



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 10:54 am BST

PDB ID : 4HNT
Title : crystal structure of F403A mutant of S. aureus Pyruvate carboxylase
Authors : Yu, L.P.C.; Tong, L.
Deposited on : 2012-10-21
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

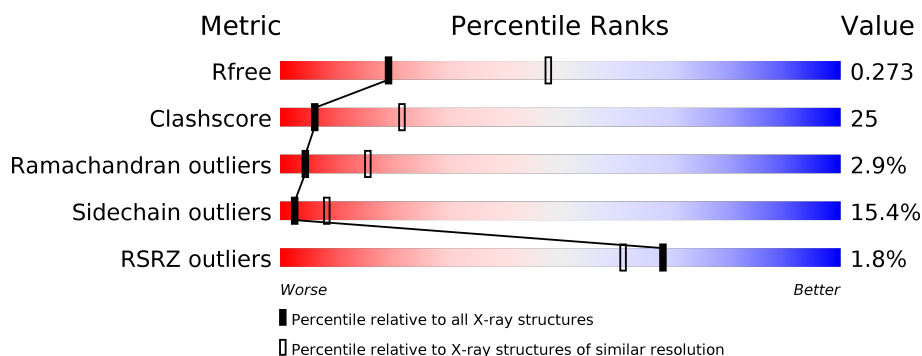
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 3140 (2.80-2.80) |
| Clashscore | 141614 | 3569 (2.80-2.80) |
| Ramachandran outliers | 138981 | 3498 (2.80-2.80) |
| Sidechain outliers | 138945 | 3500 (2.80-2.80) |
| RSRZ outliers | 127900 | 3078 (2.80-2.80) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 1173 | <div> <div>2%</div> <div> <div></div> <div>50%</div> <div>32%</div> <div>8%</div> <div>10%</div> </div> </div> |
| 1 | B | 1173 | <div> <div>2%</div> <div> <div></div> <div>47%</div> <div>30%</div> <div>6%</div> <div>16%</div> </div> </div> |
| 1 | C | 1173 | <div> <div>2%</div> <div> <div></div> <div>46%</div> <div>35%</div> <div>9%</div> <div>10%</div> </div> </div> |
| 1 | D | 1173 | <div> <div>%</div> <div> <div></div> <div>48%</div> <div>28%</div> <div>8%</div> <div>16%</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 crite-

ria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 5 | ATP | C | 1202 | - | - | X | - |

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32480 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 Pyruvate carboxylase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1 | A | 1052 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 8336 | 5286 | 1404 | 1619 | 27 | | | |
| 1 | B | 989 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 7832 | 4969 | 1321 | 1516 | 26 | | | |
| 1 | C | 1059 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 8373 | 5307 | 1412 | 1626 | 28 | | | |
| 1 | D | 989 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 7832 | 4969 | 1321 | 1516 | 26 | | | |

There are 92 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | 11 | MET | - | EXPRESSION TAG | UNP Q99UY8 |
| A | 12 | GLY | - | EXPRESSION TAG | UNP Q99UY8 |
| A | 13 | SER | - | EXPRESSION TAG | UNP Q99UY8 |
| A | 14 | SER | - | EXPRESSION TAG | UNP Q99UY8 |
| A | 15 | HIS | - | EXPRESSION TAG | UNP Q99UY8 |
| A | 16 | HIS | - | EXPRESSION TAG | UNP Q99UY8 |
| A | 17 | HIS | - | EXPRESSION TAG | UNP Q99UY8 |
| A | 18 | HIS | - | EXPRESSION TAG | UNP Q99UY8 |
| A | 19 | HIS | - | EXPRESSION TAG | UNP Q99UY8 |
| A | 20 | HIS | - | EXPRESSION TAG | UNP Q99UY8 |
| A | 21 | SER | - | EXPRESSION TAG | UNP Q99UY8 |
| A | 22 | SER | - | EXPRESSION TAG | UNP Q99UY8 |
| A | 23 | GLY | - | EXPRESSION TAG | UNP Q99UY8 |
| A | 24 | LEU | - | EXPRESSION TAG | UNP Q99UY8 |
| A | 25 | VAL | - | EXPRESSION TAG | UNP Q99UY8 |
| A | 26 | PRO | - | EXPRESSION TAG | UNP Q99UY8 |
| A | 27 | ARG | - | EXPRESSION TAG | UNP Q99UY8 |
| A | 28 | GLY | - | EXPRESSION TAG | UNP Q99UY8 |
| A | 29 | SER | - | EXPRESSION TAG | UNP Q99UY8 |
| A | 30 | HIS | - | EXPRESSION TAG | UNP Q99UY8 |
| A | 31 | MET | - | EXPRESSION TAG | UNP Q99UY8 |

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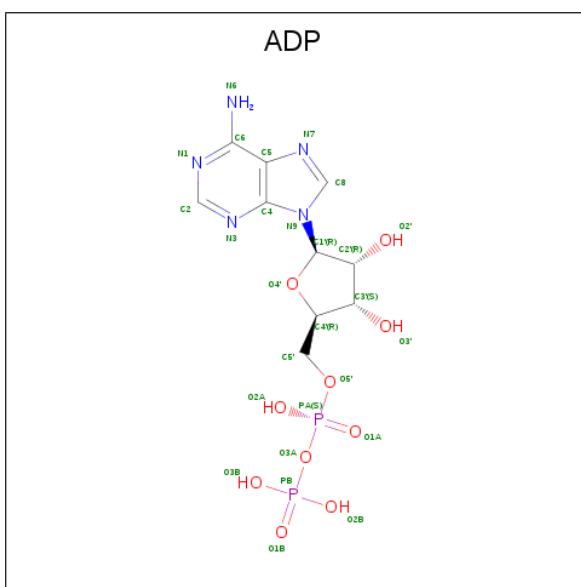
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | 32 | ALA | - | EXPRESSION TAG | UNP Q99UY8 |
| A | 33 | SER | - | EXPRESSION TAG | UNP Q99UY8 |
| B | 11 | MET | - | EXPRESSION TAG | UNP Q99UY8 |
| B | 12 | GLY | - | EXPRESSION TAG | UNP Q99UY8 |
| B | 13 | SER | - | EXPRESSION TAG | UNP Q99UY8 |
| B | 14 | SER | - | EXPRESSION TAG | UNP Q99UY8 |
| B | 15 | HIS | - | EXPRESSION TAG | UNP Q99UY8 |
| B | 16 | HIS | - | EXPRESSION TAG | UNP Q99UY8 |
| B | 17 | HIS | - | EXPRESSION TAG | UNP Q99UY8 |
| B | 18 | HIS | - | EXPRESSION TAG | UNP Q99UY8 |
| B | 19 | HIS | - | EXPRESSION TAG | UNP Q99UY8 |
| B | 20 | HIS | - | EXPRESSION TAG | UNP Q99UY8 |
| B | 21 | SER | - | EXPRESSION TAG | UNP Q99UY8 |
| B | 22 | SER | - | EXPRESSION TAG | UNP Q99UY8 |
| B | 23 | GLY | - | EXPRESSION TAG | UNP Q99UY8 |
| B | 24 | LEU | - | EXPRESSION TAG | UNP Q99UY8 |
| B | 25 | VAL | - | EXPRESSION TAG | UNP Q99UY8 |
| B | 26 | PRO | - | EXPRESSION TAG | UNP Q99UY8 |
| B | 27 | ARG | - | EXPRESSION TAG | UNP Q99UY8 |
| B | 28 | GLY | - | EXPRESSION TAG | UNP Q99UY8 |
| B | 29 | SER | - | EXPRESSION TAG | UNP Q99UY8 |
| B | 30 | HIS | - | EXPRESSION TAG | UNP Q99UY8 |
| B | 31 | MET | - | EXPRESSION TAG | UNP Q99UY8 |
| B | 32 | ALA | - | EXPRESSION TAG | UNP Q99UY8 |
| B | 33 | SER | - | EXPRESSION TAG | UNP Q99UY8 |
| C | 11 | MET | - | EXPRESSION TAG | UNP Q99UY8 |
| C | 12 | GLY | - | EXPRESSION TAG | UNP Q99UY8 |
| C | 13 | SER | - | EXPRESSION TAG | UNP Q99UY8 |
| C | 14 | SER | - | EXPRESSION TAG | UNP Q99UY8 |
| C | 15 | HIS | - | EXPRESSION TAG | UNP Q99UY8 |
| C | 16 | HIS | - | EXPRESSION TAG | UNP Q99UY8 |
| C | 17 | HIS | - | EXPRESSION TAG | UNP Q99UY8 |
| C | 18 | HIS | - | EXPRESSION TAG | UNP Q99UY8 |
| C | 19 | HIS | - | EXPRESSION TAG | UNP Q99UY8 |
| C | 20 | HIS | - | EXPRESSION TAG | UNP Q99UY8 |
| C | 21 | SER | - | EXPRESSION TAG | UNP Q99UY8 |
| C | 22 | SER | - | EXPRESSION TAG | UNP Q99UY8 |
| C | 23 | GLY | - | EXPRESSION TAG | UNP Q99UY8 |
| C | 24 | LEU | - | EXPRESSION TAG | UNP Q99UY8 |
| C | 25 | VAL | - | EXPRESSION TAG | UNP Q99UY8 |
| C | 26 | PRO | - | EXPRESSION TAG | UNP Q99UY8 |
| C | 27 | ARG | - | EXPRESSION TAG | UNP Q99UY8 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| C | 28 | GLY | - | EXPRESSION TAG | UNP Q99UY8 |
| C | 29 | SER | - | EXPRESSION TAG | UNP Q99UY8 |
| C | 30 | HIS | - | EXPRESSION TAG | UNP Q99UY8 |
| C | 31 | MET | - | EXPRESSION TAG | UNP Q99UY8 |
| C | 32 | ALA | - | EXPRESSION TAG | UNP Q99UY8 |
| C | 33 | SER | - | EXPRESSION TAG | UNP Q99UY8 |
| D | 11 | MET | - | EXPRESSION TAG | UNP Q99UY8 |
| D | 12 | GLY | - | EXPRESSION TAG | UNP Q99UY8 |
| D | 13 | SER | - | EXPRESSION TAG | UNP Q99UY8 |
| D | 14 | SER | - | EXPRESSION TAG | UNP Q99UY8 |
| D | 15 | HIS | - | EXPRESSION TAG | UNP Q99UY8 |
| D | 16 | HIS | - | EXPRESSION TAG | UNP Q99UY8 |
| D | 17 | HIS | - | EXPRESSION TAG | UNP Q99UY8 |
| D | 18 | HIS | - | EXPRESSION TAG | UNP Q99UY8 |
| D | 19 | HIS | - | EXPRESSION TAG | UNP Q99UY8 |
| D | 20 | HIS | - | EXPRESSION TAG | UNP Q99UY8 |
| D | 21 | SER | - | EXPRESSION TAG | UNP Q99UY8 |
| D | 22 | SER | - | EXPRESSION TAG | UNP Q99UY8 |
| D | 23 | GLY | - | EXPRESSION TAG | UNP Q99UY8 |
| D | 24 | LEU | - | EXPRESSION TAG | UNP Q99UY8 |
| D | 25 | VAL | - | EXPRESSION TAG | UNP Q99UY8 |
| D | 26 | PRO | - | EXPRESSION TAG | UNP Q99UY8 |
| D | 27 | ARG | - | EXPRESSION TAG | UNP Q99UY8 |
| D | 28 | GLY | - | EXPRESSION TAG | UNP Q99UY8 |
| D | 29 | SER | - | EXPRESSION TAG | UNP Q99UY8 |
| D | 30 | HIS | - | EXPRESSION TAG | UNP Q99UY8 |
| D | 31 | MET | - | EXPRESSION TAG | UNP Q99UY8 |
| D | 32 | ALA | - | EXPRESSION TAG | UNP Q99UY8 |
| D | 33 | SER | - | EXPRESSION TAG | UNP Q99UY8 |

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

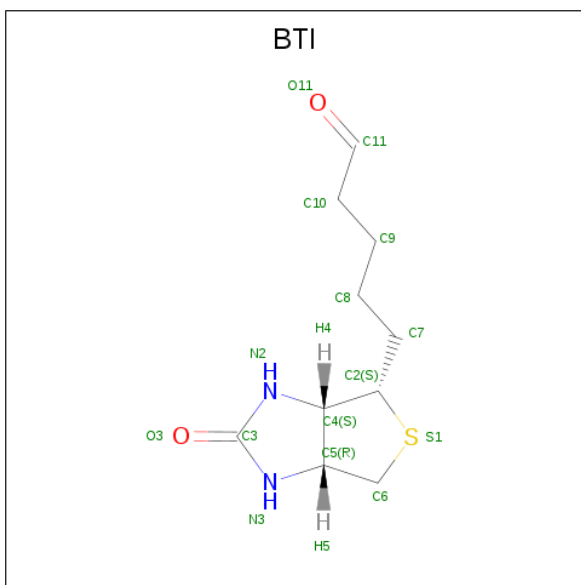


| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 2 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

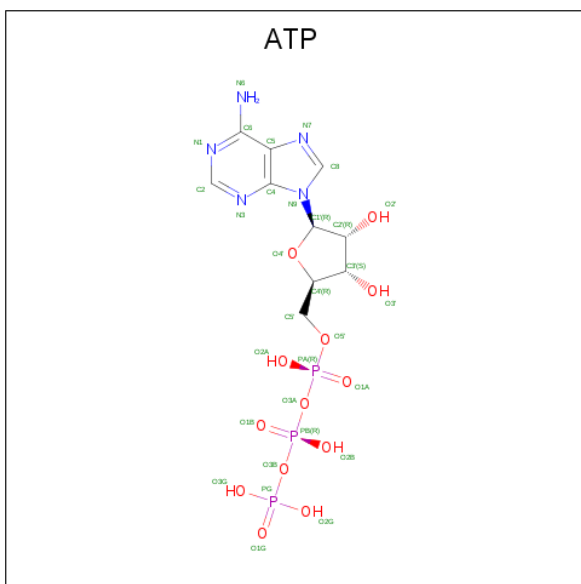
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3 | B | 1 | Total | Mn | 0 | 0 |
| | | | 1 | 1 | | |
| 3 | A | 1 | Total | Mn | 0 | 0 |
| | | | 1 | 1 | | |
| 3 | D | 1 | Total | Mn | 0 | 0 |
| | | | 1 | 1 | | |
| 3 | C | 1 | Total | Mn | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 4 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (three-letter code: BTI) (formula: C₁₀H₁₆N₂O₂S).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|--------|---------|---------|
| 4 | A | 1 | Total 15 | C 10 | N 2 | O 2 | S 1 | 0 | 0 |
| 4 | B | 1 | Total 15 | C 10 | N 2 | O 2 | S 1 | 0 | 0 |
| 4 | D | 1 | Total 15 | C 10 | N 2 | O 2 | S 1 | 0 | 0 |

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$).

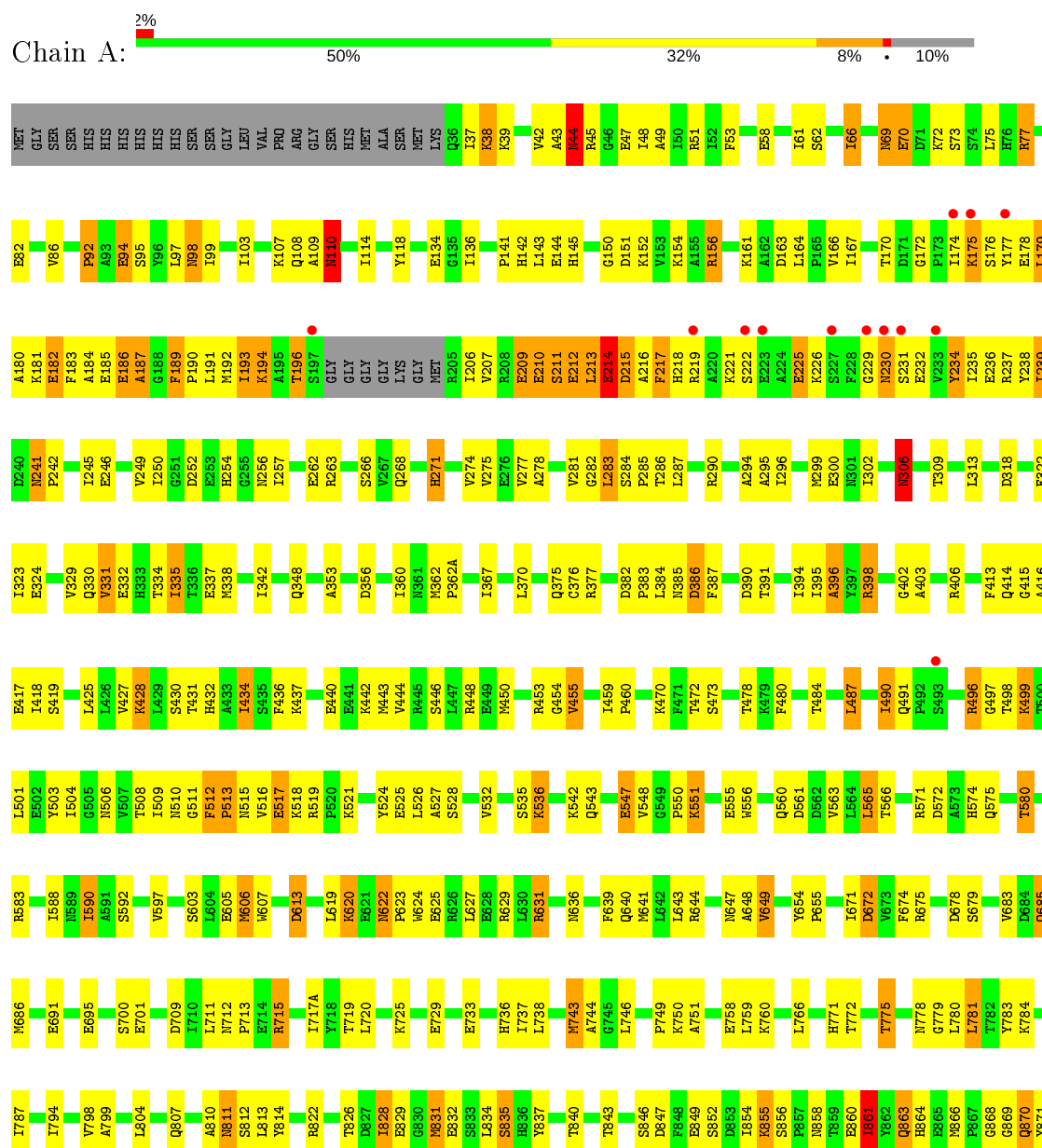


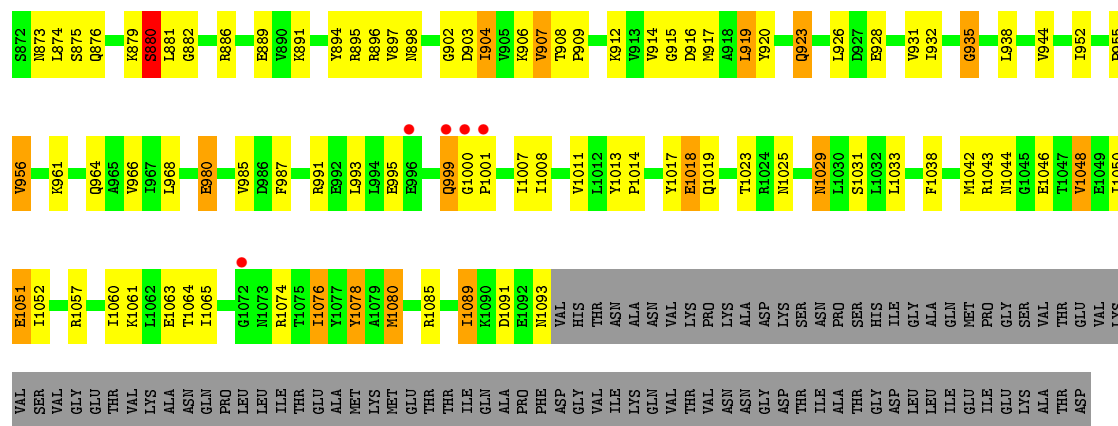
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 5 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 31 | 10 | 5 | 13 | 3 | | |

3 Residue-property plots

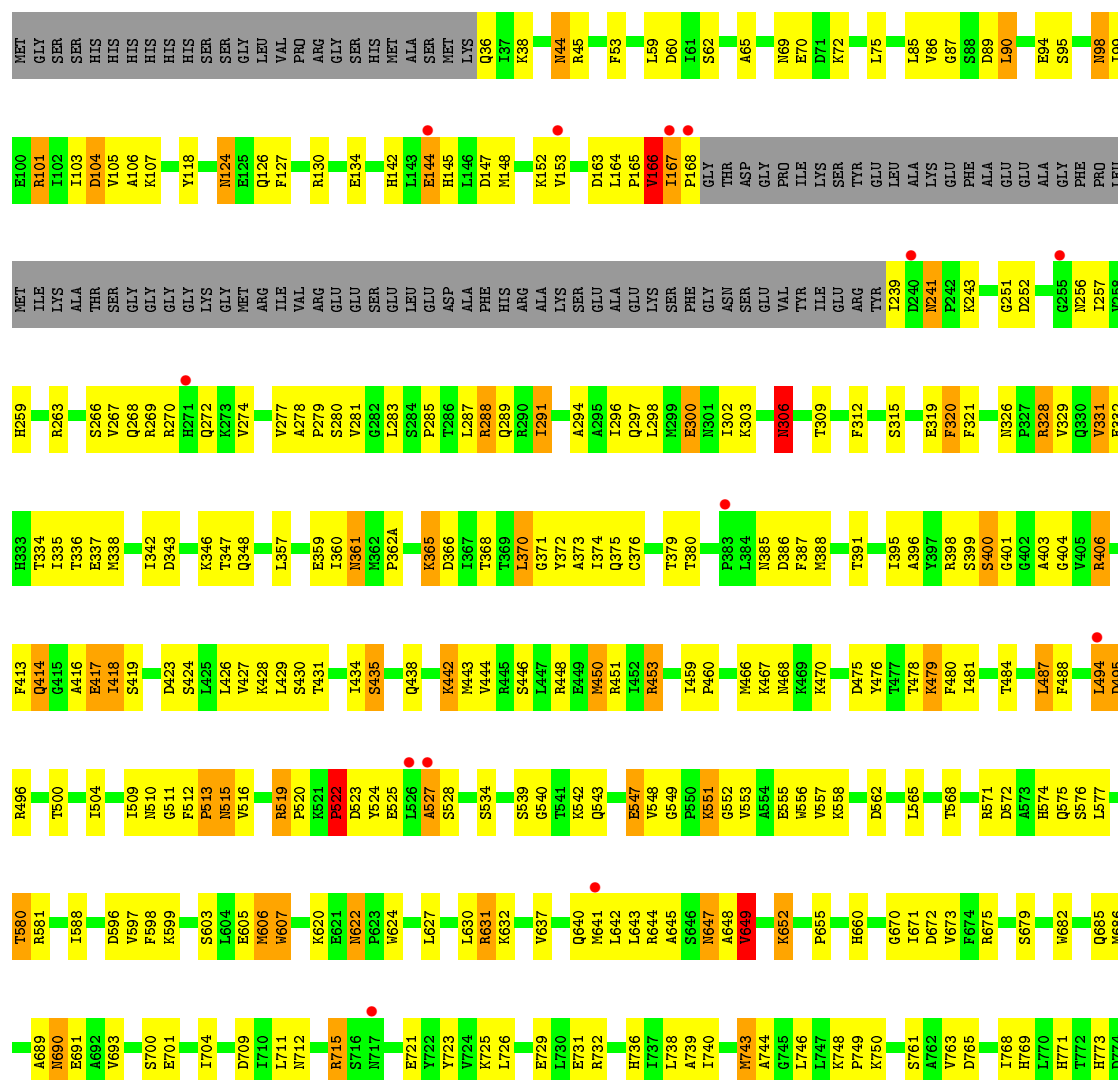
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

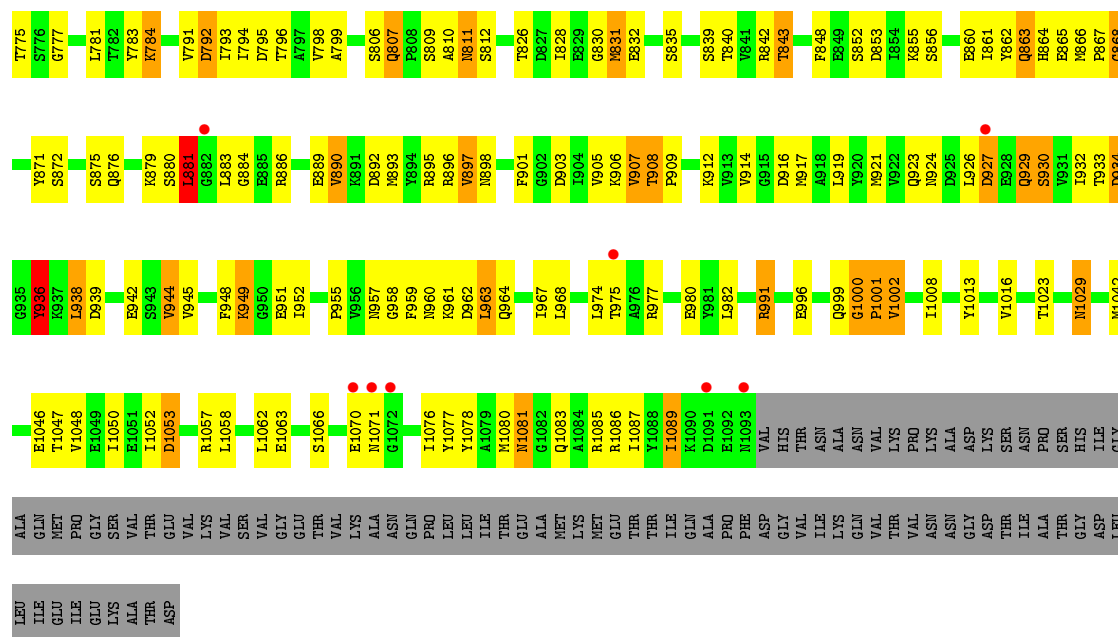
• Molecule 1: Pyruvate carboxylase



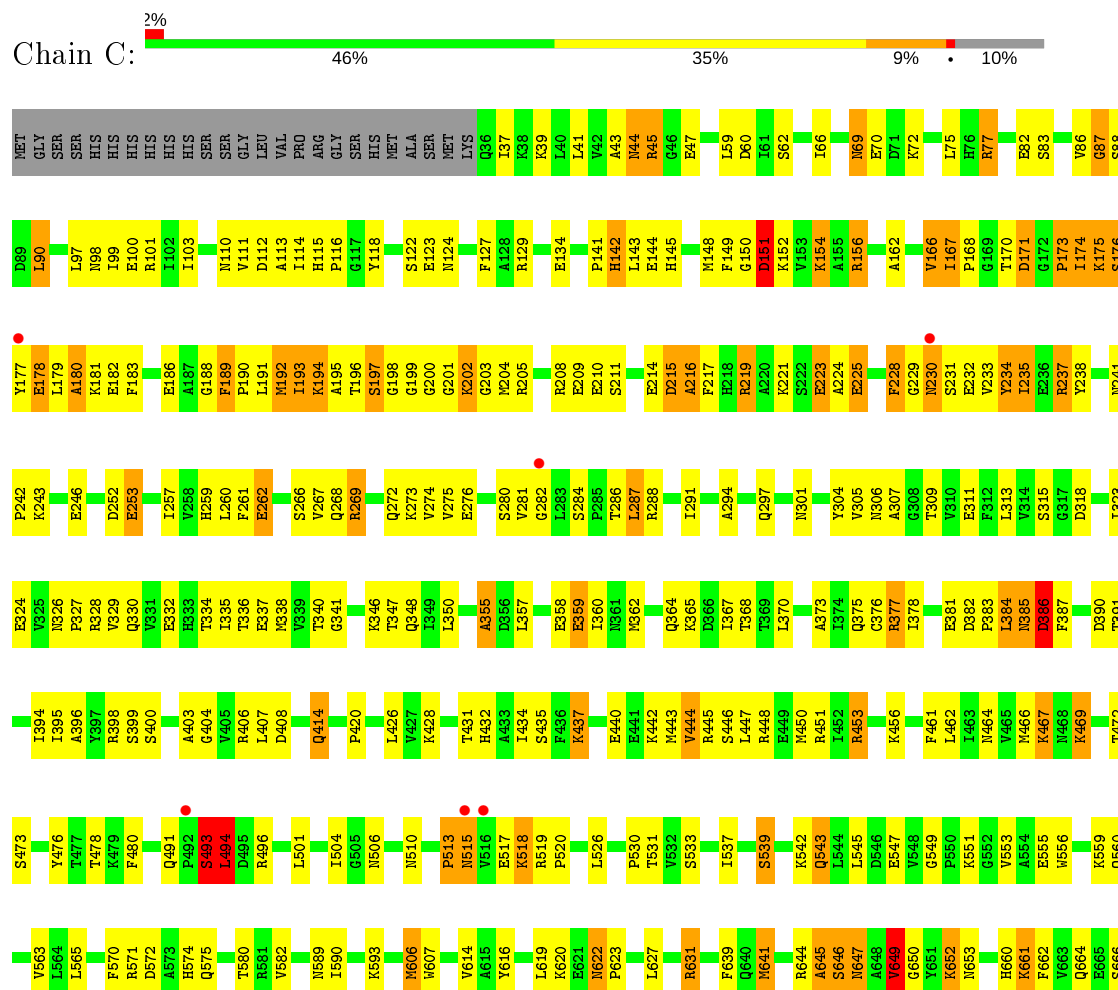


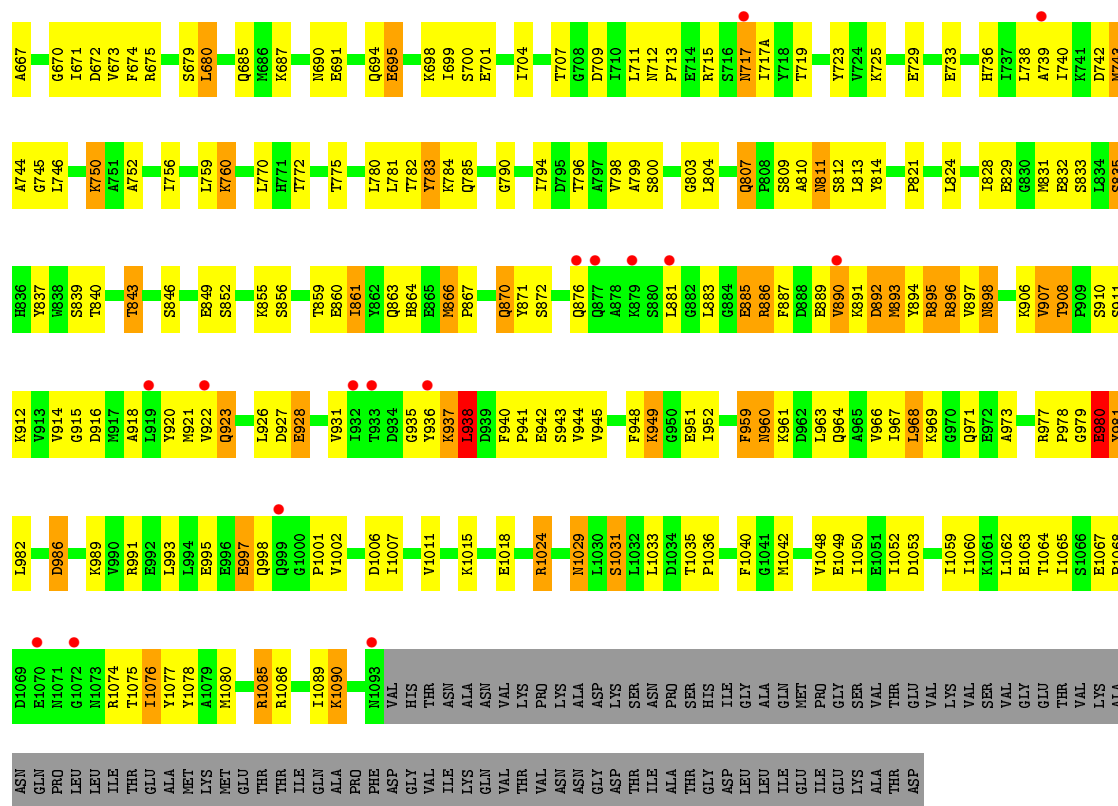
• Molecule 1: Pyruvate carboxylase



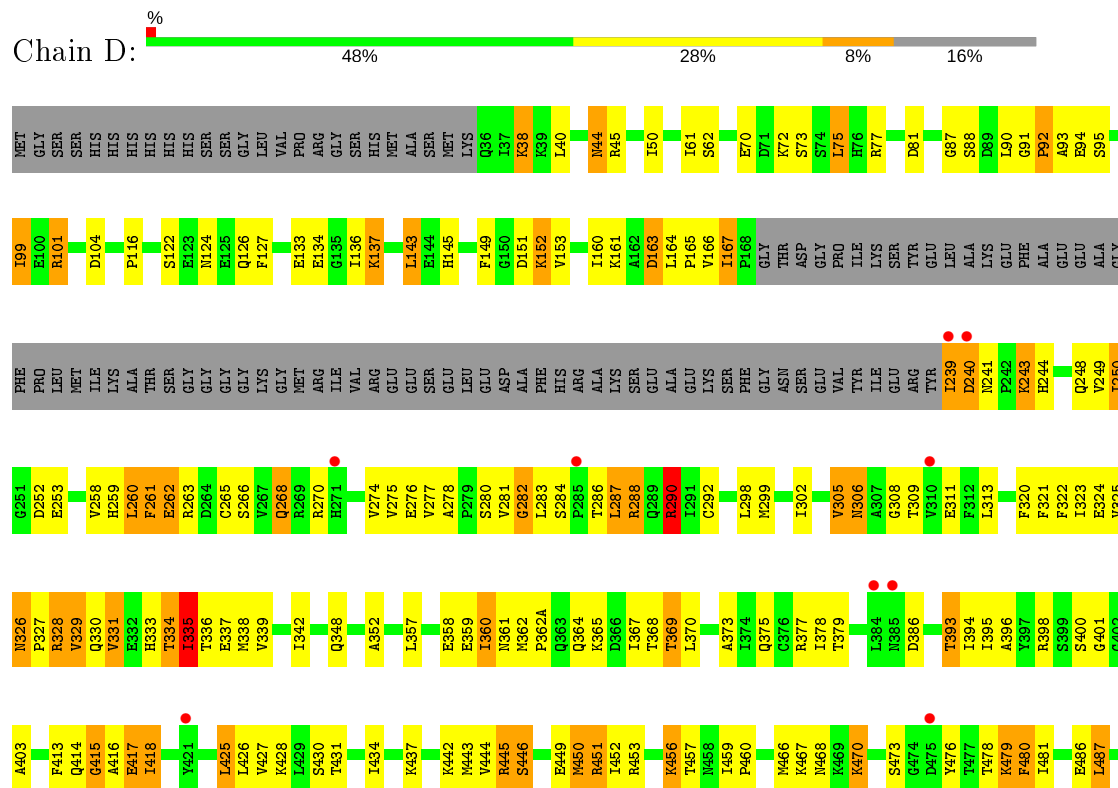


• Molecule 1: Pyruvate carboxylase





- Molecule 1: Pyruvate carboxylase



| | | | | | | | |
|-----|-------|-------|------|------|-------|------|------|
| VAL | R1057 | D939 | H864 | S776 | M690 | Q575 | I490 |
| GLY | I1060 | F940 | E865 | T782 | M690 | T580 | Q491 |
| GLU | I1061 | V944 | M866 | Y783 | Q694 | R581 | P492 |
| THR | K1061 | V945 | G869 | Y784 | K698 | V582 | S493 |
| VAL | L1062 | I952 | Q870 | Q785 | L699 | L494 | L494 |
| LYS | E1063 | I952 | Y871 | A786 | S700 | D495 | D495 |
| ALA | T1064 | I952 | Y871 | I787 | E701 | R496 | R496 |
| ASN | D1069 | N957 | L874 | V791 | T703 | Q497 | Q497 |
| GLN | E1070 | N960 | S875 | I796 | T707 | T498 | T498 |
| PRO | N1071 | N960 | S875 | I796 | T707 | K499 | K499 |
| LEU | G1072 | N960 | S875 | I796 | T707 | T500 | T500 |
| LEU | N1073 | N960 | S875 | I796 | T707 | L501 | L501 |
| ILE | N1073 | N960 | S875 | I796 | T707 | I504 | I504 |
| THR | Y1078 | N966 | S880 | A799 | L711 | G505 | G505 |
| GLU | A1079 | I967 | G881 | S800 | L711 | N506 | N506 |
| ALA | M1080 | I974 | L883 | L804 | E714 | N510 | N510 |
| LYS | L974 | I974 | G884 | L804 | E714 | G511 | G511 |
| MET | Q1083 | R977 | E885 | Q807 | S716 | F512 | F512 |
| GLU | A1084 | F978 | R886 | A810 | N717 | P513 | P513 |
| THR | R1085 | F978 | R887 | N811 | I717A | R515 | R515 |
| THR | R1086 | Y981 | D888 | N811 | I717A | V516 | V516 |
| ILE | I1087 | Y981 | D888 | N811 | L720 | E517 | E517 |
| GLN | Y1088 | D886 | K891 | Y814 | L720 | K518 | K518 |
| ALA | I1089 | F987 | D892 | Y815 | K725 | R519 | R519 |
| PRO | N1093 | E988 | M893 | A816 | L730 | P520 | P520 |
| ASP | VAL | R991 | R896 | L817 | L730 | D523 | D523 |
| GLY | HIS | R991 | R896 | L817 | L730 | Y524 | Y524 |
| THR | THR | R991 | N898 | F820 | F735 | E525 | E525 |
| ILE | ASN | R991 | N898 | F820 | H736 | L526 | L526 |
| LYS | ALA | R991 | F899 | R822 | I737 | A527 | A527 |
| GLN | ASN | R991 | L900 | I828 | L738 | S528 | S528 |
| VAL | VAL | E1004 | F901 | E829 | I740 | I529 | I529 |
| THR | LYS | E1004 | I904 | G830 | K741 | P530 | P530 |
| VAL | PRO | I1008 | I904 | M831 | D742 | T531 | T531 |
| ASN | LYS | I1008 | I904 | E832 | M743 | V532 | V532 |
| ASN | ALA | Y1013 | V907 | E832 | A744 | S533 | S533 |
| GLY | ASP | P1014 | T908 | H836 | L746 | G540 | G540 |
| ASP | LYS | K1015 | P909 | S839 | A752 | T541 | T541 |
| THR | SER | V1016 | S910 | S839 | A752 | K542 | K542 |
| ILE | ASN | T1023 | S911 | T840 | A752 | Q543 | Q543 |
| ALA | PRO | T1023 | M917 | T843 | I756 | R551 | R551 |
| THR | SER | T1023 | A818 | Y844 | G757 | E555 | E555 |
| GLY | HIS | D1034 | L919 | Y844 | G757 | D561 | D561 |
| ASP | ILE | T1035 | Y920 | Y845 | E758 | D562 | D562 |
| LEU | GLY | P1036 | M921 | Y845 | L759 | V563 | V563 |
| LEU | ALA | P1036 | M921 | Y845 | L759 | L564 | L564 |
| ILE | GLN | M1042 | N924 | F848 | K760 | L565 | L565 |
| GLU | MET | R1043 | D925 | E849 | V763 | F570 | F570 |
| ILE | PRO | N1044 | D925 | S852 | D765 | R571 | R571 |
| GLY | GLY | G1045 | L926 | D853 | L766 | D572 | D572 |
| LYS | SER | E1046 | D927 | I854 | P767 | A573 | A573 |
| ALA | VAL | T1047 | E928 | K855 | I671 | H574 | H574 |
| THR | THR | T1047 | Q929 | S856 | D672 | | |
| ASP | GLU | I1052 | S930 | P857 | H769 | | |
| | VAL | D1053 | V931 | E860 | L770 | | |
| | LYS | G1054 | G935 | I861 | H771 | | |
| | VAL | G1055 | G935 | Y862 | I772 | | |
| | SER | K1056 | L938 | Q863 | T775 | | |

4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 96.23 Å 256.28 Å 126.69 Å 90.00° 109.86° 90.00° | Depositor |
| Resolution (Å) | 30.00 – 2.80 29.79 – 2.80 | Depositor EDS |
| % Data completeness (in resolution range) | 91.0 (30.00-2.80) 91.0 (29.79-2.80) | Depositor EDS |
| R_{merge} | 0.09 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 3.17 (at 2.80 Å) | Xtriage |
| Refinement program | REFMAC 5.5.0102, CNS | Depositor |
| R, R_{free} | 0.209 , 0.279 0.207 , 0.273 | Depositor DCC |
| R_{free} test set | 6458 reflections (5.03%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 72.2 | Xtriage |
| Anisotropy | 0.060 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.31 , 48.8 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$ | Xtriage |
| Estimated twinning fraction | 0.030 for h,-k,-h-l | Xtriage |
| F_o, F_c correlation | 0.93 | EDS |
| Total number of atoms | 32480 | wwPDB-VP |
| Average B, all atoms (Å ²) | 84.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, BTI, ATP, ADP

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 | 0.68 | 1/8497 (0.0%) | 0.73 | 1/11490 (0.0%) |
| 1 | B | 0.63 | 4/7983 (0.1%) | 0.66 | 3/10801 (0.0%) |
| 1 | C | 0.65 | 4/8535 (0.0%) | 0.68 | 4/11539 (0.0%) |
| 1 | D | 0.66 | 5/7983 (0.1%) | 0.70 | 2/10801 (0.0%) |
| All | All | 0.65 | 14/32998 (0.0%) | 0.69 | 10/44631 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 6 |
| 1 | B | 0 | 3 |
| 1 | C | 0 | 7 |
| 1 | D | 0 | 2 |
| All | All | 0 | 18 |

All (14) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | C | 513 | PRO | CA-C | 14.00 | 1.80 | 1.52 |
| 1 | B | 936 | TYR | C-N | 11.65 | 1.60 | 1.34 |
| 1 | C | 513 | PRO | C-N | 10.85 | 1.58 | 1.34 |
| 1 | C | 515 | ASN | N-CA | 10.62 | 1.67 | 1.46 |
| 1 | B | 961 | LYS | C-O | 10.00 | 1.42 | 1.23 |
| 1 | C | 513 | PRO | N-CA | 8.86 | 1.62 | 1.47 |
| 1 | D | 290 | ARG | CZ-NH1 | 8.75 | 1.44 | 1.33 |
| 1 | A | 513 | PRO | CA-C | 8.56 | 1.70 | 1.52 |
| 1 | D | 513 | PRO | CA-C | 7.66 | 1.68 | 1.52 |
| 1 | D | 515 | ASN | N-CA | 7.36 | 1.61 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1 | B | 513 | PRO | CA-C | 7.18 | 1.67 | 1.52 |
| 1 | D | 513 | PRO | C-N | 6.20 | 1.48 | 1.34 |
| 1 | D | 513 | PRO | N-CA | 5.96 | 1.57 | 1.47 |
| 1 | B | 763 | VAL | N-CA | 5.78 | 1.57 | 1.46 |

All (10) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | C | 513 | PRO | C-N-CA | 8.07 | 141.87 | 121.70 |
| 1 | D | 513 | PRO | CA-C-N | 7.87 | 134.51 | 117.20 |
| 1 | C | 513 | PRO | CA-C-N | 7.83 | 134.42 | 117.20 |
| 1 | B | 763 | VAL | CA-C-N | 7.35 | 133.38 | 117.20 |
| 1 | C | 513 | PRO | N-CA-CB | -6.11 | 95.88 | 102.60 |
| 1 | A | 513 | PRO | CA-C-N | 6.09 | 130.60 | 117.20 |
| 1 | B | 763 | VAL | O-C-N | -5.91 | 113.25 | 122.70 |
| 1 | B | 513 | PRO | CA-C-N | 5.68 | 129.69 | 117.20 |
| 1 | C | 513 | PRO | O-C-N | -5.66 | 113.64 | 122.70 |
| 1 | D | 513 | PRO | O-C-N | -5.57 | 113.78 | 122.70 |

There are no chirality outliers.

All (18) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 1 | A | 1078 | TYR | Peptide |
| 1 | A | 150 | GLY | Peptide |
| 1 | A | 196 | THR | Peptide |
| 1 | A | 271 | HIS | Peptide |
| 1 | A | 415 | GLY | Peptide |
| 1 | A | 490 | ILE | Peptide |
| 1 | B | 522 | PRO | Peptide |
| 1 | B | 524 | TYR | Peptide |
| 1 | B | 936 | TYR | Sidechain |
| 1 | C | 150 | GLY | Peptide |
| 1 | C | 211 | SER | Peptide |
| 1 | C | 228 | PHE | Peptide |
| 1 | C | 262 | GLU | Peptide |
| 1 | C | 420 | PRO | Peptide |
| 1 | C | 493 | SER | Peptide |
| 1 | C | 494 | LEU | Peptide |
| 1 | D | 415 | GLY | Peptide |
| 1 | D | 416 | ALA | Peptide |

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 8336 | 0 | 8249 | 430 | 0 |
| 1 | B | 7832 | 0 | 7767 | 352 | 0 |
| 1 | C | 8373 | 0 | 8287 | 456 | 0 |
| 1 | D | 7832 | 0 | 7767 | 376 | 0 |
| 2 | A | 27 | 0 | 12 | 1 | 0 |
| 3 | A | 1 | 0 | 0 | 0 | 0 |
| 3 | B | 1 | 0 | 0 | 0 | 0 |
| 3 | C | 1 | 0 | 0 | 0 | 0 |
| 3 | D | 1 | 0 | 0 | 0 | 0 |
| 4 | A | 15 | 0 | 16 | 4 | 0 |
| 4 | B | 15 | 0 | 16 | 4 | 0 |
| 4 | D | 15 | 0 | 16 | 3 | 0 |
| 5 | C | 31 | 0 | 12 | 10 | 0 |
| All | All | 32480 | 0 | 32142 | 1586 | 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 25.

All (1586) 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:515:ASN:N | 1:C:515:ASN:CA | 1.67 | 1.56 |
| 1:C:513:PRO:CA | 1:C:513:PRO:C | 1.80 | 1.47 |
| 1:D:607:TRP:HE3 | 1:D:641:MET:CE | 1.51 | 1.23 |
| 1:C:918:ALA:O | 1:C:922:VAL:HG23 | 1.39 | 1.22 |
| 1:B:403:ALA:O | 1:B:442:LYS:HE2 | 1.42 | 1.18 |
| 1:C:334:THR:HB | 1:C:406:ARG:NH1 | 1.59 | 1.17 |
| 1:A:334:THR:HG22 | 1:A:406:ARG:HH12 | 1.06 | 1.16 |
| 1:C:893:MET:HA | 1:C:896:ARG:CD | 1.74 | 1.16 |
| 1:A:413:PHE:CZ | 1:A:416:ALA:HB2 | 1.82 | 1.14 |
| 1:C:1024:ARG:HG2 | 1:C:1024:ARG:HH11 | 1.02 | 1.14 |
| 1:B:288:ARG:HH11 | 1:B:288:ARG:HG3 | 1.00 | 1.12 |
| 1:C:396:ALA:HB3 | 1:C:453:ARG:HG3 | 1.27 | 1.11 |
| 1:D:607:TRP:CE3 | 1:D:641:MET:HE1 | 1.86 | 1.10 |
| 1:D:504:ILE:HG21 | 1:D:1042:MET:HE2 | 1.28 | 1.10 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:C:940:PHE:HB3 | 1:C:941:PRO:HD2 | 1.33 | 1.09 |
| 1:C:936:TYR:O | 1:C:937:LYS:HG3 | 1.52 | 1.09 |
| 1:B:1042:MET:HE3 | 1:B:1062:LEU:HB2 | 1.23 | 1.08 |
| 1:A:935:GLY:HA3 | 1:A:966:VAL:CG1 | 1.84 | 1.08 |
| 1:B:259:HIS:CD2 | 1:B:296:ILE:HD11 | 1.89 | 1.08 |
| 1:A:213:LEU:O | 1:A:215:ASP:N | 1.87 | 1.07 |
| 1:A:334:THR:CG2 | 1:A:406:ARG:HH12 | 1.68 | 1.06 |
| 1:C:504:ILE:HG21 | 1:C:1042:MET:HE2 | 1.36 | 1.06 |
| 1:D:268:GLN:O | 1:D:481:ILE:HD12 | 1.55 | 1.06 |
| 1:D:607:TRP:HE3 | 1:D:641:MET:HE1 | 1.17 | 1.05 |
| 1:C:1085:ARG:HH11 | 1:C:1085:ARG:HG2 | 1.17 | 1.05 |
| 1:C:1029:ASN:HD21 | 1:C:1031:SER:HB2 | 1.16 | 1.05 |
| 1:D:607:TRP:CE3 | 1:D:641:MET:CE | 2.40 | 1.05 |
| 1:C:167:ILE:HD12 | 1:C:167:ILE:H | 1.23 | 1.03 |
| 1:A:189:PHE:HB3 | 1:A:190:PRO:HD3 | 1.41 | 1.03 |
| 1:B:991:ARG:NH1 | 1:B:1002:VAL:O | 1.92 | 1.03 |
| 1:C:377:ARG:HH11 | 1:C:377:ARG:CG | 1.71 | 1.03 |
| 1:C:192:MET:HE1 | 5:C:1202:ATP:C5 | 1.95 | 1.02 |
| 1:C:940:PHE:CB | 1:C:944:VAL:HG11 | 1.92 | 1.00 |
| 1:C:893:MET:HA | 1:C:896:ARG:HD3 | 1.00 | 1.00 |
| 1:B:338:MET:CE | 1:B:430:SER:HB3 | 1.92 | 0.99 |
| 1:C:377:ARG:HG2 | 1:C:377:ARG:HH11 | 0.85 | 0.99 |
| 1:C:977:ARG:NH1 | 1:C:980:GLU:OE1 | 1.94 | 0.99 |
| 1:C:811:ASN:H | 1:C:811:ASN:HD22 | 1.10 | 0.99 |
| 1:C:170:THR:HG22 | 1:C:171:ASP:H | 1.27 | 0.98 |
| 1:D:496:ARG:HH11 | 1:D:496:ARG:HB3 | 1.26 | 0.98 |
| 1:A:935:GLY:HA3 | 1:A:966:VAL:HG11 | 1.45 | 0.98 |
| 1:A:334:THR:CG2 | 1:A:406:ARG:NH1 | 2.26 | 0.97 |
| 1:B:700:SER:H | 1:B:736:HIS:HD2 | 1.09 | 0.97 |
| 1:C:1085:ARG:HH11 | 1:C:1085:ARG:CG | 1.78 | 0.97 |
| 1:D:451:ARG:HG3 | 1:D:451:ARG:HH11 | 1.28 | 0.97 |
| 1:C:175:LYS:O | 1:C:176:SER:O | 1.83 | 0.97 |
| 1:C:377:ARG:HG2 | 1:C:377:ARG:NH1 | 1.68 | 0.97 |
| 1:B:338:MET:HE2 | 1:B:430:SER:HB3 | 1.47 | 0.97 |
| 1:A:179:LEU:H | 1:A:179:LEU:HD23 | 1.26 | 0.96 |
| 1:C:44:ASN:HD22 | 1:C:45:ARG:H | 0.96 | 0.96 |
| 1:A:156:ARG:HH11 | 1:A:156:ARG:HB3 | 1.31 | 0.95 |
| 1:D:357:LEU:O | 1:D:362:MET:HB2 | 1.66 | 0.95 |
| 1:D:44:ASN:HD22 | 1:D:45:ARG:H | 1.15 | 0.95 |
| 1:B:44:ASN:HD22 | 1:B:45:ARG:N | 1.65 | 0.94 |
| 1:C:1085:ARG:NH1 | 1:C:1085:ARG:HG2 | 1.72 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:143:LEU:H | 1:D:143:LEU:CD1 | 1.81 | 0.94 |
| 1:A:864:HIS:CD2 | 1:A:866:MET:HG3 | 2.03 | 0.93 |
| 1:B:44:ASN:ND2 | 1:B:45:ARG:H | 1.65 | 0.93 |
| 1:C:396:ALA:HA | 1:C:414:GLN:HE22 | 1.31 | 0.93 |
| 1:C:893:MET:CA | 1:C:896:ARG:HD3 | 1.95 | 0.93 |
| 1:C:895:ARG:HH11 | 1:C:895:ARG:CG | 1.82 | 0.93 |
| 1:C:334:THR:CB | 1:C:406:ARG:NH1 | 2.32 | 0.92 |
| 1:C:175:LYS:H | 1:C:175:LYS:CD | 1.82 | 0.92 |
| 1:C:1024:ARG:HH11 | 1:C:1024:ARG:CG | 1.82 | 0.92 |
| 1:C:334:THR:HB | 1:C:406:ARG:HH11 | 1.31 | 0.92 |
| 1:D:540:GLY:H | 1:D:543:GLN:HE21 | 1.08 | 0.91 |
| 1:C:940:PHE:HB2 | 1:C:944:VAL:CG1 | 2.00 | 0.91 |
| 1:B:945:VAL:HG12 | 1:B:967:ILE:HG23 | 1.52 | 0.91 |
| 1:B:44:ASN:HD22 | 1:B:45:ARG:H | 0.92 | 0.91 |
| 1:D:166:VAL:HG12 | 1:D:167:ILE:H | 1.34 | 0.91 |
| 1:D:38:LYS:HE2 | 1:D:38:LYS:HA | 1.51 | 0.90 |
| 1:D:494:LEU:HG | 1:D:499:LYS:HE2 | 1.51 | 0.90 |
| 1:C:700:SER:H | 1:C:736:HIS:HD2 | 1.03 | 0.90 |
| 1:A:334:THR:HB | 1:A:406:ARG:NH1 | 1.85 | 0.90 |
| 1:C:1029:ASN:ND2 | 1:C:1031:SER:HB2 | 1.87 | 0.90 |
| 1:C:866:MET:HE2 | 1:C:871:TYR:HD1 | 1.35 | 0.89 |
| 1:C:895:ARG:HH11 | 1:C:895:ARG:HG3 | 1.35 | 0.89 |
| 1:B:288:ARG:CG | 1:B:288:ARG:HH11 | 1.85 | 0.89 |
| 1:C:192:MET:HE1 | 5:C:1202:ATP:C6 | 2.08 | 0.89 |
| 1:A:44:ASN:HD22 | 1:A:45:ARG:H | 1.19 | 0.89 |
| 1:C:1024:ARG:NH1 | 1:C:1024:ARG:HG2 | 1.81 | 0.89 |
| 1:D:396:ALA:HB3 | 1:D:453:ARG:HB2 | 1.54 | 0.89 |
| 1:A:334:THR:HB | 1:A:406:ARG:HH11 | 1.37 | 0.88 |
| 1:B:1042:MET:CE | 1:B:1062:LEU:HB2 | 2.03 | 0.88 |
| 1:B:519:ARG:HB2 | 1:B:520:PRO:HD2 | 1.53 | 0.88 |
| 1:C:949:LYS:HD3 | 1:C:951:GLU:OE1 | 1.73 | 0.88 |
| 1:B:288:ARG:NH1 | 1:B:288:ARG:HG3 | 1.82 | 0.88 |
| 1:D:329:VAL:HG22 | 1:D:348:GLN:HE22 | 1.37 | 0.88 |
| 1:A:334:THR:CB | 1:A:406:ARG:NH1 | 2.38 | 0.87 |
| 1:B:864:HIS:HD2 | 1:B:866:MET:H | 1.18 | 0.87 |
| 1:A:334:THR:HG22 | 1:A:406:ARG:NH1 | 1.87 | 0.86 |
| 1:A:398:ARG:HH11 | 1:A:398:ARG:CG | 1.88 | 0.86 |
| 1:B:259:HIS:HD2 | 1:B:296:ILE:HD11 | 1.34 | 0.85 |
| 1:A:77:ARG:HG2 | 1:A:77:ARG:HH11 | 1.42 | 0.85 |
| 1:C:44:ASN:ND2 | 1:C:45:ARG:H | 1.75 | 0.85 |
| 1:A:402:GLY:HA2 | 1:C:408:ASP:OD1 | 1.77 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:540:GLY:H | 1:D:543:GLN:NE2 | 1.74 | 0.84 |
| 1:A:863:GLN:O | 1:A:895:ARG:HD2 | 1.77 | 0.84 |
| 1:D:250:ILE:HD11 | 1:D:260:LEU:HD11 | 1.59 | 0.84 |
| 1:B:606:MET:CE | 1:B:607:TRP:HB2 | 2.07 | 0.84 |
| 1:B:798:VAL:HG12 | 1:B:831:MET:CE | 2.07 | 0.84 |
| 1:C:700:SER:H | 1:C:736:HIS:CD2 | 1.94 | 0.84 |
| 1:D:811:ASN:H | 1:D:811:ASN:HD22 | 1.23 | 0.84 |
| 1:B:543:GLN:O | 1:B:547:GLU:HG2 | 1.77 | 0.83 |
| 1:B:999:GLN:HG2 | 1:B:1000:GLY:H | 1.43 | 0.83 |
| 1:B:704:ILE:HG23 | 1:B:726:LEU:HD23 | 1.61 | 0.82 |
| 1:D:1053:ASP:HB2 | 1:D:1056:LYS:CD | 2.08 | 0.82 |
| 1:C:198:GLY:HA3 | 1:C:228:PHE:HE2 | 1.43 | 0.82 |
| 1:B:539:SER:HA | 1:B:543:GLN:HE21 | 1.42 | 0.82 |
| 1:A:398:ARG:HH11 | 1:A:398:ARG:HG2 | 1.42 | 0.82 |
| 1:B:338:MET:HE3 | 1:B:373:ALA:HB1 | 1.61 | 0.82 |
| 1:C:87:GLY:HA3 | 1:C:90:LEU:HD22 | 1.60 | 0.82 |
| 1:C:840:THR:O | 1:C:843:THR:HB | 1.80 | 0.81 |
| 1:C:890:VAL:O | 1:C:891:LYS:HG3 | 1.79 | 0.81 |
| 1:D:1053:ASP:HB2 | 1:D:1056:LYS:HD2 | 1.60 | 0.81 |
| 1:D:935:GLY:HA3 | 1:D:966:VAL:CG1 | 2.10 | 0.81 |
| 1:C:152:LYS:H | 1:C:196:THR:CG2 | 1.94 | 0.81 |
| 1:C:334:THR:HG22 | 1:C:406:ARG:HH12 | 1.46 | 0.81 |
| 1:C:940:PHE:CB | 1:C:944:VAL:CG1 | 2.56 | 0.81 |
| 1:C:979:GLY:O | 1:C:981:TYR:N | 2.12 | 0.81 |
| 1:A:620:LYS:HG2 | 4:A:1203:BTI:H63 | 1.62 | 0.81 |
| 1:B:1066:SER:HB2 | 1:D:1064:THR:HG21 | 1.63 | 0.81 |
| 1:C:334:THR:CG2 | 1:C:406:ARG:HH12 | 1.94 | 0.81 |
| 1:D:143:LEU:H | 1:D:143:LEU:HD12 | 1.46 | 0.81 |
| 1:D:166:VAL:HG12 | 1:D:167:ILE:N | 1.96 | 0.81 |
| 1:A:504:ILE:HD13 | 1:A:1042:MET:HE3 | 1.63 | 0.80 |
| 1:C:39:LYS:HG3 | 1:C:62:SER:HB2 | 1.62 | 0.80 |
| 1:C:198:GLY:HA3 | 1:C:228:PHE:CE2 | 2.17 | 0.80 |
| 1:A:213:LEU:C | 1:A:215:ASP:H | 1.83 | 0.80 |
| 1:A:290:ARG:NH2 | 1:A:318:ASP:O | 2.13 | 0.80 |
| 1:C:892:ASP:O | 1:C:896:ARG:HD2 | 1.82 | 0.80 |
| 1:C:940:PHE:HB3 | 1:C:941:PRO:CD | 2.12 | 0.80 |
| 1:A:77:ARG:HH11 | 1:A:77:ARG:CG | 1.95 | 0.80 |
| 1:C:44:ASN:HD22 | 1:C:45:ARG:N | 1.77 | 0.79 |
| 1:C:572:ASP:HB3 | 1:C:807:GLN:NE2 | 1.97 | 0.79 |
| 1:A:700:SER:H | 1:A:736:HIS:HD2 | 1.30 | 0.79 |
| 1:D:451:ARG:HG3 | 1:D:451:ARG:NH1 | 1.96 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:396:ALA:HB3 | 1:B:453:ARG:HB2 | 1.65 | 0.79 |
| 1:D:498:THR:HG23 | 1:D:1085:ARG:HH22 | 1.47 | 0.79 |
| 1:A:622:ASN:ND2 | 1:A:624:TRP:H | 1.81 | 0.79 |
| 1:A:519:ARG:NH2 | 1:A:847:ASP:OD2 | 2.17 | 0.78 |
| 1:B:101:ARG:CG | 1:B:101:ARG:HH11 | 1.96 | 0.78 |
| 1:B:306:ASN:OD1 | 1:B:348:GLN:HG2 | 1.83 | 0.78 |
| 1:C:1062:LEU:HD12 | 1:C:1078:TYR:CE2 | 2.18 | 0.78 |
| 1:C:238:TYR:HD1 | 5:C:1202:ATP:C2 | 2.01 | 0.78 |
| 1:D:495:ASP:HB3 | 1:D:498:THR:HB | 1.66 | 0.78 |
| 1:D:504:ILE:HG21 | 1:D:1042:MET:CE | 2.13 | 0.78 |
| 1:D:513:PRO:O | 1:D:515:ASN:HB2 | 1.82 | 0.78 |
| 1:A:176:SER:O | 1:A:179:LEU:HB3 | 1.84 | 0.78 |
| 1:D:243:LYS:HZ3 | 1:D:243:LYS:HB3 | 1.47 | 0.77 |
| 1:C:921:MET:HA | 1:C:926:LEU:HB2 | 1.67 | 0.77 |
| 1:C:87:GLY:HA3 | 1:C:90:LEU:CD2 | 2.15 | 0.77 |
| 1:A:98:ASN:C | 1:A:98:ASN:HD22 | 1.88 | 0.77 |
| 1:A:1018:GLU:OE1 | 1:A:1018:GLU:HA | 1.83 | 0.77 |
| 1:C:167:ILE:HD12 | 1:C:167:ILE:N | 1.99 | 0.77 |
| 1:C:893:MET:HE1 | 1:C:918:ALA:HA | 1.67 | 0.77 |
| 1:C:183:PHE:CD2 | 1:C:183:PHE:O | 2.38 | 0.76 |
| 1:C:940:PHE:HB2 | 1:C:944:VAL:HG11 | 1.65 | 0.76 |
| 1:D:274:VAL:HG12 | 1:D:275:VAL:HG23 | 1.67 | 0.76 |
| 1:D:357:LEU:HA | 1:D:360:ILE:HD12 | 1.65 | 0.76 |
| 1:C:743:MET:HG3 | 1:C:907:VAL:HG13 | 1.66 | 0.76 |
| 1:A:720:LEU:HD21 | 1:A:758:GLU:HG3 | 1.67 | 0.76 |
| 1:B:864:HIS:CD2 | 1:B:866:MET:H | 2.03 | 0.76 |
| 1:D:259:HIS:H | 1:D:364:GLN:HE22 | 1.32 | 0.76 |
| 1:C:378:ILE:HG13 | 1:C:450:MET:HE1 | 1.67 | 0.76 |
| 1:D:620:LYS:HG2 | 1:D:1023:THR:HG21 | 1.67 | 0.76 |
| 1:D:143:LEU:N | 1:D:143:LEU:HD12 | 2.00 | 0.76 |
| 1:D:866:MET:HE2 | 1:D:871:TYR:HA | 1.68 | 0.76 |
| 1:C:188:GLY:HA3 | 1:C:237:ARG:HH22 | 1.51 | 0.76 |
| 1:D:337:GLU:HG2 | 1:D:342:ILE:O | 1.85 | 0.75 |
| 1:A:175:LYS:NZ | 1:A:232:GLU:HG3 | 2.02 | 0.75 |
| 1:A:189:PHE:HB3 | 1:A:190:PRO:CD | 2.16 | 0.75 |
| 1:C:918:ALA:O | 1:C:922:VAL:CG2 | 2.29 | 0.75 |
| 1:D:306:ASN:OD1 | 1:D:348:GLN:HG2 | 1.87 | 0.75 |
| 1:D:720:LEU:HD21 | 1:D:758:GLU:HG3 | 1.67 | 0.75 |
| 1:B:540:GLY:H | 1:B:543:GLN:NE2 | 1.84 | 0.75 |
| 1:C:644:ARG:NH1 | 1:C:650:GLY:O | 2.20 | 0.75 |
| 1:A:1060:ILE:HG12 | 1:A:1080:MET:HG3 | 1.69 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:597:VAL:HG22 | 1:B:830:GLY:HA3 | 1.68 | 0.75 |
| 1:A:1042:MET:HE1 | 1:A:1048:VAL:HG12 | 1.67 | 0.75 |
| 1:A:1051:GLU:OE1 | 1:A:1057:ARG:NH2 | 2.20 | 0.75 |
| 1:C:912:LYS:O | 1:C:916:ASP:N | 2.19 | 0.75 |
| 1:D:298:LEU:O | 1:D:302:ILE:HG13 | 1.87 | 0.75 |
| 1:D:506:ASN:ND2 | 1:D:510:ASN:HD22 | 1.85 | 0.74 |
| 1:A:167:ILE:HD11 | 1:A:323:ILE:HD11 | 1.69 | 0.74 |
| 1:D:840:THR:O | 1:D:843:THR:HB | 1.87 | 0.74 |
| 1:C:326:ASN:ND2 | 1:C:330:GLN:OE1 | 2.20 | 0.74 |
| 1:C:334:THR:CG2 | 1:C:406:ARG:NH1 | 2.49 | 0.74 |
| 1:C:178:GLU:O | 1:C:182:GLU:HG3 | 1.88 | 0.74 |
| 1:C:530:PRO:HB2 | 1:C:593:LYS:HD3 | 1.70 | 0.74 |
| 1:A:991:ARG:O | 1:A:995:GLU:HG3 | 1.88 | 0.74 |
| 1:B:1052:ILE:HG22 | 1:B:1052:ILE:O | 1.87 | 0.74 |
| 1:C:494:LEU:HB2 | 1:C:496:ARG:NH1 | 2.03 | 0.74 |
| 1:A:590:ILE:HG13 | 1:A:837:TYR:CE2 | 2.21 | 0.74 |
| 1:D:917:MET:HG2 | 1:D:944:VAL:HG11 | 1.69 | 0.74 |
| 1:C:378:ILE:HG13 | 1:C:450:MET:CE | 2.18 | 0.74 |
| 1:D:1047:THR:HG23 | 1:D:1061:LYS:HB2 | 1.70 | 0.73 |
| 1:D:278:ALA:HB2 | 1:D:335:ILE:HG23 | 1.69 | 0.73 |
| 1:A:620:LYS:HG3 | 1:A:1023:THR:HG21 | 1.71 | 0.73 |
| 1:C:238:TYR:CD1 | 5:C:1202:ATP:C2 | 2.76 | 0.73 |
| 1:C:910:SER:O | 1:C:914:VAL:HG23 | 1.88 | 0.73 |
| 1:B:269:ARG:HG2 | 1:B:481:ILE:HG21 | 1.70 | 0.73 |
| 1:B:395:ILE:HG13 | 1:B:453:ARG:HB3 | 1.69 | 0.73 |
| 1:A:406:ARG:HH21 | 1:C:403:ALA:HB2 | 1.54 | 0.73 |
| 1:A:152:LYS:NZ | 1:A:324:GLU:OE2 | 2.21 | 0.73 |
| 1:A:51:ARG:NH2 | 1:A:337:GLU:OE1 | 2.19 | 0.73 |
| 1:D:991:ARG:O | 1:D:995:GLU:HG3 | 1.89 | 0.73 |
| 1:A:470:LYS:HB2 | 1:A:480:PHE:CE1 | 2.24 | 0.73 |
| 1:A:241:ASN:N | 1:A:242:PRO:HD3 | 2.04 | 0.72 |
| 1:D:418:ILE:HD12 | 1:D:418:ILE:H | 1.54 | 0.72 |
| 1:D:456:LYS:N | 1:D:456:LYS:HD3 | 2.04 | 0.72 |
| 1:D:166:VAL:CG1 | 1:D:167:ILE:H | 2.03 | 0.72 |
| 1:A:164:LEU:HD22 | 1:A:294:ALA:HB1 | 1.71 | 0.72 |
| 1:A:864:HIS:HD2 | 1:A:866:MET:H | 1.38 | 0.72 |
| 1:A:896:ARG:HD2 | 1:A:928:GLU:OE2 | 1.89 | 0.72 |
| 1:A:206:ILE:HD11 | 1:A:238:TYR:CE1 | 2.24 | 0.71 |
| 1:B:338:MET:HE1 | 1:B:430:SER:HB3 | 1.70 | 0.71 |
| 1:C:811:ASN:HD22 | 1:C:811:ASN:N | 1.84 | 0.71 |
| 1:B:279:PRO:HD2 | 1:B:372:TYR:HD2 | 1.56 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:675:ARG:HA | 1:B:701:GLU:HB3 | 1.72 | 0.71 |
| 1:B:897:VAL:HG12 | 1:B:914:VAL:HG13 | 1.72 | 0.71 |
| 1:C:646:SER:HB2 | 1:C:685:GLN:HE22 | 1.53 | 0.71 |
| 1:D:444:VAL:HG23 | 1:D:466:MET:HB3 | 1.70 | 0.71 |
| 1:A:151:ASP:HB3 | 1:A:154:LYS:HB2 | 1.72 | 0.71 |
| 1:B:118:TYR:OH | 1:B:331:VAL:HG13 | 1.90 | 0.71 |
| 1:B:1046:GLU:HG2 | 1:B:1047:THR:N | 2.04 | 0.71 |
| 1:B:145:HIS:HE1 | 1:B:302:ILE:O | 1.72 | 0.71 |
| 1:C:200:GLY:C | 1:C:202:LYS:H | 1.92 | 0.71 |
| 1:D:917:MET:SD | 1:D:921:MET:CE | 2.79 | 0.71 |
| 1:B:999:GLN:HG2 | 1:B:1001:PRO:HD3 | 1.72 | 0.71 |
| 1:D:864:HIS:HD2 | 1:D:866:MET:H | 1.36 | 0.71 |
| 1:A:217:PHE:CE2 | 1:A:221:LYS:HE3 | 2.26 | 0.71 |
| 1:B:142:HIS:H | 1:B:145:HIS:HD2 | 1.38 | 0.71 |
| 1:B:259:HIS:HD2 | 1:B:296:ILE:CD1 | 2.02 | 0.71 |
| 1:D:116:PRO:HB2 | 1:D:122:SER:HA | 1.72 | 0.71 |
| 1:D:339:VAL:O | 1:D:369:THR:HA | 1.90 | 0.71 |
| 1:A:413:PHE:CZ | 1:A:416:ALA:CB | 2.69 | 0.70 |
| 1:A:44:ASN:HD22 | 1:A:45:ARG:N | 1.87 | 0.70 |
| 1:A:516:VAL:O | 1:A:516:VAL:HG12 | 1.89 | 0.70 |
| 1:C:170:THR:HG22 | 1:C:171:ASP:N | 2.04 | 0.70 |
| 1:D:571:ARG:HH11 | 1:D:575:GLN:NE2 | 1.88 | 0.70 |
| 1:D:901:PHE:HZ | 1:D:917:MET:HG3 | 1.56 | 0.70 |
| 1:C:175:LYS:H | 1:C:175:LYS:HD3 | 1.53 | 0.70 |
| 1:C:574:HIS:CD2 | 1:C:582:VAL:HB | 2.26 | 0.70 |
| 1:B:861:ILE:HG13 | 1:B:862:TYR:N | 2.06 | 0.70 |
| 1:D:935:GLY:HA3 | 1:D:966:VAL:HG13 | 1.73 | 0.70 |
| 1:B:1052:ILE:HD11 | 1:B:1058:LEU:HG | 1.74 | 0.70 |
| 1:D:901:PHE:CZ | 1:D:917:MET:HG3 | 2.26 | 0.70 |
| 1:A:644:ARG:HH11 | 1:A:909:PRO:HD3 | 1.56 | 0.70 |
| 1:B:577:LEU:HD13 | 1:B:842:ARG:NH2 | 2.06 | 0.70 |
| 1:C:437:LYS:HD3 | 1:C:437:LYS:H | 1.57 | 0.70 |
| 1:D:540:GLY:N | 1:D:543:GLN:HE21 | 1.87 | 0.70 |
| 1:B:744:ALA:HB3 | 1:B:746:LEU:HG | 1.74 | 0.70 |
| 1:C:359:GLU:N | 1:C:359:GLU:OE2 | 2.23 | 0.70 |
| 1:C:504:ILE:HD13 | 1:C:1042:MET:CE | 2.22 | 0.70 |
| 1:C:911:SER:O | 1:C:915:GLY:N | 2.18 | 0.70 |
| 1:C:335:ILE:HD11 | 1:C:373:ALA:O | 1.92 | 0.69 |
| 1:A:898:ASN:HD21 | 1:A:904:ILE:H | 1.40 | 0.69 |
| 1:D:263:ARG:CD | 1:D:335:ILE:HG21 | 2.23 | 0.69 |
| 1:D:358:GLU:HG2 | 1:D:359:GLU:OE2 | 1.92 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:504:ILE:CG2 | 1:D:1042:MET:HE2 | 2.17 | 0.69 |
| 1:B:571:ARG:HH11 | 1:B:575:GLN:NE2 | 1.91 | 0.69 |
| 1:C:230:ASN:HD22 | 1:C:231:SER:N | 1.90 | 0.69 |
| 1:C:940:PHE:CB | 1:C:941:PRO:HD2 | 2.19 | 0.69 |
| 1:A:338:MET:HE1 | 1:A:430:SER:HB2 | 1.73 | 0.69 |
| 1:A:691:GLU:O | 1:A:695:GLU:HG3 | 1.92 | 0.69 |
| 1:B:927:ASP:OD2 | 1:B:927:ASP:N | 2.25 | 0.69 |
| 1:A:499:LYS:HE3 | 1:A:1025:ASN:O | 1.93 | 0.69 |
| 1:A:513:PRO:O | 1:A:515:ASN:HB2 | 1.93 | 0.69 |
| 1:B:999:GLN:HG2 | 1:B:1000:GLY:N | 2.07 | 0.69 |
| 1:C:943:SER:OG | 1:C:944:VAL:N | 2.26 | 0.69 |
| 1:D:607:TRP:HE3 | 1:D:641:MET:HE3 | 1.54 | 0.69 |
| 1:C:167:ILE:CD1 | 1:C:167:ILE:H | 2.04 | 0.68 |
| 1:B:375:GLN:NE2 | 1:B:428:LYS:HD3 | 2.07 | 0.68 |
| 1:D:874:LEU:O | 1:D:887:PHE:HE1 | 1.76 | 0.68 |
| 1:A:622:ASN:HD22 | 1:A:623:PRO:HD2 | 1.58 | 0.68 |
| 1:C:590:ILE:HG12 | 1:C:837:TYR:CE2 | 2.29 | 0.68 |
| 1:A:167:ILE:CD1 | 1:A:323:ILE:HD11 | 2.24 | 0.68 |
| 1:B:631:ARG:NH2 | 1:B:672:ASP:OD1 | 2.27 | 0.68 |
| 1:B:414:GLN:HG3 | 1:D:1084:ALA:HB2 | 1.74 | 0.68 |
| 1:C:156:ARG:NH2 | 1:C:170:THR:O | 2.26 | 0.68 |
| 1:C:69:ASN:O | 1:C:72:LYS:HG3 | 1.93 | 0.68 |
| 1:C:893:MET:O | 1:C:897:VAL:N | 2.22 | 0.68 |
| 1:C:396:ALA:CB | 1:C:453:ARG:HG3 | 2.15 | 0.68 |
| 1:C:156:ARG:HG2 | 1:C:166:VAL:HG11 | 1.76 | 0.67 |
| 1:D:960:ASN:HD22 | 1:D:963:LEU:HB2 | 1.59 | 0.67 |
| 1:B:347:THR:HG23 | 1:B:360:ILE:HD13 | 1.77 | 0.67 |
| 1:D:263:ARG:HD3 | 1:D:335:ILE:CG2 | 2.24 | 0.67 |
| 1:A:840:THR:O | 1:A:843:THR:HB | 1.94 | 0.67 |
| 1:C:200:GLY:O | 1:C:202:LYS:N | 2.26 | 0.67 |
| 1:D:70:GLU:CD | 1:D:70:GLU:H | 1.96 | 0.67 |
| 1:A:194:LYS:NZ | 1:A:236:GLU:OE1 | 2.24 | 0.67 |
| 1:B:1000:GLY:H | 1:B:1001:PRO:HD3 | 1.59 | 0.67 |
| 1:C:926:LEU:CD1 | 1:C:938:LEU:HD11 | 2.25 | 0.67 |
| 1:B:519:ARG:HB2 | 1:B:520:PRO:CD | 2.25 | 0.67 |
| 1:C:152:LYS:H | 1:C:196:THR:HG23 | 1.58 | 0.67 |
| 1:D:543:GLN:HE22 | 1:D:636:ASN:HA | 1.59 | 0.67 |
| 1:B:98:ASN:C | 1:B:98:ASN:HD22 | 1.98 | 0.67 |
| 1:D:263:ARG:HH21 | 1:D:330:GLN:NE2 | 1.93 | 0.67 |
| 1:C:641:MET:HG2 | 1:C:671:ILE:HG21 | 1.75 | 0.67 |
| 1:D:362:MET:CE | 1:D:367:ILE:HD11 | 2.24 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 1:D:498:THR:HG23 | 1:D:1085:ARG:NH2 | 2.09 | 0.66 |
| 1:D:717(A):ILE:HG13 | 1:D:957:ASN:OD1 | 1.95 | 0.66 |
| 1:C:328:ARG:HG3 | 1:C:329:VAL:O | 1.96 | 0.66 |
| 1:C:978:PRO:HA | 1:C:981:TYR:CZ | 2.30 | 0.66 |
| 1:D:338:MET:CE | 1:D:430:SER:HB3 | 2.25 | 0.66 |
| 1:D:828:ILE:O | 1:D:832:GLU:HG2 | 1.96 | 0.66 |
| 1:A:504:ILE:HD13 | 1:A:1042:MET:CE | 2.26 | 0.66 |
| 1:A:334:THR:HG21 | 1:A:428:LYS:HZ2 | 1.60 | 0.66 |
| 1:A:952:ILE:O | 1:A:952:ILE:CG2 | 2.43 | 0.66 |
| 1:C:940:PHE:HB3 | 1:C:944:VAL:HG11 | 1.76 | 0.66 |
| 1:B:413:PHE:HD1 | 1:B:414:GLN:HB3 | 1.60 | 0.66 |
| 1:C:261:PHE:HE1 | 1:C:367:ILE:HG22 | 1.61 | 0.66 |
| 1:C:940:PHE:CG | 1:C:944:VAL:HG11 | 2.30 | 0.66 |
| 1:D:263:ARG:NH1 | 1:D:336:THR:OG1 | 2.28 | 0.66 |
| 1:D:917:MET:SD | 1:D:921:MET:HE1 | 2.36 | 0.66 |
| 1:C:385:ASN:O | 1:C:387:PHE:N | 2.28 | 0.66 |
| 1:D:756:ILE:HD12 | 1:D:786:ALA:HB1 | 1.77 | 0.66 |
| 1:B:268:GLN:HB3 | 1:B:272:GLN:O | 1.95 | 0.66 |
| 1:B:796:THR:HB | 1:B:810:ALA:HB2 | 1.78 | 0.66 |
| 1:C:192:MET:CE | 5:C:1202:ATP:C6 | 2.79 | 0.65 |
| 1:D:44:ASN:ND2 | 1:D:45:ARG:H | 1.92 | 0.65 |
| 1:C:646:SER:HB2 | 1:C:685:GLN:NE2 | 2.11 | 0.65 |
| 1:D:917:MET:SD | 1:D:921:MET:HE3 | 2.37 | 0.65 |
| 1:C:398:ARG:HH11 | 1:C:398:ARG:HG3 | 1.62 | 0.65 |
| 1:C:39:LYS:HG3 | 1:C:62:SER:CB | 2.27 | 0.65 |
| 1:A:206:ILE:CG2 | 1:A:207:VAL:N | 2.60 | 0.65 |
| 1:B:99:ILE:HD12 | 1:B:99:ILE:H | 1.62 | 0.65 |
| 1:A:192:MET:HE1 | 1:A:238:TYR:CE1 | 2.32 | 0.65 |
| 1:B:380:THR:HG22 | 1:B:426:LEU:HD11 | 1.78 | 0.65 |
| 1:C:396:ALA:HB3 | 1:C:453:ARG:CG | 2.17 | 0.65 |
| 1:C:572:ASP:HB3 | 1:C:807:GLN:HE22 | 1.61 | 0.65 |
| 1:C:811:ASN:H | 1:C:811:ASN:ND2 | 1.89 | 0.65 |
| 1:D:622:ASN:C | 1:D:622:ASN:HD22 | 1.98 | 0.65 |
| 1:A:207:VAL:HA | 1:A:212:GLU:OE2 | 1.96 | 0.65 |
| 1:B:927:ASP:HB2 | 1:B:929:GLN:H | 1.61 | 0.65 |
| 1:D:445:ARG:HG2 | 1:D:445:ARG:O | 1.97 | 0.65 |
| 1:A:70:GLU:HG3 | 1:A:92:PRO:HB3 | 1.80 | 0.64 |
| 1:B:268:GLN:CB | 1:B:272:GLN:O | 2.45 | 0.64 |
| 1:C:175:LYS:CD | 1:C:175:LYS:N | 2.57 | 0.64 |
| 1:C:700:SER:N | 1:C:736:HIS:HD2 | 1.87 | 0.64 |
| 1:D:1087:ILE:HG22 | 1:D:1089:ILE:HD12 | 1.80 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:173:PRO:O | 1:C:174:ILE:HD12 | 1.97 | 0.64 |
| 1:D:501:LEU:HB3 | 1:D:1078:TYR:CE1 | 2.32 | 0.64 |
| 1:A:811:ASN:H | 1:A:811:ASN:HD22 | 1.45 | 0.64 |
| 1:B:548:VAL:HG23 | 1:B:552:GLY:HA3 | 1.79 | 0.64 |
| 1:C:103:ILE:HG21 | 1:C:134:GLU:HG3 | 1.79 | 0.64 |
| 1:B:1066:SER:CB | 1:D:1064:THR:HG21 | 2.27 | 0.64 |
| 1:D:622:ASN:ND2 | 1:D:624:TRP:H | 1.95 | 0.64 |
| 1:D:715:ARG:NH1 | 1:D:865:GLU:OE2 | 2.31 | 0.64 |
| 1:A:470:LYS:HB2 | 1:A:480:PHE:HE1 | 1.63 | 0.64 |
| 1:B:892:ASP:O | 1:B:896:ARG:HG3 | 1.98 | 0.64 |
| 1:C:183:PHE:HD2 | 1:C:183:PHE:O | 1.76 | 0.64 |
| 1:D:278:ALA:CB | 1:D:335:ILE:HG23 | 2.28 | 0.64 |
| 1:D:935:GLY:HA3 | 1:D:966:VAL:HG11 | 1.77 | 0.64 |
| 1:A:362:MET:HE1 | 1:A:367:ILE:HD11 | 1.78 | 0.64 |
| 1:A:542:LYS:HE2 | 1:A:672:ASP:OD2 | 1.96 | 0.64 |
| 1:A:613:ASP:HB2 | 1:A:1013:TYR:CZ | 2.32 | 0.64 |
| 1:B:435:SER:HB3 | 1:B:438:GLN:HE21 | 1.63 | 0.64 |
| 1:D:394:ILE:HD11 | 1:D:426:LEU:HD21 | 1.79 | 0.64 |
| 1:D:498:THR:CG2 | 1:D:1085:ARG:HH22 | 2.09 | 0.64 |
| 1:B:647:ASN:O | 1:B:649:VAL:N | 2.30 | 0.64 |
| 1:C:41:LEU:HD22 | 1:C:114:ILE:HG12 | 1.79 | 0.64 |
| 1:C:170:THR:CG2 | 1:C:171:ASP:H | 2.08 | 0.64 |
| 1:C:504:ILE:HD13 | 1:C:1042:MET:HE2 | 1.79 | 0.64 |
| 1:D:685:GLN:OE1 | 1:D:978:PRO:HD2 | 1.98 | 0.64 |
| 1:D:986:ASP:OD2 | 1:D:988:GLU:HB2 | 1.97 | 0.64 |
| 1:A:179:LEU:HA | 1:A:182:GLU:OE2 | 1.96 | 0.63 |
| 1:B:540:GLY:H | 1:B:543:GLN:HE21 | 1.46 | 0.63 |
| 1:C:518:LYS:O | 1:C:518:LYS:HG3 | 1.97 | 0.63 |
| 1:D:820:PHE:HB3 | 1:D:821:PRO:CD | 2.29 | 0.63 |
| 1:A:881:LEU:HD13 | 1:A:923:GLN:HE22 | 1.62 | 0.63 |
| 1:B:606:MET:HE1 | 1:B:607:TRP:HB2 | 1.80 | 0.63 |
| 1:D:594:THR:HG23 | 1:D:598:PHE:HD1 | 1.64 | 0.63 |
| 1:A:398:ARG:NH1 | 1:A:398:ARG:HG2 | 2.12 | 0.63 |
| 1:A:216:ALA:C | 1:A:218:HIS:H | 2.01 | 0.63 |
| 1:D:492:PRO:O | 1:D:493:SER:OG | 2.16 | 0.63 |
| 1:A:1018:GLU:OE1 | 1:A:1018:GLU:CA | 2.46 | 0.63 |
| 1:A:828:ILE:O | 1:A:832:GLU:HG2 | 1.99 | 0.63 |
| 1:C:794:ILE:HD12 | 1:C:796:THR:HG23 | 1.81 | 0.63 |
| 1:D:622:ASN:HD22 | 1:D:623:PRO:N | 1.97 | 0.63 |
| 1:A:176:SER:O | 1:A:179:LEU:HD22 | 1.98 | 0.63 |
| 1:A:216:ALA:O | 1:A:218:HIS:N | 2.31 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:952:ILE:HG22 | 1:B:952:ILE:O | 1.98 | 0.63 |
| 1:C:760:LYS:HE3 | 1:C:790:GLY:O | 1.99 | 0.63 |
| 1:D:496:ARG:NH1 | 1:D:496:ARG:HB3 | 2.08 | 0.63 |
| 1:D:518:LYS:O | 1:D:518:LYS:HG3 | 1.99 | 0.63 |
| 1:A:362:MET:CE | 1:A:367:ILE:HD11 | 2.29 | 0.63 |
| 1:B:69:ASN:HD22 | 1:B:72:LYS:HE3 | 1.64 | 0.63 |
| 1:C:357:LEU:O | 1:C:362:MET:HB3 | 1.99 | 0.63 |
| 1:D:259:HIS:H | 1:D:364:GLN:NE2 | 1.95 | 0.63 |
| 1:A:334:THR:HG21 | 1:A:428:LYS:NZ | 2.13 | 0.62 |
| 1:A:44:ASN:ND2 | 1:A:45:ARG:H | 1.95 | 0.62 |
| 1:A:781:LEU:HD13 | 1:D:816:ALA:HB1 | 1.80 | 0.62 |
| 1:A:490:ILE:O | 1:A:490:ILE:CD1 | 2.47 | 0.62 |
| 1:A:583:ARG:HG2 | 1:A:619:LEU:HD22 | 1.81 | 0.62 |
| 1:C:515:ASN:N | 1:C:515:ASN:HA | 2.00 | 0.62 |
| 1:A:278:ALA:HB3 | 1:A:335:ILE:HG12 | 1.80 | 0.62 |
| 1:B:266:SER:O | 1:B:478:THR:HA | 1.99 | 0.62 |
| 1:C:377:ARG:CG | 1:C:377:ARG:NH1 | 2.43 | 0.62 |
| 1:D:364:GLN:HA | 1:D:367:ILE:HD12 | 1.82 | 0.62 |
| 1:D:565:LEU:C | 1:D:565:LEU:HD12 | 2.19 | 0.62 |
| 1:D:607:TRP:CZ3 | 1:D:641:MET:HE1 | 2.33 | 0.62 |
| 1:A:775:THR:OG1 | 1:A:861:ILE:CD1 | 2.47 | 0.62 |
| 1:B:860:GLU:O | 1:B:863:GLN:HG2 | 1.99 | 0.62 |
| 1:C:273:LYS:HB3 | 1:C:276:GLU:OE2 | 2.00 | 0.62 |
| 1:A:700:SER:H | 1:A:736:HIS:CD2 | 2.14 | 0.62 |
| 1:A:879:LYS:C | 1:A:881:LEU:H | 2.03 | 0.62 |
| 1:B:620:LYS:HG3 | 4:B:1201:BTI:H63 | 1.81 | 0.62 |
| 1:B:539:SER:HA | 1:B:543:GLN:NE2 | 2.12 | 0.62 |
| 1:B:606:MET:HE3 | 1:B:607:TRP:HB2 | 1.80 | 0.62 |
| 1:D:661:LYS:NZ | 1:D:1004:GLU:OE2 | 2.25 | 0.62 |
| 1:D:244:HIS:HD2 | 1:D:265:CYS:HB2 | 1.63 | 0.62 |
| 1:B:413:PHE:CE2 | 1:B:416:ALA:HB2 | 2.35 | 0.62 |
| 1:B:571:ARG:HH11 | 1:B:575:GLN:HE22 | 1.47 | 0.62 |
| 1:A:547:GLU:OE2 | 1:A:547:GLU:HA | 2.00 | 0.62 |
| 1:C:867:PRO:HB2 | 1:C:870:GLN:HB3 | 1.80 | 0.62 |
| 1:A:249:VAL:HG11 | 1:A:299:MET:HG3 | 1.82 | 0.62 |
| 1:B:98:ASN:ND2 | 1:B:101:ARG:H | 1.98 | 0.62 |
| 1:B:101:ARG:HH11 | 1:B:101:ARG:HG3 | 1.65 | 0.62 |
| 1:B:746:LEU:HD11 | 1:B:865:GLU:HG2 | 1.82 | 0.62 |
| 1:C:252:ASP:HB3 | 1:C:357:LEU:HB2 | 1.80 | 0.62 |
| 1:D:924:ASN:HB2 | 1:D:926:LEU:HD22 | 1.82 | 0.62 |
| 1:B:565:LEU:HD11 | 1:B:598:PHE:CE2 | 2.35 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:370:LEU:O | 1:A:432:HIS:HE1 | 1.83 | 0.61 |
| 1:B:320:PHE:N | 1:B:320:PHE:CD1 | 2.67 | 0.61 |
| 1:C:266:SER:O | 1:C:478:THR:HA | 2.00 | 0.61 |
| 1:A:935:GLY:CA | 1:A:966:VAL:CG1 | 2.72 | 0.61 |
| 1:A:406:ARG:HE | 1:C:403:ALA:HA | 1.65 | 0.61 |
| 1:D:93:ALA:O | 1:D:95:SER:N | 2.33 | 0.61 |
| 1:D:151:ASP:O | 1:D:153:VAL:N | 2.33 | 0.61 |
| 1:C:519:ARG:HG2 | 1:C:520:PRO:O | 2.00 | 0.61 |
| 1:D:143:LEU:H | 1:D:143:LEU:HD13 | 1.64 | 0.61 |
| 1:D:563:VAL:HG21 | 1:D:787:ILE:HG12 | 1.82 | 0.61 |
| 1:A:403:ALA:HA | 1:C:406:ARG:HH21 | 1.65 | 0.61 |
| 1:B:700:SER:H | 1:B:736:HIS:CD2 | 2.01 | 0.61 |
| 1:C:675:ARG:HA | 1:C:701:GLU:HB3 | 1.82 | 0.61 |
| 1:A:167:ILE:HB | 1:A:236:GLU:OE2 | 2.01 | 0.61 |
| 1:A:563:VAL:HG21 | 1:A:787:ILE:HG12 | 1.81 | 0.61 |
| 1:A:644:ARG:NH1 | 1:A:909:PRO:HD3 | 2.16 | 0.61 |
| 1:C:221:LYS:O | 1:C:224:ALA:HB3 | 2.01 | 0.61 |
| 1:D:281:VAL:O | 1:D:283:LEU:N | 2.33 | 0.61 |
| 1:A:37:ILE:HD12 | 1:A:353:ALA:HB2 | 1.82 | 0.61 |
| 1:B:644:ARG:HD3 | 1:B:909:PRO:HD3 | 1.81 | 0.61 |
| 1:D:1070:GLU:HG3 | 1:D:1071:ASN:N | 2.14 | 0.61 |
| 1:A:210:GLU:O | 1:A:212:GLU:N | 2.28 | 0.61 |
| 1:C:1033:LEU:CD2 | 1:C:1050:ILE:HD13 | 2.31 | 0.61 |
| 1:C:243:LYS:HD3 | 1:C:476:TYR:O | 2.01 | 0.61 |
| 1:D:672:ASP:HA | 1:D:698:LYS:HD2 | 1.83 | 0.61 |
| 1:A:999:GLN:HG2 | 1:A:1000:GLY:H | 1.66 | 0.60 |
| 1:A:999:GLN:HG2 | 1:A:1000:GLY:N | 2.16 | 0.60 |
| 1:A:490:ILE:O | 1:A:490:ILE:HD12 | 2.01 | 0.60 |
| 1:D:647:ASN:C | 1:D:647:ASN:HD22 | 2.03 | 0.60 |
| 1:B:338:MET:CE | 1:B:430:SER:CB | 2.75 | 0.60 |
| 1:D:335:ILE:CG2 | 1:D:336:THR:N | 2.63 | 0.60 |
| 1:D:498:THR:OG1 | 1:D:1085:ARG:NH2 | 2.34 | 0.60 |
| 1:D:335:ILE:HG22 | 1:D:336:THR:N | 2.15 | 0.60 |
| 1:A:605:GLU:HG3 | 1:A:640:GLN:HG2 | 1.83 | 0.60 |
| 1:B:337:GLU:HG2 | 1:B:342:ILE:O | 2.01 | 0.60 |
| 1:B:101:ARG:CG | 1:B:101:ARG:NH1 | 2.60 | 0.60 |
| 1:B:934:ASP:O | 1:B:938:LEU:HG | 2.00 | 0.60 |
| 1:C:141:PRO:HB2 | 1:C:145:HIS:HB2 | 1.83 | 0.60 |
| 1:D:338:MET:HE2 | 1:D:430:SER:HB3 | 1.83 | 0.60 |
| 1:A:622:ASN:HD22 | 1:A:623:PRO:CD | 2.14 | 0.60 |
| 1:D:641:MET:HB3 | 1:D:671:ILE:HD12 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:444:VAL:O | 1:A:448:ARG:HG3 | 2.01 | 0.60 |
| 1:B:1046:GLU:HG2 | 1:B:1047:THR:H | 1.64 | 0.60 |
| 1:C:69:ASN:OD1 | 1:C:69:ASN:N | 2.34 | 0.60 |
| 1:D:690:ASN:O | 1:D:694:GLN:HG2 | 2.02 | 0.60 |
| 1:A:192:MET:HE2 | 1:A:238:TYR:CD1 | 2.37 | 0.60 |
| 1:B:243:LYS:HG3 | 1:B:266:SER:OG | 2.02 | 0.60 |
| 1:B:269:ARG:O | 1:B:272:GLN:N | 2.30 | 0.60 |
| 1:C:238:TYR:CD1 | 5:C:1202:ATP:H2 | 2.20 | 0.60 |
| 1:C:556:TRP:O | 1:C:560:GLN:HG2 | 2.01 | 0.60 |
| 1:B:798:VAL:HG12 | 1:B:831:MET:HE2 | 1.83 | 0.60 |
| 1:D:622:ASN:HD22 | 1:D:623:PRO:CD | 2.15 | 0.60 |
| 1:B:917:MET:O | 1:B:921:MET:HG2 | 2.01 | 0.59 |
| 1:C:186:GLU:OE2 | 1:C:186:GLU:N | 2.35 | 0.59 |
| 1:C:323:ILE:HD11 | 5:C:1202:ATP:N7 | 2.17 | 0.59 |
| 1:D:278:ALA:HB2 | 1:D:335:ILE:CG2 | 2.32 | 0.59 |
| 1:D:885:GLU:OE2 | 1:D:885:GLU:HA | 2.02 | 0.59 |
| 1:D:960:ASN:HD22 | 1:D:963:LEU:H | 1.49 | 0.59 |
| 1:A:509:ILE:HD12 | 1:A:1089:ILE:HG21 | 1.84 | 0.59 |
| 1:A:278:ALA:CB | 1:A:335:ILE:HG12 | 2.31 | 0.59 |
| 1:A:192:MET:CE | 1:A:238:TYR:CD1 | 2.85 | 0.59 |
| 1:A:338:MET:CE | 1:A:430:SER:HB2 | 2.32 | 0.59 |
| 1:A:897:VAL:HG12 | 1:A:914:VAL:HG13 | 1.83 | 0.59 |
| 1:B:167:ILE:HG13 | 1:B:168:PRO:HD3 | 1.85 | 0.59 |
| 1:B:606:MET:HE3 | 1:B:607:TRP:N | 2.18 | 0.59 |
| 1:C:949:LYS:CD | 1:C:951:GLU:OE1 | 2.48 | 0.59 |
| 1:C:979:GLY:C | 1:C:981:TYR:H | 2.05 | 0.59 |
| 1:A:503:TYR:OH | 1:A:1038:PHE:O | 2.20 | 0.59 |
| 1:B:731:GLU:OE1 | 1:B:765:ASP:N | 2.35 | 0.59 |
| 1:C:1042:MET:HE1 | 1:C:1060:ILE:HG21 | 1.83 | 0.59 |
| 1:A:749:PRO:HG3 | 1:A:781:LEU:HB3 | 1.85 | 0.59 |
| 1:B:655:PRO:HG3 | 1:B:982:LEU:HB3 | 1.84 | 0.59 |
| 1:D:101:ARG:O | 1:D:104:ASP:HB2 | 2.01 | 0.59 |
| 1:D:512:PHE:CZ | 4:D:1201:BTI:H5 | 2.37 | 0.59 |
| 1:A:145:HIS:HE1 | 1:A:302:ILE:O | 1.86 | 0.59 |
| 1:A:382:ASP:OD1 | 1:A:384:LEU:HD13 | 2.02 | 0.59 |
| 1:B:167:ILE:CG1 | 1:B:168:PRO:HD3 | 2.31 | 0.59 |
| 1:A:434:ILE:HG13 | 1:C:341:GLY:O | 2.02 | 0.59 |
| 1:C:571:ARG:HH11 | 1:C:575:GLN:NE2 | 2.00 | 0.59 |
| 1:A:720:LEU:HD11 | 1:A:758:GLU:HG3 | 1.85 | 0.59 |
| 1:C:1068:PRO:HD3 | 1:C:1074:ARG:NH1 | 2.18 | 0.59 |
| 1:B:1052:ILE:O | 1:B:1052:ILE:CG2 | 2.49 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:243:LYS:HZ3 | 1:D:243:LYS:CB | 2.08 | 0.59 |
| 1:B:955:PRO:HG2 | 1:B:958:GLY:O | 2.02 | 0.59 |
| 1:C:193:ILE:HB | 1:C:235:ILE:HB | 1.84 | 0.59 |
| 1:A:1033:LEU:HD23 | 1:A:1050:ILE:HG12 | 1.85 | 0.59 |
| 1:A:179:LEU:CD2 | 1:A:179:LEU:H | 2.02 | 0.59 |
| 1:A:362:MET:HE3 | 1:A:362:MET:CA | 2.33 | 0.59 |
| 1:A:377:ARG:HB3 | 1:A:425:LEU:HD13 | 1.84 | 0.59 |
| 1:A:860:GLU:OE2 | 1:A:891:LYS:NZ | 2.34 | 0.59 |
| 1:D:249:VAL:HG21 | 1:D:299:MET:HG3 | 1.84 | 0.59 |
| 1:D:263:ARG:HD3 | 1:D:335:ILE:HG22 | 1.85 | 0.59 |
| 1:D:811:ASN:H | 1:D:811:ASN:ND2 | 1.94 | 0.59 |
| 1:B:380:THR:CG2 | 1:B:426:LEU:HD11 | 2.33 | 0.58 |
| 1:B:898:ASN:ND2 | 1:B:906:LYS:HE3 | 2.17 | 0.58 |
| 1:C:434:ILE:HD12 | 1:C:435:SER:N | 2.18 | 0.58 |
| 1:C:895:ARG:CG | 1:C:895:ARG:NH1 | 2.49 | 0.58 |
| 1:D:920:TYR:OH | 1:D:938:LEU:O | 2.21 | 0.58 |
| 1:A:506:ASN:OD1 | 4:A:1203:BTI:H92 | 2.03 | 0.58 |
| 1:C:886:ARG:HG2 | 1:C:889:GLU:OE1 | 2.03 | 0.58 |
| 1:C:936:TYR:O | 1:C:937:LYS:CG | 2.39 | 0.58 |
| 1:C:175:LYS:H | 1:C:175:LYS:HD2 | 1.65 | 0.58 |
| 1:C:267:VAL:HG22 | 1:C:480:PHE:HD2 | 1.68 | 0.58 |
| 1:D:679:SER:HA | 1:D:907:VAL:HG23 | 1.84 | 0.58 |
| 1:A:77:ARG:NH1 | 1:A:77:ARG:CG | 2.60 | 0.58 |
| 1:C:517:GLU:O | 1:C:519:ARG:N | 2.36 | 0.58 |
| 1:A:1029:ASN:HD22 | 1:A:1029:ASN:C | 2.07 | 0.58 |
| 1:A:181:LYS:HG2 | 1:A:185:GLU:OE2 | 2.03 | 0.58 |
| 1:B:263:ARG:HD3 | 1:B:335:ILE:CG2 | 2.32 | 0.58 |
| 1:B:864:HIS:HD2 | 1:B:866:MET:N | 1.97 | 0.58 |
| 1:C:866:MET:CE | 1:C:871:TYR:HD1 | 2.14 | 0.58 |
| 1:D:519:ARG:HB2 | 1:D:520:PRO:CD | 2.34 | 0.58 |
| 1:A:142:HIS:H | 1:A:145:HIS:HD2 | 1.51 | 0.58 |
| 1:A:590:ILE:H | 1:A:590:ILE:HD12 | 1.68 | 0.58 |
| 1:A:641:MET:HE1 | 1:A:643:LEU:HD13 | 1.86 | 0.58 |
| 1:B:279:PRO:HD2 | 1:B:372:TYR:CD2 | 2.37 | 0.58 |
| 1:C:649:VAL:CG1 | 1:C:649:VAL:O | 2.51 | 0.58 |
| 1:D:249:VAL:HG22 | 1:D:308:GLY:O | 2.03 | 0.58 |
| 1:A:384:LEU:HG | 1:A:490:ILE:CD1 | 2.33 | 0.58 |
| 1:C:622:ASN:HD22 | 1:C:623:PRO:HD2 | 1.68 | 0.58 |
| 1:C:743:MET:CG | 1:C:907:VAL:HG13 | 2.33 | 0.58 |
| 1:A:194:LYS:HE2 | 2:A:1201:ADP:N7 | 2.19 | 0.58 |
| 1:A:622:ASN:C | 1:A:622:ASN:HD22 | 2.06 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:328:ARG:HD3 | 1:B:329:VAL:O | 2.04 | 0.58 |
| 1:B:404:GLY:O | 1:B:431:THR:HA | 2.04 | 0.58 |
| 1:C:152:LYS:H | 1:C:196:THR:HG22 | 1.69 | 0.58 |
| 1:D:1034:ASP:OD1 | 1:D:1036:PRO:HD2 | 2.03 | 0.58 |
| 1:D:875:SER:OG | 1:D:887:PHE:CE1 | 2.53 | 0.58 |
| 1:C:434:ILE:HD12 | 1:C:435:SER:H | 1.69 | 0.58 |
| 1:D:513:PRO:CD | 4:D:1201:BTI:H4 | 2.34 | 0.58 |
| 1:A:572:ASP:HB3 | 1:A:807:GLN:HE22 | 1.68 | 0.57 |
| 1:B:124:ASN:C | 1:B:124:ASN:OD1 | 2.42 | 0.57 |
| 1:B:588:ILE:HD13 | 1:B:630:LEU:HD23 | 1.86 | 0.57 |
| 1:B:597:VAL:CG2 | 1:B:830:GLY:HA3 | 2.34 | 0.57 |
| 1:C:359:GLU:CD | 1:C:359:GLU:H | 2.07 | 0.57 |
| 1:A:180:ALA:O | 1:A:183:PHE:N | 2.31 | 0.57 |
| 1:A:622:ASN:HD21 | 1:A:624:TRP:HD1 | 1.49 | 0.57 |
| 1:C:1007:ILE:O | 1:C:1011:VAL:HG23 | 2.03 | 0.57 |
| 1:C:846:SER:HA | 1:C:849:GLU:HG2 | 1.84 | 0.57 |
| 1:D:243:LYS:HB3 | 1:D:243:LYS:NZ | 2.06 | 0.57 |
| 1:A:37:ILE:O | 1:A:61:ILE:HG12 | 2.04 | 0.57 |
| 1:B:338:MET:HE2 | 1:B:430:SER:CB | 2.28 | 0.57 |
| 1:B:682:TRP:CE3 | 1:B:685:GLN:HG3 | 2.39 | 0.57 |
| 1:C:959:PHE:N | 1:C:959:PHE:CD1 | 2.71 | 0.57 |
| 1:C:936:TYR:HD1 | 1:C:966:VAL:HG12 | 1.69 | 0.57 |
| 1:D:572:ASP:HB3 | 1:D:807:GLN:NE2 | 2.19 | 0.57 |
| 1:D:986:ASP:OD2 | 1:D:986:ASP:C | 2.42 | 0.57 |
| 1:A:501:LEU:HB3 | 1:A:1078:TYR:CE1 | 2.40 | 0.57 |
| 1:B:504:ILE:CG2 | 1:B:1042:MET:HG3 | 2.34 | 0.57 |
| 1:B:606:MET:C | 1:B:606:MET:HE3 | 2.24 | 0.57 |
| 1:D:542:LYS:C | 1:D:542:LYS:HD3 | 2.25 | 0.57 |
| 1:A:192:MET:HE1 | 1:A:238:TYR:HE1 | 1.68 | 0.57 |
| 1:A:206:ILE:HD11 | 1:A:238:TYR:CZ | 2.39 | 0.57 |
| 1:B:413:PHE:CD1 | 1:B:414:GLN:HB3 | 2.39 | 0.57 |
| 1:A:174:ILE:HD11 | 1:A:235:ILE:CG2 | 2.35 | 0.57 |
| 1:A:565:LEU:HD21 | 1:A:826:THR:HB | 1.87 | 0.57 |
| 1:B:334:THR:HG22 | 1:B:406:ARG:NH2 | 2.18 | 0.57 |
| 1:B:860:GLU:HA | 1:B:863:GLN:HE21 | 1.69 | 0.57 |
| 1:C:828:ILE:HD12 | 1:C:829:GLU:N | 2.19 | 0.57 |
| 1:D:288:ARG:O | 1:D:288:ARG:HG2 | 2.04 | 0.57 |
| 1:B:525:GLU:HG2 | 1:B:527:ALA:HB3 | 1.87 | 0.57 |
| 1:B:712:ASN:OD1 | 1:B:712:ASN:C | 2.43 | 0.57 |
| 1:C:192:MET:HE1 | 5:C:1202:ATP:C4 | 2.40 | 0.57 |
| 1:C:357:LEU:HA | 1:C:360:ILE:HD12 | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:622:ASN:C | 1:D:622:ASN:ND2 | 2.58 | 0.57 |
| 1:D:622:ASN:HD22 | 1:D:623:PRO:HD2 | 1.69 | 0.57 |
| 1:A:103:ILE:HG21 | 1:A:134:GLU:HG3 | 1.87 | 0.56 |
| 1:A:180:ALA:O | 1:A:184:ALA:N | 2.33 | 0.56 |
| 1:A:406:ARG:HH21 | 1:C:403:ALA:CB | 2.17 | 0.56 |
| 1:C:961:LYS:O | 1:C:964:GLN:N | 2.38 | 0.56 |
| 1:A:206:ILE:HG22 | 1:A:207:VAL:N | 2.19 | 0.56 |
| 1:A:175:LYS:HZ2 | 1:A:232:GLU:HG3 | 1.68 | 0.56 |
| 1:A:446:SER:O | 1:A:450:MET:HG2 | 2.06 | 0.56 |
| 1:B:272:GLN:HE21 | 1:B:274:VAL:HG22 | 1.71 | 0.56 |
| 1:B:332:GLU:N | 1:B:332:GLU:OE1 | 2.37 | 0.56 |
| 1:B:59:LEU:O | 1:B:60:ASP:HB2 | 2.06 | 0.56 |
| 1:D:362:MET:HE1 | 1:D:367:ILE:HD11 | 1.87 | 0.56 |
| 1:B:525:GLU:HB3 | 1:B:840:THR:HG21 | 1.87 | 0.56 |
| 1:D:260:LEU:HD22 | 1:D:342:ILE:HD13 | 1.88 | 0.56 |
| 1:D:331:VAL:O | 1:D:428:LYS:HE2 | 2.05 | 0.56 |
| 1:A:109:ALA:O | 1:A:110:ASN:HB2 | 2.04 | 0.56 |
| 1:B:396:ALA:HB3 | 1:B:453:ARG:CB | 2.35 | 0.56 |
| 1:B:622:ASN:HD21 | 1:B:624:TRP:HD1 | 1.54 | 0.56 |
| 1:C:986:ASP:OD1 | 1:C:989:LYS:HG3 | 2.06 | 0.56 |
| 1:B:403:ALA:C | 1:B:442:LYS:HE2 | 2.23 | 0.56 |
| 1:C:641:MET:HE2 | 1:C:674:PHE:CE1 | 2.41 | 0.56 |
| 1:C:756:ILE:O | 1:C:760:LYS:HB2 | 2.06 | 0.56 |
| 1:D:457:THR:OG1 | 1:D:459:ILE:HG13 | 2.05 | 0.56 |
| 1:D:675:ARG:HA | 1:D:701:GLU:HB2 | 1.88 | 0.56 |
| 1:D:799:ALA:H | 1:D:811:ASN:ND2 | 2.03 | 0.56 |
| 1:A:631:ARG:NH2 | 1:A:672:ASP:OD1 | 2.39 | 0.56 |
| 1:D:330:GLN:O | 1:D:333:HIS:ND1 | 2.30 | 0.56 |
| 1:A:382:ASP:O | 1:A:387:PHE:N | 2.38 | 0.55 |
| 1:A:396:ALA:HB3 | 1:A:453:ARG:HB2 | 1.88 | 0.55 |
| 1:A:98:ASN:C | 1:A:98:ASN:ND2 | 2.56 | 0.55 |
| 1:B:414:GLN:HE22 | 1:D:1079:ALA:HB2 | 1.70 | 0.55 |
| 1:B:504:ILE:HG21 | 1:B:1042:MET:HG3 | 1.87 | 0.55 |
| 1:C:991:ARG:NH1 | 1:C:1002:VAL:O | 2.31 | 0.55 |
| 1:C:200:GLY:C | 1:C:202:LYS:N | 2.59 | 0.55 |
| 1:B:379:THR:HG22 | 1:B:424:SER:O | 2.07 | 0.55 |
| 1:C:794:ILE:HD12 | 1:C:796:THR:CG2 | 2.36 | 0.55 |
| 1:C:679:SER:HB3 | 1:C:908:THR:O | 2.06 | 0.55 |
| 1:D:252:ASP:O | 1:D:305:VAL:HG22 | 2.05 | 0.55 |
| 1:D:866:MET:CE | 1:D:871:TYR:HA | 2.35 | 0.55 |
| 1:D:875:SER:OG | 1:D:887:PHE:CZ | 2.58 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:742:ASP:OD2 | 1:C:745:GLY:HA2 | 2.07 | 0.55 |
| 1:A:274:VAL:HG12 | 1:A:275:VAL:HG23 | 1.88 | 0.55 |
| 1:B:251:GLY:HA3 | 1:B:257:ILE:HG12 | 1.89 | 0.55 |
| 1:B:513:PRO:O | 1:B:515:ASN:HB2 | 2.06 | 0.55 |
| 1:A:641:MET:CE | 1:A:643:LEU:HD13 | 2.37 | 0.55 |
| 1:A:897:VAL:HG11 | 1:A:917:MET:HB3 | 1.88 | 0.55 |
| 1:B:101:ARG:HG2 | 1:B:101:ARG:NH1 | 2.20 | 0.55 |
| 1:B:620:LYS:CG | 4:B:1201:BTI:H63 | 2.37 | 0.55 |
| 1:B:448:ARG:HH22 | 1:B:467:LYS:HD2 | 1.72 | 0.55 |
| 1:C:230:ASN:C | 1:C:230:ASN:HD22 | 2.10 | 0.55 |
| 1:C:396:ALA:CA | 1:C:414:GLN:HE22 | 2.10 | 0.55 |
| 1:C:960:ASN:O | 1:C:963:LEU:HB3 | 2.06 | 0.55 |
| 1:D:752:ALA:HB2 | 1:D:782:THR:HG23 | 1.88 | 0.55 |
| 1:A:1065:ILE:HG12 | 1:A:1076:ILE:HD13 | 1.89 | 0.55 |
| 1:B:403:ALA:O | 1:B:442:LYS:CE | 2.35 | 0.55 |
| 1:B:577:LEU:HD13 | 1:B:842:ARG:HH22 | 1.71 | 0.55 |
| 1:C:494:LEU:HD22 | 1:C:494:LEU:H | 1.71 | 0.55 |
| 1:D:263:ARG:HG2 | 1:D:335:ILE:HG21 | 1.88 | 0.55 |
| 1:B:771:HIS:HB2 | 1:B:795:ASP:OD2 | 2.07 | 0.55 |
| 1:B:924:ASN:HB2 | 1:B:926:LEU:HD21 | 1.88 | 0.55 |
| 1:C:142:HIS:H | 1:C:145:HIS:HD2 | 1.54 | 0.55 |
| 1:D:263:ARG:HD3 | 1:D:335:ILE:HG21 | 1.86 | 0.55 |
| 1:A:991:ARG:HB2 | 1:A:1007:ILE:HD11 | 1.89 | 0.54 |
| 1:B:1080:MET:O | 1:B:1081:ASN:C | 2.45 | 0.54 |
| 1:B:343:ASP:CG | 1:B:346:LYS:HB2 | 2.28 | 0.54 |
| 1:C:313:LEU:HD22 | 1:C:323:ILE:HD12 | 1.88 | 0.54 |
| 1:C:370:LEU:O | 1:C:432:HIS:HE1 | 1.90 | 0.54 |
| 1:C:828:ILE:HD12 | 1:C:829:GLU:H | 1.73 | 0.54 |
| 1:B:263:ARG:HG2 | 1:B:278:ALA:HB2 | 1.89 | 0.54 |
| 1:D:459:ILE:HB | 1:D:460:PRO:HD3 | 1.88 | 0.54 |
| 1:A:194:LYS:HD2 | 1:A:234:TYR:OH | 2.07 | 0.54 |
| 1:A:572:ASP:HB3 | 1:A:807:GLN:NE2 | 2.22 | 0.54 |
| 1:B:334:THR:O | 1:B:338:MET:HG3 | 2.07 | 0.54 |
| 1:C:274:VAL:HG12 | 1:C:275:VAL:HG23 | 1.89 | 0.54 |
| 1:C:867:PRO:HG3 | 1:C:906:LYS:O | 2.08 | 0.54 |
| 1:C:504:ILE:HD13 | 1:C:1042:MET:HE1 | 1.89 | 0.54 |
| 1:D:960:ASN:ND2 | 1:D:963:LEU:H | 2.05 | 0.54 |
| 1:B:263:ARG:HD3 | 1:B:335:ILE:HG22 | 1.87 | 0.54 |
| 1:C:37:ILE:HG22 | 1:C:37:ILE:O | 2.06 | 0.54 |
| 1:A:216:ALA:C | 1:A:218:HIS:N | 2.59 | 0.54 |
| 1:C:43:ALA:HA | 1:C:66:ILE:HD11 | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:539:SER:HA | 1:C:543:GLN:HG3 | 1.89 | 0.54 |
| 1:C:941:PRO:C | 1:C:943:SER:H | 2.11 | 0.54 |
| 1:D:357:LEU:HD13 | 1:D:362:MET:HG3 | 1.89 | 0.54 |
| 1:D:91:GLY:O | 1:D:92:PRO:O | 2.25 | 0.54 |
| 1:A:334:THR:CG2 | 1:A:428:LYS:NZ | 2.71 | 0.54 |
| 1:B:144:GLU:O | 1:B:148:MET:HB2 | 2.08 | 0.54 |
| 1:C:1042:MET:CE | 1:C:1060:ILE:HG21 | 2.38 | 0.54 |
| 1:C:770:LEU:HB3 | 1:C:794:ILE:HG22 | 1.89 | 0.54 |
| 1:D:124:ASN:OD1 | 1:D:126:GLN:HB2 | 2.07 | 0.54 |
| 1:D:262:GLU:OE2 | 1:D:262:GLU:N | 2.33 | 0.54 |
| 1:D:446:SER:O | 1:D:450:MET:HG2 | 2.08 | 0.54 |
| 1:D:864:HIS:CD2 | 1:D:866:MET:HB2 | 2.43 | 0.54 |
| 1:A:156:ARG:NH1 | 1:A:156:ARG:HB3 | 2.12 | 0.54 |
| 1:A:186:GLU:O | 1:A:187:ALA:HB2 | 2.08 | 0.54 |
| 1:A:811:ASN:H | 1:A:811:ASN:ND2 | 2.04 | 0.54 |
| 1:B:252:ASP:OD1 | 1:B:256:ASN:HB2 | 2.08 | 0.54 |
| 1:B:312:PHE:HA | 1:B:321:PHE:O | 2.08 | 0.54 |
| 1:C:174:ILE:HG22 | 1:C:217:PHE:HE1 | 1.72 | 0.54 |
| 1:C:889:GLU:C | 1:C:891:LYS:H | 2.12 | 0.54 |
| 1:D:570:PHE:O | 1:D:574:HIS:HE1 | 1.91 | 0.54 |
| 1:D:717:ASN:HD22 | 1:D:717:ASN:N | 2.06 | 0.54 |
| 1:A:266:SER:O | 1:A:268:GLN:HG2 | 2.08 | 0.53 |
| 1:A:501:LEU:HD11 | 1:A:1080:MET:HE2 | 1.90 | 0.53 |
| 1:D:596:ASP:O | 1:D:599:LYS:HG2 | 2.08 | 0.53 |
| 1:D:776:SER:HB3 | 1:D:861:ILE:HD11 | 1.89 | 0.53 |
| 1:A:512:PHE:CZ | 4:A:1203:BTI:H5 | 2.42 | 0.53 |
| 1:A:384:LEU:HD12 | 1:A:384:LEU:H | 1.73 | 0.53 |
| 1:A:484:THR:HB | 1:A:487:LEU:HD22 | 1.90 | 0.53 |
| 1:B:624:TRP:CZ2 | 1:B:1008:ILE:CD1 | 2.91 | 0.53 |
| 1:B:773:HIS:HA | 1:B:806:SER:O | 2.09 | 0.53 |
| 1:C:385:ASN:C | 1:C:387:PHE:H | 2.12 | 0.53 |
| 1:C:738:LEU:CD2 | 1:C:759:LEU:HD13 | 2.39 | 0.53 |
| 1:C:940:PHE:HB3 | 1:C:944:VAL:CG1 | 2.37 | 0.53 |
| 1:C:959:PHE:HD1 | 1:C:959:PHE:H | 1.53 | 0.53 |
| 1:B:494:LEU:O | 1:B:496:ARG:N | 2.42 | 0.53 |
| 1:A:360:ILE:HG22 | 1:A:362:MET:H | 1.73 | 0.53 |
| 1:C:224:ALA:HB3 | 1:C:231:SER:HB2 | 1.91 | 0.53 |
| 1:C:259:HIS:O | 1:C:260:LEU:HD23 | 2.08 | 0.53 |
| 1:C:513:PRO:CB | 1:C:513:PRO:C | 2.74 | 0.53 |
| 1:D:661:LYS:HG2 | 1:D:1008:ILE:HD13 | 1.91 | 0.53 |
| 1:A:775:THR:OG1 | 1:A:861:ILE:HD13 | 2.07 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|---------------------|--------------------------|-------------------|
| 1:C:145:HIS:HA | 1:C:148:MET:HG2 | 1.91 | 0.53 |
| 1:A:406:ARG:NH2 | 1:C:403:ALA:HB2 | 2.23 | 0.53 |
| 1:A:701:GLU:HG3 | 1:A:737:ILE:HB | 1.89 | 0.53 |
| 1:B:679:SER:O | 1:B:905:VAL:HB | 2.08 | 0.53 |
| 1:A:217:PHE:HE2 | 1:A:221:LYS:HE3 | 1.71 | 0.53 |
| 1:A:398:ARG:NH1 | 1:A:398:ARG:CG | 2.59 | 0.53 |
| 1:A:874:LEU:HD11 | 1:A:919:LEU:CD2 | 2.39 | 0.53 |
| 1:B:89:ASP:OD1 | 1:B:90:LEU:HD12 | 2.09 | 0.53 |
| 1:C:551:LYS:O | 1:C:555:GLU:HG2 | 2.08 | 0.53 |
| 1:D:145:HIS:HE1 | 1:D:302:ILE:O | 1.92 | 0.53 |
| 1:A:192:MET:HE2 | 1:A:238:TYR:HD1 | 1.73 | 0.53 |
| 1:A:413:PHE:HZ | 1:A:416:ALA:HB2 | 1.61 | 0.53 |
| 1:A:543:GLN:HE22 | 1:A:636:ASN:HA | 1.73 | 0.53 |
| 1:B:495:ASP:O | 1:B:496:ARG:C | 2.47 | 0.53 |
| 1:B:924:ASN:HB2 | 1:B:926:LEU:CD2 | 2.39 | 0.53 |
| 1:C:192:MET:HB2 | 1:C:238:TYR:HB2 | 1.91 | 0.53 |
| 1:C:382:ASP:O | 1:C:387:PHE:HA | 2.08 | 0.53 |
| 1:A:194:LYS:HB3 | 1:A:234:TYR:CE2 | 2.44 | 0.53 |
| 1:A:543:GLN:NE2 | 1:A:543:GLN:H | 2.06 | 0.53 |
| 1:B:840:THR:O | 1:B:843:THR:HB | 2.09 | 0.53 |
| 1:B:945:VAL:HG12 | 1:B:967:ILE:CG2 | 2.32 | 0.53 |
| 1:C:59:LEU:O | 1:C:60:ASP:HB2 | 2.07 | 0.53 |
| 1:B:749:PRO:HG3 | 1:B:781:LEU:HB3 | 1.90 | 0.52 |
| 1:C:166:VAL:HG12 | 1:C:167:ILE:HD12 | 1.90 | 0.52 |
| 1:C:717:ASN:HD22 | 1:C:717(A):ILE:HG13 | 1.74 | 0.52 |
| 1:D:311:GLU:HG3 | 1:D:324:GLU:HG3 | 1.91 | 0.52 |
| 1:D:496:ARG:HH11 | 1:D:496:ARG:CB | 2.12 | 0.52 |
| 1:D:506:ASN:HD21 | 1:D:510:ASN:HD22 | 1.56 | 0.52 |
| 1:D:513:PRO:O | 1:D:515:ASN:CB | 2.55 | 0.52 |
| 1:D:760:LYS:HG2 | 1:D:768:ILE:HD13 | 1.91 | 0.52 |
| 1:B:167:ILE:CG1 | 1:B:168:PRO:CD | 2.87 | 0.52 |
| 1:D:519:ARG:HB2 | 1:D:520:PRO:HD2 | 1.91 | 0.52 |
| 1:A:625:GLU:O | 1:A:629:ARG:HG3 | 2.09 | 0.52 |
| 1:A:849:GLU:O | 1:A:852:SER:C | 2.44 | 0.52 |
| 1:A:879:LYS:O | 1:A:881:LEU:N | 2.42 | 0.52 |
| 1:C:519:ARG:CG | 1:C:520:PRO:O | 2.57 | 0.52 |
| 1:D:284:SER:OG | 1:D:287:LEU:HB2 | 2.09 | 0.52 |
| 1:D:451:ARG:CG | 1:D:451:ARG:HH11 | 2.08 | 0.52 |
| 1:B:863:GLN:O | 1:B:895:ARG:HG3 | 2.09 | 0.52 |
| 1:C:646:SER:O | 1:C:653:ASN:HA | 2.09 | 0.52 |
| 1:D:166:VAL:CG1 | 1:D:167:ILE:N | 2.64 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:878:ALA:O | 1:D:883:LEU:HB2 | 2.09 | 0.52 |
| 1:A:241:ASN:N | 1:A:242:PRO:CD | 2.72 | 0.52 |
| 1:B:1000:GLY:H | 1:B:1001:PRO:CD | 2.23 | 0.52 |
| 1:C:142:HIS:HB2 | 1:C:145:HIS:CD2 | 2.44 | 0.52 |
| 1:C:394:ILE:HD11 | 1:C:426:LEU:HD22 | 1.92 | 0.52 |
| 1:D:1043:ARG:O | 1:D:1046:GLU:HB2 | 2.10 | 0.52 |
| 1:D:571:ARG:HG2 | 1:D:611:THR:HG21 | 1.90 | 0.52 |
| 1:B:901:PHE:HZ | 1:B:917:MET:HG3 | 1.74 | 0.52 |
| 1:D:494:LEU:HG | 1:D:499:LYS:CE | 2.32 | 0.52 |
| 1:D:594:THR:HG23 | 1:D:598:PHE:CD1 | 2.44 | 0.52 |
| 1:D:921:MET:HG2 | 1:D:926:LEU:HB3 | 1.91 | 0.52 |
| 1:A:743:MET:HG3 | 1:A:907:VAL:HG13 | 1.91 | 0.52 |
| 1:A:804:LEU:HD13 | 1:A:854:ILE:HG22 | 1.92 | 0.52 |
| 1:A:828:ILE:HD12 | 1:A:829:GLU:H | 1.75 | 0.52 |
| 1:A:952:ILE:O | 1:A:952:ILE:HG22 | 2.10 | 0.52 |
| 1:B:624:TRP:HZ2 | 1:B:1008:ILE:HD13 | 1.74 | 0.52 |
| 1:B:540:GLY:N | 1:B:543:GLN:HE21 | 2.08 | 0.52 |
| 1:B:743:MET:SD | 1:B:907:VAL:HG13 | 2.49 | 0.52 |
| 1:C:672:ASP:HA | 1:C:698:LYS:HD2 | 1.91 | 0.52 |
| 1:A:114:ILE:HG13 | 1:A:136:ILE:HG21 | 1.92 | 0.52 |
| 1:A:655:PRO:HG2 | 1:A:985:VAL:HG23 | 1.92 | 0.52 |
| 1:B:644:ARG:HD2 | 1:B:647:ASN:OD1 | 2.09 | 0.52 |
| 1:C:1068:PRO:HD3 | 1:C:1074:ARG:CZ | 2.40 | 0.52 |
| 1:D:401:GLY:O | 1:D:445:ARG:NH2 | 2.39 | 0.52 |
| 1:D:497:GLY:O | 1:D:501:LEU:HG | 2.10 | 0.52 |
| 1:A:622:ASN:ND2 | 1:A:623:PRO:HD2 | 2.24 | 0.52 |
| 1:C:641:MET:CE | 1:C:674:PHE:CE1 | 2.93 | 0.52 |
| 1:D:593:LYS:O | 1:D:597:VAL:HG23 | 2.09 | 0.52 |
| 1:A:47:GLU:OE1 | 1:A:428:LYS:HE3 | 2.10 | 0.52 |
| 1:B:927:ASP:OD2 | 1:B:930:SER:HB2 | 2.10 | 0.52 |
| 1:C:59:LEU:HD11 | 1:C:346:LYS:HG2 | 1.91 | 0.52 |
| 1:D:431:THR:OG1 | 1:D:443:MET:HB2 | 2.10 | 0.52 |
| 1:A:858:ASN:HD21 | 1:A:860:GLU:HB2 | 1.75 | 0.51 |
| 1:B:641:MET:HB3 | 1:B:671:ILE:HD12 | 1.92 | 0.51 |
| 1:C:375:GLN:OE1 | 1:C:377:ARG:HD2 | 2.10 | 0.51 |
| 1:C:926:LEU:HD11 | 1:C:938:LEU:HD11 | 1.92 | 0.51 |
| 1:A:192:MET:CE | 1:A:238:TYR:HD1 | 2.22 | 0.51 |
| 1:A:360:ILE:CG2 | 1:A:362:MET:HG2 | 2.40 | 0.51 |
| 1:A:964:GLN:HG2 | 1:A:968:LEU:HD11 | 1.93 | 0.51 |
| 1:D:1060:ILE:HG12 | 1:D:1080:MET:HG3 | 1.91 | 0.51 |
| 1:D:313:LEU:O | 1:D:320:PHE:HA | 2.09 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:86:VAL:HG11 | 1:B:95:SER:O | 2.10 | 0.51 |
| 1:C:590:ILE:CG1 | 1:C:837:TYR:CE2 | 2.93 | 0.51 |
| 1:A:331:VAL:HG12 | 1:A:428:LYS:HE2 | 1.92 | 0.51 |
| 1:B:574:HIS:CD2 | 1:B:580:THR:HA | 2.45 | 0.51 |
| 1:C:814:TYR:CE2 | 1:C:828:ILE:HG12 | 2.45 | 0.51 |
| 1:D:513:PRO:HD2 | 4:D:1201:BTI:H4 | 1.91 | 0.51 |
| 1:D:263:ARG:CG | 1:D:335:ILE:HG21 | 2.40 | 0.51 |
| 1:D:542:LYS:HE3 | 1:D:672:ASP:OD1 | 2.11 | 0.51 |
| 1:A:118:TYR:OH | 1:A:331:VAL:HG13 | 2.10 | 0.51 |
| 1:D:495:ASP:HB3 | 1:D:498:THR:CB | 2.37 | 0.51 |
| 1:D:605:GLU:HA | 1:D:640:GLN:HB3 | 1.91 | 0.51 |
| 1:D:832:GLU:O | 1:D:836:HIS:CD2 | 2.64 | 0.51 |
| 1:C:404:GLY:O | 1:C:431:THR:HA | 2.10 | 0.51 |
| 1:C:926:LEU:HD13 | 1:C:938:LEU:HD11 | 1.90 | 0.51 |
| 1:C:948:PHE:CD2 | 1:C:959:PHE:CD2 | 2.98 | 0.51 |
| 1:D:149:PHE:HZ | 1:D:302:ILE:HD13 | 1.76 | 0.51 |
| 1:D:501:LEU:HD11 | 1:D:1080:MET:HE2 | 1.91 | 0.51 |
| 1:A:222:SER:O | 1:A:226:LYS:HB2 | 2.10 | 0.51 |
| 1:A:334:THR:CB | 1:A:406:ARG:HH11 | 2.08 | 0.51 |
| 1:A:384:LEU:HG | 1:A:490:ILE:HD11 | 1.92 | 0.51 |
| 1:A:39:LYS:HE2 | 1:A:82:GLU:OE1 | 2.11 | 0.51 |
| 1:A:521:LYS:NZ | 1:A:1046:GLU:OE1 | 2.43 | 0.51 |
| 1:A:524:TYR:HD2 | 1:A:843:THR:HG22 | 1.76 | 0.51 |
| 1:A:556:TRP:O | 1:A:560:GLN:HG2 | 2.11 | 0.51 |
| 1:C:199:GLY:HA2 | 5:C:1202:ATP:O3B | 2.10 | 0.51 |
| 1:D:811:ASN:N | 1:D:811:ASN:ND2 | 2.56 | 0.51 |
| 1:A:497:GLY:O | 1:A:501:LEU:HG | 2.11 | 0.51 |
| 1:A:794:ILE:CD1 | 1:A:813:LEU:CD2 | 2.89 | 0.51 |
| 1:B:798:VAL:CG1 | 1:B:831:MET:CE | 2.86 | 0.51 |
| 1:C:1024:ARG:NH1 | 1:C:1024:ARG:CG | 2.53 | 0.51 |
| 1:C:920:TYR:CE1 | 1:C:940:PHE:CD2 | 2.99 | 0.51 |
| 1:D:418:ILE:HD12 | 1:D:418:ILE:N | 2.23 | 0.51 |
| 1:D:449:GLU:O | 1:D:450:MET:C | 2.49 | 0.51 |
| 1:C:334:THR:CB | 1:C:406:ARG:HH12 | 2.13 | 0.51 |
| 1:D:1056:LYS:HG2 | 1:D:1056:LYS:O | 2.11 | 0.51 |
| 1:D:160:ILE:O | 1:D:161:LYS:C | 2.48 | 0.51 |
| 1:B:395:ILE:N | 1:B:453:ARG:O | 2.34 | 0.51 |
| 1:C:864:HIS:HD2 | 1:C:866:MET:H | 1.57 | 0.51 |
| 1:C:921:MET:CA | 1:C:926:LEU:HB2 | 2.40 | 0.51 |
| 1:C:989:LYS:O | 1:C:993:LEU:HB2 | 2.10 | 0.51 |
| 1:A:810:ALA:HB1 | 1:A:831:MET:HE1 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:874:LEU:CD1 | 1:A:919:LEU:HD21 | 2.41 | 0.50 |
| 1:B:124:ASN:OD1 | 1:B:127:PHE:N | 2.30 | 0.50 |
| 1:B:266:SER:HA | 1:B:478:THR:HG22 | 1.93 | 0.50 |
| 1:B:512:PHE:HB3 | 1:B:516:VAL:HB | 1.92 | 0.50 |
| 1:B:917:MET:HG2 | 1:B:944:VAL:HG11 | 1.93 | 0.50 |
| 1:C:173:PRO:C | 1:C:174:ILE:HD12 | 2.32 | 0.50 |
| 1:C:304:TYR:OH | 1:C:307:ALA:O | 2.16 | 0.50 |
| 1:A:362:MET:HE1 | 1:A:367:ILE:CD1 | 2.40 | 0.50 |
| 1:A:775:THR:OG1 | 1:A:861:ILE:HD11 | 2.10 | 0.50 |
| 1:A:874:LEU:HD11 | 1:A:919:LEU:HD22 | 1.94 | 0.50 |
| 1:B:365:LYS:HB2 | 1:B:365:LYS:HZ3 | 1.75 | 0.50 |
| 1:B:893:MET:HG2 | 1:B:921:MET:HB2 | 1.92 | 0.50 |
| 1:C:193:ILE:HG12 | 1:C:194:LYS:N | 2.25 | 0.50 |
| 1:C:334:THR:CB | 1:C:406:ARG:HH11 | 2.09 | 0.50 |
| 1:C:647:ASN:N | 1:C:647:ASN:OD1 | 2.44 | 0.50 |
| 1:B:811:ASN:H | 1:B:811:ASN:HD22 | 1.59 | 0.50 |
| 1:C:376:CYS:SG | 1:C:462:LEU:HD13 | 2.51 | 0.50 |
| 1:A:375:GLN:NE2 | 1:A:428:LYS:HZ3 | 2.10 | 0.50 |
| 1:C:1036:PRO:O | 1:C:1040:PHE:HB2 | 2.10 | 0.50 |
| 1:D:679:SER:HA | 1:D:907:VAL:CG2 | 2.42 | 0.50 |
| 1:D:740:ILE:HD13 | 1:D:740:ILE:N | 2.27 | 0.50 |
| 1:B:165:PRO:O | 1:B:166:VAL:HG13 | 2.11 | 0.50 |
| 1:C:1062:LEU:CD1 | 1:C:1078:TYR:CE2 | 2.92 | 0.50 |
| 1:D:425:LEU:HD12 | 1:D:425:LEU:C | 2.31 | 0.50 |
| 1:B:374:ILE:HG22 | 1:B:443:MET:CE | 2.41 | 0.50 |
| 1:B:571:ARG:HH21 | 1:B:605:GLU:CD | 2.15 | 0.50 |
| 1:B:285:PRO:O | 1:B:288:ARG:HG2 | 2.11 | 0.50 |
| 1:B:565:LEU:HD11 | 1:B:598:PHE:HE2 | 1.76 | 0.50 |
| 1:C:337:GLU:OE2 | 1:C:406:ARG:NH2 | 2.45 | 0.50 |
| 1:C:798:VAL:O | 1:C:799:ALA:C | 2.50 | 0.50 |
| 1:D:542:LYS:O | 1:D:542:LYS:HD3 | 2.11 | 0.50 |
| 1:A:406:ARG:HH21 | 1:C:403:ALA:CA | 2.24 | 0.50 |
| 1:A:799:ALA:H | 1:A:811:ASN:ND2 | 2.08 | 0.50 |
| 1:B:332:GLU:HA | 1:B:375:GLN:NE2 | 2.27 | 0.50 |
| 1:B:647:ASN:HB3 | 1:B:652:LYS:O | 2.12 | 0.50 |
| 1:C:1063:GLU:O | 1:C:1064:THR:HG23 | 2.12 | 0.50 |
| 1:C:189:PHE:H | 1:C:190:PRO:CD | 2.24 | 0.50 |
| 1:C:644:ARG:O | 1:C:645:ALA:C | 2.50 | 0.50 |
| 1:C:709:ASP:H | 1:C:715:ARG:HG2 | 1.77 | 0.50 |
| 1:D:122:SER:HB2 | 1:D:328:ARG:HG2 | 1.94 | 0.50 |
| 1:D:62:SER:HA | 1:D:81:ASP:OD1 | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:866:MET:HG2 | 1:A:894:TYR:CE2 | 2.47 | 0.50 |
| 1:B:385:ASN:CG | 1:B:385:ASN:O | 2.50 | 0.50 |
| 1:B:395:ILE:HD11 | 1:B:453:ARG:HG2 | 1.93 | 0.50 |
| 1:B:832:GLU:OE2 | 1:C:859:THR:OG1 | 2.28 | 0.50 |
| 1:C:396:ALA:HA | 1:C:414:GLN:NE2 | 2.13 | 0.50 |
| 1:C:398:ARG:HG3 | 1:C:398:ARG:NH1 | 2.25 | 0.50 |
| 1:C:861:ILE:HD11 | 1:C:866:MET:O | 2.12 | 0.50 |
| 1:A:334:THR:OG1 | 1:A:375:GLN:NE2 | 2.44 | 0.49 |
| 1:B:294:ALA:O | 1:B:297:GLN:HB3 | 2.11 | 0.49 |
| 1:D:746:LEU:HD11 | 1:D:865:GLU:HG2 | 1.93 | 0.49 |
| 1:A:42:VAL:HG23 | 1:A:53:PHE:HE2 | 1.77 | 0.49 |
| 1:C:1029:ASN:C | 1:C:1029:ASN:HD22 | 2.14 | 0.49 |
| 1:C:219:ARG:O | 1:C:223:GLU:HB2 | 2.13 | 0.49 |
| 1:D:459:ILE:N | 1:D:460:PRO:CD | 2.75 | 0.49 |
| 1:C:386:ASP:O | 1:C:387:PHE:HB2 | 2.11 | 0.49 |
| 1:D:1053:ASP:HB2 | 1:D:1056:LYS:HD3 | 1.94 | 0.49 |
| 1:D:164:LEU:HG | 1:D:165:PRO:HD2 | 1.95 | 0.49 |
| 1:D:167:ILE:HG23 | 1:D:321:PHE:CG | 2.48 | 0.49 |
| 1:A:141:PRO:HB2 | 1:A:145:HIS:HB2 | 1.94 | 0.49 |
| 1:C:891:LYS:HA | 1:C:894:TYR:HB2 | 1.94 | 0.49 |
| 1:D:561:ASP:O | 1:D:822:ARG:HD2 | 2.12 | 0.49 |
| 1:A:229:GLY:O | 1:A:230:ASN:HB2 | 2.12 | 0.49 |
| 1:A:375:GLN:NE2 | 1:A:428:LYS:NZ | 2.61 | 0.49 |
| 1:B:103:ILE:HG21 | 1:B:134:GLU:HG3 | 1.95 | 0.49 |
| 1:A:524:TYR:CD2 | 1:A:843:THR:HG22 | 2.46 | 0.49 |
| 1:D:90:LEU:HB2 | 1:D:95:SER:OG | 2.13 | 0.49 |
| 1:A:206:ILE:CD1 | 1:A:238:TYR:CE1 | 2.96 | 0.49 |
| 1:B:867:PRO:O | 1:B:868:GLY:C | 2.51 | 0.49 |
| 1:C:399:SER:HB3 | 1:C:400:SER:H | 1.47 | 0.49 |
| 1:C:887:PHE:HA | 1:C:890:VAL:HG23 | 1.95 | 0.49 |
| 1:B:1066:SER:HB2 | 1:D:1064:THR:CG2 | 2.39 | 0.49 |
| 1:A:239:ILE:O | 1:A:239:ILE:HG13 | 2.13 | 0.49 |
| 1:A:375:GLN:HE22 | 1:A:428:LYS:NZ | 2.11 | 0.49 |
| 1:A:454:GLY:O | 1:A:455:VAL:HG22 | 2.12 | 0.49 |
| 1:A:69:ASN:HD22 | 1:A:72:LYS:HE3 | 1.77 | 0.49 |
| 1:B:581:ARG:HG3 | 1:B:848:PHE:CD2 | 2.48 | 0.49 |
| 1:A:184:ALA:HA | 1:A:191:LEU:HD11 | 1.94 | 0.49 |
| 1:A:69:ASN:ND2 | 1:A:72:LYS:HE3 | 2.27 | 0.49 |
| 1:B:991:ARG:NH1 | 1:B:1002:VAL:HG12 | 2.28 | 0.49 |
| 1:B:949:LYS:HB2 | 1:B:951:GLU:HG3 | 1.94 | 0.49 |
| 1:C:680:LEU:HD11 | 1:C:952:ILE:HG22 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:C:687:LYS:O | 1:C:691:GLU:HG3 | 2.13 | 0.49 |
| 1:C:69:ASN:HD21 | 1:C:88:SER:HA | 1.77 | 0.49 |
| 1:A:334:THR:HG23 | 1:A:428:LYS:HZ1 | 1.78 | 0.48 |
| 1:A:627:LEU:O | 1:A:631:ARG:HB2 | 2.13 | 0.48 |
| 1:B:999:GLN:NE2 | 1:B:1001:PRO:HG3 | 2.28 | 0.48 |
| 1:D:631:ARG:NH2 | 1:D:672:ASP:OD1 | 2.46 | 0.48 |
| 1:C:944:VAL:HG13 | 1:C:945:VAL:HG13 | 1.95 | 0.48 |
| 1:D:403:ALA:O | 1:D:442:LYS:HD3 | 2.13 | 0.48 |
| 1:D:581:ARG:HG3 | 1:D:848:PHE:CG | 2.47 | 0.48 |
| 1:A:43:ALA:HA | 1:A:66:ILE:HD11 | 1.95 | 0.48 |
| 1:C:704:ILE:HB | 1:C:740:ILE:HD13 | 1.95 | 0.48 |
| 1:C:968:LEU:O | 1:C:969:LYS:C | 2.51 | 0.48 |
| 1:B:300:GLU:O | 1:B:300:GLU:HG2 | 2.12 | 0.48 |
| 1:B:948:PHE:HA | 1:B:959:PHE:CE2 | 2.48 | 0.48 |
| 1:C:1060:ILE:HG12 | 1:C:1080:MET:HG3 | 1.95 | 0.48 |
| 1:C:174:ILE:HG22 | 1:C:217:PHE:CE1 | 2.48 | 0.48 |
| 1:C:494:LEU:HB2 | 1:C:496:ARG:HH12 | 1.76 | 0.48 |
| 1:D:286:THR:O | 1:D:290:ARG:HG3 | 2.14 | 0.48 |
| 1:D:700:SER:H | 1:D:736:HIS:HD2 | 1.62 | 0.48 |
| 1:B:103:ILE:O | 1:B:107:LYS:HG3 | 2.14 | 0.48 |
| 1:C:895:ARG:HG2 | 1:C:895:ARG:NH1 | 2.25 | 0.48 |
| 1:C:948:PHE:CD2 | 1:C:959:PHE:HD2 | 2.31 | 0.48 |
| 1:D:413:PHE:O | 1:D:415:GLY:N | 2.46 | 0.48 |
| 1:A:799:ALA:H | 1:A:811:ASN:HD21 | 1.60 | 0.48 |
| 1:B:542:LYS:HE2 | 1:B:672:ASP:OD2 | 2.14 | 0.48 |
| 1:B:542:LYS:HE3 | 1:B:631:ARG:NH2 | 2.28 | 0.48 |
| 1:C:284:SER:OG | 1:C:287:LEU:HB2 | 2.13 | 0.48 |
| 1:D:338:MET:HE2 | 1:D:430:SER:CB | 2.44 | 0.48 |
| 1:A:170:THR:HG22 | 1:A:172:GLY:O | 2.13 | 0.48 |
| 1:A:332:GLU:HG2 | 1:A:332:GLU:O | 2.13 | 0.48 |
| 1:A:738:LEU:HD21 | 1:A:759:LEU:HD13 | 1.94 | 0.48 |
| 1:B:690:ASN:ND2 | 1:B:700:SER:OG | 2.47 | 0.48 |
| 1:B:711:LEU:HD11 | 1:B:750:LYS:HB3 | 1.95 | 0.48 |
| 1:A:58:GLU:HG3 | 1:C:445:ARG:HD3 | 1.96 | 0.48 |
| 1:D:38:LYS:CE | 1:D:38:LYS:HA | 2.34 | 0.48 |
| 1:A:196:THR:HG22 | 1:A:232:GLU:O | 2.14 | 0.48 |
| 1:C:1075:THR:HG22 | 1:C:1077:TYR:CE1 | 2.49 | 0.48 |
| 1:D:38:LYS:HE2 | 1:D:38:LYS:CA | 2.33 | 0.48 |
| 1:A:284:SER:HB2 | 1:A:285:PRO:HD2 | 1.96 | 0.48 |
| 1:A:571:ARG:HH11 | 1:A:575:GLN:NE2 | 2.12 | 0.48 |
| 1:B:268:GLN:HA | 1:B:274:VAL:HG23 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:C:259:HIS:C | 1:C:260:LEU:HD23 | 2.34 | 0.48 |
| 1:C:281:VAL:HG12 | 1:C:282:GLY:N | 2.29 | 0.48 |
| 1:C:253:GLU:HG2 | 1:C:305:VAL:HG11 | 1.95 | 0.48 |
| 1:C:378:ILE:HG13 | 1:C:450:MET:HE3 | 1.96 | 0.48 |
| 1:C:866:MET:HE2 | 1:C:871:TYR:CD1 | 2.28 | 0.48 |
| 1:C:883:LEU:HD11 | 1:C:923:GLN:HG2 | 1.96 | 0.48 |
| 1:D:644:ARG:NH2 | 1:D:908:THR:HB | 2.29 | 0.48 |
| 1:C:1062:LEU:HD12 | 1:C:1078:TYR:CD2 | 2.48 | 0.48 |
| 1:C:811:ASN:ND2 | 1:C:811:ASN:N | 2.51 | 0.48 |
| 1:D:431:THR:HG21 | 1:D:443:MET:HA | 1.94 | 0.48 |
| 1:D:814:TYR:C | 1:D:814:TYR:CD2 | 2.87 | 0.48 |
| 1:D:804:LEU:HD13 | 1:D:854:ILE:HG22 | 1.96 | 0.48 |
| 1:A:675:ARG:HA | 1:A:701:GLU:HB3 | 1.95 | 0.47 |
| 1:A:678:ASP:OD2 | 1:A:685:GLN:NE2 | 2.47 | 0.47 |
| 1:C:931:VAL:HG13 | 1:C:931:VAL:O | 2.14 | 0.47 |
| 1:D:504:ILE:HD13 | 1:D:1042:MET:HE1 | 1.95 | 0.47 |
| 1:D:309:THR:HB | 1:D:326:ASN:HD22 | 1.79 | 0.47 |
| 1:D:582:VAL:HA | 1:D:845:TYR:CE2 | 2.49 | 0.47 |
| 1:A:384:LEU:N | 1:A:384:LEU:HD12 | 2.29 | 0.47 |
| 1:A:42:VAL:CG2 | 1:A:53:PHE:CE2 | 2.97 | 0.47 |
| 1:A:964:GLN:HG2 | 1:A:968:LEU:CD1 | 2.44 | 0.47 |
| 1:B:309:THR:HB | 1:B:326:ASN:HB2 | 1.96 | 0.47 |
| 1:B:927:ASP:HB2 | 1:B:930:SER:H | 1.79 | 0.47 |
| 1:B:960:ASN:HD22 | 1:B:963:LEU:HB3 | 1.79 | 0.47 |
| 1:B:99:ILE:HD12 | 1:B:99:ILE:N | 2.28 | 0.47 |
| 1:C:332:GLU:HA | 1:C:375:GLN:NE2 | 2.29 | 0.47 |
| 1:C:390:ASP:OD1 | 1:C:456:LYS:HG2 | 2.14 | 0.47 |
| 1:C:649:VAL:HG13 | 1:C:649:VAL:O | 2.14 | 0.47 |
| 1:C:667:ALA:HB1 | 1:C:698:LYS:HE3 | 1.94 | 0.47 |
| 1:D:679:SER:OG | 1:D:909:PRO:HD2 | 2.14 | 0.47 |
| 1:A:175:LYS:HZ1 | 1:A:232:GLU:HG3 | 1.78 | 0.47 |
| 1:A:241:ASN:H | 1:A:242:PRO:HD3 | 1.79 | 0.47 |
| 1:A:403:ALA:CA | 1:C:406:ARG:HH21 | 2.27 | 0.47 |
| 1:C:334:THR:O | 1:C:338:MET:HG3 | 2.15 | 0.47 |
| 1:D:244:HIS:N | 1:D:266:SER:OG | 2.46 | 0.47 |
| 1:A:178:GLU:HG2 | 1:A:181:LYS:HB2 | 1.96 | 0.47 |
| 1:B:395:ILE:CD1 | 1:B:1086:ARG:O | 2.63 | 0.47 |
| 1:C:224:ALA:O | 1:C:228:PHE:HD1 | 1.98 | 0.47 |
| 1:D:152:LYS:HG2 | 1:D:152:LYS:O | 2.15 | 0.47 |
| 1:A:178:GLU:HG2 | 1:A:178:GLU:O | 2.14 | 0.47 |
| 1:C:149:PHE:O | 1:C:151:ASP:N | 2.42 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:364:GLN:HA | 1:C:367:ILE:HD12 | 1.95 | 0.47 |
| 1:D:756:ILE:HD13 | 1:D:791:VAL:HG23 | 1.97 | 0.47 |
| 1:A:1042:MET:HE1 | 1:A:1048:VAL:CG1 | 2.42 | 0.47 |
| 1:A:242:PRO:HD2 | 1:A:478:THR:OG1 | 2.14 | 0.47 |
| 1:A:383:PRO:HA | 1:A:387:PHE:CE2 | 2.49 | 0.47 |
| 1:A:516:VAL:O | 1:A:517:GLU:C | 2.51 | 0.47 |
| 1:A:70:GLU:CG | 1:A:92:PRO:HB3 | 2.44 | 0.47 |
| 1:B:1087:ILE:HG22 | 1:B:1089:ILE:HD13 | 1.95 | 0.47 |
| 1:B:641:MET:HE2 | 1:B:671:ILE:HG13 | 1.97 | 0.47 |
| 1:B:799:ALA:H | 1:B:811:ASN:ND2 | 2.13 | 0.47 |
| 1:D:1069:ASP:OD1 | 1:D:1073:ASN:HB2 | 2.14 | 0.47 |
| 1:D:1087:ILE:HG22 | 1:D:1089:ILE:CD1 | 2.43 | 0.47 |
| 1:D:756:ILE:HD11 | 1:D:770:LEU:HD22 | 1.97 | 0.47 |
| 1:B:624:TRP:O | 1:B:627:LEU:HB3 | 2.15 | 0.47 |
| 1:C:744:ALA:HB3 | 1:C:746:LEU:HG | 1.97 | 0.47 |
| 1:A:1091:ASP:OD2 | 1:A:1093:ASN:HA | 2.15 | 0.47 |
| 1:B:104:ASP:O | 1:B:105:VAL:C | 2.53 | 0.47 |
| 1:B:167:ILE:HG12 | 1:B:168:PRO:CD | 2.45 | 0.47 |
| 1:C:515:ASN:H | 1:C:515:ASN:CA | 2.06 | 0.47 |
| 1:C:701:GLU:HG2 | 1:C:739:ALA:HB2 | 1.97 | 0.47 |
| 1:C:926:LEU:HD13 | 1:C:938:LEU:CD1 | 2.44 | 0.47 |
| 1:C:948:PHE:CE2 | 1:C:959:PHE:HD2 | 2.32 | 0.47 |
| 1:D:137:LYS:HD2 | 1:D:352:ALA:HB1 | 1.97 | 0.47 |
| 1:A:846:SER:HA | 1:A:849:GLU:HG2 | 1.96 | 0.47 |
| 1:B:565:LEU:HD21 | 1:B:826:THR:HB | 1.96 | 0.47 |
| 1:B:864:HIS:CD2 | 1:B:866:MET:HB2 | 2.50 | 0.47 |
| 1:C:357:LEU:O | 1:C:362:MET:CB | 2.62 | 0.47 |
| 1:C:41:LEU:HD23 | 1:C:41:LEU:C | 2.34 | 0.47 |
| 1:C:652:LYS:HD3 | 1:C:653:ASN:O | 2.15 | 0.47 |
| 1:C:811:ASN:OD1 | 1:C:832:GLU:OE1 | 2.33 | 0.47 |
| 1:D:908:THR:HA | 1:D:909:PRO:HA | 1.57 | 0.47 |
| 1:A:334:THR:CG2 | 1:A:428:LYS:HZ1 | 2.27 | 0.47 |
| 1:B:715:ARG:HD2 | 1:B:715:ARG:O | 2.15 | 0.47 |
| 1:B:977:ARG:CZ | 1:B:980:GLU:HG3 | 2.44 | 0.47 |
| 1:B:620:LYS:NZ | 4:B:1201:BTI:HN3 | 2.13 | 0.47 |
| 1:B:624:TRP:HZ2 | 1:B:1008:ILE:CD1 | 2.28 | 0.47 |
| 1:C:1065:ILE:HG12 | 1:C:1076:ILE:HG23 | 1.96 | 0.47 |
| 1:C:1085:ARG:CG | 1:C:1085:ARG:NH1 | 2.44 | 0.47 |
| 1:C:542:LYS:HD3 | 1:C:542:LYS:C | 2.35 | 0.47 |
| 1:A:606:MET:CE | 1:A:639:PHE:HB3 | 2.45 | 0.46 |
| 1:B:948:PHE:CD2 | 1:B:964:GLN:HA | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:177:TYR:OH | 1:C:181:LYS:HE3 | 2.15 | 0.46 |
| 1:D:1013:TYR:HB3 | 1:D:1016:VAL:HB | 1.96 | 0.46 |
| 1:D:379:THR:O | 1:D:457:THR:HB | 2.14 | 0.46 |
| 1:D:532:VAL:HG21 | 1:D:596:ASP:CB | 2.45 | 0.46 |
| 1:A:674:PHE:CD2 | 1:A:674:PHE:N | 2.83 | 0.46 |
| 1:B:596:ASP:O | 1:B:599:LYS:HG2 | 2.15 | 0.46 |
| 1:C:1035:THR:N | 1:C:1036:PRO:CD | 2.77 | 0.46 |
| 1:C:936:TYR:HD1 | 1:C:966:VAL:CG1 | 2.28 | 0.46 |
| 1:D:1054:LYS:HB3 | 1:D:1054:LYS:HE2 | 1.41 | 0.46 |
| 1:D:1085:ARG:HG3 | 1:D:1085:ARG:HH11 | 1.79 | 0.46 |
| 1:D:323:ILE:HG22 | 1:D:324:GLU:HG2 | 1.97 | 0.46 |
| 1:D:927:ASP:HB3 | 1:D:930:SER:H | 1.78 | 0.46 |
| 1:A:1078:TYR:HB2 | 1:A:1085:ARG:HB3 | 1.97 | 0.46 |
| 1:A:550:PRO:HB2 | 1:A:736:HIS:CE1 | 2.49 | 0.46 |
| 1:A:572:ASP:OD1 | 1:A:771:HIS:CE1 | 2.68 | 0.46 |
| 1:A:778:ASN:O | 1:A:779:GLY:C | 2.52 | 0.46 |
| 1:A:866:MET:HE1 | 1:A:871:TYR:HA | 1.97 | 0.46 |
| 1:B:459:ILE:HB | 1:B:460:PRO:HD3 | 1.97 | 0.46 |
| 1:B:525:GLU:HG3 | 1:B:527:ALA:H | 1.80 | 0.46 |
| 1:B:744:ALA:CB | 1:B:746:LEU:HG | 2.44 | 0.46 |
| 1:C:241:ASN:N | 1:C:242:PRO:CD | 2.77 | 0.46 |
| 1:C:631:ARG:HG2 | 1:C:670:GLY:HA3 | 1.97 | 0.46 |
| 1:C:893:MET:HA | 1:C:896:ARG:HD2 | 1.86 | 0.46 |
| 1:D:258:VAL:HG21 | 1:D:362:MET:CE | 2.45 | 0.46 |
| 1:A:551:LYS:HA | 1:A:551:LYS:HD3 | 1.55 | 0.46 |
| 1:A:620:LYS:HA | 1:A:620:LYS:HD2 | 1.53 | 0.46 |
| 1:A:729:GLU:O | 1:A:733:GLU:HG2 | 2.15 | 0.46 |
| 1:C:711:LEU:HD11 | 1:C:750:LYS:HB3 | 1.98 | 0.46 |
| 1:C:885:GLU:C | 1:C:887:PHE:H | 2.18 | 0.46 |
| 1:A:398:ARG:HG3 | 1:A:398:ARG:HH11 | 1.77 | 0.46 |
| 1:A:42:VAL:HG23 | 1:A:53:PHE:CE2 | 2.51 | 0.46 |
| 1:A:880:SER:O | 1:A:881:LEU:HD23 | 2.16 | 0.46 |
| 1:B:1052:ILE:O | 1:B:1053:ASP:HB2 | 2.15 | 0.46 |
| 1:B:572:ASP:HB3 | 1:B:807:GLN:NE2 | 2.31 | 0.46 |
| 1:D:260:LEU:O | 1:D:261:PHE:HB2 | 2.15 | 0.46 |
| 1:D:527:ALA:HB2 | 1:D:840:THR:HG21 | 1.97 | 0.46 |
| 1:D:864:HIS:CD2 | 1:D:866:MET:H | 2.25 | 0.46 |
| 1:A:142:HIS:H | 1:A:145:HIS:CD2 | 2.31 | 0.46 |
| 1:A:622:ASN:HD22 | 1:A:623:PRO:N | 2.13 | 0.46 |
| 1:A:641:MET:HE2 | 1:A:674:PHE:CE1 | 2.51 | 0.46 |
| 1:B:620:LYS:HE2 | 1:B:1023:THR:OG1 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:C:1033:LEU:HD23 | 1:C:1050:ILE:HD13 | 1.97 | 0.46 |
| 1:C:570:PHE:O | 1:C:574:HIS:HE1 | 1.98 | 0.46 |
| 1:C:717:ASN:ND2 | 1:C:717(A):ILE:HG13 | 2.31 | 0.46 |
| 1:A:214:GLU:O | 1:A:218:HIS:CD2 | 2.68 | 0.46 |
| 1:A:772:THR:HG22 | 1:A:783:TYR:CE2 | 2.51 | 0.46 |
| 1:B:743:MET:HA | 1:B:773:HIS:CD2 | 2.51 | 0.46 |
| 1:C:631:ARG:HD3 | 1:C:631:ARG:HA | 1.53 | 0.46 |
| 1:C:606:MET:HE1 | 1:C:639:PHE:HB3 | 1.98 | 0.46 |
| 1:D:1044:ASN:ND2 | 1:D:1064:THR:HA | 2.30 | 0.46 |
| 1:D:248:GLN:HG2 | 1:D:260:LEU:HD12 | 1.98 | 0.46 |
| 1:D:335:ILE:HG22 | 1:D:336:THR:H | 1.79 | 0.46 |
| 1:A:879:LYS:C | 1:A:881:LEU:N | 2.68 | 0.46 |
| 1:C:347:THR:HG23 | 1:C:360:ILE:HD13 | 1.97 | 0.46 |
| 1:C:377:ARG:HD3 | 1:C:377:ARG:N | 2.30 | 0.46 |
| 1:C:382:ASP:OD1 | 1:C:384:LEU:HB2 | 2.15 | 0.46 |
| 1:C:641:MET:HE3 | 1:C:674:PHE:CD1 | 2.50 | 0.46 |
| 1:C:940:PHE:CB | 1:C:941:PRO:CD | 2.82 | 0.46 |
| 1:D:811:ASN:N | 1:D:811:ASN:HD22 | 2.00 | 0.46 |
| 1:D:878:ALA:O | 1:D:884:GLY:N | 2.49 | 0.46 |
| 1:D:927:ASP:O | 1:D:931:VAL:HG12 | 2.16 | 0.46 |
| 1:A:277:VAL:C | 1:A:335:ILE:HD11 | 2.36 | 0.46 |
| 1:A:555:GLU:OE2 | 1:A:555:GLU:HA | 2.15 | 0.46 |
| 1:B:1001:PRO:HG2 | 1:B:1002:VAL:H | 1.81 | 0.46 |
| 1:B:263:ARG:NH1 | 1:B:336:THR:OG1 | 2.49 | 0.46 |
| 1:B:547:GLU:HB2 | 1:B:548:VAL:HG13 | 1.96 | 0.46 |
| 1:C:526:LEU:HA | 1:C:526:LEU:HD23 | 1.74 | 0.46 |
| 1:C:810:ALA:HB1 | 1:C:831:MET:CE | 2.46 | 0.46 |
| 1:D:772:THR:HG22 | 1:D:783:TYR:CE2 | 2.51 | 0.46 |
| 1:B:103:ILE:O | 1:B:106:ALA:HB3 | 2.16 | 0.46 |
| 1:B:387:PHE:HE2 | 1:B:488:PHE:HE2 | 1.64 | 0.46 |
| 1:B:417:GLU:H | 1:B:417:GLU:HG2 | 1.55 | 0.46 |
| 1:C:619:LEU:O | 1:C:620:LYS:HB2 | 2.16 | 0.46 |
| 1:D:40:LEU:C | 1:D:40:LEU:HD23 | 2.36 | 0.46 |
| 1:A:1089:ILE:HG22 | 1:A:1089:ILE:O | 2.15 | 0.45 |
| 1:A:377:ARG:HB3 | 1:A:425:LEU:CD1 | 2.45 | 0.45 |
| 1:B:748:LYS:HB3 | 1:B:749:PRO:HD2 | 1.98 | 0.45 |
| 1:C:1018:GLU:OE1 | 1:C:1018:GLU:HA | 2.16 | 0.45 |
| 1:C:332:GLU:HA | 1:C:375:GLN:HE22 | 1.81 | 0.45 |
| 1:C:704:ILE:HG21 | 1:C:723:TYR:HD2 | 1.81 | 0.45 |
| 1:C:813:LEU:O | 1:C:814:TYR:C | 2.53 | 0.45 |
| 1:D:900:LEU:HD13 | 1:D:928:GLU:HG3 | 1.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:234:TYR:CE1 | 1:A:236:GLU:HG3 | 2.51 | 0.45 |
| 1:A:382:ASP:OD2 | 1:A:385:ASN:HB2 | 2.16 | 0.45 |
| 1:A:386:ASP:O | 1:A:387:PHE:HB2 | 2.16 | 0.45 |
| 1:A:418:ILE:HD12 | 1:A:418:ILE:N | 2.31 | 0.45 |
| 1:B:374:ILE:HG22 | 1:B:443:MET:HE3 | 1.98 | 0.45 |
| 1:B:565:LEU:HD12 | 1:B:565:LEU:C | 2.36 | 0.45 |
| 1:C:798:VAL:CG1 | 1:C:835:SER:HA | 2.46 | 0.45 |
| 1:A:395:ILE:O | 1:A:396:ALA:HB2 | 2.16 | 0.45 |
| 1:A:524:TYR:HD2 | 1:A:843:THR:CG2 | 2.29 | 0.45 |
| 1:B:729:GLU:HG2 | 1:B:732:ARG:NH2 | 2.31 | 0.45 |
| 1:C:234:TYR:C | 1:C:235:ILE:HG22 | 2.37 | 0.45 |
| 1:D:512:PHE:CD2 | 1:D:512:PHE:C | 2.90 | 0.45 |
| 1:D:917:MET:O | 1:D:921:MET:HB2 | 2.16 | 0.45 |
| 1:A:193:ILE:HG13 | 1:A:194:LYS:N | 2.32 | 0.45 |
| 1:A:207:VAL:HG11 | 1:A:213:LEU:HD23 | 1.97 | 0.45 |
| 1:A:920:TYR:OH | 1:A:938:LEU:HB3 | 2.16 | 0.45 |
| 1:C:1049:GLU:HG2 | 1:C:1059:ILE:HD13 | 1.98 | 0.45 |
| 1:C:192:MET:HE3 | 1:C:192:MET:HB3 | 1.87 | 0.45 |
| 1:C:385:ASN:C | 1:C:387:PHE:N | 2.69 | 0.45 |
| 1:D:529:ILE:HD13 | 1:D:589:ASN:HB3 | 1.99 | 0.45 |
| 1:D:938:LEU:O | 1:D:939:ASP:CB | 2.63 | 0.45 |
| 1:A:869:GLY:O | 1:A:871:TYR:N | 2.49 | 0.45 |
| 1:B:259:HIS:CD2 | 1:B:296:ILE:CD1 | 2.76 | 0.45 |
| 1:B:689:ALA:O | 1:B:693:VAL:HG23 | 2.16 | 0.45 |
| 1:D:337:GLU:CG | 1:D:342:ILE:O | 2.60 | 0.45 |
| 1:A:167:ILE:CD1 | 1:A:323:ILE:CD1 | 2.94 | 0.45 |
| 1:A:278:ALA:N | 1:A:335:ILE:HD11 | 2.32 | 0.45 |
| 1:A:370:LEU:O | 1:A:432:HIS:CE1 | 2.67 | 0.45 |
| 1:A:874:LEU:HD12 | 1:A:919:LEU:HD21 | 1.98 | 0.45 |
| 1:B:539:SER:CA | 1:B:543:GLN:HE21 | 2.22 | 0.45 |
| 1:B:704:ILE:HG21 | 1:B:723:TYR:HD2 | 1.82 | 0.45 |
| 1:C:1049:GLU:HG2 | 1:C:1059:ILE:CD1 | 2.46 | 0.45 |
| 1:D:305:VAL:O | 1:D:306:ASN:CB | 2.65 | 0.45 |
| 1:D:459:ILE:N | 1:D:460:PRO:HD2 | 2.32 | 0.45 |
| 1:D:574:HIS:HD2 | 1:D:580:THR:HA | 1.81 | 0.45 |
| 1:D:796:THR:HB | 1:D:810:ALA:HB2 | 1.98 | 0.45 |
| 1:A:179:LEU:HD11 | 1:A:217:PHE:CE1 | 2.51 | 0.45 |
| 1:A:873:ASN:O | 1:A:875:SER:N | 2.49 | 0.45 |
| 1:B:302:ILE:O | 1:B:303:LYS:HB2 | 2.17 | 0.45 |
| 1:B:347:THR:O | 1:B:348:GLN:C | 2.52 | 0.45 |
| 1:B:715:ARG:HD2 | 1:B:715:ARG:C | 2.32 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:309:THR:HG22 | 1:C:311:GLU:HG2 | 1.98 | 0.45 |
| 1:C:580:THR:HB | 1:C:614:VAL:HG21 | 1.98 | 0.45 |
| 1:D:262:GLU:OE1 | 1:D:288:ARG:NH1 | 2.50 | 0.45 |
| 1:D:583:ARG:HG2 | 1:D:619:LEU:HD22 | 1.98 | 0.45 |
| 1:A:174:ILE:HD11 | 1:A:235:ILE:HG22 | 1.99 | 0.45 |
| 1:A:192:MET:CE | 1:A:238:TYR:CE1 | 3.00 | 0.45 |
| 1:A:459:ILE:O | 1:A:460:PRO:C | 2.54 | 0.45 |
| 1:B:631:ARG:HG2 | 1:B:670:GLY:HA3 | 1.99 | 0.45 |
| 1:C:129:ARG:HG3 | 1:C:143:LEU:CD1 | 2.46 | 0.45 |
| 1:C:267:VAL:HG22 | 1:C:480:PHE:CD2 | 2.51 | 0.45 |
| 1:C:443:MET:HG2 | 1:C:466:MET:SD | 2.57 | 0.45 |
| 1:C:738:LEU:HD21 | 1:C:759:LEU:HD13 | 1.98 | 0.45 |
| 1:D:871:TYR:CE1 | 1:D:891:LYS:HD3 | 2.52 | 0.45 |
| 1:A:431:THR:HG21 | 1:A:443:MET:HA | 1.99 | 0.45 |
| 1:A:606:MET:CE | 1:A:639:PHE:CD2 | 3.00 | 0.45 |
| 1:B:398:ARG:HD3 | 1:B:1083:GLN:HE21 | 1.82 | 0.45 |
| 1:B:932:ILE:HG13 | 1:B:933:THR:N | 2.32 | 0.45 |
| 1:C:437:LYS:CD | 1:C:437:LYS:H | 2.22 | 0.45 |
| 1:C:440:GLU:HG3 | 1:C:472:THR:HG22 | 1.99 | 0.45 |
| 1:C:513:PRO:CA | 1:C:513:PRO:O | 2.53 | 0.45 |
| 1:C:690:ASN:O | 1:C:694:GLN:HG2 | 2.17 | 0.45 |
| 1:A:177:TYR:O | 1:A:179:LEU:N | 2.50 | 0.45 |
| 1:A:245:ILE:HG13 | 1:A:283:LEU:HD11 | 1.99 | 0.45 |
| 1:A:512:PHE:C | 1:A:512:PHE:CD2 | 2.90 | 0.45 |
| 1:A:864:HIS:HD2 | 1:A:866:MET:HG3 | 1.73 | 0.45 |
| 1:B:511:GLY:O | 4:B:1201:BTI:H102 | 2.17 | 0.45 |
| 1:B:251:GLY:HA2 | 1:B:257:ILE:HA | 1.99 | 0.45 |
| 1:B:748:LYS:O | 1:B:749:PRO:C | 2.55 | 0.45 |
| 1:C:99:ILE:HG23 | 1:C:127:PHE:HD1 | 1.82 | 0.45 |
| 1:C:173:PRO:O | 1:C:174:ILE:CD1 | 2.64 | 0.45 |
| 1:C:221:LYS:HG3 | 1:C:233:VAL:HG13 | 1.99 | 0.45 |
| 1:C:673:VAL:HG22 | 1:C:699:ILE:HB | 1.98 | 0.45 |
| 1:C:897:VAL:O | 1:C:898:ASN:C | 2.55 | 0.45 |
| 1:D:479:LYS:O | 1:D:480:PHE:C | 2.55 | 0.45 |
| 1:D:898:ASN:ND2 | 1:D:904:ILE:H | 2.15 | 0.45 |
| 1:D:907:VAL:O | 1:D:910:SER:N | 2.49 | 0.45 |
| 1:A:179:LEU:HA | 1:A:182:GLU:CD | 2.37 | 0.44 |
| 1:A:508:THR:O | 1:A:508:THR:HG22 | 2.17 | 0.44 |
| 1:A:879:LYS:HB2 | 1:A:879:LYS:HE2 | 1.66 | 0.44 |
| 1:B:267:VAL:HG12 | 1:B:481:ILE:HD11 | 1.99 | 0.44 |
| 1:C:162:ALA:HB2 | 1:C:301:ASN:HD22 | 1.82 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:662:PHE:O | 1:C:666:SER:OG | 2.29 | 0.44 |
| 1:D:167:ILE:HG23 | 1:D:321:PHE:CB | 2.47 | 0.44 |
| 1:D:259:HIS:N | 1:D:364:GLN:HE22 | 2.05 | 0.44 |
| 1:A:156:ARG:HD2 | 1:A:166:VAL:HG11 | 1.99 | 0.44 |
| 1:A:338:MET:HE1 | 1:A:430:SER:CB | 2.44 | 0.44 |
| 1:A:712:ASN:HA | 1:A:713:PRO:HD3 | 1.83 | 0.44 |
| 1:B:571:ARG:HD2 | 1:B:571:ARG:C | 2.38 | 0.44 |
| 1:B:574:HIS:HD2 | 1:B:580:THR:HA | 1.81 | 0.44 |
| 1:B:784:LYS:HE2 | 1:C:785:GLN:HE21 | 1.82 | 0.44 |
| 1:D:134:GLU:HB2 | 1:D:136:ILE:HD12 | 1.99 | 0.44 |
| 1:D:325:VAL:O | 1:D:327:PRO:HD3 | 2.18 | 0.44 |
| 1:D:787:ILE:HD13 | 1:D:817:LEU:HD11 | 1.99 | 0.44 |
| 1:D:944:VAL:O | 1:D:945:VAL:C | 2.54 | 0.44 |
| 1:A:622:ASN:HD22 | 1:A:624:TRP:H | 1.60 | 0.44 |
| 1:A:955:PRO:O | 1:A:956:VAL:C | 2.56 | 0.44 |
| 1:B:144:GLU:H | 1:B:144:GLU:HG3 | 1.53 | 0.44 |
| 1:B:709:ASP:OD1 | 1:B:748:LYS:NZ | 2.50 | 0.44 |
| 1:C:892:ASP:O | 1:C:896:ARG:CD | 2.62 | 0.44 |
| 1:D:650:GLY:HA3 | 1:D:654:TYR:CE1 | 2.53 | 0.44 |
| 1:D:917:MET:CE | 1:D:940:PHE:HD2 | 2.31 | 0.44 |
| 1:A:174:ILE:HD11 | 1:A:235:ILE:HG21 | 1.97 | 0.44 |
| 1:C:1029:ASN:C | 1:C:1029:ASN:ND2 | 2.70 | 0.44 |
| 1:A:590:ILE:CG1 | 1:A:837:TYR:CE2 | 2.98 | 0.44 |
| 1:A:873:ASN:C | 1:A:875:SER:H | 2.21 | 0.44 |
| 1:B:167:ILE:HG12 | 1:B:168:PRO:HD2 | 1.99 | 0.44 |
| 1:B:631:ARG:HA | 1:B:631:ARG:HD3 | 1.50 | 0.44 |
| 1:C:191:LEU:HD13 | 1:C:235:ILE:HD11 | 2.00 | 0.44 |
| 1:C:294:ALA:O | 1:C:297:GLN:HB3 | 2.17 | 0.44 |
| 1:C:717:ASN:C | 1:C:717:ASN:HD22 | 2.20 | 0.44 |
| 1:A:99:ILE:O | 1:A:103:ILE:HG12 | 2.17 | 0.44 |
| 1:A:1046:GLU:O | 1:A:1061:LYS:HA | 2.18 | 0.44 |
| 1:A:246:GLU:HB2 | 1:A:309:THR:CG2 | 2.48 | 0.44 |
| 1:A:413:PHE:O | 1:A:414:GLN:C | 2.56 | 0.44 |
| 1:A:641:MET:HE3 | 1:A:674:PHE:CD1 | 2.53 | 0.44 |
| 1:B:603:SER:HA | 1:B:637:VAL:HG12 | 1.99 | 0.44 |
| 1:B:792:ASP:N | 1:B:792:ASP:OD2 | 2.51 | 0.44 |
| 1:C:960:ASN:O | 1:C:961:LYS:C | 2.56 | 0.44 |
| 1:A:275:VAL:HG22 | 1:A:376:CYS:HB3 | 1.98 | 0.44 |
| 1:B:1077:TYR:OH | 1:D:1063:GLU:HB3 | 2.17 | 0.44 |
| 1:C:188:GLY:HA3 | 1:C:237:ARG:NH2 | 2.28 | 0.44 |
| 1:C:77:ARG:HD3 | 1:C:83:SER:OG | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:C:964:GLN:NE2 | 1:C:973:ALA:HB2 | 2.32 | 0.44 |
| 1:D:717:ASN:HD22 | 1:D:717:ASN:H | 1.65 | 0.44 |
| 1:B:682:TRP:HE3 | 1:B:685:GLN:HG3 | 1.81 | 0.44 |
| 1:B:912:LYS:NZ | 1:B:916:ASP:OD1 | 2.48 | 0.44 |
| 1:C:1090:LYS:HB3 | 1:C:1090:LYS:HE3 | 1.56 | 0.44 |
| 1:D:828:ILE:HD12 | 1:D:829:GLU:N | 2.33 | 0.44 |
| 1:A:866:MET:CE | 1:A:871:TYR:HA | 2.47 | 0.44 |
| 1:A:886:ARG:O | 1:A:889:GLU:N | 2.45 | 0.44 |
| 1:B:277:VAL:HA | 1:B:335:ILE:HD11 | 1.99 | 0.44 |
| 1:B:361:ASN:HA | 1:B:361:ASN:HD22 | 1.50 | 0.44 |
| 1:B:429:LEU:HD22 | 1:B:450:MET:CE | 2.48 | 0.44 |
| 1:B:556:TRP:O | 1:B:557:VAL:C | 2.56 | 0.44 |
| 1:C:775:THR:HG21 | 1:C:861:ILE:HG13 | 2.00 | 0.44 |
| 1:D:701:GLU:HG2 | 1:D:737:ILE:HB | 2.00 | 0.44 |
| 1:B:645:ALA:HB1 | 1:B:686:MET:HA | 2.00 | 0.43 |
| 1:B:99:ILE:CD1 | 1:B:99:ILE:H | 2.29 | 0.43 |
| 1:C:993:LEU:O | 1:C:997:GLU:HG2 | 2.18 | 0.43 |
| 1:D:263:ARG:HG2 | 1:D:335:ILE:CG2 | 2.48 | 0.43 |
| 1:D:283:LEU:C | 1:D:283:LEU:HD23 | 2.39 | 0.43 |
| 1:D:302:ILE:HG13 | 1:D:302:ILE:H | 1.70 | 0.43 |
| 1:D:647:ASN:HB2 | 1:D:654:TYR:CE1 | 2.53 | 0.43 |
| 1:D:898:ASN:HD21 | 1:D:904:ILE:H | 1.66 | 0.43 |
| 1:A:177:TYR:C | 1:A:179:LEU:N | 2.69 | 0.43 |
| 1:A:306:ASN:OD1 | 1:A:348:GLN:HG2 | 2.18 | 0.43 |
| 1:B:165:PRO:HB2 | 1:B:321:PHE:HD2 | 1.83 | 0.43 |
| 1:B:738:LEU:O | 1:B:768:ILE:HA | 2.19 | 0.43 |
| 1:C:493:SER:HA | 1:C:494:LEU:HD13 | 1.99 | 0.43 |
| 1:A:225:GLU:HA | 1:A:225:GLU:OE1 | 2.17 | 0.43 |
| 1:A:720:LEU:CD2 | 1:A:758:GLU:HG3 | 2.42 | 0.43 |
| 1:B:375:GLN:HG3 | 1:B:430:SER:OG | 2.18 | 0.43 |
| 1:C:115:HIS:ND1 | 1:C:116:PRO:HD2 | 2.33 | 0.43 |
| 1:C:225:GLU:HB3 | 1:C:231:SER:HB3 | 1.99 | 0.43 |
| 1:C:565:LEU:HD12 | 1:C:824:LEU:HD21 | 2.00 | 0.43 |
| 1:D:281:VAL:HG12 | 1:D:282:GLY:N | 2.33 | 0.43 |
| 1:D:338:MET:HE1 | 1:D:430:SER:HB3 | 1.98 | 0.43 |
| 1:D:487:LEU:HD12 | 1:D:487:LEU:HA | 1.82 | 0.43 |
| 1:D:50:ILE:HD11 | 1:D:75:LEU:HB3 | 1.99 | 0.43 |
| 1:A:1065:ILE:HG22 | 1:A:1074:ARG:HD3 | 2.00 | 0.43 |
| 1:A:322:PHE:O | 1:A:323:ILE:HD13 | 2.18 | 0.43 |
| 1:A:622:ASN:C | 1:A:622:ASN:ND2 | 2.70 | 0.43 |
| 1:A:858:ASN:ND2 | 1:A:860:GLU:H | 2.17 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:898:ASN:ND2 | 1:A:906:LYS:HE3 | 2.33 | 0.43 |
| 1:B:551:LYS:O | 1:B:555:GLU:HG2 | 2.19 | 0.43 |
| 1:C:241:ASN:N | 1:C:242:PRO:HD3 | 2.33 | 0.43 |
| 1:D:571:ARG:HH11 | 1:D:575:GLN:HE22 | 1.62 | 0.43 |
| 1:D:61:ILE:HG22 | 1:D:62:SER:O | 2.19 | 0.43 |
| 1:D:70:GLU:CD | 1:D:70:GLU:N | 2.69 | 0.43 |
| 1:A:856:SER:OG | 1:D:800:SER:HA | 2.19 | 0.43 |
| 1:A:561:ASP:O | 1:A:822:ARG:HD2 | 2.19 | 0.43 |
| 1:B:1063:GLU:OE1 | 1:D:1086:ARG:NH1 | 2.51 | 0.43 |
| 1:B:1042:MET:HE2 | 1:B:1078:TYR:HE2 | 1.84 | 0.43 |
| 1:B:949:LYS:HE2 | 1:B:951:GLU:OE1 | 2.18 | 0.43 |
| 1:C:118:TYR:HA | 1:C:122:SER:OG | 2.19 | 0.43 |
| 1:D:494:LEU:CD2 | 1:D:496:ARG:HA | 2.49 | 0.43 |
| 1:C:631:ARG:NH2 | 1:C:672:ASP:OD1 | 2.51 | 0.43 |
| 1:C:937:LYS:O | 1:C:938:LEU:HB2 | 2.17 | 0.43 |
| 1:D:259:HIS:NE2 | 1:D:292:CYS:HB3 | 2.34 | 0.43 |
| 1:A:38:LYS:HE2 | 1:A:38:LYS:HB3 | 1.60 | 0.43 |
| 1:A:470:LYS:CB | 1:A:480:PHE:CE1 | 3.00 | 0.43 |
| 1:A:547:GLU:HB3 | 1:A:548:VAL:HG13 | 1.99 | 0.43 |
| 1:A:711:LEU:HG | 1:A:751:ALA:HB2 | 2.00 | 0.43 |
| 1:A:798:VAL:HG11 | 1:A:835:SER:N | 2.34 | 0.43 |
| 1:B:704:ILE:CG2 | 1:B:726:LEU:HD23 | 2.40 | 0.43 |
| 1:C:43:ALA:HA | 1:C:66:ILE:CD1 | 2.49 | 0.43 |
| 1:D:164:LEU:HD22 | 1:D:298:LEU:HB2 | 2.01 | 0.43 |
| 1:D:952:ILE:HA | 1:D:952:ILE:HD12 | 1.87 | 0.43 |
| 1:A:1065:ILE:CG2 | 1:A:1074:ARG:HD3 | 2.49 | 0.43 |
| 1:A:715:ARG:HD2 | 1:A:715:ARG:HA | 1.80 | 0.43 |
| 1:A:855:LYS:O | 1:A:855:LYS:HG3 | 2.17 | 0.43 |
| 1:A:655:PRO:HG2 | 1:A:985:VAL:CG2 | 2.48 | 0.43 |
| 1:B:386:ASP:HB3 | 1:B:388:MET:HG3 | 2.01 | 0.43 |
| 1:B:883:LEU:O | 1:B:884:GLY:C | 2.56 | 0.43 |
| 1:C:148:MET:HA | 1:C:154:LYS:HD2 | 1.99 | 0.43 |
| 1:D:963:LEU:HD12 | 1:D:967:ILE:HD12 | 2.01 | 0.43 |
| 1:A:1029:ASN:ND2 | 1:A:1029:ASN:C | 2.71 | 0.43 |
| 1:A:394:ILE:O | 1:A:414:GLN:O | 2.36 | 0.43 |
| 1:B:655:PRO:HD3 | 1:B:982:LEU:CD1 | 2.49 | 0.43 |
| 1:C:142:HIS:N | 1:C:145:HIS:HD2 | 2.16 | 0.43 |
| 1:A:177:TYR:O | 1:A:178:GLU:C | 2.56 | 0.43 |
| 1:A:252:ASP:OD1 | 1:A:256:ASN:HB2 | 2.19 | 0.43 |
| 1:A:547:GLU:CA | 1:A:547:GLU:OE2 | 2.66 | 0.43 |
| 1:C:129:ARG:HG3 | 1:C:143:LEU:HD13 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:216:ALA:O | 1:C:217:PHE:C | 2.56 | 0.43 |
| 1:D:239:ILE:HD13 | 1:D:239:ILE:HA | 1.82 | 0.43 |
| 1:D:277:VAL:HG21 | 1:D:476:TYR:OH | 2.19 | 0.43 |
| 1:A:118:TYR:C | 1:A:118:TYR:CD1 | 2.91 | 0.42 |
| 1:A:814:TYR:CE2 | 1:A:828:ILE:HG12 | 2.53 | 0.42 |
| 1:B:1048:VAL:HG12 | 1:B:1050:ILE:HD12 | 2.01 | 0.42 |
| 1:B:448:ARG:NH2 | 1:B:467:LYS:HD2 | 2.32 | 0.42 |
| 1:C:347:THR:O | 1:C:348:GLN:C | 2.56 | 0.42 |
| 1:D:871:TYR:HE1 | 1:D:891:LYS:HD3 | 1.84 | 0.42 |
| 1:D:879:LYS:C | 1:D:881:LEU:H | 2.22 | 0.42 |
| 1:A:1017:TYR:O | 1:A:1018:GLU:C | 2.57 | 0.42 |
| 1:A:574:HIS:CD2 | 1:A:580:THR:HA | 2.54 | 0.42 |
| 1:B:291:ILE:HG12 | 1:B:320:PHE:HD2 | 1.84 | 0.42 |
| 1:C:1002:VAL:HG13 | 1:C:1006:ASP:OD2 | 2.19 | 0.42 |
| 1:C:238:TYR:CE1 | 5:C:1202:ATP:H2 | 2.37 | 0.42 |
| 1:C:448:ARG:HH22 | 1:C:467:LYS:HE3 | 1.84 | 0.42 |
| 1:D:456:LYS:H | 1:D:456:LYS:HD3 | 1.83 | 0.42 |
| 1:D:820:PHE:HB3 | 1:D:821:PRO:HD2 | 2.01 | 0.42 |
| 1:A:417:GLU:C | 1:A:418:ILE:HD12 | 2.40 | 0.42 |
| 1:A:532:VAL:HG13 | 1:A:536:LYS:HD2 | 2.01 | 0.42 |
| 1:B:938:LEU:HA | 1:B:938:LEU:HD23 | 1.79 | 0.42 |
| 1:C:501:LEU:HD22 | 1:C:1078:TYR:CE1 | 2.54 | 0.42 |
| 1:C:175:LYS:O | 1:C:176:SER:C | 2.49 | 0.42 |
| 1:C:661:LYS:O | 1:C:664:GLN:HB2 | 2.20 | 0.42 |
| 1:C:780:LEU:HD23 | 1:C:780:LEU:HA | 1.80 | 0.42 |
| 1:C:926:LEU:CD1 | 1:C:938:LEU:CD1 | 2.96 | 0.42 |
| 1:C:941:PRO:O | 1:C:945:VAL:HG22 | 2.19 | 0.42 |
| 1:D:796:THR:CB | 1:D:810:ALA:HB2 | 2.49 | 0.42 |
| 1:D:879:LYS:HG2 | 1:D:884:GLY:HA3 | 2.01 | 0.42 |
| 1:A:207:VAL:CG1 | 1:A:209:GLU:H | 2.33 | 0.42 |
| 1:A:506:ASN:ND2 | 1:A:510:ASN:HD22 | 2.18 | 0.42 |
| 1:A:597:VAL:HG21 | 1:A:834:LEU:HG | 1.99 | 0.42 |
| 1:A:780:LEU:HD11 | 1:A:812:SER:HB3 | 2.00 | 0.42 |
| 1:A:952:ILE:O | 1:A:952:ILE:HG23 | 2.17 | 0.42 |
| 1:B:522:PRO:HB2 | 1:B:523:ASP:H | 1.68 | 0.42 |
| 1:B:85:LEU:HG | 1:B:87:GLY:H | 1.84 | 0.42 |
| 1:B:889:GLU:O | 1:B:890:VAL:C | 2.58 | 0.42 |
| 1:D:99:ILE:HG23 | 1:D:127:PHE:HD1 | 1.84 | 0.42 |
| 1:D:258:VAL:HB | 1:D:364:GLN:NE2 | 2.34 | 0.42 |
| 1:D:378:ILE:HG23 | 1:D:459:ILE:HG12 | 2.00 | 0.42 |
| 1:D:93:ALA:C | 1:D:95:SER:H | 2.22 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:93:ALA:C | 1:D:95:SER:N | 2.73 | 0.42 |
| 1:A:213:LEU:O | 1:A:214:GLU:C | 2.55 | 0.42 |
| 1:B:278:ALA:HA | 1:B:279:PRO:HA | 1.62 | 0.42 |
| 1:B:468:ASN:OD1 | 1:B:470:LYS:HB2 | 2.19 | 0.42 |
| 1:B:631:ARG:O | 1:B:631:ARG:HD3 | 2.19 | 0.42 |
| 1:C:111:VAL:HG12 | 1:C:113:ALA:H | 1.83 | 0.42 |
| 1:C:281:VAL:HG12 | 1:C:282:GLY:H | 1.83 | 0.42 |
| 1:A:382:ASP:OD1 | 1:A:384:LEU:CD1 | 2.67 | 0.42 |
| 1:B:443:MET:HG2 | 1:B:466:MET:CE | 2.49 | 0.42 |
| 1:B:996:GLU:OE1 | 1:B:996:GLU:C | 2.58 | 0.42 |
| 1:C:1080:MET:CE | 1:C:1085:ARG:NH2 | 2.83 | 0.42 |
| 1:C:124:ASN:HB3 | 1:C:127:PHE:HB3 | 2.02 | 0.42 |
| 1:C:447:LEU:HD23 | 1:C:447:LEU:HA | 1.78 | 0.42 |
| 1:C:907:VAL:O | 1:C:911:SER:OG | 2.35 | 0.42 |
| 1:C:920:TYR:CE1 | 1:C:940:PHE:HD2 | 2.37 | 0.42 |
| 1:D:506:ASN:HD22 | 1:D:506:ASN:HA | 1.64 | 0.42 |
| 1:D:909:PRO:HG2 | 1:D:952:ILE:HG13 | 2.01 | 0.42 |
| 1:B:124:ASN:OD1 | 1:B:126:GLN:N | 2.53 | 0.42 |
| 1:B:551:LYS:HZ3 | 1:B:551:LYS:HB2 | 1.84 | 0.42 |
| 1:B:655:PRO:HD3 | 1:B:982:LEU:HD13 | 2.00 | 0.42 |
| 1:C:383:PRO:HB3 | 1:C:387:PHE:CZ | 2.54 | 0.42 |
| 1:C:572:ASP:HB3 | 1:C:807:GLN:HE21 | 1.80 | 0.42 |
| 1:C:803:GLY:O | 1:C:804:LEU:C | 2.56 | 0.42 |
| 1:C:831:MET:O | 1:C:832:GLU:C | 2.58 | 0.42 |
| 1:D:870:GLN:O | 1:D:871:TYR:C | 2.57 | 0.42 |
| 1:A:167:ILE:HD12 | 1:A:323:ILE:CD1 | 2.50 | 0.42 |
| 1:A:246:GLU:O | 1:A:262:GLU:HA | 2.19 | 0.42 |
| 1:A:384:LEU:CD1 | 1:A:384:LEU:H | 2.33 | 0.42 |
| 1:B:291:ILE:HG12 | 1:B:320:PHE:CD2 | 2.55 | 0.42 |
| 1:B:783:TYR:O | 1:B:784:LYS:C | 2.56 | 0.42 |
| 1:C:246:GLU:OE1 | 1:C:330:GLN:NE2 | 2.52 | 0.42 |
| 1:C:760:LYS:CE | 1:C:790:GLY:O | 2.67 | 0.42 |
| 1:C:794:ILE:CD1 | 1:C:796:THR:CG2 | 2.97 | 0.42 |
| 1:D:1087:ILE:HD13 | 1:D:1087:ILE:HA | 1.86 | 0.42 |
| 1:D:730:LEU:O | 1:D:735:PHE:HD1 | 2.02 | 0.42 |
| 1:D:856:SER:HB3 | 1:D:857:PRO:HD2 | 2.00 | 0.42 |
| 1:D:874:LEU:O | 1:D:887:PHE:CE1 | 2.65 | 0.42 |
| 1:A:912:LYS:NZ | 1:A:916:ASP:OD1 | 2.45 | 0.42 |
| 1:B:251:GLY:HA3 | 1:B:257:ILE:HG23 | 2.02 | 0.42 |
| 1:B:69:ASN:O | 1:B:72:LYS:HG3 | 2.19 | 0.42 |
| 1:C:336:THR:O | 1:C:340:THR:HG23 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:C:506:ASN:ND2 | 1:C:510:ASN:HD22 | 2.18 | 0.42 |
| 1:C:39:LYS:HE3 | 1:C:82:GLU:OE2 | 2.20 | 0.42 |
| 1:D:572:ASP:HB3 | 1:D:807:GLN:HE21 | 1.83 | 0.42 |
| 1:A:606:MET:HE2 | 1:A:639:PHE:CG | 2.55 | 0.42 |
| 1:A:781:LEU:HD21 | 1:D:784:LYS:HG3 | 2.01 | 0.42 |
| 1:A:902:GLY:O | 1:A:903:ASP:HB3 | 2.19 | 0.42 |
| 1:B:130:ARG:HA | 1:B:130:ARG:HD2 | 1.80 | 0.42 |
| 1:B:769:HIS:NE2 | 1:B:795:ASP:OD1 | 2.48 | 0.42 |
| 1:C:1077:TYR:N | 1:C:1077:TYR:CD1 | 2.88 | 0.42 |
| 1:C:896:ARG:NE | 1:C:928:GLU:OE1 | 2.53 | 0.42 |
| 1:D:239:ILE:O | 1:D:241:ASN:N | 2.52 | 0.42 |
| 1:D:703:THR:CG2 | 1:D:741:LYS:HB2 | 2.48 | 0.42 |
| 1:A:219:ARG:O | 1:A:219:ARG:HG2 | 2.19 | 0.41 |
| 1:A:487:LEU:HD12 | 1:A:487:LEU:HA | 1.76 | 0.41 |
| 1:A:48:ILE:HG23 | 1:A:49:ALA:N | 2.34 | 0.41 |
| 1:B:280:SER:OG | 1:B:283:LEU:HG | 2.20 | 0.41 |
| 1:B:362(A):PRO:HB2 | 1:B:366:ASP:HB2 | 2.01 | 0.41 |
| 1:B:690:ASN:O | 1:B:691:GLU:C | 2.59 | 0.41 |
| 1:C:627:LEU:O | 1:C:631:ARG:HB2 | 2.20 | 0.41 |
| 1:A:225:GLU:OE2 | 1:A:231:SER:HB3 | 2.20 | 0.41 |
| 1:A:362:MET:HE3 | 1:A:362(A):PRO:HD2 | 2.01 | 0.41 |
| 1:A:744:ALA:HB3 | 1:A:746:LEU:HG | 2.02 | 0.41 |
| 1:A:898:ASN:ND2 | 1:A:904:ILE:H | 2.12 | 0.41 |
| 1:B:251:GLY:CA | 1:B:257:ILE:HG23 | 2.50 | 0.41 |
| 1:C:772:THR:HG22 | 1:C:783:TYR:CE2 | 2.55 | 0.41 |
| 1:C:809:SER:HB3 | 1:C:812:SER:HB2 | 2.01 | 0.41 |
| 1:D:828:ILE:HD12 | 1:D:829:GLU:H | 1.85 | 0.41 |
| 1:D:860:GLU:O | 1:D:863:GLN:HG2 | 2.19 | 0.41 |
| 1:A:254:HIS:HD2 | 1:A:356:ASP:OD2 | 2.02 | 0.41 |
| 1:B:370:LEU:HD22 | 1:D:370:LEU:HB3 | 2.02 | 0.41 |
| 1:B:98:ASN:C | 1:B:98:ASN:ND2 | 2.70 | 0.41 |
| 1:C:152:LYS:HG3 | 1:C:197:SER:H | 1.84 | 0.41 |
| 1:C:59:LEU:HD22 | 1:C:350:LEU:HD21 | 2.02 | 0.41 |
| 1:C:469:LYS:HA | 1:C:469:LYS:HD2 | 1.61 | 0.41 |
| 1:C:979:GLY:O | 1:C:982:LEU:N | 2.52 | 0.41 |
| 1:A:211:SER:H | 1:A:213:LEU:HD12 | 1.85 | 0.41 |
| 1:A:743:MET:CG | 1:A:907:VAL:HG13 | 2.50 | 0.41 |
| 1:B:343:ASP:OD2 | 1:B:346:LYS:HB2 | 2.21 | 0.41 |
| 1:B:371:GLY:HA2 | 1:B:434:ILE:HA | 2.02 | 0.41 |
| 1:B:509:ILE:HG22 | 1:B:510:ASN:OD1 | 2.20 | 0.41 |
| 1:C:866:MET:HE3 | 1:C:870:GLN:HG2 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:1035:THR:N | 1:D:1036:PRO:CD | 2.84 | 0.41 |
| 1:D:276:GLU:OE2 | 1:D:377:ARG:NH1 | 2.50 | 0.41 |
| 1:D:334:THR:HB | 1:D:375:GLN:NE2 | 2.35 | 0.41 |
| 1:A:390:ASP:HB3 | 1:A:455:VAL:HG12 | 2.01 | 0.41 |
| 1:A:605:GLU:HA | 1:A:640:GLN:O | 2.20 | 0.41 |
| 1:A:641:MET:HB3 | 1:A:671:ILE:HD12 | 2.03 | 0.41 |
| 1:A:810:ALA:HB1 | 1:A:831:MET:CE | 2.50 | 0.41 |
| 1:A:915:GLY:O | 1:A:919:LEU:HD22 | 2.20 | 0.41 |
| 1:B:1029:ASN:C | 1:B:1029:ASN:HD22 | 2.23 | 0.41 |
| 1:B:509:ILE:HD12 | 1:B:1076:ILE:HD11 | 2.01 | 0.41 |
| 1:B:266:SER:HB2 | 1:B:476:TYR:HE2 | 1.85 | 0.41 |
| 1:B:400:SER:HB3 | 1:B:401:GLY:H | 1.70 | 0.41 |
| 1:B:949:LYS:O | 1:B:974:LEU:HG | 2.20 | 0.41 |
| 1:C:712:ASN:HA | 1:C:713:PRO:HD2 | 1.97 | 0.41 |
| 1:C:752:ALA:HB2 | 1:C:782:THR:HG23 | 2.03 | 0.41 |
| 1:D:322:PHE:CZ | 1:D:325:VAL:HG23 | 2.56 | 0.41 |
| 1:D:743:MET:HG2 | 1:D:744:ALA:N | 2.34 | 0.41 |
| 1:A:1052:ILE:O | 1:A:1052:ILE:HG22 | 2.20 | 0.41 |
| 1:A:152:LYS:HA | 1:A:152:LYS:HD3 | 1.83 | 0.41 |
| 1:A:987:PHE:HE2 | 1:A:1011:VAL:HG21 | 1.85 | 0.41 |
| 1:B:302:ILE:O | 1:B:303:LYS:CB | 2.68 | 0.41 |
| 1:B:53:PHE:CZ | 1:B:65:ALA:HB2 | 2.55 | 0.41 |
| 1:B:568:THR:OG1 | 1:B:807:GLN:HG3 | 2.20 | 0.41 |
| 1:C:170:THR:HG21 | 1:C:174:ILE:HD11 | 2.01 | 0.41 |
| 1:D:563:VAL:CG2 | 1:D:787:ILE:HG12 | 2.49 | 0.41 |
| 1:A:107:LYS:C | 1:A:109:ALA:H | 2.23 | 0.41 |
| 1:A:382:ASP:O | 1:A:387:PHE:HA | 2.19 | 0.41 |
| 1:C:400:SER:H | 1:C:407:LEU:HD11 | 1.86 | 0.41 |
| 1:C:606:MET:HE1 | 1:C:671:ILE:CD1 | 2.51 | 0.41 |
| 1:B:406:ARG:NH1 | 1:D:403:ALA:HA | 2.36 | 0.41 |
| 1:D:893:MET:SD | 1:D:896:ARG:NH2 | 2.94 | 0.41 |
| 1:A:375:GLN:HE22 | 1:A:428:LYS:HZ1 | 1.68 | 0.41 |
| 1:A:683:VAL:HA | 1:A:686:MET:HG3 | 2.02 | 0.41 |
| 1:B:642:LEU:HG | 1:B:643:LEU:N | 2.35 | 0.41 |
| 1:B:784:LYS:HE2 | 1:C:785:GLN:NE2 | 2.36 | 0.41 |
| 1:C:898:ASN:HD22 | 1:C:906:LYS:HD3 | 1.86 | 0.41 |
| 1:D:413:PHE:C | 1:D:415:GLY:N | 2.74 | 0.41 |
| 1:D:700:SER:H | 1:D:736:HIS:CD2 | 2.38 | 0.41 |
| 1:A:66:ILE:HB | 1:A:86:VAL:HG22 | 2.03 | 0.41 |
| 1:B:484:THR:HB | 1:B:487:LEU:HD22 | 2.01 | 0.41 |
| 1:B:640:GLN:HG3 | 1:B:673:VAL:CG1 | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:701:GLU:HG2 | 1:B:739:ALA:HB2 | 2.03 | 0.41 |
| 1:B:793:ILE:HG22 | 1:B:794:ILE:N | 2.36 | 0.41 |
| 1:B:799:ALA:HB3 | 1:B:835:SER:OG | 2.20 | 0.41 |
| 1:B:945:VAL:HA | 1:B:967:ILE:CG2 | 2.50 | 0.41 |
| 1:C:335:ILE:HG12 | 1:C:373:ALA:HB3 | 2.03 | 0.41 |
| 1:C:991:ARG:O | 1:C:995:GLU:HG2 | 2.21 | 0.41 |
| 1:D:565:LEU:C | 1:D:565:LEU:CD1 | 2.89 | 0.41 |
| 1:D:574:HIS:CD2 | 1:D:580:THR:HA | 2.56 | 0.41 |
| 1:D:650:GLY:HA3 | 1:D:654:TYR:HE1 | 1.86 | 0.41 |
| 1:D:927:ASP:H | 1:D:930:SER:HB2 | 1.85 | 0.41 |
| 1:A:1063:GLU:OE2 | 1:C:1086:ARG:NH2 | 2.54 | 0.41 |
| 1:A:606:MET:HE2 | 1:A:639:PHE:HB3 | 2.03 | 0.41 |
| 1:B:1013:TYR:HB3 | 1:B:1016:VAL:HB | 2.03 | 0.41 |
| 1:B:952:ILE:CG2 | 1:B:952:ILE:O | 2.68 | 0.41 |
| 1:D:974:LEU:HB3 | 1:D:981:TYR:CE1 | 2.56 | 0.41 |
| 1:A:295:ALA:O | 1:A:299:MET:HG2 | 2.21 | 0.41 |
| 1:A:512:PHE:CD2 | 1:A:513:PRO:N | 2.89 | 0.41 |
| 1:A:980:GLU:OE1 | 1:A:980:GLU:O | 2.39 | 0.41 |
| 1:B:338:MET:HE1 | 1:B:430:SER:CB | 2.45 | 0.41 |
| 1:B:881:LEU:HD22 | 1:B:923:GLN:NE2 | 2.35 | 0.41 |
| 1:C:549:GLY:O | 1:C:553:VAL:HG23 | 2.20 | 0.41 |
| 1:C:893:MET:O | 1:C:897:VAL:HG23 | 2.21 | 0.41 |
| 1:D:588:ILE:HD12 | 1:D:588:ILE:HG23 | 1.83 | 0.41 |
| 1:D:711:LEU:HA | 1:D:711:LEU:HD23 | 1.88 | 0.41 |
| 1:A:170:THR:HG22 | 1:A:172:GLY:H | 1.85 | 0.40 |
| 1:A:296:ILE:O | 1:A:300:GLU:HB2 | 2.21 | 0.40 |
| 1:A:47:GLU:CD | 1:A:428:LYS:HD2 | 2.41 | 0.40 |
| 1:A:498:THR:O | 1:A:499:LYS:C | 2.59 | 0.40 |
| 1:A:566:THR:HA | 1:A:603:SER:O | 2.21 | 0.40 |
| 1:A:647:ASN:O | 1:A:649:VAL:N | 2.53 | 0.40 |
| 1:B:444:VAL:CG2 | 1:B:466:MET:HB3 | 2.52 | 0.40 |
| 1:B:577:LEU:HD13 | 1:B:842:ARG:CZ | 2.51 | 0.40 |
| 1:B:798:VAL:O | 1:B:799:ALA:C | 2.59 | 0.40 |
| 1:C:189:PHE:N | 1:C:190:PRO:CD | 2.84 | 0.40 |
| 1:C:268:GLN:HA | 1:C:272:GLN:O | 2.20 | 0.40 |
| 1:C:145:HIS:CE1 | 1:C:304:TYR:HA | 2.56 | 0.40 |
| 1:C:381:GLU:O | 1:C:383:PRO:HD3 | 2.21 | 0.40 |
| 1:C:729:GLU:O | 1:C:733:GLU:HG2 | 2.21 | 0.40 |
| 1:D:281:VAL:CG1 | 1:D:282:GLY:N | 2.83 | 0.40 |
| 1:A:281:VAL:HG21 | 1:A:436:PHE:CG | 2.56 | 0.40 |
| 1:A:720:LEU:HD21 | 1:A:758:GLU:CG | 2.44 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 1:B:164:LEU:HD11 | 1:B:298:LEU:HB2 | 2.02 | 0.40 |
| 1:B:241:ASN:HA | 1:B:479:LYS:HE2 | 2.03 | 0.40 |
| 1:B:549:GLY:O | 1:B:553:VAL:HG23 | 2.22 | 0.40 |
| 1:B:908:THR:HG22 | 1:B:909:PRO:HA | 2.03 | 0.40 |
| 1:C:1089:ILE:HA | 1:C:1089:ILE:HD13 | 1.80 | 0.40 |
| 1:C:189:PHE:H | 1:C:190:PRO:HD2 | 1.86 | 0.40 |
| 1:C:350:LEU:O | 1:C:355:ALA:HB3 | 2.21 | 0.40 |
| 1:C:461:PHE:O | 1:C:464:ASN:HB2 | 2.21 | 0.40 |
| 1:B:777:GLY:O | 1:C:780:LEU:HD12 | 2.21 | 0.40 |
| 1:D:149:PHE:HZ | 1:D:302:ILE:CD1 | 2.34 | 0.40 |
| 1:D:442:LYS:HE2 | 1:D:442:LYS:HB2 | 1.66 | 0.40 |
| 1:D:468:ASN:HD22 | 1:D:470:LYS:H | 1.69 | 0.40 |
| 1:D:869:GLY:O | 1:D:870:GLN:C | 2.59 | 0.40 |
| 1:D:921:MET:HG2 | 1:D:926:LEU:CB | 2.51 | 0.40 |
| 1:D:927:ASP:HB2 | 1:D:930:SER:OG | 2.20 | 0.40 |
| 1:A:511:GLY:O | 4:A:1203:BTI:H103 | 2.20 | 0.40 |
| 1:A:250:ILE:HG21 | 1:A:250:ILE:HD13 | 1.93 | 0.40 |
| 1:A:263:ARG:HH21 | 1:A:330:GLN:HE21 | 1.69 | 0.40 |
| 1:A:335:ILE:H | 1:A:335:ILE:HG22 | 1.48 | 0.40 |
| 1:A:551:LYS:O | 1:A:555:GLU:HG2 | 2.21 | 0.40 |
| 1:B:624:TRP:CZ2 | 1:B:1008:ILE:HD11 | 2.56 | 0.40 |
| 1:B:949:LYS:HG2 | 1:B:968:LEU:HD21 | 2.03 | 0.40 |
| 1:C:444:VAL:O | 1:C:448:ARG:HG3 | 2.21 | 0.40 |
| 1:C:911:SER:HG | 1:C:911:SER:H | 1.59 | 0.40 |
| 1:D:400:SER:OG | 1:D:401:GLY:N | 2.54 | 0.40 |
| 1:D:398:ARG:NH2 | 1:D:451:ARG:HE | 2.19 | 0.40 |
| 1:A:170:THR:HG21 | 1:A:174:ILE:HG23 | 2.03 | 0.40 |
| 1:A:278:ALA:HB3 | 1:A:335:ILE:CG1 | 2.48 | 0.40 |
| 1:A:337:GLU:HG2 | 1:A:342:ILE:O | 2.21 | 0.40 |
| 1:A:622:ASN:O | 1:A:623:PRO:C | 2.60 | 0.40 |
| 1:A:647:ASN:HB2 | 1:A:654:TYR:HE1 | 1.85 | 0.40 |
| 1:A:717(A):ILE:HD12 | 1:A:717(A):ILE:N | 2.37 | 0.40 |
| 1:A:863:GLN:O | 1:A:895:ARG:CD | 2.61 | 0.40 |
| 1:B:624:TRP:CZ2 | 1:B:1008:ILE:HD13 | 2.53 | 0.40 |
| 1:B:418:ILE:HD12 | 1:B:419:SER:O | 2.21 | 0.40 |
| 1:B:856:SER:OG | 1:C:800:SER:HA | 2.21 | 0.40 |
| 1:C:180:ALA:O | 1:C:181:LYS:C | 2.60 | 0.40 |
| 1:C:47:GLU:CD | 1:C:428:LYS:HE3 | 2.41 | 0.40 |
| 1:C:480:PHE:C | 1:C:480:PHE:CD1 | 2.94 | 0.40 |
| 1:C:641:MET:HB3 | 1:C:671:ILE:HD12 | 2.04 | 0.40 |
| 1:C:691:GLU:O | 1:C:695:GLU:HB2 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:C:995:GLU:O | 1:C:998:GLN:O | 2.39 | 0.40 |
| 1:D:362:MET:HA | 1:D:362(A):PRO:HD2 | 1.97 | 0.40 |
| 1:D:393:THR:HG23 | 1:D:417:GLU:OE1 | 2.21 | 0.40 |
| 1:A:1029:ASN:ND2 | 1:A:1031:SER:H | 2.20 | 0.40 |
| 1:A:496:ARG:O | 1:A:497:GLY:C | 2.60 | 0.40 |
| 1:A:606:MET:SD | 1:A:606:MET:C | 3.00 | 0.40 |
| 1:B:266:SER:HB2 | 1:B:476:TYR:CE2 | 2.56 | 0.40 |
| 1:D:1083:GLN:HB3 | 1:D:1083:GLN:HE21 | 1.49 | 0.40 |
| 1:D:166:VAL:HG22 | 1:D:322:PHE:HB3 | 2.02 | 0.40 |
| 1:D:373:ALA:HA | 1:D:431:THR:O | 2.22 | 0.40 |
| 1:D:739:ALA:C | 1:D:740:ILE:HD13 | 2.42 | 0.40 |
| 1:D:869:GLY:O | 1:D:871:TYR:N | 2.55 | 0.40 |
| 1:D:926:LEU:HD12 | 1:D:926:LEU:HA | 1.91 | 0.40 |
| 1:D:924:ASN:CB | 1:D:926:LEU:HD22 | 2.50 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1 | A | 1048/1173 (89%) | 916 (87%) | 102 (10%) | 30 (3%) | 4 | 15 |
| 1 | B | 985/1173 (84%) | 876 (89%) | 85 (9%) | 24 (2%) | 6 | 20 |
| 1 | C | 1057/1173 (90%) | 923 (87%) | 96 (9%) | 38 (4%) | 3 | 11 |
| 1 | D | 985/1173 (84%) | 864 (88%) | 94 (10%) | 27 (3%) | 5 | 17 |
| All | All | 4075/4692 (87%) | 3579 (88%) | 377 (9%) | 119 (3%) | 4 | 15 |

All (119) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 187 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 211 | SER |
| 1 | A | 213 | LEU |
| 1 | A | 214 | GLU |
| 1 | A | 217 | PHE |
| 1 | A | 230 | ASN |
| 1 | A | 396 | ALA |
| 1 | A | 709 | ASP |
| 1 | A | 870 | GLN |
| 1 | A | 880 | SER |
| 1 | B | 163 | ASP |
| 1 | B | 270 | ARG |
| 1 | B | 414 | GLN |
| 1 | B | 495 | ASP |
| 1 | B | 522 | PRO |
| 1 | B | 975 | THR |
| 1 | C | 176 | SER |
| 1 | C | 195 | ALA |
| 1 | C | 201 | GLY |
| 1 | C | 204 | MET |
| 1 | C | 214 | GLU |
| 1 | C | 215 | ASP |
| 1 | C | 386 | ASP |
| 1 | C | 518 | LYS |
| 1 | C | 649 | VAL |
| 1 | C | 886 | ARG |
| 1 | C | 890 | VAL |
| 1 | C | 980 | GLU |
| 1 | D | 92 | PRO |
| 1 | D | 152 | LYS |
| 1 | D | 240 | ASP |
| 1 | D | 515 | ASN |
| 1 | D | 870 | GLN |
| 1 | A | 499 | LYS |
| 1 | A | 527 | ALA |
| 1 | A | 648 | ALA |
| 1 | A | 861 | ILE |
| 1 | B | 166 | VAL |
| 1 | B | 528 | SER |
| 1 | B | 868 | GLY |
| 1 | B | 881 | LEU |
| 1 | B | 903 | ASP |
| 1 | B | 1001 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | C | 87 | GLY |
| 1 | C | 203 | GLY |
| 1 | C | 229 | GLY |
| 1 | C | 385 | ASN |
| 1 | C | 645 | ALA |
| 1 | C | 937 | LYS |
| 1 | C | 938 | LEU |
| 1 | C | 942 | GLU |
| 1 | D | 87 | GLY |
| 1 | D | 94 | GLU |
| 1 | D | 163 | ASP |
| 1 | D | 306 | ASN |
| 1 | D | 414 | GLN |
| 1 | D | 450 | MET |
| 1 | D | 649 | VAL |
| 1 | D | 799 | ALA |
| 1 | D | 884 | GLY |
| 1 | D | 888 | ASP |
| 1 | A | 94 | GLU |
| 1 | A | 517 | GLU |
| 1 | B | 475 | ASP |
| 1 | B | 1002 | VAL |
| 1 | B | 1081 | ASN |
| 1 | C | 151 | ASP |
| 1 | C | 197 | SER |
| 1 | C | 981 | TYR |
| 1 | C | 1053 | ASP |
| 1 | D | 334 | THR |
| 1 | D | 517 | GLU |
| 1 | D | 518 | LYS |
| 1 | D | 1069 | ASP |
| 1 | A | 44 | ASN |
| 1 | A | 209 | GLU |
| 1 | A | 882 | GLY |
| 1 | B | 306 | ASN |
| 1 | B | 648 | ALA |
| 1 | B | 649 | VAL |
| 1 | B | 1000 | GLY |
| 1 | C | 173 | PRO |
| 1 | C | 216 | ALA |
| 1 | C | 269 | ARG |
| 1 | C | 355 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | C | 821 | PRO |
| 1 | D | 133 | GLU |
| 1 | D | 261 | PHE |
| 1 | D | 480 | PHE |
| 1 | D | 513 | PRO |
| 1 | B | 527 | ALA |
| 1 | B | 1053 | ASP |
| 1 | C | 898 | ASN |
| 1 | C | 935 | GLY |
| 1 | D | 335 | ILE |
| 1 | D | 854 | ILE |
| 1 | A | 92 | PRO |
| 1 | A | 110 | ASN |
| 1 | A | 189 | PHE |
| 1 | A | 241 | ASN |
| 1 | A | 306 | ASN |
| 1 | B | 480 | PHE |
| 1 | B | 562 | ASP |
| 1 | C | 174 | ILE |
| 1 | C | 180 | ALA |
| 1 | C | 1001 | PRO |
| 1 | A | 1001 | PRO |
| 1 | D | 282 | GLY |
| 1 | A | 282 | GLY |
| 1 | A | 1014 | PRO |
| 1 | B | 890 | VAL |
| 1 | C | 189 | PHE |
| 1 | A | 868 | GLY |
| 1 | C | 291 | ILE |
| 1 | C | 327 | PRO |
| 1 | A | 956 | VAL |
| 1 | C | 168 | PRO |
| 1 | A | 935 | GLY |
| 1 | D | 1014 | PRO |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1 | A | 907/1005 (90%) | 778 (86%) | 129 (14%) | 3 | 10 |
| 1 | B | 855/1005 (85%) | 726 (85%) | 129 (15%) | 3 | 9 |
| 1 | C | 909/1005 (90%) | 751 (83%) | 158 (17%) | 2 | 6 |
| 1 | D | 855/1005 (85%) | 727 (85%) | 128 (15%) | 3 | 9 |
| All | All | 3526/4020 (88%) | 2982 (85%) | 544 (15%) | 2 | 8 |

All (544) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 38 | LYS |
| 1 | A | 44 | ASN |
| 1 | A | 62 | SER |
| 1 | A | 66 | ILE |
| 1 | A | 69 | ASN |
| 1 | A | 70 | GLU |
| 1 | A | 73 | SER |
| 1 | A | 75 | LEU |
| 1 | A | 77 | ARG |
| 1 | A | 94 | GLU |
| 1 | A | 95 | SER |
| 1 | A | 97 | LEU |
| 1 | A | 98 | ASN |
| 1 | A | 108 | GLN |
| 1 | A | 110 | ASN |
| 1 | A | 143 | LEU |
| 1 | A | 144 | GLU |
| 1 | A | 156 | ARG |
| 1 | A | 161 | LYS |
| 1 | A | 163 | ASP |
| 1 | A | 175 | LYS |
| 1 | A | 179 | LEU |
| 1 | A | 182 | GLU |
| 1 | A | 186 | GLU |
| 1 | A | 193 | ILE |
| 1 | A | 194 | LYS |
| 1 | A | 210 | GLU |
| 1 | A | 212 | GLU |
| 1 | A | 214 | GLU |
| 1 | A | 215 | ASP |
| 1 | A | 225 | GLU |
| 1 | A | 234 | TYR |
| 1 | A | 237 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 239 | ILE |
| 1 | A | 257 | ILE |
| 1 | A | 271 | HIS |
| 1 | A | 283 | LEU |
| 1 | A | 286 | THR |
| 1 | A | 287 | LEU |
| 1 | A | 306 | ASN |
| 1 | A | 313 | LEU |
| 1 | A | 329 | VAL |
| 1 | A | 331 | VAL |
| 1 | A | 335 | ILE |
| 1 | A | 386 | ASP |
| 1 | A | 391 | THR |
| 1 | A | 398 | ARG |
| 1 | A | 419 | SER |
| 1 | A | 427 | VAL |
| 1 | A | 428 | LYS |
| 1 | A | 434 | ILE |
| 1 | A | 437 | LYS |
| 1 | A | 440 | GLU |
| 1 | A | 442 | LYS |
| 1 | A | 455 | VAL |
| 1 | A | 472 | THR |
| 1 | A | 473 | SER |
| 1 | A | 487 | LEU |
| 1 | A | 491 | GLN |
| 1 | A | 496 | ARG |
| 1 | A | 512 | PHE |
| 1 | A | 518 | LYS |
| 1 | A | 525 | GLU |
| 1 | A | 526 | LEU |
| 1 | A | 528 | SER |
| 1 | A | 535 | SER |
| 1 | A | 536 | LYS |
| 1 | A | 547 | GLU |
| 1 | A | 551 | LYS |
| 1 | A | 565 | LEU |
| 1 | A | 580 | THR |
| 1 | A | 588 | ILE |
| 1 | A | 590 | ILE |
| 1 | A | 592 | SER |
| 1 | A | 606 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 607 | TRP |
| 1 | A | 613 | ASP |
| 1 | A | 620 | LYS |
| 1 | A | 622 | ASN |
| 1 | A | 631 | ARG |
| 1 | A | 649 | VAL |
| 1 | A | 672 | ASP |
| 1 | A | 679 | SER |
| 1 | A | 685 | GLN |
| 1 | A | 715 | ARG |
| 1 | A | 719 | THR |
| 1 | A | 725 | LYS |
| 1 | A | 743 | MET |
| 1 | A | 750 | LYS |
| 1 | A | 760 | LYS |
| 1 | A | 766 | LEU |
| 1 | A | 775 | THR |
| 1 | A | 781 | LEU |
| 1 | A | 784 | LYS |
| 1 | A | 811 | ASN |
| 1 | A | 828 | ILE |
| 1 | A | 831 | MET |
| 1 | A | 835 | SER |
| 1 | A | 855 | LYS |
| 1 | A | 861 | ILE |
| 1 | A | 863 | GLN |
| 1 | A | 870 | GLN |
| 1 | A | 876 | GLN |
| 1 | A | 880 | SER |
| 1 | A | 904 | ILE |
| 1 | A | 907 | VAL |
| 1 | A | 908 | THR |
| 1 | A | 919 | LEU |
| 1 | A | 923 | GLN |
| 1 | A | 926 | LEU |
| 1 | A | 931 | VAL |
| 1 | A | 932 | ILE |
| 1 | A | 944 | VAL |
| 1 | A | 961 | LYS |
| 1 | A | 980 | GLU |
| 1 | A | 993 | LEU |
| 1 | A | 999 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1008 | ILE |
| 1 | A | 1018 | GLU |
| 1 | A | 1019 | GLN |
| 1 | A | 1029 | ASN |
| 1 | A | 1043 | ARG |
| 1 | A | 1044 | ASN |
| 1 | A | 1048 | VAL |
| 1 | A | 1051 | GLU |
| 1 | A | 1064 | THR |
| 1 | A | 1076 | ILE |
| 1 | A | 1080 | MET |
| 1 | A | 1089 | ILE |
| 1 | B | 36 | GLN |
| 1 | B | 38 | LYS |
| 1 | B | 44 | ASN |
| 1 | B | 62 | SER |
| 1 | B | 70 | GLU |
| 1 | B | 75 | LEU |
| 1 | B | 90 | LEU |
| 1 | B | 94 | GLU |
| 1 | B | 98 | ASN |
| 1 | B | 101 | ARG |
| 1 | B | 104 | ASP |
| 1 | B | 124 | ASN |
| 1 | B | 144 | GLU |
| 1 | B | 147 | ASP |
| 1 | B | 152 | LYS |
| 1 | B | 153 | VAL |
| 1 | B | 166 | VAL |
| 1 | B | 167 | ILE |
| 1 | B | 239 | ILE |
| 1 | B | 241 | ASN |
| 1 | B | 281 | VAL |
| 1 | B | 287 | LEU |
| 1 | B | 288 | ARG |
| 1 | B | 289 | GLN |
| 1 | B | 291 | ILE |
| 1 | B | 300 | GLU |
| 1 | B | 306 | ASN |
| 1 | B | 315 | SER |
| 1 | B | 319 | GLU |
| 1 | B | 320 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 328 | ARG |
| 1 | B | 331 | VAL |
| 1 | B | 357 | LEU |
| 1 | B | 359 | GLU |
| 1 | B | 361 | ASN |
| 1 | B | 365 | LYS |
| 1 | B | 368 | THR |
| 1 | B | 370 | LEU |
| 1 | B | 376 | CYS |
| 1 | B | 391 | THR |
| 1 | B | 399 | SER |
| 1 | B | 400 | SER |
| 1 | B | 406 | ARG |
| 1 | B | 417 | GLU |
| 1 | B | 418 | ILE |
| 1 | B | 423 | ASP |
| 1 | B | 427 | VAL |
| 1 | B | 435 | SER |
| 1 | B | 442 | LYS |
| 1 | B | 446 | SER |
| 1 | B | 450 | MET |
| 1 | B | 451 | ARG |
| 1 | B | 453 | ARG |
| 1 | B | 479 | LYS |
| 1 | B | 487 | LEU |
| 1 | B | 494 | LEU |
| 1 | B | 500 | THR |
| 1 | B | 515 | ASN |
| 1 | B | 519 | ARG |
| 1 | B | 534 | SER |
| 1 | B | 547 | GLU |
| 1 | B | 551 | LYS |
| 1 | B | 558 | LYS |
| 1 | B | 576 | SER |
| 1 | B | 580 | THR |
| 1 | B | 606 | MET |
| 1 | B | 607 | TRP |
| 1 | B | 622 | ASN |
| 1 | B | 631 | ARG |
| 1 | B | 632 | LYS |
| 1 | B | 647 | ASN |
| 1 | B | 649 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 652 | LYS |
| 1 | B | 660 | HIS |
| 1 | B | 690 | ASN |
| 1 | B | 715 | ARG |
| 1 | B | 721 | GLU |
| 1 | B | 725 | LYS |
| 1 | B | 740 | ILE |
| 1 | B | 743 | MET |
| 1 | B | 761 | SER |
| 1 | B | 775 | THR |
| 1 | B | 784 | LYS |
| 1 | B | 791 | VAL |
| 1 | B | 792 | ASP |
| 1 | B | 807 | GLN |
| 1 | B | 809 | SER |
| 1 | B | 811 | ASN |
| 1 | B | 812 | SER |
| 1 | B | 828 | ILE |
| 1 | B | 831 | MET |
| 1 | B | 839 | SER |
| 1 | B | 843 | THR |
| 1 | B | 852 | SER |
| 1 | B | 853 | ASP |
| 1 | B | 855 | LYS |
| 1 | B | 863 | GLN |
| 1 | B | 871 | TYR |
| 1 | B | 872 | SER |
| 1 | B | 875 | SER |
| 1 | B | 876 | GLN |
| 1 | B | 879 | LYS |
| 1 | B | 880 | SER |
| 1 | B | 881 | LEU |
| 1 | B | 886 | ARG |
| 1 | B | 897 | VAL |
| 1 | B | 907 | VAL |
| 1 | B | 908 | THR |
| 1 | B | 919 | LEU |
| 1 | B | 927 | ASP |
| 1 | B | 929 | GLN |
| 1 | B | 930 | SER |
| 1 | B | 934 | ASP |
| 1 | B | 936 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | B | 938 | LEU |
| 1 | B | 939 | ASP |
| 1 | B | 942 | GLU |
| 1 | B | 944 | VAL |
| 1 | B | 949 | LYS |
| 1 | B | 957 | ASN |
| 1 | B | 962 | ASP |
| 1 | B | 963 | LEU |
| 1 | B | 991 | ARG |
| 1 | B | 1029 | ASN |
| 1 | B | 1057 | ARG |
| 1 | B | 1070 | GLU |
| 1 | B | 1071 | ASN |
| 1 | B | 1085 | ARG |
| 1 | B | 1089 | ILE |
| 1 | C | 44 | ASN |
| 1 | C | 45 | ARG |
| 1 | C | 69 | ASN |
| 1 | C | 70 | GLU |
| 1 | C | 75 | LEU |
| 1 | C | 77 | ARG |
| 1 | C | 86 | VAL |
| 1 | C | 90 | LEU |
| 1 | C | 97 | LEU |
| 1 | C | 98 | ASN |
| 1 | C | 100 | GLU |
| 1 | C | 101 | ARG |
| 1 | C | 110 | ASN |
| 1 | C | 112 | ASP |
| 1 | C | 123 | GLU |
| 1 | C | 142 | HIS |
| 1 | C | 144 | GLU |
| 1 | C | 151 | ASP |
| 1 | C | 154 | LYS |
| 1 | C | 156 | ARG |
| 1 | C | 166 | VAL |
| 1 | C | 167 | ILE |
| 1 | C | 171 | ASP |
| 1 | C | 175 | LYS |
| 1 | C | 178 | GLU |
| 1 | C | 179 | LEU |
| 1 | C | 192 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 193 | ILE |
| 1 | C | 194 | LYS |
| 1 | C | 202 | LYS |
| 1 | C | 205 | ARG |
| 1 | C | 208 | ARG |
| 1 | C | 209 | GLU |
| 1 | C | 210 | GLU |
| 1 | C | 215 | ASP |
| 1 | C | 219 | ARG |
| 1 | C | 223 | GLU |
| 1 | C | 225 | GLU |
| 1 | C | 230 | ASN |
| 1 | C | 232 | GLU |
| 1 | C | 234 | TYR |
| 1 | C | 235 | ILE |
| 1 | C | 237 | ARG |
| 1 | C | 253 | GLU |
| 1 | C | 257 | ILE |
| 1 | C | 262 | GLU |
| 1 | C | 269 | ARG |
| 1 | C | 280 | SER |
| 1 | C | 286 | THR |
| 1 | C | 287 | LEU |
| 1 | C | 288 | ARG |
| 1 | C | 306 | ASN |
| 1 | C | 315 | SER |
| 1 | C | 318 | ASP |
| 1 | C | 324 | GLU |
| 1 | C | 358 | GLU |
| 1 | C | 359 | GLU |
| 1 | C | 365 | LYS |
| 1 | C | 368 | THR |
| 1 | C | 377 | ARG |
| 1 | C | 384 | LEU |
| 1 | C | 386 | ASP |
| 1 | C | 391 | THR |
| 1 | C | 395 | ILE |
| 1 | C | 414 | GLN |
| 1 | C | 437 | LYS |
| 1 | C | 442 | LYS |
| 1 | C | 444 | VAL |
| 1 | C | 446 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 451 | ARG |
| 1 | C | 453 | ARG |
| 1 | C | 467 | LYS |
| 1 | C | 469 | LYS |
| 1 | C | 473 | SER |
| 1 | C | 491 | GLN |
| 1 | C | 493 | SER |
| 1 | C | 494 | LEU |
| 1 | C | 531 | THR |
| 1 | C | 533 | SER |
| 1 | C | 537 | ILE |
| 1 | C | 539 | SER |
| 1 | C | 543 | GLN |
| 1 | C | 545 | LEU |
| 1 | C | 547 | GLU |
| 1 | C | 559 | LYS |
| 1 | C | 563 | VAL |
| 1 | C | 589 | ASN |
| 1 | C | 606 | MET |
| 1 | C | 607 | TRP |
| 1 | C | 616 | TYR |
| 1 | C | 622 | ASN |
| 1 | C | 631 | ARG |
| 1 | C | 641 | MET |
| 1 | C | 646 | SER |
| 1 | C | 647 | ASN |
| 1 | C | 649 | VAL |
| 1 | C | 652 | LYS |
| 1 | C | 660 | HIS |
| 1 | C | 661 | LYS |
| 1 | C | 680 | LEU |
| 1 | C | 695 | GLU |
| 1 | C | 707 | THR |
| 1 | C | 717 | ASN |
| 1 | C | 719 | THR |
| 1 | C | 725 | LYS |
| 1 | C | 743 | MET |
| 1 | C | 750 | LYS |
| 1 | C | 760 | LYS |
| 1 | C | 781 | LEU |
| 1 | C | 783 | TYR |
| 1 | C | 784 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | C | 807 | GLN |
| 1 | C | 811 | ASN |
| 1 | C | 833 | SER |
| 1 | C | 835 | SER |
| 1 | C | 839 | SER |
| 1 | C | 843 | THR |
| 1 | C | 852 | SER |
| 1 | C | 855 | LYS |
| 1 | C | 856 | SER |
| 1 | C | 860 | GLU |
| 1 | C | 861 | ILE |
| 1 | C | 863 | GLN |
| 1 | C | 866 | MET |
| 1 | C | 870 | GLN |
| 1 | C | 872 | SER |
| 1 | C | 876 | GLN |
| 1 | C | 881 | LEU |
| 1 | C | 885 | GLU |
| 1 | C | 892 | ASP |
| 1 | C | 893 | MET |
| 1 | C | 895 | ARG |
| 1 | C | 896 | ARG |
| 1 | C | 907 | VAL |
| 1 | C | 908 | THR |
| 1 | C | 923 | GLN |
| 1 | C | 927 | ASP |
| 1 | C | 928 | GLU |
| 1 | C | 938 | LEU |
| 1 | C | 949 | LYS |
| 1 | C | 959 | PHE |
| 1 | C | 960 | ASN |
| 1 | C | 967 | ILE |
| 1 | C | 968 | LEU |
| 1 | C | 971 | GLN |
| 1 | C | 980 | GLU |
| 1 | C | 986 | ASP |
| 1 | C | 997 | GLU |
| 1 | C | 1015 | LYS |
| 1 | C | 1024 | ARG |
| 1 | C | 1029 | ASN |
| 1 | C | 1031 | SER |
| 1 | C | 1048 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | C | 1052 | ILE |
| 1 | C | 1067 | GLU |
| 1 | C | 1076 | ILE |
| 1 | C | 1085 | ARG |
| 1 | C | 1090 | LYS |
| 1 | D | 38 | LYS |
| 1 | D | 44 | ASN |
| 1 | D | 72 | LYS |
| 1 | D | 73 | SER |
| 1 | D | 75 | LEU |
| 1 | D | 77 | ARG |
| 1 | D | 88 | SER |
| 1 | D | 99 | ILE |
| 1 | D | 101 | ARG |
| 1 | D | 137 | LYS |
| 1 | D | 143 | LEU |
| 1 | D | 163 | ASP |
| 1 | D | 167 | ILE |
| 1 | D | 239 | ILE |
| 1 | D | 240 | ASP |
| 1 | D | 243 | LYS |
| 1 | D | 250 | ILE |
| 1 | D | 253 | GLU |
| 1 | D | 260 | LEU |
| 1 | D | 262 | GLU |
| 1 | D | 268 | GLN |
| 1 | D | 270 | ARG |
| 1 | D | 280 | SER |
| 1 | D | 287 | LEU |
| 1 | D | 288 | ARG |
| 1 | D | 290 | ARG |
| 1 | D | 305 | VAL |
| 1 | D | 326 | ASN |
| 1 | D | 328 | ARG |
| 1 | D | 329 | VAL |
| 1 | D | 331 | VAL |
| 1 | D | 335 | ILE |
| 1 | D | 360 | ILE |
| 1 | D | 361 | ASN |
| 1 | D | 365 | LYS |
| 1 | D | 368 | THR |
| 1 | D | 369 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 386 | ASP |
| 1 | D | 393 | THR |
| 1 | D | 395 | ILE |
| 1 | D | 417 | GLU |
| 1 | D | 418 | ILE |
| 1 | D | 425 | LEU |
| 1 | D | 427 | VAL |
| 1 | D | 434 | ILE |
| 1 | D | 437 | LYS |
| 1 | D | 445 | ARG |
| 1 | D | 446 | SER |
| 1 | D | 451 | ARG |
| 1 | D | 452 | ILE |
| 1 | D | 456 | LYS |
| 1 | D | 467 | LYS |
| 1 | D | 470 | LYS |
| 1 | D | 473 | SER |
| 1 | D | 478 | THR |
| 1 | D | 479 | LYS |
| 1 | D | 486 | GLU |
| 1 | D | 487 | LEU |
| 1 | D | 491 | GLN |
| 1 | D | 496 | ARG |
| 1 | D | 506 | ASN |
| 1 | D | 513 | PRO |
| 1 | D | 519 | ARG |
| 1 | D | 523 | ASP |
| 1 | D | 525 | GLU |
| 1 | D | 526 | LEU |
| 1 | D | 528 | SER |
| 1 | D | 531 | THR |
| 1 | D | 533 | SER |
| 1 | D | 542 | LYS |
| 1 | D | 543 | GLN |
| 1 | D | 551 | LYS |
| 1 | D | 555 | GLU |
| 1 | D | 565 | LEU |
| 1 | D | 580 | THR |
| 1 | D | 607 | TRP |
| 1 | D | 620 | LYS |
| 1 | D | 622 | ASN |
| 1 | D | 629 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | D | 631 | ARG |
| 1 | D | 632 | LYS |
| 1 | D | 641 | MET |
| 1 | D | 647 | ASN |
| 1 | D | 649 | VAL |
| 1 | D | 700 | SER |
| 1 | D | 707 | THR |
| 1 | D | 714 | GLU |
| 1 | D | 715 | ARG |
| 1 | D | 725 | LYS |
| 1 | D | 743 | MET |
| 1 | D | 760 | LYS |
| 1 | D | 763 | VAL |
| 1 | D | 766 | LEU |
| 1 | D | 775 | THR |
| 1 | D | 784 | LYS |
| 1 | D | 791 | VAL |
| 1 | D | 811 | ASN |
| 1 | D | 831 | MET |
| 1 | D | 839 | SER |
| 1 | D | 852 | SER |
| 1 | D | 853 | ASP |
| 1 | D | 856 | SER |
| 1 | D | 863 | GLN |
| 1 | D | 866 | MET |
| 1 | D | 870 | GLN |
| 1 | D | 885 | GLU |
| 1 | D | 886 | ARG |
| 1 | D | 907 | VAL |
| 1 | D | 908 | THR |
| 1 | D | 911 | SER |
| 1 | D | 917 | MET |
| 1 | D | 919 | LEU |
| 1 | D | 926 | LEU |
| 1 | D | 927 | ASP |
| 1 | D | 944 | VAL |
| 1 | D | 952 | ILE |
| 1 | D | 963 | LEU |
| 1 | D | 977 | ARG |
| 1 | D | 996 | GLU |
| 1 | D | 1046 | GLU |
| 1 | D | 1052 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | D | 1054 | LYS |
| 1 | D | 1057 | ARG |
| 1 | D | 1061 | LYS |
| 1 | D | 1064 | THR |
| 1 | D | 1080 | MET |
| 1 | D | 1083 | GLN |
| 1 | D | 1085 | ARG |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (143) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 44 | ASN |
| 1 | A | 69 | ASN |
| 1 | A | 98 | ASN |
| 1 | A | 108 | GLN |
| 1 | A | 126 | GLN |
| 1 | A | 145 | HIS |
| 1 | A | 241 | ASN |
| 1 | A | 254 | HIS |
| 1 | A | 256 | ASN |
| 1 | A | 268 | GLN |
| 1 | A | 330 | GLN |
| 1 | A | 375 | GLN |
| 1 | A | 432 | HIS |
| 1 | A | 506 | ASN |
| 1 | A | 543 | GLN |
| 1 | A | 574 | HIS |
| 1 | A | 575 | GLN |
| 1 | A | 589 | ASN |
| 1 | A | 622 | ASN |
| 1 | A | 685 | GLN |
| 1 | A | 736 | HIS |
| 1 | A | 778 | ASN |
| 1 | A | 807 | GLN |
| 1 | A | 811 | ASN |
| 1 | A | 818 | ASN |
| 1 | A | 858 | ASN |
| 1 | A | 864 | HIS |
| 1 | A | 898 | ASN |
| 1 | A | 923 | GLN |
| 1 | A | 1005 | GLN |
| 1 | A | 1025 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1029 | ASN |
| 1 | A | 1044 | ASN |
| 1 | B | 36 | GLN |
| 1 | B | 44 | ASN |
| 1 | B | 69 | ASN |
| 1 | B | 98 | ASN |
| 1 | B | 108 | GLN |
| 1 | B | 145 | HIS |
| 1 | B | 256 | ASN |
| 1 | B | 272 | GLN |
| 1 | B | 301 | ASN |
| 1 | B | 326 | ASN |
| 1 | B | 330 | GLN |
| 1 | B | 361 | ASN |
| 1 | B | 363 | GLN |
| 1 | B | 375 | GLN |
| 1 | B | 432 | HIS |
| 1 | B | 438 | GLN |
| 1 | B | 515 | ASN |
| 1 | B | 543 | GLN |
| 1 | B | 574 | HIS |
| 1 | B | 575 | GLN |
| 1 | B | 589 | ASN |
| 1 | B | 622 | ASN |
| 1 | B | 690 | ASN |
| 1 | B | 736 | HIS |
| 1 | B | 778 | ASN |
| 1 | B | 811 | ASN |
| 1 | B | 863 | GLN |
| 1 | B | 864 | HIS |
| 1 | B | 898 | ASN |
| 1 | B | 923 | GLN |
| 1 | B | 960 | ASN |
| 1 | B | 998 | GLN |
| 1 | B | 1005 | GLN |
| 1 | B | 1025 | ASN |
| 1 | B | 1029 | ASN |
| 1 | B | 1044 | ASN |
| 1 | B | 1073 | ASN |
| 1 | B | 1083 | GLN |
| 1 | C | 44 | ASN |
| 1 | C | 98 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | C | 110 | ASN |
| 1 | C | 142 | HIS |
| 1 | C | 145 | HIS |
| 1 | C | 230 | ASN |
| 1 | C | 289 | GLN |
| 1 | C | 301 | ASN |
| 1 | C | 326 | ASN |
| 1 | C | 330 | GLN |
| 1 | C | 414 | GLN |
| 1 | C | 464 | ASN |
| 1 | C | 506 | ASN |
| 1 | C | 574 | HIS |
| 1 | C | 575 | GLN |
| 1 | C | 589 | ASN |
| 1 | C | 617 | ASN |
| 1 | C | 622 | ASN |
| 1 | C | 685 | GLN |
| 1 | C | 694 | GLN |
| 1 | C | 717 | ASN |
| 1 | C | 736 | HIS |
| 1 | C | 778 | ASN |
| 1 | C | 785 | GLN |
| 1 | C | 807 | GLN |
| 1 | C | 811 | ASN |
| 1 | C | 818 | ASN |
| 1 | C | 863 | GLN |
| 1 | C | 864 | HIS |
| 1 | C | 876 | GLN |
| 1 | C | 877 | GLN |
| 1 | C | 898 | ASN |
| 1 | C | 923 | GLN |
| 1 | C | 964 | GLN |
| 1 | C | 1005 | GLN |
| 1 | C | 1025 | ASN |
| 1 | C | 1029 | ASN |
| 1 | C | 1044 | ASN |
| 1 | C | 1093 | ASN |
| 1 | D | 44 | ASN |
| 1 | D | 145 | HIS |
| 1 | D | 244 | HIS |
| 1 | D | 256 | ASN |
| 1 | D | 301 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | D | 326 | ASN |
| 1 | D | 330 | GLN |
| 1 | D | 348 | GLN |
| 1 | D | 364 | GLN |
| 1 | D | 375 | GLN |
| 1 | D | 432 | HIS |
| 1 | D | 468 | ASN |
| 1 | D | 491 | GLN |
| 1 | D | 506 | ASN |
| 1 | D | 543 | GLN |
| 1 | D | 574 | HIS |
| 1 | D | 575 | GLN |
| 1 | D | 589 | ASN |
| 1 | D | 622 | ASN |
| 1 | D | 647 | ASN |
| 1 | D | 717 | ASN |
| 1 | D | 736 | HIS |
| 1 | D | 778 | ASN |
| 1 | D | 807 | GLN |
| 1 | D | 811 | ASN |
| 1 | D | 818 | ASN |
| 1 | D | 864 | HIS |
| 1 | D | 877 | GLN |
| 1 | D | 898 | ASN |
| 1 | D | 960 | ASN |
| 1 | D | 1005 | GLN |
| 1 | D | 1025 | ASN |
| 1 | D | 1083 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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 | ADP | A | 1201 | - | 24,29,29 | 1.04 | 2 (8%) | 29,45,45 | 1.46 | 6 (20%) |
| 4 | BTI | D | 1201 | - | 16,16,16 | 1.64 | 2 (12%) | 21,21,21 | 2.05 | 5 (23%) |
| 5 | ATP | C | 1202 | - | 26,33,33 | 0.99 | 2 (7%) | 31,52,52 | 1.37 | 4 (12%) |
| 4 | BTI | A | 1203 | - | 16,16,16 | 1.69 | 2 (12%) | 21,21,21 | 1.98 | 5 (23%) |
| 4 | BTI | B | 1201 | - | 16,16,16 | 1.62 | 2 (12%) | 21,21,21 | 2.49 | 5 (23%) |

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 | ADP | A | 1201 | - | - | 6/12/32/32 | 0/3/3/3 |
| 4 | BTI | D | 1201 | - | - | 1/5/27/27 | 0/2/2/2 |
| 5 | ATP | C | 1202 | - | - | 3/18/38/38 | 0/3/3/3 |
| 4 | BTI | A | 1203 | - | - | 4/5/27/27 | 0/2/2/2 |
| 4 | BTI | B | 1201 | - | - | 3/5/27/27 | 0/2/2/2 |

All (10) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 4 | A | 1203 | BTI | O3-C3 | 5.10 | 1.34 | 1.23 |
| 4 | B | 1201 | BTI | O3-C3 | 5.08 | 1.34 | 1.23 |
| 4 | D | 1201 | BTI | O3-C3 | 4.88 | 1.33 | 1.23 |
| 4 | A | 1203 | BTI | C2-S1 | -3.60 | 1.76 | 1.82 |
| 4 | D | 1201 | BTI | C2-S1 | -3.32 | 1.77 | 1.82 |
| 4 | B | 1201 | BTI | C2-S1 | -2.96 | 1.77 | 1.82 |
| 5 | C | 1202 | ATP | C5-C4 | 2.60 | 1.47 | 1.40 |
| 5 | C | 1202 | ATP | O4'-C1' | 2.53 | 1.44 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 2 | A | 1201 | ADP | C5-C4 | 2.45 | 1.47 | 1.40 |
| 2 | A | 1201 | ADP | O4'-C1' | 2.32 | 1.44 | 1.41 |

All (25) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 4 | B | 1201 | BTI | C2-C4-N2 | -8.60 | 105.42 | 113.13 |
| 4 | D | 1201 | BTI | C2-C4-N2 | -5.95 | 107.80 | 113.13 |
| 4 | A | 1203 | BTI | C5-C6-S1 | 4.96 | 110.56 | 106.31 |
| 4 | B | 1201 | BTI | C6-C5-N3 | -4.91 | 106.80 | 113.03 |
| 4 | A | 1203 | BTI | C6-C5-N3 | -4.90 | 106.80 | 113.03 |
| 4 | D | 1201 | BTI | C6-C5-N3 | -4.67 | 107.10 | 113.03 |
| 5 | C | 1202 | ATP | PA-O3A-PB | -3.82 | 119.71 | 132.83 |
| 2 | A | 1201 | ADP | N3-C2-N1 | -3.40 | 123.36 | 128.68 |
| 2 | A | 1201 | ADP | C3'-C2'-C1' | 3.31 | 105.96 | 100.98 |
| 5 | C | 1202 | ATP | N3-C2-N1 | -2.92 | 124.12 | 128.68 |
| 4 | B | 1201 | BTI | C4-C2-S1 | 2.87 | 107.94 | 105.20 |
| 5 | C | 1202 | ATP | PB-O3B-PG | -2.82 | 123.16 | 132.83 |
| 4 | D | 1201 | BTI | N2-C3-N3 | 2.81 | 111.39 | 108.76 |
| 5 | C | 1202 | ATP | C4-C5-N7 | -2.65 | 106.64 | 109.40 |
| 4 | D | 1201 | BTI | C8-C7-C2 | -2.63 | 108.52 | 113.86 |
| 2 | A | 1201 | ADP | PA-O3A-PB | -2.58 | 123.98 | 132.83 |
| 2 | A | 1201 | ADP | C4-C5-N7 | -2.40 | 106.89 | 109.40 |
| 4 | B | 1201 | BTI | N2-C3-N3 | 2.37 | 110.98 | 108.76 |
| 4 | D | 1201 | BTI | C5-C6-S1 | 2.36 | 108.33 | 106.31 |
| 4 | A | 1203 | BTI | C4-C2-S1 | 2.24 | 107.34 | 105.20 |
| 2 | A | 1201 | ADP | O3B-PB-O2B | 2.15 | 115.86 | 107.64 |
| 4 | A | 1203 | BTI | N2-C3-N3 | 2.13 | 110.76 | 108.76 |
| 4 | B | 1201 | BTI | O3-C3-N2 | -2.12 | 122.89 | 125.94 |
| 4 | A | 1203 | BTI | C8-C7-C2 | -2.06 | 109.67 | 113.86 |
| 2 | A | 1201 | ADP | C2'-C3'-C4' | 2.05 | 106.63 | 102.64 |

There are no chirality outliers.

All (17) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 2 | A | 1201 | ADP | C5'-O5'-PA-O1A |
| 2 | A | 1201 | ADP | C5'-O5'-PA-O2A |
| 2 | A | 1201 | ADP | C5'-O5'-PA-O3A |
| 5 | C | 1202 | ATP | O4'-C4'-C5'-O5' |
| 5 | C | 1202 | ATP | C3'-C4'-C5'-O5' |
| 4 | B | 1201 | BTI | C11-C10-C9-C8 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 4 | B | 1201 | BTI | S1-C2-C7-C8 |
| 4 | A | 1203 | BTI | C11-C10-C9-C8 |
| 4 | A | 1203 | BTI | S1-C2-C7-C8 |
| 4 | A | 1203 | BTI | C4-C2-C7-C8 |
| 2 | A | 1201 | ADP | C3'-C4'-C5'-O5' |
| 2 | A | 1201 | ADP | O4'-C4'-C5'-O5' |
| 4 | A | 1203 | BTI | C7-C8-C9-C10 |
| 4 | B | 1201 | BTI | C4-C2-C7-C8 |
| 5 | C | 1202 | ATP | PG-O3B-PB-O1B |
| 4 | D | 1201 | BTI | C2-C7-C8-C9 |
| 2 | A | 1201 | ADP | PB-O3A-PA-O1A |

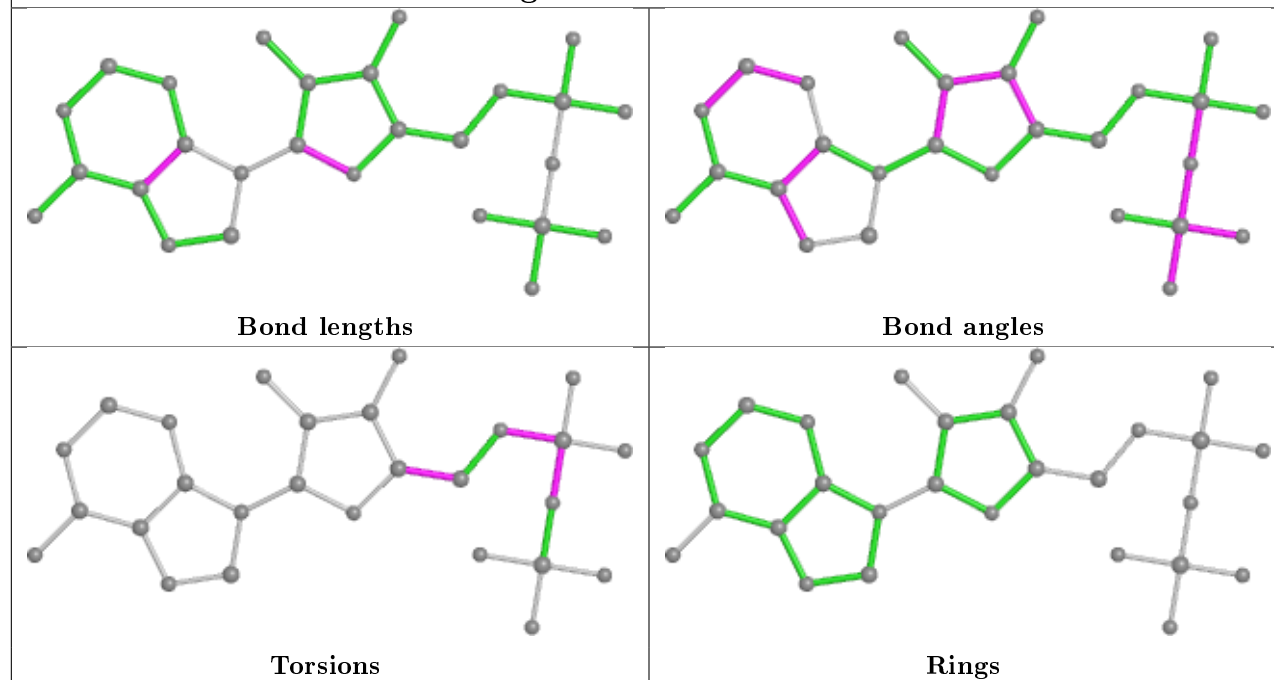
There are no ring outliers.

5 monomers are involved in 22 short contacts:

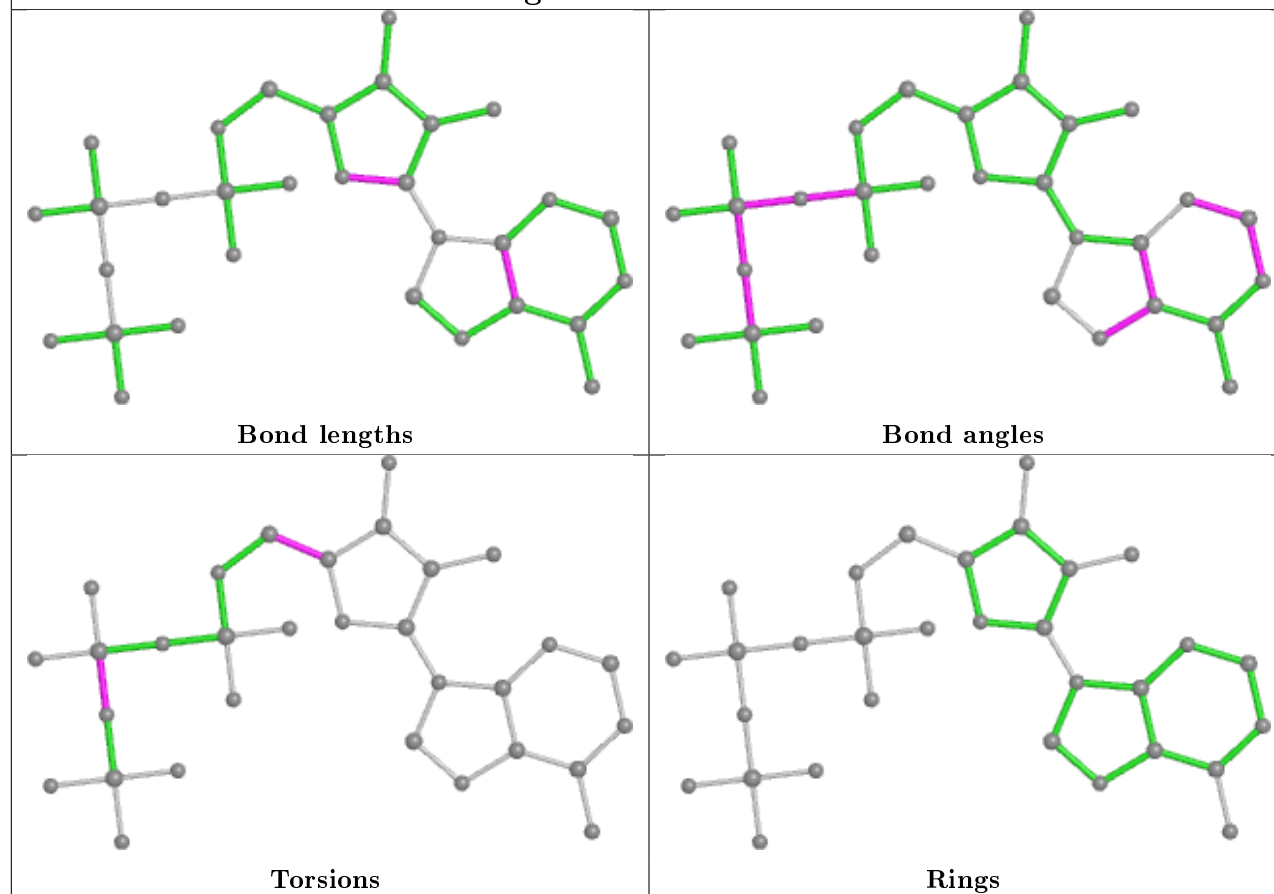
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2 | A | 1201 | ADP | 1 | 0 |
| 4 | D | 1201 | BTI | 3 | 0 |
| 5 | C | 1202 | ATP | 10 | 0 |
| 4 | A | 1203 | BTI | 4 | 0 |
| 4 | B | 1201 | BTI | 4 | 0 |

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

Ligand ADP A 1201



Ligand ATP C 1202



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

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

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | B | 936:TYR | C | 937:LYS | N | 1.60 |

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 | 1052/1173 (89%) | -0.29 | 18 (1%) | 70 63 | 49, 72, 115, 131 | 0 |
| 1 | B | 989/1173 (84%) | -0.19 | 21 (2%) | 63 54 | 55, 87, 129, 178 | 0 |
| 1 | C | 1059/1173 (90%) | -0.15 | 22 (2%) | 63 54 | 55, 84, 126, 177 | 0 |
| 1 | D | 989/1173 (84%) | -0.25 | 11 (1%) | 80 75 | 47, 78, 130, 167 | 0 |
| All | All | 4089/4692 (87%) | -0.22 | 72 (1%) | 68 61 | 47, 80, 125, 178 | 0 |

All (72) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 231 | SER | 4.8 |
| 1 | A | 233 | VAL | 4.4 |
| 1 | D | 490 | ILE | 4.3 |
| 1 | A | 229 | GLY | 4.3 |
| 1 | A | 177 | TYR | 4.1 |
| 1 | D | 240 | ASP | 3.8 |
| 1 | C | 877 | GLN | 3.7 |
| 1 | B | 168 | PRO | 3.6 |
| 1 | D | 271 | HIS | 3.4 |
| 1 | D | 475 | ASP | 3.4 |
| 1 | C | 936 | TYR | 3.3 |
| 1 | A | 230 | ASN | 3.3 |
| 1 | D | 285 | PRO | 3.3 |
| 1 | B | 526 | LEU | 3.2 |
| 1 | C | 1093 | ASN | 3.2 |
| 1 | B | 527 | ALA | 3.0 |
| 1 | A | 1000 | GLY | 2.9 |
| 1 | A | 1001 | PRO | 2.9 |
| 1 | C | 881 | LEU | 2.9 |
| 1 | C | 1070 | GLU | 2.9 |
| 1 | C | 876 | GLN | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 197 | SER | 2.8 |
| 1 | C | 890 | VAL | 2.7 |
| 1 | A | 175 | LYS | 2.7 |
| 1 | D | 310 | VAL | 2.7 |
| 1 | D | 239 | ILE | 2.7 |
| 1 | C | 515 | ASN | 2.7 |
| 1 | A | 1072 | GLY | 2.7 |
| 1 | A | 493 | SER | 2.7 |
| 1 | D | 421 | TYR | 2.7 |
| 1 | B | 240 | ASP | 2.7 |
| 1 | A | 227 | SER | 2.6 |
| 1 | C | 516 | VAL | 2.6 |
| 1 | C | 999 | GLN | 2.6 |
| 1 | A | 219 | ARG | 2.5 |
| 1 | C | 922 | VAL | 2.5 |
| 1 | B | 975 | THR | 2.5 |
| 1 | C | 492 | PRO | 2.4 |
| 1 | C | 282 | GLY | 2.4 |
| 1 | B | 271 | HIS | 2.4 |
| 1 | A | 223 | GLU | 2.4 |
| 1 | C | 177 | TYR | 2.4 |
| 1 | C | 717 | ASN | 2.4 |
| 1 | C | 933 | THR | 2.4 |
| 1 | C | 879 | LYS | 2.4 |
| 1 | A | 999 | GLN | 2.3 |
| 1 | B | 717 | ASN | 2.3 |
| 1 | C | 932 | ILE | 2.3 |
| 1 | D | 384 | LEU | 2.3 |
| 1 | B | 167 | ILE | 2.3 |
| 1 | A | 174 | ILE | 2.3 |
| 1 | A | 222 | SER | 2.2 |
| 1 | B | 255 | GLY | 2.2 |
| 1 | D | 515 | ASN | 2.2 |
| 1 | C | 739 | ALA | 2.2 |
| 1 | C | 230 | ASN | 2.2 |
| 1 | B | 1093 | ASN | 2.2 |
| 1 | B | 1091 | ASP | 2.2 |
| 1 | B | 1070 | GLU | 2.2 |
| 1 | B | 494 | LEU | 2.2 |
| 1 | A | 996 | GLU | 2.1 |
| 1 | C | 919 | LEU | 2.1 |
| 1 | B | 1071 | ASN | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | B | 383 | PRO | 2.1 |
| 1 | C | 1072 | GLY | 2.1 |
| 1 | B | 144 | GLU | 2.1 |
| 1 | B | 1072 | GLY | 2.1 |
| 1 | B | 641 | MET | 2.1 |
| 1 | B | 882 | GLY | 2.1 |
| 1 | B | 153 | VAL | 2.0 |
| 1 | D | 385 | ASN | 2.0 |
| 1 | B | 927 | ASP | 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](#)

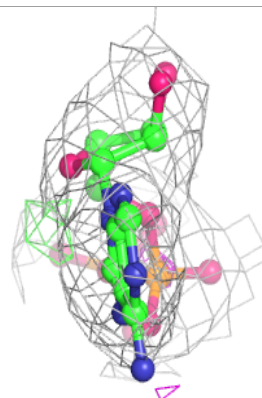
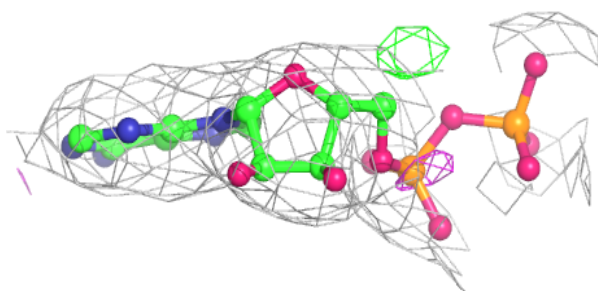
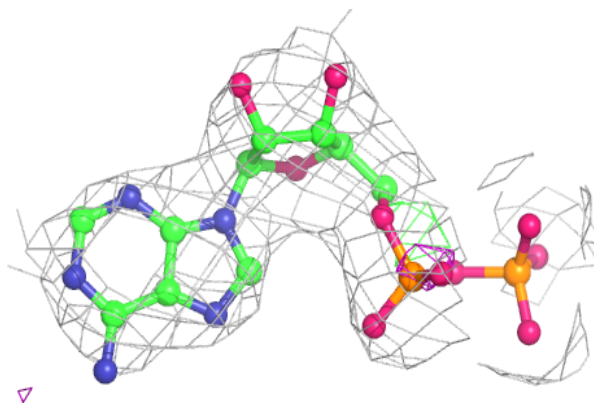
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 2 | ADP | A | 1201 | 27/27 | 0.89 | 0.18 | 86,91,110,110 | 0 |
| 4 | BTI | B | 1201 | 15/15 | 0.91 | 0.34 | 105,109,114,115 | 0 |
| 4 | BTI | D | 1201 | 15/15 | 0.92 | 0.30 | 105,109,113,116 | 0 |
| 4 | BTI | A | 1203 | 15/15 | 0.93 | 0.29 | 92,99,104,105 | 0 |
| 5 | ATP | C | 1202 | 31/31 | 0.94 | 0.14 | 102,108,115,115 | 0 |
| 3 | MN | B | 1202 | 1/1 | 0.97 | 0.18 | 82,82,82,82 | 0 |
| 3 | MN | C | 1201 | 1/1 | 0.98 | 0.26 | 76,76,76,76 | 0 |
| 3 | MN | A | 1202 | 1/1 | 0.99 | 0.19 | 74,74,74,74 | 0 |
| 3 | MN | D | 1202 | 1/1 | 0.99 | 0.19 | 74,74,74,74 | 0 |

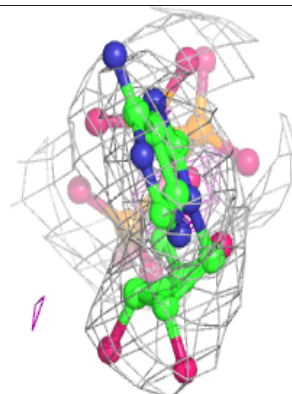
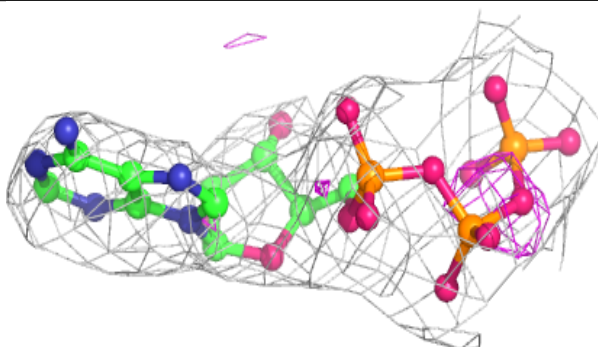
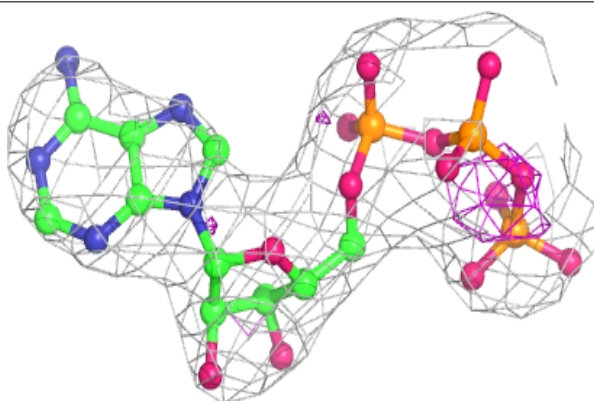
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 1201:

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

**Electron density around ATP C 1202:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.