GLU:HB3 | 2:C:1195:PO4:O3 | 2.19 | 0.42 |
| 1:B:559:GLU:OE1 | 1:B:569:ARG:NH1 | 2.50 | 0.42 |
| 1:B:773:ASN:O | 1:B:775:ILE:HD13 | 2.18 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:901:LEU:H | 1:C:981:ALA:HB2 | 1.84 | 0.42 |
| 1:A:41:GLU:HB3 | 5:A:2354:HOH:O | 2.19 | 0.42 |
| 1:C:1122:MET:HB3 | 1:D:1530:ALA:HB2 | 2.01 | 0.42 |
| 1:B:411:ILE:HG13 | 1:B:477:HIS:HE2 | 1.84 | 0.42 |
| 1:A:257:LEU:HD21 | 1:A:261:ASP:HB2 | 2.00 | 0.42 |
| 1:C:1033:VAL:CG2 | 1:D:1440:MET:HE1 | 2.50 | 0.42 |
| 1:A:13:SER:OG | 1:A:14:THR:N | 2.52 | 0.42 |
| 1:A:73:GLU:O | 1:A:73:GLU:HG3 | 2.19 | 0.42 |
| 1:C:1060:TYR:HA | 1:C:1063:LYS:HB2 | 2.00 | 0.42 |
| 1:B:410:GLY:O | 1:B:414:THR:HG23 | 2.20 | 0.42 |
| 1:C:1134:ILE:CG1 | 1:D:1520:LYS:HD3 | 2.38 | 0.42 |
| 1:C:927:VAL:O | 1:C:931:GLU:HB2 | 2.19 | 0.42 |
| 1:C:1019:VAL:HA | 1:C:1020:PRO:HD2 | 1.84 | 0.42 |
| 1:A:379:GLU:O | 1:A:383:VAL:HG23 | 2.19 | 0.42 |
| 1:B:720:LYS:HD2 | 1:B:720:LYS:HA | 1.46 | 0.42 |
| 1:A:302:LEU:O | 1:A:303:VAL:HB | 2.19 | 0.42 |
| 1:D:1583:VAL:HG12 | 1:D:1584:LEU:N | 2.35 | 0.42 |
| 1:C:984:LEU:O | 1:C:988:ALA:HB2 | 2.19 | 0.42 |
| 1:C:921:LEU:HD23 | 1:C:926:MET:HG2 | 2.01 | 0.42 |
| 1:B:500:ALA:HB2 | 4:B:796:NAD:N6A | 2.34 | 0.42 |
| 1:B:758:VAL:CG1 | 1:B:770:MET:HB2 | 2.48 | 0.42 |
| 1:B:483:LEU:O | 1:B:487:LYS:HB2 | 2.19 | 0.42 |
| 1:D:1548:LEU:O | 1:D:1552:LYS:HG3 | 2.19 | 0.42 |
| 1:B:747:LEU:HA | 1:B:747:LEU:HD23 | 1.69 | 0.42 |
| 1:C:1139:LEU:HD23 | 1:C:1139:LEU:N | 2.34 | 0.42 |
| 1:D:1506:LYS:N | 1:D:1530:ALA:O | 2.53 | 0.42 |
| 1:A:259:ASP:HB3 | 1:A:261:ASP:OD1 | 2.19 | 0.42 |
| 1:C:960:TYR:HE2 | 1:C:969:ARG:HH11 | 1.66 | 0.42 |
| 1:C:960:TYR:OH | 1:C:975:ARG:NE | 2.50 | 0.42 |
| 1:B:704:ASP:O | 1:B:706:LYS:N | 2.51 | 0.42 |
| 1:B:711:PHE:HE2 | 1:B:723:LYS:HB3 | 1.84 | 0.42 |
| 1:D:1484:LYS:HB3 | 1:D:1484:LYS:HE3 | 1.72 | 0.42 |
| 1:D:1442:ALA:HA | 5:D:1620:HOH:O | 2.20 | 0.42 |
| 1:B:412:VAL:HG11 | 1:B:547:VAL:HG21 | 2.02 | 0.42 |
| 1:B:406:VAL:HG21 | 1:B:585:TYR:CD1 | 2.54 | 0.42 |
| 1:C:1131:ILE:CG2 | 1:C:1134:ILE:HD13 | 2.50 | 0.42 |
| 1:D:1468:ARG:HG2 | 1:D:1468:ARG:HH11 | 1.85 | 0.42 |
| 1:D:1575:ILE:HA | 1:D:1580:GLN:HE21 | 1.85 | 0.42 |
| 1:A:17:MET:O | 1:A:20:ALA:HB3 | 2.20 | 0.42 |
| 1:B:501:LEU:HD12 | 1:B:523:LEU:HD11 | 2.02 | 0.42 |
| 1:D:1316:LEU:CD2 | 1:D:1326:MET:HG2 | 2.35 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:598:ASN:ND2 | 1:B:602:SER:O | 2.50 | 0.42 |
| 1:A:372:THR:HG23 | 1:A:373:ASN:N | 2.34 | 0.42 |
| 1:D:1553:LYS:HD2 | 1:D:1553:LYS:HA | 1.74 | 0.42 |
| 1:A:39:HIS:CD2 | 1:A:385:LYS:HG2 | 2.55 | 0.42 |
| 1:C:954:PRO:HG3 | 1:C:1003:PRO:HG2 | 2.01 | 0.42 |
| 1:C:870:GLU:OE2 | 1:C:1060:TYR:OH | 2.30 | 0.41 |
| 1:D:1455:ASN:ND2 | 1:D:1506:LYS:NZ | 2.68 | 0.41 |
| 1:B:501:LEU:HD23 | 1:B:501:LEU:HA | 1.89 | 0.41 |
| 1:D:1316:LEU:HD11 | 1:D:1326:MET:SD | 2.59 | 0.41 |
| 1:C:960:TYR:OH | 1:C:975:ARG:NH2 | 2.50 | 0.41 |
| 1:C:871:HIS:HE2 | 1:C:1060:TYR:HE1 | 1.64 | 0.41 |
| 1:D:1206:VAL:O | 1:D:1348:ALA:HB2 | 2.20 | 0.41 |
| 1:B:501:LEU:HD21 | 5:B:2404:HOH:O | 2.20 | 0.41 |
| 1:B:774:VAL:C | 1:B:775:ILE:HD13 | 2.41 | 0.41 |
| 1:A:276:LEU:N | 1:A:276:LEU:HD23 | 2.35 | 0.41 |
| 1:C:1024:ASN:O | 1:C:1168:SER:HB2 | 2.20 | 0.41 |
| 1:A:303:VAL:HG12 | 1:A:304:ASP:N | 2.35 | 0.41 |
| 1:B:722:MET:HB2 | 1:B:722:MET:HE3 | 1.90 | 0.41 |
| 1:B:446:TYR:CE2 | 1:B:753:LYS:HE2 | 2.56 | 0.41 |
| 1:D:1539:LEU:O | 1:D:1543:ILE:HD12 | 2.19 | 0.41 |
| 1:B:648:VAL:HG21 | 1:B:686:LEU:HD11 | 2.01 | 0.41 |
| 1:C:945:ILE:HG12 | 1:C:997:ALA:HB3 | 2.02 | 0.41 |
| 1:B:465:TYR:HB2 | 1:B:490:LEU:HB2 | 2.02 | 0.41 |
| 1:C:1084:LYS:HB3 | 1:C:1173:ASN:ND2 | 2.16 | 0.41 |
| 1:D:1559:VAL:HG21 | 1:D:1562:MET:HE1 | 2.02 | 0.41 |
| 1:A:123:LEU:CD2 | 1:A:184:LEU:HD11 | 2.50 | 0.41 |
| 1:B:750:ALA:HB1 | 1:B:755:VAL:HB | 2.02 | 0.41 |
| 1:B:615:GLU:OE1 | 1:B:615:GLU:HA | 2.20 | 0.41 |
| 1:B:739:LEU:HD23 | 1:B:739:LEU:N | 2.35 | 0.41 |
| 1:C:857:GLU:OE2 | 4:C:1196:NAD:H1B | 2.21 | 0.41 |
| 1:D:1532:ASP:CB | 4:D:1596:NAD:H72N | 2.25 | 0.41 |
| 1:A:90:LEU:HA | 1:A:90:LEU:HD22 | 1.90 | 0.41 |
| 1:D:1366:GLY:O | 1:D:1369:ARG:N | 2.50 | 0.41 |
| 1:D:1465:LEU:HB3 | 1:D:1471:LYS:HG3 | 2.02 | 0.41 |
| 1:A:378:HIS:HB3 | 5:A:1787:HOH:O | 2.19 | 0.41 |
| 1:B:775:ILE:HD13 | 1:B:775:ILE:N | 2.35 | 0.41 |
| 1:A:9:TYR:CD2 | 1:A:61:LEU:HB2 | 2.56 | 0.41 |
| 1:D:1246:TYR:HD1 | 1:D:1549:PHE:HD2 | 1.69 | 0.41 |
| 1:D:1329:ARG:CA | 1:D:1332:GLU:HB2 | 2.49 | 0.41 |
| 1:C:997:ALA:HB2 | 1:C:1147:LEU:CD1 | 2.51 | 0.41 |
| 1:B:691:TYR:OH | 1:D:1498:TYR:O | 2.30 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:923:LEU:HA | 1:C:923:LEU:HD12 | 1.85 | 0.41 |
| 1:A:235:THR:HB | 1:A:375:ILE:O | 2.21 | 0.41 |
| 5:A:2516:HOH:O | 1:D:1280:ARG:HG2 | 2.21 | 0.41 |
| 1:B:564:LEU:HB2 | 1:B:609:ALA:O | 2.21 | 0.41 |
| 1:A:116:LEU:HB3 | 1:A:117:GLU:H | 1.57 | 0.41 |
| 1:A:57:GLU:OE2 | 4:A:396:NAD:O3B | 2.30 | 0.41 |
| 1:C:990:LEU:HD22 | 1:C:1014:ALA:CB | 2.44 | 0.41 |
| 1:D:1482:LEU:HD23 | 1:D:1490:PRO:HG2 | 2.03 | 0.41 |
| 1:A:254:TYR:O | 1:A:308:ALA:HA | 2.21 | 0.41 |
| 1:D:1550:ALA:HB2 | 1:D:1587:TRP:CZ2 | 2.55 | 0.41 |
| 1:A:299:PHE:CD2 | 1:C:1093:ILE:HD12 | 2.54 | 0.41 |
| 1:A:340:ILE:HD13 | 1:A:340:ILE:N | 2.35 | 0.41 |
| 1:C:859:ARG:HG3 | 1:C:910:LEU:CD1 | 2.35 | 0.41 |
| 1:D:1455:ASN:HD22 | 1:D:1506:LYS:HZ3 | 1.68 | 0.41 |
| 1:C:1018:GLY:HA2 | 1:C:1156:LYS:CB | 2.51 | 0.41 |
| 1:D:1259:ARG:CG | 1:D:1310:LEU:HG | 2.45 | 0.41 |
| 1:C:889:ASP:OD2 | 1:C:889:ASP:N | 2.52 | 0.41 |
| 1:D:1377:GLU:HG3 | 5:D:2346:HOH:O | 2.21 | 0.41 |
| 1:C:1089:SER:HA | 1:C:1090:PRO:HD2 | 1.94 | 0.41 |
| 1:B:743:ILE:HA | 1:B:762:MET:HE1 | 2.02 | 0.41 |
| 1:A:142:THR:O | 1:A:143:VAL:HG13 | 2.20 | 0.41 |
| 1:A:142:THR:HG22 | 1:A:143:VAL:N | 2.36 | 0.41 |
| 1:D:1256:HIS:HA | 1:D:1296:ARG:O | 2.20 | 0.41 |
| 1:A:15:THR:O | 1:A:15:THR:HG22 | 2.20 | 0.41 |
| 1:A:1:MET:N | 1:A:50:SER:O | 2.50 | 0.41 |
| 1:D:1257:GLU:OE1 | 4:D:1596:NAD:O3B | 2.39 | 0.41 |
| 1:A:130:ILE:O | 1:A:130:ILE:HG22 | 2.20 | 0.41 |
| 1:A:57:GLU:OE2 | 4:A:396:NAD:H1B | 2.20 | 0.41 |
| 1:B:480:ARG:HH11 | 1:B:480:ARG:HG2 | 1.86 | 0.41 |
| 1:A:315:LYS:HG2 | 1:A:321:LEU:CD2 | 2.51 | 0.41 |
| 1:A:164:LEU:HD11 | 1:A:213:LEU:CD1 | 2.51 | 0.41 |
| 1:D:1508:ALA:O | 1:D:1527:ILE:HA | 2.20 | 0.41 |
| 1:D:1304:GLY:HA3 | 1:D:1307:ILE:CG2 | 2.51 | 0.41 |
| 1:D:1204:TRP:CE2 | 1:D:1255:GLY:HA2 | 2.56 | 0.41 |
| 1:B:411:ILE:HA | 1:B:414:THR:OG1 | 2.21 | 0.40 |
| 1:B:610:LEU:HD12 | 1:B:610:LEU:HA | 1.89 | 0.40 |
| 1:B:418:VAL:HG22 | 1:B:490:LEU:HD11 | 2.03 | 0.40 |
| 1:A:11:ILE:HD13 | 1:A:333:ALA:CB | 2.47 | 0.40 |
| 1:B:627:LYS:H | 1:B:766:PHE:HA | 1.86 | 0.40 |
| 1:B:668:ARG:O | 1:B:672:GLU:N | 2.50 | 0.40 |
| 1:B:671:LYS:HE2 | 1:B:675:VAL:CG2 | 2.46 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:551:GLU:O | 1:B:673:SER:OG | 2.30 | 0.40 |
| 1:A:239:PRO:HB3 | 1:A:243:TYR:CZ | 2.57 | 0.40 |
| 1:C:804:TRP:CD2 | 1:C:855:GLY:HA2 | 2.56 | 0.40 |
| 1:B:704:ASP:HA | 5:B:2522:HOH:O | 2.20 | 0.40 |
| 1:B:685:MET:HB2 | 1:B:685:MET:HE2 | 1.80 | 0.40 |
| 1:B:428:ALA:HA | 1:B:429:PRO:HD3 | 1.93 | 0.40 |
| 1:D:1358:GLU:HG3 | 1:D:1358:GLU:H | 1.59 | 0.40 |
| 1:A:216:LYS:HG3 | 1:A:216:LYS:O | 2.21 | 0.40 |
| 1:C:849:PHE:CE1 | 1:C:851:PHE:HE1 | 2.39 | 0.40 |
| 1:B:412:VAL:HG22 | 1:B:733:ALA:HA | 2.03 | 0.40 |
| 1:C:1131:ILE:HB | 1:C:1134:ILE:HD13 | 2.03 | 0.40 |
| 1:D:1407:ILE:HD11 | 1:D:1409:ALA:HB3 | 2.03 | 0.40 |
| 1:B:532:GLU:HG2 | 1:B:532:GLU:O | 2.21 | 0.40 |
| 1:C:954:PRO:CG | 1:C:1003:PRO:HG2 | 2.51 | 0.40 |
| 1:B:740:ILE:HD13 | 1:B:740:ILE:N | 2.35 | 0.40 |
| 1:C:1167:LYS:C | 1:C:1169:PRO:HD3 | 2.42 | 0.40 |
| 1:A:110:LEU:CB | 1:A:113:ILE:HB | 2.52 | 0.40 |
| 1:B:782:VAL:O | 1:B:786:GLU:HG3 | 2.21 | 0.40 |
| 1:C:994:LEU:O | 1:C:1019:VAL:HG11 | 2.22 | 0.40 |
| 1:D:1310:LEU:O | 1:D:1313:ILE:HB | 2.21 | 0.40 |
| 1:A:228:THR:HG22 | 1:A:339:LEU:HD11 | 2.03 | 0.40 |
| 1:B:680:LYS:HZ3 | 1:B:683:GLU:CB | 2.34 | 0.40 |
| 1:C:815:THR:OG1 | 1:C:1133:ALA:HB1 | 2.21 | 0.40 |
| 1:A:281:VAL:HG13 | 1:A:375:ILE:HG21 | 2.04 | 0.40 |
| 1:B:507:ILE:HG22 | 5:B:1774:HOH:O | 2.22 | 0.40 |
| 1:B:698:TYR:O | 1:D:1493:ILE:HD11 | 2.21 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|------------------|------------|-----------|----------|-------------|---|
| 1 | A | 390/392 (100%) | 343 (88%) | 36 (9%) | 11 (3%) | 6 | 1 |
| 1 | B | 390/392 (100%) | 331 (85%) | 43 (11%) | 16 (4%) | 3 | 0 |
| 1 | C | 390/392 (100%) | 340 (87%) | 37 (10%) | 13 (3%) | 5 | 0 |
| 1 | D | 390/392 (100%) | 324 (83%) | 43 (11%) | 23 (6%) | 2 | 0 |
| All | All | 1560/1568 (100%) | 1338 (86%) | 159 (10%) | 63 (4%) | 4 | 0 |

All (63) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 109 | GLU |
| 1 | A | 115 | THR |
| 1 | A | 224 | ASN |
| 1 | B | 505 | SER |
| 1 | B | 629 | GLY |
| 1 | B | 717 | PHE |
| 1 | C | 1024 | ASN |
| 1 | C | 1073 | SER |
| 1 | C | 1117 | PHE |
| 1 | D | 1262 | SER |
| 1 | D | 1302 | ASN |
| 1 | D | 1338 | ALA |
| 1 | D | 1339 | ASP |
| 1 | D | 1459 | ASP |
| 1 | A | 111 | GLY |
| 1 | A | 269 | ASP |
| 1 | A | 303 | VAL |
| 1 | A | 333 | ALA |
| 1 | B | 509 | GLU |
| 1 | B | 511 | GLY |
| 1 | C | 909 | GLU |
| 1 | C | 916 | LEU |
| 1 | C | 1164 | PHE |
| 1 | D | 1303 | CYS |
| 1 | D | 1355 | ASN |
| 1 | D | 1424 | ASN |
| 1 | D | 1505 | ASN |
| 1 | D | 1558 | VAL |
| 1 | A | 104 | GLY |
| 1 | B | 501 | LEU |
| 1 | C | 908 | LYS |
| 1 | C | 963 | SER |
| 1 | C | 1025 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | C | 1105 | ASN |
| 1 | D | 1287 | LYS |
| 1 | D | 1320 | GLY |
| 1 | D | 1429 | GLY |
| 1 | D | 1469 | ASP |
| 1 | B | 514 | LYS |
| 1 | B | 603 | PRO |
| 1 | B | 624 | ASN |
| 1 | B | 703 | VAL |
| 1 | B | 705 | ASN |
| 1 | C | 1103 | VAL |
| 1 | D | 1457 | LEU |
| 1 | D | 1503 | VAL |
| 1 | A | 106 | GLY |
| 1 | A | 107 | ILE |
| 1 | B | 429 | PRO |
| 1 | C | 913 | ILE |
| 1 | C | 1029 | GLY |
| 1 | D | 1307 | ILE |
| 1 | D | 1376 | LYS |
| 1 | D | 1425 | ASP |
| 1 | B | 681 | VAL |
| 1 | D | 1289 | ASP |
| 1 | B | 498 | GLY |
| 1 | D | 1583 | VAL |
| 1 | B | 658 | GLY |
| 1 | A | 220 | PRO |
| 1 | D | 1559 | VAL |
| 1 | B | 774 | VAL |
| 1 | D | 1366 | GLY |

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 | 325/325 (100%) | 247 (76%) | 78 (24%) | 1 0 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|-----------|-------------|---|
| 1 | B | 325/325 (100%) | 268 (82%) | 57 (18%) | 2 | 0 |
| 1 | C | 325/325 (100%) | 265 (82%) | 60 (18%) | 2 | 0 |
| 1 | D | 325/325 (100%) | 252 (78%) | 73 (22%) | 1 | 0 |
| All | All | 1300/1300 (100%) | 1032 (79%) | 268 (21%) | 1 | 0 |

All (268) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 11 | ILE |
| 1 | A | 13 | SER |
| 1 | A | 21 | ARG |
| 1 | A | 30 | LYS |
| 1 | A | 35 | SER |
| 1 | A | 45 | LYS |
| 1 | A | 59 | ARG |
| 1 | A | 66 | GLU |
| 1 | A | 69 | LYS |
| 1 | A | 76 | ARG |
| 1 | A | 77 | HIS |
| 1 | A | 79 | ASP |
| 1 | A | 80 | ARG |
| 1 | A | 81 | GLU |
| 1 | A | 87 | LYS |
| 1 | A | 88 | SER |
| 1 | A | 89 | ASP |
| 1 | A | 90 | LEU |
| 1 | A | 91 | GLU |
| 1 | A | 97 | LYS |
| 1 | A | 102 | ASN |
| 1 | A | 105 | SER |
| 1 | A | 107 | ILE |
| 1 | A | 108 | LYS |
| 1 | A | 110 | LEU |
| 1 | A | 112 | ASP |
| 1 | A | 113 | ILE |
| 1 | A | 114 | LYS |
| 1 | A | 116 | LEU |
| 1 | A | 117 | GLU |
| 1 | A | 121 | LEU |
| 1 | A | 125 | GLU |
| 1 | A | 128 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 132 | GLU |
| 1 | A | 136 | SER |
| 1 | A | 150 | THR |
| 1 | A | 156 | TYR |
| 1 | A | 157 | SER |
| 1 | A | 165 | GLU |
| 1 | A | 170 | MET |
| 1 | A | 172 | ASP |
| 1 | A | 173 | GLU |
| 1 | A | 174 | ASP |
| 1 | A | 175 | ARG |
| 1 | A | 180 | SER |
| 1 | A | 191 | LYS |
| 1 | A | 202 | SER |
| 1 | A | 215 | GLU |
| 1 | A | 219 | VAL |
| 1 | A | 221 | HIS |
| 1 | A | 232 | LEU |
| 1 | A | 247 | GLU |
| 1 | A | 249 | VAL |
| 1 | A | 256 | ILE |
| 1 | A | 257 | LEU |
| 1 | A | 261 | ASP |
| 1 | A | 265 | LEU |
| 1 | A | 268 | ARG |
| 1 | A | 274 | LYS |
| 1 | A | 277 | SER |
| 1 | A | 280 | LYS |
| 1 | A | 285 | MET |
| 1 | A | 286 | LEU |
| 1 | A | 289 | SER |
| 1 | A | 292 | SER |
| 1 | A | 293 | ILE |
| 1 | A | 310 | ASP |
| 1 | A | 315 | LYS |
| 1 | A | 317 | PHE |
| 1 | A | 340 | ILE |
| 1 | A | 348 | LEU |
| 1 | A | 356 | LYS |
| 1 | A | 360 | LYS |
| 1 | A | 366 | PHE |
| 1 | A | 372 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 380 | GLN |
| 1 | A | 384 | LEU |
| 1 | A | 389 | SER |
| 1 | B | 425 | ARG |
| 1 | B | 427 | ILE |
| 1 | B | 430 | LYS |
| 1 | B | 431 | ILE |
| 1 | B | 443 | ILE |
| 1 | B | 445 | LYS |
| 1 | B | 458 | ILE |
| 1 | B | 469 | LYS |
| 1 | B | 477 | HIS |
| 1 | B | 481 | GLU |
| 1 | B | 484 | GLU |
| 1 | B | 488 | SER |
| 1 | B | 491 | GLU |
| 1 | B | 496 | ARG |
| 1 | B | 497 | LYS |
| 1 | B | 499 | THR |
| 1 | B | 501 | LEU |
| 1 | B | 507 | ILE |
| 1 | B | 508 | LYS |
| 1 | B | 516 | LEU |
| 1 | B | 517 | GLU |
| 1 | B | 521 | LEU |
| 1 | B | 527 | VAL |
| 1 | B | 528 | SER |
| 1 | B | 529 | ARG |
| 1 | B | 531 | GLU |
| 1 | B | 537 | PHE |
| 1 | B | 540 | ASP |
| 1 | B | 541 | GLU |
| 1 | B | 565 | GLU |
| 1 | B | 569 | ARG |
| 1 | B | 600 | THR |
| 1 | B | 610 | LEU |
| 1 | B | 612 | GLU |
| 1 | B | 635 | THR |
| 1 | B | 640 | MET |
| 1 | B | 641 | PHE |
| 1 | B | 653 | SER |
| 1 | B | 657 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 677 | SER |
| 1 | B | 678 | LYS |
| 1 | B | 682 | LEU |
| 1 | B | 683 | GLU |
| 1 | B | 684 | LYS |
| 1 | B | 689 | SER |
| 1 | B | 693 | ILE |
| 1 | B | 701 | SER |
| 1 | B | 720 | LYS |
| 1 | B | 725 | TYR |
| 1 | B | 734 | ILE |
| 1 | B | 735 | VAL |
| 1 | B | 748 | LEU |
| 1 | B | 760 | LYS |
| 1 | B | 773 | ASN |
| 1 | B | 775 | ILE |
| 1 | B | 778 | HIS |
| 1 | B | 792 | LYS |
| 1 | C | 812 | VAL |
| 1 | C | 827 | ILE |
| 1 | C | 831 | ILE |
| 1 | C | 841 | GLU |
| 1 | C | 843 | ILE |
| 1 | C | 845 | LYS |
| 1 | C | 846 | TYR |
| 1 | C | 858 | ILE |
| 1 | C | 860 | LEU |
| 1 | C | 861 | LEU |
| 1 | C | 869 | LYS |
| 1 | C | 877 | HIS |
| 1 | C | 878 | PHE |
| 1 | C | 879 | ASP |
| 1 | C | 880 | ARG |
| 1 | C | 881 | GLU |
| 1 | C | 891 | GLU |
| 1 | C | 901 | LEU |
| 1 | C | 903 | CYS |
| 1 | C | 905 | SER |
| 1 | C | 908 | LYS |
| 1 | C | 912 | ASP |
| 1 | C | 914 | LYS |
| 1 | C | 916 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | C | 917 | GLU |
| 1 | C | 923 | LEU |
| 1 | C | 925 | GLU |
| 1 | C | 932 | GLU |
| 1 | C | 935 | LYS |
| 1 | C | 940 | ASP |
| 1 | C | 947 | VAL |
| 1 | C | 949 | SER |
| 1 | C | 951 | GLU |
| 1 | C | 957 | SER |
| 1 | C | 963 | SER |
| 1 | C | 972 | ASP |
| 1 | C | 977 | GLU |
| 1 | C | 980 | SER |
| 1 | C | 1002 | SER |
| 1 | C | 1007 | ILE |
| 1 | C | 1016 | LYS |
| 1 | C | 1017 | LYS |
| 1 | C | 1047 | GLU |
| 1 | C | 1057 | LEU |
| 1 | C | 1059 | ASP |
| 1 | C | 1063 | LYS |
| 1 | C | 1069 | ASP |
| 1 | C | 1070 | ASN |
| 1 | C | 1071 | LYS |
| 1 | C | 1073 | SER |
| 1 | C | 1077 | SER |
| 1 | C | 1084 | LYS |
| 1 | C | 1101 | SER |
| 1 | C | 1105 | ASN |
| 1 | C | 1110 | ASP |
| 1 | C | 1151 | LYS |
| 1 | C | 1167 | LYS |
| 1 | C | 1171 | ASP |
| 1 | C | 1175 | ILE |
| 1 | C | 1192 | LYS |
| 1 | D | 1213 | SER |
| 1 | D | 1227 | ILE |
| 1 | D | 1231 | ILE |
| 1 | D | 1235 | SER |
| 1 | D | 1241 | GLU |
| 1 | D | 1250 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | D | 1252 | GLU |
| 1 | D | 1253 | PHE |
| 1 | D | 1262 | SER |
| 1 | D | 1269 | LYS |
| 1 | D | 1274 | LEU |
| 1 | D | 1276 | ARG |
| 1 | D | 1280 | ARG |
| 1 | D | 1286 | VAL |
| 1 | D | 1287 | LYS |
| 1 | D | 1290 | LEU |
| 1 | D | 1303 | CYS |
| 1 | D | 1307 | ILE |
| 1 | D | 1308 | LYS |
| 1 | D | 1309 | GLU |
| 1 | D | 1310 | LEU |
| 1 | D | 1313 | ILE |
| 1 | D | 1316 | LEU |
| 1 | D | 1322 | SER |
| 1 | D | 1323 | LEU |
| 1 | D | 1326 | MET |
| 1 | D | 1332 | GLU |
| 1 | D | 1333 | ASP |
| 1 | D | 1335 | LYS |
| 1 | D | 1336 | SER |
| 1 | D | 1345 | ILE |
| 1 | D | 1346 | ASN |
| 1 | D | 1358 | GLU |
| 1 | D | 1365 | GLU |
| 1 | D | 1371 | ILE |
| 1 | D | 1372 | ASP |
| 1 | D | 1376 | LYS |
| 1 | D | 1377 | GLU |
| 1 | D | 1380 | SER |
| 1 | D | 1383 | MET |
| 1 | D | 1384 | LEU |
| 1 | D | 1402 | SER |
| 1 | D | 1410 | LEU |
| 1 | D | 1412 | GLU |
| 1 | D | 1415 | GLU |
| 1 | D | 1416 | LYS |
| 1 | D | 1421 | HIS |
| 1 | D | 1424 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | D | 1453 | SER |
| 1 | D | 1456 | ILE |
| 1 | D | 1457 | LEU |
| 1 | D | 1466 | SER |
| 1 | D | 1469 | ASP |
| 1 | D | 1470 | ASN |
| 1 | D | 1477 | SER |
| 1 | D | 1478 | LYS |
| 1 | D | 1480 | LYS |
| 1 | D | 1483 | GLU |
| 1 | D | 1484 | LYS |
| 1 | D | 1486 | LEU |
| 1 | D | 1497 | GLN |
| 1 | D | 1499 | PHE |
| 1 | D | 1505 | ASN |
| 1 | D | 1512 | VAL |
| 1 | D | 1535 | VAL |
| 1 | D | 1551 | LYS |
| 1 | D | 1556 | LYS |
| 1 | D | 1558 | VAL |
| 1 | D | 1560 | LYS |
| 1 | D | 1567 | LYS |
| 1 | D | 1568 | SER |
| 1 | D | 1580 | GLN |
| 1 | D | 1589 | SER |

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

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 71 | HIS |
| 1 | A | 77 | HIS |
| 1 | A | 102 | ASN |
| 1 | A | 161 | HIS |
| 1 | B | 624 | ASN |
| 1 | B | 697 | GLN |
| 1 | B | 778 | HIS |
| 1 | C | 839 | HIS |
| 1 | C | 877 | HIS |
| 1 | C | 1021 | HIS |
| 1 | C | 1173 | ASN |
| 1 | D | 1271 | HIS |
| 1 | D | 1277 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | D | 1302 | ASN |
| 1 | D | 1346 | ASN |
| 1 | D | 1361 | HIS |
| 1 | D | 1398 | ASN |
| 1 | D | 1424 | ASN |
| 1 | D | 1455 | ASN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 2 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 | $\# Z > 2$ |
| 2 | PO4 | A | 395 | - | 4,4,4 | 0.40 | 0 | 6,6,6 | 0.27 | 0 |
| 4 | NAD | A | 396 | - | 38,48,48 | 1.91 | 6 (15%) | 47,73,73 | 1.49 | 8 (17%) |
| 2 | PO4 | B | 795 | - | 4,4,4 | 0.41 | 0 | 6,6,6 | 0.27 | 0 |
| 4 | NAD | B | 796 | 3 | 38,48,48 | 1.11 | 3 (7%) | 47,73,73 | 1.40 | 7 (14%) |
| 2 | PO4 | C | 1195 | - | 4,4,4 | 0.39 | 0 | 6,6,6 | 0.28 | 0 |
| 4 | NAD | C | 1196 | 3 | 38,48,48 | 1.14 | 3 (7%) | 47,73,73 | 1.50 | 9 (19%) |
| 2 | PO4 | D | 1595 | - | 4,4,4 | 0.43 | 0 | 6,6,6 | 0.28 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 4 | NAD | D | 1596 | - | 38,48,48 | 1.10 | 3 (7%) | 47,73,73 | 1.41 | 8 (17%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 2 | PO4 | A | 395 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | NAD | A | 396 | - | - | 0/22/62/62 | 0/5/5/5 |
| 2 | PO4 | B | 795 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | NAD | B | 796 | 3 | - | 0/22/62/62 | 0/5/5/5 |
| 2 | PO4 | C | 1195 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | NAD | C | 1196 | 3 | - | 0/22/62/62 | 0/5/5/5 |
| 2 | PO4 | D | 1595 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | NAD | D | 1596 | - | - | 0/22/62/62 | 0/5/5/5 |

All (15) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 4 | A | 396 | NAD | C3N-C7N | -8.24 | 1.37 | 1.50 |
| 4 | C | 1196 | NAD | O4B-C1B | -3.71 | 1.36 | 1.41 |
| 4 | B | 796 | NAD | O4B-C1B | -3.46 | 1.36 | 1.41 |
| 4 | D | 1596 | NAD | O4B-C1B | -3.28 | 1.37 | 1.41 |
| 4 | A | 396 | NAD | O4B-C1B | -3.24 | 1.37 | 1.41 |
| 4 | D | 1596 | NAD | C6N-N1N | 2.07 | 1.41 | 1.35 |
| 4 | C | 1196 | NAD | C6N-N1N | 2.10 | 1.41 | 1.35 |
| 4 | B | 796 | NAD | C6N-N1N | 2.12 | 1.41 | 1.35 |
| 4 | A | 396 | NAD | C6N-N1N | 2.22 | 1.41 | 1.35 |
| 4 | A | 396 | NAD | C7N-N7N | 2.35 | 1.37 | 1.33 |
| 4 | B | 796 | NAD | C2A-N1A | 2.46 | 1.38 | 1.33 |
| 4 | A | 396 | NAD | C2A-N1A | 2.49 | 1.38 | 1.33 |
| 4 | C | 1196 | NAD | C2A-N1A | 2.51 | 1.38 | 1.33 |
| 4 | D | 1596 | NAD | C2A-N1A | 2.52 | 1.38 | 1.33 |
| 4 | A | 396 | NAD | C2N-C3N | 5.27 | 1.47 | 1.39 |

All (32) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 4 | D | 1596 | NAD | PN-O3-PA | -5.40 | 117.56 | 132.73 |
| 4 | A | 396 | NAD | PN-O3-PA | -5.27 | 117.92 | 132.73 |
| 4 | C | 1196 | NAD | O7N-C7N-C3N | -4.24 | 114.95 | 119.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 4 | B | 796 | NAD | O7N-C7N-C3N | -4.20 | 115.00 | 119.59 |
| 4 | C | 1196 | NAD | PN-O3-PA | -3.61 | 122.59 | 132.73 |
| 4 | A | 396 | NAD | C3N-C7N-N7N | -3.21 | 114.30 | 117.82 |
| 4 | D | 1596 | NAD | O7N-C7N-C3N | -2.58 | 116.77 | 119.59 |
| 4 | C | 1196 | NAD | C2B-C3B-C4B | -2.51 | 97.46 | 102.61 |
| 4 | C | 1196 | NAD | C3N-C2N-N1N | -2.48 | 117.50 | 120.36 |
| 4 | B | 796 | NAD | C3N-C2N-N1N | -2.41 | 117.58 | 120.36 |
| 4 | D | 1596 | NAD | C2B-C3B-C4B | -2.21 | 98.07 | 102.61 |
| 4 | D | 1596 | NAD | N3A-C2A-N1A | -2.19 | 127.22 | 128.89 |
| 4 | C | 1196 | NAD | C4D-O4D-C1D | -2.18 | 107.32 | 109.72 |
| 4 | A | 396 | NAD | C2B-C3B-C4B | -2.12 | 98.26 | 102.61 |
| 4 | D | 1596 | NAD | O5B-C5B-C4B | -2.11 | 101.34 | 109.12 |
| 4 | A | 396 | NAD | O5B-C5B-C4B | -2.06 | 101.53 | 109.12 |
| 4 | B | 796 | NAD | O2A-PA-O3 | 2.00 | 114.19 | 105.09 |
| 4 | A | 396 | NAD | C4A-C5A-N7A | 2.15 | 111.46 | 109.48 |
| 4 | C | 1196 | NAD | O3-PA-O5B | 2.25 | 108.90 | 102.94 |
| 4 | A | 396 | NAD | O4D-C4D-C5D | 2.35 | 117.72 | 109.32 |
| 4 | A | 396 | NAD | C4B-O4B-C1B | 2.37 | 112.32 | 109.72 |
| 4 | B | 796 | NAD | C4A-C5A-N7A | 2.44 | 111.72 | 109.48 |
| 4 | C | 1196 | NAD | C4A-C5A-N7A | 2.45 | 111.73 | 109.48 |
| 4 | D | 1596 | NAD | C4A-C5A-N7A | 2.55 | 111.82 | 109.48 |
| 4 | B | 796 | NAD | C2N-C3N-C4N | 2.60 | 121.18 | 118.29 |
| 4 | C | 1196 | NAD | C2N-C3N-C4N | 2.61 | 121.19 | 118.29 |
| 4 | B | 796 | NAD | O3-PA-O5B | 2.68 | 110.05 | 102.94 |
| 4 | D | 1596 | NAD | O3-PA-O5B | 2.70 | 110.10 | 102.94 |
| 4 | D | 1596 | NAD | O4D-C4D-C5D | 2.72 | 119.03 | 109.32 |
| 4 | C | 1196 | NAD | O4D-C1D-N1N | 3.08 | 111.51 | 108.13 |
| 4 | A | 396 | NAD | C5N-C4N-C3N | 3.12 | 124.26 | 120.33 |
| 4 | B | 796 | NAD | O4D-C1D-N1N | 3.98 | 112.50 | 108.13 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 34 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2 | A | 395 | PO4 | 1 | 0 |
| 4 | A | 396 | NAD | 6 | 0 |
| 2 | B | 795 | PO4 | 1 | 0 |
| 4 | B | 796 | NAD | 5 | 0 |
| 2 | C | 1195 | PO4 | 2 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 4 | C | 1196 | NAD | 8 | 0 |
| 2 | D | 1595 | PO4 | 2 | 0 |
| 4 | D | 1596 | NAD | 9 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|------------------|--------|----------------|-----------------------|-------|
| 1 | A | 392/392 (100%) | 0.38 | 26 (6%) 22 24 | 14, 41, 77, 131 | 0 |
| 1 | B | 392/392 (100%) | 0.51 | 43 (10%) 7 8 | 16, 42, 80, 158 | 0 |
| 1 | C | 392/392 (100%) | 0.33 | 24 (6%) 25 27 | 7, 38, 71, 131 | 0 |
| 1 | D | 392/392 (100%) | 0.53 | 35 (8%) 12 13 | 14, 43, 80, 149 | 0 |
| All | All | 1568/1568 (100%) | 0.44 | 128 (8%) 14 16 | 7, 41, 77, 158 | 0 |

All (128) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 116 | LEU | 8.9 |
| 1 | B | 504 | GLY | 8.2 |
| 1 | A | 115 | THR | 7.4 |
| 1 | C | 910 | LEU | 6.6 |
| 1 | B | 507 | ILE | 6.2 |
| 1 | B | 460 | LEU | 6.1 |
| 1 | D | 1364 | LEU | 6.1 |
| 1 | D | 1318 | GLY | 5.9 |
| 1 | D | 1313 | ILE | 5.9 |
| 1 | D | 1311 | GLY | 5.8 |
| 1 | A | 111 | GLY | 5.7 |
| 1 | B | 516 | LEU | 5.5 |
| 1 | A | 119 | GLU | 5.2 |
| 1 | D | 1314 | LYS | 5.1 |
| 1 | A | 173 | GLU | 5.1 |
| 1 | B | 513 | ILE | 5.1 |
| 1 | D | 1290 | LEU | 4.8 |
| 1 | A | 337 | ALA | 4.7 |
| 1 | C | 911 | GLY | 4.6 |
| 1 | B | 739 | LEU | 4.6 |
| 1 | D | 1468 | ARG | 4.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | B | 505 | SER | 4.5 |
| 1 | C | 907 | ILE | 4.4 |
| 1 | D | 1322 | SER | 4.4 |
| 1 | D | 1315 | THR | 4.2 |
| 1 | D | 1357 | SER | 4.0 |
| 1 | D | 1347 | VAL | 4.0 |
| 1 | C | 1058 | GLY | 3.9 |
| 1 | A | 104 | GLY | 3.8 |
| 1 | B | 514 | LYS | 3.8 |
| 1 | B | 510 | LEU | 3.8 |
| 1 | C | 916 | LEU | 3.7 |
| 1 | A | 340 | ILE | 3.7 |
| 1 | A | 339 | LEU | 3.7 |
| 1 | A | 170 | MET | 3.6 |
| 1 | B | 560 | TYR | 3.6 |
| 1 | B | 458 | ILE | 3.3 |
| 1 | B | 426 | GLY | 3.3 |
| 1 | D | 1307 | ILE | 3.3 |
| 1 | B | 566 | GLY | 3.3 |
| 1 | C | 886 | VAL | 3.3 |
| 1 | D | 1260 | LEU | 3.2 |
| 1 | B | 614 | ALA | 3.2 |
| 1 | D | 1399 | PHE | 3.2 |
| 1 | B | 740 | ILE | 3.2 |
| 1 | A | 147 | VAL | 3.2 |
| 1 | B | 490 | LEU | 3.2 |
| 1 | C | 913 | ILE | 3.1 |
| 1 | B | 599 | PHE | 3.1 |
| 1 | B | 508 | LYS | 3.1 |
| 1 | B | 669 | ASP | 3.1 |
| 1 | C | 947 | VAL | 3.1 |
| 1 | B | 743 | ILE | 3.0 |
| 1 | B | 597 | ALA | 3.0 |
| 1 | C | 962 | GLY | 2.9 |
| 1 | B | 623 | GLY | 2.9 |
| 1 | A | 107 | ILE | 2.9 |
| 1 | A | 113 | ILE | 2.9 |
| 1 | B | 545 | ILE | 2.9 |
| 1 | C | 1075 | VAL | 2.9 |
| 1 | A | 199 | PHE | 2.8 |
| 1 | D | 1359 | GLU | 2.8 |
| 1 | A | 144 | VAL | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | D | 1360 | TYR | 2.8 |
| 1 | B | 511 | GLY | 2.8 |
| 1 | C | 905 | SER | 2.8 |
| 1 | D | 1370 | MET | 2.7 |
| 1 | B | 675 | VAL | 2.7 |
| 1 | C | 969 | ARG | 2.7 |
| 1 | B | 506 | GLY | 2.7 |
| 1 | B | 582 | SER | 2.7 |
| 1 | C | 999 | PHE | 2.7 |
| 1 | C | 1143 | ILE | 2.7 |
| 1 | A | 110 | LEU | 2.7 |
| 1 | D | 1310 | LEU | 2.7 |
| 1 | B | 660 | TYR | 2.6 |
| 1 | B | 509 | GLU | 2.6 |
| 1 | D | 1319 | GLU | 2.6 |
| 1 | B | 515 | THR | 2.6 |
| 1 | B | 512 | ASP | 2.6 |
| 1 | D | 1320 | GLY | 2.6 |
| 1 | A | 105 | SER | 2.6 |
| 1 | C | 1139 | LEU | 2.5 |
| 1 | D | 1303 | CYS | 2.5 |
| 1 | A | 114 | LYS | 2.5 |
| 1 | C | 827 | ILE | 2.5 |
| 1 | B | 480 | ARG | 2.5 |
| 1 | D | 1362 | GLY | 2.5 |
| 1 | A | 258 | GLY | 2.5 |
| 1 | B | 658 | GLY | 2.5 |
| 1 | C | 973 | GLU | 2.4 |
| 1 | D | 1312 | ASP | 2.4 |
| 1 | D | 1407 | ILE | 2.4 |
| 1 | C | 923 | LEU | 2.4 |
| 1 | B | 501 | LEU | 2.4 |
| 1 | D | 1264 | ALA | 2.4 |
| 1 | B | 680 | LYS | 2.4 |
| 1 | A | 276 | LEU | 2.4 |
| 1 | B | 564 | LEU | 2.4 |
| 1 | C | 805 | LEU | 2.4 |
| 1 | B | 609 | ALA | 2.4 |
| 1 | D | 1317 | GLU | 2.3 |
| 1 | A | 120 | GLY | 2.3 |
| 1 | D | 1304 | GLY | 2.3 |
| 1 | D | 1543 | ILE | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | D | 1464 | VAL | 2.3 |
| 1 | C | 1080 | LYS | 2.3 |
| 1 | B | 735 | VAL | 2.3 |
| 1 | C | 945 | ILE | 2.3 |
| 1 | A | 375 | ILE | 2.2 |
| 1 | B | 522 | SER | 2.2 |
| 1 | B | 628 | THR | 2.2 |
| 1 | D | 1316 | LEU | 2.2 |
| 1 | B | 527 | VAL | 2.2 |
| 1 | A | 160 | TYR | 2.2 |
| 1 | B | 557 | SER | 2.2 |
| 1 | D | 1467 | ALA | 2.1 |
| 1 | C | 912 | ASP | 2.1 |
| 1 | C | 1059 | ASP | 2.1 |
| 1 | D | 1469 | ASP | 2.1 |
| 1 | D | 1375 | ARG | 2.1 |
| 1 | B | 624 | ASN | 2.1 |
| 1 | A | 167 | PHE | 2.1 |
| 1 | A | 122 | SER | 2.0 |
| 1 | D | 1326 | MET | 2.0 |
| 1 | D | 1369 | ARG | 2.0 |
| 1 | A | 162 | GLY | 2.0 |
| 1 | C | 960 | TYR | 2.0 |

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 2 | PO4 | C | 1195 | 5/5 | 0.76 | 0.23 | 2.16 | 16,36,53,92 | 0 |
| 2 | PO4 | D | 1595 | 5/5 | 0.92 | 0.19 | 1.61 | 28,51,72,87 | 0 |
| 4 | NAD | C | 1196 | 44/44 | 0.93 | 0.12 | -0.34 | 18,43,76,109 | 0 |
| 4 | NAD | A | 396 | 44/44 | 0.94 | 0.11 | -0.61 | 26,49,70,80 | 0 |
| 4 | NAD | B | 796 | 44/44 | 0.93 | 0.11 | -0.81 | 22,49,65,96 | 0 |
| 4 | NAD | D | 1596 | 44/44 | 0.94 | 0.10 | -0.82 | 14,45,64,81 | 0 |
| 2 | PO4 | B | 795 | 5/5 | 0.99 | 0.10 | -1.14 | 32,37,61,62 | 0 |
| 3 | K | B | 797 | 1/1 | 0.94 | 0.09 | -1.24 | 67,67,67,67 | 0 |
| 2 | PO4 | A | 395 | 5/5 | 0.98 | 0.07 | -1.49 | 22,27,48,78 | 0 |
| 3 | K | C | 1197 | 1/1 | 0.84 | 0.14 | - | 60,60,60,60 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.