



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 08:49 am GMT

PDB ID : 4LK1
Title : Crystal Structure Analysis of the E.coli holoenzyme
Authors : Bae, B.; Darst, S.A.
Deposited on : 2013-07-05
Resolution : 3.84 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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

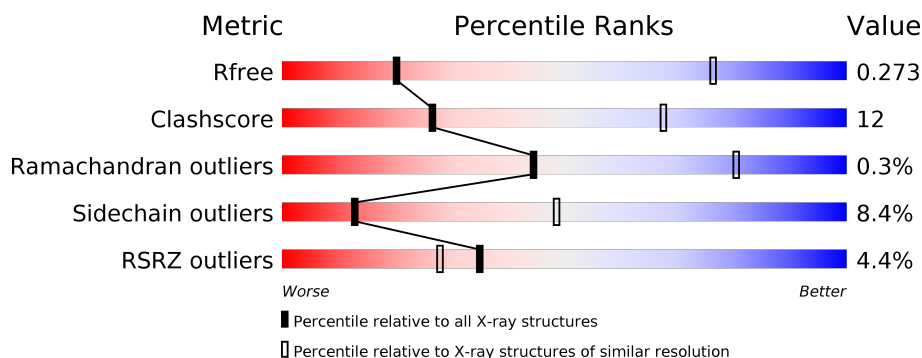
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.84 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} | 100719 | 1000 (4.12-3.56) |
| Clashscore | 112137 | 1045 (4.10-3.58) |
| Ramachandran outliers | 110173 | 1008 (4.10-3.58) |
| Sidechain outliers | 110143 | 1001 (4.10-3.58) |
| RSRZ outliers | 101464 | 1014 (4.12-3.56) |

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 | 239 | |
| 1 | B | 239 | |
| 1 | G | 239 | |
| 1 | H | 239 | |
| 2 | C | 1342 | |
| 2 | I | 1342 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3 | D | 1407 | |
| 3 | J | 1407 | |
| 4 | E | 91 | |
| 4 | K | 91 | |
| 5 | F | 613 | |
| 5 | L | 613 | |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 7 | ZN | D | 1503 | - | - | - | X |

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 57170 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 DNA-directed RNA polymerase subunit alpha.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1 | A | 224 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1730 | 1076 | 308 | 340 | 6 | | | |
| 1 | B | 220 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1687 | 1053 | 298 | 330 | 6 | | | |
| 1 | G | 228 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1750 | 1088 | 312 | 344 | 6 | | | |
| 1 | H | 217 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1667 | 1041 | 293 | 327 | 6 | | | |

There are 20 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | 235 | GLU | - | EXPRESSION TAG | UNP C9QXI7 |
| A | 236 | VAL | - | EXPRESSION TAG | UNP C9QXI7 |
| A | 237 | LEU | - | EXPRESSION TAG | UNP C9QXI7 |
| A | 238 | PHE | - | EXPRESSION TAG | UNP C9QXI7 |
| A | 239 | GLN | - | EXPRESSION TAG | UNP C9QXI7 |
| B | 235 | GLU | - | EXPRESSION TAG | UNP C9QXI7 |
| B | 236 | VAL | - | EXPRESSION TAG | UNP C9QXI7 |
| B | 237 | LEU | - | EXPRESSION TAG | UNP C9QXI7 |
| B | 238 | PHE | - | EXPRESSION TAG | UNP C9QXI7 |
| B | 239 | GLN | - | EXPRESSION TAG | UNP C9QXI7 |
| G | 235 | GLU | - | EXPRESSION TAG | UNP C9QXI7 |
| G | 236 | VAL | - | EXPRESSION TAG | UNP C9QXI7 |
| G | 237 | LEU | - | EXPRESSION TAG | UNP C9QXI7 |
| G | 238 | PHE | - | EXPRESSION TAG | UNP C9QXI7 |
| G | 239 | GLN | - | EXPRESSION TAG | UNP C9QXI7 |
| H | 235 | GLU | - | EXPRESSION TAG | UNP C9QXI7 |
| H | 236 | VAL | - | EXPRESSION TAG | UNP C9QXI7 |
| H | 237 | LEU | - | EXPRESSION TAG | UNP C9QXI7 |
| H | 238 | PHE | - | EXPRESSION TAG | UNP C9QXI7 |
| H | 239 | GLN | - | EXPRESSION TAG | UNP C9QXI7 |

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 2 | C | 1340 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 10570 | 6631 | 1841 | 2055 | 43 | | | |
| 2 | I | 1340 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 10566 | 6629 | 1840 | 2054 | 43 | | | |

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 3 | D | 1166 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 9107 | 5723 | 1634 | 1704 | 46 | | | |
| 3 | J | 1334 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 10369 | 6513 | 1850 | 1957 | 49 | | | |

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4 | E | 89 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 691 | 421 | 129 | 140 | 1 | | | |
| 4 | K | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 627 | 382 | 118 | 126 | 1 | | | |

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 5 | F | 542 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4204 | 2625 | 752 | 801 | 26 | | | |
| 5 | L | 539 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4196 | 2619 | 749 | 802 | 26 | | | |

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 6 | J | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 6 | D | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

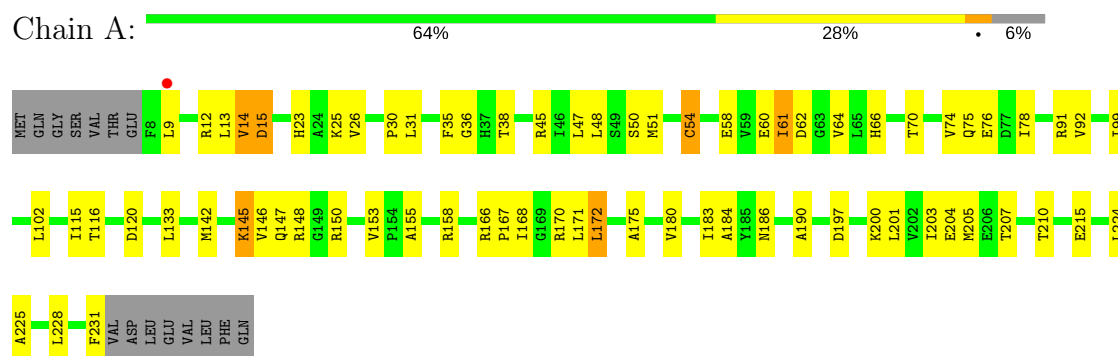
- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 7 | J | 2 | Total 2 | Zn 2 | 0 | 0 |
| 7 | D | 2 | Total 2 | Zn 2 | 0 | 0 |

3 Residue-property plots [i](#)

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

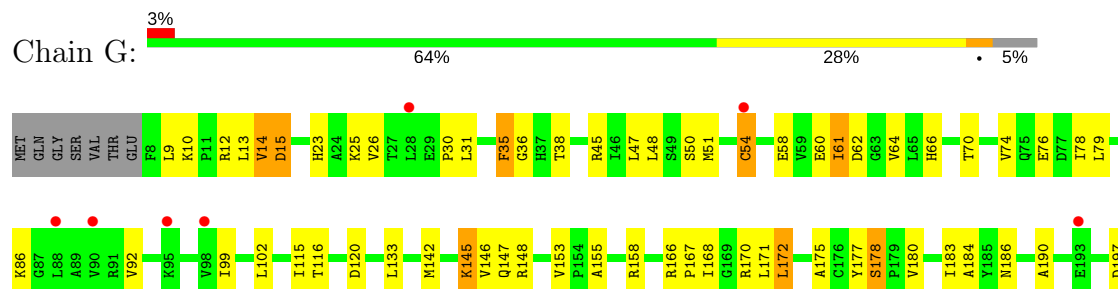
• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 1: DNA-directed RNA polymerase subunit alpha

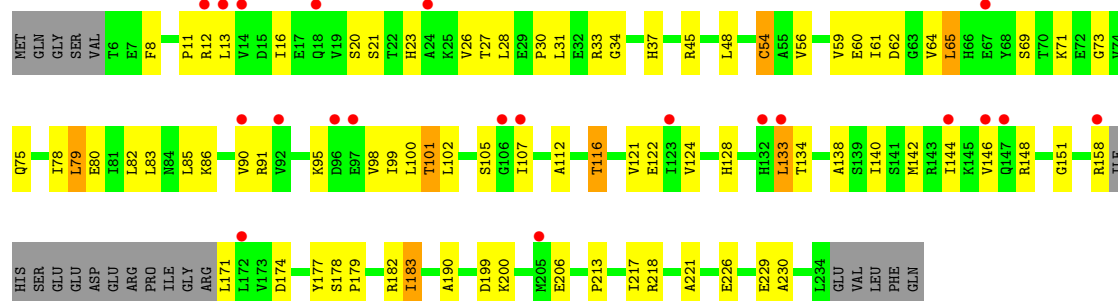


• Molecule 1: DNA-directed RNA polymerase subunit alpha

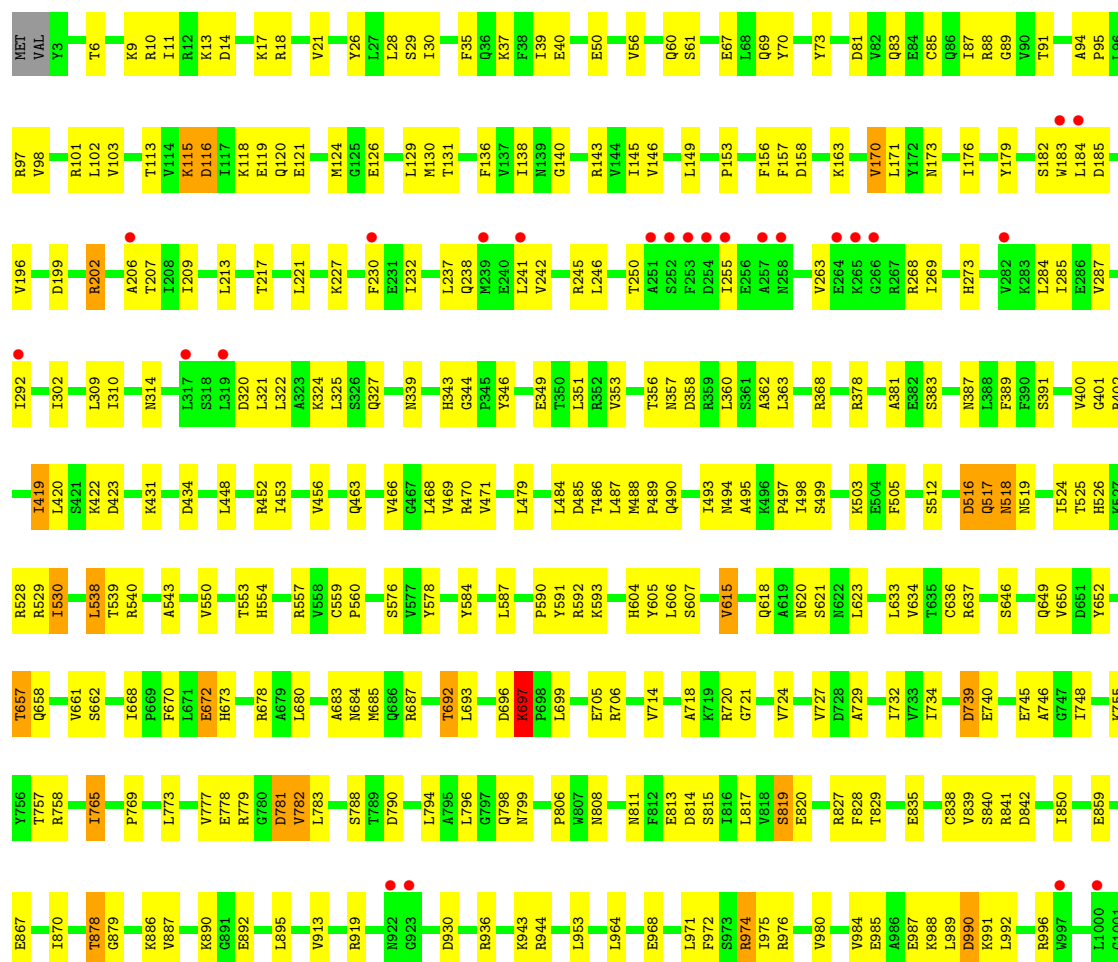


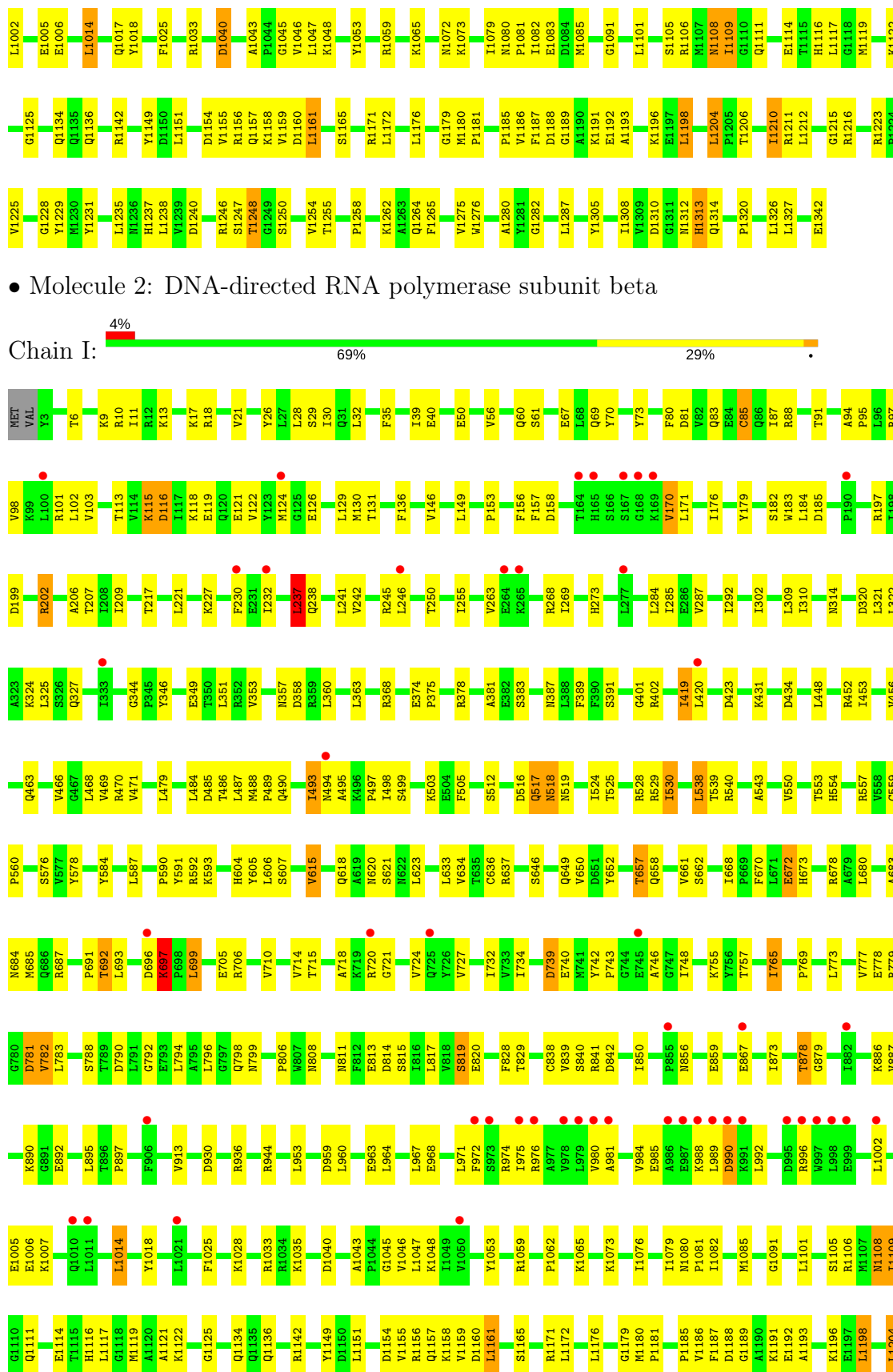


• Molecule 1: DNA-directed RNA polymerase subunit alpha

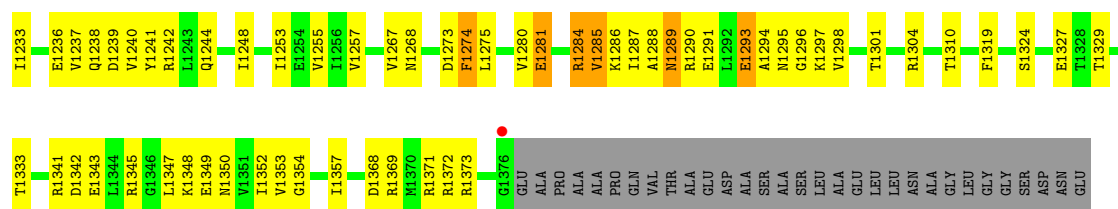


• Molecule 2: DNA-directed RNA polymerase subunit beta

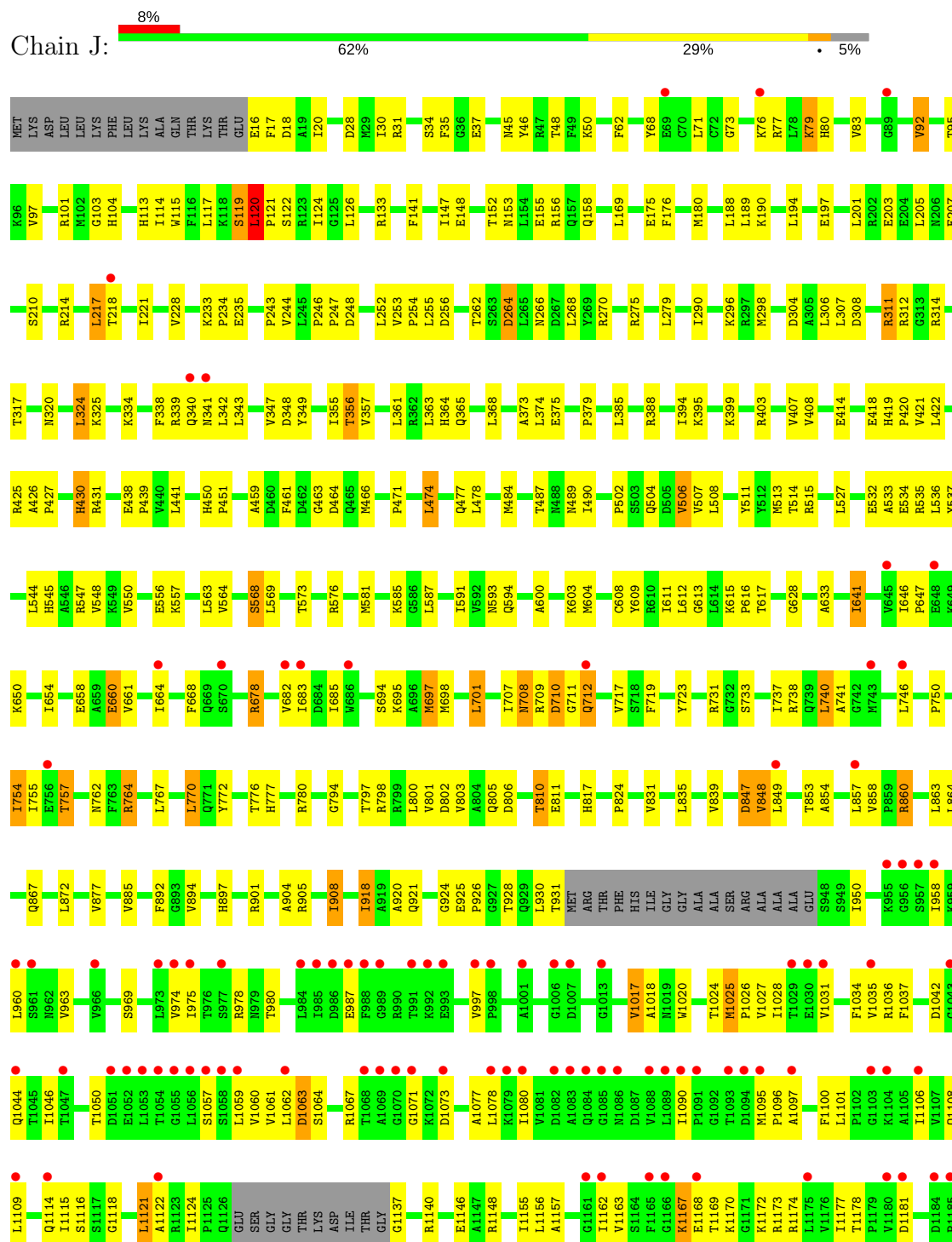


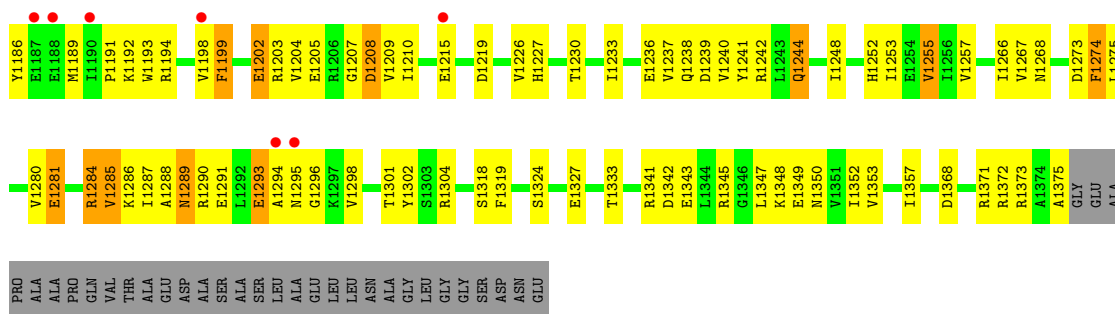




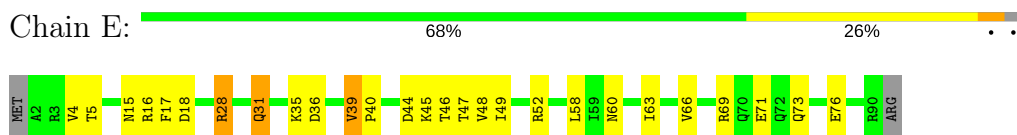


• Molecule 3: DNA-directed RNA polymerase subunit beta'

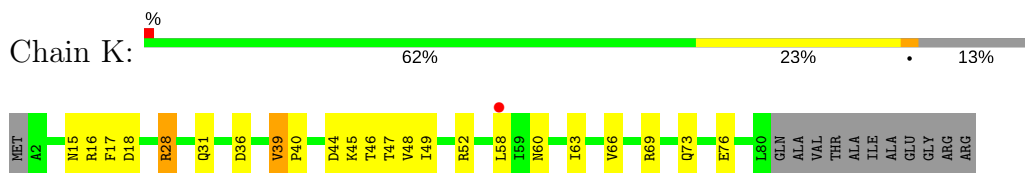




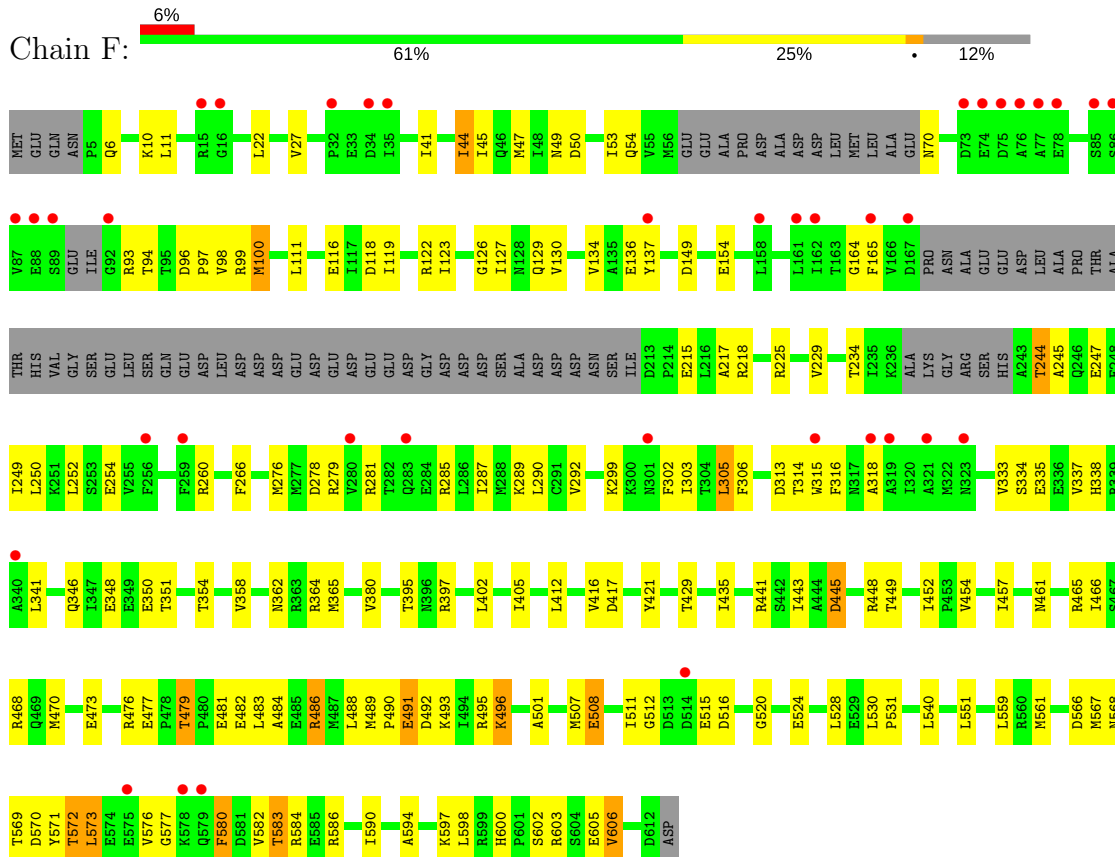
- Molecule 4: DNA-directed RNA polymerase subunit omega



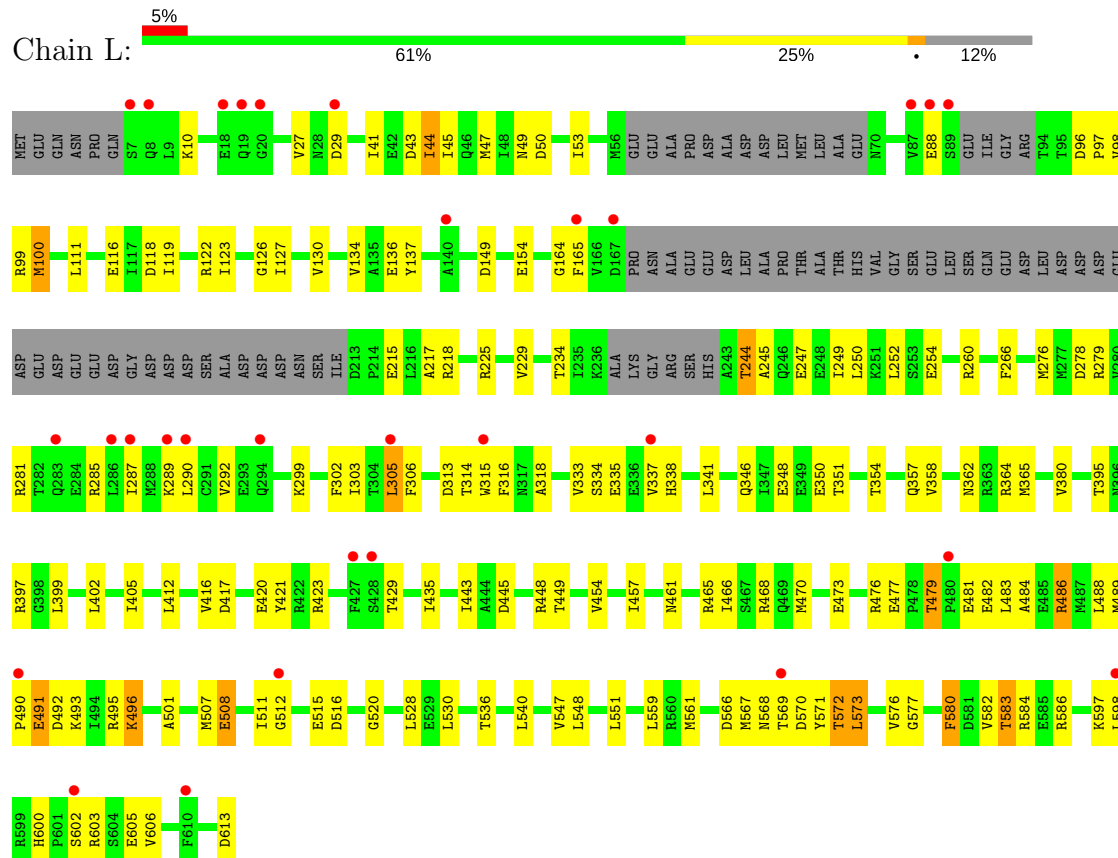
- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 5: RNA polymerase sigma factor RpoD



• Molecule 5: RNA polymerase sigma factor RpoD



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 186.68Å 206.39Å 308.84Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 44.78 – 3.84 44.78 – 3.84 | Depositor EDS |
| % Data completeness (in resolution range) | 98.2 (44.78-3.84) 98.3 (44.78-3.84) | Depositor EDS |
| R_{merge} | 0.20 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.73 (at 3.88Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: 1.8_1069) | Depositor |
| R, R_{free} | 0.224 , 0.272 0.223 , 0.273 | Depositor DCC |
| R_{free} test set | 5632 reflections (5.01%) | DCC |
| Wilson B-factor (Å ²) | 142.8 | Xtriage |
| Anisotropy | 0.442 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.26 , 63.5 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.92 | EDS |
| Total number of atoms | 57170 | wwPDB-VP |
| Average B, all atoms (Å ²) | 102.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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 | 0.25 | 0/1751 | 0.51 | 0/2373 |
| 1 | B | 0.26 | 0/1707 | 0.49 | 0/2314 |
| 1 | G | 0.25 | 0/1771 | 0.53 | 0/2401 |
| 1 | H | 0.26 | 0/1686 | 0.49 | 0/2285 |
| 2 | C | 0.26 | 0/10739 | 0.48 | 1/14489 (0.0%) |
| 2 | I | 0.26 | 0/10735 | 0.48 | 2/14484 (0.0%) |
| 3 | D | 0.26 | 0/9246 | 0.48 | 1/12478 (0.0%) |
| 3 | J | 0.26 | 0/10525 | 0.48 | 1/14212 (0.0%) |
| 4 | E | 0.24 | 0/693 | 0.48 | 0/935 |
| 4 | K | 0.24 | 0/629 | 0.48 | 0/847 |
| 5 | F | 0.29 | 0/4254 | 0.51 | 2/5731 (0.0%) |
| 5 | L | 0.29 | 0/4246 | 0.49 | 1/5720 (0.0%) |
| All | All | 0.27 | 0/57982 | 0.49 | 8/78269 (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 | C | 0 | 1 |
| 3 | D | 0 | 4 |
| 3 | J | 0 | 2 |
| 5 | F | 0 | 2 |
| 5 | L | 0 | 1 |
| All | All | 0 | 10 |

There are no bond length outliers.

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 5 | F | 11 | LEU | N-CA-C | -9.14 | 86.33 | 111.00 |
| 2 | I | 237 | LEU | N-CA-C | 5.38 | 125.53 | 111.00 |
| 3 | D | 120 | LEU | N-CA-C | 5.26 | 125.21 | 111.00 |
| 3 | J | 120 | LEU | N-CA-C | 5.25 | 125.18 | 111.00 |
| 2 | C | 516 | ASP | CB-CG-OD2 | 5.23 | 123.01 | 118.30 |
| 2 | I | 516 | ASP | CB-CG-OD2 | 5.21 | 122.99 | 118.30 |
| 5 | F | 149 | ASP | CB-CG-OD2 | 5.21 | 122.99 | 118.30 |
| 5 | L | 149 | ASP | CB-CG-OD2 | 5.19 | 122.97 | 118.30 |

There are no chirality outliers.

All (10) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-------------------|
| 2 | C | 1161 | LEU | Peptide |
| 3 | D | 119 | SER | Mainchain,Peptide |
| 3 | D | 120 | LEU | Peptide |
| 3 | D | 1296 | GLY | Peptide |
| 5 | F | 10 | LYS | Peptide |
| 5 | F | 6 | GLN | Peptide |
| 3 | J | 120 | LEU | Peptide |
| 3 | J | 1296 | GLY | Peptide |
| 5 | L | 10 | LYS | 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 | 1730 | 0 | 1756 | 48 | 0 |
| 1 | B | 1687 | 0 | 1700 | 53 | 0 |
| 1 | G | 1750 | 0 | 1764 | 54 | 0 |
| 1 | H | 1667 | 0 | 1689 | 53 | 0 |
| 2 | C | 10570 | 0 | 10582 | 254 | 0 |
| 2 | I | 10566 | 0 | 10576 | 243 | 0 |
| 3 | D | 9107 | 0 | 9308 | 249 | 0 |
| 3 | J | 10369 | 0 | 10589 | 284 | 0 |
| 4 | E | 691 | 0 | 695 | 17 | 0 |
| 4 | K | 627 | 0 | 634 | 13 | 0 |
| 5 | F | 4204 | 0 | 4106 | 90 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5 | L | 4196 | 0 | 4103 | 97 | 0 |
| 6 | D | 1 | 0 | 0 | 0 | 0 |
| 6 | J | 1 | 0 | 0 | 0 | 0 |
| 7 | D | 2 | 0 | 0 | 0 | 0 |
| 7 | J | 2 | 0 | 0 | 0 | 0 |
| All | All | 57170 | 0 | 57502 | 1328 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (1328) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:660:GLU:HB3 | 3:J:685:ILE:HD12 | 1.47 | 0.96 |
| 3:D:660:GLU:HB3 | 3:D:685:ILE:HD12 | 1.47 | 0.92 |
| 3:J:1044:GLN:HB3 | 3:J:1071:GLY:HA3 | 1.59 | 0.84 |
| 2:I:806:PRO:HA | 2:I:811:ASN:HD21 | 1.42 | 0.84 |
| 2:C:806:PRO:HA | 2:C:811:ASN:HD21 | 1.43 | 0.84 |
| 2:C:1312:ASN:HD21 | 2:C:1314:GLN:HE21 | 1.27 | 0.83 |
| 2:I:525:THR:HG21 | 2:I:687:ARG:HD2 | 1.62 | 0.82 |
| 2:I:1312:ASN:HD21 | 2:I:1314:GLN:HE21 | 1.26 | 0.82 |
| 3:D:853:THR:HG21 | 3:J:1375:ALA:HB1 | 1.62 | 0.82 |
| 2:C:525:THR:HG21 | 2:C:687:ARG:HD2 | 1.62 | 0.81 |
| 3:J:418:GLU:HG3 | 4:K:45:LYS:H | 1.45 | 0.81 |
| 3:D:418:GLU:HG3 | 4:E:45:LYS:H | 1.46 | 0.81 |
| 2:I:310:ILE:HG21 | 2:I:325:LEU:HB3 | 1.64 | 0.80 |
| 2:I:873:ILE:HG13 | 2:I:944:ARG:HH22 | 1.46 | 0.79 |
| 3:D:1280:VAL:HG21 | 3:D:1304:ARG:HE | 1.48 | 0.79 |
| 2:I:10:ARG:HD3 | 2:I:1181:PRO:HG2 | 1.64 | 0.78 |
| 3:J:1035:VAL:HG21 | 3:J:1121:LEU:HD21 | 1.67 | 0.77 |
| 2:C:10:ARG:HD3 | 2:C:1181:PRO:HG2 | 1.64 | 0.77 |
| 2:I:1105:SER:HB2 | 3:J:731:ARG:HG2 | 1.66 | 0.77 |
| 3:J:1280:VAL:HG21 | 3:J:1304:ARG:HE | 1.48 | 0.77 |
| 2:C:310:ILE:HG21 | 2:C:325:LEU:HB3 | 1.64 | 0.77 |
| 2:C:1105:SER:HB2 | 3:D:731:ARG:HG2 | 1.66 | 0.76 |
| 2:C:953:LEU:HD11 | 2:C:1033:ARG:HG3 | 1.67 | 0.76 |
| 1:A:231:PHE:HZ | 1:B:221:ALA:HB3 | 1.51 | 0.76 |
| 2:I:953:LEU:HD11 | 2:I:1033:ARG:HG3 | 1.67 | 0.75 |
| 2:I:673:HIS:HB3 | 2:I:1109:ILE:HG22 | 1.68 | 0.75 |
| 2:C:673:HIS:HB3 | 2:C:1109:ILE:HG22 | 1.69 | 0.75 |
| 5:F:561:MET:HA | 5:F:567:MET:HE1 | 1.67 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:J:155:GLU:HB2 | 3:J:158:GLN:HB2 | 1.69 | 0.74 |
| 3:J:133:ARG:HB2 | 5:L:88:GLU:HA | 1.68 | 0.74 |
| 5:F:470:MET:HA | 5:F:473:GLU:HB3 | 1.68 | 0.74 |
| 3:D:514:THR:HG23 | 3:D:576:ARG:HG2 | 1.70 | 0.74 |
| 3:J:514:THR:HG23 | 3:J:576:ARG:HG2 | 1.69 | 0.74 |
| 2:C:221:LEU:HD11 | 2:C:314:ASN:HB2 | 1.68 | 0.73 |
| 5:L:470:MET:HA | 5:L:473:GLU:HB3 | 1.69 | 0.73 |
| 2:C:559:CYS:HB2 | 2:C:662:SER:HB3 | 1.69 | 0.73 |
| 3:D:155:GLU:HB2 | 3:D:158:GLN:HB2 | 1.69 | 0.73 |
| 2:C:10:ARG:NH2 | 2:C:790:ASP:OD2 | 2.22 | 0.73 |
| 5:F:479:THR:HG22 | 5:F:482:GLU:HB2 | 1.71 | 0.73 |
| 2:I:10:ARG:NH2 | 2:I:790:ASP:OD2 | 2.22 | 0.73 |
| 3:D:806:ASP:HA | 3:D:1347:LEU:HD13 | 1.71 | 0.72 |
| 2:I:840:SER:HB2 | 2:I:850:ILE:HD11 | 1.70 | 0.72 |
| 5:L:479:THR:HG22 | 5:L:482:GLU:HB2 | 1.70 | 0.72 |
| 2:I:292:ILE:HB | 2:I:322:LEU:HD11 | 1.71 | 0.72 |
| 3:J:806:ASP:HA | 3:J:1347:LEU:HD13 | 1.71 | 0.72 |
| 1:H:59:VAL:O | 1:H:171:LEU:N | 2.23 | 0.72 |
| 2:I:559:CYS:HB2 | 2:I:662:SER:HB3 | 1.72 | 0.71 |
| 2:C:657:THR:HG21 | 2:C:1188:ASP:HB2 | 1.72 | 0.71 |
| 2:I:452:ARG:NH1 | 2:I:584:TYR:O | 2.23 | 0.71 |
| 3:J:342:LEU:HD11 | 3:J:1324:SER:HB3 | 1.72 | 0.71 |
| 3:J:1026:PRO:HB2 | 3:J:1028:ILE:HG23 | 1.73 | 0.71 |
| 2:C:840:SER:HB2 | 2:C:850:ILE:HD11 | 1.70 | 0.71 |
| 5:L:561:MET:HA | 5:L:567:MET:HE1 | 1.71 | 0.71 |
| 1:H:101:THR:HG22 | 1:H:116:THR:HB | 1.73 | 0.70 |
| 1:H:73:GLY:HA2 | 1:H:134:THR:HG22 | 1.73 | 0.70 |
| 2:C:452:ARG:NH1 | 2:C:584:TYR:O | 2.25 | 0.70 |
| 1:B:101:THR:HG22 | 1:B:116:THR:HB | 1.73 | 0.70 |
| 2:C:292:ILE:HB | 2:C:322:LEU:HD11 | 1.73 | 0.70 |
| 3:D:342:LEU:HD11 | 3:D:1324:SER:HB3 | 1.71 | 0.70 |
| 2:I:657:THR:HG21 | 2:I:1188:ASP:HB2 | 1.73 | 0.69 |
| 2:C:528:ARG:NH2 | 2:C:576:SER:O | 2.26 | 0.69 |
| 2:C:1065:LYS:HE2 | 3:D:463:GLY:HA3 | 1.74 | 0.69 |
| 1:B:73:GLY:HA2 | 1:B:134:THR:HG22 | 1.73 | 0.69 |
| 2:I:696:ASP:HB2 | 2:I:798:GLN:HG2 | 1.74 | 0.68 |
| 3:J:905:ARG:HH11 | 4:K:16:ARG:HD2 | 1.58 | 0.68 |
| 5:L:134:VAL:HG21 | 5:L:266:PHE:HE1 | 1.59 | 0.68 |
| 2:C:696:ASP:HB2 | 2:C:798:GLN:HG2 | 1.73 | 0.68 |
| 5:F:134:VAL:HG21 | 5:F:266:PHE:HE1 | 1.59 | 0.68 |
| 2:I:1065:LYS:HE2 | 3:J:463:GLY:HA3 | 1.74 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:J:664:ILE:HG22 | 3:J:678:ARG:HG2 | 1.75 | 0.68 |
| 2:I:829:THR:HA | 2:I:1059:ARG:HA | 1.76 | 0.68 |
| 2:C:732:ILE:HG21 | 2:C:783:LEU:HD12 | 1.75 | 0.68 |
| 3:D:664:ILE:HG22 | 3:D:678:ARG:HG2 | 1.76 | 0.67 |
| 2:I:528:ARG:NH2 | 2:I:576:SER:O | 2.26 | 0.67 |
| 2:I:732:ILE:HG21 | 2:I:783:LEU:HD12 | 1.75 | 0.67 |
| 3:D:532:GLU:HA | 3:D:535:ARG:HB3 | 1.76 | 0.67 |
| 2:I:618:GLN:HG3 | 3:J:770:LEU:HD21 | 1.75 | 0.67 |
| 2:C:18:ARG:NH2 | 2:C:620:ASN:OD1 | 2.27 | 0.67 |
| 2:I:734:ILE:HD11 | 2:I:783:LEU:HD11 | 1.76 | 0.67 |
| 3:J:1172:LYS:HA | 3:J:1191:PRO:HA | 1.77 | 0.67 |
| 3:D:905:ARG:HH11 | 4:E:16:ARG:HD2 | 1.59 | 0.67 |
| 2:I:18:ARG:NH2 | 2:I:620:ASN:OD1 | 2.27 | 0.66 |
| 2:I:1238:LEU:HD12 | 2:I:1238:LEU:H | 1.61 | 0.66 |
| 2:C:1238:LEU:HD12 | 2:C:1238:LEU:H | 1.61 | 0.66 |
| 3:D:1172:LYS:HA | 3:D:1191:PRO:HA | 1.77 | 0.66 |
| 3:J:489:ASN:HA | 3:J:904:ALA:HB1 | 1.78 | 0.66 |
| 2:I:197:ARG:NH2 | 5:L:29:ASP:OD2 | 2.28 | 0.66 |
| 3:D:489:ASN:HA | 3:D:904:ALA:HB1 | 1.78 | 0.66 |
| 2:C:618:GLN:HG3 | 3:D:770:LEU:HD21 | 1.76 | 0.66 |
| 1:G:31:LEU:HD11 | 1:G:201:LEU:HB2 | 1.78 | 0.66 |
| 1:A:45:ARG:NH2 | 2:C:1215:GLY:O | 2.29 | 0.66 |
| 2:C:136:PHE:O | 2:C:143:ARG:N | 2.24 | 0.66 |
| 2:I:976:ARG:HD2 | 2:I:989:LEU:HD23 | 1.77 | 0.66 |
| 3:J:527:LEU:HD23 | 3:J:532:GLU:HG3 | 1.78 | 0.66 |
| 2:C:976:ARG:HD2 | 2:C:989:LEU:HD23 | 1.77 | 0.65 |
| 1:G:190:ALA:HB2 | 1:G:200:LYS:HB2 | 1.77 | 0.65 |
| 2:I:18:ARG:NH1 | 2:I:621:SER:O | 2.29 | 0.65 |
| 3:J:646:ILE:HD11 | 3:J:764:ARG:HD2 | 1.77 | 0.65 |
| 1:G:99:ILE:HG12 | 1:G:145:LYS:HG2 | 1.78 | 0.65 |
| 3:J:532:GLU:HA | 3:J:535:ARG:HB3 | 1.76 | 0.65 |
| 2:C:829:THR:HA | 2:C:1059:ARG:HA | 1.77 | 0.65 |
| 1:A:31:LEU:HD11 | 1:A:201:LEU:HB2 | 1.78 | 0.65 |
| 3:D:527:LEU:HD23 | 3:D:532:GLU:HG3 | 1.78 | 0.65 |
| 3:D:646:ILE:HD11 | 3:D:764:ARG:HD2 | 1.77 | 0.65 |
| 3:D:797:THR:HG22 | 3:D:924:GLY:HA3 | 1.78 | 0.65 |
| 5:F:292:VAL:HG21 | 5:F:299:LYS:HG3 | 1.79 | 0.65 |
| 3:J:120:LEU:HD22 | 3:J:121:PRO:HD3 | 1.79 | 0.65 |
| 1:A:155:ALA:HA | 1:A:158:ARG:HG3 | 1.79 | 0.65 |
| 1:A:166:ARG:O | 1:A:168:ILE:N | 2.29 | 0.65 |
| 2:C:734:ILE:HD11 | 2:C:783:LEU:HD11 | 1.77 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:I:13:LYS:HZ3 | 2:I:1151:LEU:HD12 | 1.60 | 0.65 |
| 1:G:166:ARG:O | 1:G:168:ILE:N | 2.30 | 0.65 |
| 2:C:463:GLN:HG3 | 2:C:505:PHE:HB2 | 1.79 | 0.65 |
| 2:C:18:ARG:NH1 | 2:C:621:SER:O | 2.30 | 0.65 |
| 3:D:1293:GLU:H | 3:J:1226:VAL:HB | 1.62 | 0.65 |
| 3:J:478:LEU:HG | 4:K:47:THR:HG23 | 1.79 | 0.65 |
| 1:A:190:ALA:HB2 | 1:A:200:LYS:HB2 | 1.77 | 0.64 |
| 5:L:292:VAL:HG21 | 5:L:299:LYS:HG3 | 1.78 | 0.64 |
| 1:A:99:ILE:HG12 | 1:A:145:LYS:HG2 | 1.78 | 0.64 |
| 1:A:231:PHE:CZ | 1:B:221:ALA:HB3 | 2.33 | 0.64 |
| 2:I:463:GLN:HG3 | 2:I:505:PHE:HB2 | 1.79 | 0.64 |
| 3:J:1199:PHE:HB2 | 3:J:1202:GLU:HB2 | 1.80 | 0.64 |
| 3:J:797:THR:HG22 | 3:J:924:GLY:HA3 | 1.78 | 0.64 |
| 3:D:478:LEU:HG | 4:E:47:THR:HG23 | 1.79 | 0.64 |
| 3:D:1199:PHE:HB2 | 3:D:1202:GLU:HB2 | 1.80 | 0.64 |
| 3:D:755:ILE:HG22 | 3:D:757:THR:H | 1.62 | 0.64 |
| 1:G:230:ALA:HA | 1:H:12:ARG:HG2 | 1.78 | 0.64 |
| 3:D:120:LEU:HD22 | 3:D:121:PRO:HD3 | 1.78 | 0.64 |
| 2:C:13:LYS:HZ3 | 2:C:1151:LEU:HD12 | 1.61 | 0.63 |
| 1:H:33:ARG:HH11 | 2:I:1081:PRO:HG3 | 1.63 | 0.63 |
| 3:J:755:ILE:HG22 | 3:J:757:THR:H | 1.62 | 0.63 |
| 3:D:1238:GLN:NE2 | 3:D:1248:ILE:O | 2.32 | 0.63 |
| 1:G:155:ALA:HA | 1:G:158:ARG:HG3 | 1.79 | 0.63 |
| 1:A:184:ALA:HB2 | 2:C:1091:GLY:HA3 | 1.81 | 0.63 |
| 5:F:561:MET:HG2 | 5:F:576:VAL:HG22 | 1.81 | 0.63 |
| 2:I:88:ARG:NH2 | 2:I:1035:LYS:O | 2.31 | 0.63 |
| 5:L:305:LEU:HD13 | 5:L:315:TRP:HA | 1.81 | 0.63 |
| 2:C:339:ASN:HB3 | 2:C:343:HIS:H | 1.64 | 0.62 |
| 2:I:103:VAL:HG12 | 2:I:116:ASP:HB3 | 1.81 | 0.62 |
| 2:I:1106:ARG:HD2 | 2:I:1106:ARG:H | 1.63 | 0.62 |
| 2:C:1119:MET:HE3 | 2:C:1204:LEU:HD13 | 1.81 | 0.62 |
| 2:C:746:ALA:HA | 2:C:974:ARG:HH21 | 1.64 | 0.62 |
| 2:I:1119:MET:HE3 | 2:I:1204:LEU:HD13 | 1.81 | 0.62 |
| 3:J:262:THR:OG1 | 3:J:266:ASN:ND2 | 2.32 | 0.62 |
| 2:C:103:VAL:HG12 | 2:C:116:ASP:HB3 | 1.81 | 0.62 |
| 3:J:1238:GLN:NE2 | 3:J:1248:ILE:O | 2.32 | 0.62 |
| 3:D:341:ASN:HB2 | 3:D:1352:ILE:HD13 | 1.80 | 0.62 |
| 2:I:985:GLU:HB3 | 2:I:988:LYS:HB2 | 1.82 | 0.62 |
| 3:D:262:THR:OG1 | 3:D:266:ASN:ND2 | 2.32 | 0.62 |
| 3:J:1157:ALA:HB2 | 3:J:1210:ILE:HD11 | 1.82 | 0.62 |
| 2:I:518:ASN:N | 2:I:518:ASN:OD1 | 2.33 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:30:ILE:HD12 | 2:I:30:ILE:H | 1.65 | 0.61 |
| 2:C:1106:ARG:H | 2:C:1106:ARG:HD2 | 1.63 | 0.61 |
| 1:A:45:ARG:HH22 | 2:C:1216:ARG:HA | 1.65 | 0.61 |
| 5:L:561:MET:HG2 | 5:L:576:VAL:HG22 | 1.82 | 0.61 |
| 2:C:518:ASN:OD1 | 2:C:518:ASN:N | 2.33 | 0.61 |
| 2:C:985:GLU:HB3 | 2:C:988:LYS:HB2 | 1.82 | 0.61 |
| 2:I:269:ILE:HG23 | 2:I:273:HIS:HB2 | 1.83 | 0.61 |
| 2:C:138:ILE:HB | 2:C:143:ARG:HD3 | 1.83 | 0.61 |
| 1:H:182:ARG:NH1 | 3:J:581:MET:SD | 2.74 | 0.61 |
| 2:I:560:PRO:O | 3:J:780:ARG:NH2 | 2.34 | 0.61 |
| 5:L:551:LEU:HD22 | 5:L:597:LYS:HD2 | 1.83 | 0.61 |
| 2:C:841:ARG:HA | 2:C:1046:VAL:HA | 1.83 | 0.60 |
| 3:D:847:ASP:OD1 | 3:D:847:ASP:N | 2.34 | 0.60 |
| 5:F:305:LEU:HD13 | 5:F:315:TRP:HA | 1.81 | 0.60 |
| 3:D:80:HIS:HB3 | 3:D:83:VAL:HG11 | 1.83 | 0.60 |
| 2:I:221:LEU:HD11 | 2:I:314:ASN:HB2 | 1.82 | 0.60 |
| 2:C:120:GLN:HG3 | 2:C:121:GLU:HG2 | 1.81 | 0.60 |
| 3:D:304:ASP:OD2 | 3:D:312:ARG:NH2 | 2.33 | 0.60 |
| 3:J:148:GLU:H | 3:J:156:ARG:HG3 | 1.65 | 0.60 |
| 3:D:1157:ALA:HB2 | 3:D:1210:ILE:HD11 | 1.83 | 0.60 |
| 3:J:80:HIS:HB3 | 3:J:83:VAL:HG11 | 1.84 | 0.60 |
| 2:C:1313:HIS:HB2 | 3:D:474:LEU:HD13 | 1.83 | 0.60 |
| 2:C:269:ILE:HG23 | 2:C:273:HIS:HB2 | 1.83 | 0.60 |
| 2:C:494:ASN:OD1 | 2:C:495:ALA:N | 2.32 | 0.60 |
| 1:H:59:VAL:HG21 | 1:H:85:LEU:HD13 | 1.84 | 0.60 |
| 2:I:494:ASN:OD1 | 2:I:495:ALA:N | 2.33 | 0.60 |
| 3:J:304:ASP:OD2 | 3:J:312:ARG:NH2 | 2.34 | 0.60 |
| 2:I:149:LEU:HD13 | 2:I:453:ILE:HG13 | 1.84 | 0.60 |
| 3:J:1174:ARG:HG2 | 3:J:1189:MET:HG2 | 1.84 | 0.60 |
| 1:A:153:VAL:HB | 1:A:175:ALA:HB3 | 1.84 | 0.59 |
| 1:B:59:VAL:HG21 | 1:B:85:LEU:HD13 | 1.83 | 0.59 |
| 3:J:425:ARG:HD2 | 3:J:459:ALA:HB2 | 1.84 | 0.59 |
| 5:L:476:ARG:HG2 | 5:L:477:GLU:HG2 | 1.84 | 0.59 |
| 3:D:1169:THR:HG23 | 3:D:1192:LYS:HD3 | 1.84 | 0.59 |
| 1:G:26:VAL:HG22 | 1:G:203:ILE:HB | 1.84 | 0.59 |
| 3:J:1050:THR:HG23 | 3:J:1057:SER:HB3 | 1.84 | 0.59 |
| 3:D:148:GLU:H | 3:D:156:ARG:HG3 | 1.67 | 0.59 |
| 5:F:476:ARG:HG2 | 5:F:477:GLU:HG2 | 1.84 | 0.59 |
| 1:G:153:VAL:HB | 1:G:175:ALA:HB3 | 1.84 | 0.59 |
| 3:J:194:LEU:HD13 | 3:J:228:VAL:HG22 | 1.85 | 0.59 |
| 4:E:73:GLN:HA | 4:E:76:GLU:HB2 | 1.85 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:1169:THR:HG23 | 3:J:1192:LYS:HD3 | 1.84 | 0.59 |
| 1:A:26:VAL:HG22 | 1:A:203:ILE:HB | 1.84 | 0.59 |
| 2:C:145:ILE:HB | 2:C:456:VAL:HG22 | 1.85 | 0.59 |
| 1:A:38:THR:OG1 | 1:B:45:ARG:NH1 | 2.33 | 0.59 |
| 3:D:141:PHE:HD1 | 3:D:180:MET:HG3 | 1.68 | 0.59 |
| 2:I:1119:MET:HB2 | 2:I:1228:GLY:HA2 | 1.85 | 0.59 |
| 3:D:308:ASP:OD2 | 3:D:311:ARG:NH2 | 2.35 | 0.58 |
| 3:D:356:THR:OG1 | 3:D:357:VAL:N | 2.36 | 0.58 |
| 2:C:560:PRO:O | 3:D:780:ARG:NH2 | 2.35 | 0.58 |
| 2:I:1108:ASN:OD1 | 2:I:1111:GLN:NE2 | 2.36 | 0.58 |
| 2:C:149:LEU:HD13 | 2:C:453:ILE:HG13 | 1.84 | 0.58 |
| 3:D:388:ARG:NH1 | 3:D:414:GLU:OE1 | 2.36 | 0.58 |
| 3:J:308:ASP:OD2 | 3:J:311:ARG:NH2 | 2.35 | 0.58 |
| 2:C:1108:ASN:OD1 | 2:C:1111:GLN:NE2 | 2.36 | 0.58 |
| 2:C:808:ASN:H | 3:D:633:ALA:HB2 | 1.69 | 0.58 |
| 1:H:98:VAL:HG11 | 1:H:121:VAL:HG22 | 1.85 | 0.58 |
| 3:J:356:THR:OG1 | 3:J:357:VAL:N | 2.36 | 0.58 |
| 1:B:37:HIS:CE1 | 2:C:1216:ARG:HD2 | 2.37 | 0.58 |
| 3:D:1174:ARG:HG2 | 3:D:1189:MET:HG2 | 1.84 | 0.58 |
| 3:D:194:LEU:HD13 | 3:D:228:VAL:HG22 | 1.84 | 0.58 |
| 2:I:808:ASN:H | 3:J:633:ALA:HB2 | 1.68 | 0.58 |
| 5:F:551:LEU:HD22 | 5:F:597:LYS:HD2 | 1.85 | 0.58 |
| 3:J:741:ALA:O | 3:J:762:ASN:ND2 | 2.37 | 0.58 |
| 4:K:15:ASN:HB3 | 4:K:18:ASP:HB2 | 1.86 | 0.58 |
| 4:E:15:ASN:HB3 | 4:E:18:ASP:HB2 | 1.85 | 0.58 |
| 3:J:317:THR:HG23 | 3:J:320:ASN:HB3 | 1.85 | 0.58 |
| 3:J:847:ASP:N | 3:J:847:ASP:OD1 | 2.34 | 0.58 |
| 2:I:841:ARG:HA | 2:I:1046:VAL:HA | 1.85 | 0.57 |
| 3:J:506:VAL:HG23 | 3:J:628:GLY:HA3 | 1.86 | 0.57 |
| 3:D:152:THR:OG1 | 3:D:153:ASN:N | 2.37 | 0.57 |
| 3:D:741:ALA:O | 3:D:762:ASN:ND2 | 2.37 | 0.57 |
| 2:C:1185:PRO:HD2 | 2:C:1189:GLY:HA2 | 1.85 | 0.57 |
| 2:C:1275:VAL:HG13 | 2:C:1287:LEU:HD11 | 1.86 | 0.57 |
| 5:F:276:MET:SD | 5:F:279:ARG:NH1 | 2.77 | 0.57 |
| 1:B:98:VAL:HG11 | 1:B:121:VAL:HG22 | 1.85 | 0.57 |
| 1:H:16:ILE:HG13 | 1:H:26:VAL:HG22 | 1.86 | 0.57 |
| 3:J:388:ARG:NH1 | 3:J:414:GLU:OE1 | 2.37 | 0.57 |
| 3:J:77:ARG:HE | 5:L:569:THR:HA | 1.69 | 0.57 |
| 2:C:1119:MET:HB2 | 2:C:1228:GLY:HA2 | 1.85 | 0.57 |
| 2:C:30:ILE:H | 2:C:30:ILE:HD12 | 1.69 | 0.57 |
| 2:C:363:LEU:HB3 | 2:C:381:ALA:HB1 | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:425:ARG:HD2 | 3:D:459:ALA:HB2 | 1.85 | 0.57 |
| 2:I:102:LEU:HB2 | 2:I:489:PRO:HG3 | 1.87 | 0.57 |
| 1:B:33:ARG:HH11 | 2:C:1081:PRO:HG3 | 1.69 | 0.57 |
| 4:K:39:VAL:HG22 | 4:K:40:PRO:HD2 | 1.87 | 0.57 |
| 1:G:70:THR:HG21 | 2:I:755:LYS:HE2 | 1.87 | 0.57 |
| 3:J:1273:ASP:OD1 | 3:J:1274:PHE:N | 2.37 | 0.57 |
| 3:D:317:THR:HG23 | 3:D:320:ASN:HB3 | 1.85 | 0.57 |
| 3:D:650:LYS:HE2 | 3:D:654:ILE:HD11 | 1.87 | 0.57 |
| 2:I:1185:PRO:HD2 | 2:I:1189:GLY:HA2 | 1.87 | 0.57 |
| 2:I:40:GLU:O | 2:I:73:TYR:OH | 2.22 | 0.57 |
| 5:L:482:GLU:O | 5:L:486:ARG:NH2 | 2.38 | 0.57 |
| 2:C:102:LEU:HB2 | 2:C:489:PRO:HG3 | 1.87 | 0.57 |
| 1:B:191:ARG:HH22 | 3:D:409:TRP:HB3 | 1.70 | 0.57 |
| 3:D:506:VAL:HG23 | 3:D:628:GLY:HA3 | 1.86 | 0.57 |
| 4:E:39:VAL:HG22 | 4:E:40:PRO:HD2 | 1.87 | 0.57 |
| 5:L:290:LEU:HB3 | 5:L:333:VAL:HG21 | 1.87 | 0.57 |
| 1:A:60:GLU:HB2 | 1:A:170:ARG:HG2 | 1.87 | 0.56 |
| 2:C:1157:GLN:HG3 | 2:C:1159:VAL:HG13 | 1.86 | 0.56 |
| 2:C:40:GLU:O | 2:C:73:TYR:OH | 2.22 | 0.56 |
| 3:D:1140:ARG:HH21 | 3:D:1236:GLU:HG2 | 1.70 | 0.56 |
| 5:F:290:LEU:HB3 | 5:F:333:VAL:HG21 | 1.87 | 0.56 |
| 3:J:613:GLY:O | 3:J:617:THR:OG1 | 2.23 | 0.56 |
| 3:J:892:PHE:H | 3:J:1281:GLU:HG2 | 1.70 | 0.56 |
| 3:D:682:VAL:O | 3:D:685:ILE:HG12 | 2.05 | 0.56 |
| 2:I:1157:GLN:HG3 | 2:I:1159:VAL:HG13 | 1.86 | 0.56 |
| 3:J:152:THR:OG1 | 3:J:153:ASN:N | 2.37 | 0.56 |
| 3:J:141:PHE:HD1 | 3:J:180:MET:HG3 | 1.68 | 0.56 |
| 3:J:650:LYS:HE2 | 3:J:654:ILE:HD11 | 1.86 | 0.56 |
| 5:L:276:MET:SD | 5:L:279:ARG:NH1 | 2.77 | 0.56 |
| 2:I:1275:VAL:HG13 | 2:I:1287:LEU:HD11 | 1.86 | 0.56 |
| 3:D:794:GLY:O | 3:D:797:THR:OG1 | 2.21 | 0.56 |
| 2:C:1250:SER:OG | 5:F:524:GLU:OE1 | 2.24 | 0.56 |
| 1:A:14:VAL:HG22 | 1:A:15:ASP:H | 1.71 | 0.56 |
| 5:F:482:GLU:O | 5:F:486:ARG:NH2 | 2.38 | 0.56 |
| 1:B:64:VAL:HG12 | 1:B:65:LEU:H | 1.71 | 0.56 |
| 1:A:70:THR:HG21 | 2:C:755:LYS:HE2 | 1.87 | 0.56 |
| 5:F:278:ASP:OD1 | 5:F:281:ARG:NH1 | 2.38 | 0.56 |
| 5:F:515:GLU:HG2 | 5:F:516:ASP:H | 1.70 | 0.56 |
| 5:L:278:ASP:OD1 | 5:L:281:ARG:NH1 | 2.38 | 0.56 |
| 1:A:23:HIS:HB2 | 1:A:205:MET:O | 2.06 | 0.56 |
| 3:D:892:PHE:H | 3:D:1281:GLU:HG2 | 1.70 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:1198:VAL:HG23 | 3:J:1204:VAL:HG11 | 1.88 | 0.56 |
| 2:C:870:ILE:HB | 2:C:944:ARG:HD3 | 1.88 | 0.56 |
| 2:I:363:LEU:HB3 | 2:I:381:ALA:HB1 | 1.88 | 0.56 |
| 3:J:960:LEU:HB3 | 3:J:963:VAL:HG11 | 1.86 | 0.56 |
| 1:H:133:LEU:HD11 | 1:H:140:ILE:HG21 | 1.88 | 0.56 |
| 3:J:1140:ARG:HH21 | 3:J:1236:GLU:HG2 | 1.70 | 0.56 |
| 3:J:1318:SER:OG | 3:J:1342:ASP:OD2 | 2.23 | 0.56 |
| 1:B:133:LEU:HD11 | 1:B:140:ILE:HG21 | 1.88 | 0.56 |
| 2:C:1196:LYS:HD2 | 2:C:1206:THR:HG23 | 1.88 | 0.56 |
| 3:D:1273:ASP:OD1 | 3:D:1274:PHE:N | 2.38 | 0.56 |
| 3:J:609:TYR:HB2 | 3:J:617:THR:HG21 | 1.88 | 0.56 |
| 2:C:302:ILE:HG22 | 2:C:309:LEU:HA | 1.88 | 0.55 |
| 2:C:814:ASP:OD2 | 2:C:1106:ARG:NH1 | 2.36 | 0.55 |
| 3:J:682:VAL:O | 3:J:685:ILE:HG12 | 2.05 | 0.55 |
| 2:C:227:LYS:O | 2:C:245:ARG:NH2 | 2.39 | 0.55 |
| 2:C:207:THR:HG21 | 2:C:351:LEU:HG | 1.88 | 0.55 |
| 2:I:302:ILE:HG22 | 2:I:309:LEU:HA | 1.88 | 0.55 |
| 1:A:48:LEU:HA | 1:A:180:VAL:HG21 | 1.89 | 0.55 |
| 2:I:61:SER:HB3 | 2:I:479:LEU:HB3 | 1.88 | 0.55 |
| 2:C:488:MET:O | 2:C:490:GLN:N | 2.34 | 0.55 |
| 3:J:1027:VAL:HG21 | 3:J:1122:ALA:HB3 | 1.88 | 0.55 |
| 3:J:794:GLY:O | 3:J:797:THR:OG1 | 2.21 | 0.55 |
| 1:G:14:VAL:HG22 | 1:G:15:ASP:H | 1.72 | 0.55 |
| 1:B:16:ILE:HG13 | 1:B:26:VAL:HG22 | 1.88 | 0.55 |
| 1:G:60:GLU:HB2 | 1:G:170:ARG:HG2 | 1.87 | 0.55 |
| 1:H:91:ARG:HG3 | 1:H:122:GLU:HB3 | 1.89 | 0.55 |
| 2:C:61:SER:HB3 | 2:C:479:LEU:HB3 | 1.88 | 0.55 |
| 3:D:613:GLY:O | 3:D:617:THR:OG1 | 2.24 | 0.55 |
| 3:J:120:LEU:HD12 | 5:L:43:ASP:HB3 | 1.88 | 0.55 |
| 2:I:227:LYS:O | 2:I:245:ARG:NH2 | 2.40 | 0.55 |
| 3:J:958:ILE:HD11 | 3:J:1017:VAL:HG11 | 1.89 | 0.55 |
| 2:C:1314:GLN:HG2 | 4:E:28:ARG:CZ | 2.37 | 0.54 |
| 2:I:207:THR:HG21 | 2:I:351:LEU:HG | 1.88 | 0.54 |
| 3:J:872:LEU:HD22 | 3:J:877:VAL:HG11 | 1.90 | 0.54 |
| 1:B:190:ALA:HB2 | 1:B:200:LYS:HB2 | 1.89 | 0.54 |
| 1:B:62:ASP:OD2 | 1:B:71:LYS:NZ | 2.41 | 0.54 |
| 1:G:23:HIS:HB2 | 1:G:205:MET:O | 2.05 | 0.54 |
| 5:L:602:SER:H | 5:L:605:GLU:HG3 | 1.72 | 0.54 |
| 3:D:872:LEU:HD22 | 3:D:877:VAL:HG11 | 1.90 | 0.54 |
| 1:H:64:VAL:HG12 | 1:H:65:LEU:H | 1.72 | 0.54 |
| 2:I:176:ILE:HD12 | 2:I:184:LEU:HD23 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:L:515:GLU:HG2 | 5:L:516:ASP:H | 1.71 | 0.54 |
| 3:J:115:TRP:O | 3:J:119:SER:HB2 | 2.08 | 0.54 |
| 3:D:28:ASP:OD1 | 3:D:31:ARG:NH1 | 2.41 | 0.54 |
| 5:F:577:GLY:HA3 | 5:F:583:THR:HG23 | 1.90 | 0.54 |
| 2:I:488:MET:O | 2:I:490:GLN:N | 2.35 | 0.54 |
| 2:I:94:ALA:HB2 | 2:I:129:LEU:HD11 | 1.89 | 0.54 |
| 3:J:425:ARG:HG2 | 3:J:426:ALA:H | 1.72 | 0.54 |
| 3:D:770:LEU:H | 3:D:770:LEU:HD22 | 1.72 | 0.54 |
| 1:G:48:LEU:HA | 1:G:180:VAL:HG21 | 1.89 | 0.54 |
| 1:G:45:ARG:HH22 | 2:I:1216:ARG:HA | 1.71 | 0.54 |
| 3:J:279:LEU:HD11 | 3:J:296:LYS:HG2 | 1.90 | 0.54 |
| 3:J:647:PRO:HG3 | 3:J:697:MET:HB3 | 1.89 | 0.54 |
| 2:C:757:THR:HG23 | 2:C:765:ILE:HG23 | 1.89 | 0.54 |
| 3:J:1280:VAL:HG21 | 3:J:1304:ARG:NE | 2.21 | 0.54 |
| 3:D:1227:HIS:CG | 3:J:1293:GLU:HG2 | 2.42 | 0.54 |
| 2:C:1280:ALA:HB1 | 3:D:918:ILE:HG22 | 1.90 | 0.54 |
| 3:D:1198:VAL:HG23 | 3:D:1204:VAL:HG11 | 1.88 | 0.54 |
| 3:D:609:TYR:HB2 | 3:D:617:THR:HG21 | 1.89 | 0.54 |
| 3:D:647:PRO:HG3 | 3:D:697:MET:HB3 | 1.90 | 0.54 |
| 2:I:757:THR:HG23 | 2:I:765:ILE:HG23 | 1.89 | 0.54 |
| 2:I:6:THR:HG21 | 2:I:782:VAL:HG23 | 1.90 | 0.54 |
| 5:L:551:LEU:HD11 | 5:L:598:LEU:HD21 | 1.88 | 0.54 |
| 3:D:210:SER:O | 3:D:214:ARG:HG2 | 2.08 | 0.54 |
| 5:F:111:LEU:HD13 | 5:F:116:GLU:HG2 | 1.90 | 0.54 |
| 5:F:397:ARG:HG2 | 5:F:443:ILE:HG21 | 1.90 | 0.54 |
| 5:F:573:LEU:H | 5:F:573:LEU:HD23 | 1.72 | 0.54 |
| 2:I:615:VAL:HG13 | 2:I:650:VAL:HA | 1.90 | 0.54 |
| 3:J:114:ILE:HD12 | 3:J:304:ASP:HB3 | 1.89 | 0.54 |
| 2:C:176:ILE:HD12 | 2:C:184:LEU:HD23 | 1.90 | 0.54 |
| 3:D:425:ARG:HG2 | 3:D:426:ALA:H | 1.73 | 0.54 |
| 5:F:479:THR:HG23 | 5:F:481:GLU:H | 1.72 | 0.54 |
| 3:J:34:SER:OG | 3:J:104:HIS:ND1 | 2.28 | 0.54 |
| 3:J:1227:HIS:HA | 3:J:1230:THR:HG22 | 1.90 | 0.54 |
| 3:J:268:LEU:HB3 | 3:J:306:LEU:HD23 | 1.90 | 0.54 |
| 2:I:1196:LYS:HD2 | 2:I:1206:THR:HG23 | 1.90 | 0.53 |
| 3:J:210:SER:O | 3:J:214:ARG:HG2 | 2.08 | 0.53 |
| 3:J:770:LEU:HD22 | 3:J:770:LEU:H | 1.73 | 0.53 |
| 2:C:1191:LYS:HD3 | 2:C:1193:ALA:H | 1.73 | 0.53 |
| 2:C:590:PRO:HG3 | 2:C:605:TYR:CZ | 2.44 | 0.53 |
| 2:I:26:TYR:HE2 | 2:I:32:LEU:HD12 | 1.73 | 0.53 |
| 2:I:9:LYS:HA | 2:I:1171:ARG:HD2 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:L:577:GLY:HA3 | 5:L:583:THR:HG23 | 1.90 | 0.53 |
| 5:F:602:SER:H | 5:F:605:GLU:HG3 | 1.72 | 0.53 |
| 3:D:1310:THR:HG21 | 5:F:70:ASN:HA | 1.91 | 0.53 |
| 2:I:1142:ARG:HH22 | 2:I:1165:SER:HB2 | 1.73 | 0.53 |
| 2:C:745:GLU:HG3 | 2:C:1017:GLN:HB3 | 1.90 | 0.53 |
| 2:C:1142:ARG:HH22 | 2:C:1165:SER:HB2 | 1.73 | 0.53 |
| 5:L:111:LEU:HD13 | 5:L:116:GLU:HG2 | 1.90 | 0.53 |
| 5:F:165:PHE:CE2 | 5:F:217:ALA:HA | 2.44 | 0.53 |
| 2:I:718:ALA:HB2 | 2:I:783:LEU:HD23 | 1.91 | 0.53 |
| 4:K:73:GLN:HA | 4:K:76:GLU:HB3 | 1.90 | 0.53 |
| 5:L:49:ASN:HA | 5:L:53:ILE:HA | 1.90 | 0.53 |
| 2:C:758:ARG:NH1 | 2:C:835:GLU:OE1 | 2.41 | 0.53 |
| 2:C:94:ALA:HB2 | 2:C:129:LEU:HD11 | 1.89 | 0.53 |
| 1:H:64:VAL:HG21 | 1:H:69:SER:HB3 | 1.91 | 0.53 |
| 5:L:479:THR:HG23 | 5:L:481:GLU:H | 1.74 | 0.53 |
| 1:A:74:VAL:HG22 | 1:A:76:GLU:H | 1.73 | 0.53 |
| 3:D:114:ILE:HD12 | 3:D:304:ASP:HB3 | 1.89 | 0.53 |
| 5:F:511:ILE:HG13 | 5:F:512:GLY:H | 1.74 | 0.53 |
| 3:J:28:ASP:OD1 | 3:J:31:ARG:NH1 | 2.41 | 0.53 |
| 3:D:34:SER:OG | 3:D:104:HIS:ND1 | 2.29 | 0.53 |
| 3:D:268:LEU:HB3 | 3:D:306:LEU:HD23 | 1.90 | 0.53 |
| 1:H:190:ALA:HB2 | 1:H:200:LYS:HB2 | 1.89 | 0.53 |
| 1:B:11:PRO:HB3 | 1:B:30:PRO:O | 2.08 | 0.53 |
| 2:C:241:LEU:HD21 | 2:C:246:LEU:HD11 | 1.91 | 0.53 |
| 5:L:397:ARG:HG2 | 5:L:443:ILE:HG21 | 1.89 | 0.53 |
| 5:L:511:ILE:HG13 | 5:L:512:GLY:H | 1.74 | 0.53 |
| 1:B:64:VAL:HG21 | 1:B:69:SER:HB3 | 1.91 | 0.53 |
| 2:C:9:LYS:HA | 2:C:1171:ARG:HD2 | 1.91 | 0.53 |
| 2:C:324:LYS:O | 2:C:327:GLN:NE2 | 2.42 | 0.53 |
| 3:D:202:ARG:HD3 | 3:J:1181:ASP:HA | 1.90 | 0.53 |
| 5:L:548:LEU:HD21 | 5:L:559:LEU:HD23 | 1.91 | 0.53 |
| 3:D:1286:LYS:O | 3:D:1290:ARG:HB2 | 2.09 | 0.52 |
| 1:H:62:ASP:OD2 | 1:H:71:LYS:NZ | 2.42 | 0.52 |
| 2:C:615:VAL:HG13 | 2:C:650:VAL:HA | 1.90 | 0.52 |
| 3:D:1267:VAL:HB | 3:D:1301:THR:OG1 | 2.10 | 0.52 |
| 3:J:1286:LYS:O | 3:J:1290:ARG:HB2 | 2.08 | 0.52 |
| 2:C:1149:TYR:HB3 | 2:C:1159:VAL:HG11 | 1.90 | 0.52 |
| 2:C:124:MET:HB2 | 2:C:498:ILE:HD13 | 1.91 | 0.52 |
| 3:D:1227:HIS:HA | 3:D:1230:THR:HG22 | 1.90 | 0.52 |
| 2:I:591:TYR:OH | 2:I:637:ARG:NH2 | 2.43 | 0.52 |
| 3:J:1267:VAL:HB | 3:J:1301:THR:OG1 | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:172:LEU:H | 1:A:172:LEU:HD12 | 1.74 | 0.52 |
| 1:A:61:ILE:HG22 | 1:A:62:ASP:H | 1.74 | 0.52 |
| 2:I:241:LEU:HD21 | 2:I:246:LEU:HD11 | 1.92 | 0.52 |
| 2:I:734:ILE:HD12 | 2:I:777:VAL:HG21 | 1.90 | 0.52 |
| 1:H:182:ARG:NH1 | 3:J:534:GLU:OE1 | 2.43 | 0.52 |
| 5:L:165:PHE:CE2 | 5:L:217:ALA:HA | 2.44 | 0.52 |
| 5:L:489:MET:HB2 | 5:L:490:PRO:HD2 | 1.91 | 0.52 |
| 3:D:1280:VAL:HG21 | 3:D:1304:ARG:NE | 2.21 | 0.52 |
| 3:D:817:HIS:CE1 | 3:D:860:ARG:HE | 2.27 | 0.52 |
| 1:G:74:VAL:HG22 | 1:G:76:GLU:H | 1.74 | 0.52 |
| 2:I:1191:LYS:HD3 | 2:I:1193:ALA:H | 1.73 | 0.52 |
| 2:I:324:LYS:O | 2:I:327:GLN:NE2 | 2.43 | 0.52 |
| 3:J:338:PHE:CB | 3:J:343:LEU:HB2 | 2.39 | 0.52 |
| 1:B:83:LEU:HA | 1:B:86:LYS:HE2 | 1.91 | 0.52 |
| 2:C:6:THR:HG21 | 2:C:782:VAL:HG23 | 1.90 | 0.52 |
| 2:C:718:ALA:HB2 | 2:C:783:LEU:HD23 | 1.91 | 0.52 |
| 3:D:279:LEU:HD11 | 3:D:296:LYS:HG2 | 1.90 | 0.52 |
| 3:D:77:ARG:HE | 5:F:569:THR:HA | 1.74 | 0.52 |
| 2:I:124:MET:HB2 | 2:I:498:ILE:HD13 | 1.90 | 0.52 |
| 2:I:590:PRO:HG3 | 2:I:605:TYR:CZ | 2.44 | 0.52 |
| 3:J:119:SER:O | 3:J:121:PRO:HD2 | 2.10 | 0.52 |
| 1:B:91:ARG:HG3 | 1:B:122:GLU:HB3 | 1.90 | 0.52 |
| 3:D:1162:ILE:HG23 | 3:D:1178:THR:HB | 1.92 | 0.52 |
| 3:D:275:ARG:HD3 | 3:D:298:MET:HB3 | 1.92 | 0.52 |
| 5:F:126:GLY:O | 5:F:129:GLN:HB2 | 2.10 | 0.52 |
| 1:G:61:ILE:HG22 | 1:G:62:ASP:H | 1.74 | 0.52 |
| 2:I:814:ASP:OD2 | 2:I:1106:ARG:NH1 | 2.36 | 0.52 |
| 2:C:591:TYR:OH | 2:C:637:ARG:NH2 | 2.42 | 0.52 |
| 3:D:1297:LYS:HG2 | 3:J:1302:TYR:H | 1.73 | 0.52 |
| 5:F:49:ASN:HA | 5:F:53:ILE:HA | 1.91 | 0.52 |
| 1:G:12:ARG:HG3 | 1:H:230:ALA:HB1 | 1.92 | 0.52 |
| 5:L:547:VAL:HG12 | 5:L:598:LEU:HD22 | 1.92 | 0.52 |
| 2:I:820:GLU:HA | 2:I:1079:ILE:HD11 | 1.92 | 0.52 |
| 2:I:668:ILE:HD11 | 2:I:683:ALA:HB2 | 1.92 | 0.52 |
| 3:J:1162:ILE:HG23 | 3:J:1178:THR:HB | 1.92 | 0.52 |
| 5:F:441:ARG:NH1 | 5:F:445:ASP:OD1 | 2.43 | 0.52 |
| 2:I:1149:TYR:HB3 | 2:I:1159:VAL:HG11 | 1.91 | 0.52 |
| 5:L:119:ILE:HA | 5:L:122:ARG:HD3 | 1.92 | 0.52 |
| 2:C:734:ILE:HD12 | 2:C:777:VAL:HG21 | 1.92 | 0.51 |
| 5:F:489:MET:HB2 | 5:F:490:PRO:HD2 | 1.91 | 0.51 |
| 2:I:344:GLY:HA3 | 2:I:346:TYR:CZ | 2.45 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:1280:ALA:HB1 | 3:J:918:ILE:HG22 | 1.91 | 0.51 |
| 5:L:483:LEU:H | 5:L:483:LEU:HD12 | 1.74 | 0.51 |
| 3:D:73:GLY:O | 3:D:76:LYS:NZ | 2.33 | 0.51 |
| 1:G:231:PHE:HZ | 1:H:221:ALA:HB3 | 1.76 | 0.51 |
| 1:G:231:PHE:HB3 | 1:H:218:ARG:HH11 | 1.74 | 0.51 |
| 2:I:103:VAL:HB | 2:I:113:THR:HG21 | 1.91 | 0.51 |
| 3:J:1060:VAL:HG22 | 3:J:1106:ILE:HG23 | 1.92 | 0.51 |
| 3:D:585:LYS:HB2 | 3:D:612:LEU:HD21 | 1.92 | 0.51 |
| 2:C:26:TYR:CZ | 2:C:28:LEU:HB2 | 2.46 | 0.51 |
| 2:C:349:GLU:O | 2:C:353:VAL:HG23 | 2.10 | 0.51 |
| 1:H:83:LEU:HA | 1:H:86:LYS:HE2 | 1.91 | 0.51 |
| 2:I:242:VAL:HB | 2:I:245:ARG:HD2 | 1.92 | 0.51 |
| 3:J:474:LEU:HD12 | 3:J:477:GLN:HE21 | 1.75 | 0.51 |
| 2:C:103:VAL:HB | 2:C:113:THR:HG21 | 1.91 | 0.51 |
| 5:F:41:ILE:HA | 5:F:44:ILE:HG23 | 1.93 | 0.51 |
| 3:J:1078:LEU:HB3 | 3:J:1121:LEU:HD13 | 1.92 | 0.51 |
| 3:J:275:ARG:HD3 | 3:J:298:MET:HB3 | 1.92 | 0.51 |
| 3:J:798:ARG:NH1 | 3:J:802:ASP:OD2 | 2.43 | 0.51 |
| 3:D:474:LEU:HD12 | 3:D:477:GLN:HE21 | 1.75 | 0.51 |
| 1:G:50:SER:HB3 | 1:H:8:PHE:HE1 | 1.76 | 0.51 |
| 1:H:11:PRO:HB3 | 1:H:30:PRO:O | 2.10 | 0.51 |
| 3:J:189:LEU:HB3 | 3:J:234:PRO:HB2 | 1.93 | 0.51 |
| 2:C:149:LEU:HB2 | 2:C:530:ILE:HG22 | 1.93 | 0.51 |
| 2:C:28:LEU:HD21 | 2:C:524:ILE:HG13 | 1.93 | 0.51 |
| 1:G:172:LEU:HD12 | 1:G:172:LEU:H | 1.76 | 0.51 |
| 2:I:672:GLU:HG2 | 2:I:1187:PHE:HA | 1.93 | 0.51 |
| 3:J:568:SER:OG | 3:J:569:LEU:N | 2.43 | 0.51 |
| 3:J:817:HIS:CE1 | 3:J:860:ARG:HE | 2.27 | 0.51 |
| 5:L:448:ARG:NH1 | 5:L:501:ALA:O | 2.35 | 0.51 |
| 1:B:23:HIS:ND1 | 1:B:206:GLU:HG2 | 2.26 | 0.51 |
| 1:B:56:VAL:HG22 | 1:B:144:ILE:HD11 | 1.93 | 0.51 |
| 2:I:26:TYR:CZ | 2:I:28:LEU:HB2 | 2.46 | 0.51 |
| 3:J:1024:THR:HG22 | 3:J:1026:PRO:HD3 | 1.92 | 0.51 |
| 2:C:1151:LEU:HD21 | 2:C:1198:LEU:HD23 | 1.92 | 0.51 |
| 5:F:316:PHE:HZ | 5:F:334:SER:HA | 1.76 | 0.51 |
| 2:I:149:LEU:HB2 | 2:I:530:ILE:HG22 | 1.92 | 0.51 |
| 3:J:113:HIS:CE1 | 3:J:307:LEU:HD13 | 2.46 | 0.51 |
| 3:D:1268:ASN:HD22 | 3:J:1268:ASN:HD22 | 1.59 | 0.51 |
| 5:L:126:GLY:O | 5:L:130:VAL:HG13 | 2.11 | 0.51 |
| 2:C:1122:LYS:HG2 | 2:C:1229:TYR:CE1 | 2.46 | 0.51 |
| 3:D:113:HIS:CE1 | 3:D:307:LEU:HD13 | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:119:ILE:HA | 5:F:122:ARG:HD3 | 1.92 | 0.51 |
| 5:F:313:ASP:OD1 | 5:F:338:HIS:NE2 | 2.44 | 0.51 |
| 5:F:483:LEU:H | 5:F:483:LEU:HD12 | 1.75 | 0.51 |
| 1:H:56:VAL:HG22 | 1:H:144:ILE:HD11 | 1.92 | 0.51 |
| 2:I:349:GLU:O | 2:I:353:VAL:HG23 | 2.11 | 0.51 |
| 3:D:798:ARG:NH1 | 3:D:802:ASP:OD2 | 2.44 | 0.50 |
| 5:F:551:LEU:HD11 | 5:F:598:LEU:HD21 | 1.92 | 0.50 |
| 3:J:1078:LEU:HD13 | 3:J:1121:LEU:HD22 | 1.93 | 0.50 |
| 3:J:585:LYS:HB2 | 3:J:612:LEU:HD21 | 1.93 | 0.50 |
| 1:A:91:ARG:HD3 | 1:A:210:THR:O | 2.12 | 0.50 |
| 5:F:164:GLY:O | 5:F:260:ARG:HB2 | 2.10 | 0.50 |
| 5:F:402:LEU:HA | 5:F:405:ILE:HG12 | 1.94 | 0.50 |
| 3:J:73:GLY:O | 3:J:76:LYS:NZ | 2.34 | 0.50 |
| 2:I:1122:LYS:HG2 | 2:I:1229:TYR:CE1 | 2.45 | 0.50 |
| 2:C:668:ILE:HD11 | 2:C:683:ALA:HB2 | 1.92 | 0.50 |
| 3:D:568:SER:OG | 3:D:569:LEU:N | 2.44 | 0.50 |
| 2:C:820:GLU:HA | 2:C:1079:ILE:HD11 | 1.93 | 0.50 |
| 2:C:344:GLY:HA3 | 2:C:346:TYR:CZ | 2.46 | 0.50 |
| 2:C:646:SER:HB3 | 2:C:649:GLN:HG3 | 1.93 | 0.50 |
| 2:C:672:GLU:HG2 | 2:C:1187:PHE:HA | 1.93 | 0.50 |
| 2:C:867:GLU:OE1 | 2:C:943:LYS:NZ | 2.42 | 0.50 |
| 1:H:23:HIS:ND1 | 1:H:206:GLU:HG2 | 2.26 | 0.50 |
| 3:J:978:ARG:HB2 | 3:J:1199:PHE:HZ | 1.76 | 0.50 |
| 5:L:313:ASP:OD1 | 5:L:338:HIS:NE2 | 2.45 | 0.50 |
| 5:L:316:PHE:HZ | 5:L:334:SER:HA | 1.76 | 0.50 |
| 3:D:363:LEU:HD23 | 3:D:487:THR:HG22 | 1.94 | 0.50 |
| 3:J:147:ILE:HG22 | 3:J:188:LEU:HG | 1.94 | 0.50 |
| 5:L:164:GLY:O | 5:L:260:ARG:HB2 | 2.10 | 0.50 |
| 3:D:189:LEU:HB3 | 3:D:234:PRO:HB2 | 1.93 | 0.50 |
| 3:D:422:LEU:HD13 | 3:D:471:PRO:HG3 | 1.94 | 0.50 |
| 1:G:45:ARG:NH2 | 2:I:1216:ARG:HA | 2.27 | 0.50 |
| 3:J:189:LEU:HD22 | 3:J:234:PRO:HB3 | 1.93 | 0.50 |
| 5:L:573:LEU:H | 5:L:573:LEU:HD23 | 1.76 | 0.50 |
| 3:D:205:LEU:HD23 | 3:D:217:LEU:HB3 | 1.93 | 0.50 |
| 5:F:461:ASN:O | 5:F:465:ARG:HG2 | 2.11 | 0.50 |
| 2:I:28:LEU:HD21 | 2:I:524:ILE:HG13 | 1.93 | 0.50 |
| 3:J:1191:PRO:HB2 | 3:J:1194:ARG:HD3 | 1.94 | 0.50 |
| 2:C:250:THR:HA | 2:C:268:ARG:HA | 1.93 | 0.50 |
| 3:D:824:PRO:HD3 | 3:D:835:LEU:HB2 | 1.94 | 0.50 |
| 2:C:842:ASP:N | 2:C:1045:GLY:O | 2.45 | 0.49 |
| 2:I:692:THR:OG1 | 2:I:693:LEU:N | 2.45 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:L:461:ASN:O | 5:L:465:ARG:HG2 | 2.12 | 0.49 |
| 2:I:1151:LEU:HD21 | 2:I:1198:LEU:HD23 | 1.93 | 0.49 |
| 2:I:1176:LEU:HD13 | 2:I:1180:MET:HG2 | 1.94 | 0.49 |
| 3:J:950:ILE:HG13 | 3:J:1020:TRP:CH2 | 2.47 | 0.49 |
| 3:J:422:LEU:HD13 | 3:J:471:PRO:HG3 | 1.94 | 0.49 |
| 5:L:41:ILE:HA | 5:L:44:ILE:HG23 | 1.93 | 0.49 |
| 2:C:1101:LEU:HD13 | 3:D:504:GLN:HB2 | 1.95 | 0.49 |
| 2:C:1185:PRO:HB2 | 2:C:1188:ASP:HB3 | 1.93 | 0.49 |
| 3:D:147:ILE:HG22 | 3:D:188:LEU:HG | 1.94 | 0.49 |
| 3:D:800:LEU:HB3 | 3:D:920:ALA:HB1 | 1.95 | 0.49 |
| 3:D:325:LYS:HD3 | 5:F:508:GLU:HG2 | 1.95 | 0.49 |
| 2:I:739:ASP:N | 2:I:739:ASP:OD1 | 2.38 | 0.49 |
| 3:J:363:LEU:HD23 | 3:J:487:THR:HG22 | 1.94 | 0.49 |
| 3:J:800:LEU:HB3 | 3:J:920:ALA:HB1 | 1.94 | 0.49 |
| 2:C:242:VAL:HB | 2:C:245:ARG:HD2 | 1.93 | 0.49 |
| 5:F:281:ARG:O | 5:F:285:ARG:HG3 | 2.13 | 0.49 |
| 2:I:1192:GLU:O | 2:I:1196:LYS:HG2 | 2.13 | 0.49 |
| 2:I:402:ARG:NH2 | 2:I:419:ILE:O | 2.46 | 0.49 |
| 2:I:842:ASP:N | 2:I:1045:GLY:O | 2.45 | 0.49 |
| 3:J:1343:GLU:HB3 | 3:J:1345:ARG:HD3 | 1.94 | 0.49 |
| 3:J:975:ILE:HD13 | 3:J:980:THR:HG21 | 1.94 | 0.49 |
| 5:L:299:LYS:HA | 5:L:302:PHE:HB3 | 1.95 | 0.49 |
| 2:I:897:PRO:HG3 | 3:J:77:ARG:HH22 | 1.77 | 0.49 |
| 2:I:971:LEU:HG | 2:I:1014:LEU:HD23 | 1.95 | 0.49 |
| 5:L:402:LEU:HA | 5:L:405:ILE:HG12 | 1.94 | 0.49 |
| 1:A:13:LEU:H | 1:A:13:LEU:HD23 | 1.78 | 0.49 |
| 1:A:228:LEU:HD21 | 1:B:224:LEU:HD23 | 1.95 | 0.49 |
| 1:G:102:LEU:HB3 | 1:G:142:MET:HG2 | 1.95 | 0.49 |
| 1:G:231:PHE:HB3 | 1:H:218:ARG:NH1 | 2.27 | 0.49 |
| 2:I:250:THR:HA | 2:I:268:ARG:HA | 1.94 | 0.49 |
| 2:I:968:GLU:HG3 | 2:I:1018:TYR:HE1 | 1.77 | 0.49 |
| 2:I:746:ALA:HB3 | 2:I:971:LEU:HA | 1.95 | 0.49 |
| 3:J:122:SER:O | 3:J:126:LEU:HG | 2.13 | 0.49 |
| 3:J:205:LEU:HD23 | 3:J:217:LEU:HB3 | 1.95 | 0.49 |
| 5:L:281:ARG:O | 5:L:285:ARG:HG3 | 2.13 | 0.49 |
| 1:B:48:LEU:HD12 | 1:B:183:ILE:HD11 | 1.95 | 0.49 |
| 2:C:146:VAL:HG13 | 2:C:529:ARG:HB3 | 1.95 | 0.49 |
| 3:D:266:ASN:O | 3:D:270:ARG:HB2 | 2.13 | 0.49 |
| 5:F:244:THR:O | 5:F:247:GLU:HG2 | 2.13 | 0.49 |
| 2:I:856:ASN:HB3 | 5:L:613:ASP:HA | 1.93 | 0.49 |
| 3:J:1233:ILE:O | 3:J:1237:VAL:HG12 | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:202:ARG:HH22 | 2:C:368:ARG:HH12 | 1.61 | 0.49 |
| 3:D:189:LEU:HD22 | 3:D:234:PRO:HB3 | 1.94 | 0.49 |
| 2:C:968:GLU:HG3 | 2:C:1018:TYR:HE1 | 1.78 | 0.48 |
| 3:D:35:PHE:HD1 | 3:D:101:ARG:HD3 | 1.78 | 0.48 |
| 2:I:95:PRO:HA | 2:I:126:GLU:HG2 | 1.95 | 0.48 |
| 2:I:1287:LEU:HD22 | 3:J:1357:ILE:HD11 | 1.95 | 0.48 |
| 2:I:936:ARG:NH2 | 2:I:1043:ALA:O | 2.46 | 0.48 |
| 3:J:591:ILE:HG13 | 3:J:604:MET:HE2 | 1.94 | 0.48 |
| 3:J:824:PRO:HD3 | 3:J:835:LEU:HB2 | 1.94 | 0.48 |
| 2:C:238:GLN:HB3 | 2:C:284:LEU:HD11 | 1.94 | 0.48 |
| 2:C:255:ILE:HB | 2:C:263:VAL:HB | 1.96 | 0.48 |
| 2:C:878:THR:OG1 | 2:C:879:GLY:N | 2.45 | 0.48 |
| 3:D:103:GLY:HA3 | 3:D:244:VAL:HG22 | 1.95 | 0.48 |
| 3:D:1319:PHE:CE2 | 3:D:1342:ASP:HB2 | 2.48 | 0.48 |
| 3:D:392:THR:HG21 | 5:F:606:VAL:HA | 1.95 | 0.48 |
| 1:G:31:LEU:HD13 | 1:G:36:GLY:HA2 | 1.94 | 0.48 |
| 2:I:197:ARG:HH12 | 5:L:29:ASP:HB3 | 1.78 | 0.48 |
| 1:B:100:LEU:HD21 | 1:B:121:VAL:HG11 | 1.96 | 0.48 |
| 2:C:819:SER:HB2 | 2:C:1085:MET:HG3 | 1.95 | 0.48 |
| 2:C:1313:HIS:N | 4:E:31:GLN:OE1 | 2.39 | 0.48 |
| 5:F:583:THR:HG22 | 5:F:584:ARG:H | 1.79 | 0.48 |
| 2:I:238:GLN:HB3 | 2:I:284:LEU:HD11 | 1.94 | 0.48 |
| 2:I:799:ASN:HA | 2:I:1231:TYR:HA | 1.94 | 0.48 |
| 3:J:1036:ARG:HG2 | 3:J:1037:PHE:H | 1.78 | 0.48 |
| 3:J:1349:GLU:N | 3:J:1349:GLU:OE2 | 2.33 | 0.48 |
| 3:J:68:TYR:HA | 3:J:92:VAL:HG23 | 1.96 | 0.48 |
| 2:C:95:PRO:HA | 2:C:126:GLU:HG2 | 1.95 | 0.48 |
| 2:C:692:THR:OG1 | 2:C:693:LEU:N | 2.46 | 0.48 |
| 2:C:778:GLU:O | 2:C:781:ASP:HB2 | 2.14 | 0.48 |
| 3:D:1268:ASN:HD22 | 3:J:1268:ASN:ND2 | 2.11 | 0.48 |
| 1:G:13:LEU:H | 1:G:13:LEU:HD23 | 1.78 | 0.48 |
| 2:I:1185:PRO:HB2 | 2:I:1188:ASP:HB3 | 1.93 | 0.48 |
| 2:I:646:SER:HB3 | 2:I:649:GLN:HG3 | 1.95 | 0.48 |
| 3:J:1350:ASN:HA | 3:J:1353:VAL:HG12 | 1.96 | 0.48 |
| 3:J:341:ASN:HB2 | 3:J:1352:ILE:HD13 | 1.95 | 0.48 |
| 3:J:266:ASN:O | 3:J:270:ARG:HB2 | 2.13 | 0.48 |
| 3:J:35:PHE:HD1 | 3:J:101:ARG:HD3 | 1.78 | 0.48 |
| 2:C:799:ASN:HA | 2:C:1231:TYR:HA | 1.94 | 0.48 |
| 3:D:77:ARG:HG3 | 3:D:79:LYS:H | 1.78 | 0.48 |
| 5:F:165:PHE:HE2 | 5:F:217:ALA:HA | 1.77 | 0.48 |
| 2:I:136:PHE:CE2 | 2:I:456:VAL:HG11 | 2.48 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:819:SER:HB2 | 2:I:1085:MET:HG3 | 1.94 | 0.48 |
| 3:J:1077:ALA:HB2 | 3:J:1100:PHE:CD1 | 2.48 | 0.48 |
| 3:J:218:THR:HA | 3:J:221:ILE:HG22 | 1.96 | 0.48 |
| 2:I:1101:LEU:HD13 | 3:J:504:GLN:HB2 | 1.95 | 0.48 |
| 1:B:54:CYS:SG | 1:B:148:ARG:HG2 | 2.53 | 0.48 |
| 3:D:218:THR:HA | 3:D:221:ILE:HG22 | 1.96 | 0.48 |
| 3:D:750:PRO:HA | 3:D:777:HIS:CE1 | 2.49 | 0.48 |
| 5:F:448:ARG:NH1 | 5:F:501:ALA:O | 2.35 | 0.48 |
| 3:J:511:TYR:OH | 3:J:515:ARG:NH1 | 2.47 | 0.48 |
| 2:C:1192:GLU:O | 2:C:1196:LYS:HG2 | 2.14 | 0.48 |
| 3:D:1191:PRO:HB2 | 3:D:1194:ARG:HD3 | 1.94 | 0.48 |
| 2:I:878:THR:OG1 | 2:I:879:GLY:N | 2.46 | 0.48 |
| 3:J:77:ARG:HG3 | 3:J:79:LYS:H | 1.78 | 0.48 |
| 5:L:165:PHE:HE2 | 5:L:217:ALA:HA | 1.77 | 0.48 |
| 5:F:299:LYS:HA | 5:F:302:PHE:HB3 | 1.95 | 0.48 |
| 5:L:244:THR:O | 5:L:247:GLU:HG2 | 2.13 | 0.48 |
| 3:D:1227:HIS:CD2 | 3:J:1293:GLU:HG2 | 2.48 | 0.48 |
| 3:D:548:VAL:HG12 | 3:D:550:VAL:HG13 | 1.96 | 0.48 |
| 2:I:778:GLU:O | 2:I:781:ASP:HB2 | 2.14 | 0.48 |
| 3:J:708:ASN:HB3 | 3:J:712:GLN:O | 2.14 | 0.48 |
| 3:J:863:LEU:HD11 | 3:J:901:ARG:HB3 | 1.96 | 0.48 |
| 3:D:1233:ILE:O | 3:D:1237:VAL:HG12 | 2.14 | 0.48 |
| 2:I:813:GLU:HB2 | 3:J:461:PHE:HB2 | 1.95 | 0.48 |
| 1:A:102:LEU:HB3 | 1:A:142:MET:HG2 | 1.95 | 0.47 |
| 2:C:400:VAL:HG21 | 2:C:452:ARG:NH1 | 2.29 | 0.47 |
| 2:C:402:ARG:NH2 | 2:C:419:ILE:O | 2.47 | 0.47 |
| 3:D:115:TRP:O | 3:D:119:SER:HB2 | 2.14 | 0.47 |
| 1:G:184:ALA:HB2 | 2:I:1091:GLY:HA3 | 1.96 | 0.47 |
| 1:H:54:CYS:SG | 1:H:148:ARG:HG2 | 2.54 | 0.47 |
| 1:A:31:LEU:HD13 | 1:A:36:GLY:HA2 | 1.96 | 0.47 |
| 2:C:1287:LEU:HD22 | 3:D:1357:ILE:HD11 | 1.96 | 0.47 |
| 3:D:268:LEU:HD13 | 3:D:306:LEU:HA | 1.95 | 0.47 |
| 2:C:1116:HIS:HE1 | 3:D:641:ILE:H | 1.62 | 0.47 |
| 1:H:48:LEU:HD12 | 1:H:183:ILE:HD11 | 1.95 | 0.47 |
| 1:H:95:LYS:NZ | 1:H:98:VAL:HG23 | 2.29 | 0.47 |
| 3:D:733:SER:O | 3:D:737:ILE:HG12 | 2.14 | 0.47 |
| 1:G:225:ALA:HA | 1:G:228:LEU:HD23 | 1.97 | 0.47 |
| 2:I:115:LYS:HE3 | 2:I:116:ASP:H | 1.79 | 0.47 |
| 3:J:548:VAL:HG12 | 3:J:550:VAL:HG13 | 1.96 | 0.47 |
| 2:I:1116:HIS:HE1 | 3:J:641:ILE:H | 1.62 | 0.47 |
| 3:J:733:SER:O | 3:J:737:ILE:HG12 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:971:LEU:HG | 2:C:1014:LEU:HD23 | 1.95 | 0.47 |
| 3:D:13:LYS:HD3 | 3:D:13:LYS:HA | 1.70 | 0.47 |
| 5:L:137:TYR:HE1 | 5:L:351:THR:HB | 1.80 | 0.47 |
| 1:B:95:LYS:NZ | 1:B:98:VAL:HG23 | 2.29 | 0.47 |
| 2:C:813:GLU:HB2 | 3:D:461:PHE:HB2 | 1.96 | 0.47 |
| 2:I:26:TYR:CE2 | 2:I:32:LEU:HD12 | 2.49 | 0.47 |
| 2:I:202:ARG:HH22 | 2:I:368:ARG:HH12 | 1.61 | 0.47 |
| 3:D:854:ALA:HB2 | 3:J:1372:ARG:HB2 | 1.96 | 0.47 |
| 3:J:103:GLY:HA3 | 3:J:244:VAL:HG22 | 1.95 | 0.47 |
| 3:J:474:LEU:HD23 | 4:K:28:ARG:HG2 | 1.96 | 0.47 |
| 3:D:122:SER:O | 3:D:126:LEU:HG | 2.13 | 0.47 |
| 3:D:591:ILE:HG13 | 3:D:604:MET:HE2 | 1.97 | 0.47 |
| 5:F:137:TYR:HE1 | 5:F:351:THR:HB | 1.80 | 0.47 |
| 1:H:100:LEU:HD21 | 1:H:121:VAL:HG11 | 1.96 | 0.47 |
| 2:I:517:GLN:O | 2:I:517:GLN:HG2 | 2.15 | 0.47 |
| 3:J:395:LYS:HE2 | 5:L:536:THR:HG21 | 1.96 | 0.47 |
| 3:J:750:PRO:HA | 3:J:777:HIS:CE1 | 2.49 | 0.47 |
| 3:J:839:VAL:HG12 | 3:J:864:LEU:HD12 | 1.97 | 0.47 |
| 1:A:225:ALA:HA | 1:A:228:LEU:HD23 | 1.96 | 0.47 |
| 2:C:936:ARG:NH2 | 2:C:1043:ALA:O | 2.47 | 0.47 |
| 2:C:115:LYS:HE3 | 2:C:116:ASP:H | 1.78 | 0.47 |
| 2:C:560:PRO:HB3 | 3:D:776:THR:HG21 | 1.97 | 0.47 |
| 2:C:21:VAL:HG11 | 2:C:592:ARG:HD2 | 1.97 | 0.47 |
| 2:C:697:LYS:HB3 | 2:C:697:LYS:HE2 | 1.74 | 0.47 |
| 3:D:1287:ILE:HG13 | 3:D:1288:ALA:N | 2.30 | 0.47 |
| 2:C:1320:PRO:HG2 | 3:D:1354:GLY:HA3 | 1.97 | 0.47 |
| 3:D:708:ASN:HB3 | 3:D:712:GLN:O | 2.14 | 0.47 |
| 1:G:66:HIS:HA | 1:G:171:LEU:HD11 | 1.97 | 0.47 |
| 2:I:146:VAL:HG13 | 2:I:529:ARG:HB3 | 1.95 | 0.47 |
| 2:I:448:LEU:HB2 | 2:I:553:THR:HB | 1.96 | 0.47 |
| 3:J:709:ARG:C | 3:J:711:GLY:H | 2.18 | 0.47 |
| 5:L:127:ILE:O | 5:L:130:VAL:HG22 | 2.14 | 0.47 |
| 1:A:50:SER:HB3 | 1:A:150:ARG:HD2 | 1.95 | 0.47 |
| 2:C:232:ILE:HG12 | 2:C:237:LEU:HD13 | 1.96 | 0.47 |
| 3:D:1295:ASN:HB2 | 3:D:1298:VAL:HB | 1.97 | 0.47 |
| 3:D:190:LYS:HD3 | 3:D:235:GLU:HG2 | 1.97 | 0.47 |
| 3:D:511:TYR:OH | 3:D:515:ARG:NH1 | 2.47 | 0.47 |
| 2:C:1248:THR:HG21 | 5:F:531:PRO:HG3 | 1.97 | 0.47 |
| 2:I:170:VAL:HG23 | 2:I:171:LEU:H | 1.80 | 0.47 |
| 3:J:268:LEU:HD13 | 3:J:306:LEU:HA | 1.96 | 0.47 |
| 2:C:1308:ILE:HG23 | 3:D:380:PHE:CE2 | 2.50 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:217:THR:HG23 | 2:C:351:LEU:HD13 | 1.97 | 0.47 |
| 3:D:68:TYR:HA | 3:D:92:VAL:HG23 | 1.96 | 0.47 |
| 3:D:474:LEU:HD23 | 4:E:28:ARG:HG2 | 1.96 | 0.47 |
| 5:L:225:ARG:O | 5:L:229:VAL:HG13 | 2.15 | 0.47 |
| 2:C:387:ASN:HA | 2:C:391:SER:HB2 | 1.97 | 0.47 |
| 2:C:50:GLU:HG2 | 2:C:73:TYR:HE1 | 1.80 | 0.47 |
| 5:F:225:ARG:O | 5:F:229:VAL:HG13 | 2.15 | 0.47 |
| 1:H:73:GLY:HA3 | 1:H:138:ALA:HB1 | 1.96 | 0.47 |
| 3:J:950:ILE:HB | 3:J:1018:ALA:HB3 | 1.97 | 0.47 |
| 2:I:1308:ILE:HG21 | 3:J:379:PRO:HB2 | 1.96 | 0.47 |
| 5:L:583:THR:HG22 | 5:L:584:ARG:H | 1.79 | 0.47 |
| 2:C:1159:VAL:HB | 2:C:1160:ASP:H | 1.60 | 0.46 |
| 1:G:228:LEU:HD13 | 1:G:228:LEU:HA | 1.79 | 0.46 |
| 2:I:170:VAL:HG23 | 2:I:171:LEU:N | 2.30 | 0.46 |
| 3:J:1287:ILE:HG13 | 3:J:1288:ALA:N | 2.30 | 0.46 |
| 5:L:507:MET:HG2 | 5:L:520:GLY:HA3 | 1.97 | 0.46 |
| 2:C:538:LEU:HD22 | 2:C:543:ALA:HB2 | 1.97 | 0.46 |
| 3:D:349:TYR:HE2 | 3:D:379:PRO:HG2 | 1.81 | 0.46 |
| 2:I:97:ARG:HB3 | 2:I:121:GLU:HB2 | 1.97 | 0.46 |
| 3:J:1167:LYS:HE3 | 3:J:1168:GLU:H | 1.80 | 0.46 |
| 3:J:1170:LYS:C | 3:J:1172:LYS:H | 2.18 | 0.46 |
| 2:C:1176:LEU:HD13 | 2:C:1180:MET:HG2 | 1.95 | 0.46 |
| 3:D:1350:ASN:HA | 3:D:1353:VAL:HG12 | 1.96 | 0.46 |
| 3:D:133:ARG:NH2 | 5:F:93:ARG:O | 2.47 | 0.46 |
| 2:I:838:CYS:SG | 2:I:886:LYS:HD3 | 2.55 | 0.46 |
| 2:C:850:ILE:HG13 | 2:C:1048:LYS:HE2 | 1.97 | 0.46 |
| 3:D:708:ASN:N | 3:D:708:ASN:OD1 | 2.48 | 0.46 |
| 3:D:863:LEU:HD11 | 3:D:901:ARG:HB3 | 1.95 | 0.46 |
| 5:F:561:MET:HG3 | 5:F:571:TYR:CD2 | 2.50 | 0.46 |
| 2:I:560:PRO:HB3 | 3:J:776:THR:HG21 | 1.97 | 0.46 |
| 3:J:124:ILE:HG23 | 3:J:189:LEU:HD11 | 1.98 | 0.46 |
| 3:J:79:LYS:HB2 | 5:L:569:THR:N | 2.31 | 0.46 |
| 1:B:73:GLY:HA3 | 1:B:138:ALA:HB1 | 1.97 | 0.46 |
| 2:C:170:VAL:HG23 | 2:C:171:LEU:N | 2.31 | 0.46 |
| 2:C:578:TYR:HB3 | 2:C:590:PRO:HG2 | 1.97 | 0.46 |
| 2:I:578:TYR:HB3 | 2:I:590:PRO:HG2 | 1.96 | 0.46 |
| 1:A:45:ARG:NH2 | 2:C:1216:ARG:HA | 2.28 | 0.46 |
| 2:C:838:CYS:SG | 2:C:886:LYS:HD3 | 2.55 | 0.46 |
| 3:D:709:ARG:C | 3:D:711:GLY:H | 2.18 | 0.46 |
| 2:I:1125:GLY:HA3 | 2:I:1179:GLY:HA2 | 1.97 | 0.46 |
| 2:I:255:ILE:HB | 2:I:263:VAL:HB | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:385:LEU:HD11 | 3:J:408:VAL:HG12 | 1.98 | 0.46 |
| 5:L:380:VAL:HG22 | 5:L:416:VAL:HG21 | 1.98 | 0.46 |
| 2:C:448:LEU:HB2 | 2:C:553:THR:HB | 1.96 | 0.46 |
| 3:D:1170:LYS:C | 3:D:1172:LYS:H | 2.18 | 0.46 |
| 3:D:885:VAL:HG12 | 3:D:894:VAL:HG11 | 1.96 | 0.46 |
| 2:I:538:LEU:HD22 | 2:I:543:ALA:HB2 | 1.97 | 0.46 |
| 2:I:10:ARG:NH1 | 2:I:697:LYS:HD3 | 2.31 | 0.46 |
| 2:I:721:GLY:N | 2:I:740:GLU:OE1 | 2.45 | 0.46 |
| 2:I:732:ILE:HD11 | 2:I:769:PRO:HB3 | 1.98 | 0.46 |
| 3:J:611:ILE:HG22 | 3:J:612:LEU:HD12 | 1.97 | 0.46 |
| 3:J:950:ILE:HG13 | 3:J:1020:TRP:HH2 | 1.81 | 0.46 |
| 5:L:561:MET:HG3 | 5:L:571:TYR:CD2 | 2.50 | 0.46 |
| 1:G:51:MET:HB3 | 1:G:51:MET:HE3 | 1.84 | 0.46 |
| 2:I:1101:LEU:HD21 | 3:J:508:LEU:HD22 | 1.96 | 0.46 |
| 2:I:657:THR:HG1 | 2:I:1187:PHE:HB2 | 1.80 | 0.46 |
| 2:I:724:VAL:HG11 | 2:I:727:VAL:HG22 | 1.97 | 0.46 |
| 3:J:695:LYS:HA | 3:J:695:LYS:HD3 | 1.72 | 0.46 |
| 1:A:66:HIS:HA | 1:A:171:LEU:HD11 | 1.97 | 0.46 |
| 2:C:724:VAL:HG11 | 2:C:727:VAL:HG22 | 1.98 | 0.46 |
| 3:D:1341:ARG:HH22 | 3:D:1373:ARG:HH21 | 1.64 | 0.46 |
| 1:G:12:ARG:H | 1:G:30:PRO:HD2 | 1.81 | 0.46 |
| 2:I:387:ASN:HA | 2:I:391:SER:HB2 | 1.97 | 0.46 |
| 2:C:517:GLN:HG2 | 2:C:517:GLN:O | 2.15 | 0.46 |
| 3:D:611:ILE:HG22 | 3:D:612:LEU:HD12 | 1.98 | 0.46 |
| 2:I:1262:LYS:HD3 | 2:I:1262:LYS:HA | 1.78 | 0.46 |
| 3:J:1063:ASP:O | 3:J:1067:ARG:HG3 | 2.16 | 0.46 |
| 2:C:591:TYR:HD2 | 2:C:606:LEU:HD13 | 1.81 | 0.45 |
| 2:C:89:GLY:HA2 | 2:C:140:GLY:HA3 | 1.97 | 0.45 |
| 3:D:385:LEU:HD11 | 3:D:408:VAL:HG12 | 1.98 | 0.45 |
| 3:J:963:VAL:HB | 3:J:980:THR:HG23 | 1.98 | 0.45 |
| 4:K:60:ASN:ND2 | 4:K:63:ILE:HD13 | 2.32 | 0.45 |
| 2:C:206:ALA:O | 2:C:209:ILE:HG22 | 2.16 | 0.45 |
| 3:D:839:VAL:HG12 | 3:D:864:LEU:HD12 | 1.97 | 0.45 |
| 5:F:380:VAL:HG22 | 5:F:416:VAL:HG21 | 1.98 | 0.45 |
| 3:J:1095:MET:HA | 3:J:1096:PRO:HD3 | 1.81 | 0.45 |
| 3:J:190:LYS:HD3 | 3:J:235:GLU:HG2 | 1.97 | 0.45 |
| 3:J:35:PHE:CD1 | 3:J:101:ARG:HD3 | 2.51 | 0.45 |
| 1:B:51:MET:HA | 1:B:52:PRO:HD3 | 1.85 | 0.45 |
| 2:C:1125:GLY:HA3 | 2:C:1179:GLY:HA2 | 1.98 | 0.45 |
| 2:C:721:GLY:N | 2:C:740:GLU:OE1 | 2.45 | 0.45 |
| 3:D:1349:GLU:N | 3:D:1349:GLU:OE2 | 2.33 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:425:ARG:HE | 3:D:427:PRO:HD2 | 1.82 | 0.45 |
| 2:I:50:GLU:HG2 | 2:I:73:TYR:HE1 | 1.81 | 0.45 |
| 2:I:705:GLU:HB2 | 2:I:794:LEU:HB3 | 1.98 | 0.45 |
| 2:I:850:ILE:HG13 | 2:I:1048:LYS:HE2 | 1.97 | 0.45 |
| 3:J:16:GLU:HG3 | 3:J:17:PHE:HD2 | 1.81 | 0.45 |
| 3:J:264:ASP:OD2 | 3:J:264:ASP:N | 2.50 | 0.45 |
| 3:D:1193:TRP:HB2 | 3:D:1194:ARG:NH1 | 2.31 | 0.45 |
| 3:D:1239:ASP:OD1 | 3:D:1242:ARG:NH2 | 2.48 | 0.45 |
| 3:D:30:ILE:HG23 | 3:D:243:PRO:HG3 | 1.97 | 0.45 |
| 5:F:507:MET:HG2 | 5:F:520:GLY:HA3 | 1.98 | 0.45 |
| 2:I:1122:LYS:HG2 | 2:I:1229:TYR:CZ | 2.51 | 0.45 |
| 2:I:206:ALA:O | 2:I:209:ILE:HG22 | 2.16 | 0.45 |
| 3:J:1280:VAL:O | 3:J:1284:ARG:HB3 | 2.16 | 0.45 |
| 3:J:1295:ASN:HB2 | 3:J:1298:VAL:HB | 1.97 | 0.45 |
| 3:J:246:PRO:HA | 3:J:247:PRO:HD3 | 1.83 | 0.45 |
| 1:A:64:VAL:HG11 | 1:A:78:ILE:HG21 | 1.99 | 0.45 |
| 2:C:820:GLU:N | 2:C:1080:ASN:O | 2.50 | 0.45 |
| 2:C:705:GLU:HB2 | 2:C:794:LEU:HB3 | 1.97 | 0.45 |
| 3:D:1280:VAL:O | 3:D:1284:ARG:HB3 | 2.16 | 0.45 |
| 3:D:124:ILE:HG23 | 3:D:189:LEU:HD11 | 1.98 | 0.45 |
| 4:K:60:ASN:HD21 | 4:K:63:ILE:HD13 | 1.81 | 0.45 |
| 2:C:113:THR:OG1 | 2:C:116:ASP:OD2 | 2.24 | 0.45 |
| 2:C:680:LEU:O | 2:C:684:ASN:HB2 | 2.17 | 0.45 |
| 5:F:362:ASN:HB2 | 5:F:365:MET:HE2 | 1.99 | 0.45 |
| 2:I:820:GLU:N | 2:I:1080:ASN:O | 2.49 | 0.45 |
| 2:I:17:LYS:HE3 | 2:I:1154:ASP:HB3 | 1.99 | 0.45 |
| 2:I:21:VAL:HG11 | 2:I:592:ARG:HD2 | 1.98 | 0.45 |
| 2:I:389:PHE:HB3 | 2:I:420:LEU:HD12 | 1.99 | 0.45 |
| 3:J:1193:TRP:HB2 | 3:J:1194:ARG:NH1 | 2.31 | 0.45 |
| 3:J:426:ALA:HB3 | 3:J:427:PRO:HD3 | 1.99 | 0.45 |
| 5:L:287:ILE:HG12 | 5:L:337:VAL:HG13 | 1.99 | 0.45 |
| 2:C:1101:LEU:HD21 | 3:D:508:LEU:HD22 | 1.98 | 0.45 |
| 3:D:426:ALA:HB3 | 3:D:427:PRO:HD3 | 1.99 | 0.45 |
| 4:E:60:ASN:HD21 | 4:E:63:ILE:HD13 | 1.81 | 0.45 |
| 5:F:44:ILE:HA | 5:F:47:MET:HB2 | 1.98 | 0.45 |
| 2:I:1159:VAL:HB | 2:I:1160:ASP:H | 1.59 | 0.45 |
| 2:I:678:ARG:HG3 | 2:I:1108:ASN:HD22 | 1.80 | 0.45 |
| 3:D:1293:GLU:HG2 | 3:J:1227:HIS:HB2 | 1.98 | 0.45 |
| 3:J:1244:GLN:HE21 | 3:J:1244:GLN:HB3 | 1.59 | 0.45 |
| 3:J:885:VAL:HG12 | 3:J:894:VAL:HG11 | 1.98 | 0.45 |
| 5:L:466:ILE:HD13 | 5:L:486:ARG:HB3 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:136:PHE:CE2 | 2:C:456:VAL:HG11 | 2.51 | 0.45 |
| 2:C:658:GLN:O | 2:C:661:VAL:HG22 | 2.17 | 0.45 |
| 2:C:10:ARG:NH1 | 2:C:697:LYS:HD3 | 2.31 | 0.45 |
| 2:C:739:ASP:OD1 | 2:C:739:ASP:N | 2.36 | 0.45 |
| 3:D:35:PHE:CD1 | 3:D:101:ARG:HD3 | 2.51 | 0.45 |
| 3:D:1146:GLU:HB3 | 3:D:1148:ARG:HG3 | 1.99 | 0.45 |
| 3:D:264:ASP:N | 3:D:264:ASP:OD2 | 2.50 | 0.45 |
| 5:F:287:ILE:HG12 | 5:F:337:VAL:HG13 | 1.99 | 0.45 |
| 1:G:47:LEU:HD13 | 1:G:183:ILE:HG12 | 1.99 | 0.45 |
| 2:I:217:THR:HG23 | 2:I:351:LEU:HD13 | 1.97 | 0.45 |
| 3:J:1156:LEU:HB3 | 3:J:1207:GLY:HA2 | 1.99 | 0.45 |
| 3:J:368:LEU:HD22 | 3:J:373:ALA:HB2 | 1.99 | 0.45 |
| 3:J:425:ARG:HE | 3:J:427:PRO:HD2 | 1.82 | 0.45 |
| 3:J:701:LEU:HD13 | 3:J:723:TYR:HB2 | 1.99 | 0.45 |
| 2:C:97:ARG:HB3 | 2:C:121:GLU:HB2 | 1.98 | 0.45 |
| 3:D:1216:ALA:HA | 3:D:1217:PRO:HD3 | 1.85 | 0.45 |
| 3:D:16:GLU:HG3 | 3:D:1369:ARG:NH2 | 2.32 | 0.45 |
| 3:D:50:LYS:HB3 | 3:D:71:LEU:HD21 | 1.98 | 0.45 |
| 2:C:1282:GLY:HA3 | 4:E:17:PHE:CE1 | 2.52 | 0.45 |
| 3:J:654:ILE:O | 3:J:658:GLU:HB2 | 2.17 | 0.45 |
| 3:J:974:VAL:HG21 | 3:J:1118:GLY:HA2 | 1.99 | 0.45 |
| 5:L:249:ILE:O | 5:L:252:LEU:HB3 | 2.16 | 0.45 |
| 3:D:425:ARG:HH12 | 3:D:464:ASP:CG | 2.20 | 0.45 |
| 3:D:587:LEU:HD11 | 3:D:608:CYS:HA | 1.99 | 0.45 |
| 2:I:680:LEU:O | 2:I:684:ASN:HB2 | 2.17 | 0.45 |
| 3:J:1061:VAL:HG21 | 3:J:1101:LEU:HB2 | 1.99 | 0.45 |
| 3:J:1286:LYS:HD2 | 3:J:1290:ARG:NH2 | 2.32 | 0.45 |
| 3:J:425:ARG:HH12 | 3:J:464:ASP:CG | 2.19 | 0.45 |
| 3:J:708:ASN:N | 3:J:708:ASN:OD1 | 2.48 | 0.45 |
| 3:J:901:ARG:HA | 3:J:908:ILE:HA | 1.99 | 0.45 |
| 5:L:130:VAL:HB | 5:L:365:MET:HG3 | 1.99 | 0.45 |
| 5:L:412:LEU:HD13 | 5:L:435:ILE:HD11 | 1.99 | 0.45 |
| 2:C:1122:LYS:HG2 | 2:C:1229:TYR:CZ | 2.52 | 0.44 |
| 2:C:1254:VAL:HG13 | 2:C:1255:THR:H | 1.83 | 0.44 |
| 2:C:1262:LYS:HD3 | 2:C:1262:LYS:HA | 1.77 | 0.44 |
| 2:C:724:VAL:HA | 2:C:734:ILE:HD13 | 1.99 | 0.44 |
| 3:D:1198:VAL:HB | 3:D:1210:ILE:HA | 1.99 | 0.44 |
| 1:B:48:LEU:HD21 | 3:D:535:ARG:HG3 | 1.98 | 0.44 |
| 5:F:354:THR:O | 5:F:358:VAL:HG23 | 2.17 | 0.44 |
| 2:I:113:THR:OG1 | 2:I:116:ASP:OD2 | 2.23 | 0.44 |
| 3:J:421:VAL:HG13 | 3:J:439:PRO:HG3 | 1.98 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:J:62:PHE:O | 3:J:101:ARG:HD2 | 2.17 | 0.44 |
| 5:L:572:THR:O | 5:L:576:VAL:HG23 | 2.17 | 0.44 |
| 1:B:79:LEU:HD23 | 1:B:79:LEU:H | 1.82 | 0.44 |
| 4:E:60:ASN:ND2 | 4:E:63:ILE:HD13 | 2.31 | 0.44 |
| 1:G:64:VAL:HG11 | 1:G:78:ILE:HG21 | 1.99 | 0.44 |
| 1:B:102:LEU:HD23 | 1:B:102:LEU:HA | 1.76 | 0.44 |
| 2:C:519:ASN:HD21 | 2:C:796:LEU:HD23 | 1.82 | 0.44 |
| 1:H:91:ARG:HG2 | 1:H:122:GLU:O | 2.17 | 0.44 |
| 2:I:519:ASN:HD21 | 2:I:796:LEU:HD23 | 1.82 | 0.44 |
| 3:J:800:LEU:O | 3:J:803:VAL:HG12 | 2.17 | 0.44 |
| 2:C:1149:TYR:CD1 | 2:C:1159:VAL:HG11 | 2.53 | 0.44 |
| 2:C:171:LEU:HA | 2:C:171:LEU:HD23 | 1.91 | 0.44 |
| 3:D:615:LYS:HB2 | 3:D:616:PRO:HD3 | 2.00 | 0.44 |
| 5:F:346:GLN:O | 5:F:350:GLU:HG3 | 2.17 | 0.44 |
| 5:F:466:ILE:HD13 | 5:F:486:ARG:HB3 | 1.99 | 0.44 |
| 1:G:197:ASP:N | 1:G:197:ASP:OD1 | 2.51 | 0.44 |
| 2:I:98:VAL:HG21 | 2:I:124:MET:HE3 | 2.00 | 0.44 |
| 3:J:1239:ASP:OD1 | 3:J:1242:ARG:NH2 | 2.48 | 0.44 |
| 3:J:587:LEU:HD11 | 3:J:608:CYS:HA | 1.99 | 0.44 |
| 1:A:197:ASP:N | 1:A:197:ASP:OD1 | 2.51 | 0.44 |
| 2:C:156:PHE:CE2 | 2:C:158:ASP:HB2 | 2.53 | 0.44 |
| 3:D:1167:LYS:HE3 | 3:D:1168:GLU:H | 1.80 | 0.44 |
| 3:D:800:LEU:O | 3:D:803:VAL:HG12 | 2.17 | 0.44 |
| 3:D:430:HIS:HA | 3:D:921:GLN:HB3 | 1.99 | 0.44 |
| 5:F:559:LEU:HA | 5:F:559:LEU:HD12 | 1.82 | 0.44 |
| 2:I:1065:LYS:HD2 | 2:I:1235:LEU:HD12 | 1.99 | 0.44 |
| 3:J:50:LYS:HB3 | 3:J:71:LEU:HD21 | 1.99 | 0.44 |
| 3:J:709:ARG:O | 3:J:711:GLY:N | 2.50 | 0.44 |
| 5:L:215:GLU:HG2 | 5:L:218:ARG:HH21 | 1.82 | 0.44 |
| 2:C:1065:LYS:HD2 | 2:C:1235:LEU:HD12 | 1.99 | 0.44 |
| 2:C:183:TRP:HB2 | 2:C:199:ASP:HA | 2.00 | 0.44 |
| 2:C:466:VAL:O | 2:C:469:VAL:HG22 | 2.18 | 0.44 |
| 3:D:1343:GLU:HB3 | 3:D:1345:ARG:HD3 | 2.00 | 0.44 |
| 3:D:661:VAL:HG12 | 3:D:685:ILE:HD11 | 2.00 | 0.44 |
| 3:D:872:LEU:O | 3:D:877:VAL:HG12 | 2.18 | 0.44 |
| 5:F:492:ASP:HB2 | 5:F:495:ARG:HH12 | 1.82 | 0.44 |
| 2:I:1247:SER:HB3 | 3:J:375:GLU:O | 2.17 | 0.44 |
| 2:I:1282:GLY:HA3 | 4:K:17:PHE:CE1 | 2.52 | 0.44 |
| 3:J:203:GLU:O | 3:J:207:GLU:HG2 | 2.17 | 0.44 |
| 3:J:349:TYR:HE2 | 3:J:379:PRO:HG2 | 1.82 | 0.44 |
| 5:L:314:THR:O | 5:L:318:ALA:HB3 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:453:ILE:HD12 | 2:C:587:LEU:HD21 | 2.00 | 0.44 |
| 3:D:62:PHE:O | 3:D:101:ARG:HD2 | 2.18 | 0.44 |
| 2:I:591:TYR:HD2 | 2:I:606:LEU:HD13 | 1.81 | 0.44 |
| 3:J:1198:VAL:HB | 3:J:1210:ILE:HA | 1.99 | 0.44 |
| 3:J:502:PRO:HB2 | 3:J:507:VAL:HG12 | 2.00 | 0.44 |
| 5:L:346:GLN:O | 5:L:350:GLU:HG3 | 2.18 | 0.44 |
| 5:L:136:GLU:OE1 | 5:L:364:ARG:NH2 | 2.51 | 0.44 |
| 5:L:547:VAL:CG1 | 5:L:598:LEU:HD22 | 2.47 | 0.44 |
| 1:B:91:ARG:HG2 | 1:B:122:GLU:O | 2.18 | 0.44 |
| 2:C:840:SER:O | 2:C:1047:LEU:N | 2.51 | 0.44 |
| 2:C:976:ARG:NH2 | 2:C:990:ASP:OD2 | 2.51 | 0.44 |
| 3:D:1286:LYS:HD2 | 3:D:1290:ARG:NH2 | 2.33 | 0.44 |
| 3:D:334:LYS:HD2 | 3:D:334:LYS:HA | 1.50 | 0.44 |
| 3:D:421:VAL:HG13 | 3:D:439:PRO:HG3 | 1.98 | 0.44 |
| 3:D:694:SER:OG | 3:D:738:ARG:NE | 2.42 | 0.44 |
| 3:D:860:ARG:HB3 | 3:D:861:ASN:H | 1.57 | 0.44 |
| 5:F:412:LEU:HD13 | 5:F:435:ILE:HD11 | 1.99 | 0.44 |
| 1:G:25:LYS:HG2 | 1:G:204:GLU:HG3 | 2.00 | 0.44 |
| 2:I:1254:VAL:HG13 | 2:I:1255:THR:H | 1.82 | 0.44 |
| 2:I:724:VAL:HA | 2:I:734:ILE:HD13 | 1.99 | 0.44 |
| 4:K:66:VAL:HG22 | 4:K:69:ARG:HH21 | 1.83 | 0.44 |
| 5:L:97:PRO:HA | 5:L:100:MET:HG3 | 2.00 | 0.44 |
| 5:L:492:ASP:HB2 | 5:L:495:ARG:HH12 | 1.83 | 0.44 |
| 1:A:12:ARG:H | 1:A:30:PRO:HD2 | 1.82 | 0.44 |
| 2:C:678:ARG:HG3 | 2:C:1108:ASN:HD22 | 1.82 | 0.44 |
| 2:C:1211:ARG:O | 2:C:1212:LEU:HD12 | 2.18 | 0.44 |
| 3:D:368:LEU:HD22 | 3:D:373:ALA:HB2 | 1.99 | 0.44 |
| 5:F:249:ILE:O | 5:F:252:LEU:HB3 | 2.17 | 0.44 |
| 2:I:453:ILE:HD12 | 2:I:587:LEU:HD21 | 2.00 | 0.44 |
| 3:J:30:ILE:HG23 | 3:J:243:PRO:HG3 | 1.98 | 0.44 |
| 3:J:430:HIS:HA | 3:J:921:GLN:HB3 | 1.99 | 0.44 |
| 5:L:234:THR:O | 5:L:245:ALA:HB2 | 2.18 | 0.44 |
| 5:L:44:ILE:HA | 5:L:47:MET:HB2 | 2.00 | 0.44 |
| 5:L:493:LYS:HA | 5:L:496:LYS:HE2 | 2.00 | 0.44 |
| 2:C:383:SER:O | 2:C:387:ASN:HB2 | 2.18 | 0.43 |
| 2:C:453:ILE:HD11 | 2:C:530:ILE:HD12 | 2.00 | 0.43 |
| 2:C:817:LEU:HD11 | 2:C:1080:ASN:HD22 | 1.83 | 0.43 |
| 3:D:1237:VAL:HG13 | 3:D:1253:ILE:HD13 | 1.99 | 0.43 |
| 4:E:66:VAL:HG22 | 4:E:69:ARG:HH21 | 1.83 | 0.43 |
| 5:F:136:GLU:OE1 | 5:F:364:ARG:NH2 | 2.51 | 0.43 |
| 5:F:572:THR:O | 5:F:576:VAL:HG23 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:1106:ARG:HE | 3:J:731:ARG:HH21 | 1.65 | 0.43 |
| 2:I:658:GLN:O | 2:I:661:VAL:HG22 | 2.18 | 0.43 |
| 2:I:720:ARG:HA | 2:I:779:ARG:HG3 | 2.00 | 0.43 |
| 3:J:325:LYS:HD3 | 5:L:508:GLU:HG2 | 2.00 | 0.43 |
| 2:C:1151:LEU:HA | 2:C:1151:LEU:HD23 | 1.81 | 0.43 |
| 3:D:470:VAL:HA | 3:D:471:PRO:HD3 | 1.79 | 0.43 |
| 3:D:527:LEU:HD22 | 3:D:533:ALA:HA | 2.00 | 0.43 |
| 5:F:234:THR:O | 5:F:245:ALA:HB2 | 2.18 | 0.43 |
| 3:D:298:MET:SD | 5:F:402:LEU:HB3 | 2.58 | 0.43 |
| 3:J:1017:VAL:HG23 | 3:J:1018:ALA:H | 1.82 | 0.43 |
| 3:J:1034:PHE:HA | 3:J:1114:GLN:HA | 2.00 | 0.43 |
| 1:B:98:VAL:HG22 | 1:B:99:ILE:H | 1.84 | 0.43 |
| 3:D:1205:GLU:O | 3:D:1208:ASP:HB2 | 2.18 | 0.43 |
| 2:C:1276:TRP:HE1 | 3:D:1348:LYS:NZ | 2.16 | 0.43 |
| 3:D:45:ASN:HB3 | 3:D:48:THR:O | 2.18 | 0.43 |
| 1:G:145:LYS:NZ | 1:G:147:GLN:OE1 | 2.52 | 0.43 |
| 2:I:1149:TYR:CD1 | 2:I:1159:VAL:HG11 | 2.53 | 0.43 |
| 2:I:466:VAL:O | 2:I:469:VAL:HG22 | 2.18 | 0.43 |
| 2:I:634:VAL:HG13 | 2:I:636:CYS:SG | 2.58 | 0.43 |
| 3:J:314:ARG:HG2 | 3:J:314:ARG:HH11 | 1.83 | 0.43 |
| 3:D:1156:LEU:HB3 | 3:D:1207:GLY:HA2 | 1.99 | 0.43 |
| 3:D:557:LYS:HE3 | 3:D:557:LYS:HB2 | 1.78 | 0.43 |
| 3:D:654:ILE:O | 3:D:658:GLU:HB2 | 2.17 | 0.43 |
| 5:F:493:LYS:HA | 5:F:496:LYS:HE2 | 2.00 | 0.43 |
| 1:H:101:THR:HA | 1:H:142:MET:O | 2.18 | 0.43 |
| 2:I:183:TRP:HB2 | 2:I:199:ASP:HA | 2.00 | 0.43 |
| 2:I:1276:TRP:HE1 | 3:J:1348:LYS:NZ | 2.16 | 0.43 |
| 3:J:557:LYS:HA | 3:J:563:LEU:HA | 2.00 | 0.43 |
| 3:J:740:LEU:HA | 3:J:740:LEU:HD12 | 1.85 | 0.43 |
| 3:J:810:THR:HG23 | 3:J:811:GLU:H | 1.83 | 0.43 |
| 2:C:1276:TRP:CZ2 | 3:D:801:VAL:HG21 | 2.54 | 0.43 |
| 2:C:170:VAL:HG23 | 2:C:171:LEU:H | 1.81 | 0.43 |
| 3:D:557:LYS:HA | 3:D:563:LEU:HA | 2.01 | 0.43 |
| 5:F:119:ILE:O | 5:F:123:ILE:HG13 | 2.18 | 0.43 |
| 5:F:215:GLU:HG2 | 5:F:218:ARG:HH21 | 1.82 | 0.43 |
| 5:F:590:ILE:O | 5:F:594:ALA:N | 2.51 | 0.43 |
| 1:H:98:VAL:HG22 | 1:H:99:ILE:H | 1.84 | 0.43 |
| 2:I:817:LEU:HD11 | 2:I:1080:ASN:HD22 | 1.83 | 0.43 |
| 2:I:156:PHE:CE2 | 2:I:158:ASP:HB2 | 2.53 | 0.43 |
| 3:J:615:LYS:HB2 | 3:J:616:PRO:HD3 | 2.00 | 0.43 |
| 5:L:354:THR:O | 5:L:358:VAL:HG23 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:158:ARG:NH2 | 1:A:172:LEU:HD23 | 2.34 | 0.43 |
| 1:B:20:SER:OG | 1:B:21:SER:N | 2.51 | 0.43 |
| 1:A:231:PHE:HB3 | 1:B:218:ARG:HH11 | 1.82 | 0.43 |
| 1:A:224:LEU:HD22 | 1:B:228:LEU:HD11 | 2.00 | 0.43 |
| 2:C:1072:ASN:OD1 | 2:C:1072:ASN:N | 2.49 | 0.43 |
| 2:C:98:VAL:HG21 | 2:C:124:MET:HE3 | 2.01 | 0.43 |
| 2:C:593:LYS:HD3 | 2:C:652:TYR:CZ | 2.54 | 0.43 |
| 2:C:732:ILE:HD11 | 2:C:769:PRO:HB3 | 2.00 | 0.43 |
| 3:D:1280:VAL:HG11 | 3:D:1304:ARG:HH21 | 1.83 | 0.43 |
| 1:G:58:GLU:HB2 | 1:G:145:LYS:HB3 | 2.01 | 0.43 |
| 1:H:20:SER:OG | 1:H:21:SER:N | 2.51 | 0.43 |
| 1:H:79:LEU:HD23 | 1:H:79:LEU:H | 1.83 | 0.43 |
| 2:I:685:MET:SD | 2:I:1073:LYS:HG2 | 2.59 | 0.43 |
| 2:I:840:SER:O | 2:I:1047:LEU:N | 2.51 | 0.43 |
| 2:I:976:ARG:NH2 | 2:I:990:ASP:OD2 | 2.52 | 0.43 |
| 3:J:45:ASN:HB3 | 3:J:48:THR:O | 2.19 | 0.43 |
| 3:J:527:LEU:HD22 | 3:J:533:ALA:HA | 2.00 | 0.43 |
| 3:J:930:LEU:HD11 | 3:J:1241:TYR:CE2 | 2.53 | 0.43 |
| 2:C:1247:SER:HB3 | 3:D:375:GLU:O | 2.18 | 0.43 |
| 3:D:1287:ILE:O | 3:D:1291:GLU:HG3 | 2.18 | 0.43 |
| 3:D:1372:ARG:HE | 3:J:854:ALA:HB2 | 1.83 | 0.43 |
| 3:D:203:GLU:O | 3:D:207:GLU:HG2 | 2.18 | 0.43 |
| 3:D:701:LEU:HD13 | 3:D:723:TYR:HB2 | 2.00 | 0.43 |
| 3:D:930:LEU:HD11 | 3:D:1241:TYR:CE2 | 2.53 | 0.43 |
| 5:F:314:THR:O | 5:F:318:ALA:HB3 | 2.19 | 0.43 |
| 1:G:158:ARG:NH2 | 1:G:172:LEU:HD23 | 2.34 | 0.43 |
| 2:I:1223:ARG:NH2 | 3:J:719:PHE:O | 2.52 | 0.43 |
| 2:I:453:ILE:HD11 | 2:I:530:ILE:HD12 | 2.01 | 0.43 |
| 1:A:47:LEU:HD13 | 1:A:183:ILE:HG12 | 1.99 | 0.43 |
| 1:B:101:THR:HA | 1:B:142:MET:O | 2.19 | 0.43 |
| 2:C:720:ARG:HA | 2:C:779:ARG:HG3 | 2.00 | 0.43 |
| 3:D:1162:ILE:HA | 3:D:1203:ARG:HA | 2.01 | 0.43 |
| 3:D:502:PRO:HB2 | 3:D:507:VAL:HG12 | 2.01 | 0.43 |
| 3:D:848:VAL:HG22 | 3:D:858:VAL:CG2 | 2.48 | 0.43 |
| 2:I:56:VAL:HG11 | 2:I:468:LEU:HB3 | 2.01 | 0.43 |
| 3:J:661:VAL:HG12 | 3:J:685:ILE:HD11 | 2.00 | 0.43 |
| 5:L:511:ILE:HA | 5:L:511:ILE:HD12 | 1.85 | 0.43 |
| 2:C:1106:ARG:HE | 3:D:731:ARG:HH21 | 1.65 | 0.43 |
| 2:C:17:LYS:HE3 | 2:C:1154:ASP:HB3 | 2.00 | 0.43 |
| 3:D:1236:GLU:O | 3:D:1240:VAL:HG23 | 2.19 | 0.43 |
| 3:D:314:ARG:HH11 | 3:D:314:ARG:HG2 | 1.84 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:709:ARG:O | 3:D:711:GLY:N | 2.50 | 0.43 |
| 5:F:580:PHE:C | 5:F:582:VAL:H | 2.21 | 0.43 |
| 3:J:872:LEU:O | 3:J:877:VAL:HG12 | 2.18 | 0.43 |
| 5:L:348:GLU:HG2 | 5:L:354:THR:HA | 2.01 | 0.43 |
| 1:B:28:LEU:HG | 1:B:31:LEU:HD21 | 2.01 | 0.43 |
| 2:C:1210:ILE:HG22 | 2:C:1211:ARG:H | 1.83 | 0.43 |
| 2:C:980:VAL:HG13 | 2:C:984:VAL:HB | 2.01 | 0.43 |
| 3:D:497:GLU:HA | 3:D:498:PRO:HD3 | 1.86 | 0.43 |
| 3:D:537:TYR:CE1 | 3:D:544:LEU:HB2 | 2.54 | 0.43 |
| 3:D:901:ARG:HA | 3:D:908:ILE:HA | 1.99 | 0.43 |
| 5:F:561:MET:HG3 | 5:F:571:TYR:HD2 | 1.84 | 0.43 |
| 2:I:383:SER:O | 2:I:387:ASN:HB2 | 2.18 | 0.43 |
| 3:J:1319:PHE:CE2 | 3:J:1342:ASP:HB2 | 2.54 | 0.43 |
| 1:B:78:ILE:O | 1:B:82:LEU:HG | 2.19 | 0.42 |
| 1:B:34:GLY:HA3 | 2:C:1083:GLU:OE1 | 2.18 | 0.42 |
| 3:D:317:THR:HB | 3:D:324:LEU:HB3 | 2.00 | 0.42 |
| 3:D:573:THR:OG1 | 3:D:576:ARG:HG3 | 2.18 | 0.42 |
| 3:D:925:GLU:HB3 | 3:D:926:PRO:HD3 | 2.01 | 0.42 |
| 5:F:484:ALA:HB1 | 5:F:491:GLU:HB2 | 2.01 | 0.42 |
| 1:H:28:LEU:HG | 1:H:31:LEU:HD21 | 2.01 | 0.42 |
| 3:J:1287:ILE:O | 3:J:1291:GLU:HG3 | 2.19 | 0.42 |
| 3:J:298:MET:SD | 5:L:402:LEU:HB3 | 2.58 | 0.42 |
| 3:J:317:THR:HB | 3:J:324:LEU:HB3 | 2.00 | 0.42 |
| 3:J:848:VAL:HG22 | 3:J:858:VAL:CG2 | 2.48 | 0.42 |
| 1:A:115:ILE:HG22 | 1:A:116:THR:H | 1.84 | 0.42 |
| 2:C:964:LEU:HD22 | 2:C:1025:PHE:CG | 2.54 | 0.42 |
| 2:C:360:LEU:HB2 | 2:C:378:ARG:HH21 | 1.84 | 0.42 |
| 3:D:37:GLU:HB2 | 3:D:104:HIS:CE1 | 2.54 | 0.42 |
| 3:D:347:VAL:HG12 | 3:D:348:ASP:O | 2.19 | 0.42 |
| 1:G:115:ILE:HG22 | 1:G:116:THR:H | 1.84 | 0.42 |
| 1:G:219:ARG:HB2 | 1:G:219:ARG:HE | 1.56 | 0.42 |
| 1:G:45:ARG:NH2 | 2:I:1215:GLY:O | 2.42 | 0.42 |
| 2:I:26:TYR:CE2 | 2:I:28:LEU:HB2 | 2.54 | 0.42 |
| 2:I:887:VAL:HB | 2:I:913:VAL:HG21 | 2.01 | 0.42 |
| 3:J:1237:VAL:HG13 | 3:J:1253:ILE:HD13 | 2.00 | 0.42 |
| 3:J:1280:VAL:HG11 | 3:J:1304:ARG:HH21 | 1.84 | 0.42 |
| 5:L:289:LYS:HE2 | 5:L:289:LYS:HB3 | 1.88 | 0.42 |
| 1:A:51:MET:HE3 | 1:A:51:MET:HB3 | 1.88 | 0.42 |
| 2:C:634:VAL:HG13 | 2:C:636:CYS:SG | 2.59 | 0.42 |
| 2:C:692:THR:OG1 | 2:C:827:ARG:O | 2.32 | 0.42 |
| 3:D:450:HIS:HA | 3:D:451:PRO:HD3 | 1.86 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:145:LYS:HB3 | 1:G:145:LYS:HE3 | 1.84 | 0.42 |
| 3:J:1137:GLY:O | 3:J:1140:ARG:HB3 | 2.20 | 0.42 |
| 3:J:1205:GLU:O | 3:J:1208:ASP:HB2 | 2.18 | 0.42 |
| 3:J:537:TYR:CE1 | 3:J:544:LEU:HB2 | 2.54 | 0.42 |
| 5:L:580:PHE:C | 5:L:582:VAL:H | 2.22 | 0.42 |
| 1:A:145:LYS:NZ | 1:A:147:GLN:OE1 | 2.51 | 0.42 |
| 1:B:86:LYS:HD3 | 1:B:174:ASP:HB2 | 2.02 | 0.42 |
| 2:C:26:TYR:CE2 | 2:C:28:LEU:HB2 | 2.54 | 0.42 |
| 2:C:887:VAL:HB | 2:C:913:VAL:CG2 | 2.49 | 0.42 |
| 5:F:130:VAL:HB | 5:F:365:MET:HG3 | 2.00 | 0.42 |
| 3:J:1162:ILE:HA | 3:J:1203:ARG:HA | 2.01 | 0.42 |
| 4:K:49:ILE:HA | 4:K:52:ARG:HD3 | 2.01 | 0.42 |
| 1:A:25:LYS:HG2 | 1:A:204:GLU:HG3 | 2.01 | 0.42 |
| 2:C:1212:LEU:HD22 | 2:C:1225:VAL:HG21 | 2.02 | 0.42 |
| 2:C:389:PHE:HB3 | 2:C:420:LEU:HD12 | 1.99 | 0.42 |
| 5:F:97:PRO:HA | 5:F:100:MET:HG3 | 2.01 | 0.42 |
| 1:H:101:THR:H | 1:H:116:THR:HG22 | 1.84 | 0.42 |
| 1:H:37:HIS:CE1 | 2:I:1216:ARG:HD2 | 2.54 | 0.42 |
| 2:I:1211:ARG:O | 2:I:1212:LEU:HD12 | 2.19 | 0.42 |
| 3:J:1031:VAL:HG23 | 3:J:1080:ILE:HG21 | 2.01 | 0.42 |
| 3:J:1090:ILE:HG13 | 3:J:1097:ALA:HB2 | 2.01 | 0.42 |
| 3:J:573:THR:OG1 | 3:J:576:ARG:HG3 | 2.19 | 0.42 |
| 5:L:454:VAL:HA | 5:L:457:ILE:HD12 | 2.02 | 0.42 |
| 1:A:58:GLU:HB2 | 1:A:145:LYS:HB3 | 2.01 | 0.42 |
| 1:A:75:GLN:HA | 2:C:729:ALA:N | 2.35 | 0.42 |
| 2:C:357:ASN:ND2 | 2:C:358:ASP:OD2 | 2.53 | 0.42 |
| 2:C:69:GLN:HB3 | 2:C:69:GLN:HE21 | 1.67 | 0.42 |
| 2:C:758:ARG:HD3 | 2:C:835:GLU:HB2 | 2.01 | 0.42 |
| 3:D:683:ILE:HD11 | 3:D:754:ILE:HG12 | 2.01 | 0.42 |
| 5:F:348:GLU:HG2 | 5:F:354:THR:HA | 2.01 | 0.42 |
| 1:G:10:LYS:HE2 | 1:H:229:GLU:HB3 | 2.00 | 0.42 |
| 1:H:112:ALA:HB2 | 1:H:128:HIS:HB3 | 2.02 | 0.42 |
| 1:H:91:ARG:HG2 | 1:H:91:ARG:H | 1.76 | 0.42 |
| 2:I:230:PHE:HE1 | 2:I:287:VAL:HG21 | 1.85 | 0.42 |
| 3:J:1146:GLU:HB3 | 3:J:1148:ARG:HG3 | 2.00 | 0.42 |
| 3:J:925:GLU:HB3 | 3:J:926:PRO:HD3 | 2.01 | 0.42 |
| 5:L:484:ALA:HB1 | 5:L:491:GLU:HB2 | 2.00 | 0.42 |
| 1:A:54:CYS:HA | 1:A:148:ARG:HG3 | 2.02 | 0.42 |
| 1:B:90:VAL:HG11 | 1:B:146:VAL:HG11 | 2.01 | 0.42 |
| 3:D:1293:GLU:HB3 | 3:D:1294:ALA:H | 1.69 | 0.42 |
| 2:I:670:PHE:HZ | 2:I:1117:LEU:HD13 | 1.83 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:157:PHE:CZ | 2:I:431:LYS:HG2 | 2.55 | 0.42 |
| 2:I:964:LEU:HD22 | 2:I:1025:PHE:CG | 2.54 | 0.42 |
| 3:J:1046:ILE:HD12 | 3:J:1059:LEU:HB3 | 2.01 | 0.42 |
| 3:J:969:SER:HB3 | 3:J:1116:SER:HB2 | 2.00 | 0.42 |
| 2:C:14:ASP:N | 2:C:1157:GLN:OE1 | 2.34 | 0.42 |
| 2:I:981:ALA:HB1 | 2:I:1007:LYS:NZ | 2.34 | 0.42 |
| 2:I:710:VAL:HA | 2:I:715:THR:HG21 | 2.01 | 0.42 |
| 2:I:967:LEU:HA | 2:I:967:LEU:HD12 | 1.89 | 0.42 |
| 3:J:1194:ARG:HD2 | 3:J:1194:ARG:N | 2.35 | 0.42 |
| 3:J:1341:ARG:HH22 | 3:J:1373:ARG:HH21 | 1.66 | 0.42 |
| 3:J:334:LYS:HA | 3:J:334:LYS:HD2 | 1.50 | 0.42 |
| 3:J:694:SER:OG | 3:J:738:ARG:NE | 2.42 | 0.42 |
| 2:C:1080:ASN:HA | 2:C:1081:PRO:HD3 | 1.96 | 0.42 |
| 2:C:670:PHE:HZ | 2:C:1117:LEU:HD13 | 1.84 | 0.42 |
| 2:C:1223:ARG:NH2 | 3:D:719:PHE:O | 2.52 | 0.42 |
| 3:D:1194:ARG:N | 3:D:1194:ARG:HD2 | 2.35 | 0.42 |
| 3:D:1368:ASP:OD1 | 3:D:1371:ARG:NH2 | 2.53 | 0.42 |
| 5:F:454:VAL:HA | 5:F:457:ILE:HD12 | 2.02 | 0.42 |
| 1:G:61:ILE:HG23 | 1:G:142:MET:HB3 | 2.01 | 0.42 |
| 1:G:38:THR:OG1 | 1:H:45:ARG:NH1 | 2.49 | 0.42 |
| 2:I:149:LEU:HB2 | 2:I:530:ILE:CG2 | 2.50 | 0.42 |
| 2:I:374:GLU:HA | 2:I:375:PRO:HD3 | 1.91 | 0.42 |
| 3:J:438:GLU:HA | 3:J:439:PRO:HD3 | 1.87 | 0.42 |
| 1:A:61:ILE:HG23 | 1:A:142:MET:HB3 | 2.01 | 0.42 |
| 2:C:157:PHE:CZ | 2:C:431:LYS:HG2 | 2.55 | 0.42 |
| 2:C:56:VAL:HG11 | 2:C:468:LEU:HB3 | 2.01 | 0.42 |
| 2:C:1246:ARG:NE | 3:D:348:ASP:OD1 | 2.48 | 0.42 |
| 3:D:668:PHE:HB2 | 3:D:678:ARG:HG3 | 2.02 | 0.42 |
| 1:G:86:LYS:HE3 | 1:G:86:LYS:HB2 | 1.86 | 0.42 |
| 2:I:10:ARG:HA | 2:I:1172:LEU:HD23 | 2.02 | 0.42 |
| 2:I:1210:ILE:HG22 | 2:I:1211:ARG:H | 1.84 | 0.42 |
| 2:I:980:VAL:HG13 | 2:I:984:VAL:HB | 2.02 | 0.42 |
| 3:J:37:GLU:HB2 | 3:J:104:HIS:CE1 | 2.55 | 0.42 |
| 3:D:1293:GLU:HA | 3:J:1226:VAL:H | 1.85 | 0.42 |
| 5:L:119:ILE:O | 5:L:123:ILE:HG13 | 2.19 | 0.42 |
| 2:C:10:ARG:HA | 2:C:1172:LEU:HD23 | 2.02 | 0.41 |
| 2:C:153:PRO:O | 2:C:401:GLY:HA2 | 2.20 | 0.41 |
| 2:C:37:LYS:HA | 2:C:37:LYS:HD3 | 1.77 | 0.41 |
| 3:D:902:ASP:OD1 | 3:D:903:LEU:N | 2.53 | 0.41 |
| 3:D:46:TYR:CD1 | 5:F:452:ILE:HG22 | 2.55 | 0.41 |
| 1:H:178:SER:HA | 1:H:179:PRO:HD3 | 1.94 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:H:78:ILE:O | 1:H:82:LEU:HG | 2.19 | 0.41 |
| 2:I:60:GLN:HB3 | 2:I:67:GLU:HG3 | 2.02 | 0.41 |
| 2:I:782:VAL:HG11 | 2:I:792:GLY:HA2 | 2.02 | 0.41 |
| 3:J:347:VAL:HG12 | 3:J:348:ASP:O | 2.20 | 0.41 |
| 3:J:419:HIS:HA | 3:J:420:PRO:HD3 | 1.91 | 0.41 |
| 2:I:1276:TRP:CZ2 | 3:J:801:VAL:HG21 | 2.54 | 0.41 |
| 5:L:569:THR:OG1 | 5:L:570:ASP:N | 2.53 | 0.41 |
| 2:C:163:LYS:HB3 | 2:C:163:LYS:HE3 | 1.88 | 0.41 |
| 2:C:499:SER:O | 2:C:503:LYS:HB2 | 2.20 | 0.41 |
| 3:D:355:ILE:HD13 | 3:D:466:MET:HG3 | 2.02 | 0.41 |
| 5:F:289:LYS:HB3 | 5:F:289:LYS:HE2 | 1.88 | 0.41 |
| 1:G:54:CYS:HA | 1:G:148:ARG:HG3 | 2.01 | 0.41 |
| 2:I:518:ASN:O | 2:I:691:PRO:HD3 | 2.20 | 0.41 |
| 2:I:887:VAL:HB | 2:I:913:VAL:CG2 | 2.49 | 0.41 |
| 3:J:1285:VAL:O | 3:J:1289:ASN:HB3 | 2.20 | 0.41 |
| 3:J:1368:ASP:OD1 | 3:J:1371:ARG:NH2 | 2.53 | 0.41 |
| 5:L:399:LEU:HA | 5:L:399:LEU:HD12 | 1.85 | 0.41 |
| 5:L:420:GLU:OE1 | 5:L:423:ARG:NH2 | 2.50 | 0.41 |
| 5:F:511:ILE:HA | 5:F:511:ILE:HD12 | 1.86 | 0.41 |
| 1:H:158:ARG:HD2 | 1:H:158:ARG:HA | 1.91 | 0.41 |
| 1:H:151:GLY:O | 1:H:177:TYR:HD2 | 2.04 | 0.41 |
| 1:H:86:LYS:HD3 | 1:H:174:ASP:HB2 | 2.02 | 0.41 |
| 2:I:360:LEU:HB2 | 2:I:378:ARG:HH21 | 1.84 | 0.41 |
| 3:J:1025:MET:SD | 3:J:1124:ILE:HD12 | 2.60 | 0.41 |
| 3:J:1156:LEU:HD23 | 3:J:1219:ASP:HB3 | 2.02 | 0.41 |
| 3:J:124:ILE:HG13 | 3:J:124:ILE:H | 1.63 | 0.41 |
| 3:J:1293:GLU:HB3 | 3:J:1294:ALA:H | 1.69 | 0.41 |
| 5:L:299:LYS:O | 5:L:303:ILE:HG12 | 2.20 | 0.41 |
| 5:L:357:GLN:H | 5:L:357:GLN:HG3 | 1.62 | 0.41 |
| 5:L:362:ASN:HB2 | 5:L:365:MET:HE2 | 2.02 | 0.41 |
| 5:L:465:ARG:HA | 5:L:468:ARG:HH12 | 1.86 | 0.41 |
| 1:A:54:CYS:O | 1:A:146:VAL:HG13 | 2.20 | 0.41 |
| 1:B:101:THR:H | 1:B:116:THR:HG22 | 1.85 | 0.41 |
| 1:B:158:ARG:HA | 1:B:158:ARG:HD2 | 1.90 | 0.41 |
| 1:B:182:ARG:NH1 | 3:D:581:MET:SD | 2.94 | 0.41 |
| 1:B:91:ARG:H | 1:B:91:ARG:HG2 | 1.76 | 0.41 |
| 3:D:1135:THR:OG1 | 3:D:1136:GLY:N | 2.49 | 0.41 |
| 3:D:1285:VAL:O | 3:D:1289:ASN:HB3 | 2.20 | 0.41 |
| 3:D:190:LYS:HE2 | 3:D:190:LYS:HB2 | 1.87 | 0.41 |
| 3:D:361:LEU:HD22 | 3:D:365:GLN:HG3 | 2.01 | 0.41 |
| 3:D:810:THR:HG23 | 3:D:811:GLU:H | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:35:PHE:HA | 1:G:35:PHE:HD1 | 1.70 | 0.41 |
| 2:I:470:ARG:NE | 2:I:497:PRO:HB3 | 2.35 | 0.41 |
| 2:I:550:VAL:HG11 | 3:J:776:THR:HG22 | 2.02 | 0.41 |
| 1:B:68:TYR:O | 1:B:69:SER:OG | 2.34 | 0.41 |
| 2:C:88:ARG:NE | 2:C:1040:ASP:OD1 | 2.45 | 0.41 |
| 2:C:1305:TYR:CE1 | 3:D:379:PRO:HG3 | 2.55 | 0.41 |
| 2:C:158:ASP:HB3 | 2:C:173:ASN:OD1 | 2.21 | 0.41 |
| 2:C:887:VAL:HB | 2:C:913:VAL:HG21 | 2.01 | 0.41 |
| 3:D:1156:LEU:HD23 | 3:D:1219:ASP:HB3 | 2.02 | 0.41 |
| 3:D:27:PRO:O | 3:D:31:ARG:HG3 | 2.21 | 0.41 |
| 3:D:806:ASP:OD2 | 3:D:1347:LEU:N | 2.48 | 0.41 |
| 5:F:582:VAL:HG22 | 5:F:586:ARG:HG2 | 2.02 | 0.41 |
| 2:I:1062:PRO:HA | 2:I:1076:ILE:HG23 | 2.02 | 0.41 |
| 2:I:35:PHE:CD2 | 2:I:130:MET:HB3 | 2.55 | 0.41 |
| 2:I:499:SER:O | 2:I:503:LYS:HB2 | 2.20 | 0.41 |
| 2:I:593:LYS:HD3 | 2:I:652:TYR:CZ | 2.54 | 0.41 |
| 2:I:699:LEU:HA | 2:I:699:LEU:HD22 | 1.95 | 0.41 |
| 2:I:959:ASP:O | 2:I:963:GLU:HG2 | 2.21 | 0.41 |
| 3:J:1236:GLU:O | 3:J:1240:VAL:HG23 | 2.20 | 0.41 |
| 3:J:441:LEU:HA | 3:J:441:LEU:HD13 | 1.90 | 0.41 |
| 3:J:79:LYS:HG3 | 3:J:80:HIS:N | 2.35 | 0.41 |
| 5:L:561:MET:HG3 | 5:L:571:TYR:HD2 | 1.84 | 0.41 |
| 5:L:580:PHE:HA | 5:L:580:PHE:HD1 | 1.70 | 0.41 |
| 5:L:582:VAL:HG22 | 5:L:586:ARG:HG2 | 2.02 | 0.41 |
| 5:L:99:ARG:HA | 5:L:99:ARG:HD3 | 1.80 | 0.41 |
| 2:C:1280:ALA:HB3 | 3:D:431:ARG:HB3 | 2.02 | 0.41 |
| 3:D:385:LEU:HD23 | 3:D:385:LEU:HA | 1.92 | 0.41 |
| 3:D:793:SER:O | 3:D:797:THR:HG23 | 2.20 | 0.41 |
| 1:G:177:TYR:O | 1:G:178:SER:HB2 | 2.20 | 0.41 |
| 2:I:1281:TYR:CD1 | 3:J:484:MET:HG2 | 2.56 | 0.41 |
| 2:I:122:VAL:HG21 | 2:I:493:ILE:HG23 | 2.03 | 0.41 |
| 2:I:996:ARG:HA | 2:I:996:ARG:HD3 | 1.88 | 0.41 |
| 3:J:556:GLU:O | 3:J:564:VAL:N | 2.33 | 0.41 |
| 3:J:668:PHE:HB2 | 3:J:678:ARG:HG3 | 2.02 | 0.41 |
| 1:B:34:GLY:N | 1:B:199:ASP:OD2 | 2.53 | 0.41 |
| 2:C:550:VAL:HG11 | 3:D:776:THR:HG22 | 2.03 | 0.41 |
| 2:C:83:GLN:O | 2:C:87:ILE:HG13 | 2.21 | 0.41 |
| 3:D:1137:GLY:O | 3:D:1140:ARG:HB3 | 2.21 | 0.41 |
| 4:E:35:LYS:NZ | 4:E:71:GLU:OE2 | 2.46 | 0.41 |
| 1:G:10:LYS:HE3 | 1:H:226:GLU:O | 2.21 | 0.41 |
| 1:G:79:LEU:HD11 | 2:I:693:LEU:HD21 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:697:LYS:HE2 | 2:I:697:LYS:HB3 | 1.76 | 0.41 |
| 3:J:361:LEU:HD22 | 3:J:365:GLN:HG3 | 2.01 | 0.41 |
| 3:J:474:LEU:HA | 3:J:474:LEU:HD12 | 1.91 | 0.41 |
| 1:A:92:VAL:HA | 1:A:120:ASP:O | 2.21 | 0.41 |
| 1:B:51:MET:HB3 | 1:B:178:SER:HA | 2.01 | 0.41 |
| 2:C:559:CYS:HA | 2:C:560:PRO:HD3 | 1.91 | 0.41 |
| 2:C:987:GLU:O | 2:C:991:LYS:HG3 | 2.21 | 0.41 |
| 3:D:115:TRP:CE2 | 3:D:1329:THR:HG23 | 2.56 | 0.41 |
| 3:D:461:PHE:HD2 | 3:D:461:PHE:HA | 1.77 | 0.41 |
| 3:D:746:LEU:HD22 | 3:D:754:ILE:HD11 | 2.02 | 0.41 |
| 4:E:44:ASP:HB3 | 4:E:48:VAL:HB | 2.02 | 0.41 |
| 5:F:490:PRO:HG2 | 5:F:493:LYS:HE3 | 2.03 | 0.41 |
| 5:F:96:ASP:OD2 | 5:F:99:ARG:HB2 | 2.20 | 0.41 |
| 1:G:92:VAL:HA | 1:G:120:ASP:O | 2.21 | 0.41 |
| 1:H:34:GLY:N | 1:H:199:ASP:OD2 | 2.53 | 0.41 |
| 2:I:1280:ALA:HB3 | 3:J:431:ARG:HB3 | 2.03 | 0.41 |
| 3:J:450:HIS:HA | 3:J:451:PRO:HD3 | 1.86 | 0.41 |
| 3:J:355:ILE:HD13 | 3:J:466:MET:HG3 | 2.02 | 0.41 |
| 1:B:112:ALA:HB2 | 1:B:128:HIS:HB3 | 2.01 | 0.41 |
| 2:C:685:MET:SD | 2:C:1073:LYS:HG2 | 2.60 | 0.41 |
| 3:D:290:ILE:HD12 | 3:D:290:ILE:H | 1.86 | 0.41 |
| 2:I:1212:LEU:HD22 | 2:I:1225:VAL:HG21 | 2.01 | 0.41 |
| 3:J:1348:LYS:HD2 | 3:J:1348:LYS:HA | 1.87 | 0.41 |
| 3:J:253:VAL:HA | 3:J:254:PRO:HD3 | 1.74 | 0.41 |
| 3:J:385:LEU:HD23 | 3:J:385:LEU:HA | 1.92 | 0.41 |
| 5:L:96:ASP:OD2 | 5:L:99:ARG:HB2 | 2.20 | 0.41 |
| 2:C:808:ASN:OD1 | 2:C:1216:ARG:NH2 | 2.53 | 0.41 |
| 2:C:1246:ARG:CZ | 2:C:1258:PRO:HB3 | 2.51 | 0.41 |
| 2:C:470:ARG:NE | 2:C:497:PRO:HB3 | 2.36 | 0.41 |
| 2:C:498:ILE:HD12 | 2:C:498:ILE:H | 1.86 | 0.41 |
| 3:D:1163:VAL:HG23 | 3:D:1177:ILE:HA | 2.03 | 0.41 |
| 4:E:49:ILE:HA | 4:E:52:ARG:HD3 | 2.02 | 0.41 |
| 5:F:299:LYS:O | 5:F:303:ILE:HG12 | 2.20 | 0.41 |
| 5:F:22:LEU:H | 5:F:54:GLN:CB | 2.34 | 0.41 |
| 1:H:61:ILE:HB | 1:H:64:VAL:O | 2.21 | 0.41 |
| 3:J:1266:ILE:HB | 3:J:1274:PHE:O | 2.21 | 0.41 |
| 3:J:233:LYS:HA | 3:J:234:PRO:HD3 | 1.93 | 0.41 |
| 3:J:77:ARG:HG3 | 3:J:79:LYS:HB3 | 2.03 | 0.41 |
| 3:J:79:LYS:HB2 | 5:L:569:THR:H | 1.84 | 0.41 |
| 2:C:468:LEU:HA | 2:C:471:VAL:HG12 | 2.03 | 0.41 |
| 2:C:930:ASP:HB3 | 2:C:1053:TYR:HB2 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:I:1121:ALA:HB1 | 2:I:1180:MET:O | 2.21 | 0.41 |
| 2:I:357:ASN:ND2 | 2:I:358:ASP:OD2 | 2.53 | 0.41 |
| 2:I:468:LEU:HA | 2:I:471:VAL:HG12 | 2.03 | 0.41 |
| 2:I:498:ILE:H | 2:I:498:ILE:HD12 | 1.86 | 0.41 |
| 2:I:557:ARG:HH21 | 2:I:607:SER:C | 2.24 | 0.41 |
| 2:I:867:GLU:HG3 | 2:I:867:GLU:H | 1.61 | 0.41 |
| 3:J:1230:THR:OG1 | 3:J:1257:VAL:HG11 | 2.21 | 0.41 |
| 5:L:250:LEU:O | 5:L:254:GLU:HG2 | 2.21 | 0.41 |
| 1:B:71:LYS:HA | 1:B:71:LYS:HD2 | 1.90 | 0.40 |
| 2:C:516:ASP:H | 2:C:526:HIS:HD1 | 1.69 | 0.40 |
| 2:C:60:GLN:HB3 | 2:C:67:GLU:HG3 | 2.02 | 0.40 |
| 2:C:972:PHE:CD2 | 2:C:975:ILE:HD12 | 2.56 | 0.40 |
| 3:D:1230:THR:OG1 | 3:D:1257:VAL:HG11 | 2.21 | 0.40 |
| 3:D:77:ARG:HG3 | 3:D:79:LYS:HB3 | 2.03 | 0.40 |
| 1:H:90:VAL:HG11 | 1:H:146:VAL:HG11 | 2.02 | 0.40 |
| 2:I:808:ASN:OD1 | 2:I:1216:ARG:NH2 | 2.54 | 0.40 |
| 2:I:153:PRO:O | 2:I:401:GLY:HA2 | 2.21 | 0.40 |
| 2:I:232:ILE:HG12 | 2:I:237:LEU:HD13 | 2.03 | 0.40 |
| 2:I:32:LEU:HD23 | 2:I:32:LEU:HA | 1.94 | 0.40 |
| 3:J:1108:GLN:HG3 | 3:J:1109:LEU:HD13 | 2.03 | 0.40 |
| 3:J:290:ILE:HD12 | 3:J:290:ILE:H | 1.86 | 0.40 |
| 3:J:399:LYS:HG2 | 3:J:403:ARG:NH2 | 2.36 | 0.40 |
| 3:J:557:LYS:HE3 | 3:J:557:LYS:HB2 | 1.78 | 0.40 |
| 3:J:600:ALA:O | 3:J:603:LYS:HG2 | 2.21 | 0.40 |
| 3:J:490:ILE:HD11 | 3:J:609:TYR:CD2 | 2.56 | 0.40 |
| 3:J:746:LEU:HD22 | 3:J:754:ILE:HD11 | 2.02 | 0.40 |
| 3:J:683:ILE:HD11 | 3:J:754:ILE:HG12 | 2.02 | 0.40 |
| 4:K:44:ASP:HB3 | 4:K:48:VAL:HB | 2.03 | 0.40 |
| 1:A:145:LYS:HE3 | 1:A:145:LYS:HB3 | 1.85 | 0.40 |
| 1:B:133:LEU:HA | 1:B:133:LEU:HD12 | 1.86 | 0.40 |
| 2:C:101:ARG:HH21 | 2:C:118:LYS:HE3 | 1.86 | 0.40 |
| 2:C:35:PHE:CD2 | 2:C:130:MET:HB3 | 2.57 | 0.40 |
| 3:D:572:THR:OG1 | 3:D:573:THR:N | 2.54 | 0.40 |
| 3:D:79:LYS:HG3 | 3:D:80:HIS:N | 2.36 | 0.40 |
| 5:F:569:THR:OG1 | 5:F:570:ASP:N | 2.53 | 0.40 |
| 2:I:1161:LEU:HA | 2:I:1161:LEU:HD12 | 1.81 | 0.40 |
| 2:I:1246:ARG:CZ | 2:I:1258:PRO:HB3 | 2.52 | 0.40 |
| 2:I:972:PHE:CD2 | 2:I:975:ILE:HD12 | 2.56 | 0.40 |
| 2:C:213:LEU:HD13 | 2:C:422:LYS:HG2 | 2.03 | 0.40 |
| 2:C:557:ARG:HH21 | 2:C:607:SER:C | 2.24 | 0.40 |
| 2:C:996:ARG:HD3 | 2:C:996:ARG:HA | 1.88 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:197:GLU:O | 3:D:201:LEU:HG | 2.21 | 0.40 |
| 5:F:250:LEU:O | 5:F:254:GLU:HG2 | 2.21 | 0.40 |
| 5:F:465:ARG:HA | 5:F:468:ARG:HH12 | 1.87 | 0.40 |
| 1:G:54:CYS:O | 1:G:146:VAL:HG13 | 2.20 | 0.40 |
| 1:H:102:LEU:HA | 1:H:102:LEU:HD23 | 1.77 | 0.40 |
| 1:H:213:PRO:O | 1:H:217:ILE:HG13 | 2.22 | 0.40 |
| 3:J:660:GLU:O | 3:J:664:ILE:HG12 | 2.21 | 0.40 |
| 3:J:697:MET:HE1 | 3:J:737:ILE:HG22 | 2.03 | 0.40 |
| 5:L:484:ALA:HB1 | 5:L:491:GLU:CB | 2.51 | 0.40 |
| 1:B:61:ILE:HB | 1:B:64:VAL:O | 2.22 | 0.40 |
| 2:C:657:THR:HG1 | 2:C:1187:PHE:HB2 | 1.84 | 0.40 |
| 2:C:196:VAL:HG12 | 2:C:206:ALA:HA | 2.04 | 0.40 |
| 2:C:230:PHE:HE1 | 2:C:287:VAL:HG21 | 1.85 | 0.40 |
| 3:D:579:LEU:HD12 | 3:D:582:ILE:HD12 | 2.03 | 0.40 |
| 2:I:80:PHE:HB2 | 2:I:85:CYS:SG | 2.62 | 0.40 |
| 2:C:149:LEU:HB2 | 2:C:530:ILE:CG2 | 2.52 | 0.40 |
| 2:C:356:THR:HG21 | 2:C:362:ALA:HA | 2.03 | 0.40 |
| 2:C:202:ARG:NH2 | 2:C:368:ARG:HH12 | 2.20 | 0.40 |
| 3:D:600:ALA:O | 3:D:603:LYS:HG2 | 2.21 | 0.40 |
| 4:E:4:VAL:HG22 | 4:E:5:THR:HG23 | 2.04 | 0.40 |
| 2:I:960:LEU:HD11 | 2:I:1028:LYS:HE2 | 2.04 | 0.40 |
| 2:I:1109:ILE:HA | 2:I:1109:ILE:HD12 | 1.81 | 0.40 |
| 2:I:101:ARG:HH21 | 2:I:118:LYS:HE3 | 1.86 | 0.40 |
| 2:I:69:GLN:HB3 | 2:I:69:GLN:HE21 | 1.68 | 0.40 |
| 2:I:742:TYR:CD2 | 2:I:743:PRO:HD2 | 2.57 | 0.40 |
| 2:I:83:GLN:O | 2:I:87:ILE:HG13 | 2.21 | 0.40 |
| 2:I:930:ASP:HB3 | 2:I:1053:TYR:HB2 | 2.02 | 0.40 |
| 3:J:1252:HIS:O | 3:J:1255:VAL:HG13 | 2.22 | 0.40 |
| 3:J:197:GLU:O | 3:J:201:LEU:HG | 2.21 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 1 | A | 222/239 (93%) | 193 (87%) | 27 (12%) | 2 (1%) | 20 | 63 |
| 1 | B | 216/239 (90%) | 190 (88%) | 26 (12%) | 0 | 100 | 100 |
| 1 | G | 226/239 (95%) | 196 (87%) | 27 (12%) | 3 (1%) | 14 | 57 |
| 1 | H | 213/239 (89%) | 190 (89%) | 23 (11%) | 0 | 100 | 100 |
| 2 | C | 1338/1342 (100%) | 1233 (92%) | 101 (8%) | 4 (0%) | 44 | 80 |
| 2 | I | 1338/1342 (100%) | 1234 (92%) | 99 (7%) | 5 (0%) | 38 | 77 |
| 3 | D | 1162/1407 (83%) | 1061 (91%) | 97 (8%) | 4 (0%) | 44 | 80 |
| 3 | J | 1328/1407 (94%) | 1213 (91%) | 111 (8%) | 4 (0%) | 44 | 80 |
| 4 | E | 87/91 (96%) | 81 (93%) | 6 (7%) | 0 | 100 | 100 |
| 4 | K | 77/91 (85%) | 73 (95%) | 4 (5%) | 0 | 100 | 100 |
| 5 | F | 532/613 (87%) | 480 (90%) | 52 (10%) | 0 | 100 | 100 |
| 5 | L | 529/613 (86%) | 480 (91%) | 49 (9%) | 0 | 100 | 100 |
| All | All | 7268/7862 (92%) | 6624 (91%) | 622 (9%) | 22 (0%) | 44 | 80 |

All (22) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | D | 120 | LEU |
| 3 | J | 120 | LEU |
| 2 | C | 170 | VAL |
| 2 | I | 170 | VAL |
| 2 | I | 237 | LEU |
| 3 | J | 340 | GLN |
| 2 | C | 697 | LYS |
| 2 | C | 1136 | GLN |
| 3 | D | 10 | ALA |
| 3 | D | 710 | ASP |
| 1 | G | 14 | VAL |
| 2 | I | 697 | LYS |
| 2 | I | 1136 | GLN |
| 3 | J | 710 | ASP |
| 1 | A | 14 | VAL |
| 2 | C | 1186 | VAL |
| 1 | A | 167 | PRO |
| 3 | D | 831 | VAL |
| 1 | G | 167 | PRO |
| 2 | I | 1186 | VAL |
| 3 | J | 831 | VAL |
| 1 | G | 178 | SER |

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 | 191/206 (93%) | 180 (94%) | 11 (6%) | 23 | 61 |
| 1 | B | 184/206 (89%) | 168 (91%) | 16 (9%) | 12 | 46 |
| 1 | G | 191/206 (93%) | 180 (94%) | 11 (6%) | 23 | 61 |
| 1 | H | 183/206 (89%) | 168 (92%) | 15 (8%) | 13 | 49 |
| 2 | C | 1155/1157 (100%) | 1063 (92%) | 92 (8%) | 14 | 50 |
| 2 | I | 1154/1157 (100%) | 1063 (92%) | 91 (8%) | 14 | 51 |
| 3 | D | 975/1168 (84%) | 883 (91%) | 92 (9%) | 10 | 43 |
| 3 | J | 1117/1168 (96%) | 1015 (91%) | 102 (9%) | 11 | 44 |
| 4 | E | 72/75 (96%) | 66 (92%) | 6 (8%) | 13 | 49 |
| 4 | K | 67/75 (89%) | 61 (91%) | 6 (9%) | 11 | 45 |
| 5 | F | 426/540 (79%) | 387 (91%) | 39 (9%) | 11 | 44 |
| 5 | L | 428/540 (79%) | 391 (91%) | 37 (9%) | 12 | 47 |
| All | All | 6143/6704 (92%) | 5625 (92%) | 518 (8%) | 13 | 48 |

All (518) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 9 | LEU |
| 1 | A | 15 | ASP |
| 1 | A | 35 | PHE |
| 1 | A | 54 | CYS |
| 1 | A | 61 | ILE |
| 1 | A | 133 | LEU |
| 1 | A | 145 | LYS |
| 1 | A | 172 | LEU |
| 1 | A | 186 | ASN |
| 1 | A | 207 | THR |
| 1 | A | 215 | GLU |
| 1 | B | 8 | PHE |
| 1 | B | 13 | LEU |
| 1 | B | 27 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 60 | GLU |
| 1 | B | 65 | LEU |
| 1 | B | 75 | GLN |
| 1 | B | 79 | LEU |
| 1 | B | 80 | GLU |
| 1 | B | 101 | THR |
| 1 | B | 105 | SER |
| 1 | B | 107 | ILE |
| 1 | B | 116 | THR |
| 1 | B | 124 | VAL |
| 1 | B | 133 | LEU |
| 1 | B | 160 | HIS |
| 1 | B | 183 | ILE |
| 2 | C | 11 | ILE |
| 2 | C | 29 | SER |
| 2 | C | 39 | ILE |
| 2 | C | 70 | TYR |
| 2 | C | 81 | ASP |
| 2 | C | 85 | CYS |
| 2 | C | 91 | THR |
| 2 | C | 115 | LYS |
| 2 | C | 116 | ASP |
| 2 | C | 119 | GLU |
| 2 | C | 131 | THR |
| 2 | C | 179 | TYR |
| 2 | C | 182 | SER |
| 2 | C | 185 | ASP |
| 2 | C | 202 | ARG |
| 2 | C | 285 | ILE |
| 2 | C | 320 | ASP |
| 2 | C | 321 | LEU |
| 2 | C | 419 | ILE |
| 2 | C | 423 | ASP |
| 2 | C | 434 | ASP |
| 2 | C | 484 | LEU |
| 2 | C | 485 | ASP |
| 2 | C | 486 | THR |
| 2 | C | 487 | LEU |
| 2 | C | 493 | ILE |
| 2 | C | 512 | SER |
| 2 | C | 517 | GLN |
| 2 | C | 518 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | C | 530 | ILE |
| 2 | C | 538 | LEU |
| 2 | C | 539 | THR |
| 2 | C | 540 | ARG |
| 2 | C | 554 | HIS |
| 2 | C | 604 | HIS |
| 2 | C | 615 | VAL |
| 2 | C | 623 | LEU |
| 2 | C | 633 | LEU |
| 2 | C | 657 | THR |
| 2 | C | 672 | GLU |
| 2 | C | 692 | THR |
| 2 | C | 697 | LYS |
| 2 | C | 699 | LEU |
| 2 | C | 706 | ARG |
| 2 | C | 714 | VAL |
| 2 | C | 739 | ASP |
| 2 | C | 748 | ILE |
| 2 | C | 765 | ILE |
| 2 | C | 773 | LEU |
| 2 | C | 781 | ASP |
| 2 | C | 782 | VAL |
| 2 | C | 788 | SER |
| 2 | C | 815 | SER |
| 2 | C | 819 | SER |
| 2 | C | 828 | PHE |
| 2 | C | 839 | VAL |
| 2 | C | 859 | GLU |
| 2 | C | 878 | THR |
| 2 | C | 890 | LYS |
| 2 | C | 892 | GLU |
| 2 | C | 895 | LEU |
| 2 | C | 919 | ARG |
| 2 | C | 974 | ARG |
| 2 | C | 990 | ASP |
| 2 | C | 992 | LEU |
| 2 | C | 1002 | LEU |
| 2 | C | 1005 | GLU |
| 2 | C | 1006 | GLU |
| 2 | C | 1014 | LEU |
| 2 | C | 1040 | ASP |
| 2 | C | 1082 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | C | 1108 | ASN |
| 2 | C | 1109 | ILE |
| 2 | C | 1114 | GLU |
| 2 | C | 1134 | GLN |
| 2 | C | 1155 | VAL |
| 2 | C | 1156 | ARG |
| 2 | C | 1158 | LYS |
| 2 | C | 1161 | LEU |
| 2 | C | 1198 | LEU |
| 2 | C | 1204 | LEU |
| 2 | C | 1210 | ILE |
| 2 | C | 1237 | HIS |
| 2 | C | 1240 | ASP |
| 2 | C | 1248 | THR |
| 2 | C | 1264 | GLN |
| 2 | C | 1265 | PHE |
| 2 | C | 1310 | ASP |
| 2 | C | 1313 | HIS |
| 2 | C | 1326 | LEU |
| 2 | C | 1327 | LEU |
| 2 | C | 1342 | GLU |
| 3 | D | 8 | LEU |
| 3 | D | 11 | GLN |
| 3 | D | 18 | ASP |
| 3 | D | 20 | ILE |
| 3 | D | 46 | TYR |
| 3 | D | 79 | LYS |
| 3 | D | 92 | VAL |
| 3 | D | 95 | THR |
| 3 | D | 117 | LEU |
| 3 | D | 119 | SER |
| 3 | D | 120 | LEU |
| 3 | D | 169 | LEU |
| 3 | D | 172 | PHE |
| 3 | D | 175 | GLU |
| 3 | D | 176 | PHE |
| 3 | D | 217 | LEU |
| 3 | D | 248 | ASP |
| 3 | D | 252 | LEU |
| 3 | D | 255 | LEU |
| 3 | D | 256 | ASP |
| 3 | D | 264 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | D | 311 | ARG |
| 3 | D | 324 | LEU |
| 3 | D | 339 | ARG |
| 3 | D | 356 | THR |
| 3 | D | 364 | HIS |
| 3 | D | 374 | LEU |
| 3 | D | 394 | ILE |
| 3 | D | 407 | VAL |
| 3 | D | 430 | HIS |
| 3 | D | 474 | LEU |
| 3 | D | 506 | VAL |
| 3 | D | 513 | MET |
| 3 | D | 545 | HIS |
| 3 | D | 547 | ARG |
| 3 | D | 568 | SER |
| 3 | D | 593 | ASN |
| 3 | D | 594 | GLN |
| 3 | D | 641 | ILE |
| 3 | D | 660 | GLU |
| 3 | D | 678 | ARG |
| 3 | D | 697 | MET |
| 3 | D | 698 | MET |
| 3 | D | 701 | LEU |
| 3 | D | 707 | ILE |
| 3 | D | 708 | ASN |
| 3 | D | 710 | ASP |
| 3 | D | 712 | GLN |
| 3 | D | 717 | VAL |
| 3 | D | 740 | LEU |
| 3 | D | 754 | ILE |
| 3 | D | 757 | THR |
| 3 | D | 764 | ARG |
| 3 | D | 767 | LEU |
| 3 | D | 770 | LEU |
| 3 | D | 772 | TYR |
| 3 | D | 805 | GLN |
| 3 | D | 810 | THR |
| 3 | D | 847 | ASP |
| 3 | D | 848 | VAL |
| 3 | D | 849 | LEU |
| 3 | D | 853 | THR |
| 3 | D | 857 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | D | 860 | ARG |
| 3 | D | 867 | GLN |
| 3 | D | 897 | HIS |
| 3 | D | 908 | ILE |
| 3 | D | 918 | ILE |
| 3 | D | 928 | THR |
| 3 | D | 931 | THR |
| 3 | D | 1155 | ILE |
| 3 | D | 1163 | VAL |
| 3 | D | 1167 | LYS |
| 3 | D | 1173 | ARG |
| 3 | D | 1177 | ILE |
| 3 | D | 1186 | TYR |
| 3 | D | 1199 | PHE |
| 3 | D | 1202 | GLU |
| 3 | D | 1208 | ASP |
| 3 | D | 1209 | VAL |
| 3 | D | 1215 | GLU |
| 3 | D | 1244 | GLN |
| 3 | D | 1255 | VAL |
| 3 | D | 1274 | PHE |
| 3 | D | 1275 | LEU |
| 3 | D | 1281 | GLU |
| 3 | D | 1284 | ARG |
| 3 | D | 1285 | VAL |
| 3 | D | 1289 | ASN |
| 3 | D | 1293 | GLU |
| 3 | D | 1327 | GLU |
| 3 | D | 1333 | THR |
| 4 | E | 28 | ARG |
| 4 | E | 31 | GLN |
| 4 | E | 36 | ASP |
| 4 | E | 39 | VAL |
| 4 | E | 46 | THR |
| 4 | E | 58 | LEU |
| 5 | F | 27 | VAL |
| 5 | F | 44 | ILE |
| 5 | F | 45 | ILE |
| 5 | F | 50 | ASP |
| 5 | F | 94 | THR |
| 5 | F | 98 | VAL |
| 5 | F | 100 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | F | 118 | ASP |
| 5 | F | 127 | ILE |
| 5 | F | 154 | GLU |
| 5 | F | 244 | THR |
| 5 | F | 305 | LEU |
| 5 | F | 306 | PHE |
| 5 | F | 335 | GLU |
| 5 | F | 341 | LEU |
| 5 | F | 395 | THR |
| 5 | F | 417 | ASP |
| 5 | F | 421 | TYR |
| 5 | F | 429 | THR |
| 5 | F | 445 | ASP |
| 5 | F | 449 | THR |
| 5 | F | 479 | THR |
| 5 | F | 486 | ARG |
| 5 | F | 488 | LEU |
| 5 | F | 491 | GLU |
| 5 | F | 496 | LYS |
| 5 | F | 508 | GLU |
| 5 | F | 528 | LEU |
| 5 | F | 530 | LEU |
| 5 | F | 540 | LEU |
| 5 | F | 566 | ASP |
| 5 | F | 568 | ASN |
| 5 | F | 572 | THR |
| 5 | F | 573 | LEU |
| 5 | F | 580 | PHE |
| 5 | F | 583 | THR |
| 5 | F | 600 | HIS |
| 5 | F | 603 | ARG |
| 5 | F | 606 | VAL |
| 1 | G | 9 | LEU |
| 1 | G | 15 | ASP |
| 1 | G | 35 | PHE |
| 1 | G | 54 | CYS |
| 1 | G | 61 | ILE |
| 1 | G | 133 | LEU |
| 1 | G | 145 | LYS |
| 1 | G | 172 | LEU |
| 1 | G | 186 | ASN |
| 1 | G | 207 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | G | 215 | GLU |
| 1 | H | 13 | LEU |
| 1 | H | 27 | THR |
| 1 | H | 54 | CYS |
| 1 | H | 60 | GLU |
| 1 | H | 65 | LEU |
| 1 | H | 75 | GLN |
| 1 | H | 79 | LEU |
| 1 | H | 80 | GLU |
| 1 | H | 101 | THR |
| 1 | H | 105 | SER |
| 1 | H | 107 | ILE |
| 1 | H | 116 | THR |
| 1 | H | 124 | VAL |
| 1 | H | 133 | LEU |
| 1 | H | 183 | ILE |
| 2 | I | 11 | ILE |
| 2 | I | 29 | SER |
| 2 | I | 39 | ILE |
| 2 | I | 70 | TYR |
| 2 | I | 81 | ASP |
| 2 | I | 85 | CYS |
| 2 | I | 91 | THR |
| 2 | I | 115 | LYS |
| 2 | I | 116 | ASP |
| 2 | I | 119 | GLU |
| 2 | I | 131 | THR |
| 2 | I | 179 | TYR |
| 2 | I | 182 | SER |
| 2 | I | 185 | ASP |
| 2 | I | 202 | ARG |
| 2 | I | 285 | ILE |
| 2 | I | 320 | ASP |
| 2 | I | 321 | LEU |
| 2 | I | 419 | ILE |
| 2 | I | 423 | ASP |
| 2 | I | 434 | ASP |
| 2 | I | 484 | LEU |
| 2 | I | 485 | ASP |
| 2 | I | 486 | THR |
| 2 | I | 487 | LEU |
| 2 | I | 493 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | I | 512 | SER |
| 2 | I | 517 | GLN |
| 2 | I | 518 | ASN |
| 2 | I | 530 | ILE |
| 2 | I | 538 | LEU |
| 2 | I | 539 | THR |
| 2 | I | 540 | ARG |
| 2 | I | 554 | HIS |
| 2 | I | 604 | HIS |
| 2 | I | 615 | VAL |
| 2 | I | 623 | LEU |
| 2 | I | 633 | LEU |
| 2 | I | 657 | THR |
| 2 | I | 672 | GLU |
| 2 | I | 692 | THR |
| 2 | I | 697 | LYS |
| 2 | I | 699 | LEU |
| 2 | I | 706 | ARG |
| 2 | I | 714 | VAL |
| 2 | I | 739 | ASP |
| 2 | I | 748 | ILE |
| 2 | I | 765 | ILE |
| 2 | I | 773 | LEU |
| 2 | I | 781 | ASP |
| 2 | I | 782 | VAL |
| 2 | I | 788 | SER |
| 2 | I | 815 | SER |
| 2 | I | 819 | SER |
| 2 | I | 828 | PHE |
| 2 | I | 839 | VAL |
| 2 | I | 859 | GLU |
| 2 | I | 878 | THR |
| 2 | I | 890 | LYS |
| 2 | I | 892 | GLU |
| 2 | I | 895 | LEU |
| 2 | I | 974 | ARG |
| 2 | I | 990 | ASP |
| 2 | I | 992 | LEU |
| 2 | I | 1002 | LEU |
| 2 | I | 1005 | GLU |
| 2 | I | 1006 | GLU |
| 2 | I | 1014 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | I | 1040 | ASP |
| 2 | I | 1082 | ILE |
| 2 | I | 1108 | ASN |
| 2 | I | 1109 | ILE |
| 2 | I | 1114 | GLU |
| 2 | I | 1134 | GLN |
| 2 | I | 1155 | VAL |
| 2 | I | 1156 | ARG |
| 2 | I | 1158 | LYS |
| 2 | I | 1161 | LEU |
| 2 | I | 1198 | LEU |
| 2 | I | 1204 | LEU |
| 2 | I | 1210 | ILE |
| 2 | I | 1237 | HIS |
| 2 | I | 1240 | ASP |
| 2 | I | 1248 | THR |
| 2 | I | 1264 | GLN |
| 2 | I | 1265 | PHE |
| 2 | I | 1310 | ASP |
| 2 | I | 1313 | HIS |
| 2 | I | 1326 | LEU |
| 2 | I | 1327 | LEU |
| 2 | I | 1342 | GLU |
| 3 | J | 18 | ASP |
| 3 | J | 20 | ILE |
| 3 | J | 46 | TYR |
| 3 | J | 79 | LYS |
| 3 | J | 92 | VAL |
| 3 | J | 95 | THR |
| 3 | J | 97 | VAL |
| 3 | J | 117 | LEU |
| 3 | J | 119 | SER |
| 3 | J | 120 | LEU |
| 3 | J | 169 | LEU |
| 3 | J | 175 | GLU |
| 3 | J | 176 | PHE |
| 3 | J | 217 | LEU |
| 3 | J | 248 | ASP |
| 3 | J | 252 | LEU |
| 3 | J | 255 | LEU |
| 3 | J | 256 | ASP |
| 3 | J | 264 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | J | 311 | ARG |
| 3 | J | 324 | LEU |
| 3 | J | 339 | ARG |
| 3 | J | 356 | THR |
| 3 | J | 364 | HIS |
| 3 | J | 374 | LEU |
| 3 | J | 394 | ILE |
| 3 | J | 407 | VAL |
| 3 | J | 430 | HIS |
| 3 | J | 474 | LEU |
| 3 | J | 506 | VAL |
| 3 | J | 513 | MET |
| 3 | J | 536 | LEU |
| 3 | J | 545 | HIS |
| 3 | J | 547 | ARG |
| 3 | J | 568 | SER |
| 3 | J | 593 | ASN |
| 3 | J | 594 | GLN |
| 3 | J | 641 | ILE |
| 3 | J | 660 | GLU |
| 3 | J | 678 | ARG |
| 3 | J | 697 | MET |
| 3 | J | 698 | MET |
| 3 | J | 701 | LEU |
| 3 | J | 707 | ILE |
| 3 | J | 708 | ASN |
| 3 | J | 710 | ASP |
| 3 | J | 712 | GLN |
| 3 | J | 717 | VAL |
| 3 | J | 740 | LEU |
| 3 | J | 754 | ILE |
| 3 | J | 757 | THR |
| 3 | J | 764 | ARG |
| 3 | J | 767 | LEU |
| 3 | J | 770 | LEU |
| 3 | J | 772 | TYR |
| 3 | J | 805 | GLN |
| 3 | J | 810 | THR |
| 3 | J | 847 | ASP |
| 3 | J | 848 | VAL |
| 3 | J | 849 | LEU |
| 3 | J | 853 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | J | 857 | LEU |
| 3 | J | 860 | ARG |
| 3 | J | 867 | GLN |
| 3 | J | 897 | HIS |
| 3 | J | 908 | ILE |
| 3 | J | 918 | ILE |
| 3 | J | 928 | THR |
| 3 | J | 931 | THR |
| 3 | J | 987 | GLU |
| 3 | J | 997 | VAL |
| 3 | J | 1017 | VAL |
| 3 | J | 1025 | MET |
| 3 | J | 1042 | ASP |
| 3 | J | 1062 | LEU |
| 3 | J | 1063 | ASP |
| 3 | J | 1064 | SER |
| 3 | J | 1073 | ASP |
| 3 | J | 1115 | ILE |
| 3 | J | 1121 | LEU |
| 3 | J | 1155 | ILE |
| 3 | J | 1163 | VAL |
| 3 | J | 1167 | LYS |
| 3 | J | 1173 | ARG |
| 3 | J | 1177 | ILE |
| 3 | J | 1186 | TYR |
| 3 | J | 1199 | PHE |
| 3 | J | 1202 | GLU |
| 3 | J | 1208 | ASP |
| 3 | J | 1209 | VAL |
| 3 | J | 1215 | GLU |
| 3 | J | 1244 | GLN |
| 3 | J | 1255 | VAL |
| 3 | J | 1274 | PHE |
| 3 | J | 1275 | LEU |
| 3 | J | 1281 | GLU |
| 3 | J | 1284 | ARG |
| 3 | J | 1285 | VAL |
| 3 | J | 1289 | ASN |
| 3 | J | 1293 | GLU |
| 3 | J | 1327 | GLU |
| 3 | J | 1333 | THR |
| 4 | K | 28 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | K | 31 | GLN |
| 4 | K | 36 | ASP |
| 4 | K | 39 | VAL |
| 4 | K | 46 | THR |
| 4 | K | 58 | LEU |
| 5 | L | 27 | VAL |
| 5 | L | 44 | ILE |
| 5 | L | 45 | ILE |
| 5 | L | 50 | ASP |
| 5 | L | 98 | VAL |
| 5 | L | 100 | MET |
| 5 | L | 118 | ASP |
| 5 | L | 154 | GLU |
| 5 | L | 244 | THR |
| 5 | L | 305 | LEU |
| 5 | L | 306 | PHE |
| 5 | L | 335 | GLU |
| 5 | L | 341 | LEU |
| 5 | L | 395 | THR |
| 5 | L | 417 | ASP |
| 5 | L | 421 | TYR |
| 5 | L | 429 | THR |
| 5 | L | 445 | ASP |
| 5 | L | 449 | THR |
| 5 | L | 479 | THR |
| 5 | L | 486 | ARG |
| 5 | L | 488 | LEU |
| 5 | L | 491 | GLU |
| 5 | L | 496 | LYS |
| 5 | L | 508 | GLU |
| 5 | L | 528 | LEU |
| 5 | L | 530 | LEU |
| 5 | L | 540 | LEU |
| 5 | L | 566 | ASP |
| 5 | L | 568 | ASN |
| 5 | L | 572 | THR |
| 5 | L | 573 | LEU |
| 5 | L | 580 | PHE |
| 5 | L | 583 | THR |
| 5 | L | 600 | HIS |
| 5 | L | 603 | ARG |
| 5 | L | 606 | VAL |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | C | 343 | HIS |
| 2 | C | 1108 | ASN |
| 2 | C | 1111 | GLN |
| 2 | C | 1116 | HIS |
| 2 | C | 1257 | GLN |
| 2 | C | 1288 | GLN |
| 2 | C | 1312 | ASN |
| 3 | D | 340 | GLN |
| 3 | D | 364 | HIS |
| 3 | D | 419 | HIS |
| 3 | D | 477 | GLN |
| 3 | D | 560 | ASN |
| 3 | D | 1367 | GLN |
| 5 | F | 406 | GLN |
| 5 | F | 472 | GLN |
| 2 | I | 343 | HIS |
| 2 | I | 1108 | ASN |
| 2 | I | 1111 | GLN |
| 2 | I | 1116 | HIS |
| 2 | I | 1257 | GLN |
| 2 | I | 1288 | GLN |
| 2 | I | 1314 | GLN |
| 3 | J | 340 | GLN |
| 3 | J | 364 | HIS |
| 3 | J | 419 | HIS |
| 3 | J | 1268 | ASN |
| 3 | J | 1367 | GLN |
| 5 | L | 406 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|--|-----------------------|-------|
| 1 | A | 224/239 (93%) | -0.04 | 1 (0%) 92 88 | 57, 89, 134, 170 | 0 |
| 1 | B | 220/239 (92%) | 0.19 | 14 (6%) 20 15 | 57, 121, 154, 165 | 0 |
| 1 | G | 228/239 (95%) | 0.15 | 8 (3%) 44 35 | 84, 122, 155, 170 | 0 |
| 1 | H | 217/239 (90%) | 0.35 | 21 (9%) 8 7 | 90, 134, 157, 166 | 0 |
| 2 | C | 1340/1342 (99%) | -0.07 | 24 (1%) 69 60 | 31, 86, 140, 175 | 0 |
| 2 | I | 1340/1342 (99%) | 0.01 | 49 (3%) 42 34 | 41, 105, 151, 183 | 0 |
| 3 | D | 1166/1407 (82%) | -0.04 | 28 (2%) 59 49 | 28, 78, 140, 170 | 0 |
| 3 | J | 1334/1407 (94%) | 0.25 | 106 (7%) 13 11 | 33, 99, 159, 185 | 0 |
| 4 | E | 89/91 (97%) | -0.24 | 0 100 100 | 38, 82, 122, 129 | 0 |
| 4 | K | 79/91 (86%) | -0.25 | 1 (1%) 77 68 | 60, 96, 144, 154 | 0 |
| 5 | F | 542/613 (88%) | 0.16 | 38 (7%) 17 13 | 49, 127, 166, 196 | 0 |
| 5 | L | 539/613 (87%) | 0.07 | 30 (5%) 25 20 | 62, 125, 165, 179 | 0 |
| All | All | 7318/7862 (93%) | 0.06 | 320 (4%) 35 28 | 28, 102, 155, 196 | 0 |

All (320) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 3 | J | 1054 | THR | 10.1 |
| 5 | F | 89 | SER | 8.3 |
| 5 | F | 167 | ASP | 8.1 |
| 5 | L | 7 | SER | 8.1 |
| 2 | C | 265 | LYS | 7.5 |
| 2 | C | 251 | ALA | 7.3 |
| 3 | J | 1053 | LEU | 6.9 |
| 5 | L | 167 | ASP | 6.8 |
| 5 | F | 76 | ALA | 6.3 |
| 3 | J | 1007 | ASP | 6.1 |
| 5 | F | 88 | GLU | 6.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 5 | L | 480 | PRO | 5.9 |
| 2 | C | 252 | SER | 5.7 |
| 3 | J | 1088 | VAL | 5.7 |
| 3 | J | 1056 | LEU | 5.6 |
| 3 | J | 1294 | ALA | 5.6 |
| 2 | I | 998 | LEU | 5.5 |
| 2 | C | 266 | GLY | 5.3 |
| 3 | J | 1089 | LEU | 5.2 |
| 2 | I | 999 | GLU | 5.2 |
| 3 | J | 1068 | THR | 5.1 |
| 2 | I | 987 | GLU | 5.0 |
| 1 | B | 146 | VAL | 5.0 |
| 3 | J | 1295 | ASN | 5.0 |
| 5 | L | 305 | LEU | 5.0 |
| 3 | J | 1069 | ALA | 4.9 |
| 3 | J | 1055 | GLY | 4.8 |
| 2 | I | 978 | VAL | 4.7 |
| 2 | I | 165 | HIS | 4.7 |
| 1 | H | 172 | LEU | 4.7 |
| 3 | J | 991 | THR | 4.7 |
| 2 | I | 979 | LEU | 4.6 |
| 3 | J | 998 | PRO | 4.6 |
| 5 | F | 75 | ASP | 4.6 |
| 5 | L | 290 | LEU | 4.5 |
| 5 | F | 579 | GLN | 4.5 |
| 1 | B | 66 | HIS | 4.4 |
| 3 | J | 1070 | GLY | 4.3 |
| 3 | J | 1103 | GLY | 4.2 |
| 5 | F | 259 | PHE | 4.2 |
| 3 | J | 340 | GLN | 4.2 |
| 5 | F | 86 | SER | 4.2 |
| 5 | L | 294 | GLN | 4.2 |
| 3 | J | 1080 | ILE | 4.2 |
| 5 | F | 162 | ILE | 4.1 |
| 2 | I | 989 | LEU | 4.1 |
| 2 | I | 990 | ASP | 4.1 |
| 3 | J | 1097 | ALA | 4.0 |
| 3 | J | 341 | ASN | 4.0 |
| 3 | J | 1198 | VAL | 4.0 |
| 3 | J | 1095 | MET | 4.0 |
| 3 | J | 1093 | THR | 3.9 |
| 3 | J | 1058 | SER | 3.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 3 | J | 974 | VAL | 3.9 |
| 3 | J | 984 | LEU | 3.9 |
| 1 | B | 147 | GLN | 3.9 |
| 3 | J | 956 | GLY | 3.9 |
| 5 | F | 283 | GLN | 3.9 |
| 3 | J | 1059 | LEU | 3.8 |
| 3 | J | 743 | MET | 3.8 |
| 3 | J | 1215 | GLU | 3.8 |
| 5 | F | 161 | LEU | 3.8 |
| 1 | G | 193 | GLU | 3.8 |
| 5 | F | 16 | GLY | 3.8 |
| 2 | C | 241 | LEU | 3.8 |
| 5 | F | 35 | ILE | 3.8 |
| 5 | F | 578 | LYS | 3.7 |
| 5 | F | 34 | ASP | 3.7 |
| 1 | B | 67 | GLU | 3.7 |
| 3 | J | 1001 | ALA | 3.6 |
| 2 | I | 696 | ASP | 3.6 |
| 3 | J | 1030 | GLU | 3.6 |
| 5 | F | 87 | VAL | 3.6 |
| 5 | L | 610 | PHE | 3.6 |
| 3 | J | 975 | ILE | 3.5 |
| 1 | G | 90 | VAL | 3.5 |
| 3 | J | 1051 | ASP | 3.5 |
| 5 | L | 315 | TRP | 3.5 |
| 3 | D | 756 | GLU | 3.5 |
| 3 | J | 958 | ILE | 3.4 |
| 5 | F | 85 | SER | 3.4 |
| 5 | L | 490 | PRO | 3.4 |
| 3 | J | 1166 | GLY | 3.4 |
| 3 | J | 1044 | GLN | 3.4 |
| 2 | I | 976 | ARG | 3.4 |
| 3 | J | 1006 | GLY | 3.3 |
| 2 | C | 292 | ILE | 3.3 |
| 3 | J | 1085 | GLY | 3.3 |
| 1 | B | 59 | VAL | 3.2 |
| 5 | F | 165 | PHE | 3.2 |
| 5 | L | 8 | GLN | 3.2 |
| 2 | I | 164 | THR | 3.2 |
| 3 | J | 1180 | VAL | 3.2 |
| 5 | F | 315 | TRP | 3.2 |
| 1 | H | 146 | VAL | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | I | 980 | VAL | 3.2 |
| 2 | C | 230 | PHE | 3.2 |
| 3 | J | 1168 | GLU | 3.2 |
| 2 | I | 169 | LYS | 3.2 |
| 3 | J | 1161 | GLY | 3.2 |
| 3 | D | 743 | MET | 3.2 |
| 2 | I | 230 | PHE | 3.1 |
| 5 | F | 319 | ALA | 3.1 |
| 3 | J | 1090 | ILE | 3.1 |
| 3 | J | 960 | LEU | 3.1 |
| 2 | I | 981 | ALA | 3.1 |
| 5 | F | 92 | GLY | 3.1 |
| 5 | L | 88 | GLU | 3.1 |
| 5 | F | 158 | LEU | 3.1 |
| 3 | D | 1198 | VAL | 3.1 |
| 2 | I | 264 | GLU | 3.1 |
| 2 | I | 124 | MET | 3.0 |
| 2 | I | 1021 | LEU | 3.0 |
| 1 | H | 96 | ASP | 3.0 |
| 1 | H | 123 | ILE | 3.0 |
| 5 | L | 165 | PHE | 3.0 |
| 3 | J | 955 | LYS | 3.0 |
| 3 | J | 957 | SER | 3.0 |
| 1 | H | 97 | GLU | 3.0 |
| 1 | B | 173 | VAL | 3.0 |
| 3 | J | 997 | VAL | 3.0 |
| 3 | D | 1175 | LEU | 3.0 |
| 1 | H | 12 | ARG | 3.0 |
| 3 | J | 1029 | THR | 3.0 |
| 1 | H | 92 | VAL | 3.0 |
| 3 | J | 1181 | ASP | 3.0 |
| 5 | F | 73 | ASP | 3.0 |
| 5 | L | 289 | LYS | 2.9 |
| 5 | F | 575 | GLU | 2.9 |
| 3 | D | 682 | VAL | 2.9 |
| 3 | J | 1073 | ASP | 2.9 |
| 5 | L | 286 | LEU | 2.9 |
| 1 | H | 205 | MET | 2.9 |
| 3 | D | 341 | ASN | 2.9 |
| 5 | F | 77 | ALA | 2.9 |
| 1 | B | 172 | LEU | 2.9 |
| 3 | J | 1187 | GLU | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 5 | L | 427 | PHE | 2.9 |
| 1 | H | 14 | VAL | 2.9 |
| 3 | J | 992 | LYS | 2.9 |
| 2 | C | 282 | VAL | 2.9 |
| 3 | D | 1190 | ILE | 2.8 |
| 5 | F | 321 | ALA | 2.8 |
| 3 | J | 1190 | ILE | 2.8 |
| 2 | I | 1010 | GLN | 2.8 |
| 3 | D | 1180 | VAL | 2.8 |
| 3 | J | 987 | GLU | 2.8 |
| 3 | J | 1052 | GLU | 2.8 |
| 1 | B | 158 | ARG | 2.8 |
| 2 | C | 997 | TRP | 2.8 |
| 2 | I | 1050 | VAL | 2.8 |
| 3 | J | 1091 | PRO | 2.8 |
| 3 | J | 69 | GLU | 2.8 |
| 3 | J | 1057 | SER | 2.8 |
| 2 | I | 997 | TRP | 2.8 |
| 1 | G | 209 | GLY | 2.8 |
| 3 | J | 1188 | GLU | 2.8 |
| 3 | J | 1084 | GLN | 2.8 |
| 1 | G | 88 | LEU | 2.8 |
| 1 | H | 13 | LEU | 2.8 |
| 5 | L | 20 | GLY | 2.8 |
| 3 | J | 986 | ASP | 2.7 |
| 3 | D | 754 | ILE | 2.7 |
| 1 | H | 133 | LEU | 2.7 |
| 3 | J | 973 | LEU | 2.7 |
| 3 | J | 1082 | ASP | 2.7 |
| 1 | H | 144 | ILE | 2.7 |
| 5 | L | 29 | ASP | 2.7 |
| 2 | I | 988 | LYS | 2.7 |
| 5 | F | 514 | ASP | 2.7 |
| 3 | D | 1169 | THR | 2.7 |
| 2 | I | 246 | LEU | 2.7 |
| 1 | G | 95 | LYS | 2.7 |
| 1 | B | 144 | ILE | 2.7 |
| 3 | J | 1185 | PRO | 2.6 |
| 5 | F | 74 | GLU | 2.6 |
| 3 | J | 1035 | VAL | 2.6 |
| 3 | J | 988 | PHE | 2.6 |
| 1 | G | 54 | CYS | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | C | 206 | ALA | 2.6 |
| 3 | J | 1062 | LEU | 2.6 |
| 1 | A | 9 | LEU | 2.6 |
| 2 | C | 258 | ASN | 2.6 |
| 3 | J | 756 | GLU | 2.6 |
| 2 | I | 190 | PRO | 2.6 |
| 3 | J | 1083 | ALA | 2.6 |
| 3 | D | 878 | ASP | 2.6 |
| 2 | I | 167 | SER | 2.6 |
| 2 | I | 333 | ILE | 2.5 |
| 5 | F | 78 | GLU | 2.5 |
| 3 | J | 218 | THR | 2.5 |
| 3 | J | 1175 | LEU | 2.5 |
| 5 | L | 283 | GLN | 2.5 |
| 2 | I | 745 | GLU | 2.5 |
| 2 | C | 257 | ALA | 2.5 |
| 2 | C | 319 | LEU | 2.5 |
| 3 | J | 682 | VAL | 2.5 |
| 5 | L | 19 | GLN | 2.5 |
| 3 | D | 1376 | GLY | 2.5 |
| 3 | D | 753 | SER | 2.5 |
| 3 | D | 1204 | VAL | 2.5 |
| 2 | I | 168 | GLY | 2.5 |
| 3 | D | 826 | ILE | 2.5 |
| 5 | L | 569 | THR | 2.4 |
| 3 | J | 648 | GLU | 2.4 |
| 3 | J | 1114 | GLN | 2.4 |
| 3 | D | 683 | ILE | 2.4 |
| 1 | H | 147 | GLN | 2.4 |
| 3 | D | 1200 | GLU | 2.4 |
| 3 | J | 961 | SER | 2.4 |
| 1 | H | 24 | ALA | 2.4 |
| 3 | D | 340 | GLN | 2.4 |
| 2 | I | 973 | SER | 2.4 |
| 3 | J | 966 | VAL | 2.4 |
| 5 | L | 89 | SER | 2.4 |
| 3 | J | 977 | SER | 2.4 |
| 5 | L | 428 | SER | 2.4 |
| 2 | I | 991 | LYS | 2.4 |
| 2 | C | 255 | ILE | 2.4 |
| 2 | C | 923 | GLY | 2.4 |
| 2 | I | 986 | ALA | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | I | 855 | PRO | 2.4 |
| 2 | C | 317 | LEU | 2.4 |
| 2 | C | 1000 | LEU | 2.3 |
| 5 | F | 301 | ASN | 2.3 |
| 2 | I | 906 | PHE | 2.3 |
| 5 | F | 15 | ARG | 2.3 |
| 3 | J | 1079 | LYS | 2.3 |
| 3 | J | 686 | TRP | 2.3 |
| 5 | F | 137 | TYR | 2.3 |
| 3 | J | 645 | VAL | 2.3 |
| 3 | D | 1214 | PRO | 2.3 |
| 2 | I | 1011 | LEU | 2.3 |
| 5 | L | 18 | GLU | 2.3 |
| 5 | F | 318 | ALA | 2.3 |
| 1 | B | 90 | VAL | 2.3 |
| 3 | D | 77 | ARG | 2.3 |
| 2 | C | 254 | ASP | 2.3 |
| 3 | D | 1172 | LYS | 2.3 |
| 3 | J | 683 | ILE | 2.3 |
| 3 | J | 746 | LEU | 2.3 |
| 3 | J | 670 | SER | 2.3 |
| 3 | J | 664 | ILE | 2.3 |
| 5 | F | 280 | VAL | 2.3 |
| 2 | I | 996 | ARG | 2.2 |
| 3 | J | 993 | GLU | 2.2 |
| 1 | H | 90 | VAL | 2.2 |
| 2 | I | 995 | ASP | 2.2 |
| 3 | D | 674 | THR | 2.2 |
| 3 | D | 879 | ALA | 2.2 |
| 5 | F | 340 | ALA | 2.2 |
| 3 | J | 1165 | PHE | 2.2 |
| 3 | J | 1162 | ILE | 2.2 |
| 2 | C | 922 | ASN | 2.2 |
| 3 | J | 89 | GLY | 2.2 |
| 1 | H | 107 | ILE | 2.2 |
| 5 | L | 287 | ILE | 2.2 |
| 5 | L | 602 | SER | 2.2 |
| 2 | I | 882 | ILE | 2.2 |
| 5 | F | 32 | PRO | 2.2 |
| 1 | G | 28 | LEU | 2.2 |
| 3 | J | 1071 | GLY | 2.2 |
| 2 | C | 239 | MET | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | B | 69 | SER | 2.2 |
| 1 | H | 106 | GLY | 2.2 |
| 2 | I | 232 | ILE | 2.2 |
| 2 | I | 494 | ASN | 2.2 |
| 1 | B | 107 | ILE | 2.2 |
| 2 | I | 1002 | LEU | 2.2 |
| 3 | J | 1106 | ILE | 2.2 |
| 1 | B | 55 | ALA | 2.2 |
| 2 | I | 725 | GLN | 2.2 |
| 3 | J | 1109 | LEU | 2.2 |
| 2 | I | 265 | LYS | 2.2 |
| 2 | C | 184 | LEU | 2.2 |
| 5 | L | 598 | LEU | 2.2 |
| 1 | H | 158 | ARG | 2.2 |
| 3 | J | 1047 | THR | 2.2 |
| 3 | J | 76 | LYS | 2.2 |
| 3 | D | 1171 | GLY | 2.2 |
| 5 | L | 512 | GLY | 2.2 |
| 1 | H | 132 | HIS | 2.2 |
| 3 | J | 1094 | ASP | 2.2 |
| 3 | D | 1203 | ARG | 2.1 |
| 1 | H | 67 | GLU | 2.1 |
| 2 | C | 253 | PHE | 2.1 |
| 2 | I | 100 | LEU | 2.1 |
| 3 | J | 1122 | ALA | 2.1 |
| 3 | D | 849 | LEU | 2.1 |
| 3 | J | 1078 | LEU | 2.1 |
| 3 | J | 989 | GLY | 2.1 |
| 3 | J | 857 | LEU | 2.1 |
| 5 | L | 140 | ALA | 2.1 |
| 5 | F | 256 | PHE | 2.1 |
| 2 | C | 264 | GLU | 2.1 |
| 2 | I | 972 | PHE | 2.1 |
| 3 | J | 1086 | ASN | 2.1 |
| 1 | G | 98 | VAL | 2.1 |
| 1 | H | 18 | GLN | 2.1 |
| 3 | D | 679 | TYR | 2.1 |
| 2 | I | 277 | LEU | 2.1 |
| 3 | D | 1165 | PHE | 2.1 |
| 3 | J | 1031 | VAL | 2.1 |
| 3 | J | 1043 | GLY | 2.1 |
| 5 | L | 87 | VAL | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 5 | L | 337 | VAL | 2.1 |
| 2 | I | 720 | ARG | 2.1 |
| 1 | B | 98 | VAL | 2.1 |
| 3 | J | 1104 | LYS | 2.0 |
| 3 | J | 1184 | ASP | 2.0 |
| 3 | J | 1013 | GLY | 2.0 |
| 3 | J | 849 | LEU | 2.0 |
| 2 | I | 867 | GLU | 2.0 |
| 2 | I | 420 | LEU | 2.0 |
| 4 | K | 58 | LEU | 2.0 |
| 3 | J | 712 | GLN | 2.0 |
| 2 | I | 975 | ILE | 2.0 |
| 5 | F | 323 | ASN | 2.0 |
| 2 | C | 183 | TRP | 2.0 |
| 3 | J | 985 | ILE | 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 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 7 | ZN | D | 1503 | 1/1 | 0.91 | 0.40 | 1.54 | 138,138,138,138 | 0 |
| 7 | ZN | D | 1502 | 1/1 | 0.97 | 0.12 | -1.13 | 103,103,103,103 | 0 |
| 7 | ZN | J | 1502 | 1/1 | 0.94 | 0.13 | -1.29 | 107,107,107,107 | 0 |
| 7 | ZN | J | 1503 | 1/1 | 0.99 | 0.18 | -2.01 | 37,37,37,37 | 0 |
| 6 | MG | D | 1501 | 1/1 | 0.84 | 0.52 | - | 72,72,72,72 | 0 |
| 6 | MG | J | 1501 | 1/1 | 0.86 | 0.64 | - | 74,74,74,74 | 0 |

6.5 Other polymers ⓘ

There are no such residues in this entry.