



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:19 PM GMT

PDB ID : 4ZKT
Title : Crystal structure of the progenitor M complex of Clostridium botulinum type E neurotoxin
Authors : Eswaramoorthy, S.; Swaminathan, S.
Deposited on : 2015-04-30
Resolution : 3.05 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

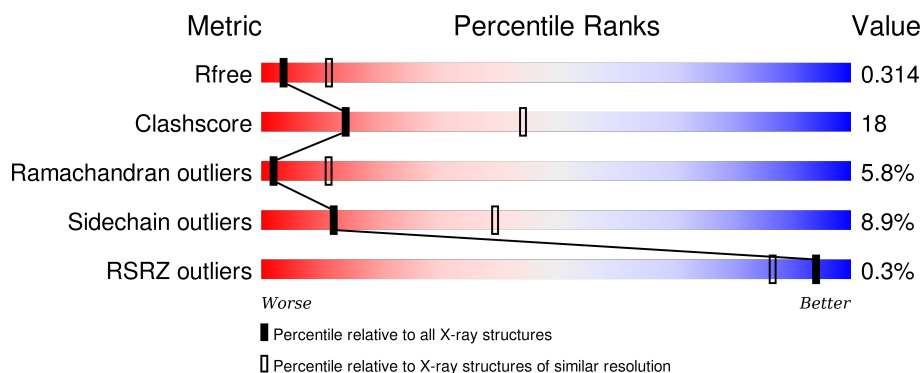
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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} | 91344 | 1191 (3.10-3.02) |
| Clashscore | 102246 | 1303 (3.10-3.02) |
| Ramachandran outliers | 100387 | 1254 (3.10-3.02) |
| Sidechain outliers | 100360 | 1254 (3.10-3.02) |
| RSRZ outliers | 91569 | 1197 (3.10-3.02) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 1252 |  |
| 1 | C | 1252 |  |
| 1 | E | 1252 |  |
| 2 | B | 1163 |  |
| 2 | D | 1163 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 2 | F | 1163 | <div><div><div>%</div><div><div></div></div><div>55%</div><div>34%</div><div>6% . .</div></div></div> |

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 56952 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 Bontoxilysin A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1 | A | 1235 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 9978 | 6351 | 1665 | 1940 | 22 | | | |
| 1 | C | 1235 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 9978 | 6351 | 1665 | 1940 | 22 | | | |
| 1 | E | 1235 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 9978 | 6351 | 1665 | 1940 | 22 | | | |

- Molecule 2 is a protein called Botulinum neurotoxin type E, nontoxic-nonhemagglutinin component, NTNH.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 2 | B | 1114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 9005 | 5804 | 1451 | 1726 | 24 | | | |
| 2 | D | 1114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 9005 | 5804 | 1451 | 1726 | 24 | | | |
| 2 | F | 1114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 9005 | 5804 | 1451 | 1726 | 24 | | | |

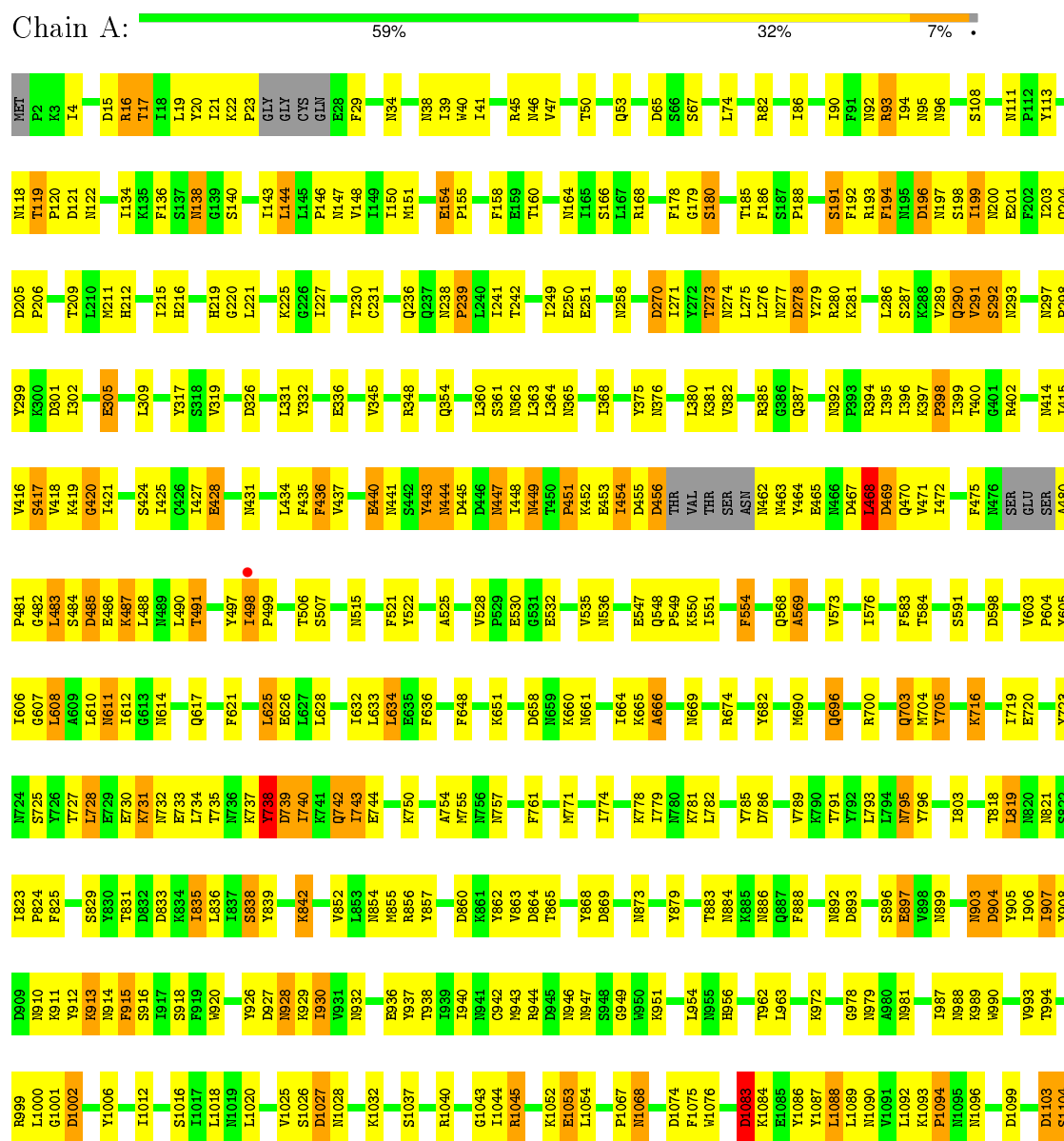
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

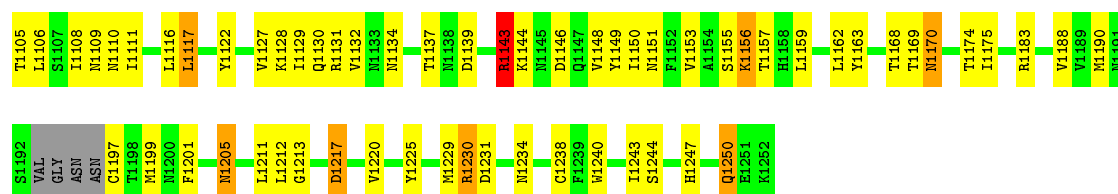
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3 | A | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 3 | C | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 3 | E | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

3 Residue-property plots

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

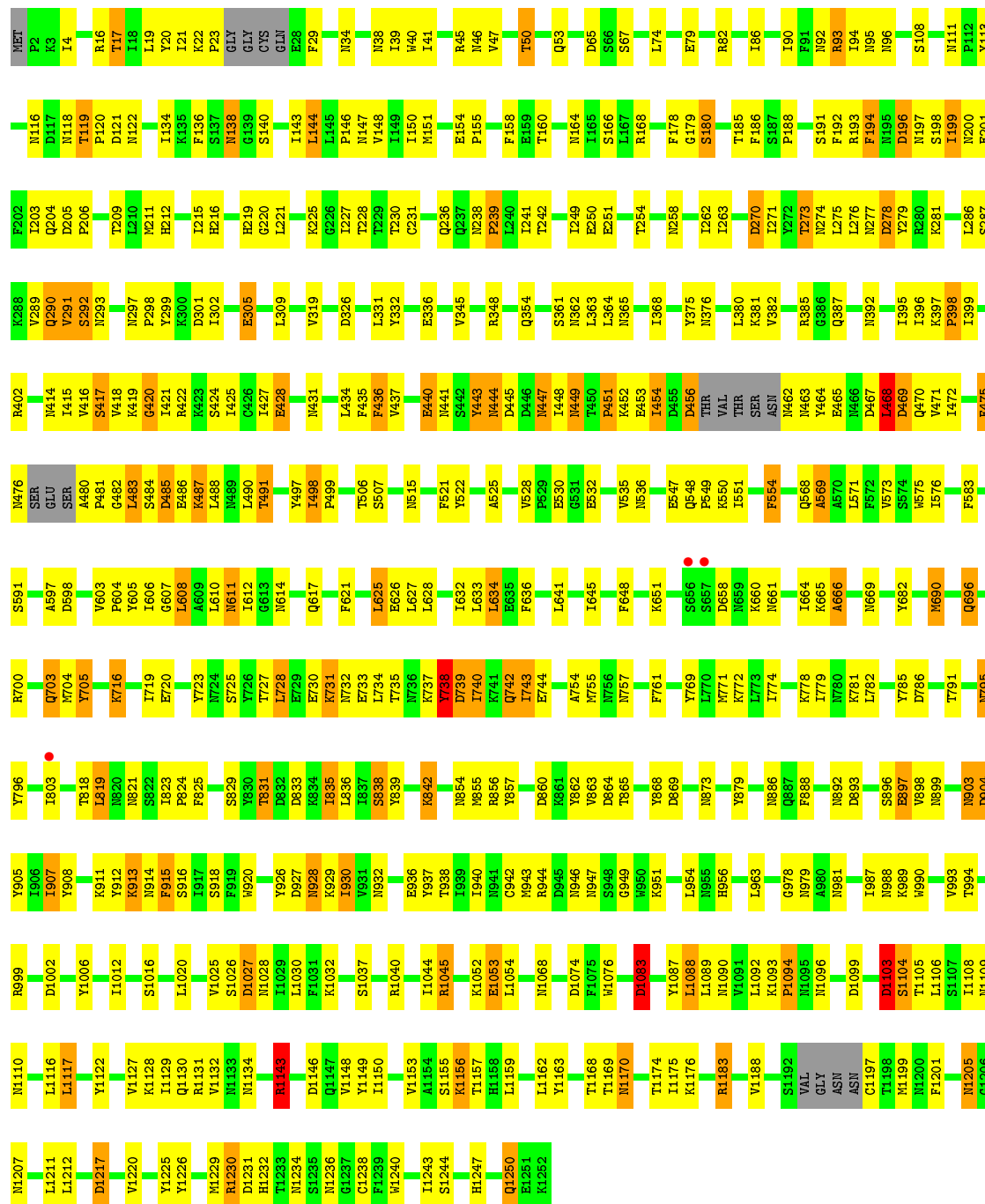
• Molecule 1: Bontoxilysin A





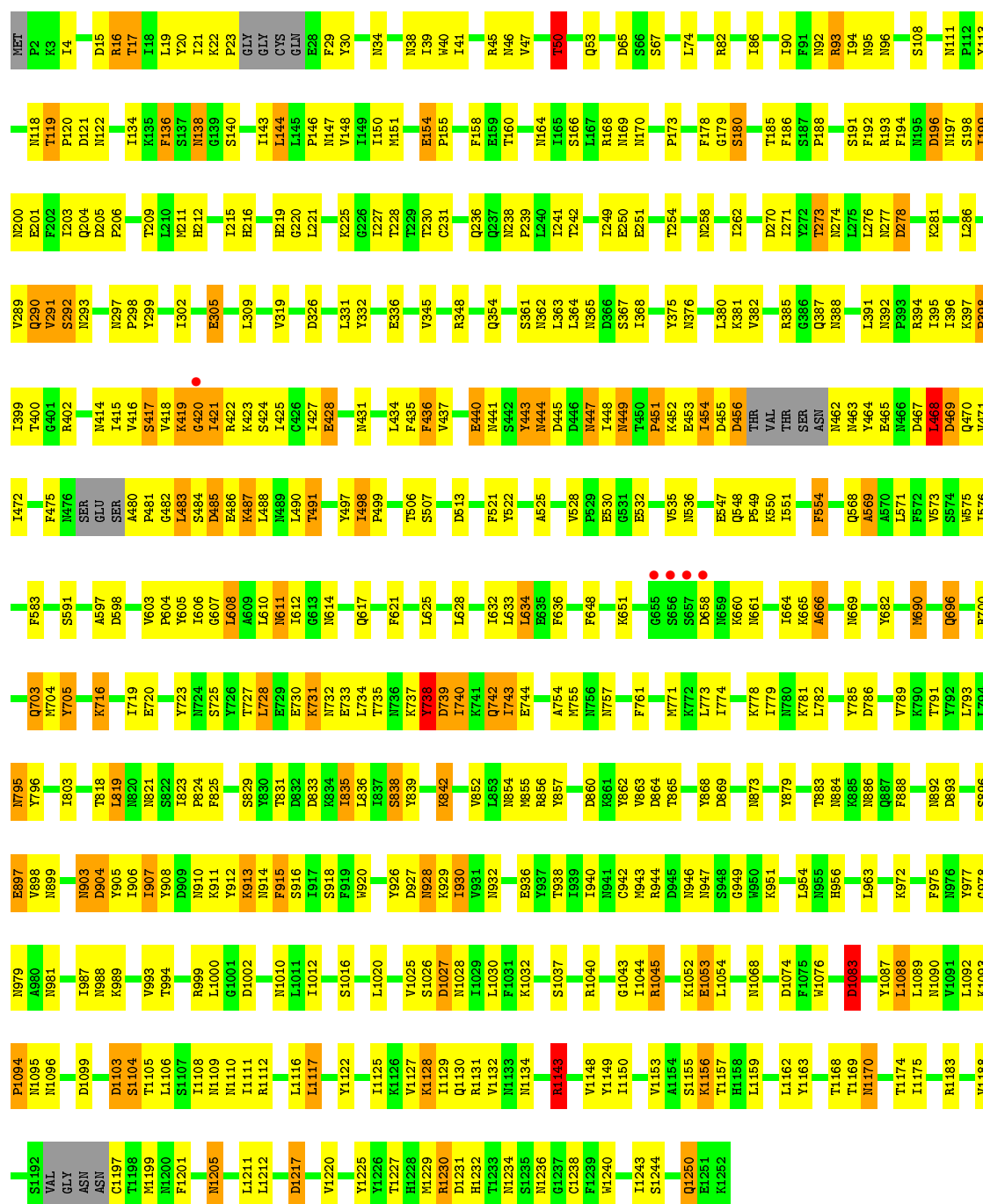
• Molecule 1: Bontoxilysin A

Chain C: 60% 32% 7%



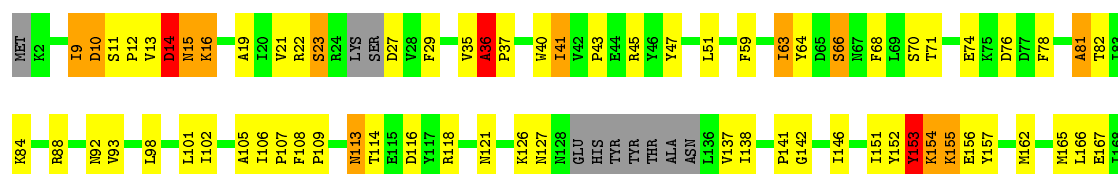
• Molecule 1: Bontoxilysin A

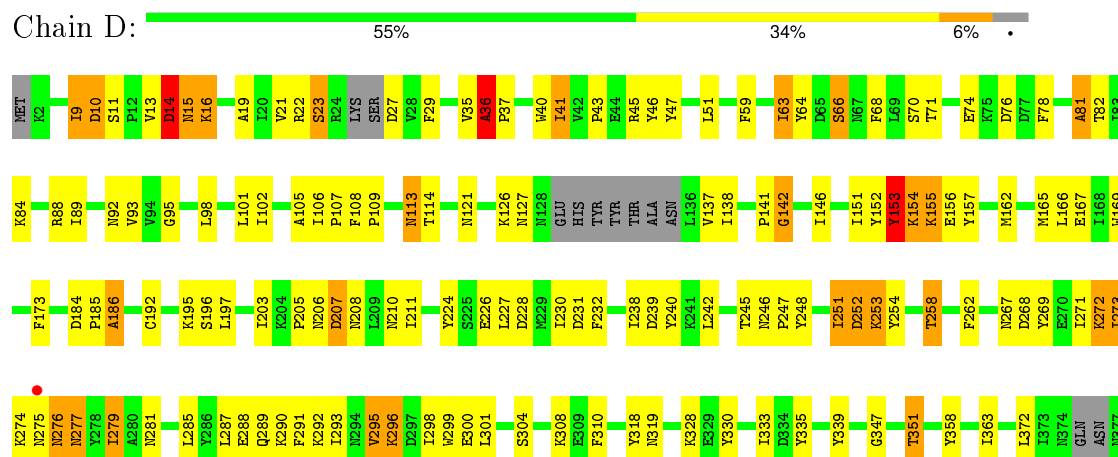
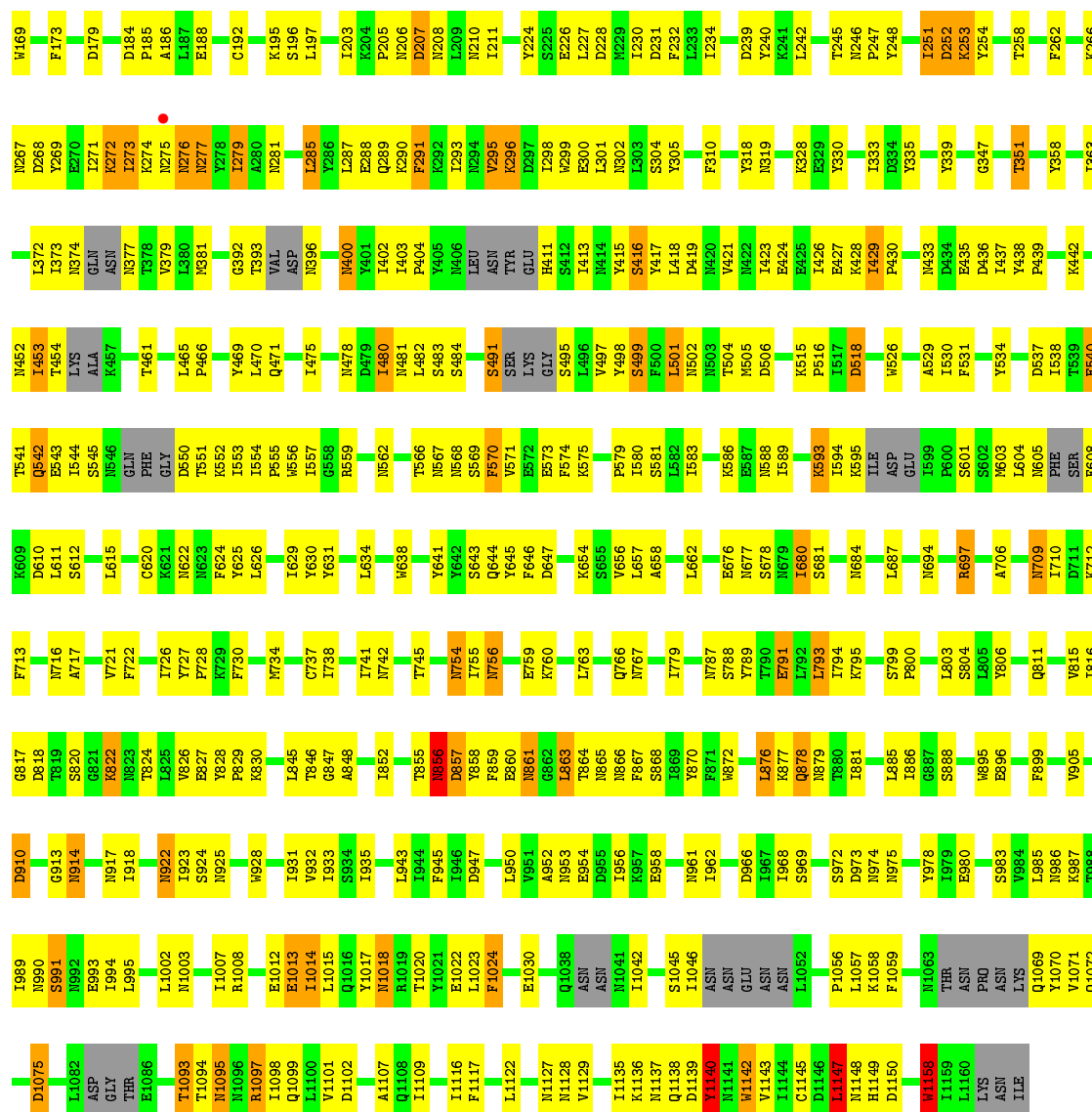
Chain E:  59% 32% 7%

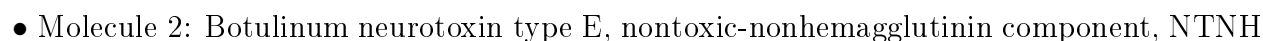


• Molecule 2: Botulinum neurotoxin type E, nontoxic-nonhemagglutinin component, NTNH

Chain B:  54% 35% 6%







| | | | | | |
|-------|-------|------|------|------|------|
| ASN | L985 | F899 | T819 | P608 | T539 |
| LYS | N986 | E900 | S820 | K609 | E540 |
| Q1069 | K987 | N901 | G821 | D610 | T541 |
| Y1070 | T988 | | K822 | L611 | Q542 |
| V1071 | I989 | D910 | N823 | S612 | E543 |
| Q1072 | N990 | S991 | T824 | F730 | I544 |
| | S992 | N914 | L825 | T731 | S545 |
| D1075 | E993 | N922 | V826 | L615 | N546 |
| L1082 | E994 | I923 | Y827 | C620 | GLN |
| ASP | L995 | S924 | Y828 | F624 | PHE |
| GLY | | N925 | K830 | Y625 | GLY |
| THR | L1002 | | T831 | L626 | D550 |
| E1086 | N1003 | W828 | I832 | | T551 |
| | | | | I629 | K552 |
| T1093 | I1007 | I931 | T843 | Y630 | I553 |
| T1094 | R1008 | V932 | H844 | Y631 | I554 |
| N1095 | | I933 | L845 | | P555 |
| M1096 | E1012 | S934 | T846 | L634 | W556 |
| R1097 | E1013 | I935 | Q847 | | I557 |
| I1098 | I1014 | | A848 | W638 | E558 |
| Q1099 | L1015 | K939 | I852 | Y641 | R559 |
| L1100 | Q1016 | | | | N562 |
| V1101 | Y1017 | L943 | K853 | Y642 | T566 |
| D1102 | N1018 | I944 | F854 | S643 | I567 |
| | R1019 | F945 | T855 | Q644 | I568 |
| A1107 | T1020 | I946 | N856 | Y645 | S569 |
| | Y1021 | D947 | I857 | | F570 |
| I1116 | E1022 | N948 | Y858 | V656 | V571 |
| F1117 | L1023 | I949 | F859 | L657 | E572 |
| | F1024 | L950 | E860 | N658 | E573 |
| L1122 | | V951 | N861 | L662 | F574 |
| | E1030 | A952 | G862 | | K575 |
| N1127 | | N953 | L863 | E676 | |
| N1128 | I1036 | E954 | T864 | N677 | P579 |
| V1129 | E1037 | D955 | N865 | S678 | I580 |
| | Q1038 | I956 | N866 | L679 | S581 |
| I1135 | ASN | K957 | F867 | I680 | L582 |
| K1136 | ASN | E958 | S868 | | I583 |
| N1137 | N1041 | | Y870 | N684 | |
| Q1138 | I1042 | I962 | F871 | | K586 |
| D1139 | | | N872 | L687 | E587 |
| | S1045 | D966 | L873 | N694 | I588 |
| N1141 | I1046 | I967 | | | |
| W1142 | ASN | I968 | L876 | | K593 |
| V1143 | ASN | S969 | K877 | R697 | I594 |
| I1144 | GLU | L970 | Q878 | P800 | K595 |
| C1145 | ASN | L971 | N879 | A706 | ILE |
| D1146 | ASN | S972 | T880 | | ASP |
| I1147 | L1052 | D973 | I881 | W709 | GLU |
| N1148 | | N974 | | I710 | I599 |
| H1149 | P1056 | N975 | L885 | F713 | P600 |
| D1150 | L1057 | | I886 | | S601 |
| | K1058 | Y978 | G887 | N716 | S602 |
| | F1059 | I979 | S888 | A717 | K603 |
| W1158 | | E980 | | V721 | L604 |
| I1159 | N1063 | | | | P605 |
| L1160 | THR | | W895 | | PHE |
| LYS | ASN | S983 | E896 | | SER |
| ASN | PRQ | V984 | | | |
| ILE | | | | | |

4 Data and refinement statistics

| Property | Value | Source |
|---|--|------------------|
| Space group | P 31 | Depositor |
| Cell constants a, b, c, α , β , γ | 192.60Å 192.60Å 286.54Å 90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 49.30 – 3.05 49.25 – 3.05 | Depositor EDS |
| % Data completeness (in resolution range) | 59.7 (49.30-3.05) 59.8 (49.25-3.05) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.46 (at 3.07Å) | Xtriage |
| Refinement program | REFMAC 5.7.0032 | Depositor |
| R, R_{free} | 0.243 , 0.321 0.247 , 0.314 | Depositor DCC |
| R_{free} test set | 1618 reflections (1.21%) | DCC |
| Wilson B-factor (Å ²) | 110.6 | Xtriage |
| Anisotropy | 0.154 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | (Not available) , (Not available) | EDS |
| Estimated twinning fraction | 0.135 for -h,-k,l 0.196 for h,-h-k,-l 0.137 for -k,-h,-l | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$ | Xtriage |
| Outliers | 0 of 134941 reflections | Xtriage |
| F_o, F_c correlation | 0.94 | EDS |
| Total number of atoms | 56952 | wwPDB-VP |
| Average B, all atoms (Å ²) | 134.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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 | 0.58 | 0/10176 | 0.74 | 2/13800 (0.0%) |
| 1 | C | 0.56 | 0/10176 | 0.73 | 1/13800 (0.0%) |
| 1 | E | 0.54 | 0/10176 | 0.72 | 2/13800 (0.0%) |
| 2 | B | 0.64 | 2/9182 (0.0%) | 0.75 | 0/12454 |
| 2 | D | 0.60 | 1/9182 (0.0%) | 0.74 | 0/12454 |
| 2 | F | 0.58 | 1/9182 (0.0%) | 0.73 | 0/12454 |
| All | All | 0.58 | 4/58074 (0.0%) | 0.73 | 5/78762 (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 |
|-----|-------|---------------------|---------------------|
| 2 | B | 0 | 1 |
| 2 | D | 0 | 1 |
| 2 | F | 0 | 2 |
| All | All | 0 | 4 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 2 | B | 1158 | TRP | CB-CG | -7.00 | 1.37 | 1.50 |
| 2 | D | 1158 | TRP | CB-CG | -5.84 | 1.39 | 1.50 |
| 2 | F | 1158 | TRP | CB-CG | -5.69 | 1.40 | 1.50 |
| 2 | B | 116 | ASP | C-O | 5.60 | 1.33 | 1.23 |

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 1143 | ARG | NE-CZ-NH2 | 7.34 | 123.97 | 120.30 |
| 1 | E | 1143 | ARG | NE-CZ-NH2 | 7.21 | 123.90 | 120.30 |
| 1 | A | 394 | ARG | NE-CZ-NH2 | -6.68 | 116.96 | 120.30 |
| 1 | C | 1143 | ARG | NE-CZ-NH2 | 6.28 | 123.44 | 120.30 |
| 1 | E | 394 | ARG | NE-CZ-NH2 | -5.63 | 117.48 | 120.30 |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|---------|
| 2 | B | 36 | ALA | Peptide |
| 2 | D | 36 | ALA | Peptide |
| 2 | F | 1138 | GLN | Peptide |
| 2 | F | 36 | 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 | 9978 | 0 | 9735 | 338 | 1 |
| 1 | C | 9978 | 0 | 9735 | 348 | 1 |
| 1 | E | 9978 | 0 | 9735 | 352 | 0 |
| 2 | B | 9005 | 0 | 8666 | 361 | 0 |
| 2 | D | 9005 | 0 | 8666 | 344 | 0 |
| 2 | F | 9005 | 0 | 8666 | 356 | 0 |
| 3 | A | 1 | 0 | 0 | 0 | 0 |
| 3 | C | 1 | 0 | 0 | 0 | 0 |
| 3 | E | 1 | 0 | 0 | 0 | 0 |
| All | All | 56952 | 0 | 55203 | 2034 | 1 |

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 18.

All (2034) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------|--------------------------|-------------------|
| 2:D:885:LEU:HG | 2:D:886:ILE:HD12 | 1.33 | 1.09 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:F:885:LEU:HG | 2:F:886:ILE:HD12 | 1.32 | 1.09 |
| 2:B:436:ASP:HA | 2:B:437:ILE:HB | 1.34 | 1.08 |
| 2:B:885:LEU:HG | 2:B:886:ILE:HD12 | 1.29 | 1.08 |
| 2:D:436:ASP:HA | 2:D:437:ILE:HB | 1.35 | 1.05 |
| 2:F:436:ASP:HA | 2:F:437:ILE:HB | 1.37 | 1.03 |
| 2:B:818:ASP:OD2 | 2:B:820:SER:OG | 1.79 | 0.99 |
| 2:F:818:ASP:OD2 | 2:F:820:SER:OG | 1.80 | 0.98 |
| 2:D:818:ASP:OD2 | 2:D:820:SER:OG | 1.80 | 0.98 |
| 1:C:1130:GLN:O | 1:C:1148:VAL:HG23 | 1.63 | 0.98 |
| 1:A:1130:GLN:O | 1:A:1148:VAL:HG23 | 1.66 | 0.96 |
| 1:E:1130:GLN:O | 1:E:1148:VAL:HG23 | 1.66 | 0.95 |
| 1:C:628:LEU:HB2 | 1:E:419:LYS:HE3 | 1.48 | 0.95 |
| 1:A:289:VAL:HB | 1:A:290:GLN:HA | 1.49 | 0.91 |
| 2:B:879:ASN:HB3 | 2:B:881:ILE:HG22 | 1.54 | 0.89 |
| 1:C:289:VAL:HB | 1:C:290:GLN:HA | 1.53 | 0.89 |
| 2:D:879:ASN:HB3 | 2:D:881:ILE:HG22 | 1.55 | 0.89 |
| 1:E:289:VAL:HB | 1:E:290:GLN:HA | 1.53 | 0.88 |
| 1:C:227:ILE:HD11 | 1:C:274:ASN:HB2 | 1.57 | 0.86 |
| 1:A:289:VAL:HB | 1:A:290:GLN:CA | 2.06 | 0.86 |
| 2:D:1045:SER:OG | 2:D:1046:ILE:N | 2.09 | 0.86 |
| 1:C:855:MET:O | 1:C:856:ARG:HD3 | 1.76 | 0.85 |
| 1:E:238:ASN:CG | 1:E:239:PRO:HD2 | 1.96 | 0.85 |
| 2:F:879:ASN:HB3 | 2:F:881:ILE:HG22 | 1.58 | 0.85 |
| 1:A:227:ILE:HD11 | 1:A:274:ASN:HB2 | 1.59 | 0.84 |
| 1:A:855:MET:O | 1:A:856:ARG:HD3 | 1.77 | 0.84 |
| 1:E:227:ILE:HD11 | 1:E:274:ASN:HB2 | 1.58 | 0.84 |
| 1:A:238:ASN:CG | 1:A:239:PRO:HD2 | 1.98 | 0.84 |
| 2:F:1045:SER:OG | 2:F:1046:ILE:N | 2.07 | 0.84 |
| 1:C:289:VAL:HB | 1:C:290:GLN:CA | 2.09 | 0.83 |
| 1:E:855:MET:O | 1:E:856:ARG:HD3 | 1.79 | 0.83 |
| 1:E:289:VAL:HB | 1:E:290:GLN:CA | 2.09 | 0.83 |
| 2:D:1137:ASN:HB3 | 2:D:1142:TRP:HE1 | 1.46 | 0.81 |
| 2:B:1045:SER:OG | 2:B:1046:ILE:N | 2.12 | 0.81 |
| 1:A:1155:SER:O | 1:A:1157:THR:N | 2.13 | 0.81 |
| 1:A:522:TYR:CE2 | 1:A:611:ASN:HB2 | 2.16 | 0.81 |
| 1:A:897:GLU:HG2 | 1:A:1032:LYS:HB2 | 1.61 | 0.81 |
| 1:E:1155:SER:O | 1:E:1157:THR:N | 2.13 | 0.81 |
| 1:E:522:TYR:CE2 | 1:E:611:ASN:HB2 | 2.17 | 0.80 |
| 1:C:238:ASN:CG | 1:C:239:PRO:HD2 | 2.03 | 0.80 |
| 1:C:1155:SER:O | 1:C:1157:THR:N | 2.14 | 0.80 |
| 2:B:1137:ASN:HB3 | 2:B:1142:TRP:HE1 | 1.47 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:421:ILE:HD11 | 2:D:510:PHE:CD1 | 2.17 | 0.79 |
| 1:E:513:ASP:OD1 | 2:D:521:LYS:NZ | 2.16 | 0.79 |
| 1:C:627:LEU:HB3 | 1:E:419:LYS:HE2 | 1.65 | 0.79 |
| 1:C:522:TYR:CE2 | 1:C:611:ASN:HB2 | 2.17 | 0.78 |
| 1:E:897:GLU:HG2 | 1:E:1032:LYS:HB2 | 1.65 | 0.77 |
| 2:F:1137:ASN:HB3 | 2:F:1142:TRP:HE1 | 1.48 | 0.77 |
| 2:F:603:MET:O | 2:F:605:ASN:N | 2.17 | 0.76 |
| 1:C:897:GLU:HG2 | 1:C:1032:LYS:HB2 | 1.67 | 0.76 |
| 1:A:199:ILE:HA | 1:A:705:TYR:HE2 | 1.50 | 0.76 |
| 2:B:815:VAL:O | 2:B:816:ILE:HG13 | 1.87 | 0.74 |
| 2:D:526:TRP:CE2 | 2:D:530:ILE:HD11 | 2.23 | 0.74 |
| 1:E:728:LEU:HA | 1:E:731:LYS:HB2 | 1.68 | 0.74 |
| 2:F:108:PHE:HB3 | 2:F:162:MET:HG3 | 1.70 | 0.73 |
| 2:B:108:PHE:HB3 | 2:B:162:MET:HG3 | 1.69 | 0.73 |
| 2:B:603:MET:O | 2:B:605:ASN:N | 2.22 | 0.73 |
| 1:A:836:LEU:HD11 | 2:B:945:PHE:CD1 | 2.24 | 0.73 |
| 2:B:526:TRP:CE2 | 2:B:530:ILE:HD11 | 2.24 | 0.73 |
| 1:C:836:LEU:HB2 | 2:D:995:LEU:HD11 | 1.69 | 0.73 |
| 1:A:728:LEU:HA | 1:A:731:LYS:HB2 | 1.70 | 0.73 |
| 2:D:603:MET:O | 2:D:605:ASN:N | 2.21 | 0.73 |
| 1:C:728:LEU:HA | 1:C:731:LYS:HB2 | 1.69 | 0.73 |
| 2:B:1127:ASN:O | 2:B:1129:VAL:N | 2.22 | 0.72 |
| 2:F:556:TRP:HA | 2:F:559:ARG:HD3 | 1.71 | 0.72 |
| 1:A:227:ILE:HD12 | 1:A:271:ILE:HA | 1.72 | 0.72 |
| 2:F:436:ASP:HA | 2:F:437:ILE:CB | 2.16 | 0.72 |
| 2:D:815:VAL:O | 2:D:816:ILE:HG13 | 1.89 | 0.72 |
| 2:D:108:PHE:HB3 | 2:D:162:MET:HG3 | 1.72 | 0.72 |
| 2:F:815:VAL:O | 2:F:816:ILE:HG13 | 1.90 | 0.71 |
| 2:D:469:TYR:CZ | 2:D:562:ASN:HB2 | 2.25 | 0.71 |
| 1:C:199:ILE:HA | 1:C:705:TYR:HE2 | 1.53 | 0.71 |
| 2:B:59:PHE:HB2 | 2:B:452:ASN:ND2 | 2.06 | 0.71 |
| 2:D:63:ILE:HD12 | 2:D:358:TYR:HB3 | 1.72 | 0.71 |
| 2:F:469:TYR:CZ | 2:F:562:ASN:HB2 | 2.26 | 0.71 |
| 1:C:118:ASN:HA | 1:C:119:THR:HB | 1.74 | 0.70 |
| 1:E:738:TYR:HA | 1:E:743:ILE:HG13 | 1.73 | 0.70 |
| 1:A:238:ASN:ND2 | 1:A:239:PRO:HD2 | 2.06 | 0.70 |
| 2:F:626:LEU:HA | 2:F:629:ILE:HD12 | 1.74 | 0.70 |
| 2:B:876:LEU:O | 2:B:877:LYS:HB2 | 1.92 | 0.70 |
| 2:B:63:ILE:HD12 | 2:B:358:TYR:HB3 | 1.73 | 0.70 |
| 2:F:21:VAL:HG13 | 2:F:121:ASN:HA | 1.72 | 0.70 |
| 1:E:199:ILE:HA | 1:E:705:TYR:HE2 | 1.56 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:526:TRP:CE2 | 2:F:530:ILE:HD11 | 2.27 | 0.69 |
| 1:C:436:PHE:HD1 | 1:C:436:PHE:C | 1.96 | 0.69 |
| 1:E:238:ASN:ND2 | 1:E:239:PRO:HD2 | 2.07 | 0.69 |
| 2:D:121:ASN:CB | 2:D:127:ASN:HA | 2.22 | 0.69 |
| 2:B:556:TRP:HA | 2:B:559:ARG:HD3 | 1.75 | 0.69 |
| 2:F:59:PHE:HB2 | 2:F:452:ASN:ND2 | 2.08 | 0.69 |
| 1:C:944:ARG:HG2 | 1:C:1026:SER:HA | 1.72 | 0.69 |
| 2:F:224:TYR:O | 2:F:392:GLY:HA2 | 1.93 | 0.69 |
| 1:A:118:ASN:HA | 1:A:119:THR:HB | 1.74 | 0.69 |
| 2:D:867:PHE:HB2 | 2:D:985:LEU:O | 1.93 | 0.68 |
| 1:C:227:ILE:HD12 | 1:C:271:ILE:HA | 1.75 | 0.68 |
| 2:D:224:TYR:O | 2:D:392:GLY:HA2 | 1.93 | 0.68 |
| 2:F:876:LEU:O | 2:F:877:LYS:HB2 | 1.93 | 0.68 |
| 2:B:21:VAL:HG13 | 2:B:121:ASN:HA | 1.75 | 0.68 |
| 1:E:436:PHE:HD1 | 1:E:436:PHE:C | 1.96 | 0.68 |
| 2:D:626:LEU:HA | 2:D:629:ILE:HD12 | 1.76 | 0.68 |
| 2:B:626:LEU:HA | 2:B:629:ILE:HD12 | 1.74 | 0.68 |
| 2:F:63:ILE:HD12 | 2:F:358:TYR:HB3 | 1.76 | 0.68 |
| 2:D:556:TRP:HA | 2:D:559:ARG:HD3 | 1.76 | 0.68 |
| 1:C:449:ASN:O | 1:C:451:PRO:HD3 | 1.94 | 0.68 |
| 2:B:469:TYR:CZ | 2:B:562:ASN:HB2 | 2.28 | 0.68 |
| 1:E:944:ARG:HG2 | 1:E:1026:SER:HA | 1.75 | 0.67 |
| 2:D:1149:HIS:CG | 2:D:1150:ASP:N | 2.62 | 0.67 |
| 1:E:449:ASN:O | 1:E:451:PRO:HD3 | 1.94 | 0.67 |
| 1:E:836:LEU:HB2 | 2:F:995:LEU:HD11 | 1.75 | 0.67 |
| 1:E:227:ILE:HD12 | 1:E:271:ILE:HA | 1.76 | 0.67 |
| 1:E:436:PHE:CD1 | 1:E:436:PHE:C | 2.67 | 0.67 |
| 1:C:1207:ASN:OD1 | 2:D:811:GLN:N | 2.28 | 0.67 |
| 2:D:876:LEU:O | 2:D:877:LYS:HB2 | 1.94 | 0.67 |
| 1:A:738:TYR:HA | 1:A:743:ILE:HG13 | 1.76 | 0.67 |
| 2:D:59:PHE:HB2 | 2:D:452:ASN:ND2 | 2.08 | 0.67 |
| 2:D:423:ILE:O | 2:D:423:ILE:HG23 | 1.94 | 0.67 |
| 2:B:1149:HIS:CG | 2:B:1150:ASP:N | 2.62 | 0.67 |
| 1:A:436:PHE:C | 1:A:436:PHE:HD1 | 1.97 | 0.67 |
| 1:C:436:PHE:CD1 | 1:C:436:PHE:C | 2.66 | 0.67 |
| 1:C:738:TYR:HA | 1:C:743:ILE:HG13 | 1.76 | 0.67 |
| 1:A:449:ASN:O | 1:A:451:PRO:HD3 | 1.94 | 0.67 |
| 2:D:1127:ASN:O | 2:D:1129:VAL:N | 2.27 | 0.66 |
| 1:E:904:ASP:HA | 1:E:907:ILE:HD11 | 1.75 | 0.66 |
| 1:A:20:TYR:HB3 | 1:A:29:PHE:HB3 | 1.77 | 0.66 |
| 2:B:393:THR:HG1 | 2:B:396:ASN:N | 1.92 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:1127:ASN:O | 2:F:1129:VAL:N | 2.27 | 0.66 |
| 2:B:295:VAL:O | 2:B:298:ILE:N | 2.29 | 0.66 |
| 2:B:436:ASP:HA | 2:B:437:ILE:CB | 2.12 | 0.66 |
| 1:A:436:PHE:C | 1:A:436:PHE:CD1 | 2.68 | 0.66 |
| 2:F:423:ILE:O | 2:F:423:ILE:HG23 | 1.94 | 0.66 |
| 2:F:867:PHE:HB2 | 2:F:985:LEU:O | 1.95 | 0.66 |
| 2:B:423:ILE:HG23 | 2:B:423:ILE:O | 1.93 | 0.66 |
| 2:F:1149:HIS:CG | 2:F:1150:ASP:N | 2.64 | 0.66 |
| 1:A:944:ARG:HG2 | 1:A:1026:SER:HA | 1.76 | 0.66 |
| 2:B:877:LYS:HB3 | 2:B:878:GLN:HB3 | 1.78 | 0.66 |
| 1:E:154:GLU:HB2 | 1:E:155:PRO:HD2 | 1.78 | 0.66 |
| 2:D:21:VAL:HG13 | 2:D:121:ASN:HA | 1.77 | 0.65 |
| 2:F:877:LYS:HB3 | 2:F:878:GLN:HB3 | 1.78 | 0.65 |
| 1:C:154:GLU:HB2 | 1:C:155:PRO:HD2 | 1.77 | 0.65 |
| 1:C:628:LEU:CB | 1:E:419:LYS:HE3 | 2.25 | 0.65 |
| 2:D:877:LYS:HB3 | 2:D:878:GLN:HB3 | 1.78 | 0.65 |
| 2:F:121:ASN:CB | 2:F:127:ASN:HA | 2.27 | 0.65 |
| 2:B:867:PHE:HB2 | 2:B:985:LEU:O | 1.97 | 0.65 |
| 2:D:1013:GLU:O | 2:D:1014:ILE:HB | 1.97 | 0.65 |
| 1:E:928:ASN:HB3 | 1:E:930:ILE:HG22 | 1.77 | 0.65 |
| 1:E:118:ASN:HA | 1:E:119:THR:HB | 1.77 | 0.65 |
| 1:C:238:ASN:ND2 | 1:C:239:PRO:HD2 | 2.11 | 0.65 |
| 2:B:121:ASN:CB | 2:B:127:ASN:HA | 2.26 | 0.65 |
| 1:E:771:MET:HA | 1:E:774:ILE:HG22 | 1.79 | 0.64 |
| 1:C:836:LEU:HD11 | 2:D:945:PHE:CD1 | 2.32 | 0.64 |
| 1:C:415:ILE:HD12 | 1:C:425:ILE:HD12 | 1.78 | 0.64 |
| 1:E:926:TYR:HB3 | 1:E:1250:GLN:CG | 2.28 | 0.64 |
| 1:A:928:ASN:HB3 | 1:A:930:ILE:HG22 | 1.79 | 0.64 |
| 1:E:236:GLN:HB3 | 1:E:241:ILE:HD13 | 1.79 | 0.64 |
| 1:A:289:VAL:CB | 1:A:290:GLN:HA | 2.23 | 0.64 |
| 1:A:216:HIS:NE2 | 1:A:251:GLU:OE1 | 2.30 | 0.64 |
| 1:A:771:MET:HA | 1:A:774:ILE:HG22 | 1.79 | 0.64 |
| 2:B:1013:GLU:O | 2:B:1014:ILE:HB | 1.97 | 0.64 |
| 1:A:926:TYR:HB3 | 1:A:1250:GLN:CG | 2.28 | 0.64 |
| 1:E:216:HIS:NE2 | 1:E:251:GLU:OE1 | 2.31 | 0.64 |
| 1:A:415:ILE:HD12 | 1:A:425:ILE:HD12 | 1.79 | 0.64 |
| 1:A:468:LEU:O | 1:A:470:GLN:N | 2.31 | 0.64 |
| 2:B:1137:ASN:HB3 | 2:B:1142:TRP:NE1 | 2.13 | 0.64 |
| 1:E:836:LEU:HD11 | 2:F:945:PHE:CD1 | 2.33 | 0.64 |
| 2:D:552:LYS:O | 2:D:713:PHE:HD1 | 1.81 | 0.64 |
| 2:B:35:VAL:HG12 | 2:B:36:ALA:H | 1.63 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:D:35:VAL:HG12 | 2:D:36:ALA:H | 1.63 | 0.64 |
| 2:F:1013:GLU:O | 2:F:1014:ILE:HB | 1.98 | 0.64 |
| 1:E:415:ILE:HD12 | 1:E:425:ILE:HD12 | 1.79 | 0.64 |
| 1:A:705:TYR:C | 1:A:705:TYR:CD1 | 2.72 | 0.63 |
| 1:E:468:LEU:O | 1:E:470:GLN:N | 2.30 | 0.63 |
| 2:B:1122:LEU:HD21 | 2:B:1158:TRP:CZ2 | 2.33 | 0.63 |
| 1:A:904:ASP:HA | 1:A:907:ILE:HD11 | 1.79 | 0.63 |
| 2:B:13:VAL:HG12 | 2:B:14:ASP:N | 2.14 | 0.63 |
| 1:C:365:ASN:O | 1:C:368:ILE:HG22 | 1.97 | 0.63 |
| 2:B:224:TYR:O | 2:B:392:GLY:HA2 | 1.97 | 0.63 |
| 1:E:454:ILE:HD13 | 1:E:666:ALA:HA | 1.79 | 0.63 |
| 2:D:1137:ASN:HB3 | 2:D:1142:TRP:NE1 | 2.12 | 0.63 |
| 2:B:608:PHE:O | 2:B:612:SER:N | 2.31 | 0.63 |
| 2:F:269:TYR:OH | 2:F:288:GLU:HB2 | 1.98 | 0.63 |
| 2:D:1122:LEU:HD21 | 2:D:1158:TRP:CZ2 | 2.33 | 0.63 |
| 1:A:154:GLU:HB2 | 1:A:155:PRO:HD2 | 1.79 | 0.63 |
| 1:C:926:TYR:HB3 | 1:C:1250:GLN:CG | 2.29 | 0.63 |
| 2:B:856:ASN:HB3 | 2:B:859:PHE:CE2 | 2.34 | 0.63 |
| 1:C:857:TYR:CZ | 1:C:860:ASP:HA | 2.33 | 0.63 |
| 2:F:1122:LEU:HD21 | 2:F:1158:TRP:CZ2 | 2.33 | 0.63 |
| 2:D:608:PHE:O | 2:D:612:SER:N | 2.32 | 0.63 |
| 1:A:926:TYR:HB3 | 1:A:1250:GLN:HG3 | 1.80 | 0.63 |
| 1:C:928:ASN:HB3 | 1:C:930:ILE:HG22 | 1.80 | 0.62 |
| 1:C:444:ASN:OD1 | 1:C:445:ASP:N | 2.33 | 0.62 |
| 2:F:961:ASN:OD1 | 2:F:962:ILE:N | 2.33 | 0.62 |
| 1:C:754:ALA:O | 1:C:757:ASN:HB2 | 1.99 | 0.62 |
| 2:F:429:ILE:N | 2:F:430:PRO:CD | 2.63 | 0.62 |
| 2:D:295:VAL:O | 2:D:298:ILE:N | 2.31 | 0.62 |
| 2:B:962:ILE:HG22 | 2:B:962:ILE:O | 1.99 | 0.62 |
| 2:B:910:ASP:HB3 | 2:B:914:ASN:HB2 | 1.81 | 0.62 |
| 1:E:219:HIS:ND1 | 1:E:250:GLU:OE2 | 2.27 | 0.62 |
| 2:D:269:TYR:OH | 2:D:288:GLU:HB2 | 1.98 | 0.62 |
| 1:C:771:MET:HA | 1:C:774:ILE:HG22 | 1.82 | 0.62 |
| 2:F:295:VAL:O | 2:F:298:ILE:N | 2.32 | 0.62 |
| 2:B:552:LYS:O | 2:B:713:PHE:HD1 | 1.83 | 0.62 |
| 1:C:216:HIS:NE2 | 1:C:251:GLU:OE1 | 2.33 | 0.62 |
| 1:C:926:TYR:HB3 | 1:C:1250:GLN:HG3 | 1.81 | 0.62 |
| 2:B:429:ILE:N | 2:B:430:PRO:CD | 2.63 | 0.62 |
| 1:A:914:ASN:O | 1:A:915:PHE:HB3 | 1.99 | 0.62 |
| 2:B:268:ASP:HA | 2:B:271:ILE:HG22 | 1.80 | 0.62 |
| 2:D:268:ASP:HA | 2:D:271:ILE:HG22 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:F:962:ILE:HG22 | 2:F:962:ILE:O | 2.00 | 0.62 |
| 1:E:926:TYR:HB3 | 1:E:1250:GLN:HG3 | 1.80 | 0.62 |
| 2:D:910:ASP:HB3 | 2:D:914:ASN:HB2 | 1.82 | 0.62 |
| 2:F:608:PHE:O | 2:F:612:SER:N | 2.32 | 0.62 |
| 2:F:35:VAL:HG12 | 2:F:36:ALA:H | 1.65 | 0.62 |
| 2:D:962:ILE:O | 2:D:962:ILE:HG22 | 2.00 | 0.62 |
| 1:A:365:ASN:O | 1:A:368:ILE:HG22 | 2.00 | 0.62 |
| 1:E:414:ASN:HA | 1:E:424:SER:HA | 1.81 | 0.62 |
| 1:A:236:GLN:HB3 | 1:A:241:ILE:HD13 | 1.82 | 0.61 |
| 1:C:20:TYR:HB3 | 1:C:29:PHE:HB3 | 1.81 | 0.61 |
| 2:D:1093:THR:HG23 | 2:D:1095:ASN:H | 1.65 | 0.61 |
| 1:E:119:THR:H | 1:E:120:PRO:CD | 2.14 | 0.61 |
| 1:C:454:ILE:HD13 | 1:C:666:ALA:HA | 1.81 | 0.61 |
| 2:F:268:ASP:HA | 2:F:271:ILE:HG22 | 1.82 | 0.61 |
| 2:F:1137:ASN:HB3 | 2:F:1142:TRP:NE1 | 2.14 | 0.61 |
| 2:B:1149:HIS:CE1 | 2:B:1150:ASP:HB3 | 2.35 | 0.61 |
| 2:F:1023:LEU:HD13 | 2:F:1158:TRP:HZ3 | 1.66 | 0.61 |
| 2:D:961:ASN:OD1 | 2:D:962:ILE:N | 2.33 | 0.61 |
| 1:E:857:TYR:CZ | 1:E:860:ASP:HA | 2.36 | 0.61 |
| 1:A:380:LEU:HA | 1:A:385:ARG:HB3 | 1.82 | 0.61 |
| 2:F:184:ASP:OD1 | 2:F:185:PRO:HD2 | 2.01 | 0.61 |
| 2:F:910:ASP:HB3 | 2:F:914:ASN:HB2 | 1.83 | 0.61 |
| 1:C:414:ASN:HA | 1:C:424:SER:HA | 1.82 | 0.61 |
| 2:F:393:THR:HG1 | 2:F:396:ASN:N | 1.99 | 0.61 |
| 1:C:1131:ARG:HD2 | 1:C:1132:VAL:N | 2.16 | 0.61 |
| 1:C:236:GLN:HB3 | 1:C:241:ILE:HD13 | 1.83 | 0.61 |
| 1:C:705:TYR:C | 1:C:705:TYR:CD1 | 2.74 | 0.61 |
| 2:D:552:LYS:HB2 | 2:D:713:PHE:HE1 | 1.65 | 0.61 |
| 1:C:468:LEU:O | 1:C:470:GLN:N | 2.33 | 0.61 |
| 1:A:454:ILE:HD13 | 1:A:666:ALA:HA | 1.82 | 0.61 |
| 2:D:956:ILE:O | 2:D:956:ILE:HG22 | 2.00 | 0.61 |
| 2:D:856:ASN:HB3 | 2:D:859:PHE:CE2 | 2.36 | 0.61 |
| 1:E:981:ASN:HD21 | 2:F:414:ASN:HB3 | 1.64 | 0.61 |
| 1:C:289:VAL:CB | 1:C:290:GLN:HA | 2.27 | 0.60 |
| 2:B:184:ASP:OD1 | 2:B:185:PRO:HD2 | 2.00 | 0.60 |
| 1:A:1131:ARG:HD2 | 1:A:1132:VAL:N | 2.15 | 0.60 |
| 1:A:854:ASN:HB2 | 1:A:865:THR:HG22 | 1.82 | 0.60 |
| 1:C:427:ILE:CD1 | 1:C:521:PHE:HA | 2.31 | 0.60 |
| 1:A:754:ALA:O | 1:A:757:ASN:HB2 | 1.99 | 0.60 |
| 2:F:956:ILE:HG22 | 2:F:956:ILE:O | 2.00 | 0.60 |
| 1:C:914:ASN:O | 1:C:915:PHE:HB3 | 2.00 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:E:365:ASN:O | 1:E:368:ILE:HG22 | 2.00 | 0.60 |
| 2:F:856:ASN:HB3 | 2:F:859:PHE:CE2 | 2.36 | 0.60 |
| 1:C:904:ASP:HA | 1:C:907:ILE:HD11 | 1.82 | 0.60 |
| 1:E:380:LEU:HA | 1:E:385:ARG:HB3 | 1.84 | 0.60 |
| 1:C:219:HIS:ND1 | 1:C:250:GLU:OE2 | 2.28 | 0.60 |
| 2:D:184:ASP:OD1 | 2:D:185:PRO:HD2 | 2.02 | 0.60 |
| 2:D:1023:LEU:HD13 | 2:D:1158:TRP:HZ3 | 1.67 | 0.60 |
| 2:B:552:LYS:HB2 | 2:B:713:PHE:HE1 | 1.65 | 0.60 |
| 2:F:246:ASN:ND2 | 2:F:413:ILE:O | 2.34 | 0.60 |
| 1:E:914:ASN:O | 1:E:915:PHE:HB3 | 2.01 | 0.60 |
| 2:F:552:LYS:O | 2:F:713:PHE:HD1 | 1.83 | 0.60 |
| 2:F:465:LEU:HB3 | 2:F:466:PRO:CD | 2.32 | 0.60 |
| 2:F:465:LEU:HB3 | 2:F:466:PRO:HD2 | 1.84 | 0.60 |
| 2:B:269:TYR:OH | 2:B:288:GLU:HB2 | 2.01 | 0.60 |
| 2:D:246:ASN:ND2 | 2:D:413:ILE:O | 2.34 | 0.60 |
| 2:D:429:ILE:N | 2:D:430:PRO:CD | 2.65 | 0.60 |
| 2:D:13:VAL:HG12 | 2:D:14:ASP:N | 2.16 | 0.60 |
| 1:E:427:ILE:CD1 | 1:E:521:PHE:HA | 2.31 | 0.60 |
| 2:B:605:ASN:HA | 2:B:754:ASN:HB2 | 1.83 | 0.60 |
| 2:F:989:ILE:HG22 | 2:F:994:ILE:HG13 | 1.82 | 0.60 |
| 1:C:1211:LEU:HD12 | 1:C:1225:TYR:HB3 | 1.83 | 0.60 |
| 1:E:754:ALA:O | 1:E:757:ASN:HB2 | 2.01 | 0.60 |
| 1:A:414:ASN:HA | 1:A:424:SER:HA | 1.84 | 0.60 |
| 2:B:544:ILE:HD12 | 2:B:553:ILE:HD12 | 1.83 | 0.59 |
| 1:C:143:ILE:HD13 | 1:C:491:THR:HG23 | 1.83 | 0.59 |
| 1:C:779:ILE:HG22 | 1:C:779:ILE:O | 2.02 | 0.59 |
| 2:D:544:ILE:HD12 | 2:D:553:ILE:HD12 | 1.82 | 0.59 |
| 1:A:987:ILE:C | 1:A:989:LYS:H | 2.06 | 0.59 |
| 2:B:411:HIS:HA | 2:B:624:PHE:HE1 | 1.66 | 0.59 |
| 1:C:417:SER:OG | 1:C:418:VAL:N | 2.33 | 0.59 |
| 1:C:836:LEU:CB | 2:D:995:LEU:HD11 | 2.31 | 0.59 |
| 2:D:989:ILE:HG22 | 2:D:994:ILE:HG13 | 1.84 | 0.59 |
| 2:F:544:ILE:HD12 | 2:F:553:ILE:HD12 | 1.83 | 0.59 |
| 2:B:498:TYR:OH | 2:B:559:ARG:O | 2.21 | 0.59 |
| 1:A:857:TYR:CZ | 1:A:860:ASP:HA | 2.36 | 0.59 |
| 2:D:605:ASN:HA | 2:D:754:ASN:HB2 | 1.84 | 0.59 |
| 1:E:705:TYR:CD1 | 1:E:705:TYR:C | 2.75 | 0.59 |
| 1:A:417:SER:OG | 1:A:418:VAL:N | 2.34 | 0.59 |
| 2:D:552:LYS:O | 2:D:713:PHE:CD1 | 2.55 | 0.59 |
| 2:B:961:ASN:OD1 | 2:B:962:ILE:N | 2.35 | 0.59 |
| 1:A:219:HIS:ND1 | 1:A:250:GLU:OE2 | 2.28 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:427:ILE:CD1 | 1:A:521:PHE:HA | 2.33 | 0.59 |
| 1:E:854:ASN:HB2 | 1:E:865:THR:HG22 | 1.85 | 0.59 |
| 2:B:1142:TRP:CD1 | 2:B:1142:TRP:N | 2.70 | 0.59 |
| 2:B:543:GLU:HA | 2:B:552:LYS:HA | 1.83 | 0.59 |
| 2:B:552:LYS:O | 2:B:713:PHE:CD1 | 2.56 | 0.59 |
| 2:B:956:ILE:O | 2:B:956:ILE:HG22 | 2.03 | 0.59 |
| 2:B:1093:THR:HG23 | 2:B:1095:ASN:H | 1.66 | 0.59 |
| 1:A:368:ILE:HD11 | 1:A:395:ILE:HA | 1.84 | 0.59 |
| 2:F:9:ILE:HG23 | 2:F:10:ASP:H | 1.67 | 0.59 |
| 1:A:462:ASN:HB3 | 1:A:463:ASN:HA | 1.85 | 0.59 |
| 2:F:543:GLU:HA | 2:F:552:LYS:HA | 1.85 | 0.59 |
| 2:B:579:PRO:C | 2:B:581:SER:H | 2.06 | 0.59 |
| 1:A:143:ILE:HD13 | 1:A:491:THR:HG23 | 1.83 | 0.59 |
| 2:D:1149:HIS:CE1 | 2:D:1150:ASP:HB3 | 2.38 | 0.58 |
| 2:B:1023:LEU:HD12 | 2:B:1024:PHE:N | 2.17 | 0.58 |
| 1:A:454:ILE:HD11 | 1:A:456:ASP:OD1 | 2.03 | 0.58 |
| 1:E:444:ASN:OD1 | 1:E:445:ASP:N | 2.36 | 0.58 |
| 1:E:198:SER:O | 1:E:200:ASN:N | 2.36 | 0.58 |
| 2:D:526:TRP:CZ2 | 2:D:530:ILE:HD11 | 2.38 | 0.58 |
| 2:D:469:TYR:CE2 | 2:D:562:ASN:HB2 | 2.38 | 0.58 |
| 1:E:628:LEU:HD23 | 1:E:632:ILE:HB | 1.85 | 0.58 |
| 1:C:854:ASN:HB2 | 1:C:865:THR:HG22 | 1.84 | 0.58 |
| 1:E:453:GLU:O | 1:E:454:ILE:HG22 | 2.04 | 0.58 |
| 1:A:453:GLU:O | 1:A:454:ILE:HG22 | 2.03 | 0.58 |
| 2:B:246:ASN:ND2 | 2:B:413:ILE:O | 2.35 | 0.58 |
| 1:E:943:MET:HB3 | 1:E:947:ASN:HA | 1.85 | 0.58 |
| 2:F:804:SER:O | 2:F:818:ASP:HA | 2.03 | 0.58 |
| 2:B:990:ASN:HB3 | 2:B:993:GLU:CD | 2.23 | 0.58 |
| 2:D:990:ASN:HB3 | 2:D:993:GLU:CD | 2.23 | 0.58 |
| 1:E:454:ILE:HD11 | 1:E:456:ASP:OD1 | 2.03 | 0.58 |
| 2:D:245:THR:O | 2:D:247:PRO:C | 2.42 | 0.58 |
| 2:D:465:LEU:HB3 | 2:D:466:PRO:HD2 | 1.86 | 0.58 |
| 1:E:779:ILE:O | 1:E:779:ILE:HG22 | 2.03 | 0.58 |
| 2:D:436:ASP:HA | 2:D:437:ILE:CB | 2.14 | 0.58 |
| 1:A:836:LEU:HB2 | 2:B:995:LEU:HD11 | 1.85 | 0.58 |
| 1:C:436:PHE:HD1 | 1:C:437:VAL:N | 2.01 | 0.58 |
| 1:A:1211:LEU:HD12 | 1:A:1225:TYR:HB3 | 1.84 | 0.58 |
| 2:F:13:VAL:HG12 | 2:F:14:ASP:N | 2.18 | 0.58 |
| 1:E:417:SER:OG | 1:E:418:VAL:N | 2.32 | 0.58 |
| 1:E:143:ILE:HD13 | 1:E:491:THR:HG23 | 1.83 | 0.58 |
| 2:B:427:GLU:C | 2:B:430:PRO:HD3 | 2.24 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:454:ILE:CD1 | 1:A:456:ASP:OD1 | 2.51 | 0.58 |
| 1:E:1131:ARG:HD2 | 1:E:1132:VAL:N | 2.18 | 0.58 |
| 1:C:164:ASN:HB3 | 1:C:180:SER:OG | 2.04 | 0.58 |
| 1:A:779:ILE:O | 1:A:779:ILE:HG22 | 2.03 | 0.58 |
| 2:F:469:TYR:CE2 | 2:F:562:ASN:HB2 | 2.39 | 0.58 |
| 1:C:168:ARG:HA | 1:C:497:TYR:HB2 | 1.86 | 0.58 |
| 1:A:164:ASN:HB3 | 1:A:180:SER:OG | 2.03 | 0.58 |
| 2:D:427:GLU:C | 2:D:430:PRO:HD3 | 2.24 | 0.58 |
| 2:F:990:ASN:HB3 | 2:F:993:GLU:CD | 2.24 | 0.58 |
| 1:C:154:GLU:HB2 | 1:C:155:PRO:CD | 2.34 | 0.58 |
| 2:D:465:LEU:HB3 | 2:D:466:PRO:CD | 2.34 | 0.58 |
| 2:D:113:ASN:HB3 | 2:D:279:ILE:CB | 2.33 | 0.58 |
| 1:A:444:ASN:OD1 | 1:A:445:ASP:N | 2.37 | 0.58 |
| 2:F:788:SER:O | 2:F:791:GLU:HB3 | 2.04 | 0.58 |
| 2:D:804:SER:O | 2:D:818:ASP:HA | 2.04 | 0.57 |
| 1:A:1044:ILE:HG22 | 1:A:1045:ARG:N | 2.19 | 0.57 |
| 2:F:411:HIS:HA | 2:F:624:PHE:HE1 | 1.69 | 0.57 |
| 1:C:824:PRO:HB3 | 2:D:952:ALA:HB2 | 1.86 | 0.57 |
| 2:D:788:SER:O | 2:D:791:GLU:HB3 | 2.04 | 0.57 |
| 2:F:227:LEU:HD11 | 2:F:231:ASP:HB2 | 1.86 | 0.57 |
| 2:B:989:ILE:HG22 | 2:B:994:ILE:HG13 | 1.86 | 0.57 |
| 2:D:1023:LEU:HD12 | 2:D:1024:PHE:N | 2.19 | 0.57 |
| 2:B:856:ASN:HB3 | 2:B:859:PHE:HE2 | 1.69 | 0.57 |
| 1:A:605:TYR:CD1 | 1:A:605:TYR:O | 2.57 | 0.57 |
| 1:C:1205:ASN:C | 1:C:1205:ASN:OD1 | 2.42 | 0.57 |
| 2:F:1142:TRP:CD1 | 2:F:1142:TRP:N | 2.72 | 0.57 |
| 2:D:498:TYR:OH | 2:D:559:ARG:O | 2.21 | 0.57 |
| 2:F:552:LYS:O | 2:F:713:PHE:CD1 | 2.57 | 0.57 |
| 2:D:756:ASN:OD1 | 2:D:756:ASN:N | 2.37 | 0.57 |
| 2:B:554:ILE:HG21 | 2:B:556:TRP:CE2 | 2.39 | 0.57 |
| 1:E:236:GLN:HB3 | 1:E:241:ILE:CD1 | 2.33 | 0.57 |
| 2:D:543:GLU:HA | 2:D:552:LYS:HA | 1.87 | 0.57 |
| 2:B:1023:LEU:HD13 | 2:B:1158:TRP:HZ3 | 1.68 | 0.57 |
| 1:E:20:TYR:HB3 | 1:E:29:PHE:HB3 | 1.84 | 0.57 |
| 1:C:628:LEU:HD23 | 1:C:632:ILE:HB | 1.86 | 0.57 |
| 2:F:1093:THR:HG23 | 2:F:1095:ASN:H | 1.69 | 0.57 |
| 1:E:368:ILE:HD11 | 1:E:395:ILE:HA | 1.85 | 0.57 |
| 1:E:168:ARG:HA | 1:E:497:TYR:HB2 | 1.87 | 0.57 |
| 1:E:824:PRO:CB | 2:F:952:ALA:HB2 | 2.35 | 0.57 |
| 1:A:168:ARG:HA | 1:A:497:TYR:HB2 | 1.87 | 0.57 |
| 1:E:154:GLU:HB2 | 1:E:155:PRO:CD | 2.35 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:E:454:ILE:CD1 | 1:E:456:ASP:OD1 | 2.52 | 0.57 |
| 1:C:416:VAL:HG13 | 1:C:420:GLY:N | 2.20 | 0.57 |
| 1:E:164:ASN:HB3 | 1:E:180:SER:OG | 2.04 | 0.57 |
| 2:D:552:LYS:HB2 | 2:D:713:PHE:CE1 | 2.40 | 0.57 |
| 1:C:857:TYR:OH | 1:C:860:ASP:HA | 2.05 | 0.57 |
| 1:C:380:LEU:HA | 1:C:385:ARG:HB3 | 1.86 | 0.57 |
| 1:C:453:GLU:O | 1:C:454:ILE:HG22 | 2.04 | 0.57 |
| 2:F:552:LYS:HB2 | 2:F:713:PHE:HE1 | 1.69 | 0.57 |
| 1:A:309:LEU:CD2 | 1:A:319:VAL:HG12 | 2.35 | 0.57 |
| 2:D:742:ASN:HA | 2:D:745:THR:HG22 | 1.87 | 0.57 |
| 2:B:166:LEU:HD12 | 2:B:196:SER:HB2 | 1.86 | 0.57 |
| 1:A:289:VAL:HB | 1:A:290:GLN:CB | 2.35 | 0.57 |
| 1:E:436:PHE:HD1 | 1:E:437:VAL:N | 2.01 | 0.57 |
| 1:E:836:LEU:HD13 | 2:F:991:SER:HA | 1.87 | 0.57 |
| 1:C:368:ILE:HD11 | 1:C:395:ILE:HA | 1.86 | 0.57 |
| 1:C:943:MET:HB3 | 1:C:947:ASN:HA | 1.86 | 0.57 |
| 2:D:9:ILE:HG23 | 2:D:10:ASP:H | 1.69 | 0.57 |
| 2:F:870:TYR:CE2 | 2:F:983:SER:OG | 2.57 | 0.57 |
| 2:F:605:ASN:HA | 2:F:754:ASN:HB2 | 1.87 | 0.56 |
| 1:E:742:GLN:O | 1:E:744:GLU:N | 2.38 | 0.56 |
| 1:A:198:SER:O | 1:A:200:ASN:N | 2.38 | 0.56 |
| 1:E:1205:ASN:C | 1:E:1205:ASN:OD1 | 2.43 | 0.56 |
| 2:F:1149:HIS:CE1 | 2:F:1150:ASP:HB3 | 2.40 | 0.56 |
| 2:F:1023:LEU:HD13 | 2:F:1158:TRP:CZ3 | 2.40 | 0.56 |
| 2:B:895:TRP:O | 2:B:896:GLU:HG2 | 2.05 | 0.56 |
| 2:F:40:TRP:O | 2:F:137:VAL:HA | 2.05 | 0.56 |
| 2:F:113:ASN:HB3 | 2:F:279:ILE:CB | 2.34 | 0.56 |
| 2:F:756:ASN:N | 2:F:756:ASN:OD1 | 2.37 | 0.56 |
| 2:B:804:SER:O | 2:B:818:ASP:HA | 2.04 | 0.56 |
| 2:F:245:THR:O | 2:F:247:PRO:C | 2.42 | 0.56 |
| 1:A:427:ILE:HG22 | 1:A:428:GLU:N | 2.19 | 0.56 |
| 1:E:1149:TYR:CD1 | 1:E:1183:ARG:HD2 | 2.40 | 0.56 |
| 2:B:943:LEU:HD23 | 2:B:953:ASN:HA | 1.88 | 0.56 |
| 1:E:452:LYS:HB2 | 1:E:651:LYS:HE2 | 1.88 | 0.56 |
| 2:B:756:ASN:N | 2:B:756:ASN:OD1 | 2.39 | 0.56 |
| 2:B:526:TRP:CZ2 | 2:B:530:ILE:HD11 | 2.40 | 0.56 |
| 1:C:481:PRO:HG2 | 1:C:483:LEU:HD21 | 1.88 | 0.56 |
| 1:A:628:LEU:HD23 | 1:A:632:ILE:HB | 1.86 | 0.56 |
| 1:A:452:LYS:HB2 | 1:A:651:LYS:HE2 | 1.87 | 0.56 |
| 1:C:454:ILE:HD11 | 1:C:456:ASP:OD1 | 2.05 | 0.56 |
| 1:C:824:PRO:CB | 2:D:952:ALA:HB2 | 2.36 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:788:SER:O | 2:B:791:GLU:HB3 | 2.04 | 0.56 |
| 2:D:393:THR:HG1 | 2:D:396:ASN:N | 2.03 | 0.56 |
| 2:D:227:LEU:HD11 | 2:D:231:ASP:HB2 | 1.88 | 0.56 |
| 2:B:465:LEU:HB3 | 2:B:466:PRO:CD | 2.36 | 0.56 |
| 1:A:1205:ASN:OD1 | 1:A:1205:ASN:C | 2.43 | 0.56 |
| 1:A:289:VAL:HB | 1:A:290:GLN:HB3 | 1.88 | 0.56 |
| 1:A:436:PHE:HD1 | 1:A:437:VAL:N | 2.03 | 0.56 |
| 2:B:822:LYS:O | 2:B:824:THR:N | 2.39 | 0.56 |
| 2:D:856:ASN:HB3 | 2:D:859:PHE:HE2 | 1.71 | 0.56 |
| 2:B:465:LEU:HB3 | 2:B:466:PRO:HD2 | 1.87 | 0.56 |
| 2:B:113:ASN:HB3 | 2:B:279:ILE:CB | 2.36 | 0.56 |
| 1:A:1150:ILE:HG22 | 1:A:1162:LEU:HD12 | 1.86 | 0.56 |
| 1:C:1163:TYR:O | 1:C:1175:ILE:HG23 | 2.05 | 0.56 |
| 1:E:462:ASN:HB3 | 1:E:463:ASN:HA | 1.87 | 0.56 |
| 1:C:1083:ASP:N | 1:C:1129:ILE:O | 2.33 | 0.56 |
| 1:A:38:ASN:HD21 | 1:A:484:SER:CB | 2.19 | 0.56 |
| 2:F:98:LEU:O | 2:F:101:LEU:HB3 | 2.06 | 0.56 |
| 1:E:416:VAL:HG13 | 1:E:420:GLY:N | 2.21 | 0.56 |
| 2:F:429:ILE:HG22 | 2:F:429:ILE:O | 2.06 | 0.56 |
| 2:B:552:LYS:HB2 | 2:B:713:PHE:CE1 | 2.40 | 0.56 |
| 1:C:454:ILE:CD1 | 1:C:456:ASP:OD1 | 2.53 | 0.56 |
| 1:C:198:SER:O | 1:C:200:ASN:N | 2.39 | 0.56 |
| 1:E:289:VAL:CB | 1:E:290:GLN:HA | 2.27 | 0.56 |
| 2:F:554:ILE:HG21 | 2:F:556:TRP:CE2 | 2.41 | 0.56 |
| 1:A:154:GLU:HB2 | 1:A:155:PRO:CD | 2.35 | 0.56 |
| 1:C:857:TYR:HA | 1:C:862:TYR:HA | 1.88 | 0.56 |
| 2:B:269:TYR:CE1 | 2:B:287:LEU:HB3 | 2.41 | 0.56 |
| 1:C:899:ASN:OD1 | 1:C:1028:ASN:HB3 | 2.05 | 0.56 |
| 2:D:870:TYR:CE2 | 2:D:983:SER:OG | 2.59 | 0.56 |
| 2:B:742:ASN:HA | 2:B:745:THR:HG22 | 1.88 | 0.56 |
| 1:C:1044:ILE:HG22 | 1:C:1045:ARG:N | 2.20 | 0.56 |
| 1:C:119:THR:H | 1:C:120:PRO:CD | 2.18 | 0.55 |
| 2:F:427:GLU:C | 2:F:430:PRO:HD3 | 2.26 | 0.55 |
| 1:E:1211:LEU:HD12 | 1:E:1225:TYR:HB3 | 1.86 | 0.55 |
| 1:E:1163:TYR:O | 1:E:1175:ILE:HG23 | 2.06 | 0.55 |
| 1:C:448:ILE:O | 1:C:449:ASN:C | 2.44 | 0.55 |
| 2:F:545:SER:HA | 2:F:550:ASP:N | 2.21 | 0.55 |
| 2:D:943:LEU:HD23 | 2:D:953:ASN:HA | 1.88 | 0.55 |
| 2:B:1015:LEU:HB2 | 2:B:1071:VAL:HB | 1.89 | 0.55 |
| 2:B:40:TRP:O | 2:B:137:VAL:HA | 2.06 | 0.55 |
| 2:D:554:ILE:HG21 | 2:D:556:TRP:CE2 | 2.41 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:F:269:TYR:CE1 | 2:F:287:LEU:HB3 | 2.41 | 0.55 |
| 2:D:1023:LEU:HD13 | 2:D:1158:TRP:CZ3 | 2.41 | 0.55 |
| 2:D:545:SER:HA | 2:D:550:ASP:N | 2.21 | 0.55 |
| 1:E:376:ASN:HB3 | 1:E:381:LYS:HA | 1.89 | 0.55 |
| 2:D:92:ASN:HB3 | 2:D:310:PHE:CZ | 2.42 | 0.55 |
| 2:F:498:TYR:OH | 2:F:559:ARG:O | 2.23 | 0.55 |
| 2:F:943:LEU:HD23 | 2:F:953:ASN:HA | 1.89 | 0.55 |
| 1:A:67:SER:HA | 1:A:158:PHE:CD2 | 2.41 | 0.55 |
| 1:C:1092:LEU:O | 1:C:1094:PRO:HD3 | 2.06 | 0.55 |
| 1:C:452:LYS:HB2 | 1:C:651:LYS:HE2 | 1.87 | 0.55 |
| 1:A:705:TYR:C | 1:A:705:TYR:HD1 | 2.09 | 0.55 |
| 2:B:1023:LEU:HD13 | 2:B:1158:TRP:CZ3 | 2.42 | 0.55 |
| 2:F:1023:LEU:HD12 | 2:F:1024:PHE:N | 2.22 | 0.55 |
| 1:C:427:ILE:HG22 | 1:C:428:GLU:N | 2.22 | 0.55 |
| 2:B:92:ASN:HB3 | 2:B:310:PHE:CZ | 2.42 | 0.55 |
| 1:A:742:GLN:O | 1:A:744:GLU:N | 2.40 | 0.55 |
| 2:D:895:TRP:O | 2:D:896:GLU:HG2 | 2.05 | 0.55 |
| 1:C:627:LEU:O | 1:E:420:GLY:N | 2.40 | 0.55 |
| 2:B:469:TYR:CE2 | 2:B:562:ASN:HB2 | 2.41 | 0.55 |
| 1:C:738:TYR:O | 1:C:739:ASP:C | 2.45 | 0.55 |
| 2:B:98:LEU:O | 2:B:101:LEU:HB3 | 2.07 | 0.55 |
| 1:A:1092:LEU:O | 1:A:1094:PRO:HD3 | 2.07 | 0.55 |
| 2:D:23:SER:OG | 2:D:29:PHE:HB2 | 2.07 | 0.55 |
| 2:B:9:ILE:HG23 | 2:B:10:ASP:H | 1.71 | 0.55 |
| 1:C:462:ASN:HB3 | 1:C:463:ASN:HA | 1.88 | 0.55 |
| 1:E:111:ASN:HA | 1:E:147:ASN:OD1 | 2.07 | 0.55 |
| 1:A:737:LYS:O | 1:A:738:TYR:O | 2.24 | 0.55 |
| 2:B:502:ASN:O | 2:B:506:ASP:HB2 | 2.06 | 0.55 |
| 2:F:579:PRO:C | 2:F:581:SER:H | 2.08 | 0.55 |
| 1:A:119:THR:H | 1:A:120:PRO:CD | 2.19 | 0.55 |
| 1:A:1025:VAL:HG12 | 1:A:1026:SER:N | 2.22 | 0.55 |
| 2:F:727:TYR:N | 2:F:728:PRO:HD2 | 2.22 | 0.55 |
| 1:C:742:GLN:O | 1:C:744:GLU:N | 2.40 | 0.55 |
| 2:B:1149:HIS:NE2 | 2:B:1150:ASP:HB3 | 2.22 | 0.55 |
| 1:E:392:ASN:O | 1:E:395:ILE:HG12 | 2.07 | 0.55 |
| 2:F:1072:GLN:O | 2:F:1075:ASP:HB2 | 2.07 | 0.55 |
| 2:B:544:ILE:HD13 | 2:B:575:LYS:HG2 | 1.88 | 0.54 |
| 2:D:98:LEU:O | 2:D:101:LEU:HB3 | 2.07 | 0.54 |
| 1:C:606:ILE:HD13 | 1:C:761:PHE:CE2 | 2.42 | 0.54 |
| 2:B:23:SER:OG | 2:B:29:PHE:HB2 | 2.08 | 0.54 |
| 1:E:1044:ILE:HG22 | 1:E:1045:ARG:N | 2.22 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:943:MET:HB3 | 1:A:947:ASN:HA | 1.88 | 0.54 |
| 2:D:1142:TRP:CD1 | 2:D:1142:TRP:N | 2.75 | 0.54 |
| 1:C:467:ASP:OD1 | 1:C:468:LEU:N | 2.40 | 0.54 |
| 1:E:824:PRO:HB3 | 2:F:952:ALA:HB2 | 1.89 | 0.54 |
| 1:E:606:ILE:HD13 | 1:E:761:PHE:CE2 | 2.42 | 0.54 |
| 1:C:67:SER:HA | 1:C:158:PHE:CD2 | 2.43 | 0.54 |
| 2:B:88:ARG:NE | 2:B:339:TYR:OH | 2.41 | 0.54 |
| 2:B:870:TYR:CE2 | 2:B:983:SER:OG | 2.59 | 0.54 |
| 2:D:579:PRO:C | 2:D:581:SER:H | 2.10 | 0.54 |
| 2:F:583:ILE:O | 2:F:586:LYS:HE3 | 2.08 | 0.54 |
| 1:C:1053:GLU:O | 1:C:1053:GLU:HG3 | 2.07 | 0.54 |
| 1:A:448:ILE:O | 1:A:449:ASN:C | 2.45 | 0.54 |
| 2:F:269:TYR:CE2 | 2:F:288:GLU:HA | 2.43 | 0.54 |
| 1:C:1150:ILE:HG22 | 1:C:1162:LEU:HD12 | 1.88 | 0.54 |
| 2:B:1072:GLN:O | 2:B:1075:ASP:HB2 | 2.07 | 0.54 |
| 1:E:480:ALA:N | 1:E:481:PRO:HD3 | 2.23 | 0.54 |
| 2:B:545:SER:HA | 2:B:550:ASP:N | 2.21 | 0.54 |
| 1:A:236:GLN:HB3 | 1:A:241:ILE:CD1 | 2.37 | 0.54 |
| 1:A:1131:ARG:HD2 | 1:A:1131:ARG:C | 2.27 | 0.54 |
| 2:D:429:ILE:HG22 | 2:D:429:ILE:O | 2.08 | 0.54 |
| 1:A:1163:TYR:O | 1:A:1175:ILE:HG23 | 2.06 | 0.54 |
| 1:E:1150:ILE:HG22 | 1:E:1162:LEU:HD12 | 1.88 | 0.54 |
| 1:E:448:ILE:O | 1:E:449:ASN:C | 2.45 | 0.54 |
| 1:C:1131:ARG:C | 1:C:1131:ARG:HD2 | 2.28 | 0.54 |
| 1:C:309:LEU:CD2 | 1:C:319:VAL:HG12 | 2.37 | 0.54 |
| 1:E:899:ASN:OD1 | 1:E:1028:ASN:HB3 | 2.07 | 0.54 |
| 2:B:429:ILE:HG22 | 2:B:429:ILE:O | 2.07 | 0.54 |
| 1:E:427:ILE:HG22 | 1:E:428:GLU:N | 2.23 | 0.54 |
| 1:A:416:VAL:HG13 | 1:A:420:GLY:N | 2.23 | 0.54 |
| 1:E:309:LEU:CD2 | 1:E:319:VAL:HG12 | 2.36 | 0.54 |
| 1:E:987:ILE:C | 1:E:989:LYS:H | 2.10 | 0.54 |
| 1:A:227:ILE:CD1 | 1:A:271:ILE:HA | 2.38 | 0.54 |
| 1:E:737:LYS:O | 1:E:738:TYR:O | 2.25 | 0.54 |
| 1:C:737:LYS:O | 1:C:738:TYR:O | 2.24 | 0.54 |
| 1:C:568:GLN:O | 1:C:569:ALA:CB | 2.56 | 0.54 |
| 2:F:502:ASN:O | 2:F:506:ASP:N | 2.38 | 0.54 |
| 1:A:892:ASN:N | 1:A:892:ASN:OD1 | 2.40 | 0.54 |
| 1:A:278:ASP:OD1 | 1:A:278:ASP:N | 2.40 | 0.54 |
| 1:A:1155:SER:O | 1:A:1156:LYS:C | 2.47 | 0.54 |
| 2:F:526:TRP:CZ2 | 2:F:530:ILE:HD11 | 2.42 | 0.54 |
| 2:B:14:ASP:OD1 | 2:B:16:LYS:N | 2.41 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:755:ILE:CG2 | 2:D:759:GLU:HB2 | 2.37 | 0.54 |
| 2:B:574:PHE:C | 2:B:574:PHE:CD2 | 2.81 | 0.54 |
| 2:B:615:LEU:HB3 | 2:B:767:ASN:ND2 | 2.23 | 0.54 |
| 2:F:742:ASN:HA | 2:F:745:THR:HG22 | 1.90 | 0.54 |
| 1:C:242:THR:HG22 | 1:C:435:PHE:O | 2.08 | 0.54 |
| 2:D:239:ASP:OD2 | 2:D:318:TYR:N | 2.41 | 0.54 |
| 1:E:857:TYR:OH | 1:E:860:ASP:HA | 2.07 | 0.54 |
| 2:F:856:ASN:HB3 | 2:F:859:PHE:HE2 | 1.72 | 0.54 |
| 1:A:857:TYR:OH | 1:A:860:ASP:HA | 2.08 | 0.54 |
| 1:A:443:TYR:CD1 | 1:A:444:ASN:N | 2.75 | 0.54 |
| 2:B:863:LEU:HD23 | 2:B:864:THR:HG23 | 1.90 | 0.54 |
| 2:B:727:TYR:N | 2:B:728:PRO:HD2 | 2.23 | 0.54 |
| 1:A:111:ASN:HA | 1:A:147:ASN:OD1 | 2.08 | 0.54 |
| 2:F:502:ASN:O | 2:F:506:ASP:HB2 | 2.08 | 0.54 |
| 2:D:1015:LEU:HB2 | 2:D:1071:VAL:HB | 1.90 | 0.54 |
| 1:C:297:ASN:N | 1:C:298:PRO:CD | 2.71 | 0.53 |
| 1:A:610:LEU:HD11 | 1:A:704:MET:HE2 | 1.90 | 0.53 |
| 1:C:86:ILE:HG13 | 1:C:364:LEU:HD21 | 1.90 | 0.53 |
| 2:B:153:TYR:HD2 | 2:B:165:MET:HB2 | 1.73 | 0.53 |
| 2:B:245:THR:O | 2:B:247:PRO:C | 2.46 | 0.53 |
| 1:E:605:TYR:O | 1:E:605:TYR:CD1 | 2.61 | 0.53 |
| 2:D:273:ILE:O | 2:D:276:ASN:HB3 | 2.08 | 0.53 |
| 1:C:289:VAL:HB | 1:C:290:GLN:CB | 2.38 | 0.53 |
| 1:A:738:TYR:O | 1:A:739:ASP:C | 2.44 | 0.53 |
| 2:B:859:PHE:CD1 | 2:B:968:ILE:HD12 | 2.43 | 0.53 |
| 1:C:480:ALA:N | 1:C:481:PRO:HD3 | 2.23 | 0.53 |
| 2:F:254:TYR:O | 2:F:258:THR:HG22 | 2.08 | 0.53 |
| 2:F:23:SER:OG | 2:F:29:PHE:HB2 | 2.07 | 0.53 |
| 2:F:755:ILE:CG2 | 2:F:759:GLU:HB2 | 2.37 | 0.53 |
| 2:D:817:GLY:HA2 | 2:D:826:VAL:HG21 | 1.91 | 0.53 |
| 1:E:289:VAL:HB | 1:E:290:GLN:CB | 2.37 | 0.53 |
| 1:E:38:ASN:HD21 | 1:E:484:SER:CB | 2.20 | 0.53 |
| 2:D:101:LEU:HD11 | 2:D:293:ILE:HD12 | 1.90 | 0.53 |
| 1:E:1083:ASP:N | 1:E:1129:ILE:O | 2.32 | 0.53 |
| 1:A:836:LEU:HD11 | 2:B:945:PHE:CE1 | 2.44 | 0.53 |
| 1:E:45:ARG:HG3 | 1:E:74:LEU:HD23 | 1.89 | 0.53 |
| 1:A:45:ARG:HG3 | 1:A:74:LEU:HD23 | 1.89 | 0.53 |
| 1:C:236:GLN:HB3 | 1:C:241:ILE:CD1 | 2.37 | 0.53 |
| 1:A:1149:TYR:CD1 | 1:A:1183:ARG:HD2 | 2.43 | 0.53 |
| 2:B:755:ILE:CG2 | 2:B:759:GLU:HB2 | 2.37 | 0.53 |
| 1:A:606:ILE:HD13 | 1:A:761:PHE:CE2 | 2.43 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:547:GLU:HB2 | 1:A:550:LYS:HG3 | 1.90 | 0.53 |
| 1:E:597:ALA:HB2 | 2:F:939:LYS:HB3 | 1.90 | 0.53 |
| 2:F:694:ASN:O | 2:F:697:ARG:HD2 | 2.08 | 0.53 |
| 1:C:447:ASN:OD1 | 1:C:447:ASN:N | 2.40 | 0.53 |
| 2:D:269:TYR:CE1 | 2:D:287:LEU:HB3 | 2.44 | 0.53 |
| 2:F:859:PHE:CD1 | 2:F:968:ILE:HD12 | 2.43 | 0.53 |
| 2:D:574:PHE:CD2 | 2:D:574:PHE:C | 2.81 | 0.53 |
| 2:D:206:ASN:ND2 | 2:D:208:ASN:HB2 | 2.23 | 0.53 |
| 1:E:382:VAL:O | 1:E:382:VAL:HG13 | 2.08 | 0.53 |
| 2:F:817:GLY:HA2 | 2:F:826:VAL:HG21 | 1.91 | 0.53 |
| 1:A:297:ASN:N | 1:A:298:PRO:CD | 2.70 | 0.53 |
| 1:C:111:ASN:HA | 1:C:147:ASN:OD1 | 2.09 | 0.53 |
| 1:C:227:ILE:CD1 | 1:C:271:ILE:HA | 2.39 | 0.53 |
| 2:F:544:ILE:HD13 | 2:F:575:LYS:HG2 | 1.91 | 0.53 |
| 2:D:277:ASN:HB3 | 2:D:281:ASN:CB | 2.39 | 0.53 |
| 2:F:895:TRP:O | 2:F:896:GLU:HG2 | 2.08 | 0.53 |
| 1:A:1012:ILE:O | 2:B:779:ILE:HD12 | 2.09 | 0.53 |
| 2:D:1072:GLN:O | 2:D:1075:ASP:HB2 | 2.09 | 0.53 |
| 2:B:554:ILE:CG2 | 2:B:556:TRP:CE2 | 2.92 | 0.53 |
| 2:D:1149:HIS:NE2 | 2:D:1150:ASP:HB3 | 2.24 | 0.53 |
| 2:F:14:ASP:O | 2:F:15:ASN:HB2 | 2.09 | 0.53 |
| 1:A:1083:ASP:N | 1:A:1129:ILE:O | 2.32 | 0.53 |
| 2:D:166:LEU:HD12 | 2:D:196:SER:HB2 | 1.89 | 0.53 |
| 1:C:382:VAL:O | 1:C:382:VAL:HG13 | 2.08 | 0.53 |
| 2:B:254:TYR:O | 2:B:258:THR:HG22 | 2.08 | 0.53 |
| 2:D:694:ASN:O | 2:D:697:ARG:HD2 | 2.09 | 0.53 |
| 2:F:206:ASN:ND2 | 2:F:208:ASN:HB2 | 2.24 | 0.53 |
| 1:C:1149:TYR:CD1 | 1:C:1183:ARG:HD2 | 2.44 | 0.53 |
| 1:C:1174:THR:HA | 1:C:1220:VAL:HG12 | 1.90 | 0.53 |
| 2:B:273:ILE:O | 2:B:276:ASN:HB3 | 2.08 | 0.53 |
| 1:A:568:GLN:O | 1:A:569:ALA:CB | 2.56 | 0.53 |
| 2:D:990:ASN:O | 2:D:991:SER:C | 2.47 | 0.53 |
| 1:E:738:TYR:O | 1:E:739:ASP:C | 2.47 | 0.53 |
| 2:B:428:LYS:C | 2:B:430:PRO:HD2 | 2.29 | 0.53 |
| 2:D:822:LYS:O | 2:D:824:THR:N | 2.41 | 0.53 |
| 2:B:239:ASP:OD2 | 2:B:318:TYR:N | 2.41 | 0.53 |
| 2:B:227:LEU:HD11 | 2:B:231:ASP:HB2 | 1.91 | 0.53 |
| 2:F:273:ILE:O | 2:F:276:ASN:HB3 | 2.08 | 0.53 |
| 1:C:605:TYR:O | 1:C:605:TYR:CD1 | 2.61 | 0.53 |
| 2:B:534:TYR:CE1 | 2:B:538:ILE:HD12 | 2.44 | 0.53 |
| 2:F:1017:TYR:O | 2:F:1018:ASN:CB | 2.57 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:551:THR:HG21 | 2:D:716:ASN:HB3 | 1.91 | 0.53 |
| 1:A:274:ASN:HA | 1:A:277:ASN:ND2 | 2.25 | 0.53 |
| 2:D:1093:THR:HG22 | 2:D:1097:ARG:O | 2.08 | 0.53 |
| 1:C:45:ARG:HG3 | 1:C:74:LEU:HD23 | 1.90 | 0.53 |
| 1:E:467:ASP:OD1 | 1:E:468:LEU:N | 2.42 | 0.53 |
| 1:A:823:ILE:HG23 | 1:A:824:PRO:HD2 | 1.91 | 0.53 |
| 2:D:863:LEU:HD23 | 2:D:864:THR:HG23 | 1.91 | 0.53 |
| 2:B:583:ILE:O | 2:B:586:LYS:HE3 | 2.09 | 0.53 |
| 1:A:467:ASP:OD1 | 1:A:468:LEU:N | 2.42 | 0.52 |
| 2:B:101:LEU:HD11 | 2:B:293:ILE:HD12 | 1.90 | 0.52 |
| 2:F:1015:LEU:HB2 | 2:F:1071:VAL:HB | 1.90 | 0.52 |
| 1:A:1108:ILE:O | 1:A:1110:ASN:N | 2.42 | 0.52 |
| 1:C:682:TYR:CE2 | 1:C:825:PHE:HA | 2.45 | 0.52 |
| 1:E:1053:GLU:O | 1:E:1053:GLU:HG3 | 2.07 | 0.52 |
| 1:E:289:VAL:HB | 1:E:290:GLN:HB3 | 1.90 | 0.52 |
| 2:D:21:VAL:CG1 | 2:D:22:ARG:N | 2.72 | 0.52 |
| 2:B:858:TYR:OH | 2:B:866:ASN:O | 2.27 | 0.52 |
| 1:A:38:ASN:HD21 | 1:A:484:SER:HB2 | 1.74 | 0.52 |
| 1:C:38:ASN:HD21 | 1:C:484:SER:CB | 2.23 | 0.52 |
| 2:D:583:ILE:O | 2:D:586:LYS:HE3 | 2.08 | 0.52 |
| 1:E:34:ASN:HB2 | 1:E:40:TRP:CH2 | 2.44 | 0.52 |
| 1:A:209:THR:O | 1:A:212:HIS:HB3 | 2.09 | 0.52 |
| 1:C:273:THR:O | 1:C:276:LEU:N | 2.42 | 0.52 |
| 1:C:443:TYR:CD1 | 1:C:444:ASN:N | 2.76 | 0.52 |
| 1:E:1174:THR:HA | 1:E:1220:VAL:HG12 | 1.92 | 0.52 |
| 2:D:40:TRP:O | 2:D:137:VAL:HA | 2.09 | 0.52 |
| 2:B:81:ALA:O | 2:B:82:THR:C | 2.47 | 0.52 |
| 1:C:1108:ILE:O | 1:C:1110:ASN:N | 2.43 | 0.52 |
| 2:F:568:ASN:OD1 | 2:F:569:SER:N | 2.42 | 0.52 |
| 2:D:254:TYR:O | 2:D:258:THR:HG22 | 2.09 | 0.52 |
| 2:F:552:LYS:HB2 | 2:F:713:PHE:CE1 | 2.44 | 0.52 |
| 1:E:443:TYR:CD1 | 1:E:444:ASN:N | 2.77 | 0.52 |
| 2:F:14:ASP:OD1 | 2:F:16:LYS:N | 2.42 | 0.52 |
| 1:A:632:ILE:HG23 | 1:A:633:LEU:N | 2.24 | 0.52 |
| 1:E:480:ALA:N | 1:E:481:PRO:CD | 2.73 | 0.52 |
| 1:E:1092:LEU:O | 1:E:1094:PRO:HD3 | 2.08 | 0.52 |
| 2:F:166:LEU:HD12 | 2:F:196:SER:HB2 | 1.90 | 0.52 |
| 1:A:818:THR:O | 1:A:819:LEU:HG | 2.09 | 0.52 |
| 2:F:574:PHE:CD2 | 2:F:574:PHE:C | 2.82 | 0.52 |
| 2:D:502:ASN:O | 2:D:506:ASP:HB2 | 2.09 | 0.52 |
| 1:A:382:VAL:HG13 | 1:A:382:VAL:O | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1053:GLU:HG3 | 1:A:1053:GLU:O | 2.09 | 0.52 |
| 2:B:421:VAL:HG12 | 2:B:421:VAL:O | 2.09 | 0.52 |
| 1:A:462:ASN:CB | 1:A:463:ASN:HA | 2.38 | 0.52 |
| 1:E:242:THR:HG22 | 1:E:435:PHE:O | 2.10 | 0.52 |
| 1:C:289:VAL:HB | 1:C:290:GLN:HB3 | 1.90 | 0.52 |
| 1:E:836:LEU:CB | 2:F:995:LEU:HD11 | 2.40 | 0.52 |
| 1:A:86:ILE:HG13 | 1:A:364:LEU:HD21 | 1.92 | 0.52 |
| 1:A:273:THR:O | 1:A:276:LEU:N | 2.42 | 0.52 |
| 2:F:1137:ASN:CB | 2:F:1142:TRP:HE1 | 2.22 | 0.52 |
| 1:E:738:TYR:HA | 1:E:743:ILE:CG1 | 2.38 | 0.52 |
| 2:F:21:VAL:CG1 | 2:F:121:ASN:HA | 2.39 | 0.52 |
| 1:E:705:TYR:HD1 | 1:E:705:TYR:C | 2.13 | 0.52 |
| 1:C:944:ARG:CG | 1:C:1026:SER:HA | 2.39 | 0.52 |
| 2:D:727:TYR:N | 2:D:728:PRO:HD2 | 2.25 | 0.52 |
| 2:B:1093:THR:HG22 | 2:B:1097:ARG:O | 2.09 | 0.52 |
| 2:B:21:VAL:CG1 | 2:B:22:ARG:N | 2.73 | 0.52 |
| 1:E:1131:ARG:HD2 | 1:E:1131:ARG:C | 2.30 | 0.52 |
| 1:A:205:ASP:OD1 | 1:A:206:PRO:HD2 | 2.10 | 0.52 |
| 1:A:1174:THR:HA | 1:A:1220:VAL:HG12 | 1.90 | 0.52 |
| 1:A:899:ASN:OD1 | 1:A:1028:ASN:HB3 | 2.09 | 0.52 |
| 2:D:411:HIS:HA | 2:D:624:PHE:HE1 | 1.74 | 0.52 |
| 2:D:421:VAL:HG12 | 2:D:421:VAL:O | 2.10 | 0.52 |
| 2:B:1137:ASN:CB | 2:B:1142:TRP:HE1 | 2.20 | 0.52 |
| 1:A:199:ILE:HA | 1:A:705:TYR:CE2 | 2.39 | 0.52 |
| 1:E:481:PRO:HG2 | 1:E:483:LEU:HD21 | 1.92 | 0.52 |
| 2:D:1017:TYR:O | 2:D:1018:ASN:CB | 2.57 | 0.52 |
| 2:B:251:ILE:O | 2:B:252:ASP:CB | 2.58 | 0.52 |
| 1:C:987:ILE:C | 1:C:989:LYS:H | 2.13 | 0.52 |
| 2:F:863:LEU:HD23 | 2:F:864:THR:HG23 | 1.92 | 0.52 |
| 2:F:1093:THR:HG22 | 2:F:1097:ARG:O | 2.09 | 0.52 |
| 1:A:738:TYR:HA | 1:A:743:ILE:CG1 | 2.40 | 0.52 |
| 2:F:277:ASN:HB3 | 2:F:281:ASN:CB | 2.39 | 0.52 |
| 1:C:209:THR:O | 1:C:212:HIS:HB3 | 2.10 | 0.52 |
| 1:E:209:THR:O | 1:E:212:HIS:HB3 | 2.10 | 0.52 |
| 1:C:41:ILE:HG22 | 1:C:150:ILE:HB | 1.92 | 0.52 |
| 1:C:1155:SER:O | 1:C:1156:LYS:C | 2.49 | 0.51 |
| 2:F:822:LYS:O | 2:F:824:THR:N | 2.42 | 0.51 |
| 1:E:462:ASN:CB | 1:E:463:ASN:HA | 2.39 | 0.51 |
| 2:F:722:PHE:HA | 2:F:726:ILE:HD12 | 1.92 | 0.51 |
| 2:D:571:VAL:O | 2:D:574:PHE:HB3 | 2.10 | 0.51 |
| 1:C:682:TYR:CD2 | 1:C:825:PHE:HD1 | 2.28 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:82:ARG:HG3 | 1:E:364:LEU:HD11 | 1.92 | 0.51 |
| 2:F:534:TYR:CE1 | 2:F:538:ILE:HD12 | 2.45 | 0.51 |
| 2:F:41:ILE:HG22 | 2:F:138:ILE:HB | 1.92 | 0.51 |
| 2:B:1140:TYR:CE2 | 2:B:1142:TRP:CD2 | 2.98 | 0.51 |
| 1:A:854:ASN:CB | 1:A:865:THR:HG22 | 2.40 | 0.51 |
| 1:A:1143:ARG:CG | 1:A:1143:ARG:HH21 | 2.23 | 0.51 |
| 1:E:568:GLN:O | 1:E:569:ALA:CB | 2.58 | 0.51 |
| 1:E:297:ASN:N | 1:E:298:PRO:CD | 2.73 | 0.51 |
| 2:B:151:ILE:HD11 | 2:B:167:GLU:HB2 | 1.91 | 0.51 |
| 2:D:534:TYR:CE1 | 2:D:538:ILE:HD12 | 2.44 | 0.51 |
| 2:F:421:VAL:O | 2:F:421:VAL:HG12 | 2.10 | 0.51 |
| 1:E:1155:SER:O | 1:E:1156:LYS:C | 2.48 | 0.51 |
| 1:A:1025:VAL:CG1 | 1:A:1026:SER:N | 2.73 | 0.51 |
| 1:A:392:ASN:O | 1:A:395:ILE:HG12 | 2.10 | 0.51 |
| 2:D:14:ASP:OD1 | 2:D:16:LYS:N | 2.43 | 0.51 |
| 2:D:502:ASN:O | 2:D:506:ASP:N | 2.41 | 0.51 |
| 1:C:205:ASP:OD1 | 1:C:206:PRO:HD2 | 2.10 | 0.51 |
| 2:D:88:ARG:NE | 2:D:339:TYR:OH | 2.43 | 0.51 |
| 2:F:88:ARG:NE | 2:F:339:TYR:OH | 2.43 | 0.51 |
| 1:C:855:MET:C | 1:C:856:ARG:HD3 | 2.31 | 0.51 |
| 1:A:166:SER:HB3 | 1:A:498:ILE:HB | 1.92 | 0.51 |
| 1:E:67:SER:HA | 1:E:158:PHE:CD2 | 2.46 | 0.51 |
| 1:A:376:ASN:HB3 | 1:A:381:LYS:HA | 1.92 | 0.51 |
| 2:B:923:ILE:O | 2:B:925:ASN:N | 2.33 | 0.51 |
| 1:E:227:ILE:CD1 | 1:E:271:ILE:HA | 2.40 | 0.51 |
| 1:C:1025:VAL:HG12 | 1:C:1026:SER:N | 2.25 | 0.51 |
| 2:B:262:PHE:CZ | 2:B:293:ILE:O | 2.63 | 0.51 |
| 1:E:38:ASN:HD21 | 1:E:484:SER:HB2 | 1.76 | 0.51 |
| 2:B:1017:TYR:O | 2:B:1018:ASN:CB | 2.59 | 0.51 |
| 2:B:1042:ILE:O | 2:B:1099:GLN:HA | 2.11 | 0.51 |
| 2:F:21:VAL:CG1 | 2:F:22:ARG:N | 2.73 | 0.51 |
| 2:F:858:TYR:OH | 2:F:866:ASN:O | 2.29 | 0.51 |
| 1:C:215:ILE:HG22 | 1:C:219:HIS:CE1 | 2.45 | 0.51 |
| 1:A:857:TYR:HA | 1:A:862:TYR:HA | 1.93 | 0.51 |
| 2:B:277:ASN:HB3 | 2:B:281:ASN:CB | 2.39 | 0.51 |
| 1:C:376:ASN:HB3 | 1:C:381:LYS:HA | 1.93 | 0.51 |
| 1:C:363:LEU:HD21 | 1:C:375:TYR:OH | 2.10 | 0.51 |
| 2:B:817:GLY:HA2 | 2:B:826:VAL:HG21 | 1.92 | 0.51 |
| 2:B:14:ASP:O | 2:B:15:ASN:HB2 | 2.11 | 0.51 |
| 1:C:462:ASN:CB | 1:C:463:ASN:HA | 2.40 | 0.51 |
| 1:E:273:THR:O | 1:E:276:LEU:N | 2.44 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:682:TYR:CD2 | 1:E:825:PHE:HD1 | 2.29 | 0.51 |
| 1:C:220:GLY:CA | 1:C:225:LYS:HE3 | 2.41 | 0.51 |
| 2:D:872:TRP:HB2 | 2:D:980:GLU:HB3 | 1.92 | 0.51 |
| 1:E:972:LYS:HB2 | 2:F:772:LEU:HD21 | 1.93 | 0.51 |
| 2:D:251:ILE:O | 2:D:252:ASP:CB | 2.59 | 0.51 |
| 2:B:22:ARG:HD2 | 2:B:27:ASP:O | 2.11 | 0.51 |
| 2:F:1022:GLU:HG2 | 2:F:1023:LEU:N | 2.25 | 0.51 |
| 1:E:144:LEU:HA | 1:E:487:LYS:HA | 1.93 | 0.51 |
| 1:E:823:ILE:HG23 | 1:E:824:PRO:HD2 | 1.92 | 0.51 |
| 2:D:9:ILE:O | 2:D:10:ASP:C | 2.49 | 0.51 |
| 1:C:480:ALA:N | 1:C:481:PRO:CD | 2.74 | 0.51 |
| 1:E:86:ILE:HG13 | 1:E:364:LEU:HD21 | 1.93 | 0.51 |
| 2:B:154:LYS:HD3 | 2:B:157:TYR:CE2 | 2.45 | 0.51 |
| 2:F:482:LEU:HD22 | 2:F:499:SER:HB3 | 1.93 | 0.51 |
| 1:A:113:TYR:HB3 | 1:A:178:PHE:HB3 | 1.93 | 0.51 |
| 1:C:392:ASN:O | 1:C:395:ILE:HG12 | 2.10 | 0.51 |
| 2:D:1122:LEU:HD21 | 2:D:1158:TRP:HZ2 | 1.75 | 0.51 |
| 2:F:428:LYS:C | 2:F:430:PRO:HD2 | 2.31 | 0.51 |
| 2:D:859:PHE:CD1 | 2:D:968:ILE:HD12 | 2.46 | 0.51 |
| 2:F:763:LEU:HA | 2:F:766:GLN:HB2 | 1.92 | 0.51 |
| 1:A:481:PRO:HG2 | 1:A:483:LEU:HD21 | 1.93 | 0.51 |
| 1:C:854:ASN:CB | 1:C:865:THR:HG22 | 2.41 | 0.51 |
| 2:B:1007:ILE:HG22 | 2:B:1015:LEU:HD12 | 1.93 | 0.51 |
| 1:C:547:GLU:HB2 | 1:C:550:LYS:HG3 | 1.92 | 0.51 |
| 1:E:363:LEU:HD21 | 1:E:375:TYR:OH | 2.11 | 0.51 |
| 2:B:146:ILE:HD13 | 2:B:330:TYR:CZ | 2.46 | 0.51 |
| 2:F:81:ALA:O | 2:F:82:THR:C | 2.48 | 0.51 |
| 1:C:47:VAL:O | 1:C:47:VAL:HG12 | 2.11 | 0.51 |
| 2:F:824:THR:HA | 2:F:856:ASN:HB2 | 1.92 | 0.50 |
| 1:C:143:ILE:HG22 | 1:C:144:LEU:N | 2.26 | 0.50 |
| 2:F:101:LEU:HD11 | 2:F:293:ILE:HD12 | 1.93 | 0.50 |
| 2:B:9:ILE:O | 2:B:11:SER:N | 2.44 | 0.50 |
| 2:B:153:TYR:CD2 | 2:B:165:MET:HB2 | 2.45 | 0.50 |
| 2:B:583:ILE:HG23 | 2:B:644:GLN:NE2 | 2.26 | 0.50 |
| 2:F:571:VAL:O | 2:F:574:PHE:HB3 | 2.11 | 0.50 |
| 2:D:568:ASN:OD1 | 2:D:569:SER:N | 2.43 | 0.50 |
| 1:A:1087:TYR:N | 1:A:1243:ILE:O | 2.45 | 0.50 |
| 1:E:1108:ILE:O | 1:E:1110:ASN:N | 2.44 | 0.50 |
| 1:A:363:LEU:HD21 | 1:A:375:TYR:OH | 2.11 | 0.50 |
| 1:C:1093:LYS:HB3 | 1:C:1096:ASN:HB2 | 1.91 | 0.50 |
| 2:B:568:ASN:OD1 | 2:B:569:SER:N | 2.44 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:154:GLU:CB | 1:C:155:PRO:HD2 | 2.41 | 0.50 |
| 1:A:215:ILE:HG22 | 1:A:219:HIS:CE1 | 2.46 | 0.50 |
| 2:F:9:ILE:O | 2:F:10:ASP:C | 2.49 | 0.50 |
| 1:E:143:ILE:HG22 | 1:E:144:LEU:N | 2.26 | 0.50 |
| 2:B:9:ILE:O | 2:B:10:ASP:C | 2.49 | 0.50 |
| 1:C:475:PHE:C | 2:D:1136:LYS:HE2 | 2.31 | 0.50 |
| 2:F:154:LYS:HD3 | 2:F:157:TYR:CE2 | 2.47 | 0.50 |
| 1:E:291:VAL:HA | 1:E:292:SER:HB2 | 1.93 | 0.50 |
| 2:B:347:GLY:O | 2:B:351:THR:HB | 2.11 | 0.50 |
| 1:C:632:ILE:HG23 | 1:C:633:LEU:N | 2.26 | 0.50 |
| 1:C:836:LEU:HD21 | 2:D:945:PHE:HE1 | 1.75 | 0.50 |
| 2:D:858:TYR:OH | 2:D:866:ASN:O | 2.30 | 0.50 |
| 2:B:1022:GLU:HG2 | 2:B:1023:LEU:N | 2.26 | 0.50 |
| 2:D:1022:GLU:HG2 | 2:D:1023:LEU:N | 2.26 | 0.50 |
| 2:D:544:ILE:HD13 | 2:D:575:LYS:HG2 | 1.92 | 0.50 |
| 1:C:823:ILE:HG23 | 1:C:824:PRO:HD2 | 1.92 | 0.50 |
| 2:B:372:LEU:O | 2:B:379:VAL:HA | 2.11 | 0.50 |
| 1:A:447:ASN:N | 1:A:447:ASN:OD1 | 2.42 | 0.50 |
| 2:F:554:ILE:CG2 | 2:F:556:TRP:CE2 | 2.94 | 0.50 |
| 2:F:1149:HIS:NE2 | 2:F:1150:ASP:HB3 | 2.26 | 0.50 |
| 2:D:269:TYR:CE2 | 2:D:288:GLU:HA | 2.47 | 0.50 |
| 1:E:857:TYR:HA | 1:E:862:TYR:HA | 1.93 | 0.50 |
| 2:D:888:SER:HB3 | 2:D:968:ILE:HG12 | 1.94 | 0.50 |
| 2:F:262:PHE:CZ | 2:F:293:ILE:O | 2.64 | 0.50 |
| 2:F:151:ILE:HD11 | 2:F:167:GLU:HB2 | 1.94 | 0.50 |
| 2:B:694:ASN:O | 2:B:697:ARG:HD2 | 2.10 | 0.50 |
| 2:B:205:PRO:HD3 | 2:B:230:ILE:HD11 | 1.94 | 0.50 |
| 2:F:22:ARG:HD2 | 2:F:27:ASP:O | 2.11 | 0.50 |
| 1:E:944:ARG:CG | 1:E:1026:SER:HA | 2.41 | 0.50 |
| 1:E:45:ARG:NH1 | 1:E:154:GLU:O | 2.45 | 0.50 |
| 1:A:154:GLU:CB | 1:A:155:PRO:HD2 | 2.42 | 0.50 |
| 1:A:143:ILE:HG22 | 1:A:144:LEU:N | 2.27 | 0.50 |
| 1:A:144:LEU:HA | 1:A:487:LYS:HA | 1.93 | 0.50 |
| 1:C:82:ARG:HG3 | 1:C:364:LEU:HD11 | 1.94 | 0.50 |
| 2:D:277:ASN:HA | 2:D:281:ASN:HA | 1.92 | 0.50 |
| 2:B:482:LEU:HD22 | 2:B:499:SER:HB3 | 1.94 | 0.50 |
| 1:E:1093:LYS:HB3 | 1:E:1096:ASN:HB2 | 1.93 | 0.50 |
| 2:F:923:ILE:O | 2:F:925:ASN:N | 2.37 | 0.50 |
| 1:E:447:ASN:OD1 | 1:E:447:ASN:N | 2.43 | 0.50 |
| 2:D:1137:ASN:CB | 2:D:1142:TRP:HE1 | 2.20 | 0.50 |
| 1:C:795:ASN:OD1 | 1:C:796:TYR:N | 2.44 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:829:SER:C | 1:A:831:THR:H | 2.15 | 0.50 |
| 1:A:661:ASN:HA | 1:A:664:ILE:HG22 | 1.94 | 0.50 |
| 1:E:278:ASP:OD1 | 1:E:278:ASP:N | 2.43 | 0.50 |
| 1:A:836:LEU:HD21 | 2:B:945:PHE:HE1 | 1.75 | 0.50 |
| 1:C:45:ARG:NH1 | 1:C:154:GLU:O | 2.44 | 0.50 |
| 2:B:9:ILE:HG13 | 2:B:10:ASP:N | 2.27 | 0.50 |
| 2:B:251:ILE:O | 2:B:252:ASP:HB2 | 2.12 | 0.50 |
| 1:C:34:ASN:HB2 | 1:C:40:TRP:CH2 | 2.47 | 0.50 |
| 1:E:661:ASN:HA | 1:E:664:ILE:HG22 | 1.93 | 0.50 |
| 1:C:1143:ARG:CG | 1:C:1143:ARG:HH21 | 2.24 | 0.50 |
| 1:E:1025:VAL:HG12 | 1:E:1026:SER:N | 2.27 | 0.50 |
| 1:E:836:LEU:HD21 | 2:F:945:PHE:HE1 | 1.76 | 0.50 |
| 1:C:738:TYR:HA | 1:C:743:ILE:CG1 | 2.42 | 0.50 |
| 2:F:1008:ARG:HA | 2:F:1014:ILE:HA | 1.94 | 0.50 |
| 1:A:45:ARG:NH1 | 1:A:154:GLU:O | 2.45 | 0.50 |
| 2:D:262:PHE:CZ | 2:D:293:ILE:O | 2.65 | 0.50 |
| 1:E:989:LYS:HG2 | 1:E:1076:TRP:HA | 1.94 | 0.50 |
| 2:F:92:ASN:HB3 | 2:F:310:PHE:CZ | 2.46 | 0.50 |
| 1:A:90:ILE:O | 1:A:93:ARG:HB3 | 2.12 | 0.50 |
| 1:E:818:THR:O | 1:E:819:LEU:HG | 2.12 | 0.50 |
| 2:F:551:THR:HG21 | 2:F:716:ASN:HB3 | 1.94 | 0.50 |
| 1:C:113:TYR:HB3 | 1:C:178:PHE:HB3 | 1.93 | 0.50 |
| 2:B:436:ASP:CA | 2:B:437:ILE:HB | 2.25 | 0.50 |
| 2:D:1140:TYR:CE2 | 2:D:1142:TRP:CD2 | 3.00 | 0.50 |
| 2:F:277:ASN:HA | 2:F:281:ASN:HA | 1.93 | 0.50 |
| 1:A:82:ARG:HG3 | 1:A:364:LEU:HD11 | 1.94 | 0.50 |
| 1:A:242:THR:HG22 | 1:A:435:PHE:O | 2.11 | 0.50 |
| 1:A:46:ASN:OD1 | 1:A:151:MET:HG3 | 2.12 | 0.50 |
| 2:D:658:ALA:O | 2:D:662:LEU:HG | 2.12 | 0.50 |
| 1:A:573:VAL:HA | 1:A:576:ILE:HD12 | 1.94 | 0.50 |
| 1:A:897:GLU:CG | 1:A:1032:LYS:HD3 | 2.42 | 0.49 |
| 1:A:897:GLU:HG2 | 1:A:1032:LYS:CB | 2.38 | 0.49 |
| 2:F:990:ASN:O | 2:F:991:SER:C | 2.50 | 0.49 |
| 2:D:877:LYS:HB3 | 2:D:878:GLN:CB | 2.42 | 0.49 |
| 2:D:9:ILE:HG21 | 2:D:76:ASP:HB2 | 1.94 | 0.49 |
| 2:D:9:ILE:O | 2:D:11:SER:N | 2.45 | 0.49 |
| 2:B:763:LEU:HA | 2:B:766:GLN:HB2 | 1.94 | 0.49 |
| 2:D:482:LEU:HD22 | 2:D:499:SER:HB3 | 1.93 | 0.49 |
| 1:A:607:GLY:HA2 | 1:A:612:ILE:HG13 | 1.94 | 0.49 |
| 1:A:1090:ASN:HB2 | 1:A:1240:TRP:CZ3 | 2.47 | 0.49 |
| 1:E:41:ILE:HG22 | 1:E:150:ILE:HB | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:21:VAL:HG12 | 2:D:22:ARG:N | 2.26 | 0.49 |
| 2:F:888:SER:HB3 | 2:F:968:ILE:HG12 | 1.94 | 0.49 |
| 2:D:14:ASP:O | 2:D:15:ASN:HB2 | 2.12 | 0.49 |
| 2:F:251:ILE:O | 2:F:252:ASP:CB | 2.60 | 0.49 |
| 2:B:41:ILE:HG22 | 2:B:138:ILE:HB | 1.94 | 0.49 |
| 2:D:388:ASP:N | 2:D:388:ASP:OD1 | 2.42 | 0.49 |
| 1:A:836:LEU:HD13 | 2:B:991:SER:HA | 1.94 | 0.49 |
| 2:D:554:ILE:CG2 | 2:D:556:TRP:CE2 | 2.95 | 0.49 |
| 2:B:888:SER:HB3 | 2:B:968:ILE:HG12 | 1.95 | 0.49 |
| 1:E:547:GLU:HB2 | 1:E:550:LYS:HG3 | 1.94 | 0.49 |
| 1:A:940:ILE:O | 1:A:951:LYS:HA | 2.13 | 0.49 |
| 1:C:705:TYR:C | 1:C:705:TYR:HD1 | 2.12 | 0.49 |
| 2:F:877:LYS:HB3 | 2:F:878:GLN:CB | 2.42 | 0.49 |
| 2:D:824:THR:HA | 2:D:856:ASN:HB2 | 1.94 | 0.49 |
| 1:E:143:ILE:CG2 | 1:E:144:LEU:N | 2.75 | 0.49 |
| 2:F:1007:ILE:HG22 | 2:F:1015:LEU:HD12 | 1.93 | 0.49 |
| 2:D:290:LYS:HG2 | 2:D:290:LYS:O | 2.13 | 0.49 |
| 2:D:347:GLY:O | 2:D:351:THR:HB | 2.13 | 0.49 |
| 2:B:803:LEU:C | 2:B:803:LEU:HD23 | 2.33 | 0.49 |
| 2:B:990:ASN:O | 2:B:991:SER:C | 2.50 | 0.49 |
| 2:D:706:ALA:O | 2:D:709:ASN:HB2 | 2.13 | 0.49 |
| 1:C:38:ASN:HD21 | 1:C:484:SER:HB2 | 1.77 | 0.49 |
| 2:D:827:GLU:O | 2:D:852:ILE:HG23 | 2.12 | 0.49 |
| 1:A:795:ASN:OD1 | 1:A:796:TYR:N | 2.45 | 0.49 |
| 1:C:1188:VAL:CG1 | 1:C:1199:MET:HB2 | 2.43 | 0.49 |
| 1:C:90:ILE:O | 1:C:93:ARG:HB3 | 2.13 | 0.49 |
| 2:D:151:ILE:HD11 | 2:D:167:GLU:HB2 | 1.94 | 0.49 |
| 1:E:607:GLY:HA2 | 1:E:612:ILE:CG1 | 2.42 | 0.49 |
| 2:D:755:ILE:HG23 | 2:D:759:GLU:HB2 | 1.95 | 0.49 |
| 2:B:722:PHE:HA | 2:B:726:ILE:HD12 | 1.93 | 0.49 |
| 2:B:755:ILE:HG23 | 2:B:759:GLU:HB2 | 1.95 | 0.49 |
| 2:B:717:ALA:O | 2:B:721:VAL:HG23 | 2.12 | 0.49 |
| 1:A:41:ILE:HG22 | 1:A:150:ILE:HB | 1.93 | 0.49 |
| 1:A:1093:LYS:HB3 | 1:A:1096:ASN:HB2 | 1.94 | 0.49 |
| 1:C:607:GLY:HA2 | 1:C:612:ILE:HG13 | 1.95 | 0.49 |
| 1:E:166:SER:HB3 | 1:E:498:ILE:HB | 1.94 | 0.49 |
| 2:B:1095:ASN:HB2 | 2:B:1097:ARG:HB2 | 1.95 | 0.49 |
| 1:C:199:ILE:HA | 1:C:705:TYR:CE2 | 2.42 | 0.49 |
| 2:D:22:ARG:HD2 | 2:D:27:ASP:O | 2.12 | 0.49 |
| 2:F:424:GLU:O | 2:F:428:LYS:N | 2.44 | 0.49 |
| 1:A:989:LYS:HG2 | 1:A:1076:TRP:HA | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1122:TYR:HE1 | 1:A:1244:SER:O | 1.95 | 0.49 |
| 2:D:717:ALA:O | 2:D:721:VAL:HG23 | 2.13 | 0.49 |
| 1:A:607:GLY:HA2 | 1:A:612:ILE:CG1 | 2.43 | 0.49 |
| 1:E:607:GLY:HA2 | 1:E:612:ILE:HG13 | 1.95 | 0.49 |
| 2:F:347:GLY:O | 2:F:351:THR:HB | 2.12 | 0.49 |
| 1:E:113:TYR:HB3 | 1:E:178:PHE:HB3 | 1.93 | 0.49 |
| 2:D:41:ILE:HG22 | 2:D:138:ILE:HB | 1.94 | 0.49 |
| 2:B:64:TYR:HE2 | 2:B:363:ILE:HD12 | 1.78 | 0.49 |
| 2:D:154:LYS:HD3 | 2:D:157:TYR:CE2 | 2.47 | 0.49 |
| 2:F:518:ASP:O | 2:F:680:ILE:HD11 | 2.12 | 0.49 |
| 2:D:153:TYR:HD2 | 2:D:165:MET:HB2 | 1.77 | 0.49 |
| 1:C:892:ASN:N | 1:C:892:ASN:OD1 | 2.45 | 0.49 |
| 2:B:806:TYR:O | 2:B:806:TYR:CD1 | 2.65 | 0.49 |
| 2:B:541:THR:O | 2:B:542:GLN:CB | 2.60 | 0.49 |
| 1:E:154:GLU:CB | 1:E:155:PRO:HD2 | 2.40 | 0.49 |
| 1:A:854:ASN:HB2 | 1:A:865:THR:CG2 | 2.43 | 0.49 |
| 1:A:700:ARG:HA | 1:A:703:GLN:HB2 | 1.95 | 0.49 |
| 2:D:23:SER:HB2 | 2:D:47:TYR:CZ | 2.47 | 0.49 |
| 2:F:203:ILE:HG22 | 2:F:254:TYR:OH | 2.12 | 0.49 |
| 2:F:755:ILE:HG23 | 2:F:759:GLU:HB2 | 1.95 | 0.49 |
| 1:E:205:ASP:OD1 | 1:E:206:PRO:HD2 | 2.13 | 0.49 |
| 1:A:34:ASN:HB2 | 1:A:40:TRP:CH2 | 2.48 | 0.49 |
| 2:B:393:THR:OG1 | 2:B:396:ASN:N | 2.46 | 0.49 |
| 1:C:143:ILE:CG2 | 1:C:144:LEU:N | 2.75 | 0.49 |
| 1:C:940:ILE:O | 1:C:951:LYS:HA | 2.12 | 0.49 |
| 2:D:763:LEU:HA | 2:D:766:GLN:HB2 | 1.95 | 0.49 |
| 2:B:872:TRP:HB2 | 2:B:980:GLU:HB3 | 1.94 | 0.49 |
| 1:C:331:LEU:HB2 | 1:C:332:TYR:HD2 | 1.77 | 0.49 |
| 2:B:815:VAL:HG12 | 2:B:816:ILE:N | 2.28 | 0.49 |
| 1:A:143:ILE:CG2 | 1:A:144:LEU:N | 2.76 | 0.49 |
| 2:B:277:ASN:HA | 2:B:281:ASN:HA | 1.94 | 0.49 |
| 2:F:153:TYR:HD2 | 2:F:165:MET:HB2 | 1.77 | 0.49 |
| 1:C:627:LEU:O | 1:E:419:LYS:HG2 | 2.12 | 0.48 |
| 1:C:1025:VAL:CG1 | 1:C:1026:SER:N | 2.76 | 0.48 |
| 1:E:944:ARG:O | 1:E:946:ASN:N | 2.46 | 0.48 |
| 1:C:854:ASN:HB2 | 1:C:865:THR:CG2 | 2.43 | 0.48 |
| 1:C:1108:ILE:CG2 | 1:C:1217:ASP:HA | 2.43 | 0.48 |
| 2:B:1020:THR:HA | 2:B:1059:PHE:O | 2.12 | 0.48 |
| 1:C:879:TYR:O | 1:C:888:PHE:HA | 2.13 | 0.48 |
| 1:C:278:ASP:OD1 | 1:C:278:ASP:N | 2.43 | 0.48 |
| 2:B:877:LYS:HB3 | 2:B:878:GLN:CB | 2.42 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:428:LYS:C | 2:D:430:PRO:HD2 | 2.33 | 0.48 |
| 2:D:251:ILE:O | 2:D:252:ASP:HB2 | 2.13 | 0.48 |
| 1:E:46:ASN:OD1 | 1:E:151:MET:HG3 | 2.12 | 0.48 |
| 1:E:47:VAL:O | 1:E:47:VAL:HG12 | 2.12 | 0.48 |
| 2:D:518:ASP:O | 2:D:680:ILE:HD11 | 2.12 | 0.48 |
| 2:F:658:ALA:O | 2:F:662:LEU:HG | 2.13 | 0.48 |
| 2:F:803:LEU:C | 2:F:803:LEU:HD23 | 2.33 | 0.48 |
| 2:F:207:ASP:OD1 | 2:F:207:ASP:N | 2.46 | 0.48 |
| 2:F:1140:TYR:CE2 | 2:F:1142:TRP:CD2 | 3.02 | 0.48 |
| 2:F:21:VAL:HG12 | 2:F:22:ARG:N | 2.28 | 0.48 |
| 2:B:424:GLU:O | 2:B:428:LYS:N | 2.46 | 0.48 |
| 2:F:9:ILE:O | 2:F:11:SER:N | 2.46 | 0.48 |
| 1:A:480:ALA:N | 1:A:481:PRO:HD3 | 2.29 | 0.48 |
| 1:A:17:THR:HG22 | 1:A:34:ASN:HB3 | 1.94 | 0.48 |
| 2:B:206:ASN:ND2 | 2:B:208:ASN:HB2 | 2.27 | 0.48 |
| 1:A:220:GLY:CA | 1:A:225:LYS:HE3 | 2.43 | 0.48 |
| 1:C:1087:TYR:N | 1:C:1243:ILE:O | 2.46 | 0.48 |
| 1:E:940:ILE:O | 1:E:951:LYS:HA | 2.13 | 0.48 |
| 1:C:818:THR:O | 1:C:819:LEU:HG | 2.13 | 0.48 |
| 1:C:548:GLN:HB2 | 1:C:549:PRO:HD3 | 1.95 | 0.48 |
| 2:D:64:TYR:HE2 | 2:D:363:ILE:HD12 | 1.79 | 0.48 |
| 2:D:1008:ARG:HA | 2:D:1014:ILE:HA | 1.96 | 0.48 |
| 2:B:552:LYS:CB | 2:B:713:PHE:HE1 | 2.26 | 0.48 |
| 1:E:376:ASN:O | 1:E:381:LYS:HB3 | 2.13 | 0.48 |
| 1:E:17:THR:HG22 | 1:E:34:ASN:HB3 | 1.95 | 0.48 |
| 1:C:607:GLY:HA2 | 1:C:612:ILE:CG1 | 2.43 | 0.48 |
| 2:D:372:LEU:O | 2:D:379:VAL:HA | 2.14 | 0.48 |
| 1:C:573:VAL:HA | 1:C:576:ILE:HD12 | 1.95 | 0.48 |
| 1:C:829:SER:C | 1:C:831:THR:H | 2.17 | 0.48 |
| 2:D:552:LYS:CB | 2:D:713:PHE:HE1 | 2.26 | 0.48 |
| 2:D:1007:ILE:HG22 | 2:D:1015:LEU:HD12 | 1.95 | 0.48 |
| 1:E:972:LYS:CB | 2:F:772:LEU:HD11 | 2.44 | 0.48 |
| 2:B:827:GLU:O | 2:B:852:ILE:HG23 | 2.12 | 0.48 |
| 2:F:615:LEU:HB3 | 2:F:767:ASN:ND2 | 2.28 | 0.48 |
| 2:B:402:ILE:HG12 | 2:B:593:LYS:CB | 2.44 | 0.48 |
| 1:A:1212:LEU:O | 1:A:1238:CYS:HA | 2.12 | 0.48 |
| 1:A:936:GLU:HA | 1:A:954:LEU:O | 2.14 | 0.48 |
| 1:C:46:ASN:OD1 | 1:C:151:MET:HG3 | 2.12 | 0.48 |
| 1:E:892:ASN:N | 1:E:892:ASN:OD1 | 2.45 | 0.48 |
| 1:C:231:CYS:CB | 1:C:249:ILE:HD12 | 2.43 | 0.48 |
| 1:E:854:ASN:CB | 1:E:865:THR:HG22 | 2.43 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:E:440:GLU:O | 1:E:443:TYR:CD1 | 2.67 | 0.48 |
| 2:B:502:ASN:O | 2:B:506:ASP:N | 2.42 | 0.48 |
| 2:B:570:PHE:O | 2:B:573:GLU:HB2 | 2.13 | 0.48 |
| 1:C:1122:TYR:HE1 | 1:C:1244:SER:O | 1.97 | 0.48 |
| 1:E:1122:TYR:HE1 | 1:E:1244:SER:O | 1.97 | 0.48 |
| 2:F:570:PHE:O | 2:F:573:GLU:HB2 | 2.14 | 0.48 |
| 1:A:47:VAL:HG12 | 1:A:47:VAL:O | 2.13 | 0.48 |
| 1:E:423:LYS:HD2 | 2:D:510:PHE:CE2 | 2.48 | 0.48 |
| 1:E:700:ARG:HA | 1:E:703:GLN:HB2 | 1.95 | 0.48 |
| 2:F:23:SER:HB2 | 2:F:47:TYR:CZ | 2.49 | 0.48 |
| 1:E:220:GLY:CA | 1:E:225:LYS:HE3 | 2.44 | 0.48 |
| 2:B:518:ASP:O | 2:B:680:ILE:HD11 | 2.13 | 0.48 |
| 1:A:944:ARG:CG | 1:A:1026:SER:HA | 2.42 | 0.48 |
| 1:E:215:ILE:HG22 | 1:E:219:HIS:CE1 | 2.48 | 0.48 |
| 2:B:1122:LEU:HD21 | 2:B:1158:TRP:HZ2 | 1.76 | 0.48 |
| 2:D:153:TYR:CD2 | 2:D:165:MET:HB2 | 2.48 | 0.48 |
| 2:D:1042:ILE:O | 2:D:1099:GLN:HA | 2.13 | 0.48 |
| 1:E:548:GLN:HB2 | 1:E:549:PRO:HD3 | 1.96 | 0.48 |
| 2:F:232:PHE:CZ | 2:F:240:TYR:HA | 2.49 | 0.48 |
| 2:D:1138:GLN:HB3 | 2:D:1139:ASP:C | 2.34 | 0.48 |
| 1:A:291:VAL:HA | 1:A:292:SER:HB2 | 1.95 | 0.48 |
| 1:E:897:GLU:CG | 1:E:1032:LYS:HD3 | 2.44 | 0.48 |
| 1:C:836:LEU:HD13 | 2:D:991:SER:HA | 1.96 | 0.48 |
| 1:A:944:ARG:O | 1:A:946:ASN:N | 2.47 | 0.48 |
| 2:F:15:ASN:OD1 | 2:F:126:LYS:CB | 2.62 | 0.48 |
| 2:B:203:ILE:O | 2:B:203:ILE:HG22 | 2.13 | 0.48 |
| 2:D:615:LEU:HB3 | 2:D:767:ASN:ND2 | 2.29 | 0.48 |
| 2:D:684:ASN:O | 2:D:687:LEU:N | 2.47 | 0.48 |
| 2:F:1020:THR:HA | 2:F:1059:PHE:O | 2.14 | 0.48 |
| 2:F:475:ILE:HG21 | 2:F:497:VAL:HG22 | 1.95 | 0.48 |
| 2:D:146:ILE:HD13 | 2:D:330:TYR:CZ | 2.49 | 0.48 |
| 2:D:1095:ASN:HB2 | 2:D:1097:ARG:HB2 | 1.95 | 0.48 |
| 1:C:944:ARG:O | 1:C:946:ASN:N | 2.47 | 0.48 |
| 2:B:21:VAL:HG12 | 2:B:22:ARG:N | 2.29 | 0.48 |
| 2:B:1008:ARG:HA | 2:B:1014:ILE:HA | 1.96 | 0.48 |
| 2:B:571:VAL:O | 2:B:574:PHE:HB3 | 2.14 | 0.48 |
| 2:B:64:TYR:N | 2:B:64:TYR:CD2 | 2.81 | 0.48 |
| 1:C:661:ASN:HA | 1:C:664:ILE:HG22 | 1.95 | 0.48 |
| 1:C:1088:LEU:HD23 | 1:C:1089:LEU:N | 2.29 | 0.48 |
| 2:F:1042:ILE:O | 2:F:1099:GLN:HA | 2.14 | 0.48 |
| 1:E:1143:ARG:HH21 | 1:E:1143:ARG:CG | 2.26 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:F:815:VAL:HG12 | 2:F:816:ILE:N | 2.29 | 0.47 |
| 2:F:726:ILE:C | 2:F:728:PRO:HD2 | 2.34 | 0.47 |
| 2:F:583:ILE:HG23 | 2:F:644:GLN:NE2 | 2.29 | 0.47 |
| 2:B:203:ILE:HG22 | 2:B:254:TYR:OH | 2.13 | 0.47 |
| 1:C:166:SER:HB3 | 1:C:498:ILE:HB | 1.95 | 0.47 |
| 2:B:232:PHE:CZ | 2:B:240:TYR:HA | 2.49 | 0.47 |
| 2:F:381:MET:HE3 | 2:F:471:GLN:HB3 | 1.95 | 0.47 |
| 1:E:90:ILE:O | 1:E:93:ARG:HB3 | 2.14 | 0.47 |
| 2:D:945:PHE:CD1 | 2:D:950:LEU:HA | 2.49 | 0.47 |
| 2:D:991:SER:O | 2:D:994:ILE:HB | 2.13 | 0.47 |
| 2:F:1122:LEU:HD21 | 2:F:1158:TRP:HZ2 | 1.75 | 0.47 |
| 1:E:682:TYR:CE2 | 1:E:825:PHE:HA | 2.49 | 0.47 |
| 2:F:631:TYR:O | 2:F:634:LEU:HB2 | 2.14 | 0.47 |
| 2:D:205:PRO:HD3 | 2:D:230:ILE:HD11 | 1.96 | 0.47 |
| 1:A:929:LYS:HA | 1:A:932:ASN:HB2 | 1.96 | 0.47 |
| 2:B:551:THR:HG21 | 2:B:716:ASN:HB3 | 1.95 | 0.47 |
| 1:E:879:TYR:O | 1:E:888:PHE:HA | 2.13 | 0.47 |
| 2:B:541:THR:HA | 2:B:553:ILE:O | 2.14 | 0.47 |
| 2:B:554:ILE:HB | 2:B:557:ILE:CD1 | 2.44 | 0.47 |
| 1:E:1025:VAL:CG1 | 1:E:1026:SER:N | 2.78 | 0.47 |
| 2:F:269:TYR:HD1 | 2:F:287:LEU:HD23 | 1.79 | 0.47 |
| 1:E:854:ASN:HB2 | 1:E:865:THR:CG2 | 2.43 | 0.47 |
| 2:F:717:ALA:O | 2:F:721:VAL:HG23 | 2.14 | 0.47 |
| 1:A:270:ASP:O | 1:A:273:THR:HG22 | 2.14 | 0.47 |
| 2:B:402:ILE:HG12 | 2:B:593:LYS:HB2 | 1.96 | 0.47 |
| 1:C:936:GLU:HA | 1:C:954:LEU:O | 2.14 | 0.47 |
| 1:A:138:ASN:ND2 | 1:A:140:SER:OG | 2.47 | 0.47 |
| 2:B:290:LYS:HG2 | 2:B:290:LYS:O | 2.14 | 0.47 |
| 1:E:911:LYS:O | 1:E:999:ARG:NE | 2.47 | 0.47 |
| 2:D:1020:THR:HA | 2:D:1059:PHE:O | 2.14 | 0.47 |
| 2:F:205:PRO:HD3 | 2:F:230:ILE:HD11 | 1.96 | 0.47 |
| 2:F:1095:ASN:HB2 | 2:F:1097:ARG:HB2 | 1.96 | 0.47 |
| 2:D:815:VAL:HG12 | 2:D:816:ILE:N | 2.29 | 0.47 |
| 1:A:203:ILE:HD13 | 1:A:396:ILE:HG21 | 1.96 | 0.47 |
| 1:A:603:VAL:CG1 | 1:A:605:TYR:CE2 | 2.98 | 0.47 |
| 1:C:716:LYS:O | 1:C:719:ILE:HG22 | 2.14 | 0.47 |
| 2:D:192:CYS:O | 2:D:195:LYS:HB3 | 2.14 | 0.47 |
| 1:E:231:CYS:HB2 | 1:E:249:ILE:HD12 | 1.97 | 0.47 |
| 1:A:456:ASP:HA | 1:A:669:ASN:HD21 | 1.79 | 0.47 |
| 1:E:1108:ILE:CG2 | 1:E:1217:ASP:HA | 2.44 | 0.47 |
| 1:C:17:THR:HG22 | 1:C:34:ASN:HB3 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:949:GLY:O | 1:C:963:LEU:HD12 | 2.15 | 0.47 |
| 1:C:138:ASN:ND2 | 1:C:140:SER:OG | 2.47 | 0.47 |
| 2:F:239:ASP:OD2 | 2:F:318:TYR:N | 2.43 | 0.47 |
| 2:D:794:ILE:O | 2:D:795:LYS:C | 2.53 | 0.47 |
| 2:F:827:GLU:O | 2:F:852:ILE:HG23 | 2.14 | 0.47 |
| 2:F:402:ILE:HG12 | 2:F:593:LYS:HB2 | 1.97 | 0.47 |
| 1:E:1087:TYR:N | 1:E:1243:ILE:O | 2.47 | 0.47 |
| 1:A:528:VAL:O | 1:A:528:VAL:HG13 | 2.15 | 0.47 |
| 1:A:855:MET:C | 1:A:856:ARG:HD3 | 2.33 | 0.47 |
| 1:C:897:GLU:CG | 1:C:1032:LYS:HD3 | 2.44 | 0.47 |
| 2:B:991:SER:O | 2:B:994:ILE:HB | 2.15 | 0.47 |
| 2:B:706:ALA:O | 2:B:709:ASN:HB2 | 2.13 | 0.47 |
| 2:D:271:ILE:HG23 | 2:D:272:LYS:N | 2.30 | 0.47 |
| 2:D:424:GLU:O | 2:D:428:LYS:N | 2.47 | 0.47 |
| 1:E:1043:GLY:C | 1:E:1044:ILE:HG13 | 2.35 | 0.47 |
| 2:B:726:ILE:C | 2:B:728:PRO:HD2 | 2.35 | 0.47 |
| 1:A:1229:MET:O | 1:A:1231:ASP:N | 2.48 | 0.47 |
| 1:E:186:PHE:CE2 | 1:E:188:PRO:HB3 | 2.48 | 0.47 |
| 2:B:1138:GLN:HB3 | 2:B:1139:ASP:C | 2.34 | 0.47 |
| 2:F:173:PHE:HA | 2:F:333:ILE:HB | 1.96 | 0.47 |
| 1:A:431:ASN:O | 1:A:434:LEU:HB2 | 2.14 | 0.47 |
| 1:A:912:TYR:O | 1:A:913:LYS:HB3 | 2.15 | 0.47 |
| 1:C:203:ILE:HD13 | 1:C:396:ILE:HG21 | 1.97 | 0.47 |
| 2:F:706:ALA:O | 2:F:709:ASN:HB2 | 2.14 | 0.47 |
| 2:B:269:TYR:HD1 | 2:B:287:LEU:HD23 | 1.79 | 0.47 |
| 2:D:541:THR:HA | 2:D:553:ILE:O | 2.15 | 0.47 |
| 2:F:9:ILE:HG21 | 2:F:76:ASP:HB2 | 1.97 | 0.47 |
| 1:E:633:LEU:O | 1:E:700:ARG:NH2 | 2.45 | 0.47 |
| 2:D:203:ILE:HG22 | 2:D:254:TYR:OH | 2.14 | 0.47 |
| 1:C:376:ASN:O | 1:C:381:LYS:HB3 | 2.15 | 0.47 |
| 1:E:270:ASP:O | 1:E:273:THR:HG22 | 2.15 | 0.47 |
| 1:A:716:LYS:O | 1:A:719:ILE:HG22 | 2.15 | 0.47 |
| 1:A:778:LYS:HA | 1:A:782:LEU:HB2 | 1.96 | 0.47 |
| 2:B:210:ASN:HB3 | 2:B:228:ASP:HA | 1.97 | 0.47 |
| 1:E:829:SER:C | 1:E:831:THR:H | 2.18 | 0.47 |
| 2:F:388:ASP:OD1 | 2:F:388:ASP:N | 2.44 | 0.47 |
| 2:B:1069:GLN:O | 2:B:1070:TYR:CD2 | 2.68 | 0.47 |
| 1:A:548:GLN:HB2 | 1:A:549:PRO:HD3 | 1.96 | 0.47 |
| 1:C:911:LYS:O | 1:C:999:ARG:NE | 2.47 | 0.47 |
| 1:C:291:VAL:HA | 1:C:292:SER:HB2 | 1.97 | 0.47 |
| 2:D:917:ASN:C | 2:D:918:ILE:HG13 | 2.35 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:F:290:LYS:O | 2:F:290:LYS:HG2 | 2.15 | 0.47 |
| 1:A:286:LEU:O | 1:A:287:SER:C | 2.52 | 0.47 |
| 2:B:13:VAL:HG12 | 2:B:14:ASP:H | 1.77 | 0.47 |
| 2:B:185:PRO:O | 2:B:186:ALA:C | 2.53 | 0.47 |
| 1:E:632:ILE:HG23 | 1:E:633:LEU:N | 2.28 | 0.47 |
| 1:C:1092:LEU:HD11 | 1:C:1234:ASN:O | 2.15 | 0.47 |
| 2:F:251:ILE:O | 2:F:252:ASP:HB2 | 2.14 | 0.47 |
| 1:A:231:CYS:HB2 | 1:A:249:ILE:HD12 | 1.97 | 0.47 |
| 2:D:868:SER:HA | 2:D:933:ILE:O | 2.14 | 0.47 |
| 1:E:795:ASN:OD1 | 1:E:796:TYR:N | 2.48 | 0.47 |
| 2:B:876:LEU:HD21 | 2:B:978:TYR:CD2 | 2.50 | 0.47 |
| 2:B:15:ASN:OD1 | 2:B:126:LYS:CB | 2.63 | 0.47 |
| 1:C:857:TYR:HB2 | 1:C:862:TYR:CE1 | 2.50 | 0.47 |
| 2:D:9:ILE:HG13 | 2:D:10:ASP:N | 2.29 | 0.47 |
| 1:E:1092:LEU:HD11 | 1:E:1234:ASN:O | 2.15 | 0.47 |
| 2:B:658:ALA:O | 2:B:662:LEU:HG | 2.14 | 0.47 |
| 1:A:911:LYS:O | 1:A:999:ARG:NE | 2.47 | 0.47 |
| 1:E:331:LEU:HB2 | 1:E:332:TYR:HD2 | 1.80 | 0.47 |
| 2:F:541:THR:HA | 2:F:553:ILE:O | 2.15 | 0.47 |
| 2:F:876:LEU:HD21 | 2:F:978:TYR:CD2 | 2.50 | 0.47 |
| 1:A:942:CYS:SG | 1:A:1025:VAL:CG1 | 3.03 | 0.47 |
| 1:C:231:CYS:HB2 | 1:C:249:ILE:HD12 | 1.97 | 0.47 |
| 1:C:270:ASP:O | 1:C:273:THR:HG22 | 2.15 | 0.47 |
| 2:B:1116:ILE:HG23 | 2:B:1117:PHE:N | 2.29 | 0.47 |
| 1:A:949:GLY:O | 1:A:963:LEU:HD12 | 2.15 | 0.47 |
| 2:B:475:ILE:HG21 | 2:B:497:VAL:HG22 | 1.96 | 0.47 |
| 2:B:305:TYR:CE1 | 2:B:418:LEU:CD1 | 2.97 | 0.47 |
| 1:E:896:SER:C | 1:E:897:GLU:HG3 | 2.35 | 0.46 |
| 2:F:185:PRO:O | 2:F:186:ALA:C | 2.53 | 0.46 |
| 1:A:1132:VAL:HG23 | 1:A:1149:TYR:CE2 | 2.50 | 0.46 |
| 1:A:480:ALA:N | 1:A:481:PRO:CD | 2.78 | 0.46 |
| 2:B:106:ILE:HG22 | 2:B:107:PRO:O | 2.14 | 0.46 |
| 2:F:146:ILE:HD13 | 2:F:330:TYR:CZ | 2.50 | 0.46 |
| 2:B:45:ARG:HG3 | 2:B:141:PRO:O | 2.15 | 0.46 |
| 2:B:155:LYS:O | 2:B:156:GLU:C | 2.54 | 0.46 |
| 1:A:1188:VAL:CG1 | 1:A:1199:MET:HB2 | 2.45 | 0.46 |
| 1:C:535:VAL:HG12 | 1:C:536:ASN:N | 2.30 | 0.46 |
| 2:D:1093:THR:OG1 | 2:D:1094:THR:N | 2.49 | 0.46 |
| 1:E:154:GLU:CB | 1:E:155:PRO:CD | 2.94 | 0.46 |
| 1:C:440:GLU:O | 1:C:443:TYR:CD1 | 2.68 | 0.46 |
| 1:C:470:GLN:HG3 | 2:D:1028:PHE:CE1 | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:D:631:TYR:O | 2:D:634:LEU:HB2 | 2.15 | 0.46 |
| 1:E:824:PRO:HB2 | 2:F:952:ALA:HB2 | 1.97 | 0.46 |
| 1:A:297:ASN:N | 1:A:298:PRO:HD3 | 2.30 | 0.46 |
| 2:D:722:PHE:HA | 2:D:726:ILE:HD12 | 1.96 | 0.46 |
| 2:D:570:PHE:O | 2:D:573:GLU:HB2 | 2.15 | 0.46 |
| 2:D:81:ALA:O | 2:D:82:THR:C | 2.53 | 0.46 |
| 1:A:186:PHE:CE2 | 1:A:188:PRO:HB3 | 2.51 | 0.46 |
| 1:C:1090:ASN:HB2 | 1:C:1240:TRP:CZ3 | 2.50 | 0.46 |
| 1:E:528:VAL:HG13 | 1:E:528:VAL:O | 2.15 | 0.46 |
| 1:E:855:MET:C | 1:E:856:ARG:HD3 | 2.36 | 0.46 |
| 2:D:990:ASN:O | 2:D:993:GLU:N | 2.48 | 0.46 |
| 1:E:920:TRP:HB2 | 1:E:1045:ARG:CD | 2.45 | 0.46 |
| 2:B:567:ASN:O | 2:B:568:ASN:C | 2.53 | 0.46 |
| 1:E:1188:VAL:CG1 | 1:E:1199:MET:HB2 | 2.45 | 0.46 |
| 2:F:45:ARG:HG3 | 2:F:141:PRO:O | 2.15 | 0.46 |
| 1:C:528:VAL:HG13 | 1:C:528:VAL:O | 2.15 | 0.46 |
| 2:F:989:ILE:HG22 | 2:F:990:ASN:N | 2.31 | 0.46 |
| 2:F:867:PHE:CZ | 2:F:935:ILE:HD12 | 2.50 | 0.46 |
| 2:F:859:PHE:HD1 | 2:F:968:ILE:HD12 | 1.80 | 0.46 |
| 1:E:1132:VAL:HG23 | 1:E:1149:TYR:CE2 | 2.50 | 0.46 |
| 1:C:606:ILE:CG2 | 1:C:621:PHE:CE2 | 2.98 | 0.46 |
| 2:B:23:SER:HB2 | 2:B:47:TYR:CZ | 2.50 | 0.46 |
| 1:A:376:ASN:O | 1:A:381:LYS:HB3 | 2.15 | 0.46 |
| 1:C:795:ASN:C | 1:C:795:ASN:OD1 | 2.54 | 0.46 |
| 2:D:106:ILE:HG22 | 2:D:107:PRO:O | 2.15 | 0.46 |
| 2:F:153:TYR:CD2 | 2:F:165:MET:HB2 | 2.50 | 0.46 |
| 1:E:573:VAL:HA | 1:E:576:ILE:HD12 | 1.97 | 0.46 |
| 1:A:785:TYR:O | 1:A:786:ASP:C | 2.53 | 0.46 |
| 1:A:879:TYR:O | 1:A:888:PHE:HA | 2.16 | 0.46 |
| 2:D:846:THR:HG23 | 2:D:847:GLY:N | 2.31 | 0.46 |
| 1:E:345:VAL:HG13 | 1:E:387:GLN:HE22 | 1.81 | 0.46 |
| 1:C:469:ASP:O | 1:C:472:ILE:HB | 2.15 | 0.46 |
| 1:A:453:GLU:C | 1:A:454:ILE:HG22 | 2.36 | 0.46 |
| 2:D:13:VAL:HG12 | 2:D:14:ASP:H | 1.80 | 0.46 |
| 2:F:14:ASP:O | 2:F:15:ASN:CB | 2.64 | 0.46 |
| 2:B:305:TYR:CZ | 2:B:418:LEU:CD1 | 2.99 | 0.46 |
| 2:B:141:PRO:HA | 2:B:169:TRP:HB3 | 1.96 | 0.46 |
| 1:C:571:LEU:O | 1:C:575:TRP:N | 2.42 | 0.46 |
| 2:B:868:SER:HA | 2:B:933:ILE:O | 2.16 | 0.46 |
| 1:A:1088:LEU:HD23 | 1:A:1089:LEU:N | 2.30 | 0.46 |
| 1:A:22:LYS:CG | 1:A:23:PRO:HD2 | 2.45 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:22:LYS:CG | 1:C:23:PRO:HD2 | 2.45 | 0.46 |
| 2:B:192:CYS:O | 2:B:195:LYS:HB3 | 2.15 | 0.46 |
| 2:D:610:ASP:OD1 | 2:D:611:LEU:HD13 | 2.15 | 0.46 |
| 2:F:872:TRP:HB2 | 2:F:980:GLU:HB3 | 1.97 | 0.46 |
| 2:B:989:ILE:HG22 | 2:B:990:ASN:N | 2.30 | 0.46 |
| 2:D:815:VAL:C | 2:D:816:ILE:HG13 | 2.36 | 0.46 |
| 1:E:453:GLU:C | 1:E:454:ILE:HG22 | 2.35 | 0.46 |
| 2:F:271:ILE:HG23 | 2:F:272:LYS:N | 2.30 | 0.46 |
| 2:B:269:TYR:CE2 | 2:B:288:GLU:HA | 2.51 | 0.46 |
| 2:D:203:ILE:HG22 | 2:D:203:ILE:O | 2.16 | 0.46 |
| 1:C:989:LYS:HG2 | 1:C:1076:TRP:HA | 1.97 | 0.46 |
| 1:C:179:GLY:HA2 | 1:C:220:GLY:O | 2.15 | 0.46 |
| 1:E:664:ILE:HG23 | 1:E:665:LYS:N | 2.30 | 0.46 |
| 1:A:179:GLY:HA2 | 1:A:220:GLY:O | 2.15 | 0.46 |
| 2:F:806:TYR:CD1 | 2:F:806:TYR:O | 2.69 | 0.46 |
| 1:C:932:ASN:HA | 1:C:956:HIS:CE1 | 2.51 | 0.46 |
| 2:D:1003:ASN:HB3 | 2:D:1116:ILE:CD1 | 2.46 | 0.46 |
| 1:A:286:LEU:O | 1:A:289:VAL:HG13 | 2.16 | 0.46 |
| 1:C:942:CYS:SG | 1:C:1025:VAL:CG1 | 3.04 | 0.46 |
| 2:D:475:ILE:HG21 | 2:D:497:VAL:HG22 | 1.96 | 0.46 |
| 2:F:991:SER:O | 2:F:994:ILE:HB | 2.16 | 0.46 |
| 1:E:981:ASN:ND2 | 2:F:414:ASN:HB3 | 2.28 | 0.46 |
| 2:F:586:LYS:O | 2:F:641:TYR:CZ | 2.69 | 0.46 |
| 1:E:873:ASN:N | 1:E:899:ASN:O | 2.39 | 0.46 |
| 1:A:231:CYS:CB | 1:A:249:ILE:HD12 | 2.46 | 0.46 |
| 1:E:949:GLY:O | 1:E:963:LEU:HD12 | 2.16 | 0.46 |
| 2:B:207:ASP:N | 2:B:207:ASP:OD1 | 2.48 | 0.46 |
| 1:E:286:LEU:O | 1:E:289:VAL:HG13 | 2.16 | 0.46 |
| 1:E:610:LEU:HD11 | 1:E:704:MET:HE2 | 1.98 | 0.46 |
| 2:B:815:VAL:C | 2:B:816:ILE:HG13 | 2.36 | 0.46 |
| 2:F:554:ILE:HB | 2:F:557:ILE:CD1 | 2.45 | 0.46 |
| 1:E:456:ASP:HA | 1:E:669:ASN:HD21 | 1.80 | 0.46 |
| 2:B:1007:ILE:CG2 | 2:B:1015:LEU:HD12 | 2.46 | 0.46 |
| 1:A:1108:ILE:CG2 | 1:A:1217:ASP:HA | 2.46 | 0.46 |
| 1:A:382:VAL:HG11 | 1:A:868:TYR:CE1 | 2.51 | 0.46 |
| 2:D:726:ILE:C | 2:D:728:PRO:HD2 | 2.36 | 0.46 |
| 2:D:1003:ASN:HB3 | 2:D:1116:ILE:HD13 | 1.97 | 0.46 |
| 2:D:515:LYS:HB3 | 2:D:516:PRO:HD2 | 1.97 | 0.46 |
| 2:B:867:PHE:CZ | 2:B:935:ILE:HD12 | 2.51 | 0.46 |
| 1:A:468:LEU:HD12 | 1:A:471:VAL:HG22 | 1.98 | 0.46 |
| 1:C:297:ASN:N | 1:C:298:PRO:HD3 | 2.31 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:937:TYR:CE1 | 1:A:954:LEU:HB2 | 2.51 | 0.46 |
| 1:E:231:CYS:CB | 1:E:249:ILE:HD12 | 2.45 | 0.46 |
| 2:F:402:ILE:HG12 | 2:F:593:LYS:CB | 2.45 | 0.46 |
| 2:D:173:PHE:HA | 2:D:333:ILE:HB | 1.98 | 0.46 |
| 1:E:1010:ASN:HB3 | 2:F:780:GLN:HG3 | 1.97 | 0.46 |
| 2:F:51:LEU:HB3 | 2:F:66:SER:HA | 1.97 | 0.46 |
| 1:E:1212:LEU:O | 1:E:1238:CYS:HA | 2.16 | 0.46 |
| 2:F:1003:ASN:HB3 | 2:F:1116:ILE:CD1 | 2.46 | 0.46 |
| 2:F:1138:GLN:HB3 | 2:F:1139:ASP:C | 2.36 | 0.46 |
| 1:C:627:LEU:O | 1:E:420:GLY:HA3 | 2.16 | 0.46 |
| 2:D:298:ILE:HA | 2:D:301:LEU:HD12 | 1.98 | 0.46 |
| 1:A:1127:VAL:HG11 | 1:A:1150:ILE:HG23 | 1.97 | 0.46 |
| 2:D:1135:ILE:HG22 | 2:D:1136:LYS:N | 2.31 | 0.46 |
| 1:A:664:ILE:HG23 | 1:A:665:LYS:N | 2.31 | 0.46 |
| 2:F:106:ILE:HG22 | 2:F:107:PRO:O | 2.16 | 0.46 |
| 2:B:610:ASP:OD1 | 2:B:611:LEU:HD13 | 2.16 | 0.46 |
| 1:C:1168:THR:HG22 | 1:C:1170:ASN:H | 1.80 | 0.46 |
| 2:D:806:TYR:CD1 | 2:D:806:TYR:O | 2.69 | 0.46 |
| 1:A:896:SER:C | 1:A:897:GLU:HG3 | 2.36 | 0.45 |
| 2:B:21:VAL:CG1 | 2:B:121:ASN:HA | 2.43 | 0.45 |
| 2:F:298:ILE:HA | 2:F:301:LEU:HD12 | 1.97 | 0.45 |
| 1:A:456:ASP:HA | 1:A:669:ASN:ND2 | 2.31 | 0.45 |
| 1:E:972:LYS:CD | 2:F:772:LEU:HD11 | 2.46 | 0.45 |
| 1:E:972:LYS:HB2 | 2:F:772:LEU:HD11 | 1.98 | 0.45 |
| 1:A:482:GLY:C | 1:A:483:LEU:HG | 2.36 | 0.45 |
| 1:C:664:ILE:HG23 | 1:C:665:LYS:N | 2.31 | 0.45 |
| 2:B:846:THR:HG23 | 2:B:847:GLY:N | 2.31 | 0.45 |
| 1:C:778:LYS:HA | 1:C:782:LEU:HB2 | 1.98 | 0.45 |
| 2:F:868:SER:HA | 2:F:933:ILE:O | 2.16 | 0.45 |
| 1:C:345:VAL:HG13 | 1:C:387:GLN:HE22 | 1.81 | 0.45 |
| 2:B:51:LEU:HB3 | 2:B:66:SER:HA | 1.98 | 0.45 |
| 1:C:897:GLU:HG2 | 1:C:1032:LYS:CB | 2.44 | 0.45 |
| 2:B:1149:HIS:CE1 | 2:B:1150:ASP:CB | 3.00 | 0.45 |
| 2:F:269:TYR:HE2 | 2:F:288:GLU:CG | 2.29 | 0.45 |
| 2:D:269:TYR:HD1 | 2:D:287:LEU:HD23 | 1.81 | 0.45 |
| 2:F:552:LYS:CB | 2:F:713:PHE:HE1 | 2.30 | 0.45 |
| 1:E:606:ILE:CG2 | 1:E:621:PHE:CE2 | 2.99 | 0.45 |
| 1:A:912:TYR:O | 1:A:913:LYS:CB | 2.64 | 0.45 |
| 1:A:535:VAL:HG12 | 1:A:536:ASN:N | 2.32 | 0.45 |
| 1:E:1168:THR:HG22 | 1:E:1170:ASN:H | 1.80 | 0.45 |
| 1:C:942:CYS:SG | 1:C:1026:SER:HB3 | 2.56 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:867:PHE:CB | 2:D:985:LEU:O | 2.64 | 0.45 |
| 2:B:298:ILE:O | 2:B:301:LEU:HB2 | 2.17 | 0.45 |
| 2:F:866:ASN:O | 2:F:867:PHE:HB3 | 2.16 | 0.45 |
| 1:A:771:MET:HA | 1:A:774:ILE:CG2 | 2.46 | 0.45 |
| 2:D:15:ASN:OD1 | 2:D:126:LYS:CB | 2.64 | 0.45 |
| 1:C:1106:LEU:HD12 | 1:C:1175:ILE:HB | 1.97 | 0.45 |
| 1:E:482:GLY:C | 1:E:483:LEU:HG | 2.37 | 0.45 |
| 1:E:603:VAL:CG1 | 1:E:605:TYR:CE2 | 2.99 | 0.45 |
| 2:F:65:ASP:O | 2:F:66:SER:OG | 2.31 | 0.45 |
| 1:A:94:ILE:HG23 | 1:A:211:MET:HE3 | 1.98 | 0.45 |
| 1:A:469:ASP:O | 1:A:472:ILE:HB | 2.15 | 0.45 |
| 2:B:990:ASN:O | 2:B:993:GLU:N | 2.49 | 0.45 |
| 1:C:448:ILE:O | 1:C:449:ASN:O | 2.35 | 0.45 |
| 1:E:942:CYS:SG | 1:E:1026:SER:HB3 | 2.57 | 0.45 |
| 1:E:836:LEU:HD11 | 2:F:945:PHE:CE1 | 2.52 | 0.45 |
| 1:A:1092:LEU:HD11 | 1:A:1234:ASN:O | 2.16 | 0.45 |
| 2:F:932:VAL:C | 2:F:933:ILE:HG13 | 2.37 | 0.45 |
| 1:C:597:ALA:HB2 | 2:D:939:LYS:HB3 | 1.98 | 0.45 |
| 1:A:864:ASP:C | 1:A:864:ASP:OD1 | 2.55 | 0.45 |
| 1:E:778:LYS:HA | 1:E:782:LEU:HB2 | 1.97 | 0.45 |
| 1:C:21:ILE:HG12 | 1:C:134:ILE:HG22 | 1.98 | 0.45 |
| 2:F:594:ILE:CG2 | 2:F:595:LYS:N | 2.79 | 0.45 |
| 2:B:374:ASN:C | 2:B:374:ASN:OD1 | 2.54 | 0.45 |
| 2:B:1142:TRP:HD1 | 2:B:1142:TRP:H | 1.65 | 0.45 |
| 1:E:199:ILE:HA | 1:E:705:TYR:CE2 | 2.45 | 0.45 |
| 1:A:203:ILE:CD1 | 1:A:396:ILE:HG21 | 2.46 | 0.45 |
| 1:E:203:ILE:HD13 | 1:E:396:ILE:HG21 | 1.97 | 0.45 |
| 1:A:440:GLU:O | 1:A:443:TYR:CD1 | 2.69 | 0.45 |
| 1:E:1127:VAL:HG11 | 1:E:1150:ILE:HG23 | 1.99 | 0.45 |
| 1:A:606:ILE:CG2 | 1:A:621:PHE:CE2 | 3.00 | 0.45 |
| 1:C:576:ILE:HG12 | 1:C:719:ILE:HD11 | 1.97 | 0.45 |
| 2:D:932:VAL:C | 2:D:933:ILE:HG13 | 2.36 | 0.45 |
| 1:E:716:LYS:O | 1:E:719:ILE:HG22 | 2.16 | 0.45 |
| 1:C:1012:ILE:O | 2:D:779:ILE:HD12 | 2.17 | 0.45 |
| 2:F:192:CYS:O | 2:F:195:LYS:HB3 | 2.16 | 0.45 |
| 2:B:173:PHE:HA | 2:B:333:ILE:HB | 1.98 | 0.45 |
| 1:A:192:PHE:CE1 | 1:A:204:GLN:HB3 | 2.51 | 0.45 |
| 1:C:160:THR:HA | 1:C:185:THR:O | 2.17 | 0.45 |
| 1:C:275:LEU:HD11 | 1:C:279:TYR:CE2 | 2.51 | 0.45 |
| 1:E:981:ASN:HB3 | 1:E:1117:LEU:HB3 | 1.99 | 0.45 |
| 1:C:427:ILE:HD12 | 1:C:521:PHE:CD1 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:857:TYR:HB2 | 1:A:862:TYR:CE1 | 2.51 | 0.45 |
| 2:F:203:ILE:HG22 | 2:F:203:ILE:O | 2.15 | 0.45 |
| 2:B:43:PRO:HA | 2:B:78:PHE:CE2 | 2.51 | 0.45 |
| 1:A:92:ASN:O | 1:A:96:ASN:HB2 | 2.17 | 0.45 |
| 2:D:402:ILE:HG12 | 2:D:593:LYS:CB | 2.46 | 0.45 |
| 1:C:720:GLU:HA | 1:C:723:TYR:HB3 | 1.99 | 0.45 |
| 2:B:541:THR:O | 2:B:542:GLN:HB3 | 2.16 | 0.45 |
| 1:C:453:GLU:C | 1:C:454:ILE:HG22 | 2.37 | 0.45 |
| 1:C:456:ASP:HA | 1:C:669:ASN:HD21 | 1.81 | 0.45 |
| 2:B:727:TYR:N | 2:B:728:PRO:CD | 2.80 | 0.45 |
| 1:C:484:SER:O | 1:C:485:ASP:CB | 2.64 | 0.45 |
| 2:D:102:ILE:HG12 | 2:D:197:LEU:HD11 | 1.98 | 0.45 |
| 2:F:734:MET:HA | 2:F:737:CYS:SG | 2.57 | 0.45 |
| 1:A:275:LEU:HD11 | 1:A:279:TYR:CE2 | 2.51 | 0.45 |
| 1:A:345:VAL:HG13 | 1:A:387:GLN:HE22 | 1.80 | 0.45 |
| 2:F:684:ASN:O | 2:F:687:LEU:N | 2.50 | 0.45 |
| 2:B:738:ILE:HA | 2:B:741:ILE:HD12 | 1.99 | 0.45 |
| 2:B:730:PHE:O | 2:B:734:MET:HG2 | 2.17 | 0.45 |
| 1:A:427:ILE:CG2 | 1:A:428:GLU:N | 2.79 | 0.45 |
| 1:C:416:VAL:CG1 | 1:C:420:GLY:N | 2.80 | 0.45 |
| 2:B:9:ILE:HG21 | 2:B:76:ASP:HB2 | 1.98 | 0.45 |
| 2:B:631:TYR:O | 2:B:634:LEU:HB2 | 2.16 | 0.45 |
| 2:D:583:ILE:HG23 | 2:D:644:GLN:NE2 | 2.32 | 0.45 |
| 2:F:1003:ASN:HB3 | 2:F:1116:ILE:HD13 | 1.98 | 0.45 |
| 2:D:730:PHE:O | 2:D:734:MET:HG2 | 2.17 | 0.45 |
| 1:A:634:LEU:HD23 | 1:A:696:GLN:CD | 2.37 | 0.45 |
| 1:A:1168:THR:HG22 | 1:A:1170:ASN:H | 1.82 | 0.45 |
| 2:D:43:PRO:HA | 2:D:78:PHE:CE2 | 2.52 | 0.45 |
| 1:C:92:ASN:O | 1:C:96:ASN:HB2 | 2.16 | 0.45 |
| 1:E:416:VAL:CG1 | 1:E:420:GLY:N | 2.80 | 0.45 |
| 1:C:610:LEU:HD11 | 1:C:704:MET:HE2 | 1.98 | 0.45 |
| 2:B:867:PHE:C | 2:B:867:PHE:CD1 | 2.91 | 0.45 |
| 1:C:203:ILE:CD1 | 1:C:396:ILE:HG21 | 2.47 | 0.45 |
| 1:C:144:LEU:HA | 1:C:487:LYS:HA | 1.99 | 0.45 |
| 1:A:206:PRO:O | 1:A:209:THR:N | 2.50 | 0.45 |
| 2:D:64:TYR:N | 2:D:64:TYR:CD2 | 2.85 | 0.45 |
| 1:E:576:ILE:HG12 | 1:E:719:ILE:HD11 | 1.98 | 0.45 |
| 2:D:402:ILE:HG12 | 2:D:593:LYS:HB2 | 1.99 | 0.45 |
| 2:F:610:ASP:OD1 | 2:F:611:LEU:HD13 | 2.17 | 0.45 |
| 1:E:852:VAL:HG11 | 1:E:906:ILE:HG23 | 1.99 | 0.45 |
| 2:B:684:ASN:O | 2:B:687:LEU:N | 2.49 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:F:738:ILE:HA | 2:F:741:ILE:HD12 | 1.98 | 0.45 |
| 1:E:94:ILE:HG23 | 1:E:211:MET:HE3 | 1.99 | 0.45 |
| 2:D:232:PHE:CZ | 2:D:240:TYR:HA | 2.52 | 0.45 |
| 1:C:194:PHE:N | 1:C:194:PHE:CD1 | 2.85 | 0.45 |
| 1:E:423:LYS:HD2 | 2:D:510:PHE:CZ | 2.52 | 0.45 |
| 1:C:896:SER:C | 1:C:897:GLU:HG3 | 2.36 | 0.45 |
| 2:F:989:ILE:CG2 | 2:F:994:ILE:HG13 | 2.47 | 0.45 |
| 2:F:423:ILE:O | 2:F:423:ILE:CG2 | 2.64 | 0.45 |
| 1:A:942:CYS:SG | 1:A:1026:SER:HB3 | 2.57 | 0.45 |
| 2:B:14:ASP:O | 2:B:15:ASN:CB | 2.64 | 0.45 |
| 1:A:154:GLU:CB | 1:A:155:PRO:CD | 2.94 | 0.45 |
| 2:B:856:ASN:O | 2:B:857:ASP:C | 2.55 | 0.45 |
| 2:D:298:ILE:O | 2:D:301:LEU:HB2 | 2.17 | 0.45 |
| 2:F:870:TYR:HA | 2:F:931:ILE:O | 2.17 | 0.45 |
| 1:C:920:TRP:HB2 | 1:C:1045:ARG:CD | 2.47 | 0.45 |
| 2:B:274:LYS:C | 2:B:276:ASN:H | 2.19 | 0.45 |
| 2:D:1116:ILE:HG23 | 2:D:1117:PHE:N | 2.32 | 0.45 |
| 1:E:1088:LEU:HD23 | 1:E:1089:LEU:N | 2.31 | 0.45 |
| 1:E:193:ARG:NH2 | 1:E:196:ASP:OD1 | 2.50 | 0.45 |
| 2:D:210:ASN:HB3 | 2:D:228:ASP:HA | 1.99 | 0.45 |
| 1:C:1212:LEU:O | 1:C:1238:CYS:HA | 2.16 | 0.45 |
| 1:A:682:TYR:CE2 | 1:A:825:PHE:HA | 2.52 | 0.45 |
| 2:D:803:LEU:HD23 | 2:D:803:LEU:C | 2.37 | 0.45 |
| 1:C:738:TYR:C | 1:C:740:ILE:N | 2.70 | 0.44 |
| 1:C:154:GLU:CB | 1:C:155:PRO:CD | 2.94 | 0.44 |
| 2:B:824:THR:HA | 2:B:856:ASN:HB2 | 1.99 | 0.44 |
| 2:D:14:ASP:O | 2:D:15:ASN:CB | 2.65 | 0.44 |
| 1:A:427:ILE:HD12 | 1:A:521:PHE:CD1 | 2.52 | 0.44 |
| 1:A:633:LEU:O | 1:A:700:ARG:NH2 | 2.46 | 0.44 |
| 1:E:484:SER:O | 1:E:485:ASP:CB | 2.65 | 0.44 |
| 2:B:870:TYR:HA | 2:B:931:ILE:O | 2.17 | 0.44 |
| 2:D:274:LYS:C | 2:D:276:ASN:H | 2.20 | 0.44 |
| 2:B:677:ASN:CG | 2:D:849:ASN:ND2 | 2.70 | 0.44 |
| 2:D:51:LEU:HB3 | 2:D:66:SER:HA | 1.98 | 0.44 |
| 1:A:614:ASN:CB | 1:A:617:GLN:OE1 | 2.66 | 0.44 |
| 2:B:1056:PRO:O | 2:B:1058:LYS:N | 2.50 | 0.44 |
| 1:C:1229:MET:O | 1:C:1231:ASP:N | 2.50 | 0.44 |
| 2:F:1056:PRO:O | 2:F:1058:LYS:N | 2.50 | 0.44 |
| 1:E:785:TYR:O | 1:E:786:ASP:C | 2.55 | 0.44 |
| 2:B:866:ASN:O | 2:B:867:PHE:HB3 | 2.18 | 0.44 |
| 2:D:35:VAL:O | 2:D:36:ALA:HB2 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:271:ILE:HG23 | 2:B:272:LYS:N | 2.32 | 0.44 |
| 2:D:859:PHE:HD1 | 2:D:968:ILE:HD12 | 1.82 | 0.44 |
| 1:A:1076:TRP:HZ3 | 1:A:1244:SER:HG | 1.66 | 0.44 |
| 1:A:603:VAL:HG13 | 1:A:605:TYR:CE2 | 2.52 | 0.44 |
| 1:C:1127:VAL:HG11 | 1:C:1150:ILE:HG23 | 1.99 | 0.44 |
| 2:B:922:ASN:C | 2:B:923:ILE:HG13 | 2.37 | 0.44 |
| 1:A:576:ILE:HG12 | 1:A:719:ILE:HD11 | 1.99 | 0.44 |
| 2:F:155:LYS:O | 2:F:156:GLU:C | 2.55 | 0.44 |
| 1:E:535:VAL:HG11 | 1:E:551:ILE:HD12 | 1.99 | 0.44 |
| 1:E:554:PHE:HB3 | 1:E:608:LEU:HD12 | 1.99 | 0.44 |
| 2:F:64:TYR:HE2 | 2:F:363:ILE:HD12 | 1.81 | 0.44 |
| 2:D:594:ILE:CG2 | 2:D:595:LYS:N | 2.80 | 0.44 |
| 2:D:415:TYR:O | 2:D:416:SER:CB | 2.65 | 0.44 |
| 1:C:700:ARG:HA | 1:C:703:GLN:HB2 | 1.98 | 0.44 |
| 2:D:866:ASN:O | 2:D:867:PHE:HB3 | 2.18 | 0.44 |
| 2:B:27:ASP:OD1 | 2:B:27:ASP:N | 2.50 | 0.44 |
| 1:E:448:ILE:O | 1:E:449:ASN:O | 2.36 | 0.44 |
| 1:C:220:GLY:HA2 | 1:C:225:LYS:HE3 | 1.99 | 0.44 |
| 1:A:795:ASN:C | 1:A:795:ASN:OD1 | 2.55 | 0.44 |
| 1:E:22:LYS:CG | 1:E:23:PRO:HD2 | 2.47 | 0.44 |
| 1:E:912:TYR:O | 1:E:913:LYS:CB | 2.65 | 0.44 |
| 1:A:331:LEU:HB2 | 1:A:332:TYR:HD2 | 1.81 | 0.44 |
| 2:F:372:LEU:O | 2:F:379:VAL:HA | 2.17 | 0.44 |
| 1:C:94:ILE:HG23 | 1:C:211:MET:HE3 | 1.99 | 0.44 |
| 2:B:622:ASN:O | 2:B:625:TYR:N | 2.50 | 0.44 |
| 1:E:864:ASP:C | 1:E:864:ASP:OD1 | 2.55 | 0.44 |
| 2:D:45:ARG:HG3 | 2:D:141:PRO:O | 2.18 | 0.44 |
| 2:F:1036:ILE:HD12 | 2:F:1045:SER:HB3 | 1.99 | 0.44 |
| 1:C:908:TYR:HB3 | 1:C:1025:VAL:CG2 | 2.47 | 0.44 |
| 1:A:738:TYR:C | 1:A:740:ILE:N | 2.71 | 0.44 |
| 1:A:908:TYR:HB3 | 1:A:1025:VAL:CG2 | 2.47 | 0.44 |
| 1:E:469:ASP:O | 1:E:472:ILE:HB | 2.17 | 0.44 |
| 2:B:1122:LEU:HD21 | 2:B:1158:TRP:CE2 | 2.53 | 0.44 |
| 1:C:331:LEU:CB | 1:C:332:TYR:CD2 | 3.01 | 0.44 |
| 2:F:480:ILE:HG21 | 2:F:497:VAL:HG23 | 2.00 | 0.44 |
| 1:A:535:VAL:HG11 | 1:A:551:ILE:HD12 | 1.99 | 0.44 |
| 1:E:1090:ASN:HB2 | 1:E:1240:TRP:CZ3 | 2.53 | 0.44 |
| 2:F:880:THR:CB | 2:F:901:ASN:HA | 2.48 | 0.44 |
| 2:F:846:THR:HG23 | 2:F:847:GLY:N | 2.32 | 0.44 |
| 2:D:1056:PRO:O | 2:D:1058:LYS:N | 2.50 | 0.44 |
| 1:C:286:LEU:O | 1:C:289:VAL:HG13 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:522:TYR:O | 1:A:525:ALA:HB3 | 2.16 | 0.44 |
| 2:D:554:ILE:HB | 2:D:557:ILE:CD1 | 2.48 | 0.44 |
| 2:F:1013:GLU:O | 2:F:1014:ILE:CB | 2.66 | 0.44 |
| 2:B:932:VAL:C | 2:B:933:ILE:HG13 | 2.37 | 0.44 |
| 1:A:636:PHE:HD2 | 1:A:696:GLN:OE1 | 2.01 | 0.44 |
| 1:E:21:ILE:HG12 | 1:E:134:ILE:HG22 | 2.00 | 0.44 |
| 2:B:1135:ILE:HG22 | 2:B:1136:LYS:N | 2.32 | 0.44 |
| 2:B:211:ILE:O | 2:B:226:GLU:HA | 2.18 | 0.44 |
| 1:C:785:TYR:O | 1:C:786:ASP:C | 2.54 | 0.44 |
| 1:C:186:PHE:CE2 | 1:C:188:PRO:HB3 | 2.53 | 0.44 |
| 2:F:815:VAL:C | 2:F:816:ILE:HG13 | 2.37 | 0.44 |
| 2:B:298:ILE:HA | 2:B:301:LEU:HD12 | 1.99 | 0.44 |
| 2:F:727:TYR:N | 2:F:728:PRO:CD | 2.80 | 0.44 |
| 2:F:1007:ILE:CG2 | 2:F:1015:LEU:HD12 | 2.47 | 0.44 |
| 2:D:141:PRO:HA | 2:D:169:TRP:HB3 | 1.99 | 0.44 |
| 2:B:102:ILE:HG12 | 2:B:197:LEU:HD11 | 1.99 | 0.44 |
| 1:A:916:SER:OG | 1:A:1054:LEU:HG | 2.18 | 0.44 |
| 2:D:990:ASN:HB3 | 2:D:993:GLU:OE2 | 2.17 | 0.44 |
| 2:B:877:LYS:CB | 2:B:878:GLN:HB3 | 2.47 | 0.44 |
| 1:E:203:ILE:CD1 | 1:E:396:ILE:HG21 | 2.47 | 0.44 |
| 2:B:285:LEU:O | 2:B:288:GLU:N | 2.51 | 0.44 |
| 2:F:8:ASN:O | 2:F:9:ILE:C | 2.55 | 0.44 |
| 1:A:920:TRP:HB2 | 1:A:1045:ARG:CD | 2.48 | 0.44 |
| 1:C:1044:ILE:CG2 | 1:C:1045:ARG:N | 2.80 | 0.44 |
| 1:C:912:TYR:O | 1:C:913:LYS:HB3 | 2.18 | 0.44 |
| 1:A:287:SER:HA | 1:A:317:TYR:CD2 | 2.53 | 0.44 |
| 1:A:395:ILE:HG13 | 1:A:396:ILE:HG23 | 2.00 | 0.44 |
| 1:C:1132:VAL:HG23 | 1:C:1149:TYR:CE2 | 2.52 | 0.44 |
| 2:F:552:LYS:C | 2:F:713:PHE:CE1 | 2.91 | 0.44 |
| 1:A:987:ILE:O | 1:A:989:LYS:N | 2.51 | 0.44 |
| 1:A:1044:ILE:CG2 | 1:A:1045:ARG:N | 2.80 | 0.44 |
| 1:C:380:LEU:HD23 | 1:C:385:ARG:HD3 | 2.00 | 0.44 |
| 1:A:484:SER:O | 1:A:485:ASP:CB | 2.66 | 0.44 |
| 2:B:153:TYR:HB2 | 2:B:165:MET:O | 2.18 | 0.44 |
| 1:C:864:ASP:OD1 | 1:C:864:ASP:C | 2.56 | 0.44 |
| 1:E:299:TYR:HA | 1:E:302:ILE:HG22 | 1.99 | 0.44 |
| 1:C:916:SER:OG | 1:C:1054:LEU:HG | 2.18 | 0.44 |
| 1:C:1153:VAL:HG23 | 1:C:1159:LEU:CD2 | 2.48 | 0.44 |
| 1:A:193:ARG:NH2 | 1:A:196:ASP:OD1 | 2.51 | 0.44 |
| 1:C:431:ASN:O | 1:C:434:LEU:HB2 | 2.17 | 0.44 |
| 2:B:400:ASN:N | 2:B:400:ASN:OD1 | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:F:1142:TRP:H | 2:F:1142:TRP:HD1 | 1.66 | 0.44 |
| 2:F:108:PHE:HB3 | 2:F:162:MET:CG | 2.46 | 0.44 |
| 2:D:867:PHE:CZ | 2:D:935:ILE:HD12 | 2.52 | 0.44 |
| 1:E:942:CYS:SG | 1:E:1025:VAL:CG1 | 3.06 | 0.44 |
| 2:F:945:PHE:CD1 | 2:F:950:LEU:HA | 2.53 | 0.44 |
| 2:B:579:PRO:C | 2:B:581:SER:N | 2.71 | 0.44 |
| 1:C:482:GLY:C | 1:C:483:LEU:HG | 2.38 | 0.44 |
| 2:F:274:LYS:C | 2:F:276:ASN:H | 2.21 | 0.44 |
| 1:C:476:ASN:N | 2:D:1136:LYS:CE | 2.81 | 0.44 |
| 2:B:106:ILE:N | 2:B:290:LYS:HD3 | 2.33 | 0.44 |
| 1:E:571:LEU:O | 1:E:575:TRP:N | 2.42 | 0.44 |
| 1:A:21:ILE:HG12 | 1:A:134:ILE:HG22 | 2.00 | 0.44 |
| 1:A:554:PHE:HB3 | 1:A:608:LEU:HD12 | 1.99 | 0.44 |
| 1:E:431:ASN:O | 1:E:434:LEU:HB2 | 2.17 | 0.44 |
| 1:E:1229:MET:O | 1:E:1231:ASP:N | 2.51 | 0.44 |
| 1:E:92:ASN:O | 1:E:96:ASN:HB2 | 2.18 | 0.44 |
| 1:C:727:THR:O | 1:C:728:LEU:CB | 2.65 | 0.43 |
| 2:F:298:ILE:O | 2:F:301:LEU:HB2 | 2.17 | 0.43 |
| 1:C:427:ILE:CG2 | 1:C:428:GLU:N | 2.81 | 0.43 |
| 2:F:227:LEU:HD11 | 2:F:231:ASP:CB | 2.48 | 0.43 |
| 2:D:870:TYR:HA | 2:D:931:ILE:O | 2.18 | 0.43 |
| 2:B:1003:ASN:HB3 | 2:B:1116:ILE:HD13 | 2.00 | 0.43 |
| 2:B:173:PHE:O | 2:B:333:ILE:N | 2.51 | 0.43 |
| 1:E:535:VAL:HG12 | 1:E:536:ASN:N | 2.31 | 0.43 |
| 2:F:305:TYR:CE1 | 2:F:418:LEU:CD1 | 3.01 | 0.43 |
| 1:A:398:PRO:C | 1:A:399:ILE:HG13 | 2.38 | 0.43 |
| 1:C:636:PHE:HD2 | 1:C:696:GLN:OE1 | 2.00 | 0.43 |
| 2:D:804:SER:HB3 | 2:D:819:THR:HG22 | 1.99 | 0.43 |
| 1:C:522:TYR:O | 1:C:525:ALA:HB3 | 2.18 | 0.43 |
| 2:D:962:ILE:O | 2:D:962:ILE:CG2 | 2.66 | 0.43 |
| 1:E:857:TYR:HB2 | 1:E:862:TYR:CE1 | 2.53 | 0.43 |
| 1:A:416:VAL:CG1 | 1:A:420:GLY:N | 2.81 | 0.43 |
| 2:F:141:PRO:HA | 2:F:169:TRP:HB3 | 2.00 | 0.43 |
| 1:C:554:PHE:HB3 | 1:C:608:LEU:HD12 | 2.00 | 0.43 |
| 1:E:361:SER:OG | 1:E:397:LYS:HE2 | 2.17 | 0.43 |
| 2:D:381:MET:HE3 | 2:D:471:GLN:CD | 2.39 | 0.43 |
| 2:F:501:LEU:HD22 | 2:F:537:ASP:HB3 | 2.00 | 0.43 |
| 2:F:415:TYR:O | 2:F:416:SER:CB | 2.65 | 0.43 |
| 2:B:501:LEU:HD22 | 2:B:537:ASP:HB3 | 2.00 | 0.43 |
| 1:A:299:TYR:HA | 1:A:302:ILE:HG22 | 1.99 | 0.43 |
| 1:E:522:TYR:O | 1:E:525:ALA:HB3 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:F:867:PHE:C | 2:F:867:PHE:CD1 | 2.91 | 0.43 |
| 2:B:962:ILE:O | 2:B:962:ILE:CG2 | 2.65 | 0.43 |
| 2:B:645:TYR:O | 2:B:646:PHE:C | 2.56 | 0.43 |
| 2:F:567:ASN:O | 2:F:568:ASN:C | 2.57 | 0.43 |
| 1:A:873:ASN:N | 1:A:899:ASN:O | 2.39 | 0.43 |
| 1:C:299:TYR:HA | 1:C:302:ILE:HG22 | 2.00 | 0.43 |
| 2:F:540:GLU:HB3 | 2:F:555:PRO:CD | 2.49 | 0.43 |
| 2:B:799:SER:HB2 | 2:B:800:PRO:HD2 | 1.99 | 0.43 |
| 1:E:993:VAL:HG12 | 1:E:994:THR:N | 2.33 | 0.43 |
| 2:F:1135:ILE:HG22 | 2:F:1136:LYS:N | 2.33 | 0.43 |
| 2:B:806:TYR:O | 2:B:816:ILE:HA | 2.19 | 0.43 |
| 1:C:836:LEU:HD11 | 2:D:945:PHE:CE1 | 2.54 | 0.43 |
| 1:A:727:THR:O | 1:A:728:LEU:CB | 2.66 | 0.43 |
| 1:E:771:MET:HA | 1:E:774:ILE:CG2 | 2.45 | 0.43 |
| 2:D:552:LYS:C | 2:D:713:PHE:CE1 | 2.92 | 0.43 |
| 1:A:454:ILE:HD12 | 1:A:456:ASP:OD1 | 2.19 | 0.43 |
| 2:F:645:TYR:OH | 2:F:721:VAL:HG21 | 2.19 | 0.43 |
| 2:F:89:ILE:O | 2:F:95:GLY:HA3 | 2.18 | 0.43 |
| 1:C:929:LYS:HA | 1:C:932:ASN:HB2 | 1.99 | 0.43 |
| 1:C:398:PRO:C | 1:C:399:ILE:HG13 | 2.38 | 0.43 |
| 1:E:1095:ASN:O | 1:E:1112:ARG:N | 2.40 | 0.43 |
| 2:D:296:LYS:HA | 2:D:299:TRP:HE3 | 1.84 | 0.43 |
| 2:B:794:ILE:O | 2:B:795:LYS:C | 2.56 | 0.43 |
| 1:E:833:ASP:HB3 | 1:E:835:ILE:HD12 | 2.01 | 0.43 |
| 2:B:515:LYS:HB3 | 2:B:516:PRO:HD2 | 1.98 | 0.43 |
| 2:F:794:ILE:O | 2:F:795:LYS:C | 2.56 | 0.43 |
| 2:B:1142:TRP:HD1 | 2:B:1142:TRP:N | 2.16 | 0.43 |
| 1:A:836:LEU:CB | 2:B:995:LEU:HD11 | 2.47 | 0.43 |
| 2:D:876:LEU:HD21 | 2:D:978:TYR:CD2 | 2.53 | 0.43 |
| 2:D:35:VAL:CG1 | 2:D:36:ALA:H | 2.29 | 0.43 |
| 1:E:456:ASP:HA | 1:E:669:ASN:ND2 | 2.34 | 0.43 |
| 2:D:246:ASN:HA | 2:D:247:PRO:HA | 1.83 | 0.43 |
| 2:B:146:ILE:HD13 | 2:B:330:TYR:CE2 | 2.54 | 0.43 |
| 2:D:567:ASN:O | 2:D:568:ASN:C | 2.54 | 0.43 |
| 2:B:105:ALA:HA | 2:B:290:LYS:CD | 2.48 | 0.43 |
| 2:D:738:ILE:HA | 2:D:741:ILE:HD12 | 1.99 | 0.43 |
| 1:E:634:LEU:HD23 | 1:E:696:GLN:CD | 2.39 | 0.43 |
| 1:A:361:SER:OG | 1:A:397:LYS:HE2 | 2.18 | 0.43 |
| 1:A:981:ASN:HB3 | 1:A:1117:LEU:HB3 | 2.01 | 0.43 |
| 1:E:522:TYR:CZ | 1:E:611:ASN:HB2 | 2.53 | 0.43 |
| 2:D:21:VAL:CG1 | 2:D:121:ASN:HA | 2.46 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:269:TYR:HE2 | 2:D:288:GLU:CG | 2.31 | 0.43 |
| 1:A:380:LEU:HD23 | 1:A:385:ARG:HD3 | 2.01 | 0.43 |
| 1:E:632:ILE:HG23 | 1:E:633:LEU:HG | 2.01 | 0.43 |
| 2:D:645:TYR:O | 2:D:646:PHE:C | 2.55 | 0.43 |
| 2:B:81:ALA:O | 2:B:84:LYS:N | 2.52 | 0.43 |
| 1:E:179:GLY:HA2 | 1:E:220:GLY:O | 2.17 | 0.43 |
| 1:C:4:ILE:HD11 | 1:C:95:ASN:HB2 | 2.01 | 0.43 |
| 1:C:193:ARG:NH2 | 1:C:196:ASP:OD1 | 2.51 | 0.43 |
| 1:E:617:GLN:OE1 | 1:E:617:GLN:N | 2.47 | 0.43 |
| 1:E:883:THR:HG23 | 1:E:884:ASN:H | 1.84 | 0.43 |
| 1:C:633:LEU:O | 1:C:700:ARG:NH2 | 2.47 | 0.43 |
| 2:B:1013:GLU:O | 2:B:1014:ILE:CB | 2.66 | 0.43 |
| 1:C:456:ASP:HA | 1:C:669:ASN:ND2 | 2.34 | 0.43 |
| 2:F:856:ASN:O | 2:F:857:ASP:C | 2.56 | 0.43 |
| 1:E:1106:LEU:HD12 | 1:E:1175:ILE:HB | 1.99 | 0.43 |
| 1:E:912:TYR:O | 1:E:913:LYS:HB3 | 2.16 | 0.43 |
| 1:E:863:VAL:HG12 | 1:E:864:ASP:N | 2.33 | 0.43 |
| 1:E:1232:HIS:CB | 1:E:1236:ASN:HD21 | 2.32 | 0.43 |
| 1:C:627:LEU:HG | 1:E:419:LYS:O | 2.18 | 0.43 |
| 1:E:423:LYS:NZ | 2:D:514:ASP:OD1 | 2.41 | 0.43 |
| 1:E:897:GLU:HG2 | 1:E:1032:LYS:CB | 2.42 | 0.43 |
| 2:F:990:ASN:O | 2:F:993:GLU:N | 2.51 | 0.43 |
| 1:E:118:ASN:HA | 1:E:119:THR:CB | 2.41 | 0.43 |
| 1:A:468:LEU:C | 1:A:468:LEU:HD12 | 2.39 | 0.43 |
| 2:B:13:VAL:CG1 | 2:B:14:ASP:N | 2.82 | 0.43 |
| 2:B:913:GLY:O | 2:B:914:ASN:C | 2.57 | 0.43 |
| 1:C:990:TRP:HZ3 | 1:C:1044:ILE:HA | 1.83 | 0.43 |
| 1:E:38:ASN:HB3 | 1:E:147:ASN:HB2 | 2.00 | 0.43 |
| 1:E:603:VAL:HG13 | 1:E:605:TYR:CE2 | 2.54 | 0.43 |
| 1:A:824:PRO:HB3 | 2:B:952:ALA:HB2 | 2.00 | 0.43 |
| 1:A:660:LYS:CG | 1:A:661:ASN:N | 2.82 | 0.43 |
| 1:E:47:VAL:C | 1:E:50:THR:HG1 | 2.22 | 0.43 |
| 2:B:1003:ASN:HB3 | 2:B:1116:ILE:CD1 | 2.48 | 0.43 |
| 1:C:863:VAL:HG12 | 1:C:864:ASP:N | 2.34 | 0.43 |
| 1:E:262:ILE:CD1 | 1:E:690:MET:HB3 | 2.49 | 0.43 |
| 1:C:898:VAL:O | 1:C:1030:LEU:HA | 2.18 | 0.43 |
| 2:F:43:PRO:HA | 2:F:78:PHE:CE2 | 2.54 | 0.43 |
| 1:C:994:THR:HB | 1:C:1006:TYR:HB2 | 2.00 | 0.43 |
| 2:F:400:ASN:N | 2:F:400:ASN:OD1 | 2.51 | 0.43 |
| 2:D:1093:THR:HG23 | 2:D:1095:ASN:N | 2.34 | 0.43 |
| 2:F:867:PHE:CB | 2:F:985:LEU:O | 2.65 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:423:ILE:CG2 | 2:B:423:ILE:O | 2.64 | 0.43 |
| 2:B:859:PHE:HD1 | 2:B:968:ILE:HD12 | 1.81 | 0.43 |
| 1:C:250:GLU:O | 1:C:254:THR:N | 2.43 | 0.43 |
| 2:D:13:VAL:HG13 | 2:D:19:ALA:HA | 2.01 | 0.43 |
| 2:F:13:VAL:HG12 | 2:F:14:ASP:H | 1.82 | 0.43 |
| 1:C:943:MET:CE | 1:C:947:ASN:HB3 | 2.49 | 0.43 |
| 1:A:452:LYS:CB | 1:A:651:LYS:HE2 | 2.49 | 0.43 |
| 1:C:682:TYR:HE2 | 1:C:825:PHE:HA | 1.83 | 0.43 |
| 2:D:917:ASN:O | 2:D:918:ILE:HG13 | 2.19 | 0.43 |
| 1:E:795:ASN:C | 1:E:795:ASN:OD1 | 2.57 | 0.43 |
| 2:D:854:PHE:HE2 | 2:D:970:LEU:HB2 | 1.83 | 0.43 |
| 2:F:306:PHE:O | 2:F:307:SER:C | 2.57 | 0.43 |
| 1:C:632:ILE:HG23 | 1:C:633:LEU:HG | 2.01 | 0.43 |
| 2:F:554:ILE:HG21 | 2:F:556:TRP:CZ2 | 2.54 | 0.43 |
| 2:B:289:GLN:NE2 | 2:B:423:ILE:HG22 | 2.34 | 0.43 |
| 2:F:429:ILE:N | 2:F:430:PRO:HD3 | 2.34 | 0.43 |
| 2:D:1007:ILE:CG2 | 2:D:1015:LEU:HD12 | 2.49 | 0.43 |
| 2:B:923:ILE:C | 2:B:925:ASN:N | 2.72 | 0.43 |
| 1:C:475:PHE:C | 2:D:1136:LYS:CE | 2.87 | 0.43 |
| 2:F:923:ILE:C | 2:F:925:ASN:H | 2.21 | 0.43 |
| 1:E:173:PRO:HB2 | 1:E:178:PHE:HB2 | 2.01 | 0.43 |
| 1:C:634:LEU:HD23 | 1:C:696:GLN:CD | 2.38 | 0.43 |
| 1:E:916:SER:OG | 1:E:1054:LEU:HG | 2.18 | 0.43 |
| 1:E:838:SER:O | 1:E:842:LYS:HB3 | 2.19 | 0.43 |
| 1:A:994:THR:HB | 1:A:1006:TYR:HB2 | 2.00 | 0.43 |
| 2:F:289:GLN:NE2 | 2:F:292:LYS:HE3 | 2.34 | 0.43 |
| 1:A:730:GLU:O | 1:A:732:ASN:N | 2.52 | 0.43 |
| 1:C:1226:TYR:CD2 | 1:C:1226:TYR:N | 2.87 | 0.43 |
| 1:C:286:LEU:O | 1:C:287:SER:C | 2.58 | 0.42 |
| 2:D:989:ILE:HG22 | 2:D:990:ASN:N | 2.34 | 0.42 |
| 1:A:448:ILE:O | 1:A:449:ASN:O | 2.36 | 0.42 |
| 2:B:35:VAL:O | 2:B:36:ALA:HB2 | 2.19 | 0.42 |
| 1:E:468:LEU:HD12 | 1:E:471:VAL:HG22 | 2.01 | 0.42 |
| 1:A:1106:LEU:HD12 | 1:A:1175:ILE:HB | 2.00 | 0.42 |
| 1:A:610:LEU:CD1 | 1:A:704:MET:HE2 | 2.48 | 0.42 |
| 1:C:382:VAL:HG11 | 1:C:868:TYR:CE1 | 2.54 | 0.42 |
| 2:B:586:LYS:O | 2:B:641:TYR:CZ | 2.72 | 0.42 |
| 2:D:254:TYR:O | 2:D:258:THR:HB | 2.19 | 0.42 |
| 1:E:660:LYS:CG | 1:E:661:ASN:N | 2.82 | 0.42 |
| 1:A:912:TYR:CD1 | 1:A:912:TYR:N | 2.83 | 0.42 |
| 1:C:196:ASP:N | 1:C:196:ASP:OD2 | 2.52 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:E:936:GLU:HA | 1:E:954:LEU:O | 2.19 | 0.42 |
| 2:F:973:ASP:O | 2:F:975:ASN:N | 2.51 | 0.42 |
| 2:D:211:ILE:O | 2:D:226:GLU:HA | 2.19 | 0.42 |
| 1:A:191:SER:HB2 | 1:A:360:LEU:HD11 | 2.01 | 0.42 |
| 1:E:1153:VAL:HG23 | 1:E:1159:LEU:CD2 | 2.48 | 0.42 |
| 2:B:989:ILE:CG2 | 2:B:994:ILE:HG13 | 2.50 | 0.42 |
| 2:B:428:LYS:C | 2:B:430:PRO:CD | 2.88 | 0.42 |
| 1:A:453:GLU:HG3 | 1:A:454:ILE:HB | 2.01 | 0.42 |
| 2:F:9:ILE:HG13 | 2:F:10:ASP:N | 2.34 | 0.42 |
| 2:D:106:ILE:N | 2:D:290:LYS:HD3 | 2.34 | 0.42 |
| 2:D:1003:ASN:CG | 2:D:1003:ASN:O | 2.57 | 0.42 |
| 2:D:976:ASN:C | 2:D:977:VAL:HG23 | 2.40 | 0.42 |
| 1:E:138:ASN:ND2 | 1:E:140:SER:OG | 2.52 | 0.42 |
| 2:F:211:ILE:O | 2:F:226:GLU:HA | 2.19 | 0.42 |
| 2:B:296:LYS:HA | 2:B:299:TRP:HE3 | 1.84 | 0.42 |
| 1:E:274:ASN:HA | 1:E:277:ASN:ND2 | 2.34 | 0.42 |
| 2:D:238:ILE:O | 2:D:239:ASP:C | 2.55 | 0.42 |
| 2:B:645:TYR:OH | 2:B:721:VAL:HG21 | 2.19 | 0.42 |
| 1:C:1188:VAL:HG22 | 1:C:1201:PHE:CE1 | 2.54 | 0.42 |
| 2:B:480:ILE:HG21 | 2:B:497:VAL:HG23 | 2.01 | 0.42 |
| 1:C:912:TYR:O | 1:C:913:LYS:CB | 2.67 | 0.42 |
| 1:C:361:SER:OG | 1:C:397:LYS:HE2 | 2.19 | 0.42 |
| 2:F:210:ASN:HB3 | 2:F:228:ASP:HA | 1.99 | 0.42 |
| 2:B:381:MET:HE3 | 2:B:471:GLN:CD | 2.38 | 0.42 |
| 2:B:266:LYS:HA | 2:B:291:PHE:CE1 | 2.55 | 0.42 |
| 1:A:194:PHE:N | 1:A:194:PHE:CD1 | 2.87 | 0.42 |
| 2:D:1098:ILE:HD12 | 2:D:1143:VAL:CG1 | 2.50 | 0.42 |
| 2:F:877:LYS:CB | 2:F:878:GLN:HB3 | 2.47 | 0.42 |
| 2:D:877:LYS:CB | 2:D:878:GLN:HB3 | 2.47 | 0.42 |
| 2:D:289:GLN:NE2 | 2:D:423:ILE:HG22 | 2.35 | 0.42 |
| 2:B:1122:LEU:HD12 | 2:B:1122:LEU:C | 2.40 | 0.42 |
| 2:F:962:ILE:CG2 | 2:F:962:ILE:O | 2.66 | 0.42 |
| 1:C:467:ASP:C | 1:C:467:ASP:OD1 | 2.57 | 0.42 |
| 1:A:990:TRP:HZ3 | 1:A:1044:ILE:HA | 1.84 | 0.42 |
| 2:F:411:HIS:CA | 2:F:624:PHE:HE1 | 2.32 | 0.42 |
| 1:C:416:VAL:HG13 | 1:C:420:GLY:CA | 2.50 | 0.42 |
| 1:C:920:TRP:O | 1:C:1044:ILE:HA | 2.19 | 0.42 |
| 1:E:1083:ASP:HB2 | 1:E:1128:LYS:HE3 | 2.01 | 0.42 |
| 1:E:597:ALA:HA | 2:F:939:LYS:HD3 | 2.01 | 0.42 |
| 1:E:297:ASN:N | 1:E:298:PRO:HD3 | 2.33 | 0.42 |
| 2:F:1116:ILE:HG23 | 2:F:1117:PHE:N | 2.34 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:160:THR:HA | 1:A:185:THR:O | 2.19 | 0.42 |
| 2:D:855:THR:HG22 | 2:D:967:ILE:HG12 | 2.02 | 0.42 |
| 2:D:155:LYS:O | 2:D:156:GLU:C | 2.57 | 0.42 |
| 1:E:727:THR:O | 1:E:728:LEU:CB | 2.66 | 0.42 |
| 1:A:1043:GLY:C | 1:A:1044:ILE:HG13 | 2.39 | 0.42 |
| 1:E:1044:ILE:CG2 | 1:E:1045:ARG:N | 2.82 | 0.42 |
| 1:E:987:ILE:O | 1:E:989:LYS:N | 2.52 | 0.42 |
| 1:C:535:VAL:HG11 | 1:C:551:ILE:HD12 | 2.00 | 0.42 |
| 1:C:194:PHE:N | 1:C:194:PHE:HD1 | 2.18 | 0.42 |
| 2:B:234:ILE:O | 2:B:302:ASN:HB2 | 2.19 | 0.42 |
| 2:B:415:TYR:O | 2:B:416:SER:CB | 2.67 | 0.42 |
| 2:B:242:LEU:CD1 | 2:B:638:TRP:CG | 3.03 | 0.42 |
| 1:E:1012:ILE:O | 2:F:779:ILE:HD12 | 2.19 | 0.42 |
| 1:A:287:SER:HB3 | 1:A:317:TYR:H | 1.84 | 0.42 |
| 1:E:738:TYR:C | 1:E:740:ILE:N | 2.72 | 0.42 |
| 1:E:427:ILE:CG2 | 1:E:428:GLU:N | 2.82 | 0.42 |
| 1:C:1127:VAL:CG1 | 1:C:1128:LYS:N | 2.82 | 0.42 |
| 2:F:276:ASN:O | 2:F:277:ASN:HB3 | 2.20 | 0.42 |
| 2:D:727:TYR:N | 2:D:728:PRO:CD | 2.82 | 0.42 |
| 1:A:993:VAL:HG12 | 1:A:994:THR:N | 2.35 | 0.42 |
| 2:F:242:LEU:CD1 | 2:F:638:TRP:CG | 3.02 | 0.42 |
| 1:A:720:GLU:HA | 1:A:723:TYR:HB3 | 2.02 | 0.42 |
| 1:E:15:ASP:HA | 1:E:16:ARG:HA | 1.77 | 0.42 |
| 1:A:1002:ASP:N | 1:A:1002:ASP:OD1 | 2.53 | 0.42 |
| 2:B:1097:ARG:NE | 2:B:1142:TRP:CE3 | 2.87 | 0.42 |
| 2:B:629:ILE:O | 2:B:630:TYR:C | 2.58 | 0.42 |
| 2:F:945:PHE:HA | 2:F:949:ILE:O | 2.20 | 0.42 |
| 1:E:250:GLU:O | 1:E:254:THR:N | 2.44 | 0.42 |
| 1:C:926:TYR:HD1 | 1:C:1247:HIS:O | 2.03 | 0.42 |
| 2:D:586:LYS:O | 2:D:641:TYR:CZ | 2.73 | 0.42 |
| 1:A:932:ASN:HA | 1:A:956:HIS:CE1 | 2.55 | 0.42 |
| 1:A:1190:MET:HE1 | 1:A:1199:MET:HB3 | 2.02 | 0.42 |
| 1:A:617:GLN:N | 1:A:617:GLN:OE1 | 2.47 | 0.42 |
| 2:D:923:ILE:O | 2:D:925:ASN:N | 2.39 | 0.42 |
| 1:E:730:GLU:O | 1:E:732:ASN:N | 2.52 | 0.42 |
| 1:E:170:ASN:HD21 | 2:B:377:ASN:ND2 | 2.18 | 0.42 |
| 1:A:436:PHE:CD1 | 1:A:437:VAL:N | 2.86 | 0.42 |
| 2:B:13:VAL:HG13 | 2:B:19:ALA:HA | 2.01 | 0.42 |
| 1:C:452:LYS:CB | 1:C:651:LYS:HE2 | 2.50 | 0.42 |
| 2:B:755:ILE:HG22 | 2:B:760:LYS:HG3 | 2.01 | 0.42 |
| 2:D:153:TYR:HB2 | 2:D:165:MET:O | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:660:LYS:CG | 1:C:661:ASN:N | 2.82 | 0.42 |
| 2:F:238:ILE:O | 2:F:239:ASP:C | 2.57 | 0.42 |
| 2:F:738:ILE:O | 2:F:739:LYS:C | 2.58 | 0.42 |
| 1:E:15:ASP:HA | 1:E:136:PHE:HZ | 1.85 | 0.42 |
| 2:D:922:ASN:C | 2:D:923:ILE:HG13 | 2.40 | 0.42 |
| 1:C:262:ILE:CD1 | 1:C:690:MET:HB3 | 2.50 | 0.42 |
| 1:C:1232:HIS:CB | 1:C:1236:ASN:HD21 | 2.32 | 0.42 |
| 1:C:981:ASN:HB3 | 1:C:1117:LEU:HB3 | 2.02 | 0.42 |
| 1:C:617:GLN:OE1 | 1:C:617:GLN:N | 2.48 | 0.42 |
| 2:B:905:VAL:HA | 2:B:918:ILE:O | 2.20 | 0.42 |
| 1:A:305:GLU:HA | 1:A:305:GLU:OE1 | 2.20 | 0.42 |
| 2:B:1093:THR:HG23 | 2:B:1095:ASN:N | 2.35 | 0.42 |
| 2:B:108:PHE:CG | 2:B:109:PRO:HD2 | 2.55 | 0.42 |
| 2:B:945:PHE:CD1 | 2:B:950:LEU:HA | 2.55 | 0.42 |
| 2:D:554:ILE:HG21 | 2:D:556:TRP:CZ2 | 2.54 | 0.42 |
| 2:D:1149:HIS:CE1 | 2:D:1150:ASP:CB | 3.02 | 0.42 |
| 1:C:395:ILE:HG13 | 1:C:396:ILE:HG23 | 2.02 | 0.42 |
| 2:F:709:ASN:O | 2:F:713:PHE:HD2 | 2.02 | 0.42 |
| 1:C:38:ASN:HB3 | 1:C:147:ASN:HB2 | 2.02 | 0.42 |
| 2:B:276:ASN:O | 2:B:277:ASN:HB3 | 2.20 | 0.42 |
| 2:F:922:ASN:C | 2:F:923:ILE:HG13 | 2.39 | 0.42 |
| 1:A:220:GLY:HA2 | 1:A:225:LYS:HE3 | 2.01 | 0.42 |
| 1:E:196:ASP:OD2 | 1:E:196:ASP:N | 2.53 | 0.42 |
| 2:F:515:LYS:HB3 | 2:F:516:PRO:HD2 | 2.01 | 0.42 |
| 1:C:838:SER:O | 1:C:842:LYS:HB3 | 2.20 | 0.42 |
| 1:A:1153:VAL:HG23 | 1:A:1159:LEU:CD2 | 2.50 | 0.42 |
| 1:E:398:PRO:C | 1:E:399:ILE:HG13 | 2.40 | 0.42 |
| 2:F:266:LYS:HA | 2:F:291:PHE:CE1 | 2.55 | 0.42 |
| 1:A:903:ASN:OD1 | 1:A:903:ASN:C | 2.59 | 0.42 |
| 1:A:1111:ILE:HG23 | 1:A:1111:ILE:O | 2.20 | 0.42 |
| 1:A:522:TYR:CZ | 1:A:611:ASN:HB2 | 2.53 | 0.42 |
| 2:B:1093:THR:OG1 | 2:B:1094:THR:N | 2.52 | 0.42 |
| 2:B:990:ASN:HB3 | 2:B:993:GLU:OE2 | 2.19 | 0.42 |
| 2:F:629:ILE:O | 2:F:630:TYR:C | 2.58 | 0.42 |
| 2:D:27:ASP:OD1 | 2:D:27:ASP:N | 2.52 | 0.42 |
| 2:B:734:MET:HA | 2:B:737:CYS:SG | 2.60 | 0.42 |
| 1:E:908:TYR:HB3 | 1:E:1025:VAL:CG2 | 2.49 | 0.42 |
| 2:D:1122:LEU:HD21 | 2:D:1158:TRP:CE2 | 2.55 | 0.42 |
| 2:B:552:LYS:C | 2:B:713:PHE:CE1 | 2.93 | 0.42 |
| 1:A:427:ILE:CD1 | 1:A:521:PHE:CD1 | 3.03 | 0.42 |
| 2:D:81:ALA:O | 2:D:84:LYS:N | 2.52 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:E:1227:THR:HG22 | 2:F:806:TYR:CD2 | 2.54 | 0.42 |
| 1:C:993:VAL:HG12 | 1:C:994:THR:N | 2.35 | 0.42 |
| 1:E:4:ILE:HD11 | 1:E:95:ASN:HB2 | 2.02 | 0.42 |
| 2:D:308:LYS:HA | 2:D:789:TYR:CE2 | 2.55 | 0.42 |
| 1:E:39:ILE:HG12 | 1:E:148:VAL:HB | 2.02 | 0.42 |
| 1:C:1103:ASP:OD1 | 1:C:1103:ASP:N | 2.36 | 0.42 |
| 2:F:1122:LEU:HD21 | 2:F:1158:TRP:CE2 | 2.54 | 0.41 |
| 2:D:856:ASN:O | 2:D:857:ASP:C | 2.58 | 0.41 |
| 1:C:427:ILE:CD1 | 1:C:521:PHE:CD1 | 3.02 | 0.41 |
| 1:E:943:MET:CE | 1:E:947:ASN:HB3 | 2.50 | 0.41 |
| 2:F:1003:ASN:CG | 2:F:1003:ASN:O | 2.58 | 0.41 |
| 1:E:636:PHE:HD2 | 1:E:696:GLN:OE1 | 2.03 | 0.41 |
| 2:B:917:ASN:C | 2:B:918:ILE:HG13 | 2.40 | 0.41 |
| 2:B:973:ASP:O | 2:B:975:ASN:N | 2.50 | 0.41 |
| 2:F:855:THR:HA | 2:F:966:ASP:O | 2.19 | 0.41 |
| 2:F:855:THR:HG22 | 2:F:967:ILE:HG12 | 2.02 | 0.41 |
| 2:F:71:THR:OG1 | 2:F:74:GLU:HG2 | 2.20 | 0.41 |
| 2:D:1097:ARG:NE | 2:D:1142:TRP:CE3 | 2.89 | 0.41 |
| 1:C:522:TYR:CZ | 1:C:611:ASN:HB2 | 2.54 | 0.41 |
| 2:B:530:ILE:O | 2:B:531:PHE:C | 2.59 | 0.41 |
| 1:E:216:HIS:CE1 | 1:E:250:GLU:HG3 | 2.54 | 0.41 |
| 2:B:1122:LEU:HD21 | 2:B:1158:TRP:NE1 | 2.35 | 0.41 |
| 1:C:468:LEU:HD12 | 1:C:471:VAL:HG22 | 2.02 | 0.41 |
| 2:F:321:ALA:HB1 | 2:F:388:ASP:HB3 | 2.02 | 0.41 |
| 2:B:917:ASN:O | 2:B:918:ILE:HG13 | 2.20 | 0.41 |
| 2:D:828:TYR:HB2 | 2:D:829:PRO:HD2 | 2.02 | 0.41 |
| 2:B:71:THR:OG1 | 2:B:74:GLU:HG2 | 2.19 | 0.41 |
| 1:E:720:GLU:HA | 1:E:723:TYR:HB3 | 2.02 | 0.41 |
| 1:C:192:PHE:CE1 | 1:C:204:GLN:HB3 | 2.55 | 0.41 |
| 2:D:89:ILE:O | 2:D:95:GLY:HA3 | 2.21 | 0.41 |
| 2:B:453:ILE:CG1 | 2:B:454:THR:H | 2.32 | 0.41 |
| 2:D:622:ASN:O | 2:D:625:TYR:N | 2.53 | 0.41 |
| 2:F:580:ILE:H | 2:F:580:ILE:HG13 | 1.66 | 0.41 |
| 1:E:436:PHE:CD1 | 1:E:437:VAL:N | 2.85 | 0.41 |
| 2:D:185:PRO:O | 2:D:186:ALA:C | 2.57 | 0.41 |
| 1:A:987:ILE:C | 1:A:989:LYS:N | 2.73 | 0.41 |
| 2:B:1007:ILE:HG12 | 2:B:1072:GLN:C | 2.41 | 0.41 |
| 2:F:502:ASN:O | 2:F:505:MET:N | 2.54 | 0.41 |
| 2:B:245:THR:HB | 2:B:631:TYR:CE1 | 2.55 | 0.41 |
| 1:A:1143:ARG:HB2 | 1:A:1146:ASP:OD1 | 2.20 | 0.41 |
| 1:A:22:LYS:HG3 | 1:A:23:PRO:HD2 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:1010:ASN:HB3 | 2:F:780:GLN:CG | 2.50 | 0.41 |
| 1:E:778:LYS:HA | 1:E:782:LEU:HD12 | 2.02 | 0.41 |
| 2:F:730:PHE:O | 2:F:734:MET:HG2 | 2.20 | 0.41 |
| 1:C:912:TYR:CD1 | 1:C:912:TYR:N | 2.87 | 0.41 |
| 1:C:1232:HIS:HB3 | 1:C:1236:ASN:HD21 | 1.85 | 0.41 |
| 2:D:308:LYS:HA | 2:D:789:TYR:CD2 | 2.56 | 0.41 |
| 2:D:799:SER:HB2 | 2:D:800:PRO:HD2 | 2.02 | 0.41 |
| 2:F:308:LYS:HA | 2:F:789:TYR:CE2 | 2.55 | 0.41 |
| 2:B:885:LEU:HG | 2:B:886:ILE:CD1 | 2.22 | 0.41 |
| 2:B:526:TRP:O | 2:B:529:ALA:HB3 | 2.20 | 0.41 |
| 2:B:554:ILE:HG21 | 2:B:556:TRP:CZ2 | 2.54 | 0.41 |
| 2:D:289:GLN:NE2 | 2:D:292:LYS:HE3 | 2.36 | 0.41 |
| 2:F:423:ILE:HG23 | 2:F:426:ILE:HB | 2.02 | 0.41 |
| 2:F:269:TYR:CZ | 2:F:288:GLU:HB2 | 2.55 | 0.41 |
| 2:F:35:VAL:O | 2:F:36:ALA:HB2 | 2.19 | 0.41 |
| 1:C:903:ASN:OD1 | 1:C:903:ASN:C | 2.59 | 0.41 |
| 1:C:249:ILE:HG23 | 1:C:263:ILE:CD1 | 2.51 | 0.41 |
| 1:A:38:ASN:HB3 | 1:A:147:ASN:HB2 | 2.03 | 0.41 |
| 2:D:645:TYR:OH | 2:D:721:VAL:HG21 | 2.21 | 0.41 |
| 2:D:254:TYR:O | 2:D:258:THR:CG2 | 2.69 | 0.41 |
| 1:E:1188:VAL:HG22 | 1:E:1201:PHE:CE1 | 2.55 | 0.41 |
| 1:E:614:ASN:CB | 1:E:617:GLN:OE1 | 2.68 | 0.41 |
| 2:F:1069:GLN:O | 2:F:1070:TYR:CD2 | 2.74 | 0.41 |
| 2:B:860:GLU:O | 2:B:861:ASN:HB2 | 2.20 | 0.41 |
| 1:A:789:VAL:HG12 | 1:A:793:LEU:HD12 | 2.03 | 0.41 |
| 2:D:71:THR:OG1 | 2:D:74:GLU:HG2 | 2.19 | 0.41 |
| 2:F:46:TYR:HB3 | 2:F:142:GLY:HA2 | 2.03 | 0.41 |
| 1:A:852:VAL:HG11 | 1:A:906:ILE:HG23 | 2.03 | 0.41 |
| 2:D:46:TYR:HB3 | 2:D:142:GLY:HA2 | 2.02 | 0.41 |
| 2:B:540:GLU:HB3 | 2:B:555:PRO:CD | 2.50 | 0.41 |
| 1:A:838:SER:O | 1:A:842:LYS:HB3 | 2.21 | 0.41 |
| 2:F:860:GLU:O | 2:F:861:ASN:HB2 | 2.21 | 0.41 |
| 1:A:584:THR:HG22 | 1:A:750:LYS:HD2 | 2.02 | 0.41 |
| 1:A:1000:LEU:N | 1:A:1000:LEU:HD12 | 2.36 | 0.41 |
| 1:C:274:ASN:HA | 1:C:277:ASN:ND2 | 2.36 | 0.41 |
| 1:C:835:ILE:HG23 | 2:D:949:ILE:HA | 2.03 | 0.41 |
| 2:B:730:PHE:CE2 | 2:B:734:MET:HG3 | 2.55 | 0.41 |
| 2:D:423:ILE:HG23 | 2:D:426:ILE:HB | 2.01 | 0.41 |
| 1:E:456:ASP:OD1 | 1:E:456:ASP:N | 2.52 | 0.41 |
| 2:B:709:ASN:O | 2:B:712:LYS:N | 2.53 | 0.41 |
| 1:E:395:ILE:HG13 | 1:E:396:ILE:HG23 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:1127:VAL:CG1 | 1:E:1128:LYS:N | 2.84 | 0.41 |
| 2:F:755:ILE:HG22 | 2:F:760:LYS:HG3 | 2.03 | 0.41 |
| 1:A:297:ASN:N | 1:A:297:ASN:OD1 | 2.49 | 0.41 |
| 2:F:88:ARG:O | 2:F:91:ASN:HB2 | 2.20 | 0.41 |
| 1:C:614:ASN:HB2 | 1:C:617:GLN:HE22 | 1.85 | 0.41 |
| 1:C:730:GLU:O | 1:C:732:ASN:N | 2.53 | 0.41 |
| 2:B:594:ILE:CG2 | 2:B:595:LYS:N | 2.83 | 0.41 |
| 2:D:654:LYS:HA | 2:D:657:LEU:HD12 | 2.02 | 0.41 |
| 2:F:799:SER:HB2 | 2:F:800:PRO:HD2 | 2.02 | 0.41 |
| 1:E:932:ASN:HA | 1:E:956:HIS:CE1 | 2.56 | 0.41 |
| 2:F:1098:ILE:HD12 | 2:F:1143:VAL:CG1 | 2.51 | 0.41 |
| 1:A:1001:GLY:HA2 | 1:A:1018:LEU:HD21 | 2.02 | 0.41 |
| 2:B:1140:TYR:CE2 | 2:B:1142:TRP:CE2 | 3.09 | 0.41 |
| 2:F:1097:ARG:NE | 2:F:1142:TRP:CE3 | 2.89 | 0.41 |
| 2:D:945:PHE:HA | 2:D:949:ILE:O | 2.20 | 0.41 |
| 2:F:553:ILE:CG2 | 2:F:554:ILE:N | 2.83 | 0.41 |
| 2:B:626:LEU:HD22 | 2:B:734:MET:HE3 | 2.01 | 0.41 |
| 2:B:709:ASN:O | 2:B:713:PHE:HD2 | 2.03 | 0.41 |
| 2:B:185:PRO:O | 2:B:188:GLU:N | 2.53 | 0.41 |
| 1:A:1083:ASP:HB2 | 1:A:1128:LYS:HE3 | 2.02 | 0.41 |
| 1:A:1127:VAL:CG1 | 1:A:1128:LYS:N | 2.83 | 0.41 |
| 2:D:755:ILE:HG22 | 2:D:760:LYS:HG3 | 2.03 | 0.41 |
| 1:C:603:VAL:CG1 | 1:C:605:TYR:CE2 | 3.04 | 0.41 |
| 2:B:583:ILE:HD11 | 2:B:645:TYR:CE2 | 2.55 | 0.41 |
| 1:A:863:VAL:HG12 | 1:A:864:ASP:N | 2.36 | 0.41 |
| 1:A:883:THR:HG23 | 1:A:884:ASN:H | 1.85 | 0.41 |
| 2:D:501:LEU:HD22 | 2:D:537:ASP:HB3 | 2.01 | 0.41 |
| 2:F:731:THR:O | 2:F:735:GLU:HG3 | 2.21 | 0.41 |
| 2:B:828:TYR:HB2 | 2:B:829:PRO:HD2 | 2.02 | 0.41 |
| 1:E:1111:ILE:O | 1:E:1111:ILE:HG23 | 2.20 | 0.41 |
| 2:B:423:ILE:HG23 | 2:B:426:ILE:HB | 2.02 | 0.41 |
| 2:B:35:VAL:CG1 | 2:B:36:ALA:H | 2.30 | 0.41 |
| 2:F:185:PRO:O | 2:F:188:GLU:N | 2.53 | 0.41 |
| 1:C:470:GLN:HG3 | 2:D:1028:PHE:HE1 | 1.86 | 0.41 |
| 2:B:11:SER:CB | 2:B:12:PRO:HA | 2.51 | 0.41 |
| 2:B:254:TYR:O | 2:B:258:THR:HB | 2.21 | 0.41 |
| 2:F:182:TYR:CE2 | 2:F:351:THR:HG22 | 2.56 | 0.41 |
| 1:A:682:TYR:CD2 | 1:A:825:PHE:HD1 | 2.38 | 0.41 |
| 2:F:102:ILE:HG12 | 2:F:197:LEU:HD11 | 2.03 | 0.41 |
| 1:E:416:VAL:HG13 | 1:E:420:GLY:CA | 2.51 | 0.41 |
| 1:C:436:PHE:CD1 | 1:C:437:VAL:N | 2.83 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:D:480:ILE:HG21 | 2:D:497:VAL:HG23 | 2.02 | 0.41 |
| 1:A:143:ILE:CD1 | 1:A:491:THR:HG23 | 2.50 | 0.41 |
| 2:F:13:VAL:HG13 | 2:F:19:ALA:HA | 2.03 | 0.41 |
| 1:A:1127:VAL:HG13 | 1:A:1151:ASN:O | 2.21 | 0.41 |
| 1:C:1083:ASP:HB2 | 1:C:1128:LYS:HE3 | 2.03 | 0.41 |
| 2:D:583:ILE:HD11 | 2:D:645:TYR:CE2 | 2.55 | 0.41 |
| 1:A:1188:VAL:HG22 | 1:A:1201:PHE:CE1 | 2.55 | 0.41 |
| 2:B:681:SER:HB3 | 2:B:684:ASN:HD22 | 1.85 | 0.41 |
| 2:B:381:MET:HE3 | 2:B:471:GLN:HB3 | 2.03 | 0.41 |
| 1:A:15:ASP:HA | 1:A:16:ARG:HA | 1.75 | 0.41 |
| 1:E:903:ASN:C | 1:E:903:ASN:OD1 | 2.59 | 0.41 |
| 1:C:627:LEU:O | 1:E:419:LYS:CG | 2.69 | 0.41 |
| 1:C:610:LEU:O | 1:C:611:ASN:C | 2.58 | 0.41 |
| 2:D:108:PHE:CG | 2:D:109:PRO:HD2 | 2.55 | 0.41 |
| 2:F:27:ASP:N | 2:F:27:ASP:OD1 | 2.54 | 0.41 |
| 1:C:74:LEU:N | 1:C:79:GLU:OE1 | 2.49 | 0.41 |
| 2:D:1008:ARG:HD2 | 2:D:1012:GLU:HB3 | 2.02 | 0.41 |
| 1:E:773:LEU:O | 1:E:774:ILE:C | 2.59 | 0.41 |
| 2:D:710:ILE:HG23 | 2:D:714:PHE:CE2 | 2.56 | 0.41 |
| 2:D:709:ASN:O | 2:D:713:PHE:HD2 | 2.03 | 0.41 |
| 1:E:468:LEU:O | 1:E:469:ASP:C | 2.60 | 0.41 |
| 2:F:35:VAL:CG1 | 2:F:36:ALA:H | 2.31 | 0.41 |
| 1:C:468:LEU:O | 1:C:469:ASP:C | 2.59 | 0.41 |
| 1:C:468:LEU:C | 1:C:468:LEU:HD12 | 2.41 | 0.41 |
| 2:F:709:ASN:O | 2:F:710:ILE:C | 2.60 | 0.41 |
| 2:F:552:LYS:C | 2:F:713:PHE:HE1 | 2.24 | 0.41 |
| 1:A:989:LYS:HE2 | 1:A:1075:PHE:CE2 | 2.55 | 0.41 |
| 1:E:989:LYS:CG | 1:E:1076:TRP:HA | 2.50 | 0.41 |
| 1:E:382:VAL:HG11 | 1:E:868:TYR:CE1 | 2.56 | 0.41 |
| 2:D:105:ALA:HA | 2:D:290:LYS:CD | 2.50 | 0.41 |
| 1:C:331:LEU:HB2 | 1:C:332:TYR:CD2 | 2.55 | 0.41 |
| 1:E:220:GLY:HA2 | 1:E:225:LYS:HE3 | 2.03 | 0.41 |
| 2:F:106:ILE:N | 2:F:290:LYS:HD3 | 2.36 | 0.41 |
| 2:F:146:ILE:HD13 | 2:F:330:TYR:CE2 | 2.56 | 0.41 |
| 1:A:1190:MET:CE | 1:A:1199:MET:HB3 | 2.51 | 0.41 |
| 2:D:734:MET:HA | 2:D:737:CYS:SG | 2.60 | 0.41 |
| 1:E:912:TYR:N | 1:E:912:TYR:CD1 | 2.87 | 0.41 |
| 1:C:645:ILE:HD12 | 1:C:785:TYR:HB2 | 2.03 | 0.41 |
| 2:B:197:LEU:HD12 | 2:B:197:LEU:N | 2.36 | 0.41 |
| 1:C:641:LEU:HD12 | 1:E:614:ASN:ND2 | 2.35 | 0.41 |
| 2:D:855:THR:HA | 2:D:966:ASP:O | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:929:LYS:HA | 1:E:932:ASN:HB2 | 2.02 | 0.41 |
| 1:A:962:THR:HA | 1:A:972:LYS:HG2 | 2.03 | 0.41 |
| 2:B:789:TYR:CE2 | 2:B:793:LEU:CD1 | 3.03 | 0.41 |
| 2:D:453:ILE:CG1 | 2:D:454:THR:H | 2.33 | 0.41 |
| 1:C:116:ASN:N | 1:C:116:ASN:OD1 | 2.54 | 0.41 |
| 2:D:207:ASP:N | 2:D:207:ASP:OD1 | 2.52 | 0.41 |
| 2:F:832:ILE:HG13 | 2:F:832:ILE:H | 1.75 | 0.41 |
| 2:B:491:SER:O | 2:B:495:SER:N | 2.54 | 0.41 |
| 1:A:1137:THR:OG1 | 2:B:1109:ILE:HG21 | 2.21 | 0.41 |
| 1:C:769:TYR:O | 1:C:772:LYS:HB2 | 2.21 | 0.41 |
| 1:E:192:PHE:CE1 | 1:E:204:GLN:HB3 | 2.56 | 0.41 |
| 2:D:242:LEU:CD1 | 2:D:638:TRP:CG | 3.04 | 0.41 |
| 2:B:1147:LEU:HD12 | 2:B:1147:LEU:N | 2.36 | 0.41 |
| 2:F:285:LEU:O | 2:F:288:GLU:N | 2.54 | 0.41 |
| 2:B:269:TYR:HE2 | 2:B:288:GLU:CG | 2.34 | 0.41 |
| 1:E:452:LYS:CB | 1:E:651:LYS:HE2 | 2.50 | 0.41 |
| 2:B:502:ASN:O | 2:B:505:MET:N | 2.54 | 0.41 |
| 1:C:297:ASN:N | 1:C:297:ASN:OD1 | 2.49 | 0.41 |
| 2:D:276:ASN:O | 2:D:277:ASN:HB3 | 2.21 | 0.41 |
| 1:A:1143:ARG:O | 1:A:1144:LYS:C | 2.59 | 0.41 |
| 1:A:778:LYS:HA | 1:A:782:LEU:HD12 | 2.02 | 0.41 |
| 2:B:855:THR:HA | 2:B:966:ASP:O | 2.21 | 0.41 |
| 1:E:160:THR:HA | 1:E:185:THR:O | 2.21 | 0.41 |
| 1:A:1067:PRO:O | 1:A:1068:ASN:O | 2.38 | 0.41 |
| 2:B:1098:ILE:HD12 | 2:B:1143:VAL:CG1 | 2.50 | 0.41 |
| 1:C:625:LEU:O | 1:C:626:GLU:C | 2.59 | 0.41 |
| 2:D:1069:GLN:O | 2:D:1070:TYR:CD2 | 2.74 | 0.41 |
| 2:D:400:ASN:OD1 | 2:D:400:ASN:N | 2.54 | 0.41 |
| 2:F:108:PHE:CG | 2:F:109:PRO:HD2 | 2.56 | 0.40 |
| 2:D:108:PHE:HB3 | 2:D:162:MET:CG | 2.47 | 0.40 |
| 2:B:554:ILE:CG2 | 2:B:556:TRP:NE1 | 2.84 | 0.40 |
| 2:F:428:LYS:C | 2:F:430:PRO:CD | 2.89 | 0.40 |
| 1:A:989:LYS:CG | 1:A:1076:TRP:HA | 2.50 | 0.40 |
| 1:E:20:TYR:HA | 1:E:30:TYR:O | 2.21 | 0.40 |
| 2:F:254:TYR:O | 2:F:258:THR:HB | 2.21 | 0.40 |
| 1:C:225:LYS:HA | 1:C:228:THR:OG1 | 2.21 | 0.40 |
| 1:A:196:ASP:N | 1:A:196:ASP:OD2 | 2.54 | 0.40 |
| 1:E:388:ASN:HB3 | 1:E:391:LEU:HB3 | 2.01 | 0.40 |
| 1:E:898:VAL:O | 1:E:1030:LEU:HA | 2.22 | 0.40 |
| 1:A:4:ILE:HD11 | 1:A:95:ASN:HB2 | 2.02 | 0.40 |
| 1:C:833:ASP:HB3 | 1:C:835:ILE:HD12 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:D:497:VAL:HG12 | 2:D:498:TYR:N | 2.35 | 0.40 |
| 2:F:990:ASN:HB3 | 2:F:993:GLU:OE2 | 2.20 | 0.40 |
| 2:B:429:ILE:N | 2:B:430:PRO:HD3 | 2.34 | 0.40 |
| 2:F:583:ILE:HD11 | 2:F:645:TYR:CE2 | 2.56 | 0.40 |
| 2:F:880:THR:HB | 2:F:901:ASN:HA | 2.03 | 0.40 |
| 1:C:614:ASN:CB | 1:C:617:GLN:OE1 | 2.68 | 0.40 |
| 2:F:854:PHE:HE2 | 2:F:970:LEU:HB2 | 1.87 | 0.40 |
| 2:B:470:LEU:HD11 | 2:B:654:LYS:HB3 | 2.04 | 0.40 |
| 1:C:897:GLU:HG2 | 1:C:1032:LYS:HD3 | 2.04 | 0.40 |
| 2:F:541:THR:O | 2:F:542:GLN:HB3 | 2.21 | 0.40 |
| 2:F:469:TYR:CE1 | 2:F:562:ASN:HB2 | 2.55 | 0.40 |
| 2:B:553:ILE:CG2 | 2:B:554:ILE:N | 2.83 | 0.40 |
| 1:A:926:TYR:HD1 | 1:A:1247:HIS:O | 2.04 | 0.40 |
| 2:D:709:ASN:O | 2:D:710:ILE:C | 2.60 | 0.40 |
| 2:F:298:ILE:HA | 2:F:301:LEU:CD1 | 2.52 | 0.40 |
| 1:C:903:ASN:OD1 | 1:C:904:ASP:N | 2.54 | 0.40 |
| 2:F:246:ASN:HA | 2:F:247:PRO:HA | 1.84 | 0.40 |
| 1:A:1213:GLY:HA3 | 1:A:1225:TYR:CE2 | 2.57 | 0.40 |
| 1:A:632:ILE:HG23 | 1:A:633:LEU:HG | 2.02 | 0.40 |
| 2:F:254:TYR:O | 2:F:258:THR:CG2 | 2.69 | 0.40 |
| 2:B:107:PRO:HG2 | 2:B:118:ARG:CB | 2.50 | 0.40 |
| 2:F:205:PRO:CD | 2:F:230:ILE:HD11 | 2.52 | 0.40 |
| 2:D:197:LEU:HD12 | 2:D:197:LEU:N | 2.36 | 0.40 |
| 1:A:625:LEU:O | 1:A:626:GLU:C | 2.60 | 0.40 |
| 1:C:39:ILE:HG12 | 1:C:148:VAL:HB | 2.04 | 0.40 |
| 1:C:305:GLU:HA | 1:C:305:GLU:OE1 | 2.20 | 0.40 |
| 1:E:1125:ILE:HD12 | 1:E:1125:ILE:HA | 1.93 | 0.40 |
| 1:E:216:HIS:CE1 | 1:E:254:THR:HG1 | 2.39 | 0.40 |
| 1:A:467:ASP:OD1 | 1:A:467:ASP:C | 2.58 | 0.40 |
| 1:C:824:PRO:HB2 | 2:D:952:ALA:HB2 | 2.03 | 0.40 |
| 2:F:99:LEU:C | 2:F:101:LEU:N | 2.75 | 0.40 |
| 1:E:920:TRP:O | 1:E:1044:ILE:HA | 2.21 | 0.40 |
| 2:B:589:ILE:HG13 | 2:B:641:TYR:OH | 2.22 | 0.40 |
| 2:B:646:PHE:O | 2:B:647:ASP:C | 2.59 | 0.40 |
| 2:D:646:PHE:O | 2:D:647:ASP:C | 2.60 | 0.40 |
| 1:E:225:LYS:HA | 1:E:228:THR:OG1 | 2.22 | 0.40 |
| 1:C:937:TYR:CE1 | 1:C:954:LEU:HB2 | 2.57 | 0.40 |
| 1:A:614:ASN:HB2 | 1:A:617:GLN:HE22 | 1.86 | 0.40 |
| 2:D:1106:ASN:O | 2:D:1107:ALA:C | 2.59 | 0.40 |
| 2:F:828:TYR:HB2 | 2:F:829:PRO:HD2 | 2.04 | 0.40 |
| 1:A:1084:LYS:HB3 | 1:A:1086:TYR:CE2 | 2.57 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:833:ASP:HB3 | 1:A:835:ILE:HD12 | 2.03 | 0.40 |
| 1:E:789:VAL:HG12 | 1:E:793:LEU:HD12 | 2.03 | 0.40 |
| 1:E:305:GLU:HA | 1:E:305:GLU:OE1 | 2.21 | 0.40 |
| 1:E:610:LEU:O | 1:E:611:ASN:C | 2.60 | 0.40 |
| 2:D:271:ILE:CG2 | 2:D:272:LYS:N | 2.84 | 0.40 |
| 1:C:249:ILE:O | 1:C:250:GLU:C | 2.57 | 0.40 |
| 2:D:245:THR:HB | 2:D:631:TYR:CE1 | 2.56 | 0.40 |
| 2:D:13:VAL:CG1 | 2:D:14:ASP:N | 2.84 | 0.40 |
| 1:E:427:ILE:HD12 | 1:E:521:PHE:CD1 | 2.56 | 0.40 |
| 1:C:1163:TYR:CZ | 1:C:1176:LYS:HB2 | 2.56 | 0.40 |
| 1:C:873:ASN:N | 1:C:899:ASN:O | 2.41 | 0.40 |
| 2:F:579:PRO:C | 2:F:581:SER:N | 2.74 | 0.40 |
| 2:D:589:ILE:HG13 | 2:D:641:TYR:OH | 2.21 | 0.40 |
| 2:B:373:ILE:HG22 | 2:B:379:VAL:HG22 | 2.04 | 0.40 |
| 2:F:92:ASN:O | 2:F:95:GLY:N | 2.55 | 0.40 |
| 2:F:153:TYR:HB2 | 2:F:165:MET:O | 2.21 | 0.40 |
| 1:C:22:LYS:HG3 | 1:C:23:PRO:HD2 | 2.02 | 0.40 |
| 2:B:654:LYS:HA | 2:B:657:LEU:HD12 | 2.02 | 0.40 |
| 2:B:403:ILE:HA | 2:B:404:PRO:HD3 | 1.95 | 0.40 |
| 1:A:39:ILE:HG12 | 1:A:148:VAL:HB | 2.04 | 0.40 |
| 1:E:975:PHE:CE2 | 1:E:977:TYR:HB3 | 2.57 | 0.40 |
| 2:D:540:GLU:HB3 | 2:D:555:PRO:CD | 2.52 | 0.40 |
| 1:E:169:ASN:OD1 | 2:B:461:THR:HA | 2.20 | 0.40 |
| 1:E:1000:LEU:N | 1:E:1000:LEU:HD12 | 2.36 | 0.40 |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|----------------------|--------------------------|-------------------|
| 1:A:280:ARG:NH2 | 1:C:420:GLY:O[3_564] | 2.16 | 0.04 |

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|------------|----------|-------------|----|
| 1 | A | 1225/1252 (98%) | 999 (82%) | 159 (13%) | 67 (6%) | 2 | 13 |
| 1 | C | 1225/1252 (98%) | 995 (81%) | 166 (14%) | 64 (5%) | 2 | 14 |
| 1 | E | 1225/1252 (98%) | 997 (81%) | 162 (13%) | 66 (5%) | 2 | 13 |
| 2 | B | 1084/1163 (93%) | 832 (77%) | 183 (17%) | 69 (6%) | 2 | 9 |
| 2 | D | 1084/1163 (93%) | 835 (77%) | 179 (16%) | 70 (6%) | 1 | 9 |
| 2 | F | 1084/1163 (93%) | 838 (77%) | 177 (16%) | 69 (6%) | 2 | 9 |
| All | All | 6927/7245 (96%) | 5496 (79%) | 1026 (15%) | 405 (6%) | 2 | 11 |

All (405) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 119 | THR |
| 1 | A | 199 | ILE |
| 1 | A | 291 | VAL |
| 1 | A | 419 | LYS |
| 1 | A | 449 | ASN |
| 1 | A | 469 | ASP |
| 1 | A | 483 | LEU |
| 1 | A | 485 | ASP |
| 1 | A | 490 | LEU |
| 1 | A | 499 | PRO |
| 1 | A | 738 | TYR |
| 1 | A | 740 | ILE |
| 1 | A | 743 | ILE |
| 1 | A | 928 | ASN |
| 1 | A | 978 | GLY |
| 1 | A | 979 | ASN |
| 1 | A | 1068 | ASN |
| 1 | A | 1074 | ASP |
| 1 | A | 1103 | ASP |
| 1 | A | 1104 | SER |
| 1 | A | 1109 | ASN |
| 1 | A | 1156 | LYS |
| 1 | C | 119 | THR |
| 1 | C | 199 | ILE |
| 1 | C | 291 | VAL |
| 1 | C | 419 | LYS |
| 1 | C | 449 | ASN |
| 1 | C | 469 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | C | 483 | LEU |
| 1 | C | 485 | ASP |
| 1 | C | 490 | LEU |
| 1 | C | 499 | PRO |
| 1 | C | 738 | TYR |
| 1 | C | 740 | ILE |
| 1 | C | 743 | ILE |
| 1 | C | 928 | ASN |
| 1 | C | 978 | GLY |
| 1 | C | 979 | ASN |
| 1 | C | 1068 | ASN |
| 1 | C | 1074 | ASP |
| 1 | C | 1103 | ASP |
| 1 | C | 1104 | SER |
| 1 | C | 1109 | ASN |
| 1 | C | 1156 | LYS |
| 1 | E | 119 | THR |
| 1 | E | 199 | ILE |
| 1 | E | 291 | VAL |
| 1 | E | 419 | LYS |
| 1 | E | 449 | ASN |
| 1 | E | 469 | ASP |
| 1 | E | 483 | LEU |
| 1 | E | 485 | ASP |
| 1 | E | 490 | LEU |
| 1 | E | 499 | PRO |
| 1 | E | 738 | TYR |
| 1 | E | 740 | ILE |
| 1 | E | 743 | ILE |
| 1 | E | 928 | ASN |
| 1 | E | 978 | GLY |
| 1 | E | 979 | ASN |
| 1 | E | 1068 | ASN |
| 1 | E | 1074 | ASP |
| 1 | E | 1103 | ASP |
| 1 | E | 1104 | SER |
| 1 | E | 1109 | ASN |
| 1 | E | 1156 | LYS |
| 2 | B | 9 | ILE |
| 2 | B | 10 | ASP |
| 2 | B | 36 | ALA |
| 2 | B | 37 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | B | 155 | LYS |
| 2 | B | 252 | ASP |
| 2 | B | 253 | LYS |
| 2 | B | 273 | ILE |
| 2 | B | 277 | ASN |
| 2 | B | 279 | ILE |
| 2 | B | 285 | LEU |
| 2 | B | 416 | SER |
| 2 | B | 439 | PRO |
| 2 | B | 480 | ILE |
| 2 | B | 604 | LEU |
| 2 | B | 709 | ASN |
| 2 | B | 848 | ALA |
| 2 | B | 856 | ASN |
| 2 | B | 861 | ASN |
| 2 | B | 914 | ASN |
| 2 | B | 991 | SER |
| 2 | B | 1057 | LEU |
| 2 | B | 1102 | ASP |
| 2 | B | 1107 | ALA |
| 2 | B | 1128 | ASN |
| 2 | D | 9 | ILE |
| 2 | D | 10 | ASP |
| 2 | D | 36 | ALA |
| 2 | D | 37 | PRO |
| 2 | D | 155 | LYS |
| 2 | D | 252 | ASP |
| 2 | D | 253 | LYS |
| 2 | D | 273 | ILE |
| 2 | D | 277 | ASN |
| 2 | D | 279 | ILE |
| 2 | D | 285 | LEU |
| 2 | D | 416 | SER |
| 2 | D | 439 | PRO |
| 2 | D | 480 | ILE |
| 2 | D | 604 | LEU |
| 2 | D | 709 | ASN |
| 2 | D | 848 | ALA |
| 2 | D | 856 | ASN |
| 2 | D | 861 | ASN |
| 2 | D | 914 | ASN |
| 2 | D | 991 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | D | 1057 | LEU |
| 2 | D | 1102 | ASP |
| 2 | D | 1128 | ASN |
| 2 | F | 9 | ILE |
| 2 | F | 10 | ASP |
| 2 | F | 36 | ALA |
| 2 | F | 37 | PRO |
| 2 | F | 155 | LYS |
| 2 | F | 252 | ASP |
| 2 | F | 253 | LYS |
| 2 | F | 273 | ILE |
| 2 | F | 277 | ASN |
| 2 | F | 279 | ILE |
| 2 | F | 285 | LEU |
| 2 | F | 416 | SER |
| 2 | F | 439 | PRO |
| 2 | F | 480 | ILE |
| 2 | F | 604 | LEU |
| 2 | F | 709 | ASN |
| 2 | F | 848 | ALA |
| 2 | F | 856 | ASN |
| 2 | F | 861 | ASN |
| 2 | F | 914 | ASN |
| 2 | F | 991 | SER |
| 2 | F | 1057 | LEU |
| 2 | F | 1102 | ASP |
| 2 | F | 1107 | ALA |
| 2 | F | 1128 | ASN |
| 1 | A | 362 | ASN |
| 1 | A | 417 | SER |
| 1 | A | 420 | GLY |
| 1 | A | 444 | ASN |
| 1 | A | 530 | GLU |
| 1 | A | 569 | ALA |
| 1 | A | 611 | ASN |
| 1 | A | 728 | LEU |
| 1 | A | 731 | LYS |
| 1 | A | 739 | ASP |
| 1 | A | 742 | GLN |
| 1 | A | 819 | LEU |
| 1 | A | 835 | ILE |
| 1 | A | 1116 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1230 | ARG |
| 1 | C | 362 | ASN |
| 1 | C | 417 | SER |
| 1 | C | 420 | GLY |
| 1 | C | 444 | ASN |
| 1 | C | 530 | GLU |
| 1 | C | 569 | ALA |
| 1 | C | 611 | ASN |
| 1 | C | 728 | LEU |
| 1 | C | 731 | LYS |
| 1 | C | 739 | ASP |
| 1 | C | 742 | GLN |
| 1 | C | 819 | LEU |
| 1 | C | 835 | ILE |
| 1 | C | 1027 | ASP |
| 1 | C | 1116 | LEU |
| 1 | C | 1230 | ARG |
| 1 | E | 362 | ASN |
| 1 | E | 417 | SER |
| 1 | E | 420 | GLY |
| 1 | E | 444 | ASN |
| 1 | E | 530 | GLU |
| 1 | E | 569 | ALA |
| 1 | E | 611 | ASN |
| 1 | E | 728 | LEU |
| 1 | E | 731 | LYS |
| 1 | E | 739 | ASP |
| 1 | E | 742 | GLN |
| 1 | E | 819 | LEU |
| 1 | E | 835 | ILE |
| 1 | E | 1116 | LEU |
| 1 | E | 1230 | ARG |
| 2 | B | 15 | ASN |
| 2 | B | 81 | ALA |
| 2 | B | 114 | THR |
| 2 | B | 419 | ASP |
| 2 | B | 501 | LEU |
| 2 | B | 540 | GLU |
| 2 | B | 676 | GLU |
| 2 | B | 710 | ILE |
| 2 | B | 811 | GLN |
| 2 | B | 822 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | B | 947 | ASP |
| 2 | B | 1012 | GLU |
| 2 | B | 1014 | ILE |
| 2 | D | 15 | ASN |
| 2 | D | 81 | ALA |
| 2 | D | 114 | THR |
| 2 | D | 419 | ASP |
| 2 | D | 501 | LEU |
| 2 | D | 540 | GLU |
| 2 | D | 676 | GLU |
| 2 | D | 710 | ILE |
| 2 | D | 811 | GLN |
| 2 | D | 822 | LYS |
| 2 | D | 947 | ASP |
| 2 | D | 1012 | GLU |
| 2 | D | 1014 | ILE |
| 2 | D | 1107 | ALA |
| 2 | F | 15 | ASN |
| 2 | F | 81 | ALA |
| 2 | F | 114 | THR |
| 2 | F | 419 | ASP |
| 2 | F | 501 | LEU |
| 2 | F | 540 | GLU |
| 2 | F | 676 | GLU |
| 2 | F | 710 | ILE |
| 2 | F | 811 | GLN |
| 2 | F | 822 | LYS |
| 2 | F | 947 | ASP |
| 2 | F | 1012 | GLU |
| 2 | F | 1014 | ILE |
| 1 | A | 138 | ASN |
| 1 | A | 293 | ASN |
| 1 | A | 398 | PRO |
| 1 | A | 451 | PRO |
| 1 | A | 507 | SER |
| 1 | A | 583 | PHE |
| 1 | A | 648 | PHE |
| 1 | A | 666 | ALA |
| 1 | A | 1027 | ASP |
| 1 | C | 138 | ASN |
| 1 | C | 293 | ASN |
| 1 | C | 398 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | C | 451 | PRO |
| 1 | C | 507 | SER |
| 1 | C | 583 | PHE |
| 1 | C | 648 | PHE |
| 1 | C | 666 | ALA |
| 1 | E | 138 | ASN |
| 1 | E | 293 | ASN |
| 1 | E | 398 | PRO |
| 1 | E | 451 | PRO |
| 1 | E | 507 | SER |
| 1 | E | 583 | PHE |
| 1 | E | 648 | PHE |
| 1 | E | 666 | ALA |
| 1 | E | 1027 | ASP |
| 1 | E | 1083 | ASP |
| 2 | B | 16 | LYS |
| 2 | B | 113 | ASN |
| 2 | B | 153 | TYR |
| 2 | B | 154 | LYS |
| 2 | B | 276 | ASN |
| 2 | B | 542 | GLN |
| 2 | B | 857 | ASP |
| 2 | B | 922 | ASN |
| 2 | B | 924 | SER |
| 2 | B | 972 | SER |
| 2 | B | 1018 | ASN |
| 2 | D | 16 | LYS |
| 2 | D | 113 | ASN |
| 2 | D | 153 | TYR |
| 2 | D | 154 | LYS |
| 2 | D | 276 | ASN |
| 2 | D | 296 | LYS |
| 2 | D | 417 | TYR |
| 2 | D | 542 | GLN |
| 2 | D | 922 | ASN |
| 2 | D | 924 | SER |
| 2 | D | 972 | SER |
| 2 | D | 1018 | ASN |
| 2 | F | 16 | LYS |
| 2 | F | 113 | ASN |
| 2 | F | 154 | LYS |
| 2 | F | 276 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | F | 417 | TYR |
| 2 | F | 922 | ASN |
| 2 | F | 924 | SER |
| 2 | F | 972 | SER |
| 2 | F | 1018 | ASN |
| 1 | A | 454 | ILE |
| 1 | A | 488 | LEU |
| 1 | A | 498 | ILE |
| 1 | A | 913 | LYS |
| 1 | A | 915 | PHE |
| 1 | A | 927 | ASP |
| 1 | A | 1083 | ASP |
| 1 | A | 1117 | LEU |
| 1 | C | 454 | ILE |
| 1 | C | 488 | LEU |
| 1 | C | 498 | ILE |
| 1 | C | 913 | LYS |
| 1 | C | 927 | ASP |
| 1 | C | 1083 | ASP |
| 1 | C | 1117 | LEU |
| 1 | E | 468 | LEU |
| 1 | E | 498 | ILE |
| 1 | E | 913 | LYS |
| 1 | E | 927 | ASP |
| 1 | E | 988 | ASN |
| 2 | B | 66 | SER |
| 2 | B | 296 | LYS |
| 2 | B | 417 | TYR |
| 2 | B | 442 | LYS |
| 2 | B | 680 | ILE |
| 2 | B | 1093 | THR |
| 2 | B | 1140 | TYR |
| 2 | B | 1147 | LEU |
| 2 | D | 275 | ASN |
| 2 | D | 295 | VAL |
| 2 | D | 442 | LYS |
| 2 | D | 680 | ILE |
| 2 | D | 857 | ASP |
| 2 | D | 878 | GLN |
| 2 | D | 1093 | THR |
| 2 | D | 1140 | TYR |
| 2 | D | 1147 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | F | 153 | TYR |
| 2 | F | 275 | ASN |
| 2 | F | 295 | VAL |
| 2 | F | 296 | LYS |
| 2 | F | 442 | LYS |
| 2 | F | 542 | GLN |
| 2 | F | 857 | ASP |
| 2 | F | 1140 | TYR |
| 2 | F | 1147 | LEU |
| 1 | A | 146 | PRO |
| 1 | A | 292 | SER |
| 1 | A | 400 | THR |
| 1 | A | 468 | LEU |
| 1 | A | 791 | THR |
| 1 | A | 910 | ASN |
| 1 | A | 988 | ASN |
| 1 | A | 1139 | ASP |
| 1 | C | 50 | THR |
| 1 | C | 146 | PRO |
| 1 | C | 292 | SER |
| 1 | C | 468 | LEU |
| 1 | C | 791 | THR |
| 1 | C | 915 | PHE |
| 1 | C | 988 | ASN |
| 1 | C | 1094 | PRO |
| 1 | E | 146 | PRO |
| 1 | E | 292 | SER |
| 1 | E | 400 | THR |
| 1 | E | 454 | ILE |
| 1 | E | 488 | LEU |
| 1 | E | 791 | THR |
| 1 | E | 910 | ASN |
| 1 | E | 915 | PHE |
| 1 | E | 1094 | PRO |
| 1 | E | 1117 | LEU |
| 2 | B | 275 | ASN |
| 2 | B | 295 | VAL |
| 2 | B | 433 | ASN |
| 2 | B | 478 | ASN |
| 2 | B | 878 | GLN |
| 2 | D | 14 | ASP |
| 2 | D | 66 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | D | 328 | LYS |
| 2 | D | 433 | ASN |
| 2 | D | 478 | ASN |
| 2 | F | 66 | SER |
| 2 | F | 433 | ASN |
| 2 | F | 478 | ASN |
| 2 | F | 680 | ILE |
| 2 | F | 878 | GLN |
| 2 | F | 1093 | THR |
| 1 | A | 1094 | PRO |
| 1 | E | 50 | THR |
| 2 | B | 14 | ASP |
| 2 | B | 328 | LYS |
| 2 | B | 429 | ILE |
| 2 | B | 1101 | VAL |
| 2 | D | 186 | ALA |
| 2 | D | 429 | ILE |
| 2 | D | 1101 | VAL |
| 2 | F | 14 | ASP |
| 2 | F | 328 | LYS |
| 2 | F | 1101 | VAL |
| 1 | C | 604 | PRO |
| 2 | B | 251 | ILE |
| 2 | D | 142 | GLY |
| 2 | D | 251 | ILE |
| 2 | F | 142 | GLY |
| 2 | F | 251 | ILE |
| 2 | F | 429 | ILE |
| 1 | A | 604 | PRO |
| 1 | C | 239 | PRO |
| 2 | B | 93 | VAL |
| 2 | B | 142 | GLY |
| 2 | D | 93 | VAL |
| 2 | F | 93 | VAL |
| 1 | A | 154 | GLU |
| 1 | A | 803 | ILE |
| 1 | C | 803 | ILE |
| 1 | E | 604 | PRO |
| 1 | A | 239 | PRO |
| 1 | E | 803 | ILE |
| 1 | E | 154 | GLU |

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 | 1125/1155 (97%) | 1013 (90%) | 112 (10%) | 9 | 32 |
| 1 | C | 1125/1155 (97%) | 1011 (90%) | 114 (10%) | 9 | 32 |
| 1 | E | 1125/1155 (97%) | 1014 (90%) | 111 (10%) | 10 | 33 |
| 2 | B | 990/1103 (90%) | 915 (92%) | 75 (8%) | 16 | 49 |
| 2 | D | 990/1103 (90%) | 915 (92%) | 75 (8%) | 16 | 49 |
| 2 | F | 990/1103 (90%) | 914 (92%) | 76 (8%) | 16 | 48 |
| All | All | 6345/6774 (94%) | 5782 (91%) | 563 (9%) | 12 | 39 |

All (563) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 16 | ARG |
| 1 | A | 17 | THR |
| 1 | A | 19 | LEU |
| 1 | A | 50 | THR |
| 1 | A | 53 | GLN |
| 1 | A | 65 | ASP |
| 1 | A | 93 | ARG |
| 1 | A | 108 | SER |
| 1 | A | 121 | ASP |
| 1 | A | 122 | ASN |
| 1 | A | 136 | PHE |
| 1 | A | 144 | LEU |
| 1 | A | 180 | SER |
| 1 | A | 191 | SER |
| 1 | A | 194 | PHE |
| 1 | A | 196 | ASP |
| 1 | A | 197 | ASN |
| 1 | A | 201 | GLU |
| 1 | A | 221 | LEU |
| 1 | A | 230 | THR |
| 1 | A | 258 | ASN |
| 1 | A | 270 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 273 | THR |
| 1 | A | 278 | ASP |
| 1 | A | 281 | LYS |
| 1 | A | 290 | GLN |
| 1 | A | 301 | ASP |
| 1 | A | 305 | GLU |
| 1 | A | 326 | ASP |
| 1 | A | 336 | GLU |
| 1 | A | 348 | ARG |
| 1 | A | 354 | GLN |
| 1 | A | 402 | ARG |
| 1 | A | 421 | ILE |
| 1 | A | 428 | GLU |
| 1 | A | 436 | PHE |
| 1 | A | 440 | GLU |
| 1 | A | 441 | ASN |
| 1 | A | 443 | TYR |
| 1 | A | 447 | ASN |
| 1 | A | 455 | ASP |
| 1 | A | 456 | ASP |
| 1 | A | 464 | TYR |
| 1 | A | 465 | GLU |
| 1 | A | 468 | LEU |
| 1 | A | 475 | PHE |
| 1 | A | 486 | GLU |
| 1 | A | 487 | LYS |
| 1 | A | 491 | THR |
| 1 | A | 506 | THR |
| 1 | A | 515 | ASN |
| 1 | A | 532 | GLU |
| 1 | A | 554 | PHE |
| 1 | A | 591 | SER |
| 1 | A | 598 | ASP |
| 1 | A | 608 | LEU |
| 1 | A | 625 | LEU |
| 1 | A | 634 | LEU |
| 1 | A | 658 | ASP |
| 1 | A | 674 | ARG |
| 1 | A | 690 | MET |
| 1 | A | 696 | GLN |
| 1 | A | 703 | GLN |
| 1 | A | 705 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 716 | LYS |
| 1 | A | 725 | SER |
| 1 | A | 733 | GLU |
| 1 | A | 734 | LEU |
| 1 | A | 735 | THR |
| 1 | A | 738 | TYR |
| 1 | A | 755 | MET |
| 1 | A | 781 | LYS |
| 1 | A | 795 | ASN |
| 1 | A | 821 | ASN |
| 1 | A | 838 | SER |
| 1 | A | 839 | TYR |
| 1 | A | 842 | LYS |
| 1 | A | 869 | ASP |
| 1 | A | 886 | ASN |
| 1 | A | 893 | ASP |
| 1 | A | 897 | GLU |
| 1 | A | 903 | ASN |
| 1 | A | 904 | ASP |
| 1 | A | 905 | TYR |
| 1 | A | 907 | ILE |
| 1 | A | 918 | SER |
| 1 | A | 930 | ILE |
| 1 | A | 938 | THR |
| 1 | A | 1002 | ASP |
| 1 | A | 1016 | SER |
| 1 | A | 1020 | LEU |
| 1 | A | 1027 | ASP |
| 1 | A | 1037 | SER |
| 1 | A | 1040 | ARG |
| 1 | A | 1045 | ARG |
| 1 | A | 1052 | LYS |
| 1 | A | 1053 | GLU |
| 1 | A | 1083 | ASP |
| 1 | A | 1088 | LEU |
| 1 | A | 1099 | ASP |
| 1 | A | 1103 | ASP |
| 1 | A | 1104 | SER |
| 1 | A | 1105 | THR |
| 1 | A | 1134 | ASN |
| 1 | A | 1143 | ARG |
| 1 | A | 1169 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1170 | ASN |
| 1 | A | 1197 | CYS |
| 1 | A | 1205 | ASN |
| 1 | A | 1217 | ASP |
| 1 | A | 1230 | ARG |
| 1 | A | 1250 | GLN |
| 1 | C | 16 | ARG |
| 1 | C | 17 | THR |
| 1 | C | 19 | LEU |
| 1 | C | 50 | THR |
| 1 | C | 53 | GLN |
| 1 | C | 65 | ASP |
| 1 | C | 93 | ARG |
| 1 | C | 108 | SER |
| 1 | C | 121 | ASP |
| 1 | C | 122 | ASN |
| 1 | C | 136 | PHE |
| 1 | C | 144 | LEU |
| 1 | C | 180 | SER |
| 1 | C | 191 | SER |
| 1 | C | 194 | PHE |
| 1 | C | 196 | ASP |
| 1 | C | 197 | ASN |
| 1 | C | 201 | GLU |
| 1 | C | 221 | LEU |
| 1 | C | 230 | THR |
| 1 | C | 258 | ASN |
| 1 | C | 270 | ASP |
| 1 | C | 273 | THR |
| 1 | C | 278 | ASP |
| 1 | C | 281 | LYS |
| 1 | C | 290 | GLN |
| 1 | C | 301 | ASP |
| 1 | C | 305 | GLU |
| 1 | C | 326 | ASP |
| 1 | C | 336 | GLU |
| 1 | C | 348 | ARG |
| 1 | C | 354 | GLN |
| 1 | C | 402 | ARG |
| 1 | C | 421 | ILE |
| 1 | C | 422 | ARG |
| 1 | C | 428 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 436 | PHE |
| 1 | C | 440 | GLU |
| 1 | C | 441 | ASN |
| 1 | C | 443 | TYR |
| 1 | C | 447 | ASN |
| 1 | C | 456 | ASP |
| 1 | C | 464 | TYR |
| 1 | C | 465 | GLU |
| 1 | C | 468 | LEU |
| 1 | C | 475 | PHE |
| 1 | C | 486 | GLU |
| 1 | C | 487 | LYS |
| 1 | C | 491 | THR |
| 1 | C | 506 | THR |
| 1 | C | 515 | ASN |
| 1 | C | 532 | GLU |
| 1 | C | 554 | PHE |
| 1 | C | 591 | SER |
| 1 | C | 598 | ASP |
| 1 | C | 608 | LEU |
| 1 | C | 625 | LEU |
| 1 | C | 634 | LEU |
| 1 | C | 658 | ASP |
| 1 | C | 690 | MET |
| 1 | C | 696 | GLN |
| 1 | C | 703 | GLN |
| 1 | C | 705 | TYR |
| 1 | C | 716 | LYS |
| 1 | C | 725 | SER |
| 1 | C | 733 | GLU |
| 1 | C | 734 | LEU |
| 1 | C | 735 | THR |
| 1 | C | 738 | TYR |
| 1 | C | 755 | MET |
| 1 | C | 781 | LYS |
| 1 | C | 795 | ASN |
| 1 | C | 821 | ASN |
| 1 | C | 831 | THR |
| 1 | C | 838 | SER |
| 1 | C | 839 | TYR |
| 1 | C | 842 | LYS |
| 1 | C | 869 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | C | 886 | ASN |
| 1 | C | 893 | ASP |
| 1 | C | 897 | GLU |
| 1 | C | 903 | ASN |
| 1 | C | 904 | ASP |
| 1 | C | 905 | TYR |
| 1 | C | 907 | ILE |
| 1 | C | 918 | SER |
| 1 | C | 930 | ILE |
| 1 | C | 938 | THR |
| 1 | C | 1002 | ASP |
| 1 | C | 1016 | SER |
| 1 | C | 1020 | LEU |
| 1 | C | 1027 | ASP |
| 1 | C | 1037 | SER |
| 1 | C | 1040 | ARG |
| 1 | C | 1045 | ARG |
| 1 | C | 1052 | LYS |
| 1 | C | 1053 | GLU |
| 1 | C | 1083 | ASP |
| 1 | C | 1088 | LEU |
| 1 | C | 1099 | ASP |
| 1 | C | 1103 | ASP |
| 1 | C | 1104 | SER |
| 1 | C | 1105 | THR |
| 1 | C | 1134 | ASN |
| 1 | C | 1143 | ARG |
| 1 | C | 1146 | ASP |
| 1 | C | 1169 | THR |
| 1 | C | 1170 | ASN |
| 1 | C | 1183 | ARG |
| 1 | C | 1197 | CYS |
| 1 | C | 1205 | ASN |
| 1 | C | 1217 | ASP |
| 1 | C | 1230 | ARG |
| 1 | C | 1250 | GLN |
| 1 | E | 16 | ARG |
| 1 | E | 17 | THR |
| 1 | E | 19 | LEU |
| 1 | E | 50 | THR |
| 1 | E | 53 | GLN |
| 1 | E | 65 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 93 | ARG |
| 1 | E | 108 | SER |
| 1 | E | 121 | ASP |
| 1 | E | 122 | ASN |
| 1 | E | 136 | PHE |
| 1 | E | 144 | LEU |
| 1 | E | 180 | SER |
| 1 | E | 191 | SER |
| 1 | E | 194 | PHE |
| 1 | E | 196 | ASP |
| 1 | E | 197 | ASN |
| 1 | E | 201 | GLU |
| 1 | E | 221 | LEU |
| 1 | E | 230 | THR |
| 1 | E | 258 | ASN |
| 1 | E | 273 | THR |
| 1 | E | 278 | ASP |
| 1 | E | 281 | LYS |
| 1 | E | 290 | GLN |
| 1 | E | 305 | GLU |
| 1 | E | 326 | ASP |
| 1 | E | 336 | GLU |
| 1 | E | 348 | ARG |
| 1 | E | 354 | GLN |
| 1 | E | 367 | SER |
| 1 | E | 402 | ARG |
| 1 | E | 421 | ILE |
| 1 | E | 422 | ARG |
| 1 | E | 428 | GLU |
| 1 | E | 436 | PHE |
| 1 | E | 440 | GLU |
| 1 | E | 441 | ASN |
| 1 | E | 443 | TYR |
| 1 | E | 447 | ASN |
| 1 | E | 455 | ASP |
| 1 | E | 456 | ASP |
| 1 | E | 464 | TYR |
| 1 | E | 465 | GLU |
| 1 | E | 468 | LEU |
| 1 | E | 475 | PHE |
| 1 | E | 486 | GLU |
| 1 | E | 487 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | E | 491 | THR |
| 1 | E | 506 | THR |
| 1 | E | 532 | GLU |
| 1 | E | 554 | PHE |
| 1 | E | 591 | SER |
| 1 | E | 598 | ASP |
| 1 | E | 608 | LEU |
| 1 | E | 625 | LEU |
| 1 | E | 634 | LEU |
| 1 | E | 658 | ASP |
| 1 | E | 690 | MET |
| 1 | E | 696 | GLN |
| 1 | E | 703 | GLN |
| 1 | E | 705 | TYR |
| 1 | E | 716 | LYS |
| 1 | E | 725 | SER |
| 1 | E | 733 | GLU |
| 1 | E | 734 | LEU |
| 1 | E | 735 | THR |
| 1 | E | 738 | TYR |
| 1 | E | 755 | MET |
| 1 | E | 781 | LYS |
| 1 | E | 795 | ASN |
| 1 | E | 821 | ASN |
| 1 | E | 838 | SER |
| 1 | E | 839 | TYR |
| 1 | E | 842 | LYS |
| 1 | E | 869 | ASP |
| 1 | E | 886 | ASN |
| 1 | E | 893 | ASP |
| 1 | E | 897 | GLU |
| 1 | E | 903 | ASN |
| 1 | E | 904 | ASP |
| 1 | E | 905 | TYR |
| 1 | E | 907 | ILE |
| 1 | E | 918 | SER |
| 1 | E | 930 | ILE |
| 1 | E | 938 | THR |
| 1 | E | 1002 | ASP |
| 1 | E | 1016 | SER |
| 1 | E | 1020 | LEU |
| 1 | E | 1027 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | E | 1037 | SER |
| 1 | E | 1040 | ARG |
| 1 | E | 1045 | ARG |
| 1 | E | 1052 | LYS |
| 1 | E | 1053 | GLU |
| 1 | E | 1083 | ASP |
| 1 | E | 1088 | LEU |
| 1 | E | 1099 | ASP |
| 1 | E | 1103 | ASP |
| 1 | E | 1104 | SER |
| 1 | E | 1105 | THR |
| 1 | E | 1128 | LYS |
| 1 | E | 1134 | ASN |
| 1 | E | 1143 | ARG |
| 1 | E | 1169 | THR |
| 1 | E | 1170 | ASN |
| 1 | E | 1197 | CYS |
| 1 | E | 1205 | ASN |
| 1 | E | 1217 | ASP |
| 1 | E | 1230 | ARG |
| 1 | E | 1250 | GLN |
| 2 | B | 14 | ASP |
| 2 | B | 23 | SER |
| 2 | B | 41 | ILE |
| 2 | B | 63 | ILE |
| 2 | B | 68 | PHE |
| 2 | B | 70 | SER |
| 2 | B | 152 | TYR |
| 2 | B | 153 | TYR |
| 2 | B | 179 | ASP |
| 2 | B | 207 | ASP |
| 2 | B | 248 | TYR |
| 2 | B | 253 | LYS |
| 2 | B | 267 | ASN |
| 2 | B | 272 | LYS |
| 2 | B | 291 | PHE |
| 2 | B | 300 | GLU |
| 2 | B | 304 | SER |
| 2 | B | 319 | ASN |
| 2 | B | 335 | TYR |
| 2 | B | 351 | THR |
| 2 | B | 400 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | B | 435 | GLU |
| 2 | B | 438 | TYR |
| 2 | B | 453 | ILE |
| 2 | B | 481 | ASN |
| 2 | B | 483 | SER |
| 2 | B | 484 | SER |
| 2 | B | 491 | SER |
| 2 | B | 499 | SER |
| 2 | B | 504 | THR |
| 2 | B | 518 | ASP |
| 2 | B | 566 | THR |
| 2 | B | 570 | PHE |
| 2 | B | 580 | ILE |
| 2 | B | 588 | ASN |
| 2 | B | 593 | LYS |
| 2 | B | 601 | SER |
| 2 | B | 620 | CYS |
| 2 | B | 643 | SER |
| 2 | B | 656 | VAL |
| 2 | B | 678 | SER |
| 2 | B | 697 | ARG |
| 2 | B | 754 | ASN |
| 2 | B | 756 | ASN |
| 2 | B | 787 | ASN |
| 2 | B | 791 | GLU |
| 2 | B | 793 | LEU |
| 2 | B | 830 | LYS |
| 2 | B | 845 | LEU |
| 2 | B | 856 | ASN |
| 2 | B | 863 | LEU |
| 2 | B | 865 | ASN |
| 2 | B | 876 | LEU |
| 2 | B | 899 | PHE |
| 2 | B | 910 | ASP |
| 2 | B | 928 | TRP |
| 2 | B | 954 | GLU |
| 2 | B | 958 | GLU |
| 2 | B | 969 | SER |
| 2 | B | 974 | ASN |
| 2 | B | 986 | ASN |
| 2 | B | 987 | LYS |
| 2 | B | 1002 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | B | 1013 | GLU |
| 2 | B | 1024 | PHE |
| 2 | B | 1030 | GLU |
| 2 | B | 1075 | ASP |
| 2 | B | 1095 | ASN |
| 2 | B | 1097 | ARG |
| 2 | B | 1140 | TYR |
| 2 | B | 1142 | TRP |
| 2 | B | 1145 | CYS |
| 2 | B | 1147 | LEU |
| 2 | B | 1148 | ASN |
| 2 | B | 1158 | TRP |
| 2 | D | 14 | ASP |
| 2 | D | 23 | SER |
| 2 | D | 41 | ILE |
| 2 | D | 63 | ILE |
| 2 | D | 68 | PHE |
| 2 | D | 70 | SER |
| 2 | D | 152 | TYR |
| 2 | D | 153 | TYR |
| 2 | D | 207 | ASP |
| 2 | D | 248 | TYR |
| 2 | D | 253 | LYS |
| 2 | D | 258 | THR |
| 2 | D | 267 | ASN |
| 2 | D | 272 | LYS |
| 2 | D | 291 | PHE |
| 2 | D | 300 | GLU |
| 2 | D | 304 | SER |
| 2 | D | 319 | ASN |
| 2 | D | 335 | TYR |
| 2 | D | 351 | THR |
| 2 | D | 400 | ASN |
| 2 | D | 438 | TYR |
| 2 | D | 445 | ASP |
| 2 | D | 453 | ILE |
| 2 | D | 481 | ASN |
| 2 | D | 483 | SER |
| 2 | D | 484 | SER |
| 2 | D | 491 | SER |
| 2 | D | 499 | SER |
| 2 | D | 504 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | D | 518 | ASP |
| 2 | D | 566 | THR |
| 2 | D | 570 | PHE |
| 2 | D | 580 | ILE |
| 2 | D | 588 | ASN |
| 2 | D | 593 | LYS |
| 2 | D | 601 | SER |
| 2 | D | 620 | CYS |
| 2 | D | 643 | SER |
| 2 | D | 656 | VAL |
| 2 | D | 678 | SER |
| 2 | D | 697 | ARG |
| 2 | D | 703 | SER |
| 2 | D | 754 | ASN |
| 2 | D | 756 | ASN |
| 2 | D | 787 | ASN |
| 2 | D | 791 | GLU |
| 2 | D | 793 | LEU |
| 2 | D | 830 | LYS |
| 2 | D | 845 | LEU |
| 2 | D | 863 | LEU |
| 2 | D | 865 | ASN |
| 2 | D | 876 | LEU |
| 2 | D | 899 | PHE |
| 2 | D | 910 | ASP |
| 2 | D | 928 | TRP |
| 2 | D | 954 | GLU |
| 2 | D | 958 | GLU |
| 2 | D | 969 | SER |
| 2 | D | 974 | ASN |
| 2 | D | 986 | ASN |
| 2 | D | 987 | LYS |
| 2 | D | 1002 | LEU |
| 2 | D | 1013 | GLU |
| 2 | D | 1024 | PHE |
| 2 | D | 1030 | GLU |
| 2 | D | 1075 | ASP |
| 2 | D | 1095 | ASN |
| 2 | D | 1097 | ARG |
| 2 | D | 1140 | TYR |
| 2 | D | 1142 | TRP |
| 2 | D | 1145 | CYS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | D | 1147 | LEU |
| 2 | D | 1148 | ASN |
| 2 | D | 1158 | TRP |
| 2 | F | 14 | ASP |
| 2 | F | 23 | SER |
| 2 | F | 41 | ILE |
| 2 | F | 56 | ASP |
| 2 | F | 63 | ILE |
| 2 | F | 68 | PHE |
| 2 | F | 70 | SER |
| 2 | F | 74 | GLU |
| 2 | F | 152 | TYR |
| 2 | F | 153 | TYR |
| 2 | F | 207 | ASP |
| 2 | F | 248 | TYR |
| 2 | F | 253 | LYS |
| 2 | F | 267 | ASN |
| 2 | F | 272 | LYS |
| 2 | F | 291 | PHE |
| 2 | F | 300 | GLU |
| 2 | F | 304 | SER |
| 2 | F | 319 | ASN |
| 2 | F | 335 | TYR |
| 2 | F | 351 | THR |
| 2 | F | 400 | ASN |
| 2 | F | 438 | TYR |
| 2 | F | 445 | ASP |
| 2 | F | 453 | ILE |
| 2 | F | 481 | ASN |
| 2 | F | 483 | SER |
| 2 | F | 484 | SER |
| 2 | F | 491 | SER |
| 2 | F | 499 | SER |
| 2 | F | 504 | THR |
| 2 | F | 518 | ASP |
| 2 | F | 566 | THR |
| 2 | F | 570 | PHE |
| 2 | F | 580 | ILE |
| 2 | F | 588 | ASN |
| 2 | F | 593 | LYS |
| 2 | F | 601 | SER |
| 2 | F | 620 | CYS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | F | 643 | SER |
| 2 | F | 656 | VAL |
| 2 | F | 678 | SER |
| 2 | F | 697 | ARG |
| 2 | F | 754 | ASN |
| 2 | F | 756 | ASN |
| 2 | F | 791 | GLU |
| 2 | F | 793 | LEU |
| 2 | F | 830 | LYS |
| 2 | F | 845 | LEU |
| 2 | F | 855 | THR |
| 2 | F | 856 | ASN |
| 2 | F | 863 | LEU |
| 2 | F | 865 | ASN |
| 2 | F | 876 | LEU |
| 2 | F | 899 | PHE |
| 2 | F | 910 | ASP |
| 2 | F | 928 | TRP |
| 2 | F | 954 | GLU |
| 2 | F | 958 | GLU |
| 2 | F | 969 | SER |
| 2 | F | 974 | ASN |
| 2 | F | 986 | ASN |
| 2 | F | 987 | LYS |
| 2 | F | 1002 | LEU |
| 2 | F | 1013 | GLU |
| 2 | F | 1024 | PHE |
| 2 | F | 1030 | GLU |
| 2 | F | 1075 | ASP |
| 2 | F | 1095 | ASN |
| 2 | F | 1097 | ARG |
| 2 | F | 1140 | TYR |
| 2 | F | 1142 | TRP |
| 2 | F | 1145 | CYS |
| 2 | F | 1147 | LEU |
| 2 | F | 1148 | ASN |
| 2 | F | 1158 | TRP |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (110) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 111 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 122 | ASN |
| 1 | A | 125 | HIS |
| 1 | A | 195 | ASN |
| 1 | A | 197 | ASN |
| 1 | A | 204 | GLN |
| 1 | A | 235 | GLN |
| 1 | A | 261 | ASN |
| 1 | A | 379 | ASN |
| 1 | A | 441 | ASN |
| 1 | A | 661 | ASN |
| 1 | A | 669 | ASN |
| 1 | A | 711 | GLN |
| 1 | A | 957 | ASN |
| 1 | A | 1060 | GLN |
| 1 | A | 1170 | ASN |
| 1 | A | 1228 | HIS |
| 1 | C | 111 | ASN |
| 1 | C | 122 | ASN |
| 1 | C | 125 | HIS |
| 1 | C | 195 | ASN |
| 1 | C | 197 | ASN |
| 1 | C | 235 | GLN |
| 1 | C | 261 | ASN |
| 1 | C | 379 | ASN |
| 1 | C | 441 | ASN |
| 1 | C | 661 | ASN |
| 1 | C | 669 | ASN |
| 1 | C | 841 | ASN |
| 1 | C | 932 | ASN |
| 1 | C | 956 | HIS |
| 1 | C | 957 | ASN |
| 1 | C | 1060 | GLN |
| 1 | C | 1170 | ASN |
| 1 | E | 111 | ASN |
| 1 | E | 122 | ASN |
| 1 | E | 125 | HIS |
| 1 | E | 142 | HIS |
| 1 | E | 195 | ASN |
| 1 | E | 197 | ASN |
| 1 | E | 204 | GLN |
| 1 | E | 235 | GLN |
| 1 | E | 261 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | E | 379 | ASN |
| 1 | E | 441 | ASN |
| 1 | E | 661 | ASN |
| 1 | E | 669 | ASN |
| 1 | E | 711 | GLN |
| 1 | E | 932 | ASN |
| 1 | E | 956 | HIS |
| 1 | E | 957 | ASN |
| 1 | E | 1060 | GLN |
| 1 | E | 1170 | ASN |
| 1 | E | 1228 | HIS |
| 2 | B | 67 | ASN |
| 2 | B | 171 | GLN |
| 2 | B | 208 | ASN |
| 2 | B | 289 | GLN |
| 2 | B | 324 | HIS |
| 2 | B | 377 | ASN |
| 2 | B | 452 | ASN |
| 2 | B | 636 | GLN |
| 2 | B | 644 | GLN |
| 2 | B | 677 | ASN |
| 2 | B | 684 | ASN |
| 2 | B | 704 | GLN |
| 2 | B | 762 | HIS |
| 2 | B | 849 | ASN |
| 2 | B | 865 | ASN |
| 2 | B | 1003 | ASN |
| 2 | B | 1034 | ASN |
| 2 | B | 1130 | ASN |
| 2 | B | 1137 | ASN |
| 2 | D | 67 | ASN |
| 2 | D | 171 | GLN |
| 2 | D | 208 | ASN |
| 2 | D | 289 | GLN |
| 2 | D | 324 | HIS |
| 2 | D | 452 | ASN |
| 2 | D | 636 | GLN |
| 2 | D | 644 | GLN |
| 2 | D | 677 | ASN |
| 2 | D | 684 | ASN |
| 2 | D | 704 | GLN |
| 2 | D | 762 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | D | 849 | ASN |
| 2 | D | 865 | ASN |
| 2 | D | 925 | ASN |
| 2 | D | 1003 | ASN |
| 2 | D | 1034 | ASN |
| 2 | D | 1130 | ASN |
| 2 | D | 1137 | ASN |
| 2 | F | 67 | ASN |
| 2 | F | 92 | ASN |
| 2 | F | 171 | GLN |
| 2 | F | 208 | ASN |
| 2 | F | 289 | GLN |
| 2 | F | 324 | HIS |
| 2 | F | 452 | ASN |
| 2 | F | 636 | GLN |
| 2 | F | 644 | GLN |
| 2 | F | 677 | ASN |
| 2 | F | 684 | ASN |
| 2 | F | 704 | GLN |
| 2 | F | 762 | HIS |
| 2 | F | 865 | ASN |
| 2 | F | 1003 | ASN |
| 2 | F | 1034 | ASN |
| 2 | F | 1130 | ASN |
| 2 | F | 1137 | ASN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | A | 1235/1252 (98%) | -0.69 | 1 (0%) 95 91 | 53, 120, 189, 296 | 0 |
| 1 | C | 1235/1252 (98%) | -0.66 | 3 (0%) 95 89 | 46, 129, 207, 365 | 0 |
| 1 | E | 1235/1252 (98%) | -0.67 | 5 (0%) 93 84 | 62, 143, 214, 391 | 0 |
| 2 | B | 1114/1163 (95%) | -0.69 | 1 (0%) 95 91 | 37, 109, 179, 274 | 0 |
| 2 | D | 1114/1163 (95%) | -0.68 | 4 (0%) 93 84 | 48, 129, 194, 278 | 0 |
| 2 | F | 1114/1163 (95%) | -0.61 | 10 (0%) 85 69 | 51, 143, 220, 328 | 0 |
| All | All | 7047/7245 (97%) | -0.67 | 24 (0%) 94 87 | 37, 129, 203, 391 | 0 |

All (24) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | C | 657 | SER | 9.4 |
| 1 | E | 655 | GLY | 7.5 |
| 1 | E | 657 | SER | 7.4 |
| 2 | B | 275 | ASN | 6.8 |
| 1 | E | 656 | SER | 4.7 |
| 2 | F | 852 | ILE | 4.4 |
| 1 | E | 658 | ASP | 4.2 |
| 1 | C | 656 | SER | 3.9 |
| 2 | F | 434 | ASP | 3.7 |
| 2 | F | 1158 | TRP | 3.4 |
| 1 | C | 803 | ILE | 3.4 |
| 1 | E | 420 | GLY | 3.2 |
| 2 | F | 843 | ILE | 3.2 |
| 1 | A | 498 | ILE | 2.9 |
| 2 | D | 275 | ASN | 2.8 |
| 2 | F | 275 | ASN | 2.3 |
| 2 | F | 279 | ILE | 2.2 |
| 2 | F | 278 | TYR | 2.2 |
| 2 | F | 380 | LEU | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | D | 843 | ILE | 2.1 |
| 2 | D | 1158 | TRP | 2.1 |
| 2 | F | 873 | LEU | 2.1 |
| 2 | F | 979 | ILE | 2.0 |
| 2 | D | 863 | LEU | 2.0 |

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|----------------------------|-------|
| 3 | ZN | E | 1301 | 1/1 | 0.98 | 0.14 | - | 99,99,99,99 | 0 |
| 3 | ZN | A | 1301 | 1/1 | 0.99 | 0.18 | - | 86,86,86,86 | 0 |
| 3 | ZN | C | 1301 | 1/1 | 0.98 | 0.17 | - | 83,83,83,83 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.