



Full wwPDB EM Validation Report ⓘ

Nov 9, 2022 – 07:45 AM EST

PDB ID : 6OUL
EMDB ID : EMD-20203
Title : Cryo-EM structure of Escherichia coli RNAP polymerase bound to rpsTP2 promoter DNA
Authors : Chen, J.; Chiu, C.E.; Campbell, E.A.; Darst, S.A.
Deposited on : 2019-05-04
Resolution : 3.40 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

| | | |
|--------------------------------|---|--|
| EMDB validation analysis | : | 0.0.1.dev43 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.31.2 |

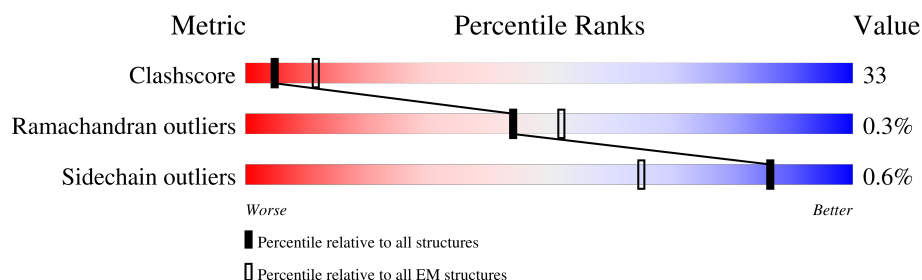
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | G | 329 | |
| 1 | H | 329 | |
| 1 | R | 329 | |
| 2 | I | 1342 | |
| 3 | J | 1430 | |
| 4 | K | 91 | |
| 5 | L | 616 | |
| 6 | P | 85 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 7 | Q | 85 | <div><div><div></div><div></div><div></div></div><div>24%15%51%34%</div></div> |

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 32044 atoms, of which 117 are hydrogens and 0 are deuteriums.

In the tables below, 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 | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1 | G | 231 | Total | C | N | O | S | 0 | 0 |
| | | | 1785 | 1112 | 318 | 349 | 6 | | |
| 1 | H | 219 | Total | C | N | O | S | 0 | 0 |
| | | | 1681 | 1050 | 295 | 330 | 6 | | |
| 1 | R | 73 | Total | C | N | O | S | 0 | 0 |
| | | | 572 | 362 | 100 | 108 | 2 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 2 | I | 1341 | Total | C | N | O | S | 0 | 0 |
| | | | 10575 | 6634 | 1842 | 2056 | 43 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 3 | J | 1337 | Total | C | N | O | S | 0 | 0 |
| | | | 10386 | 6525 | 1851 | 1961 | 49 | | |

There are 24 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| J | 1 | VAL | - | expression tag | UNP U9YPW3 |
| J | 1408 | LEU | - | expression tag | UNP U9YPW3 |
| J | 1409 | GLU | - | expression tag | UNP U9YPW3 |
| J | 1410 | LEU | - | expression tag | UNP U9YPW3 |
| J | 1411 | GLU | - | expression tag | UNP U9YPW3 |
| J | 1412 | VAL | - | expression tag | UNP U9YPW3 |
| J | 1413 | LEU | - | expression tag | UNP U9YPW3 |
| J | 1414 | PHE | - | expression tag | UNP U9YPW3 |
| J | 1415 | GLN | - | expression tag | UNP U9YPW3 |
| J | 1416 | GLY | - | expression tag | UNP U9YPW3 |
| J | 1417 | PRO | - | expression tag | UNP U9YPW3 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| J | 1418 | SER | - | expression tag | UNP U9YPW3 |
| J | 1419 | SER | - | expression tag | UNP U9YPW3 |
| J | 1420 | GLY | - | expression tag | UNP U9YPW3 |
| J | 1421 | HIS | - | expression tag | UNP U9YPW3 |
| J | 1422 | HIS | - | expression tag | UNP U9YPW3 |
| J | 1423 | HIS | - | expression tag | UNP U9YPW3 |
| J | 1424 | HIS | - | expression tag | UNP U9YPW3 |
| J | 1425 | HIS | - | expression tag | UNP U9YPW3 |
| J | 1426 | HIS | - | expression tag | UNP U9YPW3 |
| J | 1427 | HIS | - | expression tag | UNP U9YPW3 |
| J | 1428 | HIS | - | expression tag | UNP U9YPW3 |
| J | 1429 | HIS | - | expression tag | UNP U9YPW3 |
| J | 1430 | HIS | - | expression tag | UNP U9YPW3 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4 | K | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 627 | 382 | 118 | 126 | 1 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5 | L | 471 | Total | C | N | O | S | 0 | 0 |
| | | | 3821 | 2397 | 681 | 720 | 23 | | |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| L | -2 | SER | - | expression tag | UNP Q0P6L9 |
| L | -1 | GLU | - | expression tag | UNP Q0P6L9 |
| L | 0 | PHE | - | expression tag | UNP Q0P6L9 |

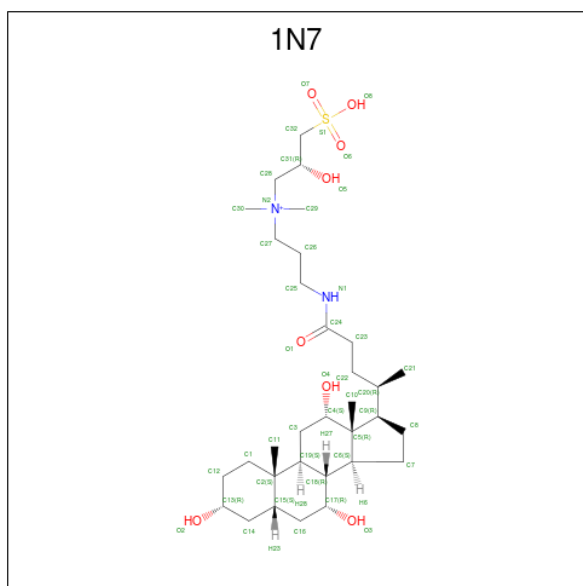
- Molecule 6 is a DNA chain called Non-template strand of rpsTP2 DNA promoter.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 6 | P | 61 | Total | C | N | O | P | 0 | 0 |
| | | | 1253 | 599 | 235 | 358 | 61 | | |

- Molecule 7 is a DNA chain called Template strand of rpsTP2 DNA promoter.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 7 | Q | 56 | Total | C | N | O | P | 0 | 0 |
| | | | 1143 | 549 | 192 | 346 | 56 | | |

- Molecule 8 is CHAPSO (three-letter code: 1N7) (formula: $\text{C}_{32}\text{H}_{59}\text{N}_2\text{O}_8\text{S}$).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|
| 8 | I | 1 | Total 66 | C 24 | H 39 | O 3 | 0 |
| 8 | J | 1 | Total 66 | C 24 | H 39 | O 3 | 0 |
| 8 | L | 1 | Total 66 | C 24 | H 39 | O 3 | 0 |

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 9 | J | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

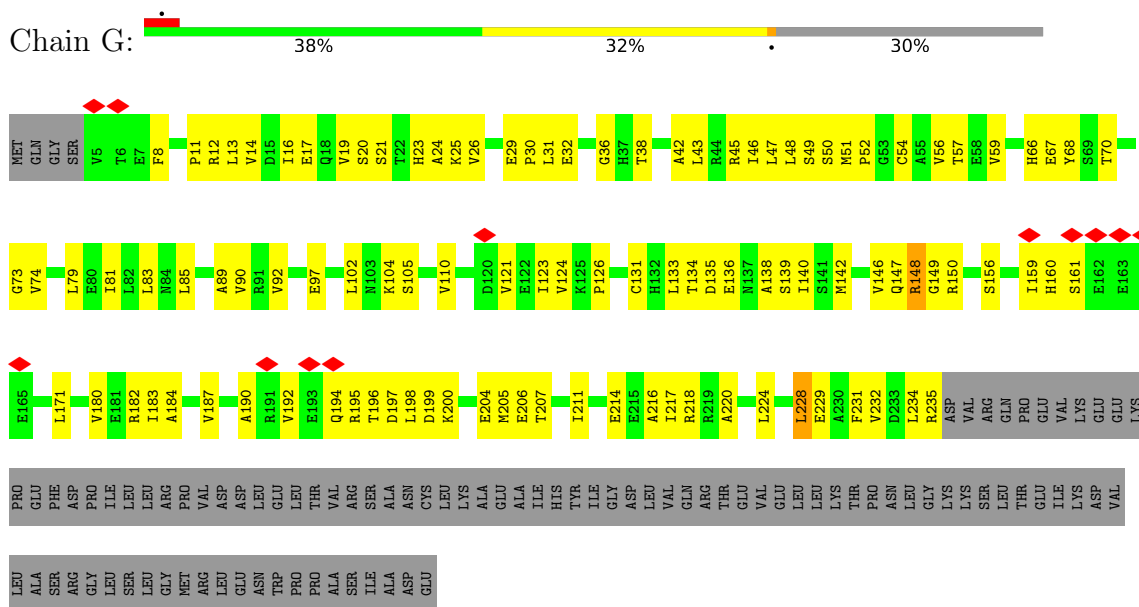
- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|-----------------|---------|
| 10 | J | 2 | Total Zn 2 2 | 0 |

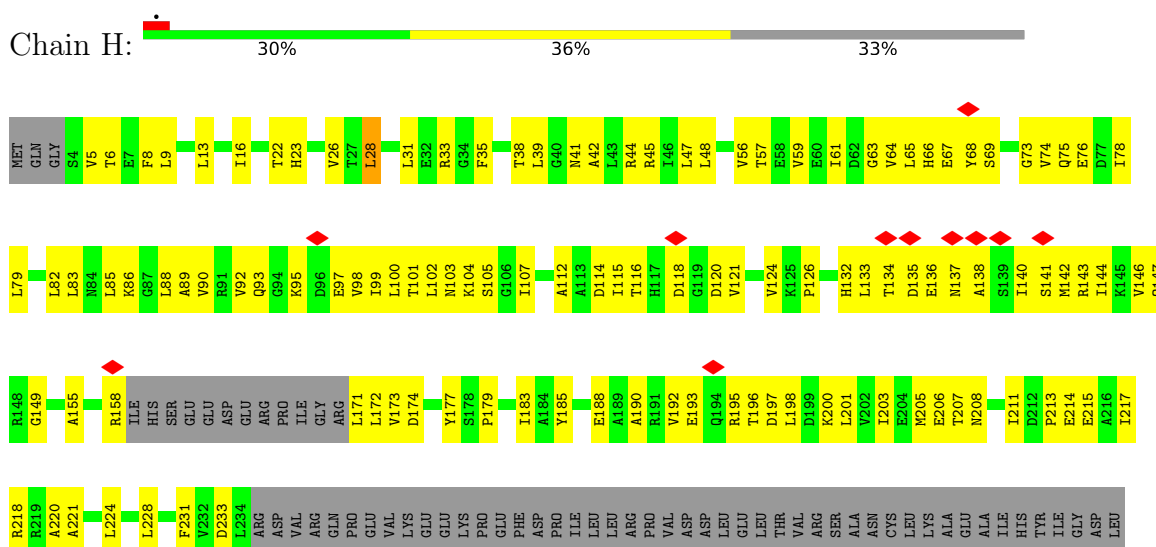
3 Residue-property plots

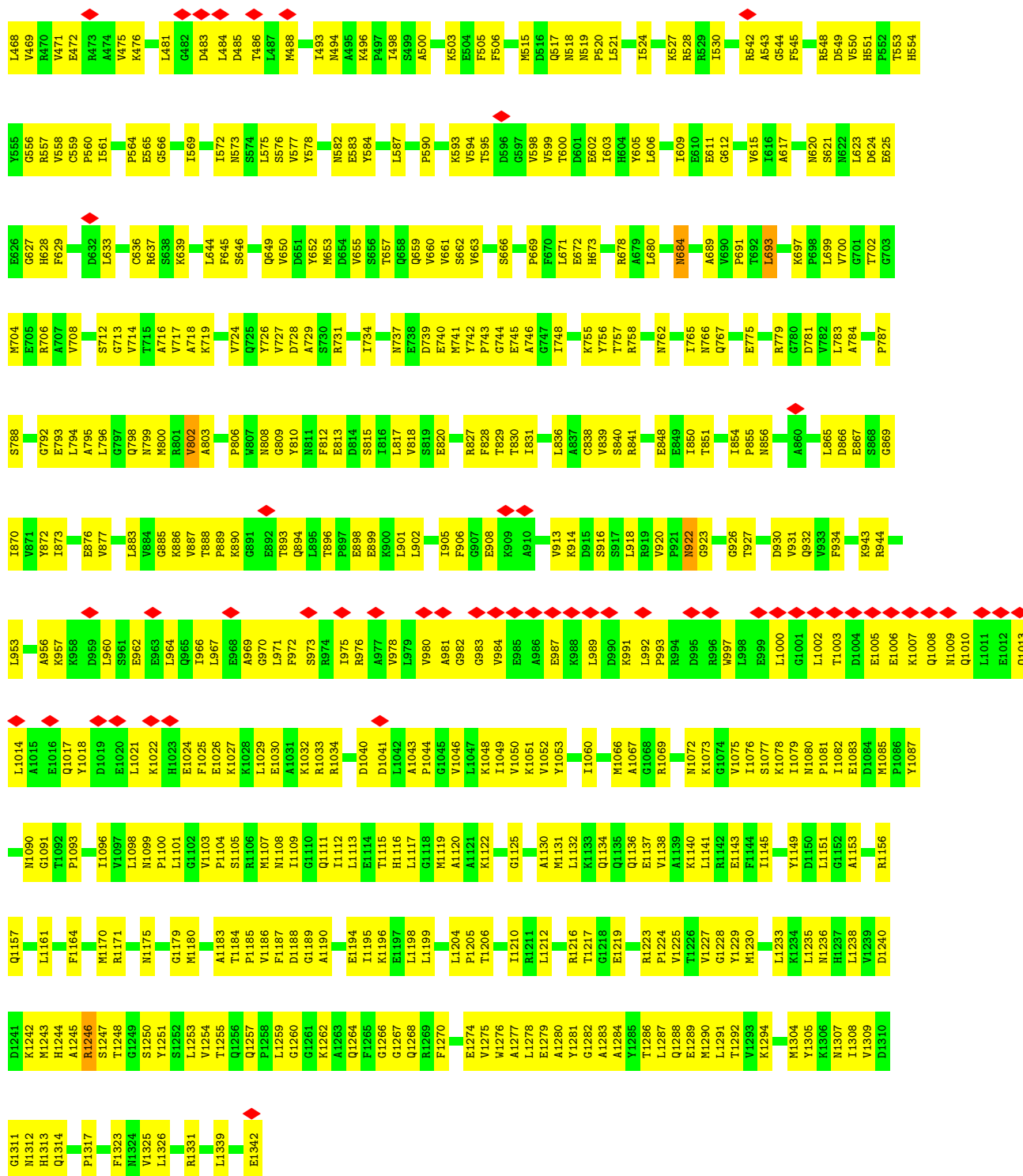
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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

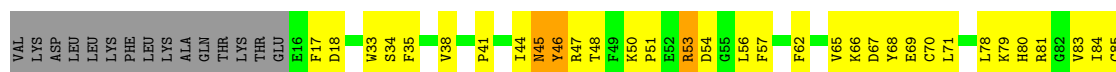
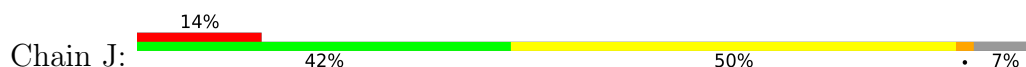


• Molecule 1: DNA-directed RNA polymerase subunit alpha

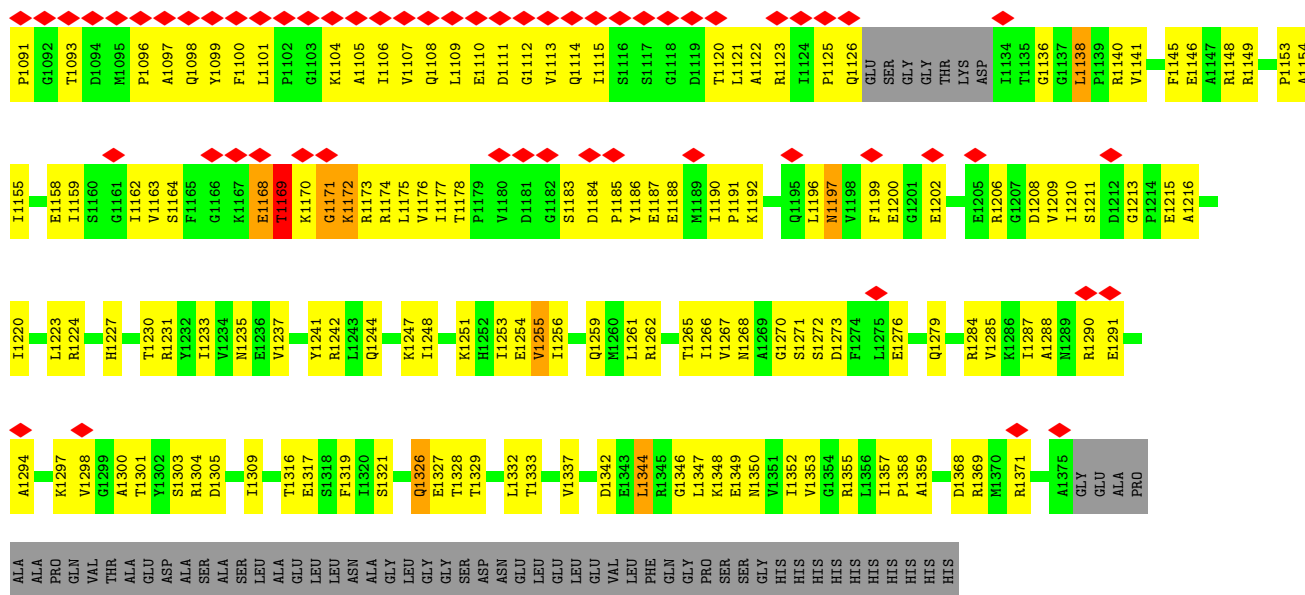




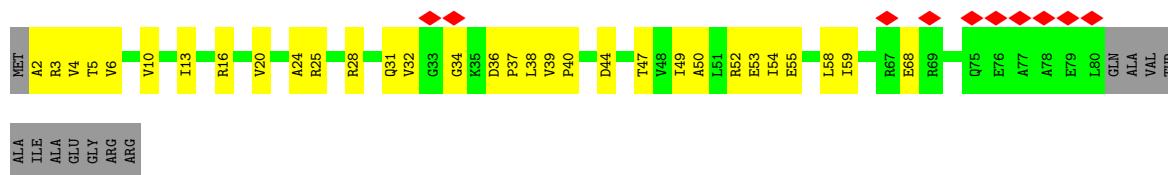
• Molecule 3: DNA-directed RNA polymerase subunit beta'



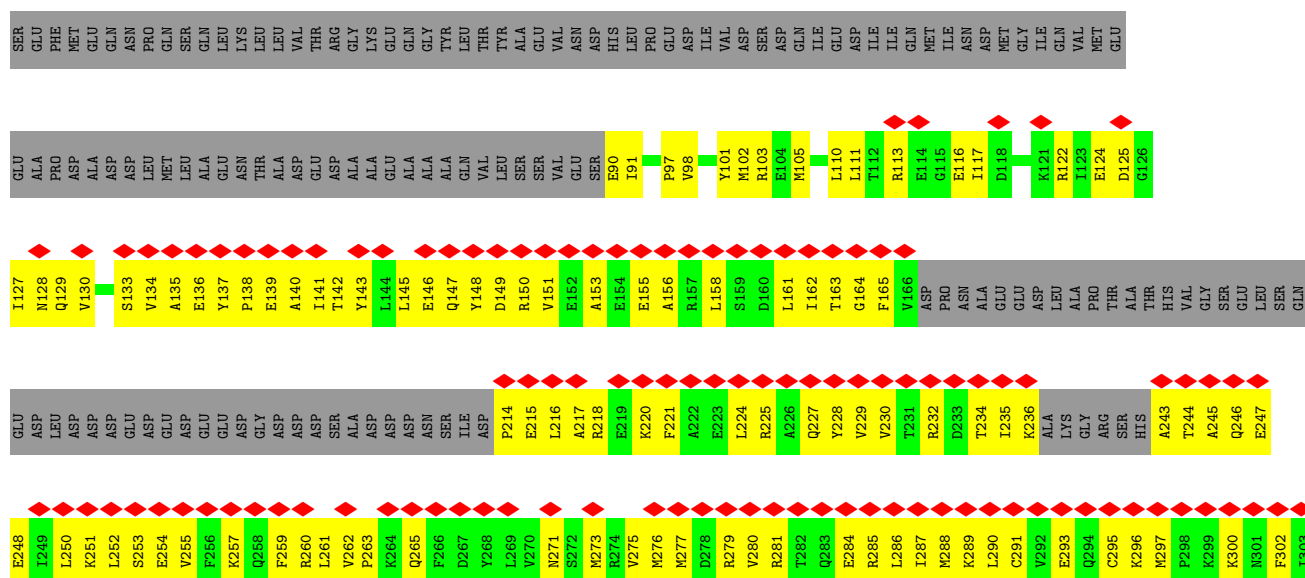


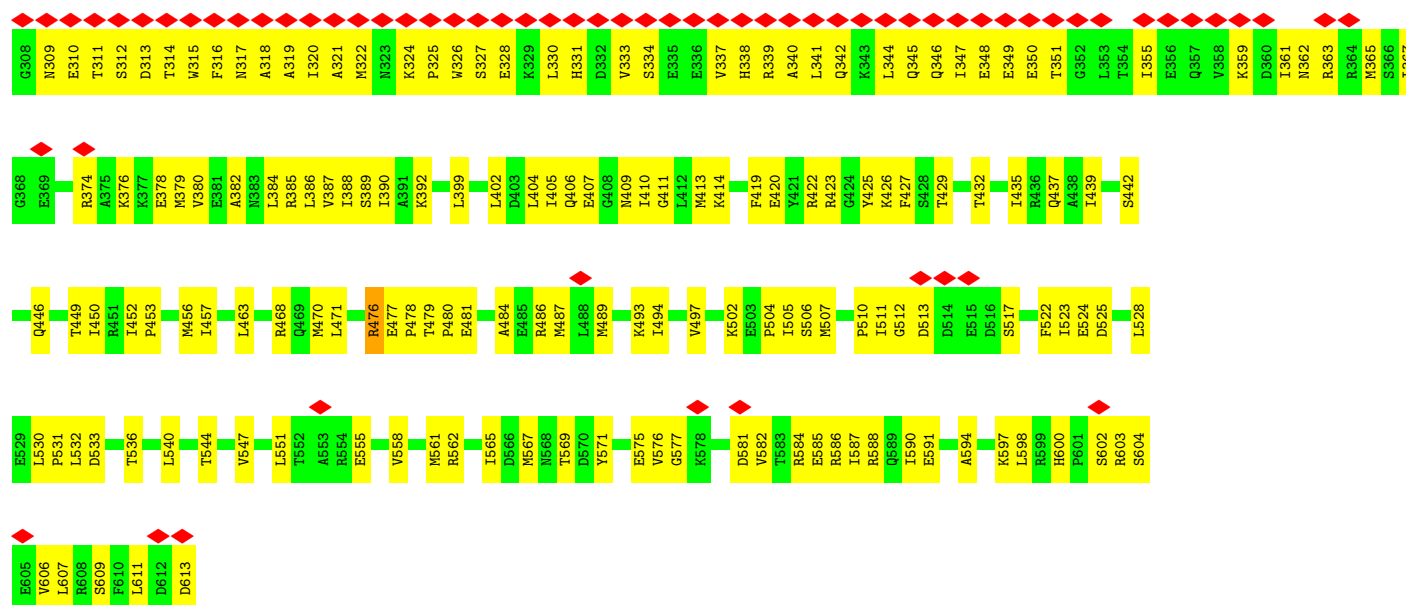


• Molecule 4: DNA-directed RNA polymerase subunit omega

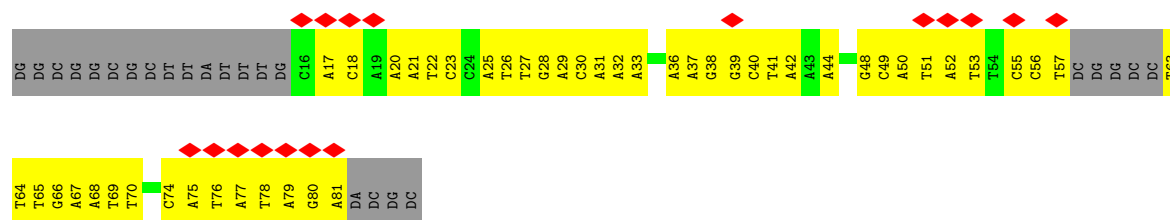
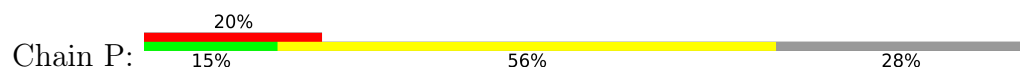


• Molecule 5: RNA polymerase sigma factor RpoD

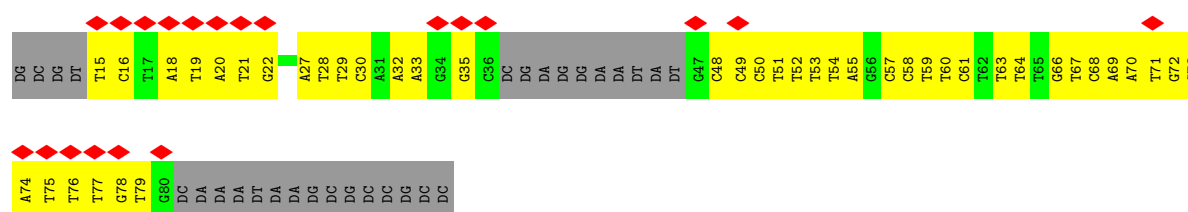
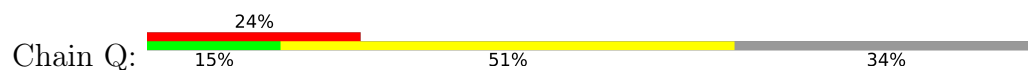




- Molecule 6: Non-template strand of rpsTP2 DNA promoter



- Molecule 7: Template strand of rpsTP2 DNA promoter



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 289670 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 1.0 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 0.251 | Depositor |
| Minimum map value | -0.158 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.007 | Depositor |
| Recommended contour level | 0.025 | Depositor |
| Map size (Å) | 332.8, 332.8, 332.8 | wwPDB |
| Map dimensions | 256, 256, 256 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.3, 1.3, 1.3 | Depositor |

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: 1N7, MG, ZN

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|----------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | G | 0.71 | 0/1807 | 0.69 | 1/2449 (0.0%) |
| 1 | H | 0.55 | 0/1700 | 0.65 | 1/2305 (0.0%) |
| 1 | R | 0.26 | 0/579 | 0.51 | 0/784 |
| 2 | I | 0.75 | 0/10744 | 0.68 | 3/14496 (0.0%) |
| 3 | J | 0.70 | 2/10543 (0.0%) | 0.69 | 3/14239 (0.0%) |
| 4 | K | 0.50 | 0/629 | 0.59 | 0/847 |
| 5 | L | 0.42 | 0/3872 | 0.55 | 0/5204 |
| 6 | P | 0.75 | 0/1407 | 0.97 | 0/2166 |
| 7 | Q | 0.73 | 0/1276 | 0.99 | 0/1965 |
| All | All | 0.68 | 2/32557 (0.0%) | 0.70 | 8/44455 (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 | I | 0 | 1 |
| 3 | J | 0 | 10 |
| All | All | 0 | 11 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 3 | J | 1255 | VAL | CB-CG1 | -5.31 | 1.41 | 1.52 |
| 3 | J | 453 | VAL | CB-CG1 | -5.03 | 1.42 | 1.52 |

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3 | J | 1344 | LEU | CA-CB-CG | -6.66 | 99.97 | 115.30 |
| 3 | J | 903 | LEU | CA-CB-CG | 6.38 | 129.96 | 115.30 |
| 2 | I | 693 | LEU | CA-CB-CG | 5.57 | 128.10 | 115.30 |
| 3 | J | 807 | LEU | CA-CB-CG | -5.45 | 102.77 | 115.30 |
| 2 | I | 28 | LEU | CA-CB-CG | -5.36 | 102.98 | 115.30 |
| 1 | H | 28 | LEU | CA-CB-CG | 5.34 | 127.58 | 115.30 |
| 2 | I | 575 | LEU | CA-CB-CG | 5.27 | 127.41 | 115.30 |
| 1 | G | 228 | LEU | CA-CB-CG | 5.03 | 126.86 | 115.30 |

There are no chirality outliers.

All (11) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|---------|
| 2 | I | 1185 | PRO | Peptide |
| 3 | J | 1138 | LEU | Peptide |
| 3 | J | 1168 | GLU | Peptide |
| 3 | J | 1169 | THR | Peptide |
| 3 | J | 1171 | GLY | Peptide |
| 3 | J | 1326 | GLN | Peptide |
| 3 | J | 320 | ASN | Peptide |
| 3 | J | 416 | ILE | Peptide |
| 3 | J | 853 | THR | Peptide |
| 3 | J | 855 | ASP | Peptide |
| 3 | J | 902 | ASP | Peptide |

5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | G | 1785 | 0 | 1806 | 120 | 0 |
| 1 | H | 1681 | 0 | 1708 | 148 | 0 |
| 1 | R | 572 | 0 | 602 | 84 | 0 |
| 2 | I | 10575 | 0 | 10584 | 682 | 0 |
| 3 | J | 10386 | 0 | 10594 | 791 | 0 |
| 4 | K | 627 | 0 | 634 | 39 | 0 |
| 5 | L | 3821 | 0 | 3891 | 312 | 0 |
| 6 | P | 1253 | 0 | 689 | 72 | 0 |
| 7 | Q | 1143 | 0 | 640 | 50 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 8 | I | 27 | 39 | 37 | 6 | 0 |
| 8 | J | 27 | 39 | 37 | 4 | 0 |
| 8 | L | 27 | 39 | 38 | 4 | 0 |
| 9 | J | 1 | 0 | 0 | 0 | 0 |
| 10 | J | 2 | 0 | 0 | 0 | 0 |
| All | All | 31927 | 117 | 31260 | 2115 | 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 33.

All (2115) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:I:1401:1N7:C3 | 8:I:1401:1N7:C19 | 1.83 | 1.55 |
| 8:J:1504:1N7:C19 | 8:J:1504:1N7:C3 | 1.84 | 1.54 |
| 8:L:701:1N7:C19 | 8:L:701:1N7:C3 | 1.84 | 1.52 |
| 1:H:105:SER:HA | 1:H:138:ALA:HB2 | 1.42 | 1.01 |
| 2:I:75:LEU:HD11 | 2:I:127:ILE:HD11 | 1.43 | 1.00 |
| 5:L:98:VAL:HG22 | 5:L:402:LEU:HD11 | 1.46 | 0.98 |
| 3:J:1081:VAL:HG12 | 3:J:1087:ASP:HA | 1.43 | 0.97 |
| 2:I:1212:LEU:HD22 | 2:I:1225:VAL:HG21 | 1.48 | 0.96 |
| 1:H:74:VAL:HG12 | 1:H:76:GLU:H | 1.30 | 0.96 |
| 5:L:262:VAL:HB | 5:L:265:GLN:HG2 | 1.48 | 0.95 |
| 5:L:135:ALA:HB1 | 5:L:253:SER:HB3 | 1.48 | 0.95 |
| 3:J:155:GLU:HB2 | 3:J:158:GLN:HB2 | 1.48 | 0.94 |
| 2:I:718:ALA:HB2 | 2:I:783:LEU:HD21 | 1.48 | 0.94 |
| 2:I:1120:ALA:HB1 | 2:I:1198:LEU:HD12 | 1.50 | 0.94 |
| 1:H:103:ASN:HB3 | 1:H:141:SER:HA | 1.49 | 0.92 |
| 3:J:518:VAL:HG11 | 3:J:707:ILE:HD13 | 1.47 | 0.92 |
| 2:I:1136:GLN:HE21 | 2:I:1140:LYS:HD3 | 1.34 | 0.91 |
| 3:J:1090:ILE:HD11 | 3:J:1097:ALA:HB2 | 1.53 | 0.91 |
| 3:J:271:ARG:HH11 | 3:J:316:ILE:HD12 | 1.35 | 0.90 |
| 3:J:960:LEU:HD23 | 3:J:963:VAL:HG21 | 1.51 | 0.90 |
| 3:J:1079:LYS:HD3 | 3:J:1098:GLN:HB3 | 1.50 | 0.90 |
| 1:R:300:LEU:HA | 1:R:303:ILE:HD12 | 1.50 | 0.90 |
| 3:J:559:ALA:HB3 | 3:J:562:GLU:HB2 | 1.51 | 0.90 |
| 3:J:797:THR:HG22 | 3:J:924:GLY:HA3 | 1.54 | 0.90 |
| 2:I:870:ILE:HG21 | 2:I:931:VAL:HG11 | 1.55 | 0.89 |
| 3:J:547:ARG:HA | 3:J:573:THR:HG22 | 1.52 | 0.89 |
| 5:L:290:LEU:HB3 | 5:L:333:VAL:HG21 | 1.55 | 0.89 |
| 3:J:1060:VAL:HG22 | 3:J:1106:ILE:HG12 | 1.52 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:R:287:VAL:HG12 | 1:R:291:LYS:HE3 | 1.53 | 0.88 |
| 5:L:309:ASN:HD21 | 5:L:312:SER:HB3 | 1.39 | 0.88 |
| 3:J:311:ARG:HH22 | 3:J:1329:THR:HG21 | 1.38 | 0.88 |
| 1:H:44:ARG:HB2 | 1:H:183:ILE:HD13 | 1.55 | 0.87 |
| 2:I:1279:GLU:HG2 | 3:J:1357:ILE:HD13 | 1.57 | 0.87 |
| 5:L:151:VAL:HG22 | 5:L:156:ALA:HB3 | 1.56 | 0.87 |
| 3:J:1272:SER:HB3 | 3:J:1273:ASP:HB3 | 1.56 | 0.86 |
| 2:I:806:PRO:HD3 | 2:I:1100:PRO:HG2 | 1.57 | 0.86 |
| 2:I:748:ILE:HD11 | 2:I:966:ILE:HG12 | 1.58 | 0.86 |
| 2:I:1151:LEU:HD22 | 2:I:1198:LEU:HD23 | 1.56 | 0.86 |
| 1:R:283:GLN:HE21 | 1:R:318:LEU:HD22 | 1.41 | 0.86 |
| 2:I:1111:GLN:HB2 | 2:I:1230:MET:HE1 | 1.58 | 0.86 |
| 3:J:527:LEU:HB2 | 3:J:550:VAL:HG12 | 1.58 | 0.86 |
| 2:I:251:ALA:HB2 | 2:I:269:ILE:HD11 | 1.57 | 0.85 |
| 3:J:1104:LYS:HD2 | 3:J:1125:PRO:HG2 | 1.55 | 0.85 |
| 2:I:519:ASN:HD21 | 2:I:796:LEU:HG | 1.41 | 0.85 |
| 5:L:318:ALA:HA | 5:L:321:ALA:HB3 | 1.57 | 0.84 |
| 2:I:452:ARG:NH1 | 2:I:584:TYR:O | 2.10 | 0.84 |
| 3:J:520:ALA:HB3 | 3:J:546:ALA:HB2 | 1.58 | 0.84 |
| 1:R:283:GLN:HG2 | 1:R:318:LEU:HD13 | 1.58 | 0.84 |
| 3:J:974:VAL:HG12 | 3:J:1002:VAL:HG22 | 1.60 | 0.84 |
| 3:J:514:THR:HG21 | 3:J:596:LEU:HB2 | 1.58 | 0.83 |
| 5:L:218:ARG:HA | 5:L:221:PHE:HD2 | 1.43 | 0.83 |
| 1:G:16:ILE:HD13 | 1:G:214:GLU:HB2 | 1.60 | 0.83 |
| 5:L:313:ASP:HA | 5:L:316:PHE:HB3 | 1.61 | 0.83 |
| 4:K:2:ALA:HB1 | 4:K:3:ARG:HB2 | 1.60 | 0.82 |
| 3:J:1061:VAL:HG11 | 3:J:1101:LEU:HB2 | 1.60 | 0.82 |
| 5:L:588:ARG:HD3 | 7:Q:67:DT:H73 | 1.62 | 0.82 |
| 2:I:600:THR:HG22 | 2:I:602:GLU:H | 1.43 | 0.81 |
| 5:L:148:TYR:OH | 5:L:218:ARG:HG2 | 1.80 | 0.81 |
| 1:R:260:LEU:HD21 | 1:R:278:ILE:HG12 | 1.63 | 0.81 |
| 3:J:741:ALA:O | 3:J:762:ASN:ND2 | 2.12 | 0.81 |
| 5:L:215:GLU:HG2 | 5:L:218:ARG:HH21 | 1.44 | 0.81 |
| 3:J:475:GLU:HG3 | 4:K:24:ALA:HB1 | 1.63 | 0.81 |
| 2:I:980:VAL:HG22 | 2:I:984:VAL:HG23 | 1.62 | 0.80 |
| 1:R:250:ASP:HB3 | 1:R:253:LEU:HB2 | 1.64 | 0.80 |
| 3:J:56:LEU:HD11 | 3:J:273:ILE:HD12 | 1.64 | 0.80 |
| 3:J:984:LEU:HB3 | 3:J:993:GLU:HB2 | 1.64 | 0.80 |
| 1:H:112:ALA:HB3 | 1:H:126:PRO:HA | 1.63 | 0.79 |
| 3:J:1173:ARG:HE | 3:J:1192:LYS:HA | 1.47 | 0.79 |
| 1:G:70:THR:HG21 | 2:I:755:LYS:HE2 | 1.64 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:950:ILE:HB | 3:J:1018:ALA:HB3 | 1.64 | 0.79 |
| 2:I:103:VAL:HG12 | 2:I:117:ILE:HG22 | 1.64 | 0.79 |
| 3:J:202:ARG:NH2 | 3:J:225:GLU:OE2 | 2.14 | 0.79 |
| 2:I:528:ARG:NH2 | 2:I:576:SER:O | 2.16 | 0.79 |
| 1:G:182:ARG:NH1 | 2:I:1090:ASN:O | 2.14 | 0.79 |
| 3:J:1075:ARG:HH21 | 3:J:1168:GLU:HG2 | 1.46 | 0.79 |
| 3:J:1078:LEU:HD11 | 3:J:1101:LEU:HD11 | 1.62 | 0.79 |
| 3:J:1046:ILE:HD12 | 3:J:1059:LEU:HD13 | 1.65 | 0.79 |
| 2:I:617:ALA:HB3 | 2:I:653:MET:HA | 1.63 | 0.78 |
| 2:I:400:VAL:HG22 | 2:I:584:TYR:HB3 | 1.64 | 0.78 |
| 3:J:833:GLU:OE1 | 3:J:1242:ARG:NH2 | 2.17 | 0.78 |
| 2:I:1210:ILE:HD12 | 2:I:1227:VAL:HG21 | 1.65 | 0.78 |
| 3:J:128:LEU:HA | 3:J:192:MET:HE1 | 1.66 | 0.78 |
| 2:I:1280:ALA:HB1 | 3:J:918:ILE:HG22 | 1.64 | 0.78 |
| 3:J:322:ARG:HG3 | 3:J:323:PRO:HD2 | 1.64 | 0.78 |
| 2:I:887:VAL:HG22 | 2:I:913:VAL:HG22 | 1.64 | 0.77 |
| 1:R:269:CYS:HB3 | 1:R:295:LEU:HD12 | 1.64 | 0.77 |
| 3:J:576:ARG:HD3 | 3:J:593:ASN:HA | 1.65 | 0.77 |
| 3:J:1344:LEU:HD22 | 3:J:1349:GLU:HB3 | 1.67 | 0.77 |
| 3:J:201:LEU:HD11 | 3:J:220:ARG:HH11 | 1.49 | 0.77 |
| 2:I:590:PRO:HB2 | 2:I:655:VAL:HG21 | 1.67 | 0.77 |
| 1:G:211:ILE:HG21 | 1:G:216:ALA:HB2 | 1.66 | 0.77 |
| 7:Q:60:DT:H1' | 7:Q:61:DC:H5' | 1.66 | 0.77 |
| 2:I:39:ILE:HD11 | 2:I:75:LEU:HG | 1.66 | 0.77 |
| 5:L:392:LYS:HD3 | 6:P:56:DC:H5'' | 1.65 | 0.77 |
| 2:I:257:ALA:HB3 | 2:I:262:TYR:HE2 | 1.48 | 0.76 |
| 5:L:585:GLU:OE2 | 5:L:588:ARG:NH2 | 2.16 | 0.76 |
| 3:J:91:GLU:OE1 | 3:J:101:ARG:NH2 | 2.18 | 0.76 |
| 1:H:214:GLU:HG2 | 1:H:218:ARG:HH12 | 1.49 | 0.76 |
| 3:J:789:LYS:NZ | 3:J:931:THR:O | 2.18 | 0.76 |
| 1:G:110:VAL:HG21 | 1:G:133:LEU:HD23 | 1.67 | 0.76 |
| 3:J:401:VAL:HA | 3:J:408:VAL:HG11 | 1.68 | 0.76 |
| 3:J:518:VAL:HG11 | 3:J:707:ILE:CD1 | 2.16 | 0.76 |
| 3:J:1081:VAL:HA | 3:J:1088:VAL:HG23 | 1.66 | 0.76 |
| 5:L:277:MET:SD | 5:L:362:ASN:ND2 | 2.58 | 0.76 |
| 2:I:883:LEU:HD11 | 2:I:920:VAL:HG22 | 1.68 | 0.75 |
| 3:J:1220:ILE:HD12 | 3:J:1224:ARG:HH21 | 1.51 | 0.75 |
| 3:J:1268:ASN:OD1 | 3:J:1301:THR:OG1 | 2.01 | 0.75 |
| 5:L:402:LEU:HA | 5:L:405:ILE:HG12 | 1.66 | 0.75 |
| 5:L:456:MET:HE1 | 5:L:497:VAL:HG22 | 1.68 | 0.75 |
| 2:I:238:GLN:HG2 | 2:I:286:GLU:HG2 | 1.67 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:I:980:VAL:HA | 2:I:984:VAL:HB | 1.68 | 0.75 |
| 2:I:1006:GLU:HA | 2:I:1009:ASN:HB3 | 1.69 | 0.75 |
| 3:J:799:ARG:NH1 | 3:J:1146:GLU:OE2 | 2.20 | 0.75 |
| 3:J:807:LEU:HD11 | 3:J:894:VAL:HG23 | 1.67 | 0.75 |
| 3:J:1199:PHE:HB2 | 3:J:1202:GLU:HG2 | 1.67 | 0.75 |
| 3:J:363:LEU:HD21 | 3:J:618:VAL:HG13 | 1.68 | 0.75 |
| 5:L:429:THR:HA | 6:P:53:DT:H72 | 1.67 | 0.75 |
| 1:H:107:ILE:HG12 | 1:H:135:ASP:HA | 1.67 | 0.75 |
| 3:J:510:LEU:O | 3:J:514:THR:HG22 | 1.86 | 0.75 |
| 3:J:857:LEU:HG | 3:J:858:VAL:H | 1.51 | 0.75 |
| 1:H:190:ALA:HB2 | 1:H:200:LYS:HB2 | 1.69 | 0.75 |
| 1:R:270:LEU:O | 1:R:274:ALA:N | 2.17 | 0.75 |
| 1:H:206:GLU:OE1 | 3:J:531:LYS:NZ | 2.20 | 0.74 |
| 2:I:742:TYR:HB3 | 2:I:743:PRO:HD2 | 1.67 | 0.74 |
| 3:J:1042:ASP:HA | 3:J:1046:ILE:HG13 | 1.66 | 0.74 |
| 1:G:83:LEU:HD21 | 2:I:693:LEU:HD21 | 1.68 | 0.74 |
| 2:I:44:GLU:HG3 | 2:I:46:GLN:HG2 | 1.69 | 0.74 |
| 3:J:141:PHE:HE2 | 3:J:296:LYS:HB2 | 1.51 | 0.74 |
| 3:J:429:LEU:HB3 | 3:J:925:GLU:HB2 | 1.67 | 0.74 |
| 3:J:982:LEU:HB2 | 3:J:997:VAL:HG23 | 1.67 | 0.74 |
| 6:P:63:DT:H4' | 6:P:64:DT:H5' | 1.68 | 0.74 |
| 3:J:902:ASP:HA | 3:J:903:LEU:HG | 1.69 | 0.74 |
| 3:J:255:LEU:HD23 | 3:J:261:ALA:HB2 | 1.68 | 0.74 |
| 1:G:51:MET:HE1 | 1:G:216:ALA:HA | 1.70 | 0.74 |
| 5:L:407:GLU:OE2 | 5:L:446:GLN:NE2 | 2.21 | 0.74 |
| 1:H:196:THR:HG21 | 3:J:443:GLU:HG2 | 1.70 | 0.73 |
| 5:L:387:VAL:HG22 | 5:L:435:ILE:HD13 | 1.70 | 0.73 |
| 1:G:90:VAL:HG11 | 1:G:146:VAL:HG11 | 1.70 | 0.73 |
| 1:H:22:THR:OG1 | 1:H:207:THR:O | 2.06 | 0.73 |
| 3:J:859:PRO:HD2 | 3:J:862:THR:HG21 | 1.70 | 0.73 |
| 1:R:250:ASP:OD2 | 1:R:253:LEU:N | 2.16 | 0.73 |
| 2:I:471:VAL:HG21 | 2:I:493:ILE:HG13 | 1.71 | 0.73 |
| 3:J:1041:ILE:N | 3:J:1045:THR:OG1 | 2.22 | 0.73 |
| 2:I:972:PHE:HA | 2:I:975:ILE:HD12 | 1.69 | 0.73 |
| 3:J:279:LEU:HD12 | 3:J:295:GLU:HG3 | 1.70 | 0.73 |
| 1:H:13:LEU:HA | 1:H:28:LEU:HD23 | 1.70 | 0.72 |
| 5:L:147:GLN:HB3 | 5:L:161:LEU:HD11 | 1.70 | 0.72 |
| 2:I:11:ILE:O | 2:I:1149:TYR:OH | 2.06 | 0.72 |
| 2:I:1131:MET:HE2 | 2:I:1141:LEU:HA | 1.71 | 0.72 |
| 2:I:6:THR:OG1 | 2:I:781:ASP:OD1 | 2.02 | 0.72 |
| 2:I:817:LEU:HD11 | 2:I:1080:ASN:HD22 | 1.52 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:1117:LEU:HD12 | 2:I:1195:ILE:HG12 | 1.71 | 0.72 |
| 2:I:302:ILE:HG22 | 2:I:309:LEU:HA | 1.69 | 0.72 |
| 2:I:758:ARG:NH2 | 2:I:762:ASN:OD1 | 2.20 | 0.72 |
| 2:I:953:LEU:HD11 | 2:I:1033:ARG:HG2 | 1.71 | 0.72 |
| 3:J:1061:VAL:HG21 | 3:J:1101:LEU:HD12 | 1.71 | 0.72 |
| 2:I:12:ARG:NH2 | 2:I:793:GLU:OE1 | 2.23 | 0.72 |
| 3:J:958:ILE:HD13 | 3:J:984:LEU:HD13 | 1.71 | 0.72 |
| 2:I:303:ASP:HB2 | 2:I:310:ILE:HD11 | 1.72 | 0.72 |
| 2:I:689:ALA:CB | 2:I:1233:LEU:HD12 | 2.21 | 0.71 |
| 3:J:1326:GLN:HE21 | 7:Q:32:DA:H5'' | 1.56 | 0.71 |
| 5:L:320:ILE:HG23 | 5:L:327:SER:HB3 | 1.72 | 0.71 |
| 1:H:35:PHE:HA | 1:H:38:THR:HG22 | 1.72 | 0.71 |
| 3:J:902:ASP:HA | 3:J:903:LEU:CG | 2.20 | 0.71 |
| 3:J:844:THR:OG1 | 3:J:860:ARG:O | 2.08 | 0.71 |
| 5:L:163:THR:O | 5:L:260:ARG:NE | 2.23 | 0.71 |
| 7:Q:77:DT:H3' | 1:R:296:GLY:HA3 | 1.72 | 0.71 |
| 1:G:38:THR:OG1 | 1:H:45:ARG:NH1 | 2.23 | 0.71 |
| 2:I:617:ALA:N | 2:I:652:TYR:O | 2.22 | 0.71 |
| 4:K:25:ARG:NH2 | 4:K:68:GLU:OE1 | 2.23 | 0.71 |
| 2:I:22:LEU:HD13 | 2:I:603:ILE:HD13 | 1.73 | 0.71 |
| 3:J:665:GLN:OE1 | 3:J:678:ARG:NH2 | 2.21 | 0.71 |
| 5:L:533:ASP:HA | 5:L:536:THR:HG22 | 1.71 | 0.71 |
| 1:G:135:ASP:HB3 | 1:G:138:ALA:HB3 | 1.73 | 0.71 |
| 3:J:680:ASN:HA | 3:J:683:ILE:HG22 | 1.73 | 0.70 |
| 3:J:1107:VAL:HG22 | 3:J:1122:ALA:HB2 | 1.73 | 0.70 |
| 2:I:254:ASP:OD1 | 2:I:265:LYS:N | 2.24 | 0.70 |
| 2:I:594:VAL:HG22 | 2:I:599:VAL:HG22 | 1.72 | 0.70 |
| 3:J:1031:VAL:HG12 | 3:J:1091:PRO:HD3 | 1.73 | 0.70 |
| 3:J:1109:LEU:HD23 | 3:J:1113:VAL:HG12 | 1.74 | 0.70 |
| 2:I:1254:VAL:O | 3:J:99:ARG:NH2 | 2.23 | 0.70 |
| 3:J:822:MET:HE3 | 3:J:838:ARG:HB3 | 1.72 | 0.70 |
| 5:L:151:VAL:HG21 | 5:L:161:LEU:HB2 | 1.74 | 0.70 |
| 2:I:560:PRO:O | 3:J:780:ARG:NH2 | 2.25 | 0.70 |
| 2:I:975:ILE:HG12 | 2:I:1014:LEU:HG | 1.75 | 0.69 |
| 3:J:141:PHE:HA | 3:J:180:MET:HE2 | 1.73 | 0.69 |
| 3:J:977:SER:OG | 3:J:980:THR:OG1 | 2.09 | 0.69 |
| 3:J:1062:LEU:O | 3:J:1067:ARG:NH2 | 2.25 | 0.69 |
| 3:J:1174:ARG:NH2 | 3:J:1187:GLU:OE1 | 2.25 | 0.69 |
| 3:J:930:LEU:HD11 | 3:J:1241:TYR:CE1 | 2.27 | 0.69 |
| 2:I:1103:VAL:HG22 | 2:I:1111:GLN:HE21 | 1.57 | 0.69 |
| 2:I:1219:GLU:OE2 | 3:J:538:ARG:NH1 | 2.26 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:218:THR:HA | 3:J:221:ILE:HG22 | 1.75 | 0.69 |
| 1:G:23:HIS:HB2 | 1:G:205:MET:O | 1.92 | 0.69 |
| 3:J:951:GLN:OE1 | 3:J:1016:THR:OG1 | 2.10 | 0.69 |
| 3:J:963:VAL:HG23 | 3:J:975:ILE:HG12 | 1.75 | 0.69 |
| 3:J:1206:ARG:HH21 | 3:J:1223:LEU:HD13 | 1.56 | 0.69 |
| 2:I:1122:LYS:HG2 | 2:I:1229:TYR:CZ | 2.28 | 0.69 |
| 1:R:273:GLU:OE1 | 1:R:284:ARG:NH1 | 2.26 | 0.69 |
| 1:H:105:SER:HA | 1:H:138:ALA:CB | 2.21 | 0.69 |
| 2:I:657:THR:HG21 | 2:I:1188:ASP:HB2 | 1.73 | 0.69 |
| 3:J:872:LEU:HD23 | 3:J:877:VAL:HG21 | 1.75 | 0.69 |
| 5:L:598:LEU:O | 5:L:604:SER:OG | 2.05 | 0.69 |
| 3:J:270:ARG:NH1 | 5:L:449:THR:OG1 | 2.25 | 0.69 |
| 2:I:176:ILE:HD11 | 2:I:428:VAL:HG21 | 1.74 | 0.69 |
| 3:J:318:GLY:N | 3:J:322:ARG:O | 2.16 | 0.69 |
| 3:J:1038:THR:OG1 | 3:J:1077:ALA:O | 2.11 | 0.69 |
| 3:J:1072:LYS:O | 3:J:1075:ARG:NH1 | 2.24 | 0.69 |
| 7:Q:19:DT:H3' | 7:Q:19:DT:OP2 | 1.93 | 0.69 |
| 2:I:214:ASN:HB3 | 2:I:359:ARG:HD2 | 1.75 | 0.68 |
| 5:L:137:TYR:CE2 | 5:L:139:GLU:HB2 | 2.27 | 0.68 |
| 1:R:255:ARG:HB3 | 1:R:278:ILE:HD12 | 1.75 | 0.68 |
| 2:I:60:GLN:O | 2:I:476:LYS:NZ | 2.25 | 0.68 |
| 3:J:385:LEU:HD21 | 3:J:411:ILE:HG13 | 1.75 | 0.68 |
| 1:G:90:VAL:HG23 | 1:G:123:ILE:HD13 | 1.74 | 0.68 |
| 3:J:255:LEU:HD11 | 3:J:259:ARG:HB2 | 1.74 | 0.68 |
| 3:J:1108:GLN:HG3 | 3:J:1109:LEU:HD12 | 1.75 | 0.68 |
| 2:I:714:VAL:HB | 2:I:787:PRO:HD2 | 1.73 | 0.68 |
| 2:I:1116:HIS:HE1 | 3:J:641:ILE:H | 1.41 | 0.68 |
| 2:I:453:ILE:HD11 | 2:I:587:LEU:HD11 | 1.73 | 0.68 |
| 3:J:930:LEU:HD11 | 3:J:1241:TYR:HE1 | 1.58 | 0.68 |
| 3:J:554:GLU:OE1 | 3:J:589:TYR:N | 2.24 | 0.68 |
| 5:L:261:LEU:HD23 | 5:L:265:GLN:HB3 | 1.76 | 0.68 |
| 6:P:39:DG:H1' | 6:P:40:DC:H5' | 1.76 | 0.68 |
| 1:H:64:VAL:HG12 | 1:H:66:HIS:H | 1.57 | 0.68 |
| 3:J:1028:ILE:HG22 | 3:J:1120:THR:HA | 1.75 | 0.68 |
| 2:I:704:MET:O | 2:I:708:VAL:HG23 | 1.93 | 0.68 |
| 3:J:490:ILE:HG13 | 3:J:491:LEU:HD12 | 1.76 | 0.68 |
| 2:I:1212:LEU:HD11 | 2:I:1227:VAL:HG11 | 1.75 | 0.67 |
| 3:J:134:ASP:OD1 | 3:J:159:ILE:HD12 | 1.93 | 0.67 |
| 3:J:1046:ILE:HB | 3:J:1059:LEU:HB3 | 1.76 | 0.67 |
| 1:G:192:VAL:HG11 | 1:G:198:LEU:HD12 | 1.76 | 0.67 |
| 3:J:807:LEU:HD23 | 3:J:1255:VAL:HG23 | 1.75 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:46:GLN:O | 2:I:51:ALA:HB2 | 1.94 | 0.67 |
| 2:I:483:ASP:HB2 | 2:I:486:THR:HG22 | 1.76 | 0.67 |
| 2:I:131:THR:HG22 | 2:I:132:ASP:H | 1.60 | 0.67 |
| 3:J:914:ALA:HB2 | 3:J:1359:ALA:HB1 | 1.76 | 0.67 |
| 4:K:3:ARG:NH2 | 4:K:55:GLU:OE1 | 2.22 | 0.67 |
| 2:I:5:TYR:OH | 2:I:1171:ARG:NH1 | 2.23 | 0.67 |
| 2:I:1314:GLN:HG2 | 4:K:28:ARG:NH2 | 2.08 | 0.67 |
| 5:L:407:GLU:OE1 | 5:L:442:SER:OG | 2.08 | 0.67 |
| 3:J:514:THR:CG2 | 3:J:596:LEU:HB2 | 2.25 | 0.67 |
| 3:J:1233:ILE:O | 3:J:1237:VAL:HG12 | 1.95 | 0.67 |
| 3:J:801:VAL:HG12 | 3:J:920:ALA:HB3 | 1.77 | 0.67 |
| 3:J:1175:LEU:HD22 | 3:J:1190:ILE:HD11 | 1.76 | 0.67 |
| 3:J:962:ASN:O | 3:J:980:THR:OG1 | 2.13 | 0.67 |
| 5:L:456:MET:CE | 5:L:497:VAL:HG22 | 2.24 | 0.67 |
| 2:I:877:VAL:HG21 | 2:I:920:VAL:HG21 | 1.77 | 0.66 |
| 5:L:162:ILE:HD13 | 5:L:221:PHE:HZ | 1.60 | 0.66 |
| 2:I:975:ILE:HG23 | 2:I:1014:LEU:HD21 | 1.77 | 0.66 |
| 5:L:287:ILE:HD13 | 5:L:341:LEU:HD12 | 1.77 | 0.66 |
| 2:I:810:TYR:O | 2:I:1077:SER:OG | 2.12 | 0.66 |
| 2:I:838:CYS:HB2 | 2:I:918:LEU:HD22 | 1.78 | 0.66 |
| 2:I:902:LEU:HD21 | 5:L:611:LEU:HD21 | 1.76 | 0.66 |
| 3:J:759:ILE:HG23 | 3:J:771:GLN:HB3 | 1.77 | 0.66 |
| 5:L:98:VAL:O | 5:L:102:MET:HG2 | 1.95 | 0.66 |
| 2:I:207:THR:OG1 | 2:I:354:ASP:OD2 | 2.12 | 0.66 |
| 3:J:1031:VAL:CG1 | 3:J:1090:ILE:HA | 2.25 | 0.66 |
| 3:J:1044:GLN:HG2 | 3:J:1068:THR:OG1 | 1.95 | 0.66 |
| 2:I:30:ILE:HD12 | 2:I:30:ILE:H | 1.60 | 0.66 |
| 2:I:565:GLU:HA | 2:I:569:ILE:HG12 | 1.78 | 0.66 |
| 3:J:79:LYS:HG2 | 5:L:569:THR:HG22 | 1.77 | 0.66 |
| 5:L:309:ASN:ND2 | 5:L:312:SER:HB3 | 2.10 | 0.66 |
| 2:I:484:LEU:HD12 | 2:I:485:ASP:HB2 | 1.77 | 0.66 |
| 3:J:822:MET:CE | 3:J:838:ARG:HB3 | 2.26 | 0.66 |
| 2:I:840:SER:HB2 | 2:I:850:ILE:HD11 | 1.78 | 0.66 |
| 3:J:1199:PHE:HB2 | 3:J:1202:GLU:CG | 2.26 | 0.66 |
| 3:J:1348:LYS:O | 3:J:1352:ILE:HG12 | 1.95 | 0.66 |
| 1:G:218:ARG:NH2 | 1:H:233:ASP:OD1 | 2.28 | 0.66 |
| 2:I:590:PRO:HG3 | 2:I:605:TYR:CE1 | 2.31 | 0.66 |
| 3:J:141:PHE:CE1 | 3:J:181:GLY:HA3 | 2.31 | 0.66 |
| 3:J:515:ARG:HG2 | 3:J:516:ASP:H | 1.61 | 0.66 |
| 4:K:38:LEU:HD22 | 4:K:58:LEU:HD13 | 1.76 | 0.66 |
| 5:L:420:GLU:HG3 | 5:L:422:ARG:HH21 | 1.61 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:I:744:GLY:O | 2:I:745:GLU:HG3 | 1.95 | 0.65 |
| 2:I:983:GLY:HA3 | 2:I:1002:LEU:HD11 | 1.78 | 0.65 |
| 3:J:357:VAL:HG22 | 3:J:461:PHE:CD2 | 2.31 | 0.65 |
| 3:J:650:LYS:HE3 | 3:J:654:ILE:HD11 | 1.77 | 0.65 |
| 5:L:227:GLN:HA | 5:L:230:VAL:HG12 | 1.78 | 0.65 |
| 5:L:289:LYS:HA | 5:L:293:GLU:OE1 | 1.95 | 0.65 |
| 2:I:324:LYS:O | 2:I:327:GLN:NE2 | 2.23 | 0.65 |
| 3:J:384:LYS:HE3 | 3:J:415:VAL:HG12 | 1.78 | 0.65 |
| 2:I:269:ILE:HG23 | 2:I:273:HIS:HB2 | 1.77 | 0.65 |
| 3:J:510:LEU:HD22 | 3:J:601:ILE:HD11 | 1.78 | 0.65 |
| 3:J:516:ASP:HA | 3:J:545:HIS:HB2 | 1.79 | 0.65 |
| 5:L:470:MET:SD | 5:L:486:ARG:NH1 | 2.70 | 0.65 |
| 2:I:13:LYS:HB2 | 2:I:1180:MET:CE | 2.27 | 0.65 |
| 2:I:1283:ALA:HB1 | 2:I:1286:THR:HB | 1.77 | 0.65 |
| 1:R:257:VAL:HG12 | 1:R:260:LEU:HD11 | 1.78 | 0.65 |
| 2:I:794:LEU:HG | 2:I:796:LEU:HD13 | 1.79 | 0.65 |
| 3:J:966:VAL:O | 3:J:974:VAL:HG22 | 1.97 | 0.65 |
| 7:Q:27:DA:H2'' | 7:Q:28:DT:H5' | 1.77 | 0.65 |
| 2:I:975:ILE:CG2 | 2:I:1014:LEU:HD21 | 2.27 | 0.65 |
| 1:R:297:LYS:O | 1:R:301:THR:OG1 | 2.07 | 0.65 |
| 1:G:110:VAL:CG2 | 1:G:133:LEU:HD23 | 2.27 | 0.65 |
| 2:I:559:CYS:HB2 | 2:I:662:SER:HB3 | 1.78 | 0.64 |
| 3:J:264:ASP:OD1 | 5:L:506:SER:OG | 2.14 | 0.64 |
| 2:I:9:LYS:NZ | 2:I:775:GLU:OE2 | 2.26 | 0.64 |
| 3:J:156:ARG:NH2 | 3:J:191:SER:OG | 2.27 | 0.64 |
| 3:J:430:HIS:HB3 | 3:J:925:GLU:HG2 | 1.78 | 0.64 |
| 3:J:863:LEU:HD22 | 3:J:908:ILE:HG23 | 1.79 | 0.64 |
| 3:J:1057:SER:OG | 3:J:1110:GLU:OE2 | 2.08 | 0.64 |
| 5:L:113:ARG:O | 5:L:117:ILE:HG12 | 1.97 | 0.64 |
| 2:I:796:LEU:HB3 | 2:I:1233:LEU:CD1 | 2.27 | 0.64 |
| 3:J:527:LEU:HD13 | 3:J:548:VAL:CG1 | 2.27 | 0.64 |
| 3:J:1022:PRO:O | 3:J:1126:GLN:NE2 | 2.30 | 0.64 |
| 3:J:661:VAL:HG12 | 3:J:685:ILE:HG21 | 1.80 | 0.64 |
| 4:K:36:ASP:OD1 | 4:K:37:PRO:HD2 | 1.97 | 0.64 |
| 3:J:511:TYR:OH | 3:J:515:ARG:NH1 | 2.31 | 0.64 |
| 3:J:697:MET:CE | 3:J:741:ALA:HB3 | 2.28 | 0.64 |
| 1:G:135:ASP:HB3 | 1:G:138:ALA:CB | 2.28 | 0.64 |
| 3:J:214:ARG:NH2 | 3:J:1276:GLU:OE2 | 2.31 | 0.64 |
| 3:J:385:LEU:CD2 | 3:J:411:ILE:HG13 | 2.28 | 0.64 |
| 3:J:520:ALA:HB3 | 3:J:546:ALA:CB | 2.28 | 0.64 |
| 3:J:654:ILE:HG12 | 3:J:743:MET:HE1 | 1.79 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:J:1267:VAL:O | 3:J:1276:GLU:HB2 | 1.98 | 0.64 |
| 5:L:512:GLY:HA3 | 5:L:513:ASP:CG | 2.18 | 0.64 |
| 2:I:518:ASN:O | 2:I:691:PRO:HD3 | 1.98 | 0.64 |
| 2:I:673:HIS:HB3 | 2:I:1109:ILE:CG2 | 2.28 | 0.64 |
| 3:J:848:VAL:O | 3:J:857:LEU:HB3 | 1.97 | 0.64 |
| 5:L:234:THR:OG1 | 5:L:248:GLU:OE1 | 2.07 | 0.64 |
| 5:L:248:GLU:HA | 5:L:251:LYS:HZ2 | 1.61 | 0.64 |
| 5:L:463:LEU:HD23 | 5:L:487:MET:SD | 2.38 | 0.64 |
| 1:H:82:LEU:HD22 | 1:H:173:VAL:HG22 | 1.80 | 0.64 |
| 1:H:107:ILE:CG1 | 1:H:135:ASP:HA | 2.27 | 0.64 |
| 2:I:240:GLU:CG | 2:I:284:LEU:HD13 | 2.28 | 0.64 |
| 6:P:56:DC:H2' | 6:P:57:DT:H71 | 1.80 | 0.64 |
| 2:I:1130:ALA:O | 2:I:1134:GLN:NE2 | 2.30 | 0.64 |
| 1:H:69:SER:HB2 | 1:H:78:ILE:CD1 | 2.28 | 0.63 |
| 3:J:510:LEU:HD22 | 3:J:601:ILE:CD1 | 2.28 | 0.63 |
| 2:I:1223:ARG:NH2 | 3:J:721:SER:OG | 2.31 | 0.63 |
| 3:J:259:ARG:NH1 | 5:L:502:LYS:HB2 | 2.14 | 0.63 |
| 3:J:423:LEU:HB3 | 3:J:466:MET:CE | 2.29 | 0.63 |
| 6:P:27:DT:H1' | 6:P:28:DG:H5' | 1.81 | 0.63 |
| 1:G:187:VAL:HA | 1:G:200:LYS:O | 1.98 | 0.63 |
| 2:I:3:TYR:OH | 2:I:1157:GLN:OE1 | 2.17 | 0.63 |
| 2:I:149:LEU:HD12 | 2:I:452:ARG:O | 1.98 | 0.63 |
| 2:I:241:LEU:N | 2:I:283:LYS:O | 2.28 | 0.63 |
| 2:I:373:GLY:O | 5:L:103:ARG:HD3 | 1.99 | 0.63 |
| 3:J:823:THR:HG22 | 3:J:879:ALA:HB1 | 1.80 | 0.63 |
| 5:L:246:GLN:O | 5:L:250:LEU:HG | 1.98 | 0.63 |
| 2:I:930:ASP:HB3 | 2:I:1053:TYR:HD2 | 1.63 | 0.63 |
| 3:J:80:HIS:O | 3:J:83:VAL:HG12 | 1.99 | 0.63 |
| 3:J:1090:ILE:CD1 | 3:J:1097:ALA:HB2 | 2.28 | 0.63 |
| 5:L:314:THR:O | 5:L:318:ALA:HB3 | 1.98 | 0.63 |
| 1:H:69:SER:HB2 | 1:H:78:ILE:HD12 | 1.80 | 0.63 |
| 1:H:83:LEU:HD11 | 3:J:526:VAL:HB | 1.80 | 0.63 |
| 3:J:416:ILE:HG13 | 3:J:441:LEU:HD21 | 1.81 | 0.63 |
| 1:G:45:ARG:HH21 | 2:I:1216:ARG:HA | 1.64 | 0.63 |
| 3:J:1259:GLN:OE1 | 3:J:1262:ARG:NH1 | 2.31 | 0.63 |
| 1:G:29:GLU:HB2 | 1:G:30:PRO:HD3 | 1.79 | 0.63 |
| 3:J:850:LYS:HB3 | 3:J:854:ALA:HB3 | 1.80 | 0.63 |
| 2:I:865:LEU:HD22 | 2:I:869:GLY:O | 1.98 | 0.62 |
| 5:L:338:HIS:O | 5:L:342:GLN:HG2 | 1.98 | 0.62 |
| 1:H:98:VAL:HG11 | 1:H:121:VAL:HG22 | 1.81 | 0.62 |
| 2:I:56:VAL:HG11 | 2:I:468:LEU:HB3 | 1.79 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:960:LEU:HB3 | 2:I:1025:PHE:CE1 | 2.33 | 0.62 |
| 3:J:853:THR:O | 3:J:855:ASP:N | 2.32 | 0.62 |
| 2:I:699:LEU:HB2 | 2:I:799:ASN:ND2 | 2.14 | 0.62 |
| 3:J:210:SER:HB3 | 3:J:213:LYS:HB3 | 1.81 | 0.62 |
| 5:L:420:GLU:HG3 | 5:L:422:ARG:HE | 1.63 | 0.62 |
| 1:G:45:ARG:NH2 | 2:I:1216:ARG:HA | 2.14 | 0.62 |
| 5:L:437:GLN:HB2 | 6:P:49:DC:N4 | 2.15 | 0.62 |
| 1:G:235:ARG:H | 1:H:13:LEU:HD23 | 1.64 | 0.62 |
| 2:I:594:VAL:HG22 | 2:I:599:VAL:HA | 1.81 | 0.62 |
| 2:I:1242:LYS:HD2 | 3:J:465:GLN:NE2 | 2.14 | 0.62 |
| 3:J:810:THR:HG22 | 3:J:893:GLY:HA3 | 1.81 | 0.62 |
| 5:L:561:MET:HA | 5:L:567:MET:CE | 2.29 | 0.62 |
| 1:R:257:VAL:HG13 | 1:R:276:HIS:O | 2.00 | 0.62 |
| 1:G:57:THR:HG21 | 1:G:147:GLN:HE21 | 1.63 | 0.62 |
| 3:J:259:ARG:HH12 | 5:L:502:LYS:HB2 | 1.64 | 0.62 |
| 1:G:59:VAL:HG21 | 1:G:85:LEU:HD12 | 1.81 | 0.62 |
| 2:I:593:LYS:HA | 2:I:652:TYR:CD1 | 2.34 | 0.62 |
| 5:L:493:LYS:O | 5:L:497:VAL:HG23 | 2.00 | 0.62 |
| 2:I:1060:ILE:HD11 | 2:I:1076:ILE:HD11 | 1.81 | 0.62 |
| 2:I:1259:LEU:HD23 | 2:I:1264:GLN:HB3 | 1.80 | 0.62 |
| 5:L:165:PHE:HD1 | 5:L:259:PHE:HA | 1.65 | 0.62 |
| 5:L:333:VAL:HG22 | 5:L:337:VAL:HG23 | 1.82 | 0.62 |
| 3:J:872:LEU:CD2 | 3:J:877:VAL:HG21 | 2.30 | 0.62 |
| 3:J:1175:LEU:HB2 | 3:J:1190:ILE:HD12 | 1.80 | 0.62 |
| 7:Q:32:DA:H2'' | 7:Q:33:DA:C5' | 2.29 | 0.62 |
| 1:H:59:VAL:O | 1:H:171:LEU:HB2 | 2.00 | 0.61 |
| 3:J:1077:ALA:HB2 | 3:J:1100:PHE:CE1 | 2.35 | 0.61 |
| 3:J:1162:ILE:HG22 | 3:J:1178:THR:O | 1.99 | 0.61 |
| 5:L:547:VAL:HG21 | 5:L:607:LEU:HD21 | 1.82 | 0.61 |
| 2:I:318:SER:OG | 2:I:320:ASP:OD1 | 2.12 | 0.61 |
| 2:I:854:ILE:HD11 | 2:I:885:GLY:HA2 | 1.81 | 0.61 |
| 2:I:1277:ALA:HB3 | 3:J:434:ILE:HD12 | 1.82 | 0.61 |
| 7:Q:15:DT:H2'' | 7:Q:16:DC:OP2 | 1.99 | 0.61 |
| 1:R:275:ILE:HG23 | 1:R:280:ASP:HB3 | 1.82 | 0.61 |
| 1:G:8:PHE:HA | 1:G:32:GLU:OE2 | 2.01 | 0.61 |
| 2:I:235:ASN:OD1 | 2:I:236:LYS:HG2 | 2.01 | 0.61 |
| 2:I:1018:TYR:O | 2:I:1022:LYS:HG2 | 1.99 | 0.61 |
| 3:J:697:MET:HE3 | 3:J:741:ALA:HB3 | 1.82 | 0.61 |
| 3:J:1186:TYR:OH | 3:J:1188:GLU:OE1 | 2.18 | 0.61 |
| 2:I:229:ILE:HG23 | 2:I:332:ARG:HD2 | 1.82 | 0.61 |
| 2:I:1248:THR:HG21 | 5:L:531:PRO:HG3 | 1.82 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:1347:LEU:HG | 3:J:1357:ILE:HG23 | 1.83 | 0.61 |
| 7:Q:21:DT:H2" | 7:Q:22:DG:C8 | 2.36 | 0.61 |
| 1:G:12:ARG:O | 1:G:14:VAL:HG23 | 2.00 | 0.61 |
| 1:G:224:LEU:HD22 | 1:H:228:LEU:CD1 | 2.30 | 0.61 |
| 3:J:1046:ILE:CD1 | 3:J:1059:LEU:HD13 | 2.31 | 0.61 |
| 1:R:300:LEU:CD1 | 1:R:304:LYS:HE2 | 2.31 | 0.61 |
| 2:I:611:GLU:OE2 | 2:I:637:ARG:NH2 | 2.31 | 0.61 |
| 3:J:1355:ARG:HH12 | 3:J:1369:ARG:HH22 | 1.47 | 0.61 |
| 1:R:300:LEU:HD21 | 1:R:314:LEU:HD11 | 1.82 | 0.61 |
| 2:I:726:TYR:CE2 | 2:I:728:ASP:HB2 | 2.35 | 0.61 |
| 2:I:817:LEU:HD11 | 2:I:1080:ASN:ND2 | 2.15 | 0.61 |
| 3:J:368:LEU:CD2 | 3:J:373:ALA:HB2 | 2.30 | 0.61 |
| 2:I:796:LEU:HB3 | 2:I:1233:LEU:HD11 | 1.82 | 0.61 |
| 3:J:253:VAL:HG11 | 5:L:523:ILE:HG21 | 1.81 | 0.61 |
| 3:J:268:LEU:HB3 | 3:J:306:LEU:HD23 | 1.82 | 0.61 |
| 3:J:975:ILE:HD13 | 3:J:980:THR:HG21 | 1.82 | 0.61 |
| 5:L:261:LEU:HB3 | 5:L:265:GLN:HB2 | 1.83 | 0.61 |
| 1:G:13:LEU:CD2 | 1:G:214:GLU:HG3 | 2.30 | 0.61 |
| 1:G:81:ILE:HG12 | 1:G:131:CYS:HB3 | 1.81 | 0.61 |
| 1:H:33:ARG:NH1 | 2:I:1081:PRO:HG3 | 2.15 | 0.61 |
| 2:I:992:LEU:HB2 | 2:I:993:PRO:HD2 | 1.82 | 0.61 |
| 3:J:1173:ARG:HG3 | 3:J:1190:ILE:HB | 1.81 | 0.61 |
| 2:I:1113:LEU:HD11 | 3:J:641:ILE:HD13 | 1.83 | 0.60 |
| 5:L:216:LEU:O | 5:L:220:LYS:HG2 | 2.01 | 0.60 |
| 5:L:287:ILE:HG23 | 5:L:337:VAL:HG13 | 1.83 | 0.60 |
| 2:I:560:PRO:HB3 | 3:J:776:THR:HG21 | 1.83 | 0.60 |
| 3:J:68:TYR:HA | 3:J:92:VAL:HG23 | 1.82 | 0.60 |
| 2:I:971:LEU:HD23 | 2:I:975:ILE:HD11 | 1.83 | 0.60 |
| 2:I:1305:TYR:CE1 | 3:J:379:PRO:HG3 | 2.37 | 0.60 |
| 2:I:1312:ASN:OD1 | 2:I:1314:GLN:HG3 | 2.01 | 0.60 |
| 4:K:3:ARG:HD2 | 4:K:5:THR:O | 2.01 | 0.60 |
| 1:G:42:ALA:O | 1:G:46:ILE:HG12 | 2.00 | 0.60 |
| 1:H:101:THR:HG22 | 1:H:116:THR:HG21 | 1.82 | 0.60 |
| 2:I:216:THR:OG1 | 2:I:219:GLN:OE1 | 2.19 | 0.60 |
| 2:I:517:GLN:O | 2:I:517:GLN:HG3 | 2.00 | 0.60 |
| 2:I:848:GLU:OE1 | 2:I:886:LYS:NZ | 2.28 | 0.60 |
| 2:I:1132:LEU:HD21 | 2:I:1141:LEU:HD21 | 1.82 | 0.60 |
| 3:J:964:LYS:O | 3:J:976:THR:OG1 | 2.11 | 0.60 |
| 5:L:101:TYR:CE2 | 5:L:405:ILE:HD12 | 2.36 | 0.60 |
| 7:Q:74:DA:C8 | 7:Q:75:DT:H72 | 2.37 | 0.60 |
| 2:I:296:VAL:HA | 2:I:316:GLU:HA | 1.82 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:H:102:LEU:HD23 | 1:H:142:MET:SD | 2.42 | 0.60 |
| 2:I:118:LYS:CE | 2:I:488:MET:HG2 | 2.32 | 0.60 |
| 3:J:38:VAL:HG11 | 3:J:56:LEU:HD12 | 1.83 | 0.60 |
| 3:J:1148:ARG:NH1 | 6:P:66:DG:H5" | 2.17 | 0.60 |
| 5:L:463:LEU:HD21 | 5:L:494:ILE:HG12 | 1.83 | 0.60 |
| 2:I:150:HIS:NE2 | 2:I:454:ARG:HG3 | 2.16 | 0.60 |
| 2:I:1243:MET:HA | 3:J:353:SER:HB3 | 1.82 | 0.60 |
| 3:J:800:LEU:HB3 | 3:J:920:ALA:HB1 | 1.83 | 0.60 |
| 3:J:1071:GLY:HA2 | 3:J:1074:LEU:HB2 | 1.83 | 0.60 |
| 3:J:1267:VAL:N | 3:J:1301:THR:O | 2.33 | 0.60 |
| 5:L:271:ASN:O | 5:L:275:VAL:HG23 | 2.02 | 0.60 |
| 1:R:290:LEU:HA | 1:R:295:LEU:HD22 | 1.84 | 0.60 |
| 2:I:1006:GLU:O | 2:I:1009:ASN:C | 2.40 | 0.60 |
| 3:J:279:LEU:HD11 | 3:J:296:LYS:HG2 | 1.83 | 0.60 |
| 3:J:407:VAL:O | 3:J:411:ILE:HG12 | 2.01 | 0.60 |
| 3:J:98:ARG:O | 3:J:247:PRO:HD2 | 2.02 | 0.60 |
| 3:J:823:THR:HG22 | 3:J:879:ALA:CB | 2.32 | 0.60 |
| 3:J:1149:ARG:NH2 | 3:J:1153:PRO:HG3 | 2.17 | 0.60 |
| 5:L:606:VAL:O | 5:L:609:SER:OG | 2.11 | 0.60 |
| 2:I:269:ILE:HG23 | 2:I:273:HIS:CB | 2.31 | 0.60 |
| 3:J:646:ILE:HD12 | 3:J:762:ASN:HD21 | 1.65 | 0.60 |
| 5:L:137:TYR:HE2 | 5:L:139:GLU:HB2 | 1.66 | 0.60 |
| 5:L:561:MET:HG2 | 5:L:576:VAL:HG22 | 1.83 | 0.60 |
| 3:J:398:LYS:HD2 | 5:L:532:LEU:CD2 | 2.31 | 0.59 |
| 3:J:1227:HIS:HA | 3:J:1230:THR:HG22 | 1.84 | 0.59 |
| 5:L:339:ARG:HA | 5:L:342:GLN:CG | 2.31 | 0.59 |
| 1:G:68:TYR:HB3 | 2:I:756:TYR:HD2 | 1.66 | 0.59 |
| 2:I:27:LEU:HB2 | 2:I:524:ILE:HD11 | 1.82 | 0.59 |
| 2:I:118:LYS:HE2 | 2:I:488:MET:HA | 1.84 | 0.59 |
| 1:G:224:LEU:HD22 | 1:H:228:LEU:HD11 | 1.84 | 0.59 |
| 3:J:268:LEU:CB | 3:J:306:LEU:HD23 | 2.31 | 0.59 |
| 3:J:1109:LEU:HD22 | 3:J:1115:ILE:HG22 | 1.84 | 0.59 |
| 5:L:148:TYR:CE1 | 5:L:158:LEU:HD21 | 2.37 | 0.59 |
| 1:H:35:PHE:HA | 1:H:38:THR:CG2 | 2.31 | 0.59 |
| 2:I:33:ASP:O | 2:I:37:LYS:HG2 | 2.02 | 0.59 |
| 2:I:905:ILE:HG22 | 2:I:906:PHE:CD1 | 2.36 | 0.59 |
| 3:J:197:GLU:OE2 | 3:J:220:ARG:NH2 | 2.29 | 0.59 |
| 5:L:505:ILE:H | 5:L:505:ILE:HD12 | 1.66 | 0.59 |
| 1:G:234:LEU:HD22 | 1:H:13:LEU:HD22 | 1.85 | 0.59 |
| 2:I:854:ILE:HD11 | 2:I:885:GLY:CA | 2.33 | 0.59 |
| 1:R:260:LEU:HD13 | 1:R:281:LEU:HD22 | 1.82 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:145:ILE:CG2 | 2:I:456:VAL:HG22 | 2.33 | 0.59 |
| 3:J:114:ILE:HD12 | 3:J:304:ASP:OD1 | 2.02 | 0.59 |
| 3:J:515:ARG:NH2 | 3:J:718:SER:O | 2.36 | 0.59 |
| 3:J:682:VAL:O | 3:J:685:ILE:HG22 | 2.02 | 0.59 |
| 3:J:1155:ILE:HD12 | 3:J:1210:ILE:HB | 1.83 | 0.59 |
| 6:P:21:DA:H2'' | 6:P:22:DT:H5' | 1.83 | 0.59 |
| 1:G:160:HIS:CD2 | 1:G:161:SER:HB2 | 2.38 | 0.59 |
| 1:H:56:VAL:HG22 | 1:H:146:VAL:HG12 | 1.83 | 0.59 |
| 1:H:158:ARG:CB | 1:H:172:LEU:HD23 | 2.33 | 0.59 |
| 3:J:1058:SER:HB3 | 3:J:1106:ILE:HG23 | 1.83 | 0.59 |
| 3:J:1170:LYS:CB | 6:P:75:DA:H3' | 2.33 | 0.59 |
| 5:L:584:ARG:O | 5:L:587:ILE:HG22 | 2.02 | 0.59 |
| 7:Q:52:DT:H2'' | 7:Q:53:DT:C6 | 2.38 | 0.59 |
| 2:I:719:LYS:O | 2:I:779:ARG:HG3 | 2.03 | 0.59 |
| 3:J:546:ALA:O | 3:J:548:VAL:HG23 | 2.03 | 0.59 |
| 3:J:641:ILE:HD12 | 3:J:644:MET:CE | 2.33 | 0.59 |
| 5:L:309:ASN:HB3 | 5:L:315:TRP:CD1 | 2.37 | 0.59 |
| 2:I:564:PRO:CG | 2:I:572:ILE:HB | 2.33 | 0.59 |
| 3:J:1287:ILE:HG22 | 3:J:1290:ARG:NH2 | 2.18 | 0.59 |
| 4:K:38:LEU:HB2 | 4:K:53:GLU:OE1 | 2.03 | 0.59 |
| 5:L:110:LEU:HD21 | 5:L:385:ARG:HD2 | 1.85 | 0.58 |
| 2:I:1255:THR:O | 2:I:1257:GLN:N | 2.36 | 0.58 |
| 3:J:282:LEU:HD21 | 5:L:410:ILE:HG12 | 1.85 | 0.58 |
| 3:J:1155:ILE:CD1 | 3:J:1210:ILE:HB | 2.33 | 0.58 |
| 1:R:252:ILE:O | 1:R:278:ILE:HB | 2.03 | 0.58 |
| 2:I:130:MET:CG | 2:I:134:GLY:HA2 | 2.33 | 0.58 |
| 2:I:424:ASP:O | 2:I:428:VAL:HG23 | 2.03 | 0.58 |
| 2:I:447:HIS:HE1 | 2:I:609:ILE:HG22 | 1.68 | 0.58 |
| 3:J:301:GLU:OE1 | 5:L:97:PRO:HG2 | 2.02 | 0.58 |
| 5:L:148:TYR:CE1 | 5:L:158:LEU:CD2 | 2.86 | 0.58 |
| 5:L:311:THR:O | 5:L:341:LEU:HD23 | 2.04 | 0.58 |
| 2:I:594:VAL:CG2 | 2:I:599:VAL:HG22 | 2.33 | 0.58 |
| 3:J:1155:ILE:HD12 | 3:J:1155:ILE:O | 2.03 | 0.58 |
| 5:L:295:CYS:SG | 5:L:330:LEU:HD23 | 2.44 | 0.58 |
| 2:I:556:GLY:HA2 | 2:I:659:GLN:O | 2.03 | 0.58 |
| 2:I:1278:LEU:HB2 | 2:I:1287:LEU:HD12 | 1.84 | 0.58 |
| 3:J:475:GLU:OE2 | 4:K:28:ARG:NH1 | 2.36 | 0.58 |
| 3:J:1216:ALA:O | 3:J:1220:ILE:HG12 | 2.03 | 0.58 |
| 1:H:82:LEU:HD22 | 1:H:173:VAL:CG2 | 2.33 | 0.58 |
| 2:I:297:VAL:HG12 | 2:I:315:MET:H | 1.68 | 0.58 |
| 2:I:798:GLN:NE2 | 2:I:827:ARG:O | 2.36 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:1260:GLY:O | 2:I:1266:GLY:HA3 | 2.04 | 0.58 |
| 3:J:51:PRO:HB3 | 3:J:57:PHE:O | 2.03 | 0.58 |
| 5:L:288:MET:HA | 5:L:302:PHE:CZ | 2.39 | 0.58 |
| 7:Q:54:DT:H2'' | 7:Q:55:DA:C8 | 2.38 | 0.58 |
| 1:G:23:HIS:CB | 1:G:206:GLU:HA | 2.34 | 0.58 |
| 2:I:551:HIS:HB3 | 2:I:554:HIS:CE1 | 2.37 | 0.58 |
| 2:I:1080:ASN:HD22 | 2:I:1085:MET:HE3 | 1.69 | 0.58 |
| 3:J:195:GLU:OE2 | 3:J:228:VAL:HG11 | 2.03 | 0.58 |
| 3:J:984:LEU:CB | 3:J:993:GLU:HB2 | 2.33 | 0.58 |
| 1:H:211:ILE:HD11 | 1:H:215:GLU:OE1 | 2.03 | 0.58 |
| 2:I:240:GLU:HG3 | 2:I:284:LEU:HD13 | 1.86 | 0.58 |
| 2:I:1294:LYS:HG2 | 3:J:472:LEU:HD11 | 1.86 | 0.58 |
| 3:J:473:THR:HG23 | 3:J:476:ALA:H | 1.68 | 0.58 |
| 1:G:140:ILE:HD12 | 1:G:142:MET:CE | 2.33 | 0.58 |
| 2:I:1161:LEU:HA | 2:I:1164:PHE:CD2 | 2.38 | 0.58 |
| 3:J:44:ILE:HG12 | 5:L:450:ILE:HG22 | 1.86 | 0.58 |
| 3:J:1033:GLY:C | 3:J:1114:GLN:HG3 | 2.24 | 0.58 |
| 3:J:1048:ARG:HD2 | 3:J:1059:LEU:HD21 | 1.85 | 0.58 |
| 5:L:315:TRP:HZ2 | 5:L:341:LEU:HD21 | 1.68 | 0.58 |
| 6:P:29:DA:H1' | 6:P:30:DC:H5' | 1.86 | 0.58 |
| 2:I:802:VAL:HG21 | 2:I:1098:LEU:HD22 | 1.86 | 0.58 |
| 2:I:1005:GLU:H | 2:I:1008:GLN:HB3 | 1.68 | 0.58 |
| 2:I:1275:VAL:O | 2:I:1279:GLU:HG3 | 2.03 | 0.58 |
| 3:J:322:ARG:HH12 | 5:L:510:PRO:HG3 | 1.69 | 0.58 |
| 4:K:32:VAL:O | 4:K:34:GLY:N | 2.37 | 0.58 |
| 5:L:253:SER:O | 5:L:257:LYS:HG3 | 2.04 | 0.58 |
| 5:L:530:LEU:HD23 | 5:L:530:LEU:H | 1.69 | 0.58 |
| 3:J:271:ARG:NH1 | 3:J:316:ILE:HD12 | 2.13 | 0.57 |
| 3:J:1034:PHE:HD1 | 3:J:1114:GLN:HB2 | 1.69 | 0.57 |
| 5:L:577:GLY:O | 5:L:581:ASP:N | 2.37 | 0.57 |
| 1:G:134:THR:HG21 | 2:I:727:VAL:O | 2.04 | 0.57 |
| 5:L:571:TYR:HD1 | 5:L:575:GLU:HG2 | 1.68 | 0.57 |
| 2:I:184:LEU:HB2 | 2:I:389:PHE:CE1 | 2.39 | 0.57 |
| 2:I:712:SER:OG | 2:I:713:GLY:N | 2.35 | 0.57 |
| 3:J:200:GLN:O | 3:J:203:GLU:HG2 | 2.05 | 0.57 |
| 5:L:324:LYS:HB3 | 5:L:325:PRO:HD2 | 1.86 | 0.57 |
| 5:L:555:GLU:HA | 5:L:558:VAL:HG12 | 1.86 | 0.57 |
| 1:H:61:ILE:HG22 | 1:H:63:GLY:H | 1.69 | 0.57 |
| 2:I:4:SER:HB2 | 2:I:7:GLU:HB2 | 1.86 | 0.57 |
| 2:I:22:LEU:HB3 | 2:I:655:VAL:HG11 | 1.86 | 0.57 |
| 2:I:184:LEU:HD13 | 2:I:389:PHE:CZ | 2.39 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:232:ILE:HG12 | 2:I:237:LEU:CD2 | 2.34 | 0.57 |
| 2:I:322:LEU:O | 2:I:325:LEU:HG | 2.04 | 0.57 |
| 3:J:527:LEU:HD13 | 3:J:548:VAL:HG11 | 1.85 | 0.57 |
| 3:J:641:ILE:HD12 | 3:J:644:MET:HE1 | 1.86 | 0.57 |
| 3:J:744:ARG:O | 3:J:744:ARG:HD3 | 2.04 | 0.57 |
| 6:P:20:DA:H2'' | 6:P:21:DA:C8 | 2.39 | 0.57 |
| 1:R:283:GLN:CG | 1:R:318:LEU:HD13 | 2.32 | 0.57 |
| 1:R:318:LEU:HD23 | 1:R:321:TRP:CB | 2.34 | 0.57 |
| 1:G:235:ARG:N | 1:H:13:LEU:HD23 | 2.19 | 0.57 |
| 2:I:302:ILE:HD12 | 2:I:302:ILE:O | 2.05 | 0.57 |
| 2:I:1073:LYS:HG3 | 3:J:462:ASP:HB2 | 1.87 | 0.57 |
| 2:I:1082:ILE:H | 2:I:1082:ILE:HD12 | 1.69 | 0.57 |
| 2:I:1212:LEU:HD13 | 2:I:1225:VAL:CG2 | 2.35 | 0.57 |
| 3:J:325:LYS:HG2 | 3:J:330:MET:HE2 | 1.86 | 0.57 |
| 3:J:693:VAL:HG21 | 3:J:743:MET:HE2 | 1.85 | 0.57 |
| 3:J:840:LEU:HD13 | 3:J:869:CYS:SG | 2.45 | 0.57 |
| 3:J:883:ARG:NH2 | 3:J:898:CYS:SG | 2.77 | 0.57 |
| 1:H:205:MET:CE | 1:H:217:ILE:HG13 | 2.34 | 0.57 |
| 4:K:3:ARG:HD3 | 4:K:4:VAL:H | 1.70 | 0.57 |
| 5:L:328:GLU:HA | 5:L:331:HIS:HD2 | 1.68 | 0.57 |
| 8:L:701:1N7:C3 | 8:L:701:1N7:C2 | 2.74 | 0.57 |
| 1:R:302:GLU:HA | 1:R:305:ASP:OD2 | 2.05 | 0.57 |
| 1:R:318:LEU:HD23 | 1:R:321:TRP:HB3 | 1.87 | 0.57 |
| 2:I:748:ILE:HD11 | 2:I:966:ILE:CG1 | 2.33 | 0.57 |
| 2:I:1009:ASN:O | 2:I:1010:GLN:HG2 | 2.04 | 0.57 |
| 3:J:478:LEU:HG | 4:K:47:THR:HG23 | 1.87 | 0.57 |
| 3:J:1319:PHE:CE1 | 3:J:1342:ASP:HB2 | 2.40 | 0.57 |
| 2:I:13:LYS:HB2 | 2:I:1180:MET:HE1 | 1.86 | 0.57 |
| 2:I:184:LEU:HB2 | 2:I:389:PHE:HE1 | 1.70 | 0.57 |
| 2:I:289:VAL:HG22 | 2:I:322:LEU:HD13 | 1.87 | 0.57 |
| 2:I:371:ARG:NH1 | 6:P:57:DT:O4 | 2.37 | 0.57 |
| 2:I:672:GLU:HB3 | 2:I:1187:PHE:HD1 | 1.69 | 0.57 |
| 2:I:700:VAL:HG22 | 2:I:1117:LEU:HD23 | 1.86 | 0.57 |
| 2:I:1246:ARG:NH1 | 2:I:1266:GLY:HA2 | 2.19 | 0.57 |
| 3:J:667:GLN:O | 3:J:673:VAL:HG22 | 2.05 | 0.57 |
| 3:J:1173:ARG:NE | 3:J:1192:LYS:HA | 2.18 | 0.57 |
| 5:L:345:GLN:O | 5:L:349:GLU:HG3 | 2.05 | 0.57 |
| 2:I:1040:ASP:OD1 | 2:I:1041:ASP:N | 2.36 | 0.57 |
| 2:I:1119:MET:CE | 2:I:1210:ILE:HD11 | 2.34 | 0.57 |
| 5:L:313:ASP:CA | 5:L:316:PHE:HB3 | 2.34 | 0.57 |
| 1:H:136:GLU:HG2 | 1:H:137:ASN:H | 1.69 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:432:LEU:O | 3:J:435:GLN:NE2 | 2.37 | 0.56 |
| 3:J:1215:GLU:HB3 | 3:J:1220:ILE:HD11 | 1.86 | 0.56 |
| 5:L:318:ALA:HA | 5:L:321:ALA:CB | 2.30 | 0.56 |
| 1:R:282:VAL:HG11 | 1:R:312:LEU:HD22 | 1.87 | 0.56 |
| 3:J:201:LEU:HD11 | 3:J:220:ARG:NH1 | 2.19 | 0.56 |
| 3:J:559:ALA:CB | 3:J:562:GLU:HB2 | 2.31 | 0.56 |
| 3:J:901:ARG:HD3 | 3:J:906:GLY:O | 2.05 | 0.56 |
| 2:I:130:MET:SD | 2:I:134:GLY:HA2 | 2.45 | 0.56 |
| 2:I:646:SER:HB3 | 2:I:649:GLN:HG3 | 1.86 | 0.56 |
| 2:I:728:ASP:OD1 | 2:I:729:ALA:N | 2.38 | 0.56 |
| 2:I:877:VAL:CG2 | 2:I:920:VAL:HG21 | 2.36 | 0.56 |
| 3:J:347:VAL:HG12 | 3:J:348:ASP:O | 2.05 | 0.56 |
| 3:J:475:GLU:HG3 | 4:K:24:ALA:CB | 2.35 | 0.56 |
| 3:J:701:LEU:CD1 | 3:J:723:TYR:HB2 | 2.35 | 0.56 |
| 3:J:746:LEU:HG | 3:J:758:PRO:HG3 | 1.87 | 0.56 |
| 3:J:810:THR:CG2 | 3:J:893:GLY:HA3 | 2.35 | 0.56 |
| 3:J:952:VAL:HG12 | 3:J:1015:GLU:O | 2.05 | 0.56 |
| 3:J:965:SER:HA | 3:J:975:ILE:HA | 1.86 | 0.56 |
| 3:J:1159:ILE:O | 3:J:1177:ILE:HG21 | 2.05 | 0.56 |
| 3:J:1183:SER:OG | 3:J:1185:PRO:HD3 | 2.05 | 0.56 |
| 3:J:1261:LEU:HD13 | 3:J:1304:ARG:HH11 | 1.70 | 0.56 |
| 3:J:1326:GLN:HG2 | 3:J:1327:GLU:H | 1.71 | 0.56 |
| 5:L:392:LYS:CD | 6:P:56:DC:H5" | 2.32 | 0.56 |
| 1:G:25:LYS:HE2 | 1:G:204:GLU:OE1 | 2.06 | 0.56 |
| 2:I:289:VAL:CG2 | 2:I:322:LEU:HD13 | 2.35 | 0.56 |
| 3:J:180:MET:N | 3:J:184:ALA:HB2 | 2.20 | 0.56 |
| 3:J:697:MET:O | 3:J:701:LEU:HB2 | 2.06 | 0.56 |
| 3:J:1031:VAL:HG11 | 3:J:1090:ILE:HA | 1.88 | 0.56 |
| 3:J:1220:ILE:HD12 | 3:J:1224:ARG:NH2 | 2.21 | 0.56 |
| 5:L:286:LEU:HD23 | 5:L:340:ALA:HB2 | 1.87 | 0.56 |
| 1:R:260:LEU:O | 1:R:306:VAL:HG21 | 2.06 | 0.56 |
| 1:H:205:MET:HE3 | 1:H:213:PRO:HA | 1.88 | 0.56 |
| 2:I:629:PHE:CZ | 2:I:650:VAL:HG21 | 2.40 | 0.56 |
| 2:I:953:LEU:CD1 | 2:I:1033:ARG:HG2 | 2.36 | 0.56 |
| 3:J:532:GLU:O | 3:J:536:LEU:HD23 | 2.04 | 0.56 |
| 3:J:821:MET:SD | 3:J:881:LYS:HB2 | 2.46 | 0.56 |
| 3:J:863:LEU:HD22 | 3:J:908:ILE:CG2 | 2.35 | 0.56 |
| 3:J:1162:ILE:CG2 | 3:J:1178:THR:HB | 2.35 | 0.56 |
| 5:L:148:TYR:HE1 | 5:L:158:LEU:CD2 | 2.18 | 0.56 |
| 5:L:310:GLU:OE1 | 5:L:355:ILE:HG21 | 2.06 | 0.56 |
| 5:L:320:ILE:HD13 | 5:L:331:HIS:CE1 | 2.39 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:498:ILE:H | 2:I:498:ILE:HD12 | 1.71 | 0.56 |
| 2:I:908:GLU:OE2 | 5:L:611:LEU:HD13 | 2.06 | 0.56 |
| 2:I:1304:MET:HE2 | 2:I:1308:ILE:HD11 | 1.87 | 0.56 |
| 2:I:1313:HIS:HE2 | 3:J:380:PHE:HE1 | 1.52 | 0.56 |
| 3:J:70:CYS:SG | 3:J:71:LEU:N | 2.78 | 0.56 |
| 5:L:522:PHE:HB3 | 8:L:701:1N7:H17 | 1.88 | 0.56 |
| 5:L:586:ARG:HB2 | 6:P:26:DT:C7 | 2.36 | 0.56 |
| 2:I:123:TYR:OH | 2:I:126:GLU:HG3 | 2.06 | 0.56 |
| 2:I:494:ASN:OD1 | 5:L:468:ARG:HD2 | 2.05 | 0.56 |
| 2:I:564:PRO:CD | 2:I:572:ILE:HB | 2.35 | 0.56 |
| 5:L:319:ALA:HB1 | 5:L:326:TRP:HZ3 | 1.71 | 0.56 |
| 2:I:1072:ASN:ND2 | 2:I:1111:GLN:OE1 | 2.38 | 0.56 |
| 6:P:26:DT:H2'' | 6:P:27:DT:O5' | 2.06 | 0.56 |
| 2:I:866:ASP:HB3 | 2:I:872:TYR:CE1 | 2.40 | 0.56 |
| 2:I:876:GLU:HG2 | 2:I:927:THR:OG1 | 2.06 | 0.56 |
| 2:I:1326:LEU:HD21 | 3:J:338:PHE:CZ | 2.41 | 0.56 |
| 3:J:825:VAL:HG22 | 3:J:833:GLU:HB3 | 1.87 | 0.56 |
| 3:J:959:LYS:HD2 | 3:J:1007:ASP:OD1 | 2.06 | 0.56 |
| 5:L:277:MET:CE | 5:L:359:LYS:HG2 | 2.36 | 0.56 |
| 1:R:257:VAL:N | 1:R:276:HIS:O | 2.38 | 0.56 |
| 2:I:888:THR:HG23 | 2:I:916:SER:HB2 | 1.87 | 0.56 |
| 3:J:1079:LYS:HB2 | 3:J:1098:GLN:HA | 1.86 | 0.56 |
| 1:G:13:LEU:HB2 | 1:H:231:PHE:HE1 | 1.71 | 0.55 |
| 1:H:112:ALA:HB3 | 1:H:126:PRO:CA | 2.36 | 0.55 |
| 2:I:1103:VAL:HG22 | 2:I:1111:GLN:NE2 | 2.20 | 0.55 |
| 3:J:972:LYS:HE2 | 3:J:972:LYS:HA | 1.87 | 0.55 |
| 3:J:1047:THR:O | 3:J:1059:LEU:HA | 2.05 | 0.55 |
| 4:K:58:LEU:HD12 | 4:K:59:ILE:HG12 | 1.88 | 0.55 |
| 5:L:290:LEU:HD13 | 5:L:333:VAL:CG2 | 2.36 | 0.55 |
| 1:H:44:ARG:HH22 | 3:J:538:ARG:HB3 | 1.71 | 0.55 |
| 2:I:38:PHE:CZ | 2:I:49:LEU:HD21 | 2.41 | 0.55 |
| 3:J:839:VAL:HG12 | 3:J:864:LEU:HD12 | 1.89 | 0.55 |
| 3:J:848:VAL:HB | 3:J:858:VAL:CG2 | 2.36 | 0.55 |
| 5:L:148:TYR:HE1 | 5:L:158:LEU:HD22 | 1.71 | 0.55 |
| 5:L:561:MET:HA | 5:L:567:MET:HE1 | 1.87 | 0.55 |
| 5:L:582:VAL:HG21 | 5:L:586:ARG:HG2 | 1.88 | 0.55 |
| 7:Q:77:DT:P | 1:R:298:LYS:HD3 | 2.47 | 0.55 |
| 1:R:255:ARG:O | 1:R:278:ILE:HG13 | 2.05 | 0.55 |
| 1:G:19:VAL:HG11 | 1:G:23:HIS:CE1 | 2.41 | 0.55 |
| 2:I:435:ILE:HD11 | 2:I:442:VAL:HG12 | 1.88 | 0.55 |
| 2:I:1029:LEU:HD21 | 2:I:1033:ARG:HD2 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:255:LEU:CD1 | 3:J:259:ARG:HB2 | 2.35 | 0.55 |
| 3:J:384:LYS:CE | 3:J:415:VAL:HG12 | 2.36 | 0.55 |
| 3:J:694:SER:O | 3:J:697:MET:HG3 | 2.07 | 0.55 |
| 3:J:749:LYS:HG2 | 3:J:753:SER:O | 2.06 | 0.55 |
| 3:J:1173:ARG:HD2 | 3:J:1196:LEU:HD21 | 1.87 | 0.55 |
| 8:J:1504:1N7:C3 | 8:J:1504:1N7:C18 | 2.75 | 0.55 |
| 1:R:255:ARG:HD3 | 1:R:256:PRO:HD2 | 1.87 | 0.55 |
| 1:R:292:THR:OG1 | 1:R:295:LEU:HD13 | 2.07 | 0.55 |
| 2:I:902:LEU:CD2 | 5:L:611:LEU:HD21 | 2.36 | 0.55 |
| 3:J:262:THR:O | 5:L:507:MET:HB2 | 2.06 | 0.55 |
| 3:J:709:ARG:NH1 | 3:J:710:ASP:HB3 | 2.21 | 0.55 |
| 3:J:1035:VAL:O | 3:J:1111:ASP:HA | 2.07 | 0.55 |
| 6:P:64:DT:C2' | 6:P:65:DT:H71 | 2.36 | 0.55 |
| 1:R:279:GLY:O | 1:R:283:GLN:HG3 | 2.07 | 0.55 |
| 1:G:13:LEU:HD21 | 1:G:214:GLU:HG3 | 1.87 | 0.55 |
| 2:I:680:LEU:HD13 | 3:J:783:LEU:CD1 | 2.36 | 0.55 |
| 2:I:983:GLY:HA3 | 2:I:1002:LEU:CD1 | 2.36 | 0.55 |
| 3:J:525:MET:O | 3:J:548:VAL:HG13 | 2.07 | 0.55 |
| 3:J:1061:VAL:HG13 | 3:J:1076:PRO:CG | 2.36 | 0.55 |
| 3:J:1090:ILE:HB | 3:J:1093:THR:OG1 | 2.06 | 0.55 |
| 5:L:280:VAL:O | 5:L:284:GLU:HG3 | 2.06 | 0.55 |
| 7:Q:28:DT:C2' | 7:Q:29:DT:H71 | 2.36 | 0.55 |
| 1:R:254:LEU:HB3 | 1:R:321:TRP:CH2 | 2.42 | 0.55 |
| 1:H:179:PRO:HA | 1:H:208:ASN:HD22 | 1.72 | 0.55 |
| 2:I:91:THR:HG22 | 2:I:138:ILE:O | 2.06 | 0.55 |
| 2:I:193:ASN:OD1 | 2:I:349:GLU:HG2 | 2.06 | 0.55 |
| 2:I:957:LYS:HG3 | 2:I:1029:LEU:HD11 | 1.88 | 0.55 |
| 3:J:103:GLY:O | 3:J:244:VAL:N | 2.27 | 0.55 |
| 1:G:17:GLU:O | 1:G:24:ALA:HB1 | 2.07 | 0.55 |
| 1:G:23:HIS:HB2 | 1:G:206:GLU:HA | 1.89 | 0.55 |
| 1:G:184:ALA:O | 1:G:204:GLU:HG2 | 2.05 | 0.55 |
| 2:I:629:PHE:CE2 | 2:I:650:VAL:HG21 | 2.42 | 0.55 |
| 2:I:1120:ALA:CB | 2:I:1198:LEU:HD12 | 2.31 | 0.55 |
| 3:J:336:GLY:O | 3:J:340:GLN:HB3 | 2.07 | 0.55 |
| 3:J:836:ARG:HG3 | 3:J:869:CYS:HB3 | 1.89 | 0.55 |
| 3:J:1347:LEU:HG | 3:J:1357:ILE:CG2 | 2.37 | 0.55 |
| 4:K:39:VAL:HG12 | 4:K:53:GLU:OE2 | 2.06 | 0.55 |
| 5:L:328:GLU:HA | 5:L:331:HIS:CD2 | 2.41 | 0.55 |
| 5:L:450:ILE:HG13 | 5:L:450:ILE:O | 2.07 | 0.55 |
| 2:I:901:LEU:HD11 | 2:I:905:ILE:HD11 | 1.89 | 0.55 |
| 2:I:901:LEU:HD22 | 5:L:565:ILE:HD11 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:89:ALA:O | 1:G:124:VAL:HG22 | 2.07 | 0.55 |
| 2:I:9:LYS:O | 2:I:1175:ASN:ND2 | 2.37 | 0.55 |
| 2:I:256:GLU:CB | 2:I:261:VAL:HA | 2.36 | 0.55 |
| 2:I:316:GLU:OE1 | 2:I:316:GLU:N | 2.33 | 0.55 |
| 2:I:548:ARG:HG2 | 2:I:569:ILE:O | 2.07 | 0.55 |
| 3:J:93:THR:HG22 | 3:J:94:GLN:H | 1.72 | 0.55 |
| 3:J:782:GLY:O | 3:J:786:THR:HG23 | 2.07 | 0.55 |
| 3:J:1075:ARG:NH2 | 3:J:1168:GLU:HG2 | 2.20 | 0.55 |
| 5:L:135:ALA:O | 5:L:253:SER:OG | 2.11 | 0.55 |
| 5:L:165:PHE:CD1 | 5:L:259:PHE:HA | 2.42 | 0.55 |
| 3:J:355:ILE:HG12 | 3:J:464:ASP:O | 2.07 | 0.55 |
| 3:J:1327:GLU:OE1 | 3:J:1327:GLU:N | 2.40 | 0.55 |
| 5:L:423:ARG:HG2 | 5:L:425:TYR:CE2 | 2.42 | 0.55 |
| 2:I:447:HIS:O | 2:I:450:ASN:N | 2.28 | 0.54 |
| 2:I:1161:LEU:HA | 2:I:1164:PHE:HD2 | 1.72 | 0.54 |
| 3:J:527:LEU:HD23 | 3:J:533:ALA:HB2 | 1.88 | 0.54 |
| 3:J:707:ILE:O | 3:J:713:GLU:HA | 2.08 | 0.54 |
| 5:L:470:MET:SD | 5:L:486:ARG:HG3 | 2.47 | 0.54 |
| 7:Q:32:DA:H2'' | 7:Q:33:DA:H5' | 1.88 | 0.54 |
| 1:R:286:GLU:O | 1:R:290:LEU:HG | 2.07 | 0.54 |
| 1:G:73:GLY:O | 1:G:134:THR:HG22 | 2.07 | 0.54 |
| 1:G:228:LEU:HD11 | 1:H:224:LEU:HD23 | 1.90 | 0.54 |
| 3:J:378:LYS:HE3 | 3:J:382:TYR:OH | 2.07 | 0.54 |
| 8:J:1504:1N7:C3 | 8:J:1504:1N7:C2 | 2.75 | 0.54 |
| 3:J:147:ILE:HG22 | 3:J:188:LEU:HD21 | 1.89 | 0.54 |
| 4:K:10:VAL:HG21 | 4:K:16:ARG:HD3 | 1.90 | 0.54 |
| 1:G:156:SER:O | 1:G:159:ILE:HG22 | 2.06 | 0.54 |
| 2:I:1067:ALA:HB3 | 2:I:1235:LEU:HD11 | 1.88 | 0.54 |
| 3:J:1081:VAL:CA | 3:J:1088:VAL:HG23 | 2.34 | 0.54 |
| 2:I:39:ILE:HD11 | 2:I:75:LEU:CG | 2.36 | 0.54 |
| 2:I:887:VAL:HG22 | 2:I:913:VAL:CG2 | 2.34 | 0.54 |
| 3:J:679:TYR:OH | 3:J:754:ILE:HG23 | 2.08 | 0.54 |
| 3:J:974:VAL:CG1 | 3:J:1002:VAL:HG22 | 2.34 | 0.54 |
| 5:L:136:GLU:OE1 | 5:L:361:ILE:HG12 | 2.08 | 0.54 |
| 5:L:426:LYS:NZ | 6:P:53:DT:OP1 | 2.37 | 0.54 |
| 7:Q:63:DT:H2' | 7:Q:64:DT:H72 | 1.89 | 0.54 |
| 2:I:519:ASN:ND2 | 2:I:796:LEU:HG | 2.18 | 0.54 |
| 3:J:255:LEU:CD2 | 3:J:261:ALA:HB2 | 2.38 | 0.54 |
| 1:R:284:ARG:HG3 | 1:R:289:LEU:HD21 | 1.90 | 0.54 |
| 2:I:163:LYS:HA | 2:I:163:LYS:HE2 | 1.89 | 0.54 |
| 2:I:549:ASP:OD2 | 3:J:750:PRO:HB3 | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:41:PRO:HG3 | 3:J:274:ASN:OD1 | 2.08 | 0.54 |
| 3:J:85:CYS:SG | 3:J:86:GLU:N | 2.81 | 0.54 |
| 3:J:1241:TYR:CD2 | 3:J:1248:ILE:HD12 | 2.43 | 0.54 |
| 4:K:50:ALA:O | 4:K:54:ILE:HG12 | 2.08 | 0.54 |
| 5:L:164:GLY:O | 5:L:260:ARG:HB3 | 2.08 | 0.54 |
| 5:L:276:MET:SD | 5:L:347:ILE:HG23 | 2.47 | 0.54 |
| 2:I:224:PHE:CG | 2:I:347:ILE:HG13 | 2.43 | 0.54 |
| 5:L:489:MET:SD | 5:L:493:LYS:HD2 | 2.48 | 0.54 |
| 7:Q:78:DG:H1' | 7:Q:79:DT:H5' | 1.88 | 0.54 |
| 2:I:136:PHE:CE2 | 2:I:145:ILE:HD13 | 2.43 | 0.54 |
| 8:I:1401:1N7:C3 | 8:I:1401:1N7:C2 | 2.74 | 0.54 |
| 3:J:1079:LYS:HD2 | 3:J:1096:PRO:HB3 | 1.90 | 0.54 |
| 3:J:1146:GLU:OE1 | 3:J:1148:ARG:NH2 | 2.41 | 0.54 |
| 5:L:148:TYR:HA | 5:L:161:LEU:CD2 | 2.38 | 0.54 |
| 1:G:54:CYS:SG | 1:G:148:ARG:HG3 | 2.47 | 0.54 |
| 1:G:192:VAL:CG1 | 1:G:198:LEU:HD12 | 2.37 | 0.54 |
| 2:I:215:TYR:OH | 2:I:422:LYS:HD2 | 2.08 | 0.54 |
| 2:I:693:LEU:HB2 | 2:I:829:THR:O | 2.07 | 0.54 |
| 3:J:334:LYS:NZ | 7:Q:35:DG:OP2 | 2.24 | 0.54 |
| 3:J:925:GLU:HG3 | 3:J:926:PRO:HD3 | 1.88 | 0.54 |
| 3:J:1169:THR:HG22 | 3:J:1170:LYS:N | 2.23 | 0.54 |
| 1:H:86:LYS:HD3 | 1:H:174:ASP:HB2 | 1.90 | 0.53 |
| 5:L:250:LEU:O | 5:L:254:GLU:HG2 | 2.08 | 0.53 |
| 2:I:673:HIS:HB3 | 2:I:1109:ILE:HG22 | 1.89 | 0.53 |
| 3:J:1027:VAL:HG23 | 3:J:1122:ALA:O | 2.07 | 0.53 |
| 2:I:1138:VAL:HG12 | 2:I:1170:MET:SD | 2.48 | 0.53 |
| 3:J:393:THR:HG23 | 3:J:396:ALA:H | 1.71 | 0.53 |
| 3:J:482:ALA:O | 3:J:488:ASN:ND2 | 2.42 | 0.53 |
| 3:J:490:ILE:C | 3:J:491:LEU:HD12 | 2.29 | 0.53 |
| 3:J:1061:VAL:HG13 | 3:J:1076:PRO:HG3 | 1.90 | 0.53 |
| 7:Q:73:DG:H2'' | 7:Q:74:DA:C8 | 2.44 | 0.53 |
| 3:J:368:LEU:HD21 | 3:J:373:ALA:HB2 | 1.89 | 0.53 |
| 3:J:1003:LEU:HD23 | 3:J:1018:ALA:HA | 1.89 | 0.53 |
| 3:J:1169:THR:HG21 | 3:J:1172:LYS:CB | 2.38 | 0.53 |
| 2:I:133:ASN:HB3 | 2:I:527:LYS:NZ | 2.23 | 0.53 |
| 2:I:671:LEU:HB3 | 2:I:1186:VAL:CG1 | 2.38 | 0.53 |
| 2:I:1101:LEU:HB3 | 3:J:731:ARG:HG3 | 1.90 | 0.53 |
| 3:J:668:PHE:HD1 | 3:J:673:VAL:HG23 | 1.73 | 0.53 |
| 3:J:712:GLN:HG2 | 3:J:713:GLU:N | 2.24 | 0.53 |
| 3:J:858:VAL:HG12 | 3:J:868:TRP:CZ3 | 2.43 | 0.53 |
| 5:L:602:SER:HB3 | 1:R:259:ASP:OD1 | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:H:68:TYR:O | 1:H:69:SER:OG | 2.26 | 0.53 |
| 2:I:245:ARG:HB3 | 2:I:337:PHE:CE1 | 2.44 | 0.53 |
| 2:I:264:GLU:HB2 | 2:I:267:ARG:HG3 | 1.91 | 0.53 |
| 2:I:818:VAL:HG21 | 2:I:1066:MET:HE1 | 1.91 | 0.53 |
| 6:P:28:DG:H2'' | 6:P:29:DA:C5' | 2.39 | 0.53 |
| 1:R:269:CYS:CB | 1:R:295:LEU:HD12 | 2.35 | 0.53 |
| 1:R:317:ARG:C | 1:R:318:LEU:HD12 | 2.29 | 0.53 |
| 2:I:621:SER:HB2 | 2:I:653:MET:HE3 | 1.90 | 0.53 |
| 2:I:1103:VAL:HB | 2:I:1104:PRO:HD3 | 1.91 | 0.53 |
| 2:I:1287:LEU:HD13 | 3:J:1357:ILE:CD1 | 2.38 | 0.53 |
| 5:L:511:ILE:O | 5:L:513:ASP:HB2 | 2.09 | 0.53 |
| 1:H:33:ARG:HH12 | 2:I:1081:PRO:HG3 | 1.72 | 0.53 |
| 1:H:100:LEU:HD23 | 1:H:115:ILE:CG2 | 2.38 | 0.53 |
| 2:I:746:ALA:HB2 | 2:I:970:GLY:N | 2.23 | 0.53 |
| 2:I:1325:VAL:HG22 | 3:J:249:LEU:HD22 | 1.91 | 0.53 |
| 3:J:1169:THR:HG22 | 3:J:1171:GLY:H | 1.73 | 0.53 |
| 3:J:1291:GLU:O | 3:J:1294:ALA:HB3 | 2.08 | 0.53 |
| 5:L:399:LEU:HD23 | 5:L:404:LEU:CD2 | 2.38 | 0.53 |
| 1:G:211:ILE:CG2 | 1:G:216:ALA:HB2 | 2.36 | 0.53 |
| 5:L:232:ARG:O | 5:L:235:ILE:HG12 | 2.08 | 0.53 |
| 1:G:104:LYS:O | 1:G:139:SER:OG | 2.17 | 0.53 |
| 2:I:1268:GLN:NE2 | 3:J:352:ARG:HD2 | 2.23 | 0.53 |
| 3:J:745:GLY:O | 3:J:758:PRO:HB3 | 2.09 | 0.53 |
| 3:J:759:ILE:CG2 | 3:J:771:GLN:HB3 | 2.37 | 0.53 |
| 3:J:955:LYS:HE2 | 3:J:1010:GLN:NE2 | 2.24 | 0.53 |
| 3:J:960:LEU:HD23 | 3:J:963:VAL:CG2 | 2.33 | 0.53 |
| 3:J:1011:VAL:HB | 3:J:1015:GLU:OE1 | 2.09 | 0.53 |
| 5:L:319:ALA:HB1 | 5:L:326:TRP:CZ3 | 2.44 | 0.53 |
| 5:L:374:ARG:O | 5:L:378:GLU:HG3 | 2.08 | 0.53 |
| 2:I:396:ASP:HA | 2:I:418:GLY:O | 2.09 | 0.52 |
| 2:I:432:LEU:HA | 2:I:435:ILE:HG22 | 1.89 | 0.52 |
| 2:I:1115:THR:HG23 | 2:I:1228:GLY:HA3 | 1.92 | 0.52 |
| 3:J:580:TRP:CZ3 | 3:J:589:TYR:HA | 2.43 | 0.52 |
| 3:J:1048:ARG:CZ | 3:J:1057:SER:HB2 | 2.39 | 0.52 |
| 5:L:134:VAL:HG13 | 5:L:273:MET:HE3 | 1.90 | 0.52 |
| 5:L:295:CYS:SG | 5:L:330:LEU:HA | 2.49 | 0.52 |
| 5:L:297:MET:HE1 | 5:L:302:PHE:HA | 1.91 | 0.52 |
| 6:P:37:DA:H2' | 6:P:37:DA:OP2 | 2.09 | 0.52 |
| 1:H:158:ARG:HB2 | 1:H:172:LEU:HD23 | 1.92 | 0.52 |
| 2:I:103:VAL:CG1 | 2:I:117:ILE:HG22 | 2.36 | 0.52 |
| 2:I:987:GLU:HG2 | 2:I:991:LYS:HE3 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:382:TYR:HB3 | 3:J:394:ILE:HD11 | 1.91 | 0.52 |
| 3:J:574:VAL:O | 3:J:578:ILE:HG13 | 2.09 | 0.52 |
| 5:L:571:TYR:CD1 | 5:L:575:GLU:HG2 | 2.45 | 0.52 |
| 1:H:205:MET:HE3 | 1:H:213:PRO:HB3 | 1.92 | 0.52 |
| 2:I:558:VAL:CG1 | 2:I:573:ASN:HB3 | 2.39 | 0.52 |
| 2:I:1141:LEU:O | 2:I:1145:ILE:HD12 | 2.10 | 0.52 |
| 2:I:1268:GLN:HE22 | 3:J:352:ARG:HD2 | 1.74 | 0.52 |
| 3:J:384:LYS:HG2 | 3:J:411:ILE:HG23 | 1.90 | 0.52 |
| 3:J:514:THR:HG21 | 3:J:596:LEU:CB | 2.36 | 0.52 |
| 3:J:621:ALA:O | 3:J:624:ILE:HG22 | 2.09 | 0.52 |
| 3:J:1149:ARG:HH22 | 3:J:1153:PRO:HG3 | 1.75 | 0.52 |
| 5:L:512:GLY:HA3 | 5:L:513:ASP:CB | 2.39 | 0.52 |
| 1:R:299:SER:O | 1:R:303:ILE:HG13 | 2.10 | 0.52 |
| 1:G:68:TYR:HA | 2:I:756:TYR:HE2 | 1.74 | 0.52 |
| 2:I:39:ILE:O | 2:I:39:ILE:HG23 | 2.09 | 0.52 |
| 2:I:699:LEU:HD13 | 2:I:699:LEU:O | 2.09 | 0.52 |
| 2:I:1281:TYR:CD2 | 3:J:484:MET:HG2 | 2.44 | 0.52 |
| 5:L:138:PRO:O | 5:L:142:THR:HG23 | 2.10 | 0.52 |
| 5:L:315:TRP:CZ2 | 5:L:341:LEU:HD21 | 2.44 | 0.52 |
| 5:L:339:ARG:HA | 5:L:342:GLN:HG2 | 1.90 | 0.52 |
| 6:P:75:DA:H2'' | 6:P:76:DT:OP2 | 2.09 | 0.52 |
| 1:H:88:LEU:O | 1:H:90:VAL:HG23 | 2.10 | 0.52 |
| 2:I:93:SER:OG | 2:I:126:GLU:OE1 | 2.15 | 0.52 |
| 2:I:765:ILE:HG13 | 2:I:787:PRO:HG3 | 1.91 | 0.52 |
| 2:I:800:MET:HE1 | 2:I:828:PHE:CE2 | 2.44 | 0.52 |
| 2:I:1131:MET:CE | 2:I:1141:LEU:HA | 2.40 | 0.52 |
| 3:J:129:ASP:HB2 | 3:J:220:ARG:NE | 2.24 | 0.52 |
| 3:J:516:ASP:HB3 | 3:J:573:THR:HG21 | 1.90 | 0.52 |
| 5:L:215:GLU:HG2 | 5:L:218:ARG:NH2 | 2.20 | 0.52 |
| 1:H:79:LEU:HD23 | 1:H:79:LEU:H | 1.75 | 0.52 |
| 2:I:1043:ALA:O | 2:I:1046:VAL:HG12 | 2.10 | 0.52 |
| 5:L:145:LEU:HD21 | 5:L:224:LEU:HG | 1.90 | 0.52 |
| 1:R:280:ASP:OD1 | 1:R:283:GLN:NE2 | 2.43 | 0.52 |
| 1:R:287:VAL:O | 1:R:291:LYS:HG3 | 2.10 | 0.52 |
| 1:G:183:ILE:O | 2:I:1091:GLY:HA3 | 2.10 | 0.52 |
| 1:G:214:GLU:O | 1:G:218:ARG:HG2 | 2.10 | 0.52 |
| 1:H:173:VAL:HG12 | 1:H:174:ASP:O | 2.10 | 0.52 |
| 2:I:714:VAL:O | 2:I:767:GLN:NE2 | 2.42 | 0.52 |
| 2:I:739:ASP:OD1 | 2:I:740:GLU:N | 2.43 | 0.52 |
| 2:I:1279:GLU:HG2 | 3:J:1357:ILE:CD1 | 2.37 | 0.52 |
| 3:J:712:GLN:HG2 | 3:J:713:GLU:H | 1.74 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:J:1504:1N7:H9 | 5:L:511:ILE:HD13 | 1.92 | 0.52 |
| 1:H:85:LEU:HD22 | 1:H:144:ILE:HD11 | 1.91 | 0.52 |
| 2:I:398:SER:O | 2:I:401:GLY:N | 2.42 | 0.52 |
| 2:I:1109:ILE:HD11 | 3:J:644:MET:CE | 2.40 | 0.52 |
| 2:I:1113:LEU:CD1 | 3:J:641:ILE:HD13 | 2.40 | 0.52 |
| 8:I:1401:1N7:H31 | 8:I:1401:1N7:H5 | 1.90 | 0.52 |
| 3:J:902:ASP:HB2 | 3:J:903:LEU:O | 2.09 | 0.52 |
| 3:J:1136:GLY:HA2 | 3:J:1140:ARG:HB2 | 1.92 | 0.52 |
| 3:J:1267:VAL:HB | 3:J:1301:THR:OG1 | 2.09 | 0.52 |
| 2:I:515:MET:HE2 | 2:I:517:GLN:HB3 | 1.92 | 0.52 |
| 2:I:617:ALA:HB3 | 2:I:653:MET:HG3 | 1.92 | 0.52 |
| 2:I:1268:GLN:HE22 | 3:J:352:ARG:HH11 | 1.58 | 0.52 |
| 3:J:424:ASN:OD1 | 3:J:425:ARG:N | 2.43 | 0.52 |
| 3:J:716:GLN:HG2 | 3:J:717:VAL:O | 2.10 | 0.52 |
| 3:J:982:LEU:HB2 | 3:J:997:VAL:CG2 | 2.39 | 0.52 |
| 6:P:38:DG:H2'' | 6:P:39:DG:C8 | 2.44 | 0.52 |
| 1:G:192:VAL:HG13 | 1:G:195:ARG:HB3 | 1.92 | 0.52 |
| 1:H:104:LYS:H | 1:H:140:ILE:CG2 | 2.23 | 0.52 |
| 2:I:731:ARG:NH1 | 2:I:962:GLU:OE1 | 2.34 | 0.52 |
| 3:J:848:VAL:HB | 3:J:858:VAL:HG22 | 1.91 | 0.52 |
| 3:J:870:ASP:O | 3:J:874:GLU:HG2 | 2.09 | 0.52 |
| 3:J:968:ASN:HD21 | 3:J:972:LYS:HB2 | 1.74 | 0.52 |
| 4:K:39:VAL:HG23 | 4:K:40:PRO:HD2 | 1.92 | 0.52 |
| 1:H:41:ASN:ND2 | 2:I:1217:THR:HA | 2.25 | 0.51 |
| 2:I:4:SER:HB2 | 2:I:7:GLU:CB | 2.39 | 0.51 |
| 2:I:521:LEU:HD23 | 2:I:708:VAL:HG11 | 1.92 | 0.51 |
| 2:I:564:PRO:HG3 | 2:I:572:ILE:HB | 1.92 | 0.51 |
| 2:I:1136:GLN:HG2 | 2:I:1137:GLU:H | 1.74 | 0.51 |
| 3:J:429:LEU:HB3 | 3:J:925:GLU:CB | 2.38 | 0.51 |
| 3:J:664:ILE:HD12 | 3:J:681:LYS:HG2 | 1.92 | 0.51 |
| 3:J:1034:PHE:CD1 | 3:J:1114:GLN:HB2 | 2.45 | 0.51 |
| 3:J:45:ASN:O | 3:J:47:ARG:N | 2.42 | 0.51 |
| 5:L:291:CYS:O | 5:L:295:CYS:HB2 | 2.10 | 0.51 |
| 5:L:389:SER:HA | 5:L:392:LYS:HE2 | 1.92 | 0.51 |
| 6:P:69:DT:H1' | 6:P:70:DT:H5' | 1.92 | 0.51 |
| 7:Q:19:DT:H2'' | 7:Q:20:DA:O5' | 2.10 | 0.51 |
| 1:R:290:LEU:HA | 1:R:295:LEU:CD2 | 2.40 | 0.51 |
| 2:I:384:LEU:O | 2:I:388:LEU:HG | 2.10 | 0.51 |
| 2:I:1119:MET:HE3 | 2:I:1210:ILE:HD11 | 1.92 | 0.51 |
| 2:I:1311:GLY:O | 4:K:31:GLN:NE2 | 2.38 | 0.51 |
| 3:J:126:LEU:HD11 | 3:J:223:LEU:HD22 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:287:ALA:HB1 | 3:J:288:PRO:HD2 | 1.91 | 0.51 |
| 3:J:294:ASN:ND2 | 5:L:406:GLN:HE21 | 2.08 | 0.51 |
| 3:J:660:GLU:HB3 | 3:J:685:ILE:HD11 | 1.93 | 0.51 |
| 3:J:697:MET:HE1 | 3:J:737:ILE:HG22 | 1.91 | 0.51 |
| 3:J:807:LEU:HD23 | 3:J:1255:VAL:CG2 | 2.39 | 0.51 |
| 3:J:961:SER:O | 3:J:980:THR:HA | 2.10 | 0.51 |
| 5:L:471:LEU:HA | 5:L:476:ARG:O | 2.10 | 0.51 |
| 1:R:256:PRO:HA | 1:R:276:HIS:O | 2.11 | 0.51 |
| 1:H:74:VAL:HG13 | 1:H:132:HIS:O | 2.09 | 0.51 |
| 1:H:76:GLU:OE2 | 1:H:132:HIS:HB2 | 2.10 | 0.51 |
| 2:I:118:LYS:CE | 2:I:488:MET:HA | 2.41 | 0.51 |
| 2:I:171:LEU:HD22 | 2:I:188:PHE:O | 2.10 | 0.51 |
| 3:J:482:ALA:HA | 4:K:6:VAL:HG21 | 1.93 | 0.51 |
| 3:J:526:VAL:HG12 | 3:J:549:LYS:HB2 | 1.91 | 0.51 |
| 3:J:733:SER:O | 3:J:737:ILE:HG12 | 2.10 | 0.51 |
| 3:J:785:ASP:O | 3:J:788:LEU:N | 2.39 | 0.51 |
| 3:J:1267:VAL:HG22 | 3:J:1303:SER:HB2 | 1.91 | 0.51 |
| 5:L:234:THR:O | 5:L:245:ALA:HB2 | 2.11 | 0.51 |
| 5:L:429:THR:HA | 6:P:53:DT:C7 | 2.40 | 0.51 |
| 5:L:452:ILE:HG13 | 5:L:457:ILE:HG13 | 1.92 | 0.51 |
| 1:R:307:LEU:HA | 1:R:312:LEU:HB2 | 1.91 | 0.51 |
| 3:J:1037:PHE:CE2 | 3:J:1059:LEU:HD12 | 2.46 | 0.51 |
| 5:L:122:ARG:NH1 | 5:L:378:GLU:OE1 | 2.44 | 0.51 |
| 5:L:151:VAL:CG2 | 5:L:161:LEU:HD22 | 2.40 | 0.51 |
| 5:L:388:ILE:O | 5:L:392:LYS:HG3 | 2.10 | 0.51 |
| 1:G:50:SER:HB3 | 1:H:8:PHE:HZ | 1.76 | 0.51 |
| 1:H:100:LEU:HG | 1:H:118:ASP:OD2 | 2.11 | 0.51 |
| 2:I:75:LEU:HD11 | 2:I:127:ILE:CD1 | 2.29 | 0.51 |
| 2:I:689:ALA:HB2 | 2:I:1233:LEU:HD12 | 1.93 | 0.51 |
| 2:I:901:LEU:HD22 | 5:L:565:ILE:CD1 | 2.41 | 0.51 |
| 3:J:79:LYS:HG2 | 5:L:569:THR:HA | 1.92 | 0.51 |
| 3:J:291:ILE:HD13 | 5:L:409:ASN:HB3 | 1.93 | 0.51 |
| 3:J:416:ILE:HG21 | 3:J:441:LEU:CD2 | 2.41 | 0.51 |
| 3:J:902:ASP:HA | 3:J:903:LEU:CD2 | 2.40 | 0.51 |
| 5:L:98:VAL:HG22 | 5:L:402:LEU:CD1 | 2.30 | 0.51 |
| 6:P:75:DA:H1' | 6:P:76:DT:H5' | 1.93 | 0.51 |
| 1:H:185:TYR:HB2 | 1:H:201:LEU:CD1 | 2.41 | 0.51 |
| 2:I:135:THR:OG1 | 2:I:142:GLU:OE2 | 2.11 | 0.51 |
| 2:I:1153:ALA:HB3 | 2:I:1194:GLU:OE2 | 2.11 | 0.51 |
| 3:J:54:ASP:OD1 | 3:J:54:ASP:N | 2.42 | 0.51 |
| 3:J:139:LEU:HA | 3:J:181:GLY:HA2 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:J:360:TYR:OH | 3:J:448:GLN:OE1 | 2.12 | 0.51 |
| 3:J:369:PRO:HA | 3:J:442:ILE:O | 2.11 | 0.51 |
| 3:J:978:ARG:NH1 | 3:J:999:TYR:H | 2.07 | 0.51 |
| 5:L:276:MET:O | 5:L:280:VAL:HG23 | 2.11 | 0.51 |
| 1:G:57:THR:HG21 | 1:G:147:GLN:NE2 | 2.26 | 0.51 |
| 1:G:234:LEU:HD22 | 1:H:13:LEU:CD2 | 2.40 | 0.51 |
| 1:H:115:ILE:HG22 | 1:H:116:THR:O | 2.10 | 0.51 |
| 1:H:196:THR:HG21 | 3:J:443:GLU:CG | 2.39 | 0.51 |
| 2:I:699:LEU:HB2 | 2:I:799:ASN:HD22 | 1.75 | 0.51 |
| 2:I:1136:GLN:HG2 | 2:I:1137:GLU:N | 2.26 | 0.51 |
| 3:J:140:TYR:O | 3:J:297:ARG:HD3 | 2.11 | 0.51 |
| 3:J:670:SER:O | 3:J:672:LEU:HD12 | 2.10 | 0.51 |
| 3:J:788:LEU:O | 3:J:788:LEU:HD23 | 2.11 | 0.51 |
| 3:J:902:ASP:HB2 | 3:J:903:LEU:C | 2.31 | 0.51 |
| 4:K:38:LEU:CD2 | 4:K:58:LEU:HD13 | 2.41 | 0.51 |
| 5:L:320:ILE:HG12 | 5:L:327:SER:O | 2.11 | 0.51 |
| 5:L:551:LEU:CD2 | 5:L:597:LYS:HD2 | 2.40 | 0.51 |
| 6:P:40:DC:H2" | 6:P:41:DT:C6 | 2.46 | 0.51 |
| 1:H:205:MET:HE1 | 1:H:217:ILE:HG13 | 1.91 | 0.51 |
| 1:H:214:GLU:HG2 | 1:H:218:ARG:NH1 | 2.21 | 0.51 |
| 2:I:877:VAL:HG11 | 2:I:883:LEU:HD21 | 1.91 | 0.51 |
| 3:J:153:ASN:O | 3:J:154:LEU:HD12 | 2.10 | 0.51 |
| 3:J:282:LEU:HD13 | 3:J:291:ILE:HG22 | 1.91 | 0.51 |
| 3:J:876:SER:HA | 3:J:990:ARG:HH21 | 1.75 | 0.51 |
| 3:J:968:ASN:ND2 | 3:J:972:LYS:HB2 | 2.26 | 0.51 |
| 3:J:1271:SER:OG | 3:J:1297:LYS:HD3 | 2.10 | 0.51 |
| 3:J:1287:ILE:HD12 | 3:J:1288:ALA:N | 2.26 | 0.51 |
| 2:I:13:LYS:HB2 | 2:I:1180:MET:HE2 | 1.92 | 0.51 |
| 2:I:94:ALA:HB2 | 2:I:129:LEU:HD11 | 1.93 | 0.51 |
| 2:I:856:ASN:HA | 5:L:613:ASP:HB2 | 1.93 | 0.51 |
| 2:I:1267:GLY:HA3 | 3:J:347:VAL:O | 2.10 | 0.51 |
| 3:J:1350:ASN:HD22 | 3:J:1358:PRO:HD3 | 1.76 | 0.51 |
| 5:L:225:ARG:O | 5:L:229:VAL:HG22 | 2.11 | 0.51 |
| 6:P:78:DT:H2" | 6:P:79:DA:C8 | 2.46 | 0.51 |
| 6:P:80:DG:H2" | 6:P:81:DA:C8 | 2.45 | 0.51 |
| 1:G:228:LEU:HD21 | 1:H:221:ALA:O | 2.10 | 0.50 |
| 1:G:231:PHE:HZ | 1:H:201:LEU:HD23 | 1.75 | 0.50 |
| 2:I:452:ARG:NH2 | 2:I:458:GLU:OE1 | 2.43 | 0.50 |
| 2:I:809:GLY:O | 3:J:357:VAL:HG11 | 2.10 | 0.50 |
| 3:J:412:LEU:HD23 | 3:J:416:ILE:HG13 | 1.93 | 0.50 |
| 3:J:611:ILE:HG22 | 3:J:612:LEU:HD12 | 1.92 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:707:ILE:HD11 | 3:J:714:GLU:HB3 | 1.93 | 0.50 |
| 1:R:270:LEU:HD21 | 1:R:281:LEU:HD13 | 1.94 | 0.50 |
| 1:G:25:LYS:HG2 | 1:G:204:GLU:HB3 | 1.93 | 0.50 |
| 1:H:155:ALA:N | 1:H:174:ASP:OD1 | 2.44 | 0.50 |
| 2:I:297:VAL:HG12 | 2:I:315:MET:O | 2.12 | 0.50 |
| 2:I:964:LEU:HD22 | 2:I:1025:PHE:CD2 | 2.45 | 0.50 |
| 2:I:1245:ALA:HB3 | 3:J:375:GLU:HG2 | 1.93 | 0.50 |
| 3:J:144:TYR:N | 3:J:160:LEU:O | 2.44 | 0.50 |
| 3:J:658:GLU:O | 3:J:661:VAL:HG22 | 2.11 | 0.50 |
| 3:J:807:LEU:CD2 | 3:J:1255:VAL:HG23 | 2.41 | 0.50 |
| 1:G:54:CYS:SG | 1:G:92:VAL:HG22 | 2.51 | 0.50 |
| 2:I:71:VAL:HB | 2:I:99:LYS:O | 2.10 | 0.50 |
| 2:I:636:CYS:HB2 | 2:I:645:PHE:HD2 | 1.75 | 0.50 |
| 2:I:1101:LEU:HD23 | 3:J:725:MET:SD | 2.52 | 0.50 |
| 3:J:391:ALA:HB2 | 3:J:400:MET:SD | 2.51 | 0.50 |
| 3:J:679:TYR:OH | 3:J:754:ILE:O | 2.27 | 0.50 |
| 3:J:707:ILE:CD1 | 3:J:714:GLU:HB3 | 2.41 | 0.50 |
| 3:J:1169:THR:CG2 | 3:J:1171:GLY:H | 2.24 | 0.50 |
| 5:L:300:LYS:O | 5:L:304:THR:OG1 | 2.14 | 0.50 |
| 1:R:300:LEU:HA | 1:R:303:ILE:CD1 | 2.33 | 0.50 |
| 1:R:321:TRP:CD2 | 1:R:322:PRO:HA | 2.46 | 0.50 |
| 1:H:158:ARG:HB3 | 1:H:172:LEU:HD23 | 1.93 | 0.50 |
| 2:I:818:VAL:CG2 | 2:I:1066:MET:HE1 | 2.41 | 0.50 |
| 2:I:934:PHE:O | 2:I:1048:LYS:HA | 2.11 | 0.50 |
| 2:I:970:GLY:O | 2:I:973:SER:OG | 2.22 | 0.50 |
| 3:J:528:THR:HG22 | 3:J:532:GLU:CD | 2.32 | 0.50 |
| 3:J:1319:PHE:CD1 | 3:J:1342:ASP:HB2 | 2.47 | 0.50 |
| 1:G:124:VAL:O | 1:G:126:PRO:HD3 | 2.11 | 0.50 |
| 1:G:182:ARG:HB3 | 1:G:206:GLU:HB3 | 1.94 | 0.50 |
| 1:H:59:VAL:HG21 | 1:H:85:LEU:CD1 | 2.41 | 0.50 |
| 2:I:39:ILE:HD12 | 2:I:127:ILE:CD1 | 2.41 | 0.50 |
| 2:I:192:ASP:HB3 | 2:I:346:TYR:CD1 | 2.47 | 0.50 |
| 3:J:298:MET:SD | 5:L:402:LEU:HB3 | 2.52 | 0.50 |
| 3:J:701:LEU:HD11 | 3:J:723:TYR:HB2 | 1.93 | 0.50 |
| 5:L:347:ILE:O | 5:L:351:THR:HG23 | 2.11 | 0.50 |
| 7:Q:75:DT:C6 | 7:Q:76:DT:H72 | 2.46 | 0.50 |
| 1:R:253:LEU:HD22 | 1:R:279:GLY:HA2 | 1.94 | 0.50 |
| 1:H:16:ILE:HG13 | 1:H:26:VAL:HG22 | 1.93 | 0.50 |
| 2:I:269:ILE:HG22 | 2:I:274:ILE:HG13 | 1.94 | 0.50 |
| 2:I:978:VAL:HG11 | 2:I:1010:GLN:OE1 | 2.11 | 0.50 |
| 2:I:1109:ILE:HG21 | 3:J:763:PHE:O | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:481:ARG:O | 3:J:485:MET:HB2 | 2.12 | 0.50 |
| 3:J:1163:VAL:HG13 | 3:J:1200:GLU:O | 2.12 | 0.50 |
| 1:H:99:ILE:HG13 | 1:H:144:ILE:O | 2.10 | 0.50 |
| 2:I:812:PHE:CD2 | 2:I:813:GLU:HG2 | 2.47 | 0.50 |
| 2:I:1101:LEU:O | 3:J:731:ARG:HG3 | 2.11 | 0.50 |
| 2:I:1308:ILE:HG21 | 3:J:379:PRO:HB2 | 1.92 | 0.50 |
| 3:J:126:LEU:HD22 | 3:J:219:LYS:HE2 | 1.92 | 0.50 |
| 3:J:1141:VAL:HG22 | 3:J:1237:VAL:HG23 | 1.93 | 0.50 |
| 5:L:248:GLU:HA | 5:L:251:LYS:NZ | 2.27 | 0.50 |
| 2:I:159:SER:OG | 2:I:161:LYS:HB3 | 2.12 | 0.50 |
| 2:I:1212:LEU:HD11 | 2:I:1227:VAL:CG1 | 2.41 | 0.50 |
| 3:J:62:PHE:O | 3:J:98:ARG:HA | 2.11 | 0.50 |
| 3:J:320:ASN:O | 3:J:321:LYS:HG2 | 2.11 | 0.50 |
| 3:J:657:ALA:O | 3:J:661:VAL:HG13 | 2.12 | 0.50 |
| 3:J:805:GLN:OE1 | 3:J:1321:SER:OG | 2.24 | 0.50 |
| 3:J:958:ILE:HD13 | 3:J:984:LEU:CD1 | 2.42 | 0.50 |
| 5:L:230:VAL:O | 5:L:234:THR:HG23 | 2.12 | 0.50 |
| 5:L:296:LYS:HE2 | 5:L:296:LYS:HA | 1.94 | 0.50 |
| 1:G:16:ILE:CD1 | 1:G:214:GLU:HB2 | 2.38 | 0.50 |
| 2:I:1022:LYS:O | 2:I:1026:GLU:HG2 | 2.11 | 0.50 |
| 2:I:1122:LYS:HG2 | 2:I:1229:TYR:CE2 | 2.46 | 0.50 |
| 3:J:38:VAL:CG1 | 3:J:56:LEU:HD12 | 2.41 | 0.50 |
| 3:J:473:THR:OG1 | 3:J:474:LEU:N | 2.44 | 0.50 |
| 3:J:487:THR:O | 3:J:614:LEU:HD21 | 2.12 | 0.50 |
| 3:J:547:ARG:CA | 3:J:573:THR:HG22 | 2.33 | 0.50 |
| 2:I:520:PRO:HG3 | 2:I:714:VAL:HG21 | 1.94 | 0.49 |
| 2:I:967:LEU:CD2 | 2:I:1021:LEU:HD22 | 2.42 | 0.49 |
| 2:I:1304:MET:CE | 2:I:1308:ILE:HD11 | 2.42 | 0.49 |
| 3:J:128:LEU:HD23 | 3:J:192:MET:CE | 2.42 | 0.49 |
| 5:L:124:GLU:O | 5:L:127:ILE:HG13 | 2.11 | 0.49 |
| 5:L:399:LEU:HD23 | 5:L:404:LEU:HD23 | 1.94 | 0.49 |
| 2:I:817:LEU:O | 2:I:817:LEU:HD13 | 2.12 | 0.49 |
| 2:I:1010:GLN:HA | 2:I:1013:GLN:CG | 2.43 | 0.49 |
| 2:I:1024:GLU:O | 2:I:1027:LYS:HG2 | 2.11 | 0.49 |
| 2:I:1253:LEU:HD23 | 5:L:525:ASP:HA | 1.94 | 0.49 |
| 3:J:80:HIS:HB3 | 3:J:83:VAL:CG1 | 2.41 | 0.49 |
| 3:J:268:LEU:O | 3:J:272:VAL:HG23 | 2.11 | 0.49 |
| 3:J:1111:ASP:OD1 | 3:J:1112:GLY:N | 2.44 | 0.49 |
| 3:J:1171:GLY:HA3 | 3:J:1172:LYS:CB | 2.41 | 0.49 |
| 4:K:38:LEU:HD22 | 4:K:58:LEU:CD1 | 2.42 | 0.49 |
| 6:P:25:DA:H2' | 6:P:26:DT:H72 | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:50:SER:HB3 | 1:H:8:PHE:CZ | 2.48 | 0.49 |
| 1:H:103:ASN:HB3 | 1:H:141:SER:CA | 2.33 | 0.49 |
| 2:I:866:ASP:HB3 | 2:I:872:TYR:CZ | 2.47 | 0.49 |
| 2:I:976:ARG:HB2 | 2:I:997:TRP:HZ2 | 1.78 | 0.49 |
| 2:I:1307:ASN:HB3 | 2:I:1312:ASN:O | 2.12 | 0.49 |
| 2:I:1339:LEU:HD23 | 3:J:17:PHE:CG | 2.47 | 0.49 |
| 3:J:79:LYS:CG | 5:L:569:THR:HG22 | 2.41 | 0.49 |
| 3:J:978:ARG:HE | 3:J:1197:ASN:HD21 | 1.59 | 0.49 |
| 6:P:27:DT:C1' | 6:P:28:DG:H5' | 2.42 | 0.49 |
| 2:I:149:LEU:HG | 2:I:451:ARG:HG2 | 1.94 | 0.49 |
| 2:I:240:GLU:HG2 | 2:I:284:LEU:HD13 | 1.93 | 0.49 |
| 2:I:1108:ASN:OD1 | 2:I:1111:GLN:NE2 | 2.45 | 0.49 |
| 2:I:1276:TRP:CE2 | 3:J:801:VAL:HG21 | 2.47 | 0.49 |
| 3:J:78:LEU:HD12 | 3:J:81:ARG:HB2 | 1.94 | 0.49 |
| 3:J:279:LEU:HD11 | 3:J:296:LYS:CG | 2.41 | 0.49 |
| 3:J:1028:ILE:HG22 | 3:J:1120:THR:CA | 2.41 | 0.49 |
| 1:G:133:LEU:HD21 | 1:G:140:ILE:HG12 | 1.94 | 0.49 |
| 1:H:214:GLU:O | 1:H:218:ARG:NH1 | 2.46 | 0.49 |
| 2:I:81:ASP:N | 2:I:81:ASP:OD1 | 2.43 | 0.49 |
| 2:I:577:VAL:HG23 | 2:I:661:VAL:O | 2.12 | 0.49 |
| 2:I:594:VAL:HG13 | 2:I:598:VAL:O | 2.12 | 0.49 |
| 2:I:978:VAL:O | 2:I:1007:LYS:HE2 | 2.13 | 0.49 |
| 3:J:357:VAL:HG22 | 3:J:461:PHE:HD2 | 1.74 | 0.49 |
| 3:J:442:ILE:HG22 | 3:J:443:GLU:O | 2.13 | 0.49 |
| 3:J:796:LEU:O | 3:J:800:LEU:HD13 | 2.12 | 0.49 |
| 3:J:822:MET:CB | 3:J:839:VAL:HG22 | 2.42 | 0.49 |
| 3:J:1272:SER:CB | 3:J:1273:ASP:HB3 | 2.38 | 0.49 |
| 1:R:260:LEU:CD1 | 1:R:281:LEU:HD22 | 2.43 | 0.49 |
| 1:R:265:ARG:HE | 1:R:294:ASN:HB3 | 1.77 | 0.49 |
| 1:H:85:LEU:HD22 | 1:H:144:ILE:CD1 | 2.43 | 0.49 |
| 2:I:145:ILE:HG22 | 2:I:456:VAL:HG22 | 1.95 | 0.49 |
| 2:I:155:VAL:HA | 2:I:175:ARG:O | 2.12 | 0.49 |
| 2:I:447:HIS:CE1 | 2:I:609:ILE:HG22 | 2.48 | 0.49 |
| 2:I:521:LEU:HB2 | 2:I:794:LEU:HD21 | 1.95 | 0.49 |
| 2:I:680:LEU:O | 2:I:684:ASN:HB2 | 2.13 | 0.49 |
| 2:I:808:ASN:OD1 | 2:I:1216:ARG:NH2 | 2.45 | 0.49 |
| 2:I:971:LEU:CD2 | 2:I:975:ILE:HD11 | 2.43 | 0.49 |
| 2:I:982:GLY:O | 2:I:1007:LYS:NZ | 2.36 | 0.49 |
| 2:I:1250:SER:OG | 5:L:524:GLU:OE1 | 2.23 | 0.49 |
| 3:J:537:TYR:CE1 | 3:J:544:LEU:HB2 | 2.48 | 0.49 |
| 3:J:836:ARG:O | 3:J:840:LEU:HB2 | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:L:315:TRP:O | 5:L:319:ALA:HB2 | 2.11 | 0.49 |
| 1:R:303:ILE:O | 1:R:307:LEU:HG | 2.13 | 0.49 |
| 1:G:195:ARG:HG2 | 1:G:198:LEU:HG | 1.94 | 0.49 |
| 2:I:270:THR:H | 2:I:273:HIS:HD2 | 1.59 | 0.49 |
| 2:I:375:PRO:HD3 | 5:L:103:ARG:HG2 | 1.95 | 0.49 |
| 3:J:154:LEU:HD22 | 3:J:176:PHE:HE1 | 1.77 | 0.49 |
| 3:J:252:LEU:O | 3:J:252:LEU:HD23 | 2.13 | 0.49 |
| 3:J:514:THR:HG23 | 3:J:595:ALA:O | 2.13 | 0.49 |
| 5:L:105:MET:CE | 5:L:388:ILE:HD12 | 2.42 | 0.49 |
| 5:L:125:ASP:O | 5:L:129:GLN:HG3 | 2.11 | 0.49 |
| 1:G:67:GLU:HB3 | 1:G:171:LEU:CD1 | 2.43 | 0.49 |
| 1:H:183:ILE:HD12 | 1:H:183:ILE:O | 2.12 | 0.49 |
| 2:I:14:ASP:HA | 2:I:1183:ALA:HB3 | 1.94 | 0.49 |
| 2:I:1331:ARG:HG3 | 3:J:33:TRP:CH2 | 2.48 | 0.49 |
| 3:J:596:LEU:HD11 | 3:J:604:MET:HE3 | 1.95 | 0.49 |
| 3:J:809:VAL:HG21 | 3:J:909:ILE:HG12 | 1.95 | 0.49 |
| 1:G:45:ARG:HD3 | 2:I:1083:GLU:HB3 | 1.95 | 0.49 |
| 2:I:74:ARG:NH2 | 2:I:97:ARG:HG3 | 2.28 | 0.49 |
| 2:I:1120:ALA:HA | 2:I:1199:LEU:HD23 | 1.95 | 0.49 |
| 2:I:1304:MET:O | 2:I:1308:ILE:HG12 | 2.12 | 0.49 |
| 3:J:34:SER:OG | 3:J:103:GLY:HA2 | 2.13 | 0.49 |
| 3:J:149:GLY:O | 3:J:152:THR:OG1 | 2.22 | 0.49 |
| 3:J:468:VAL:HG23 | 3:J:468:VAL:O | 2.13 | 0.49 |
| 3:J:1184:ASP:N | 3:J:1185:PRO:HD3 | 2.27 | 0.49 |
| 1:R:307:LEU:O | 1:R:312:LEU:N | 2.26 | 0.49 |
| 1:G:36:GLY:HA3 | 1:G:187:VAL:HG11 | 1.95 | 0.49 |
| 1:H:205:MET:HE3 | 1:H:213:PRO:CA | 2.43 | 0.49 |
| 2:I:636:CYS:SG | 2:I:650:VAL:HG12 | 2.52 | 0.49 |
| 3:J:950:ILE:O | 3:J:1016:THR:HG23 | 2.12 | 0.49 |
| 3:J:1035:VAL:HG21 | 3:J:1115:ILE:HG23 | 1.95 | 0.49 |
| 5:L:165:PHE:HE2 | 5:L:217:ALA:HB1 | 1.78 | 0.49 |
| 5:L:286:LEU:O | 5:L:290:LEU:HG | 2.13 | 0.49 |
| 5:L:402:LEU:HG | 5:L:405:ILE:HD11 | 1.95 | 0.49 |
| 1:R:250:ASP:HB2 | 1:R:253:LEU:HD12 | 1.95 | 0.49 |
| 1:G:190:ALA:HB2 | 1:G:200:LYS:HB2 | 1.95 | 0.48 |
| 2:I:133:ASN:HB3 | 2:I:527:LYS:HZ3 | 1.77 | 0.48 |
| 2:I:299:LYS:HG3 | 2:I:334:GLU:OE2 | 2.13 | 0.48 |
| 2:I:1030:GLU:O | 2:I:1034:ARG:HG2 | 2.13 | 0.48 |
| 3:J:105:ILE:HD13 | 3:J:273:ILE:HG12 | 1.95 | 0.48 |
| 3:J:1071:GLY:HA2 | 3:J:1074:LEU:HD12 | 1.95 | 0.48 |
| 3:J:1328:THR:HG22 | 3:J:1332:LEU:HD23 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:L:142:THR:O | 5:L:146:GLU:HG3 | 2.13 | 0.48 |
| 7:Q:49:DC:H2'' | 7:Q:50:DC:C5' | 2.43 | 0.48 |
| 2:I:839:VAL:HG21 | 2:I:841:ARG:HH12 | 1.78 | 0.48 |
| 3:J:423:LEU:HB3 | 3:J:466:MET:HE2 | 1.95 | 0.48 |
| 3:J:536:LEU:HD13 | 3:J:541:LEU:HB2 | 1.95 | 0.48 |
| 1:H:47:LEU:CD2 | 1:H:220:ALA:HB2 | 2.43 | 0.48 |
| 2:I:251:ALA:HB3 | 2:I:263:VAL:HG11 | 1.95 | 0.48 |
| 2:I:1010:GLN:HA | 2:I:1013:GLN:HG2 | 1.95 | 0.48 |
| 2:I:1289:GLU:OE1 | 3:J:473:THR:HG22 | 2.13 | 0.48 |
| 3:J:647:PRO:HG3 | 3:J:697:MET:HA | 1.94 | 0.48 |
| 3:J:800:LEU:O | 3:J:803:VAL:HG12 | 2.13 | 0.48 |
| 5:L:363:ARG:O | 5:L:367:ILE:HG13 | 2.13 | 0.48 |
| 1:R:300:LEU:HD13 | 1:R:304:LYS:HE2 | 1.94 | 0.48 |
| 1:R:307:LEU:CA | 1:R:312:LEU:HB2 | 2.44 | 0.48 |
| 1:H:98:VAL:HG22 | 1:H:100:LEU:HD11 | 1.94 | 0.48 |
| 1:H:101:THR:HG22 | 1:H:116:THR:CG2 | 2.43 | 0.48 |
| 2:I:251:ALA:CB | 2:I:263:VAL:HG11 | 2.43 | 0.48 |
| 2:I:360:LEU:HD22 | 2:I:378:ARG:NH2 | 2.28 | 0.48 |
| 2:I:624:ASP:OD1 | 2:I:625:GLU:HG2 | 2.12 | 0.48 |
| 2:I:1085:MET:CE | 2:I:1085:MET:HA | 2.43 | 0.48 |
| 5:L:470:MET:HB2 | 5:L:478:PRO:HG3 | 1.95 | 0.48 |
| 1:R:257:VAL:HA | 1:R:260:LEU:HG | 1.95 | 0.48 |
| 1:H:98:VAL:HG22 | 1:H:100:LEU:CD1 | 2.44 | 0.48 |
| 2:I:557:ARG:NH2 | 2:I:611:GLU:OE1 | 2.46 | 0.48 |
| 2:I:646:SER:HB3 | 2:I:649:GLN:CG | 2.43 | 0.48 |
| 3:J:401:VAL:HG12 | 3:J:408:VAL:CG1 | 2.44 | 0.48 |
| 3:J:742:GLY:O | 3:J:762:ASN:HB3 | 2.12 | 0.48 |
| 3:J:850:LYS:CG | 3:J:851:PRO:HD2 | 2.44 | 0.48 |
| 5:L:139:GLU:HA | 5:L:142:THR:OG1 | 2.13 | 0.48 |
| 5:L:287:ILE:CD1 | 5:L:341:LEU:HD12 | 2.41 | 0.48 |
| 5:L:425:TYR:CE1 | 6:P:51:DT:H5'' | 2.49 | 0.48 |
| 8:L:701:1N7:H31 | 8:L:701:1N7:H14 | 1.96 | 0.48 |
| 2:I:148:GLN:O | 2:I:453:ILE:HA | 2.13 | 0.48 |
| 2:I:560:PRO:CB | 3:J:776:THR:HG21 | 2.42 | 0.48 |
| 3:J:960:LEU:HD23 | 3:J:963:VAL:HG11 | 1.95 | 0.48 |
| 3:J:1108:GLN:HG3 | 3:J:1109:LEU:CD1 | 2.42 | 0.48 |
| 3:J:1155:ILE:HG13 | 3:J:1211:SER:OG | 2.12 | 0.48 |
| 5:L:127:ILE:HD12 | 5:L:128:ASN:N | 2.28 | 0.48 |
| 7:Q:32:DA:H2'' | 7:Q:33:DA:O5' | 2.14 | 0.48 |
| 1:G:43:LEU:HD13 | 1:G:217:ILE:HD11 | 1.96 | 0.48 |
| 1:G:104:LYS:HG2 | 1:G:110:VAL:HG22 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:56:VAL:HG13 | 2:I:57:PHE:CD2 | 2.48 | 0.48 |
| 2:I:689:ALA:HB1 | 2:I:1233:LEU:HD12 | 1.96 | 0.48 |
| 2:I:1003:THR:O | 2:I:1008:GLN:HB2 | 2.14 | 0.48 |
| 2:I:1250:SER:OG | 5:L:524:GLU:HB2 | 2.14 | 0.48 |
| 3:J:66:LYS:HE2 | 3:J:69:GLU:OE1 | 2.12 | 0.48 |
| 3:J:518:VAL:HG11 | 3:J:707:ILE:CG1 | 2.44 | 0.48 |
| 3:J:770:LEU:HD22 | 3:J:770:LEU:HA | 1.56 | 0.48 |
| 3:J:950:ILE:HG13 | 3:J:1020:TRP:CH2 | 2.49 | 0.48 |
| 5:L:555:GLU:O | 5:L:558:VAL:HG12 | 2.13 | 0.48 |
| 1:R:252:ILE:HG12 | 1:R:278:ILE:CD1 | 2.44 | 0.48 |
| 1:G:90:VAL:CG1 | 1:G:146:VAL:HG11 | 2.42 | 0.48 |
| 2:I:242:VAL:HG12 | 2:I:244:GLU:OE1 | 2.14 | 0.48 |
| 2:I:274:ILE:O | 2:I:278:GLU:HG3 | 2.14 | 0.48 |
| 2:I:303:ASP:OD1 | 2:I:328:SER:HB2 | 2.13 | 0.48 |
| 2:I:431:LYS:O | 2:I:435:ILE:HG22 | 2.13 | 0.48 |
| 2:I:757:THR:HG23 | 2:I:765:ILE:HG23 | 1.95 | 0.48 |
| 2:I:975:ILE:HG12 | 2:I:1014:LEU:CG | 2.43 | 0.48 |
| 2:I:1184:THR:HG23 | 2:I:1189:GLY:CA | 2.44 | 0.48 |
| 2:I:1259:LEU:HD23 | 2:I:1264:GLN:HG2 | 1.96 | 0.48 |
| 3:J:103:GLY:O | 3:J:244:VAL:HG22 | 2.14 | 0.48 |
| 3:J:262:THR:HG23 | 3:J:263:SER:O | 2.14 | 0.48 |
| 3:J:668:PHE:HA | 3:J:673:VAL:HG22 | 1.95 | 0.48 |
| 6:P:66:DG:H2'' | 6:P:67:DA:H5' | 1.94 | 0.48 |
| 7:Q:20:DA:H2'' | 7:Q:21:DT:O5' | 2.14 | 0.48 |
| 1:G:184:ALA:HB2 | 2:I:1090:ASN:O | 2.14 | 0.48 |
| 2:I:124:MET:HE1 | 2:I:493:ILE:CD1 | 2.44 | 0.48 |
| 2:I:232:ILE:HG12 | 2:I:237:LEU:HD22 | 1.95 | 0.48 |
| 3:J:80:HIS:HB3 | 3:J:83:VAL:HG11 | 1.96 | 0.48 |
| 3:J:925:GLU:HG3 | 3:J:926:PRO:CD | 2.44 | 0.48 |
| 6:P:17:DA:H2'' | 6:P:18:DC:C6 | 2.49 | 0.48 |
| 2:I:141:THR:O | 2:I:143:ARG:HG3 | 2.13 | 0.48 |
| 2:I:322:LEU:HA | 2:I:325:LEU:HD21 | 1.95 | 0.48 |
| 2:I:636:CYS:HB2 | 2:I:645:PHE:CD2 | 2.49 | 0.48 |
| 2:I:1212:LEU:HD22 | 2:I:1225:VAL:CG2 | 2.31 | 0.48 |
| 4:K:44:ASP:HB2 | 4:K:49:ILE:HG13 | 1.96 | 0.48 |
| 5:L:151:VAL:CG2 | 5:L:156:ALA:HB3 | 2.35 | 0.48 |
| 5:L:227:GLN:HA | 5:L:230:VAL:CG1 | 2.42 | 0.48 |
| 5:L:244:THR:HA | 5:L:247:GLU:OE1 | 2.14 | 0.48 |
| 7:Q:70:DA:H2' | 7:Q:71:DT:H72 | 1.95 | 0.48 |
| 1:H:74:VAL:HG12 | 1:H:76:GLU:N | 2.14 | 0.47 |
| 1:H:188:GLU:O | 1:H:200:LYS:HB3 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:I:53:PHE:O | 2:I:57:PHE:HB2 | 2.14 | 0.47 |
| 2:I:463:GLN:HG3 | 2:I:505:PHE:HB2 | 1.96 | 0.47 |
| 2:I:854:ILE:HG23 | 2:I:855:PRO:HD2 | 1.95 | 0.47 |
| 2:I:1342:GLU:HG3 | 3:J:18:ASP:OD2 | 2.14 | 0.47 |
| 3:J:513:MET:CE | 3:J:579:LEU:HB2 | 2.43 | 0.47 |
| 3:J:606:ASN:O | 3:J:610:ARG:HG2 | 2.14 | 0.47 |
| 3:J:680:ASN:HA | 3:J:683:ILE:CG2 | 2.41 | 0.47 |
| 3:J:839:VAL:HG12 | 3:J:864:LEU:CD1 | 2.43 | 0.47 |
| 3:J:955:LYS:HE2 | 3:J:1010:GLN:HE22 | 1.79 | 0.47 |
| 3:J:1163:VAL:HA | 3:J:1176:VAL:O | 2.14 | 0.47 |
| 5:L:133:SER:CB | 5:L:365:MET:HB2 | 2.44 | 0.47 |
| 5:L:318:ALA:O | 5:L:322:MET:HG3 | 2.14 | 0.47 |
| 5:L:385:ARG:HH22 | 6:P:55:DC:N4 | 2.12 | 0.47 |
| 5:L:561:MET:HG3 | 5:L:571:TYR:CD2 | 2.48 | 0.47 |
| 1:H:9:LEU:HD23 | 1:H:9:LEU:H | 1.79 | 0.47 |
| 2:I:257:ALA:HB3 | 2:I:262:TYR:CE2 | 2.38 | 0.47 |
| 2:I:396:ASP:OD2 | 2:I:398:SER:HB3 | 2.13 | 0.47 |
| 2:I:599:VAL:HG21 | 2:I:623:LEU:HD22 | 1.97 | 0.47 |
| 2:I:669:PRO:HG3 | 2:I:1069:ARG:NH2 | 2.30 | 0.47 |
| 2:I:757:THR:CG2 | 2:I:765:ILE:HG23 | 2.43 | 0.47 |
| 3:J:46:TYR:CE1 | 5:L:453:PRO:HD3 | 2.49 | 0.47 |
| 3:J:83:VAL:O | 3:J:92:VAL:HG12 | 2.13 | 0.47 |
| 3:J:1328:THR:CG2 | 3:J:1332:LEU:HD23 | 2.44 | 0.47 |
| 4:K:3:ARG:HD3 | 4:K:4:VAL:N | 2.29 | 0.47 |
| 5:L:130:VAL:O | 5:L:134:VAL:HG23 | 2.13 | 0.47 |
| 5:L:227:GLN:HG3 | 5:L:252:LEU:HD13 | 1.96 | 0.47 |
| 5:L:287:ILE:HD13 | 5:L:341:LEU:CD1 | 2.42 | 0.47 |
| 5:L:437:GLN:HB2 | 6:P:49:DC:H41 | 1.80 | 0.47 |
| 1:H:79:LEU:HD12 | 3:J:526:VAL:HG11 | 1.95 | 0.47 |
| 2:I:84:GLU:OE1 | 2:I:84:GLU:N | 2.36 | 0.47 |
| 2:I:91:THR:HG21 | 2:I:503:LYS:NZ | 2.29 | 0.47 |
| 2:I:445:ILE:HG12 | 2:I:451:ARG:HH21 | 1.78 | 0.47 |
| 3:J:53:ARG:O | 3:J:53:ARG:HD3 | 2.15 | 0.47 |
| 3:J:351:GLY:O | 3:J:467:ALA:HA | 2.15 | 0.47 |
| 3:J:683:ILE:HD11 | 3:J:754:ILE:HG21 | 1.96 | 0.47 |
| 3:J:968:ASN:OD1 | 3:J:972:LYS:N | 2.43 | 0.47 |
| 5:L:281:ARG:HA | 5:L:284:GLU:HB2 | 1.95 | 0.47 |
| 5:L:586:ARG:HD3 | 6:P:25:DA:OP2 | 2.13 | 0.47 |
| 6:P:63:DT:C6 | 6:P:64:DT:H72 | 2.49 | 0.47 |
| 1:G:31:LEU:HB2 | 1:G:199:ASP:O | 2.13 | 0.47 |
| 2:I:599:VAL:HG21 | 2:I:623:LEU:CD2 | 2.45 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:623:LEU:HB2 | 2:I:628:HIS:O | 2.15 | 0.47 |
| 2:I:718:ALA:HB2 | 2:I:783:LEU:CD2 | 2.32 | 0.47 |
| 2:I:737:ASN:O | 2:I:741:MET:HB2 | 2.14 | 0.47 |
| 2:I:817:LEU:HD23 | 2:I:1078:LYS:HB3 | 1.96 | 0.47 |
| 2:I:1140:LYS:O | 2:I:1143:GLU:HG3 | 2.14 | 0.47 |
| 2:I:1275:VAL:HG13 | 2:I:1287:LEU:HD11 | 1.95 | 0.47 |
| 3:J:482:ALA:CB | 4:K:6:VAL:HG21 | 2.45 | 0.47 |
| 3:J:744:ARG:HD3 | 3:J:759:ILE:HB | 1.95 | 0.47 |
| 3:J:1077:ALA:HB2 | 3:J:1100:PHE:CD1 | 2.49 | 0.47 |
| 4:K:6:VAL:O | 4:K:10:VAL:HG23 | 2.14 | 0.47 |
| 5:L:161:LEU:HD12 | 5:L:265:GLN:NE2 | 2.29 | 0.47 |
| 5:L:286:LEU:HD23 | 5:L:340:ALA:CB | 2.44 | 0.47 |
| 6:P:77:DA:H2'' | 6:P:78:DT:OP2 | 2.14 | 0.47 |
| 1:G:68:TYR:HB3 | 2:I:756:TYR:CD2 | 2.48 | 0.47 |
| 2:I:250:THR:HA | 2:I:268:ARG:HA | 1.96 | 0.47 |
| 2:I:660:VAL:HG11 | 3:J:769:VAL:HG13 | 1.97 | 0.47 |
| 2:I:820:GLU:HB2 | 2:I:1080:ASN:O | 2.15 | 0.47 |
| 2:I:1002:LEU:HD23 | 2:I:1003:THR:N | 2.29 | 0.47 |
| 2:I:1067:ALA:CB | 2:I:1235:LEU:HD11 | 2.45 | 0.47 |
| 3:J:720:ASN:HB3 | 3:J:723:TYR:HB3 | 1.95 | 0.47 |
| 3:J:1101:LEU:HB3 | 3:J:1105:ALA:CB | 2.43 | 0.47 |
| 5:L:141:ILE:O | 5:L:145:LEU:HG | 2.14 | 0.47 |
| 6:P:27:DT:H1' | 6:P:28:DG:O4' | 2.14 | 0.47 |
| 1:H:89:ALA:HB3 | 1:H:124:VAL:CG1 | 2.45 | 0.47 |
| 2:I:322:LEU:HA | 2:I:325:LEU:CD2 | 2.45 | 0.47 |
| 2:I:615:VAL:HG21 | 2:I:645:PHE:CD2 | 2.50 | 0.47 |
| 2:I:1251:TYR:HB2 | 5:L:528:LEU:HD11 | 1.97 | 0.47 |
| 3:J:872:LEU:O | 3:J:877:VAL:HG23 | 2.15 | 0.47 |
| 3:J:1005:LYS:HA | 3:J:1009:GLU:OE1 | 2.15 | 0.47 |
| 3:J:1037:PHE:HE2 | 3:J:1059:LEU:HD12 | 1.79 | 0.47 |
| 5:L:387:VAL:HG22 | 5:L:435:ILE:CD1 | 2.42 | 0.47 |
| 5:L:562:ARG:HG2 | 5:L:591:GLU:CD | 2.35 | 0.47 |
| 7:Q:20:DA:H2'' | 7:Q:21:DT:C5' | 2.44 | 0.47 |
| 2:I:39:ILE:HD11 | 2:I:75:LEU:CD1 | 2.44 | 0.47 |
| 2:I:101:ARG:HG3 | 2:I:118:LYS:O | 2.14 | 0.47 |
| 2:I:322:LEU:HD23 | 2:I:325:LEU:HD21 | 1.97 | 0.47 |
| 2:I:515:MET:CE | 2:I:517:GLN:HB3 | 2.45 | 0.47 |
| 2:I:1283:ALA:HA | 3:J:479:GLU:OE1 | 2.15 | 0.47 |
| 3:J:45:ASN:O | 3:J:45:ASN:ND2 | 2.47 | 0.47 |
| 3:J:48:THR:O | 3:J:50:LYS:N | 2.47 | 0.47 |
| 3:J:147:ILE:HG22 | 3:J:188:LEU:CD2 | 2.44 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:518:VAL:HG23 | 3:J:547:ARG:HH12 | 1.79 | 0.47 |
| 3:J:603:LYS:O | 3:J:607:THR:HG23 | 2.14 | 0.47 |
| 3:J:950:ILE:HG13 | 3:J:1020:TRP:HH2 | 1.80 | 0.47 |
| 3:J:952:VAL:CG2 | 3:J:984:LEU:HD22 | 2.44 | 0.47 |
| 3:J:1041:ILE:O | 3:J:1046:ILE:HG12 | 2.14 | 0.47 |
| 3:J:1178:THR:HG23 | 3:J:1184:ASP:OD2 | 2.14 | 0.47 |
| 5:L:341:LEU:O | 5:L:345:GLN:HG3 | 2.14 | 0.47 |
| 6:P:36:DA:H2'' | 6:P:37:DA:C8 | 2.50 | 0.47 |
| 2:I:398:SER:O | 2:I:400:VAL:N | 2.48 | 0.47 |
| 2:I:484:LEU:HD12 | 2:I:485:ASP:N | 2.30 | 0.47 |
| 2:I:551:HIS:CE1 | 2:I:553:THR:HG23 | 2.50 | 0.47 |
| 2:I:1212:LEU:HD13 | 2:I:1225:VAL:HG22 | 1.96 | 0.47 |
| 3:J:647:PRO:HG3 | 3:J:697:MET:CA | 2.44 | 0.47 |
| 3:J:665:GLN:O | 3:J:669:GLN:HG3 | 2.15 | 0.47 |
| 3:J:1237:VAL:HG13 | 3:J:1253:ILE:HD13 | 1.96 | 0.47 |
| 6:P:28:DG:H2'' | 6:P:29:DA:O5' | 2.15 | 0.47 |
| 6:P:51:DT:H2'' | 6:P:52:DA:OP1 | 2.15 | 0.47 |
| 2:I:161:LYS:O | 2:I:161:LYS:HG2 | 2.15 | 0.47 |
| 2:I:766:ASN:OD1 | 2:I:767:GLN:N | 2.47 | 0.47 |
| 2:I:802:VAL:CG2 | 2:I:1098:LEU:HD13 | 2.45 | 0.47 |
| 2:I:1250:SER:HG | 5:L:524:GLU:HB2 | 1.79 | 0.47 |
| 3:J:203:GLU:O | 3:J:206:ASN:HB3 | 2.14 | 0.47 |
| 3:J:490:ILE:O | 3:J:491:LEU:HD12 | 2.14 | 0.47 |
| 3:J:825:VAL:O | 3:J:831:VAL:HG23 | 2.14 | 0.47 |
| 3:J:1047:THR:HG22 | 3:J:1060:VAL:HB | 1.97 | 0.47 |
| 7:Q:27:DA:H2' | 7:Q:28:DT:H72 | 1.96 | 0.47 |
| 1:G:25:LYS:HG2 | 1:G:204:GLU:CB | 2.45 | 0.47 |
| 2:I:145:ILE:HB | 2:I:456:VAL:HG22 | 1.97 | 0.47 |
| 2:I:975:ILE:CD1 | 2:I:1014:LEU:HG | 2.45 | 0.47 |
| 2:I:1243:MET:HG3 | 3:J:372:MET:SD | 2.55 | 0.47 |
| 3:J:491:LEU:O | 3:J:904:ALA:HB2 | 2.15 | 0.47 |
| 3:J:700:ASN:O | 3:J:704:GLU:HB2 | 2.14 | 0.47 |
| 3:J:1026:PRO:HB2 | 3:J:1028:ILE:HG23 | 1.96 | 0.47 |
| 3:J:1163:VAL:HG23 | 3:J:1175:LEU:CD1 | 2.45 | 0.47 |
| 3:J:1163:VAL:HG23 | 3:J:1175:LEU:HD11 | 1.97 | 0.47 |
| 3:J:1190:ILE:HG22 | 3:J:1191:PRO:O | 2.15 | 0.47 |
| 3:J:1327:GLU:HG2 | 3:J:1327:GLU:O | 2.15 | 0.47 |
| 5:L:111:LEU:HD13 | 5:L:116:GLU:HG2 | 1.97 | 0.47 |
| 6:P:25:DA:H2' | 6:P:26:DT:C7 | 2.45 | 0.47 |
| 1:R:269:CYS:SG | 1:R:295:LEU:HD12 | 2.55 | 0.47 |
| 1:R:286:GLU:HG2 | 1:R:290:LEU:HD11 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:H:65:LEU:O | 1:H:65:LEU:HD13 | 2.16 | 0.46 |
| 1:H:195:ARG:HB3 | 1:H:198:LEU:HD21 | 1.97 | 0.46 |
| 2:I:16:GLY:HA3 | 2:I:1156:ARG:NH1 | 2.30 | 0.46 |
| 2:I:453:ILE:HD11 | 2:I:587:LEU:CD1 | 2.44 | 0.46 |
| 2:I:691:PRO:HA | 2:I:788:SER:OG | 2.15 | 0.46 |
| 2:I:956:ALA:HB1 | 2:I:1032:LYS:HG2 | 1.97 | 0.46 |
| 3:J:51:PRO:HG2 | 3:J:65:VAL:CG2 | 2.45 | 0.46 |
| 3:J:127:LEU:HD23 | 3:J:189:LEU:HD22 | 1.97 | 0.46 |
| 3:J:479:GLU:CG | 4:K:20:VAL:HG11 | 2.45 | 0.46 |
| 5:L:346:GLN:O | 5:L:350:GLU:HG3 | 2.15 | 0.46 |
| 5:L:511:ILE:O | 5:L:511:ILE:HG23 | 2.14 | 0.46 |
| 1:R:287:VAL:CG1 | 1:R:291:LYS:HE3 | 2.36 | 0.46 |
| 1:R:307:LEU:HD22 | 1:R:312:LEU:HB3 | 1.97 | 0.46 |
| 2:I:633:LEU:O | 2:I:633:LEU:HD12 | 2.14 | 0.46 |
| 3:J:141:PHE:CD1 | 3:J:180:MET:HG3 | 2.50 | 0.46 |
| 3:J:306:LEU:O | 3:J:326:SER:HB2 | 2.15 | 0.46 |
| 3:J:680:ASN:O | 3:J:683:ILE:HG22 | 2.15 | 0.46 |
| 5:L:290:LEU:HD13 | 5:L:333:VAL:HG22 | 1.96 | 0.46 |
| 5:L:420:GLU:OE1 | 5:L:423:ARG:NH1 | 2.45 | 0.46 |
| 5:L:452:ILE:CG1 | 5:L:457:ILE:HG13 | 2.45 | 0.46 |
| 7:Q:77:DT:OP1 | 1:R:298:LYS:HD3 | 2.14 | 0.46 |
| 1:G:229:GLU:HA | 1:G:232:VAL:HG12 | 1.96 | 0.46 |
| 2:I:26:TYR:HE2 | 2:I:32:LEU:HD12 | 1.79 | 0.46 |
| 2:I:148:GLN:OE1 | 2:I:454:ARG:HD2 | 2.15 | 0.46 |
| 2:I:148:GLN:HB3 | 2:I:454:ARG:HB2 | 1.97 | 0.46 |
| 2:I:1109:ILE:HA | 2:I:1109:ILE:HD12 | 1.66 | 0.46 |
| 3:J:17:PHE:HZ | 3:J:1353:VAL:HG21 | 1.79 | 0.46 |
| 3:J:189:LEU:HB3 | 3:J:234:PRO:HB2 | 1.97 | 0.46 |
| 3:J:693:VAL:HG21 | 3:J:743:MET:CE | 2.44 | 0.46 |
| 3:J:813:ASP:OD1 | 3:J:814:CYS:N | 2.48 | 0.46 |
| 3:J:960:LEU:HD13 | 3:J:1007:ASP:CA | 2.45 | 0.46 |
| 5:L:236:LYS:O | 5:L:243:ALA:N | 2.49 | 0.46 |
| 7:Q:48:DC:H2" | 7:Q:49:DC:C6 | 2.51 | 0.46 |
| 1:G:160:HIS:HA | 1:G:161:SER:HA | 1.71 | 0.46 |
| 1:H:67:GLU:OE2 | 1:H:79:LEU:HB3 | 2.15 | 0.46 |
| 3:J:62:PHE:HZ | 3:J:244:VAL:HG21 | 1.79 | 0.46 |
| 3:J:129:ASP:HB2 | 3:J:220:ARG:CZ | 2.46 | 0.46 |
| 3:J:479:GLU:HG3 | 4:K:20:VAL:HG11 | 1.96 | 0.46 |
| 3:J:509:GLY:CA | 3:J:632:ALA:HB2 | 2.46 | 0.46 |
| 5:L:576:VAL:HB | 5:L:587:ILE:CD1 | 2.46 | 0.46 |
| 1:G:135:ASP:OD1 | 1:G:136:GLU:N | 2.49 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:H:100:LEU:HD11 | 1:H:121:VAL:HG21 | 1.96 | 0.46 |
| 1:H:112:ALA:CB | 1:H:126:PRO:HA | 2.40 | 0.46 |
| 1:H:179:PRO:HA | 1:H:208:ASN:ND2 | 2.31 | 0.46 |
| 2:I:56:VAL:HG11 | 2:I:468:LEU:HD13 | 1.98 | 0.46 |
| 2:I:338:THR:HG21 | 2:I:345:PRO:HB3 | 1.97 | 0.46 |
| 3:J:807:LEU:HB2 | 3:J:1259:GLN:NE2 | 2.31 | 0.46 |
| 3:J:1175:LEU:HB2 | 3:J:1190:ILE:CD1 | 2.44 | 0.46 |
| 1:H:185:TYR:HB2 | 1:H:201:LEU:HD12 | 1.98 | 0.46 |
| 2:I:678:ARG:HA | 2:I:678:ARG:HD3 | 1.72 | 0.46 |
| 2:I:1132:LEU:CD2 | 2:I:1141:LEU:HD21 | 2.45 | 0.46 |
| 3:J:128:LEU:HD23 | 3:J:192:MET:HE3 | 1.98 | 0.46 |
| 3:J:327:LEU:O | 3:J:330:MET:HB2 | 2.15 | 0.46 |
| 5:L:479:THR:OG1 | 5:L:480:PRO:HD2 | 2.16 | 0.46 |
| 1:H:76:GLU:N | 1:H:76:GLU:OE1 | 2.48 | 0.46 |
| 2:I:204:LEU:HD13 | 2:I:208:ILE:HD13 | 1.96 | 0.46 |
| 2:I:960:LEU:HB3 | 2:I:1025:PHE:CZ | 2.50 | 0.46 |
| 3:J:141:PHE:HE1 | 3:J:181:GLY:HA3 | 1.77 | 0.46 |
| 3:J:370:LYS:HA | 3:J:441:LEU:HD12 | 1.98 | 0.46 |
| 3:J:829:GLY:HA2 | 3:J:993:GLU:OE1 | 2.16 | 0.46 |
| 3:J:1048:ARG:NE | 3:J:1048:ARG:HA | 2.31 | 0.46 |
| 3:J:1071:GLY:CA | 3:J:1074:LEU:HB2 | 2.44 | 0.46 |
| 1:H:59:VAL:HG21 | 1:H:85:LEU:HD13 | 1.98 | 0.46 |
| 2:I:1253:LEU:HD12 | 3:J:251:PRO:HG3 | 1.98 | 0.46 |
| 3:J:646:ILE:CD1 | 3:J:762:ASN:HD21 | 2.27 | 0.46 |
| 3:J:806:ASP:O | 3:J:808:VAL:HG23 | 2.15 | 0.46 |
| 3:J:1061:VAL:HB | 3:J:1105:ALA:HB3 | 1.98 | 0.46 |
| 5:L:420:GLU:HG3 | 5:L:422:ARG:NH2 | 2.30 | 0.46 |
| 5:L:511:ILE:HG22 | 5:L:517:SER:O | 2.16 | 0.46 |
| 1:R:278:ILE:O | 1:R:282:VAL:HG13 | 2.16 | 0.46 |
| 1:G:97:GLU:HA | 1:G:147:GLN:HA | 1.97 | 0.46 |
| 1:G:140:ILE:HD12 | 1:G:142:MET:HE2 | 1.97 | 0.46 |
| 2:I:103:VAL:HA | 2:I:116:ASP:O | 2.16 | 0.46 |
| 2:I:192:ASP:HB3 | 2:I:346:TYR:CE1 | 2.51 | 0.46 |
| 2:I:1105:SER:HB2 | 3:J:731:ARG:HB3 | 1.98 | 0.46 |
| 3:J:291:ILE:CD1 | 5:L:409:ASN:HB3 | 2.46 | 0.46 |
| 3:J:491:LEU:HD23 | 3:J:496:GLY:O | 2.16 | 0.46 |
| 3:J:712:GLN:N | 3:J:712:GLN:OE1 | 2.48 | 0.46 |
| 3:J:844:THR:CG2 | 3:J:864:LEU:HD11 | 2.46 | 0.46 |
| 6:P:21:DA:C8 | 6:P:22:DT:H72 | 2.50 | 0.46 |
| 6:P:64:DT:H2" | 6:P:65:DT:H71 | 1.98 | 0.46 |
| 6:P:79:DA:H2" | 6:P:80:DG:C8 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:47:LEU:O | 1:G:180:VAL:HG21 | 2.16 | 0.46 |
| 1:G:67:GLU:HB3 | 1:G:171:LEU:HD12 | 1.98 | 0.46 |
| 1:G:83:LEU:HD21 | 2:I:693:LEU:CD2 | 2.44 | 0.46 |
| 2:I:815:SER:HB3 | 2:I:1077:SER:HB3 | 1.98 | 0.46 |
| 2:I:980:VAL:HG22 | 2:I:984:VAL:CG2 | 2.41 | 0.46 |
| 3:J:103:GLY:C | 3:J:244:VAL:HG22 | 2.36 | 0.46 |
| 3:J:735:ALA:O | 3:J:738:ARG:HB3 | 2.16 | 0.46 |
| 3:J:1078:LEU:CD1 | 3:J:1101:LEU:HD11 | 2.40 | 0.46 |
| 5:L:261:LEU:HD23 | 5:L:265:GLN:CB | 2.45 | 0.46 |
| 5:L:290:LEU:HD12 | 5:L:337:VAL:HG22 | 1.98 | 0.46 |
| 6:P:32:DA:H1' | 6:P:33:DA:H5' | 1.98 | 0.46 |
| 1:G:79:LEU:HD13 | 1:G:83:LEU:HD13 | 1.98 | 0.45 |
| 1:H:13:LEU:HA | 1:H:28:LEU:CD2 | 2.43 | 0.45 |
| 1:H:13:LEU:O | 1:H:13:LEU:HG | 2.16 | 0.45 |
| 2:I:292:ILE:O | 2:I:292:ILE:HG22 | 2.16 | 0.45 |
| 2:I:666:SER:O | 2:I:702:THR:OG1 | 2.29 | 0.45 |
| 2:I:830:THR:OG1 | 2:I:831:ILE:N | 2.48 | 0.45 |
| 2:I:886:LYS:HE3 | 2:I:916:SER:O | 2.16 | 0.45 |
| 4:K:39:VAL:CG2 | 4:K:40:PRO:HD2 | 2.46 | 0.45 |
| 5:L:285:ARG:HD3 | 5:L:288:MET:CE | 2.46 | 0.45 |
| 5:L:287:ILE:HG23 | 5:L:337:VAL:CG1 | 2.45 | 0.45 |
| 1:H:107:ILE:HG12 | 1:H:136:GLU:H | 1.81 | 0.45 |
| 1:H:197:ASP:C | 1:H:198:LEU:HD22 | 2.37 | 0.45 |
| 3:J:526:VAL:HA | 3:J:549:LYS:O | 2.16 | 0.45 |
| 3:J:1158:GLU:HG3 | 3:J:1186:TYR:CE1 | 2.51 | 0.45 |
| 6:P:74:DC:H5' | 6:P:74:DC:C6 | 2.51 | 0.45 |
| 1:R:321:TRP:CE3 | 1:R:322:PRO:HA | 2.50 | 0.45 |
| 1:H:31:LEU:O | 1:H:198:LEU:HD12 | 2.16 | 0.45 |
| 2:I:364:VAL:HG13 | 2:I:376:PRO:CG | 2.46 | 0.45 |
| 2:I:905:ILE:HG22 | 2:I:906:PHE:CE1 | 2.52 | 0.45 |
| 2:I:1087:TYR:HD2 | 2:I:1091:GLY:HA2 | 1.80 | 0.45 |
| 2:I:1091:GLY:O | 2:I:1093:PRO:HD3 | 2.16 | 0.45 |
| 3:J:807:LEU:HD22 | 3:J:1259:GLN:HE21 | 1.81 | 0.45 |
| 3:J:1115:ILE:HD12 | 3:J:1115:ILE:O | 2.17 | 0.45 |
| 5:L:254:GLU:OE1 | 5:L:257:LYS:HD3 | 2.17 | 0.45 |
| 5:L:316:PHE:CZ | 5:L:334:SER:HB3 | 2.50 | 0.45 |
| 5:L:411:GLY:O | 5:L:414:LYS:HB3 | 2.16 | 0.45 |
| 3:J:161:THR:HG22 | 3:J:164:GLN:HG3 | 1.99 | 0.45 |
| 3:J:355:ILE:HG21 | 3:J:466:MET:SD | 2.57 | 0.45 |
| 3:J:516:ASP:N | 3:J:516:ASP:OD1 | 2.48 | 0.45 |
| 3:J:708:ASN:N | 3:J:708:ASN:OD1 | 2.48 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:J:955:LYS:HD3 | 3:J:956:GLY:N | 2.31 | 0.45 |
| 3:J:1329:THR:O | 3:J:1333:THR:HG22 | 2.16 | 0.45 |
| 5:L:151:VAL:HG21 | 5:L:161:LEU:CB | 2.44 | 0.45 |
| 5:L:162:ILE:HD13 | 5:L:221:PHE:CZ | 2.46 | 0.45 |
| 6:P:31:DA:H2'' | 6:P:32:DA:C8 | 2.51 | 0.45 |
| 7:Q:28:DT:H2'' | 7:Q:29:DT:H71 | 1.98 | 0.45 |
| 7:Q:78:DG:H1' | 7:Q:79:DT:C5' | 2.47 | 0.45 |
| 1:R:250:ASP:OD2 | 1:R:252:ILE:HG22 | 2.17 | 0.45 |
| 1:H:73:GLY:O | 1:H:133:LEU:HD12 | 2.16 | 0.45 |
| 2:I:702:THR:HG22 | 2:I:1184:THR:O | 2.16 | 0.45 |
| 2:I:889:PRO:HA | 2:I:913:VAL:HG23 | 1.98 | 0.45 |
| 2:I:971:LEU:HD11 | 2:I:1017:GLN:HB3 | 1.97 | 0.45 |
| 2:I:1281:TYR:CE2 | 3:J:484:MET:HG2 | 2.52 | 0.45 |
| 3:J:868:TRP:CE3 | 3:J:871:LEU:HD12 | 2.51 | 0.45 |
| 5:L:380:VAL:O | 5:L:384:LEU:HG | 2.17 | 0.45 |
| 1:G:43:LEU:O | 1:G:47:LEU:HG | 2.17 | 0.45 |
| 1:H:92:VAL:HG12 | 1:H:93:GLN:O | 2.17 | 0.45 |
| 2:I:287:VAL:HG13 | 2:I:288:PRO:HD2 | 1.99 | 0.45 |
| 2:I:301:TYR:HB2 | 2:I:311:CYS:SG | 2.57 | 0.45 |
| 2:I:483:ASP:OD2 | 2:I:486:THR:HG21 | 2.17 | 0.45 |
| 2:I:543:ALA:HA | 2:I:544:GLY:HA3 | 1.60 | 0.45 |
| 2:I:898:GLU:HG2 | 5:L:544:THR:OG1 | 2.17 | 0.45 |
| 3:J:485:MET:HG3 | 3:J:486:SER:H | 1.80 | 0.45 |
| 3:J:579:LEU:HD12 | 3:J:579:LEU:O | 2.17 | 0.45 |
| 3:J:653:ILE:HG21 | 3:J:693:VAL:HG23 | 1.99 | 0.45 |
| 3:J:1027:VAL:O | 3:J:1027:VAL:HG12 | 2.16 | 0.45 |
| 3:J:1029:THR:CG2 | 3:J:1121:LEU:HD11 | 2.47 | 0.45 |
| 5:L:533:ASP:HA | 5:L:536:THR:CG2 | 2.44 | 0.45 |
| 2:I:876:GLU:HA | 2:I:926:GLY:O | 2.16 | 0.45 |
| 2:I:975:ILE:CG1 | 2:I:1014:LEU:HG | 2.43 | 0.45 |
| 2:I:1119:MET:HE1 | 2:I:1210:ILE:HD11 | 1.98 | 0.45 |
| 2:I:1120:ALA:HB2 | 2:I:1199:LEU:CD2 | 2.47 | 0.45 |
| 3:J:140:TYR:O | 3:J:141:PHE:HB2 | 2.16 | 0.45 |
| 3:J:352:ARG:HA | 3:J:466:MET:O | 2.17 | 0.45 |
| 5:L:280:VAL:HG22 | 5:L:347:ILE:HG21 | 1.99 | 0.45 |
| 1:R:257:VAL:HG12 | 1:R:260:LEU:CD1 | 2.46 | 0.45 |
| 1:R:280:ASP:HA | 1:R:283:GLN:HG3 | 1.98 | 0.45 |
| 1:G:92:VAL:HG12 | 1:G:121:VAL:HG22 | 1.99 | 0.45 |
| 1:H:39:LEU:HA | 1:H:39:LEU:HD23 | 1.69 | 0.45 |
| 1:H:98:VAL:HG11 | 1:H:121:VAL:CG2 | 2.46 | 0.45 |
| 1:H:105:SER:CA | 1:H:138:ALA:HB2 | 2.31 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:I:24:VAL:HA | 2:I:578:TYR:HE1 | 1.81 | 0.45 |
| 2:I:303:ASP:CB | 2:I:310:ILE:HD11 | 2.45 | 0.45 |
| 2:I:468:LEU:HA | 2:I:471:VAL:HG12 | 1.98 | 0.45 |
| 2:I:623:LEU:HD12 | 2:I:623:LEU:O | 2.16 | 0.45 |
| 2:I:672:GLU:OE1 | 2:I:672:GLU:N | 2.32 | 0.45 |
| 2:I:960:LEU:HB3 | 2:I:1025:PHE:HE1 | 1.79 | 0.45 |
| 3:J:287:ALA:HA | 5:L:413:MET:HE1 | 1.99 | 0.45 |
| 3:J:298:MET:SD | 5:L:406:GLN:HG3 | 2.56 | 0.45 |
| 3:J:816:THR:HG22 | 3:J:889:ASP:OD2 | 2.17 | 0.45 |
| 3:J:820:ILE:O | 3:J:881:LYS:HA | 2.16 | 0.45 |
| 3:J:884:SER:OG | 3:J:1254:GLU:OE1 | 2.26 | 0.45 |
| 3:J:1061:VAL:HG13 | 3:J:1076:PRO:HG2 | 1.99 | 0.45 |
| 3:J:1208:ASP:OD1 | 3:J:1209:VAL:N | 2.50 | 0.45 |
| 4:K:13:ILE:HD12 | 4:K:54:ILE:CG2 | 2.46 | 0.45 |
| 5:L:218:ARG:HA | 5:L:221:PHE:CD2 | 2.36 | 0.45 |
| 2:I:669:PRO:HD3 | 2:I:1069:ARG:NH1 | 2.31 | 0.45 |
| 2:I:1288:GLN:NE2 | 2:I:1317:PRO:HB3 | 2.31 | 0.45 |
| 3:J:125:GLY:HA2 | 3:J:135:ILE:CD1 | 2.47 | 0.45 |
| 3:J:623:GLN:O | 3:J:627:THR:HG22 | 2.16 | 0.45 |
| 3:J:876:SER:HA | 3:J:990:ARG:NH2 | 2.31 | 0.45 |
| 6:P:50:DA:OP2 | 6:P:50:DA:H2' | 2.17 | 0.45 |
| 1:R:252:ILE:HG12 | 1:R:278:ILE:HD12 | 1.99 | 0.45 |
| 2:I:15:PHE:CD2 | 2:I:1190:ALA:HB2 | 2.52 | 0.45 |
| 2:I:364:VAL:HG13 | 2:I:376:PRO:HG3 | 1.98 | 0.45 |
| 2:I:818:VAL:O | 2:I:1079:ILE:HA | 2.17 | 0.45 |
| 3:J:198:CYS:SG | 3:J:221:ILE:HD11 | 2.57 | 0.45 |
| 3:J:657:ALA:HB2 | 3:J:689:ALA:HB2 | 1.98 | 0.45 |
| 3:J:961:SER:O | 3:J:980:THR:HG23 | 2.16 | 0.45 |
| 3:J:1344:LEU:CD2 | 3:J:1349:GLU:HB3 | 2.41 | 0.45 |
| 5:L:489:MET:HG3 | 5:L:494:ILE:HD11 | 1.99 | 0.45 |
| 7:Q:49:DC:H2'' | 7:Q:50:DC:O5' | 2.16 | 0.45 |
| 1:G:47:LEU:CD2 | 1:G:220:ALA:HB2 | 2.47 | 0.44 |
| 1:G:52:PRO:HA | 1:G:149:GLY:O | 2.16 | 0.44 |
| 1:H:69:SER:HB2 | 1:H:78:ILE:HD11 | 1.98 | 0.44 |
| 2:I:812:PHE:O | 3:J:504:GLN:NE2 | 2.46 | 0.44 |
| 2:I:980:VAL:CA | 2:I:984:VAL:HB | 2.43 | 0.44 |
| 3:J:1346:GLY:O | 3:J:1350:ASN:ND2 | 2.49 | 0.44 |
| 1:H:57:THR:O | 1:H:173:VAL:HB | 2.16 | 0.44 |
| 1:H:102:LEU:HD12 | 1:H:114:ASP:O | 2.17 | 0.44 |
| 1:H:192:VAL:HG12 | 1:H:193:GLU:H | 1.82 | 0.44 |
| 2:I:252:SER:C | 2:I:265:LYS:HG3 | 2.37 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:560:PRO:HG3 | 3:J:773:PHE:HE1 | 1.82 | 0.44 |
| 2:I:893:THR:OG1 | 2:I:894:GLN:N | 2.50 | 0.44 |
| 2:I:1043:ALA:HB1 | 2:I:1044:PRO:HD2 | 2.00 | 0.44 |
| 2:I:1080:ASN:HD22 | 2:I:1085:MET:CE | 2.29 | 0.44 |
| 2:I:1125:GLY:HA3 | 2:I:1179:GLY:HA2 | 1.99 | 0.44 |
| 2:I:1326:LEU:HD12 | 2:I:1326:LEU:HA | 1.73 | 0.44 |
| 3:J:478:LEU:HD23 | 3:J:478:LEU:HA | 1.78 | 0.44 |
| 3:J:485:MET:HB3 | 3:J:488:ASN:ND2 | 2.32 | 0.44 |
| 3:J:812:ASP:HB2 | 3:J:911:LYS:HE2 | 1.99 | 0.44 |
| 5:L:286:LEU:HG | 5:L:290:LEU:HD11 | 1.99 | 0.44 |
| 1:H:104:LYS:H | 1:H:140:ILE:HG23 | 1.82 | 0.44 |
| 2:I:62:TYR:CE1 | 2:I:476:LYS:HE3 | 2.51 | 0.44 |
| 2:I:1075:VAL:HB | 3:J:461:PHE:O | 2.17 | 0.44 |
| 2:I:1113:LEU:HD11 | 3:J:641:ILE:CD1 | 2.47 | 0.44 |
| 2:I:1204:LEU:HB3 | 2:I:1205:PRO:HD2 | 2.00 | 0.44 |
| 3:J:506:VAL:HG23 | 3:J:628:GLY:HA3 | 1.99 | 0.44 |
| 3:J:965:SER:OG | 3:J:973:LEU:HD11 | 2.17 | 0.44 |
| 3:J:1265:THR:OG1 | 3:J:1303:SER:HB3 | 2.17 | 0.44 |
| 5:L:275:VAL:O | 5:L:279:ARG:HG3 | 2.16 | 0.44 |
| 6:P:39:DG:OP2 | 6:P:39:DG:H2' | 2.17 | 0.44 |
| 1:G:102:LEU:HD11 | 1:G:110:VAL:HG11 | 2.00 | 0.44 |
| 1:H:107:ILE:CG2 | 1:H:135:ASP:HA | 2.48 | 0.44 |
| 2:I:469:VAL:HA | 2:I:472:GLU:HG2 | 2.00 | 0.44 |
| 2:I:980:VAL:HG13 | 2:I:984:VAL:HG21 | 1.98 | 0.44 |
| 2:I:1115:THR:CG2 | 2:I:1228:GLY:HA3 | 2.48 | 0.44 |
| 3:J:218:THR:HA | 3:J:221:ILE:CG2 | 2.47 | 0.44 |
| 3:J:930:LEU:HD23 | 3:J:1244:GLN:HG2 | 1.98 | 0.44 |
| 3:J:1353:VAL:O | 3:J:1353:VAL:HG22 | 2.17 | 0.44 |
| 5:L:286:LEU:HG | 5:L:290:LEU:CD1 | 2.47 | 0.44 |
| 6:P:29:DA:H2'' | 6:P:30:DC:O5' | 2.17 | 0.44 |
| 7:Q:20:DA:H2'' | 7:Q:21:DT:H5' | 1.98 | 0.44 |
| 1:G:52:PRO:HB3 | 1:H:5:VAL:HG11 | 2.00 | 0.44 |
| 1:G:207:THR:HG21 | 1:G:211:ILE:HB | 1.99 | 0.44 |
| 1:H:26:VAL:O | 1:H:203:ILE:N | 2.51 | 0.44 |
| 1:H:103:ASN:CB | 1:H:141:SER:HA | 2.35 | 0.44 |
| 3:J:93:THR:HG22 | 3:J:94:GLN:N | 2.33 | 0.44 |
| 3:J:902:ASP:N | 3:J:902:ASP:OD1 | 2.47 | 0.44 |
| 3:J:1273:ASP:OD1 | 3:J:1273:ASP:N | 2.51 | 0.44 |
| 5:L:141:ILE:HG23 | 5:L:224:LEU:HD11 | 2.00 | 0.44 |
| 5:L:419:PHE:CE1 | 5:L:427:PHE:HA | 2.52 | 0.44 |
| 6:P:37:DA:H2'' | 6:P:38:DG:C8 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:I:303:ASP:OD1 | 2:I:304:GLU:N | 2.50 | 0.44 |
| 2:I:558:VAL:HG13 | 2:I:573:ASN:HB3 | 2.00 | 0.44 |
| 2:I:890:LYS:HB2 | 2:I:914:LYS:HB2 | 2.00 | 0.44 |
| 2:I:989:LEU:HD13 | 2:I:1000:LEU:CD1 | 2.48 | 0.44 |
| 2:I:1236:ASN:HA | 2:I:1238:LEU:CD1 | 2.48 | 0.44 |
| 2:I:1274:GLU:HG2 | 3:J:424:ASN:ND2 | 2.33 | 0.44 |
| 3:J:165:TYR:OH | 3:J:169:LEU:HD12 | 2.17 | 0.44 |
| 3:J:1005:LYS:HE3 | 3:J:1015:GLU:OE2 | 2.18 | 0.44 |
| 6:P:77:DA:H2'' | 6:P:78:DT:C6 | 2.53 | 0.44 |
| 2:I:39:ILE:HD13 | 2:I:129:LEU:HD21 | 2.00 | 0.44 |
| 2:I:118:LYS:NZ | 2:I:488:MET:HA | 2.32 | 0.44 |
| 2:I:244:GLU:OE1 | 2:I:244:GLU:N | 2.36 | 0.44 |
| 2:I:551:HIS:HB3 | 2:I:554:HIS:HE1 | 1.82 | 0.44 |
| 2:I:572:ILE:O | 2:I:572:ILE:HG22 | 2.17 | 0.44 |
| 2:I:1305:TYR:O | 2:I:1309:VAL:HG22 | 2.18 | 0.44 |
| 3:J:490:ILE:HG13 | 3:J:491:LEU:CD1 | 2.47 | 0.44 |
| 3:J:747:MET:O | 3:J:755:ILE:HD12 | 2.18 | 0.44 |
| 3:J:1270:GLY:C | 3:J:1298:VAL:HG13 | 2.38 | 0.44 |
| 4:K:39:VAL:HG22 | 4:K:52:ARG:HH21 | 1.83 | 0.44 |
| 2:I:69:GLN:NE2 | 2:I:101:ARG:HH21 | 2.15 | 0.44 |
| 2:I:468:LEU:HA | 2:I:468:LEU:HD23 | 1.60 | 0.44 |
| 2:I:621:SER:HB2 | 2:I:653:MET:CE | 2.46 | 0.44 |
| 2:I:757:THR:O | 2:I:765:ILE:HG22 | 2.17 | 0.44 |
| 2:I:969:ALA:HB1 | 8:I:1401:1N7:C24 | 2.47 | 0.44 |
| 3:J:56:LEU:HD11 | 3:J:273:ILE:CD1 | 2.40 | 0.44 |
| 3:J:275:ARG:HD3 | 3:J:298:MET:HB3 | 2.00 | 0.44 |
| 3:J:325:LYS:HG3 | 3:J:329:ASP:HB3 | 2.00 | 0.44 |
| 3:J:664:ILE:HD11 | 3:J:681:LYS:HE3 | 2.00 | 0.44 |
| 3:J:842:ARG:HB2 | 3:J:882:VAL:HG21 | 1.99 | 0.44 |
| 3:J:1028:ILE:CG2 | 3:J:1120:THR:HG22 | 2.48 | 0.44 |
| 7:Q:19:DT:H3' | 7:Q:19:DT:P | 2.57 | 0.44 |
| 7:Q:72:DG:H2' | 7:Q:73:DG:C8 | 2.52 | 0.44 |
| 2:I:131:THR:HG22 | 2:I:132:ASP:N | 2.30 | 0.44 |
| 2:I:794:LEU:HG | 2:I:796:LEU:CD1 | 2.46 | 0.44 |
| 3:J:83:VAL:O | 3:J:83:VAL:HG13 | 2.18 | 0.44 |
| 3:J:432:LEU:CD1 | 3:J:499:ILE:HG21 | 2.48 | 0.44 |
| 3:J:1162:ILE:O | 3:J:1177:ILE:HA | 2.18 | 0.44 |
| 3:J:1261:LEU:O | 3:J:1261:LEU:HD12 | 2.18 | 0.44 |
| 3:J:1368:ASP:O | 3:J:1371:ARG:HG2 | 2.18 | 0.44 |
| 5:L:133:SER:HB3 | 5:L:365:MET:HB2 | 2.00 | 0.44 |
| 5:L:404:LEU:HD22 | 5:L:439:ILE:HG23 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:192:VAL:CG1 | 1:G:195:ARG:HB3 | 2.48 | 0.43 |
| 2:I:151:ARG:HD2 | 2:I:445:ILE:HD12 | 1.99 | 0.43 |
| 2:I:572:ILE:HD12 | 2:I:572:ILE:HG23 | 1.78 | 0.43 |
| 2:I:1136:GLN:OE1 | 2:I:1136:GLN:N | 2.38 | 0.43 |
| 8:I:1401:1N7:H17 | 8:I:1401:1N7:H4 | 2.00 | 0.43 |
| 3:J:67:ASP:OD1 | 3:J:95:THR:N | 2.33 | 0.43 |
| 3:J:120:LEU:HB3 | 3:J:121:PRO:HD3 | 1.99 | 0.43 |
| 3:J:123:ARG:HG2 | 3:J:1337:VAL:HG11 | 1.99 | 0.43 |
| 3:J:858:VAL:HA | 3:J:859:PRO:HD3 | 1.89 | 0.43 |
| 3:J:963:VAL:HG13 | 3:J:963:VAL:O | 2.18 | 0.43 |
| 3:J:1104:LYS:HB3 | 3:J:1125:PRO:CD | 2.48 | 0.43 |
| 3:J:1270:GLY:H | 3:J:1300:ALA:HA | 1.83 | 0.43 |
| 5:L:311:THR:C | 5:L:341:LEU:HD23 | 2.38 | 0.43 |
| 7:Q:59:DT:C2' | 7:Q:60:DT:H71 | 2.48 | 0.43 |
| 7:Q:69:DA:H2'' | 7:Q:70:DA:O5' | 2.18 | 0.43 |
| 1:G:140:ILE:HD12 | 1:G:142:MET:HE3 | 1.99 | 0.43 |
| 1:H:57:THR:OG1 | 1:H:147:GLN:HB3 | 2.18 | 0.43 |
| 2:I:257:ALA:O | 2:I:260:LYS:HB3 | 2.19 | 0.43 |
| 2:I:615:VAL:HG13 | 2:I:615:VAL:O | 2.18 | 0.43 |
| 3:J:287:ALA:HA | 5:L:413:MET:CE | 2.48 | 0.43 |
| 3:J:876:SER:CB | 3:J:990:ARG:HH21 | 2.31 | 0.43 |
| 3:J:1105:ALA:HA | 3:J:1123:ARG:O | 2.18 | 0.43 |
| 6:P:31:DA:H2'' | 6:P:32:DA:H8 | 1.83 | 0.43 |
| 7:Q:49:DC:OP2 | 7:Q:49:DC:H6 | 2.01 | 0.43 |
| 7:Q:70:DA:H2' | 7:Q:71:DT:C7 | 2.49 | 0.43 |
| 1:R:279:GLY:HA2 | 1:R:282:VAL:HG22 | 2.00 | 0.43 |
| 1:R:282:VAL:HB | 1:R:316:MET:SD | 2.59 | 0.43 |
| 1:G:11:PRO:HB3 | 1:G:31:LEU:CD2 | 2.48 | 0.43 |
| 2:I:734:ILE:HD12 | 2:I:734:ILE:HG23 | 1.71 | 0.43 |
| 3:J:401:VAL:HG12 | 3:J:408:VAL:HG12 | 1.98 | 0.43 |
| 3:J:582:ILE:HG22 | 3:J:620:PHE:CD1 | 2.53 | 0.43 |
| 3:J:1078:LEU:O | 3:J:1099:TYR:N | 2.46 | 0.43 |
| 1:H:73:GLY:HA2 | 1:H:134:THR:HB | 2.01 | 0.43 |
| 1:H:74:VAL:HG22 | 1:H:133:LEU:HD12 | 2.00 | 0.43 |
| 2:I:21:VAL:CG1 | 2:I:655:VAL:HG13 | 2.49 | 0.43 |
| 2:I:186:PHE:HZ | 2:I:425:ILE:HG23 | 1.82 | 0.43 |
| 2:I:316:GLU:O | 2:I:316:GLU:HG2 | 2.18 | 0.43 |
| 3:J:142:GLU:HB3 | 5:L:91:ILE:CG2 | 2.49 | 0.43 |
| 3:J:430:HIS:CD2 | 3:J:432:LEU:HB2 | 2.53 | 0.43 |
| 4:K:13:ILE:HD12 | 4:K:54:ILE:HG23 | 2.00 | 0.43 |
| 4:K:38:LEU:HD13 | 4:K:53:GLU:OE1 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:L:291:CYS:HA | 5:L:295:CYS:HB2 | 2.00 | 0.43 |
| 1:G:90:VAL:HG11 | 1:G:146:VAL:CG1 | 2.45 | 0.43 |
| 1:G:182:ARG:O | 1:G:183:ILE:HD13 | 2.19 | 0.43 |
| 1:G:196:THR:OG1 | 1:G:197:ASP:N | 2.52 | 0.43 |
| 1:H:89:ALA:HB3 | 1:H:124:VAL:HG12 | 2.00 | 0.43 |
| 2:I:22:LEU:HD13 | 2:I:603:ILE:CD1 | 2.45 | 0.43 |
| 2:I:27:LEU:HD22 | 2:I:663:VAL:HG11 | 2.00 | 0.43 |
| 2:I:218:GLU:HG2 | 2:I:299:LYS:HA | 1.99 | 0.43 |
| 2:I:969:ALA:HB2 | 8:I:1401:1N7:H34 | 2.00 | 0.43 |
| 2:I:976:ARG:HB2 | 2:I:997:TRP:CZ2 | 2.53 | 0.43 |
| 3:J:194:LEU:HD22 | 3:J:224:LEU:HD22 | 2.00 | 0.43 |
| 3:J:697:MET:HE2 | 3:J:741:ALA:HB3 | 2.00 | 0.43 |
| 3:J:930:LEU:HA | 3:J:1244:GLN:HG2 | 1.99 | 0.43 |
| 3:J:1279:GLN:NE2 | 3:J:1305:ASP:OD2 | 2.51 | 0.43 |
| 5:L:313:ASP:HA | 5:L:316:PHE:CB | 2.42 | 0.43 |
| 5:L:390:ILE:CD1 | 5:L:432:THR:HG23 | 2.48 | 0.43 |
| 2:I:312:ALA:H | 2:I:315:MET:CE | 2.31 | 0.43 |
| 2:I:566:GLY:O | 2:I:569:ILE:HG13 | 2.17 | 0.43 |
| 3:J:53:ARG:HA | 3:J:54:ASP:HA | 1.56 | 0.43 |
| 3:J:960:LEU:CD2 | 3:J:963:VAL:HG11 | 2.49 | 0.43 |
| 4:K:4:VAL:HG22 | 4:K:5:THR:HG23 | 2.01 | 0.43 |
| 5:L:124:GLU:HA | 5:L:127:ILE:CG1 | 2.48 | 0.43 |
| 5:L:150:ARG:O | 5:L:155:GLU:HB2 | 2.18 | 0.43 |
| 6:P:68:DA:H1' | 6:P:69:DT:H5' | 1.99 | 0.43 |
| 1:G:105:SER:CB | 1:G:139:SER:HB2 | 2.49 | 0.43 |
| 2:I:281:ASP:OD1 | 2:I:283:LYS:HE3 | 2.19 | 0.43 |
| 2:I:971:LEU:O | 2:I:975:ILE:HG13 | 2.18 | 0.43 |
| 2:I:1120:ALA:CA | 2:I:1199:LEU:HD23 | 2.49 | 0.43 |
| 2:I:1196:LYS:HD2 | 2:I:1206:THR:HG23 | 2.00 | 0.43 |
| 3:J:166:LEU:HD12 | 3:J:166:LEU:HA | 1.86 | 0.43 |
| 3:J:268:LEU:HB2 | 3:J:306:LEU:HD23 | 2.01 | 0.43 |
| 3:J:537:TYR:HE2 | 3:J:634:ARG:HH12 | 1.65 | 0.43 |
| 3:J:902:ASP:HA | 3:J:903:LEU:HD23 | 1.98 | 0.43 |
| 5:L:281:ARG:HA | 5:L:284:GLU:CD | 2.38 | 0.43 |
| 5:L:452:ILE:HD11 | 5:L:457:ILE:CG1 | 2.48 | 0.43 |
| 5:L:481:GLU:O | 5:L:484:ALA:HB3 | 2.18 | 0.43 |
| 1:G:74:VAL:HG13 | 1:G:74:VAL:O | 2.19 | 0.43 |
| 2:I:221:LEU:HD11 | 2:I:314:ASN:HB2 | 2.00 | 0.43 |
| 2:I:716:ALA:HB3 | 2:I:784:ALA:HB3 | 2.01 | 0.43 |
| 2:I:922:ASN:HD22 | 2:I:923:GLY:H | 1.66 | 0.43 |
| 3:J:394:ILE:HG13 | 5:L:532:LEU:HD11 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:513:MET:HE2 | 3:J:579:LEU:HB2 | 2.00 | 0.43 |
| 3:J:718:SER:OG | 3:J:719:PHE:N | 2.51 | 0.43 |
| 5:L:533:ASP:CA | 5:L:536:THR:HG22 | 2.45 | 0.43 |
| 1:H:56:VAL:HA | 1:H:146:VAL:HA | 2.00 | 0.43 |
| 2:I:18:ARG:NH1 | 2:I:620:ASN:HA | 2.34 | 0.43 |
| 2:I:230:PHE:HB3 | 2:I:237:LEU:HD12 | 2.01 | 0.43 |
| 2:I:237:LEU:HD11 | 2:I:333:ILE:HD13 | 2.00 | 0.43 |
| 2:I:582:ASN:OD1 | 2:I:583:GLU:N | 2.49 | 0.43 |
| 3:J:79:LYS:CB | 5:L:569:THR:HG22 | 2.49 | 0.43 |
| 3:J:213:LYS:O | 3:J:217:LEU:HG | 2.19 | 0.43 |
| 3:J:841:GLY:O | 3:J:863:LEU:HD11 | 2.18 | 0.43 |
| 3:J:1046:ILE:HD12 | 3:J:1059:LEU:CD1 | 2.44 | 0.43 |
| 3:J:1164:SER:HA | 3:J:1200:GLU:OE2 | 2.19 | 0.43 |
| 3:J:1332:LEU:HD13 | 3:J:1332:LEU:HA | 1.83 | 0.43 |
| 5:L:386:LEU:O | 5:L:389:SER:OG | 2.27 | 0.43 |
| 7:Q:28:DT:H2' | 7:Q:29:DT:H71 | 2.01 | 0.43 |
| 1:R:300:LEU:CA | 1:R:303:ILE:HD12 | 2.34 | 0.43 |
| 2:I:300:ASP:HB2 | 2:I:309:LEU:HD11 | 2.00 | 0.43 |
| 2:I:344:GLY:HA3 | 2:I:346:TYR:CE2 | 2.54 | 0.43 |
| 2:I:612:GLY:O | 2:I:639:LYS:HG2 | 2.19 | 0.43 |
| 2:I:1225:VAL:HA | 3:J:638:SER:HB3 | 2.01 | 0.43 |
| 3:J:84:ILE:O | 3:J:84:ILE:HG13 | 2.18 | 0.43 |
| 3:J:422:LEU:CD1 | 3:J:471:PRO:HG3 | 2.49 | 0.43 |
| 3:J:511:TYR:HE2 | 3:J:724:MET:HG2 | 1.83 | 0.43 |
| 3:J:1046:ILE:HD12 | 3:J:1059:LEU:HB3 | 2.00 | 0.43 |
| 5:L:143:TYR:O | 5:L:147:GLN:HG2 | 2.19 | 0.43 |
| 7:Q:78:DG:H2'' | 7:Q:79:DT:OP2 | 2.19 | 0.43 |
| 1:R:265:ARG:NE | 1:R:294:ASN:O | 2.49 | 0.43 |
| 1:G:56:VAL:HA | 1:G:146:VAL:HA | 2.01 | 0.42 |
| 1:H:107:ILE:HA | 1:H:134:THR:O | 2.19 | 0.42 |
| 2:I:39:ILE:HD12 | 2:I:127:ILE:HD12 | 2.01 | 0.42 |
| 2:I:127:ILE:HG13 | 2:I:127:ILE:O | 2.19 | 0.42 |
| 2:I:432:LEU:HA | 2:I:435:ILE:CG2 | 2.49 | 0.42 |
| 2:I:542:ARG:O | 6:P:63:DT:H5'' | 2.19 | 0.42 |
| 2:I:1247:SER:HB3 | 3:J:375:GLU:O | 2.19 | 0.42 |
| 3:J:111:THR:HG21 | 3:J:303:VAL:HB | 2.01 | 0.42 |
| 3:J:596:LEU:HD11 | 3:J:604:MET:CE | 2.49 | 0.42 |
| 3:J:793:SER:OG | 3:J:927:GLY:HA3 | 2.19 | 0.42 |
| 3:J:807:LEU:HA | 3:J:807:LEU:HD12 | 1.54 | 0.42 |
| 3:J:842:ARG:CB | 3:J:882:VAL:HG21 | 2.49 | 0.42 |
| 3:J:1251:LYS:O | 3:J:1255:VAL:HG12 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:L:101:TYR:CD2 | 5:L:405:ILE:HD12 | 2.54 | 0.42 |
| 5:L:318:ALA:CA | 5:L:321:ALA:HB3 | 2.40 | 0.42 |
| 2:I:367:TYR:CD2 | 2:I:376:PRO:HB3 | 2.53 | 0.42 |
| 2:I:496:LYS:O | 2:I:500:ALA:CB | 2.67 | 0.42 |
| 2:I:717:VAL:HA | 2:I:781:ASP:O | 2.19 | 0.42 |
| 2:I:1288:GLN:O | 2:I:1292:THR:HB | 2.19 | 0.42 |
| 3:J:134:ASP:CG | 3:J:159:ILE:HD12 | 2.40 | 0.42 |
| 3:J:266:ASN:O | 3:J:270:ARG:HB2 | 2.19 | 0.42 |
| 3:J:500:ILE:HG22 | 3:J:500:ILE:O | 2.19 | 0.42 |
| 3:J:530:PRO:HB3 | 3:J:581:MET:HG3 | 2.00 | 0.42 |
| 3:J:966:VAL:N | 3:J:974:VAL:O | 2.51 | 0.42 |
| 3:J:1096:PRO:HB2 | 3:J:1098:GLN:OE1 | 2.19 | 0.42 |
| 3:J:1261:LEU:HD13 | 3:J:1304:ARG:NH1 | 2.33 | 0.42 |
| 3:J:1266:ILE:CD1 | 3:J:1285:VAL:HG21 | 2.49 | 0.42 |
| 5:L:142:THR:HG22 | 5:L:228:TYR:OH | 2.19 | 0.42 |
| 5:L:165:PHE:CE2 | 5:L:217:ALA:HB1 | 2.54 | 0.42 |
| 5:L:585:GLU:OE1 | 7:Q:68:DC:N4 | 2.49 | 0.42 |
| 1:G:48:LEU:HD23 | 1:G:48:LEU:HA | 1.62 | 0.42 |
| 1:G:228:LEU:CD1 | 1:H:224:LEU:HD23 | 2.48 | 0.42 |
| 2:I:706:ARG:HD3 | 2:I:792:GLY:O | 2.19 | 0.42 |
| 2:I:1312:ASN:HD21 | 2:I:1314:GLN:NE2 | 2.17 | 0.42 |
| 3:J:680:ASN:CA | 3:J:683:ILE:HG22 | 2.46 | 0.42 |
| 5:L:214:PRO:O | 5:L:218:ARG:HG3 | 2.18 | 0.42 |
| 5:L:262:VAL:HG13 | 5:L:263:PRO:HD2 | 2.01 | 0.42 |
| 2:I:151:ARG:HD2 | 2:I:445:ILE:CD1 | 2.50 | 0.42 |
| 2:I:561:ILE:HG21 | 3:J:772:TYR:HE2 | 1.85 | 0.42 |
| 2:I:561:ILE:CD1 | 2:I:671:LEU:HD21 | 2.50 | 0.42 |
| 2:I:971:LEU:HD11 | 2:I:1017:GLN:CB | 2.49 | 0.42 |
| 3:J:1064:SER:HB3 | 3:J:1192:LYS:NZ | 2.34 | 0.42 |
| 3:J:1098:GLN:HG2 | 3:J:1098:GLN:O | 2.18 | 0.42 |
| 3:J:1172:LYS:O | 3:J:1192:LYS:HE2 | 2.19 | 0.42 |
| 5:L:137:TYR:O | 5:L:140:ALA:HB3 | 2.19 | 0.42 |
| 5:L:252:LEU:O | 5:L:255:VAL:HG22 | 2.20 | 0.42 |
| 5:L:606:VAL:HG13 | 5:L:607:LEU:HD22 | 2.00 | 0.42 |
| 6:P:66:DG:H1' | 6:P:67:DA:H5' | 2.00 | 0.42 |
| 1:H:75:GLN:OE1 | 1:H:75:GLN:N | 2.40 | 0.42 |
| 1:H:112:ALA:HB3 | 1:H:126:PRO:O | 2.19 | 0.42 |
| 2:I:118:LYS:HE2 | 2:I:488:MET:HG2 | 2.00 | 0.42 |
| 2:I:1099:ASN:OD1 | 2:I:1100:PRO:HD2 | 2.19 | 0.42 |
| 2:I:1240:ASP:OD1 | 2:I:1240:ASP:N | 2.49 | 0.42 |
| 3:J:218:THR:CA | 3:J:221:ILE:HG22 | 2.48 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:262:THR:H | 5:L:504:PRO:HB2 | 1.84 | 0.42 |
| 3:J:612:LEU:HB3 | 3:J:616:PRO:HG2 | 2.02 | 0.42 |
| 3:J:1172:LYS:O | 3:J:1192:LYS:HB3 | 2.19 | 0.42 |
| 7:Q:51:DT:C6 | 7:Q:52:DT:H72 | 2.55 | 0.42 |
| 1:H:97:GLU:HG2 | 1:H:147:GLN:HG3 | 2.01 | 0.42 |
| 2:I:14:ASP:HB3 | 2:I:1157:GLN:HB2 | 2.01 | 0.42 |
| 2:I:157:PHE:O | 2:I:442:VAL:HB | 2.20 | 0.42 |
| 2:I:788:SER:HB3 | 2:I:795:ALA:O | 2.19 | 0.42 |
| 2:I:1006:GLU:O | 2:I:1009:ASN:O | 2.37 | 0.42 |
| 2:I:1270:PHE:CE2 | 2:I:1290:MET:HG2 | 2.54 | 0.42 |
| 3:J:423:LEU:HB3 | 3:J:466:MET:HE1 | 2.01 | 0.42 |
| 3:J:426:ALA:HB3 | 3:J:427:PRO:CD | 2.50 | 0.42 |
| 3:J:845:ALA:HB2 | 3:J:883:ARG:HG3 | 2.01 | 0.42 |
| 3:J:982:LEU:HD12 | 3:J:982:LEU:HA | 1.93 | 0.42 |
| 1:R:289:LEU:O | 1:R:295:LEU:HD22 | 2.20 | 0.42 |
| 1:G:228:LEU:HD11 | 1:H:224:LEU:HB3 | 2.02 | 0.42 |
| 2:I:128:PRO:HG2 | 2:I:506:PHE:CD2 | 2.55 | 0.42 |
| 2:I:850:ILE:O | 2:I:850:ILE:HG22 | 2.20 | 0.42 |
| 2:I:851:THR:HG22 | 2:I:887:VAL:HG12 | 2.01 | 0.42 |
| 2:I:888:THR:HG23 | 2:I:916:SER:CB | 2.50 | 0.42 |
| 2:I:898:GLU:HB3 | 5:L:540:LEU:CD2 | 2.50 | 0.42 |
| 2:I:1096:ILE:HD13 | 2:I:1096:ILE:HG21 | 1.81 | 0.42 |
| 2:I:1276:TRP:CD2 | 3:J:801:VAL:HG21 | 2.54 | 0.42 |
| 3:J:1037:PHE:HA | 3:J:1040:MET:SD | 2.60 | 0.42 |
| 3:J:1097:ALA:HB1 | 3:J:1099:TYR:CZ | 2.55 | 0.42 |
| 6:P:63:DT:H6 | 6:P:63:DT:H2' | 1.72 | 0.42 |
| 7:Q:50:DC:C6 | 7:Q:51:DT:H72 | 2.54 | 0.42 |
| 2:I:339:ASN:N | 2:I:343:HIS:O | 2.43 | 0.42 |
| 2:I:817:LEU:HD21 | 2:I:1080:ASN:ND2 | 2.34 | 0.42 |
| 2:I:975:ILE:CG2 | 2:I:997:TRP:HE1 | 2.32 | 0.42 |
| 3:J:68:TYR:CA | 3:J:92:VAL:HG23 | 2.50 | 0.42 |
| 3:J:716:GLN:OE1 | 3:J:716:GLN:N | 2.53 | 0.42 |
| 3:J:812:ASP:HB2 | 3:J:911:LYS:CE | 2.49 | 0.42 |
| 3:J:886:VAL:O | 3:J:886:VAL:HG22 | 2.19 | 0.42 |
| 3:J:1035:VAL:CG2 | 3:J:1115:ILE:HG23 | 2.49 | 0.42 |
| 3:J:1040:MET:HA | 3:J:1045:THR:HG21 | 2.02 | 0.42 |
| 3:J:1145:PHE:HB3 | 3:J:1309:ILE:HD13 | 2.01 | 0.42 |
| 3:J:1256:ILE:HD13 | 3:J:1256:ILE:HA | 1.84 | 0.42 |
| 5:L:134:VAL:HA | 5:L:273:MET:HE1 | 2.00 | 0.42 |
| 5:L:330:LEU:O | 5:L:334:SER:N | 2.53 | 0.42 |
| 5:L:423:ARG:HG2 | 5:L:425:TYR:CD2 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:P:22:DT:H5' | 6:P:22:DT:H6 | 1.83 | 0.42 |
| 6:P:25:DA:H2' | 6:P:26:DT:C6 | 2.55 | 0.42 |
| 1:G:66:HIS:HB2 | 2:I:927:THR:HG21 | 2.01 | 0.42 |
| 1:H:98:VAL:O | 1:H:146:VAL:HG22 | 2.20 | 0.42 |
| 2:I:237:LEU:HD13 | 2:I:237:LEU:HA | 1.86 | 0.42 |
| 2:I:359:ARG:O | 2:I:363:LEU:HG | 2.20 | 0.42 |
| 2:I:453:ILE:HG21 | 2:I:453:ILE:HD13 | 1.75 | 0.42 |
| 2:I:593:LYS:O | 2:I:600:THR:HB | 2.19 | 0.42 |
| 2:I:620:ASN:HD21 | 3:J:768:ASN:HB2 | 1.84 | 0.42 |
| 2:I:971:LEU:HD23 | 2:I:975:ILE:CD1 | 2.48 | 0.42 |
| 2:I:1282:GLY:O | 2:I:1284:ALA:N | 2.52 | 0.42 |
| 3:J:294:ASN:HD22 | 5:L:406:GLN:HE21 | 1.67 | 0.42 |
| 3:J:363:LEU:HB3 | 3:J:450:HIS:CE1 | 2.55 | 0.42 |
| 3:J:709:ARG:HD3 | 3:J:710:ASP:CG | 2.40 | 0.42 |
| 3:J:843:VAL:C | 3:J:882:VAL:HG23 | 2.39 | 0.42 |
| 3:J:849:LEU:HA | 3:J:849:LEU:HD13 | 1.80 | 0.42 |
| 3:J:1037:PHE:HB3 | 3:J:1040:MET:HB2 | 2.02 | 0.42 |
| 3:J:1051:ASP:HB2 | 3:J:1054:THR:OG1 | 2.20 | 0.42 |
| 3:J:1231:ARG:HG2 | 3:J:1235:ASN:OD1 | 2.19 | 0.42 |
| 3:J:1284:ARG:O | 3:J:1287:ILE:HG13 | 2.20 | 0.42 |
| 5:L:313:ASP:HB3 | 5:L:317:ASN:OD1 | 2.19 | 0.42 |
| 5:L:313:ASP:O | 5:L:317:ASN:N | 2.51 | 0.42 |
| 5:L:376:LYS:O | 5:L:380:VAL:HG23 | 2.20 | 0.42 |
| 5:L:390:ILE:HD13 | 5:L:432:THR:HG23 | 2.01 | 0.42 |
| 5:L:453:PRO:HG2 | 6:P:44:DA:OP2 | 2.19 | 0.42 |
| 6:P:41:DT:H2'' | 6:P:42:DA:C8 | 2.55 | 0.42 |
| 1:R:250:ASP:CB | 1:R:253:LEU:HD12 | 2.50 | 0.42 |
| 1:R:264:VAL:HA | 1:R:267:ALA:HB3 | 2.01 | 0.42 |
| 2:I:311:CYS:HB2 | 2:I:315:MET:SD | 2.59 | 0.42 |
| 2:I:325:LEU:HD12 | 2:I:326:SER:N | 2.34 | 0.42 |
| 2:I:444:ASP:OD1 | 2:I:444:ASP:N | 2.47 | 0.42 |
| 2:I:633:LEU:CD1 | 2:I:644:LEU:HD12 | 2.50 | 0.42 |
| 2:I:867:GLU:OE2 | 2:I:943:LYS:HG3 | 2.19 | 0.42 |
| 2:I:1277:ALA:HB3 | 3:J:434:ILE:CD1 | 2.48 | 0.42 |
| 3:J:142:GLU:OE1 | 5:L:91:ILE:HG23 | 2.19 | 0.42 |
| 3:J:316:ILE:HD13 | 3:J:316:ILE:HG21 | 1.82 | 0.42 |
| 3:J:420:PRO:O | 3:J:471:PRO:HD2 | 2.20 | 0.42 |
| 3:J:963:VAL:HG23 | 3:J:975:ILE:CG1 | 2.48 | 0.42 |
| 3:J:1035:VAL:HG22 | 3:J:1115:ILE:HG12 | 2.00 | 0.42 |
| 5:L:311:THR:HG22 | 5:L:344:LEU:CD2 | 2.49 | 0.42 |
| 6:P:56:DC:H2' | 6:P:57:DT:C7 | 2.50 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:H:192:VAL:HG12 | 1:H:193:GLU:N | 2.35 | 0.41 |
| 2:I:90:VAL:HG12 | 2:I:91:THR:N | 2.35 | 0.41 |
| 2:I:484:LEU:HD12 | 2:I:485:ASP:CB | 2.48 | 0.41 |
| 2:I:558:VAL:HG11 | 2:I:573:ASN:HB3 | 2.02 | 0.41 |
| 2:I:1103:VAL:HG11 | 2:I:1112:ILE:HD12 | 2.02 | 0.41 |
| 3:J:141:PHE:HA | 3:J:180:MET:CE | 2.48 | 0.41 |
| 3:J:550:VAL:O | 3:J:569:LEU:HA | 2.20 | 0.41 |
| 3:J:584:PRO:O | 3:J:586:GLY:N | 2.53 | 0.41 |
| 3:J:1158:GLU:HG3 | 3:J:1186:TYR:OH | 2.20 | 0.41 |
| 5:L:149:ASP:O | 5:L:153:ALA:N | 2.52 | 0.41 |
| 1:G:49:SER:HB3 | 2:I:1083:GLU:OE2 | 2.20 | 0.41 |
| 1:G:160:HIS:NE2 | 1:G:161:SER:HB2 | 2.35 | 0.41 |
| 1:H:48:LEU:HD13 | 1:H:183:ILE:HD11 | 2.01 | 0.41 |
| 1:H:100:LEU:HB2 | 1:H:144:ILE:CG2 | 2.49 | 0.41 |
| 2:I:131:THR:OG1 | 2:I:135:THR:O | 2.26 | 0.41 |
| 2:I:195:PHE:HA | 2:I:204:LEU:O | 2.20 | 0.41 |
| 2:I:666:SER:HA | 2:I:1186:VAL:HG21 | 2.00 | 0.41 |
| 2:I:1291:LEU:HB2 | 3:J:345:LYS:HD2 | 2.02 | 0.41 |
| 3:J:114:ILE:HD11 | 3:J:311:ARG:CG | 2.50 | 0.41 |
| 3:J:551:ARG:O | 3:J:551:ARG:HG2 | 2.20 | 0.41 |
| 3:J:668:PHE:HB2 | 3:J:678:ARG:HG3 | 2.02 | 0.41 |
| 3:J:830:ASP:OD2 | 3:J:953:LYS:NZ | 2.51 | 0.41 |
| 1:G:150:ARG:HD2 | 1:H:8:PHE:CZ | 2.54 | 0.41 |
| 1:G:214:GLU:O | 1:G:217:ILE:HG22 | 2.21 | 0.41 |
| 2:I:149:LEU:HG | 2:I:451:ARG:CG | 2.51 | 0.41 |
| 2:I:561:ILE:HG21 | 2:I:561:ILE:HD13 | 1.75 | 0.41 |
| 2:I:976:ARG:HG2 | 2:I:980:VAL:CG2 | 2.50 | 0.41 |
| 3:J:35:PHE:CE2 | 3:J:101:ARG:HG2 | 2.55 | 0.41 |
| 3:J:605:LEU:HD23 | 3:J:605:LEU:HA | 1.79 | 0.41 |
| 5:L:90:GLU:O | 5:L:90:GLU:HG2 | 2.20 | 0.41 |
| 5:L:600:HIS:O | 5:L:603:ARG:HB3 | 2.20 | 0.41 |
| 6:P:23:DC:H6 | 6:P:23:DC:O5' | 2.03 | 0.41 |
| 6:P:39:DG:C1' | 6:P:40:DC:H5' | 2.49 | 0.41 |
| 1:H:42:ALA:HB1 | 1:H:224:LEU:CD2 | 2.50 | 0.41 |
| 1:H:100:LEU:HD23 | 1:H:115:ILE:HG21 | 2.03 | 0.41 |
| 2:I:113:THR:HG22 | 2:I:114:VAL:N | 2.35 | 0.41 |
| 2:I:114:VAL:HG23 | 2:I:114:VAL:O | 2.20 | 0.41 |
| 2:I:413:GLU:OE1 | 2:I:413:GLU:N | 2.53 | 0.41 |
| 2:I:757:THR:HG23 | 2:I:765:ILE:CG2 | 2.50 | 0.41 |
| 2:I:839:VAL:HG12 | 2:I:1049:ILE:HG12 | 2.01 | 0.41 |
| 2:I:1107:MET:HG2 | 3:J:740:LEU:HD11 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:113:HIS:CE1 | 3:J:115:TRP:HB2 | 2.56 | 0.41 |
| 3:J:246:PRO:O | 3:J:250:ARG:NE | 2.53 | 0.41 |
| 3:J:283:LEU:HD23 | 3:J:283:LEU:HA | 1.86 | 0.41 |
| 3:J:343:LEU:HD23 | 3:J:343:LEU:HA | 1.79 | 0.41 |
| 3:J:480:ALA:HA | 3:J:484:MET:HB2 | 2.02 | 0.41 |
| 5:L:139:GLU:OE1 | 5:L:142:THR:OG1 | 2.28 | 0.41 |
| 7:Q:52:DT:H2' | 7:Q:53:DT:H72 | 2.01 | 0.41 |
| 1:R:300:LEU:O | 1:R:303:ILE:HB | 2.19 | 0.41 |
| 1:H:95:LYS:HB2 | 1:H:120:ASP:OD2 | 2.21 | 0.41 |
| 1:H:99:ILE:HD11 | 1:H:143:ARG:HB3 | 2.03 | 0.41 |
| 1:H:149:GLY:HA3 | 1:H:177:TYR:CE1 | 2.56 | 0.41 |
| 2:I:124:MET:O | 2:I:124:MET:HG3 | 2.21 | 0.41 |
| 2:I:594:VAL:HG12 | 2:I:595:THR:O | 2.20 | 0.41 |
| 2:I:873:ILE:HG13 | 2:I:944:ARG:NH2 | 2.35 | 0.41 |
| 2:I:976:ARG:HG2 | 2:I:980:VAL:HG23 | 2.02 | 0.41 |
| 3:J:322:ARG:NH1 | 5:L:510:PRO:HG3 | 2.34 | 0.41 |
| 3:J:419:HIS:O | 3:J:439:PRO:HD3 | 2.21 | 0.41 |
| 3:J:495:ASN:OD1 | 3:J:495:ASN:N | 2.53 | 0.41 |
| 3:J:1047:THR:O | 3:J:1059:LEU:HD23 | 2.20 | 0.41 |
| 4:K:38:LEU:HB2 | 4:K:53:GLU:CD | 2.41 | 0.41 |
| 5:L:489:MET:HG3 | 5:L:494:ILE:CG1 | 2.51 | 0.41 |
| 6:P:68:DA:C8 | 6:P:69:DT:H72 | 2.56 | 0.41 |
| 7:Q:29:DT:H2'' | 7:Q:30:DC:C6 | 2.55 | 0.41 |
| 1:G:16:ILE:HG23 | 1:G:26:VAL:HG12 | 2.03 | 0.41 |
| 2:I:303:ASP:O | 2:I:307:GLY:HA2 | 2.20 | 0.41 |
| 2:I:471:VAL:CG2 | 2:I:493:ILE:HG13 | 2.48 | 0.41 |
| 2:I:471:VAL:HB | 2:I:498:ILE:HD11 | 2.03 | 0.41 |
| 3:J:364:HIS:CD2 | 4:K:4:VAL:HG23 | 2.55 | 0.41 |
| 3:J:822:MET:HB3 | 3:J:839:VAL:HG22 | 2.02 | 0.41 |
| 3:J:961:SER:HB2 | 3:J:981:GLU:O | 2.21 | 0.41 |
| 3:J:1048:ARG:NH1 | 3:J:1050:THR:OG1 | 2.49 | 0.41 |
| 3:J:1316:THR:HG22 | 3:J:1317:GLU:N | 2.36 | 0.41 |
| 4:K:2:ALA:HA | 4:K:3:ARG:HA | 1.82 | 0.41 |
| 5:L:127:ILE:HA | 5:L:130:VAL:HG22 | 2.02 | 0.41 |
| 5:L:432:THR:HG21 | 6:P:53:DT:C4 | 2.56 | 0.41 |
| 6:P:63:DT:H3' | 6:P:63:DT:OP2 | 2.20 | 0.41 |
| 1:R:255:ARG:HG2 | 1:R:259:ASP:OD2 | 2.21 | 0.41 |
| 1:R:265:ARG:HH21 | 1:R:294:ASN:HA | 1.86 | 0.41 |
| 1:H:197:ASP:OD1 | 1:H:197:ASP:N | 2.54 | 0.41 |
| 2:I:459:MET:HB2 | 2:I:459:MET:HE3 | 1.98 | 0.41 |
| 2:I:545:PHE:HE1 | 3:J:784:ALA:HB3 | 1.84 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:1323:PHE:O | 2:I:1326:LEU:HB3 | 2.20 | 0.41 |
| 3:J:141:PHE:CE2 | 3:J:296:LYS:HB2 | 2.42 | 0.41 |
| 5:L:348:GLU:OE2 | 5:L:355:ILE:HG12 | 2.20 | 0.41 |
| 5:L:555:GLU:CG | 5:L:594:ALA:HB2 | 2.51 | 0.41 |
| 6:P:26:DT:H2'' | 6:P:27:DT:C5' | 2.51 | 0.41 |
| 2:I:165:HIS:CD2 | 2:I:167:SER:H | 2.38 | 0.41 |
| 2:I:520:PRO:HB2 | 2:I:794:LEU:CD1 | 2.51 | 0.41 |
| 2:I:883:LEU:HD13 | 2:I:1052:VAL:HG11 | 2.02 | 0.41 |
| 2:I:1104:PRO:HG2 | 3:J:725:MET:HE3 | 2.03 | 0.41 |
| 3:J:514:THR:HG23 | 3:J:514:THR:O | 2.21 | 0.41 |
| 3:J:527:LEU:HD13 | 3:J:548:VAL:HG13 | 1.98 | 0.41 |
| 3:J:850:LYS:HG2 | 3:J:851:PRO:HD2 | 2.01 | 0.41 |
| 3:J:903:LEU:HA | 3:J:904:ALA:HA | 1.87 | 0.41 |
| 6:P:48:DG:H2'' | 6:P:49:DC:O5' | 2.20 | 0.41 |
| 1:G:45:ARG:CD | 2:I:1083:GLU:HB3 | 2.50 | 0.41 |
| 1:G:183:ILE:HG23 | 1:G:183:ILE:HD12 | 1.71 | 0.41 |
| 1:G:194:GLN:O | 1:G:195:ARG:HB2 | 2.21 | 0.41 |
| 1:H:112:ALA:HB3 | 1:H:126:PRO:C | 2.42 | 0.41 |
| 2:I:60:GLN:HA | 2:I:67:GLU:CB | 2.51 | 0.41 |
| 2:I:251:ALA:HB2 | 2:I:269:ILE:CD1 | 2.40 | 0.41 |
| 2:I:471:VAL:O | 2:I:475:VAL:HG23 | 2.21 | 0.41 |
| 2:I:481:LEU:O | 2:I:481:LEU:HD12 | 2.21 | 0.41 |
| 2:I:550:VAL:O | 2:I:550:VAL:HG13 | 2.21 | 0.41 |
| 2:I:576:SER:HA | 2:I:662:SER:HA | 2.02 | 0.41 |
| 2:I:599:VAL:N | 2:I:627:GLY:O | 2.50 | 0.41 |
| 2:I:742:TYR:HB3 | 2:I:743:PRO:CD | 2.44 | 0.41 |
| 2:I:981:ALA:O | 2:I:1007:LYS:NZ | 2.45 | 0.41 |
| 2:I:1119:MET:HB2 | 2:I:1228:GLY:HA2 | 2.02 | 0.41 |
| 2:I:1244:HIS:CD2 | 2:I:1262:LYS:HA | 2.55 | 0.41 |
| 2:I:1246:ARG:HH11 | 2:I:1267:GLY:N | 2.19 | 0.41 |
| 3:J:97:VAL:CG1 | 3:J:101:ARG:HE | 2.33 | 0.41 |
| 3:J:145:VAL:O | 3:J:178:ALA:HA | 2.21 | 0.41 |
| 3:J:179:LYS:HB2 | 3:J:184:ALA:HA | 2.03 | 0.41 |
| 3:J:868:TRP:CZ3 | 3:J:871:LEU:HD12 | 2.56 | 0.41 |
| 3:J:963:VAL:CG2 | 3:J:975:ILE:HG12 | 2.46 | 0.41 |
| 3:J:1162:ILE:HG22 | 3:J:1178:THR:HB | 2.02 | 0.41 |
| 5:L:139:GLU:HA | 5:L:142:THR:HG23 | 2.03 | 0.41 |
| 5:L:150:ARG:NE | 5:L:155:GLU:OE1 | 2.40 | 0.41 |
| 5:L:227:GLN:CA | 5:L:230:VAL:HG12 | 2.48 | 0.41 |
| 5:L:586:ARG:O | 5:L:590:ILE:HG13 | 2.20 | 0.41 |
| 7:Q:57:DC:H2'' | 7:Q:58:DC:C6 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:R:290:LEU:HD21 | 1:R:300:LEU:HB3 | 2.03 | 0.41 |
| 1:H:6:THR:HG22 | 1:H:6:THR:O | 2.21 | 0.41 |
| 2:I:606:LEU:HD11 | 2:I:652:TYR:HE2 | 1.86 | 0.41 |
| 2:I:724:VAL:HG11 | 2:I:727:VAL:CG2 | 2.51 | 0.41 |
| 2:I:787:PRO:O | 2:I:788:SER:HB2 | 2.21 | 0.41 |
| 2:I:1274:GLU:HG2 | 3:J:424:ASN:HD21 | 1.85 | 0.41 |
| 3:J:361:LEU:HB2 | 3:J:450:HIS:HD2 | 1.85 | 0.41 |
| 3:J:528:THR:HG22 | 3:J:532:GLU:HG2 | 2.02 | 0.41 |
| 3:J:586:GLY:HA3 | 3:J:612:LEU:HD11 | 2.02 | 0.41 |
| 3:J:792:ASN:O | 3:J:795:TYR:N | 2.44 | 0.41 |
| 3:J:1220:ILE:HG23 | 3:J:1224:ARG:HH21 | 1.85 | 0.41 |
| 1:H:22:THR:O | 1:H:206:GLU:HA | 2.20 | 0.40 |
| 1:H:73:GLY:O | 1:H:134:THR:N | 2.54 | 0.40 |
| 2:I:102:LEU:HD12 | 2:I:103:VAL:H | 1.84 | 0.40 |
| 2:I:189:ASP:O | 2:I:192:ASP:N | 2.37 | 0.40 |
| 2:I:273:HIS:O | 2:I:277:LEU:HG | 2.21 | 0.40 |
| 2:I:817:LEU:HD11 | 2:I:1085:MET:HE3 | 2.03 | 0.40 |
| 2:I:1184:THR:O | 2:I:1184:THR:HG22 | 2.20 | 0.40 |
| 2:I:1287:LEU:HD22 | 3:J:1357:ILE:CD1 | 2.51 | 0.40 |
| 3:J:442:ILE:HD13 | 3:J:442:ILE:HA | 1.90 | 0.40 |
| 1:R:286:GLU:HG2 | 1:R:290:LEU:CD1 | 2.51 | 0.40 |
| 1:H:33:ARG:HD3 | 1:H:197:ASP:CG | 2.42 | 0.40 |
| 2:I:149:LEU:HB2 | 2:I:530:ILE:CG2 | 2.50 | 0.40 |
| 2:I:208:ILE:HD11 | 2:I:365:GLU:CG | 2.52 | 0.40 |
| 2:I:802:VAL:HG13 | 2:I:803:ALA:N | 2.35 | 0.40 |
| 2:I:836:LEU:O | 2:I:1051:LYS:HA | 2.21 | 0.40 |
| 2:I:1103:VAL:HG11 | 2:I:1112:ILE:CD1 | 2.51 | 0.40 |
| 3:J:423:LEU:CD1 | 3:J:468:VAL:HG12 | 2.51 | 0.40 |
| 3:J:473:THR:O | 3:J:477:GLN:HG3 | 2.22 | 0.40 |
| 3:J:497:GLU:OE2 | 3:J:1247:LYS:HE2 | 2.22 | 0.40 |
| 3:J:573:THR:HG23 | 3:J:576:ARG:NH1 | 2.36 | 0.40 |
| 3:J:797:THR:HG22 | 3:J:924:GLY:CA | 2.38 | 0.40 |
| 3:J:842:ARG:NH1 | 3:J:1251:LYS:HG2 | 2.36 | 0.40 |
| 5:L:105:MET:HE3 | 5:L:388:ILE:HD12 | 2.02 | 0.40 |
| 5:L:277:MET:HE3 | 5:L:359:LYS:HG2 | 2.03 | 0.40 |
| 5:L:489:MET:HG3 | 5:L:494:ILE:HG13 | 2.04 | 0.40 |
| 5:L:562:ARG:NH2 | 7:Q:66:DG:H5" | 2.36 | 0.40 |
| 1:R:282:VAL:O | 1:R:316:MET:HB2 | 2.22 | 0.40 |
| 1:H:23:HIS:ND1 | 1:H:206:GLU:OE2 | 2.49 | 0.40 |
| 2:I:239:MET:C | 2:I:284:LEU:HD12 | 2.42 | 0.40 |
| 2:I:896:THR:O | 2:I:899:GLU:HB2 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:932:GLN:O | 2:I:1050:VAL:HA | 2.21 | 0.40 |
| 2:I:1246:ARG:HH12 | 2:I:1266:GLY:HA2 | 1.86 | 0.40 |
| 2:I:1339:LEU:HD23 | 3:J:17:PHE:CD1 | 2.57 | 0.40 |
| 3:J:694:SER:OG | 3:J:738:ARG:NE | 2.55 | 0.40 |
| 3:J:827:GLU:HB3 | 3:J:832:LYS:HD2 | 2.02 | 0.40 |
| 3:J:956:GLY:C | 3:J:984:LEU:HD11 | 2.41 | 0.40 |
| 3:J:1061:VAL:HG11 | 3:J:1101:LEU:CB | 2.42 | 0.40 |
| 3:J:1272:SER:HB3 | 3:J:1273:ASP:CB | 2.39 | 0.40 |
| 3:J:1355:ARG:NH1 | 3:J:1369:ARG:HH12 | 2.19 | 0.40 |
| 4:K:49:ILE:O | 4:K:53:GLU:HG2 | 2.22 | 0.40 |
| 5:L:290:LEU:CB | 5:L:333:VAL:HG21 | 2.39 | 0.40 |
| 5:L:420:GLU:HG3 | 5:L:422:ARG:NE | 2.33 | 0.40 |
| 5:L:476:ARG:HD2 | 5:L:477:GLU:N | 2.36 | 0.40 |
| 7:Q:71:DT:H2'' | 7:Q:72:DG:C8 | 2.55 | 0.40 |
| 1:R:265:ARG:HH21 | 1:R:294:ASN:CA | 2.35 | 0.40 |
| 1:G:20:SER:OG | 1:G:21:SER:N | 2.54 | 0.40 |
| 1:H:203:ILE:HG23 | 1:H:203:ILE:HD12 | 1.68 | 0.40 |
| 2:I:232:ILE:HG12 | 2:I:237:LEU:HD21 | 2.03 | 0.40 |
| 3:J:364:HIS:HB2 | 3:J:485:MET:HE3 | 2.03 | 0.40 |
| 3:J:382:TYR:HB3 | 3:J:394:ILE:CD1 | 2.51 | 0.40 |
| 3:J:450:HIS:HA | 3:J:451:PRO:HD3 | 1.93 | 0.40 |
| 3:J:1034:PHE:HA | 3:J:1114:GLN:HA | 2.03 | 0.40 |
| 3:J:1058:SER:CB | 3:J:1106:ILE:HG23 | 2.49 | 0.40 |
| 3:J:1154:ALA:HB2 | 3:J:1213:GLY:O | 2.22 | 0.40 |
| 5:L:379:MET:O | 5:L:382:ALA:HB3 | 2.21 | 0.40 |
| 6:P:74:DC:H5' | 6:P:74:DC:H6 | 1.86 | 0.40 |
| 7:Q:18:DA:H2'' | 7:Q:19:DT:C6 | 2.56 | 0.40 |
| 1:R:250:ASP:OD2 | 1:R:252:ILE:N | 2.55 | 0.40 |
| 1:G:45:ARG:HD3 | 1:G:45:ARG:HA | 1.86 | 0.40 |
| 1:G:56:VAL:H | 1:G:56:VAL:HG12 | 1.67 | 0.40 |
| 1:H:107:ILE:HG23 | 1:H:134:THR:C | 2.42 | 0.40 |
| 2:I:453:ILE:HD13 | 2:I:530:ILE:CD1 | 2.51 | 0.40 |
| 2:I:799:ASN:OD1 | 2:I:799:ASN:N | 2.35 | 0.40 |
| 2:I:1132:LEU:HD21 | 2:I:1141:LEU:CD2 | 2.50 | 0.40 |
| 2:I:1325:VAL:HG22 | 3:J:249:LEU:CD2 | 2.51 | 0.40 |
| 3:J:755:ILE:HG22 | 3:J:757:THR:H | 1.86 | 0.40 |
| 5:L:555:GLU:HG2 | 5:L:594:ALA:HB2 | 2.04 | 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 PDB entries followed by that with respect to all EM entries.

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 | G | 229/329 (70%) | 194 (85%) | 35 (15%) | 0 | 100 | 100 |
| 1 | H | 215/329 (65%) | 185 (86%) | 30 (14%) | 0 | 100 | 100 |
| 1 | R | 71/329 (22%) | 62 (87%) | 9 (13%) | 0 | 100 | 100 |
| 2 | I | 1339/1342 (100%) | 1161 (87%) | 175 (13%) | 3 (0%) | 47 | 78 |
| 3 | J | 1331/1430 (93%) | 1167 (88%) | 157 (12%) | 7 (0%) | 29 | 61 |
| 4 | K | 77/91 (85%) | 67 (87%) | 10 (13%) | 0 | 100 | 100 |
| 5 | L | 465/616 (76%) | 428 (92%) | 37 (8%) | 0 | 100 | 100 |
| All | All | 3727/4466 (84%) | 3264 (88%) | 453 (12%) | 10 (0%) | 44 | 72 |

All (10) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | J | 854 | ALA |
| 3 | J | 1169 | THR |
| 2 | I | 399 | ALA |
| 3 | J | 320 | ASN |
| 3 | J | 1172 | LYS |
| 3 | J | 46 | TYR |
| 2 | I | 1224 | PRO |
| 3 | J | 906 | GLY |
| 3 | J | 1138 | LEU |
| 2 | I | 697 | LYS |

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 PDB entries followed by that with respect to all EM entries.

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 | G | 196/286 (68%) | 195 (100%) | 1 (0%) | 88 | 94 |
| 1 | H | 186/286 (65%) | 186 (100%) | 0 | 100 | 100 |
| 1 | R | 65/286 (23%) | 65 (100%) | 0 | 100 | 100 |
| 2 | I | 1155/1157 (100%) | 1149 (100%) | 6 (0%) | 88 | 94 |
| 3 | J | 1118/1189 (94%) | 1108 (99%) | 10 (1%) | 78 | 90 |
| 4 | K | 67/75 (89%) | 67 (100%) | 0 | 100 | 100 |
| 5 | L | 415/543 (76%) | 414 (100%) | 1 (0%) | 93 | 98 |
| All | All | 3202/3822 (84%) | 3184 (99%) | 18 (1%) | 86 | 94 |

All (18) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | G | 148 | ARG |
| 2 | I | 161 | LYS |
| 2 | I | 272 | ARG |
| 2 | I | 684 | ASN |
| 2 | I | 802 | VAL |
| 2 | I | 922 | ASN |
| 2 | I | 1246 | ARG |
| 3 | J | 45 | ASN |
| 3 | J | 53 | ARG |
| 3 | J | 431 | ARG |
| 3 | J | 709 | ARG |
| 3 | J | 720 | ASN |
| 3 | J | 744 | ARG |
| 3 | J | 770 | LEU |
| 3 | J | 901 | ARG |
| 3 | J | 903 | LEU |
| 3 | J | 1197 | ASN |
| 5 | L | 476 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | G | 23 | HIS |
| 1 | G | 132 | HIS |
| 1 | G | 147 | GLN |
| 1 | H | 84 | ASN |
| 1 | H | 208 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | I | 31 | GLN |
| 2 | I | 69 | GLN |
| 2 | I | 165 | HIS |
| 2 | I | 273 | HIS |
| 2 | I | 276 | GLN |
| 2 | I | 447 | HIS |
| 2 | I | 618 | GLN |
| 2 | I | 673 | HIS |
| 2 | I | 684 | ASN |
| 2 | I | 760 | ASN |
| 2 | I | 922 | ASN |
| 2 | I | 1080 | ASN |
| 2 | I | 1116 | HIS |
| 2 | I | 1134 | GLN |
| 2 | I | 1237 | HIS |
| 2 | I | 1268 | GLN |
| 2 | I | 1314 | GLN |
| 3 | J | 45 | ASN |
| 3 | J | 294 | ASN |
| 3 | J | 341 | ASN |
| 3 | J | 450 | HIS |
| 3 | J | 488 | ASN |
| 3 | J | 720 | ASN |
| 3 | J | 817 | HIS |
| 3 | J | 1010 | GLN |
| 3 | J | 1197 | ASN |
| 3 | J | 1227 | HIS |
| 3 | J | 1326 | GLN |
| 3 | J | 1350 | ASN |
| 3 | J | 1367 | GLN |
| 5 | L | 265 | GLN |
| 5 | L | 309 | ASN |
| 5 | L | 331 | HIS |
| 1 | R | 283 | 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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | # $ Z > 2$ | Counts | RMSZ | # $ Z > 2$ |
| 8 | 1N7 | J | 1504 | - | 30,30,46 | 5.12 | 15 (50%) | 47,48,72 | 2.84 | 25 (53%) |
| 8 | 1N7 | I | 1401 | - | 30,30,46 | 5.03 | 16 (53%) | 47,48,72 | 2.59 | 17 (36%) |
| 8 | 1N7 | L | 701 | - | 30,30,46 | 5.03 | 14 (46%) | 47,48,72 | 2.67 | 16 (34%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 8 | 1N7 | J | 1504 | - | - | 7/7/72/92 | 0/4/4/4 |
| 8 | 1N7 | I | 1401 | - | - | 1/7/72/92 | 0/4/4/4 |
| 8 | 1N7 | L | 701 | - | - | 0/7/72/92 | 0/4/4/4 |

All (45) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 8 | J | 1504 | 1N7 | C3-C19 | 18.52 | 1.84 | 1.53 |
| 8 | L | 701 | 1N7 | C3-C19 | 18.49 | 1.84 | 1.53 |
| 8 | I | 1401 | 1N7 | C3-C19 | 17.99 | 1.83 | 1.53 |
| 8 | I | 1401 | 1N7 | C3-C4 | 12.22 | 1.73 | 1.53 |
| 8 | L | 701 | 1N7 | C3-C4 | 11.66 | 1.73 | 1.53 |
| 8 | J | 1504 | 1N7 | C3-C4 | 11.13 | 1.72 | 1.53 |
| 8 | J | 1504 | 1N7 | C5-C4 | -9.35 | 1.39 | 1.54 |
| 8 | I | 1401 | 1N7 | C5-C4 | -8.64 | 1.41 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 8 | L | 701 | 1N7 | C5-C4 | -8.52 | 1.41 | 1.54 |
| 8 | L | 701 | 1N7 | C2-C19 | -7.51 | 1.42 | 1.56 |
| 8 | I | 1401 | 1N7 | C2-C19 | -6.84 | 1.43 | 1.56 |
| 8 | J | 1504 | 1N7 | C2-C19 | -6.43 | 1.44 | 1.56 |
| 8 | J | 1504 | 1N7 | C8-C7 | 6.06 | 1.70 | 1.54 |
| 8 | L | 701 | 1N7 | C8-C7 | 5.79 | 1.69 | 1.54 |
| 8 | I | 1401 | 1N7 | C8-C7 | 5.73 | 1.69 | 1.54 |
| 8 | J | 1504 | 1N7 | C2-C15 | 4.93 | 1.63 | 1.55 |
| 8 | I | 1401 | 1N7 | C2-C15 | 4.83 | 1.63 | 1.55 |
| 8 | J | 1504 | 1N7 | O4-C4 | -4.50 | 1.36 | 1.43 |
| 8 | L | 701 | 1N7 | C5-C9 | 4.31 | 1.62 | 1.55 |
| 8 | I | 1401 | 1N7 | O4-C4 | -4.27 | 1.36 | 1.43 |
| 8 | I | 1401 | 1N7 | C5-C9 | 4.00 | 1.62 | 1.55 |
| 8 | J | 1504 | 1N7 | C5-C6 | -3.87 | 1.48 | 1.55 |
| 8 | L | 701 | 1N7 | C14-C15 | -3.82 | 1.47 | 1.53 |
| 8 | L | 701 | 1N7 | O4-C4 | -3.60 | 1.37 | 1.43 |
| 8 | L | 701 | 1N7 | C18-C6 | -3.48 | 1.47 | 1.53 |
| 8 | J | 1504 | 1N7 | C14-C15 | -3.47 | 1.48 | 1.53 |
| 8 | J | 1504 | 1N7 | C18-C6 | -3.43 | 1.47 | 1.53 |
| 8 | L | 701 | 1N7 | C2-C15 | 3.39 | 1.60 | 1.55 |
| 8 | J | 1504 | 1N7 | C1-C2 | 3.28 | 1.60 | 1.54 |
| 8 | I | 1401 | 1N7 | C14-C15 | -3.16 | 1.48 | 1.53 |
| 8 | J | 1504 | 1N7 | C10-C5 | 3.15 | 1.59 | 1.54 |
| 8 | J | 1504 | 1N7 | C5-C9 | 3.12 | 1.60 | 1.55 |
| 8 | J | 1504 | 1N7 | C7-C6 | 3.08 | 1.60 | 1.54 |
| 8 | I | 1401 | 1N7 | C7-C6 | 2.95 | 1.60 | 1.54 |
| 8 | L | 701 | 1N7 | C5-C6 | -2.87 | 1.50 | 1.55 |
| 8 | L | 701 | 1N7 | C1-C2 | 2.85 | 1.59 | 1.54 |
| 8 | I | 1401 | 1N7 | C1-C2 | 2.78 | 1.59 | 1.54 |
| 8 | L | 701 | 1N7 | C7-C6 | 2.78 | 1.60 | 1.54 |
| 8 | I | 1401 | 1N7 | C5-C6 | -2.72 | 1.50 | 1.55 |
| 8 | I | 1401 | 1N7 | C18-C6 | -2.65 | 1.48 | 1.53 |
| 8 | L | 701 | 1N7 | O2-C13 | -2.56 | 1.35 | 1.43 |
| 8 | I | 1401 | 1N7 | C10-C5 | 2.50 | 1.58 | 1.54 |
| 8 | I | 1401 | 1N7 | O2-C13 | -2.46 | 1.36 | 1.43 |
| 8 | J | 1504 | 1N7 | O2-C13 | -2.34 | 1.36 | 1.43 |
| 8 | I | 1401 | 1N7 | C16-C15 | 2.30 | 1.57 | 1.53 |

All (58) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 8 | J | 1504 | 1N7 | C9-C5-C4 | -8.57 | 109.84 | 117.67 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 8 | L | 701 | 1N7 | C7-C6-C18 | -7.10 | 108.40 | 118.33 |
| 8 | L | 701 | 1N7 | C9-C5-C6 | 6.82 | 106.97 | 100.09 |
| 8 | I | 1401 | 1N7 | C9-C5-C6 | 6.44 | 106.59 | 100.09 |
| 8 | L | 701 | 1N7 | C9-C5-C4 | -6.15 | 112.05 | 117.67 |
| 8 | I | 1401 | 1N7 | C16-C15-C14 | -6.13 | 104.13 | 111.19 |
| 8 | J | 1504 | 1N7 | C16-C17-C18 | -5.35 | 105.77 | 111.48 |
| 8 | I | 1401 | 1N7 | C11-C2-C1 | -5.15 | 99.96 | 108.26 |
| 8 | I | 1401 | 1N7 | C9-C5-C4 | -5.15 | 112.96 | 117.67 |
| 8 | I | 1401 | 1N7 | C16-C17-C18 | -4.97 | 106.18 | 111.48 |
| 8 | L | 701 | 1N7 | C19-C18-C17 | -4.92 | 106.00 | 111.88 |
| 8 | J | 1504 | 1N7 | C1-C2-C15 | 4.83 | 114.91 | 107.77 |
| 8 | I | 1401 | 1N7 | C7-C6-C18 | -4.77 | 111.66 | 118.33 |
| 8 | J | 1504 | 1N7 | C14-C13-C12 | -4.71 | 104.93 | 110.55 |
| 8 | L | 701 | 1N7 | C16-C17-C18 | -4.41 | 106.77 | 111.48 |
| 8 | J | 1504 | 1N7 | C7-C6-C18 | -4.39 | 112.20 | 118.33 |
| 8 | I | 1401 | 1N7 | C14-C13-C12 | -4.23 | 105.50 | 110.55 |
| 8 | L | 701 | 1N7 | C11-C2-C15 | -4.19 | 103.26 | 110.36 |
| 8 | J | 1504 | 1N7 | C15-C14-C13 | -4.12 | 106.71 | 112.76 |
| 8 | L | 701 | 1N7 | C14-C13-C12 | -3.98 | 105.81 | 110.55 |
| 8 | L | 701 | 1N7 | C16-C15-C14 | -3.97 | 106.61 | 111.19 |
| 8 | J | 1504 | 1N7 | C19-C18-C17 | -3.90 | 107.21 | 111.88 |
| 8 | L | 701 | 1N7 | C6-C5-C4 | 3.86 | 111.00 | 107.40 |
| 8 | I | 1401 | 1N7 | C21-C20-C22 | -3.84 | 104.34 | 110.36 |
| 8 | J | 1504 | 1N7 | C11-C2-C15 | -3.79 | 103.93 | 110.36 |
| 8 | I | 1401 | 1N7 | C19-C18-C17 | -3.79 | 107.34 | 111.88 |
| 8 | L | 701 | 1N7 | C5-C6-C18 | 3.77 | 119.55 | 114.74 |
| 8 | J | 1504 | 1N7 | C16-C15-C14 | -3.76 | 106.86 | 111.19 |
| 8 | L | 701 | 1N7 | C21-C20-C22 | -3.72 | 104.53 | 110.36 |
| 8 | J | 1504 | 1N7 | C21-C20-C9 | -3.69 | 107.27 | 112.92 |
| 8 | J | 1504 | 1N7 | C5-C9-C20 | -3.48 | 115.34 | 119.50 |
| 8 | J | 1504 | 1N7 | C9-C5-C6 | 3.42 | 103.54 | 100.09 |
| 8 | J | 1504 | 1N7 | C22-C20-C9 | 3.22 | 116.94 | 110.28 |
| 8 | J | 1504 | 1N7 | C6-C5-C4 | 3.10 | 110.29 | 107.40 |
| 8 | L | 701 | 1N7 | C10-C5-C9 | -3.08 | 106.39 | 111.21 |
| 8 | J | 1504 | 1N7 | C11-C2-C1 | -3.04 | 103.36 | 108.26 |
| 8 | J | 1504 | 1N7 | C8-C9-C20 | 2.98 | 116.76 | 112.15 |
| 8 | I | 1401 | 1N7 | C16-C15-C2 | 2.94 | 115.78 | 112.66 |
| 8 | L | 701 | 1N7 | C1-C12-C13 | -2.93 | 106.71 | 110.47 |
| 8 | I | 1401 | 1N7 | C10-C5-C9 | -2.90 | 106.67 | 111.21 |
| 8 | L | 701 | 1N7 | C6-C18-C17 | 2.89 | 115.63 | 111.81 |
| 8 | J | 1504 | 1N7 | C11-C2-C19 | 2.85 | 115.11 | 111.18 |
| 8 | I | 1401 | 1N7 | C6-C18-C17 | 2.72 | 115.42 | 111.81 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 8 | J | 1504 | 1N7 | C2-C19-C18 | 2.71 | 114.73 | 111.82 |
| 8 | J | 1504 | 1N7 | C16-C15-C2 | 2.66 | 115.48 | 112.66 |
| 8 | J | 1504 | 1N7 | C1-C2-C19 | -2.65 | 107.19 | 111.35 |
| 8 | J | 1504 | 1N7 | C19-C2-C15 | 2.60 | 112.23 | 108.58 |
| 8 | J | 1504 | 1N7 | O4-C4-C3 | -2.38 | 104.28 | 109.12 |
| 8 | I | 1401 | 1N7 | C8-C9-C20 | -2.37 | 108.48 | 112.15 |
| 8 | L | 701 | 1N7 | C8-C9-C20 | -2.37 | 108.48 | 112.15 |
| 8 | J | 1504 | 1N7 | C12-C1-C2 | 2.36 | 116.83 | 112.78 |
| 8 | I | 1401 | 1N7 | C5-C6-C18 | 2.34 | 117.73 | 114.74 |
| 8 | I | 1401 | 1N7 | C7-C6-C5 | 2.32 | 105.82 | 103.55 |
| 8 | I | 1401 | 1N7 | C12-C1-C2 | 2.28 | 116.69 | 112.78 |
| 8 | J | 1504 | 1N7 | C5-C6-C18 | 2.13 | 117.46 | 114.74 |
| 8 | J | 1504 | 1N7 | C21-C20-C22 | -2.11 | 107.06 | 110.36 |
| 8 | I | 1401 | 1N7 | C3-C4-C5 | 2.05 | 113.35 | 111.24 |
| 8 | L | 701 | 1N7 | O3-C17-C18 | 2.03 | 113.97 | 109.43 |

There are no chirality outliers.

All (8) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 8 | J | 1504 | 1N7 | C21-C20-C9-C5 |
| 8 | J | 1504 | 1N7 | C21-C20-C9-C8 |
| 8 | J | 1504 | 1N7 | C22-C20-C9-C5 |
| 8 | J | 1504 | 1N7 | C22-C20-C9-C8 |
| 8 | J | 1504 | 1N7 | C9-C20-C22-C23 |
| 8 | J | 1504 | 1N7 | C21-C20-C22-C23 |
| 8 | J | 1504 | 1N7 | C20-C22-C23-C24 |
| 8 | I | 1401 | 1N7 | C20-C22-C23-C24 |

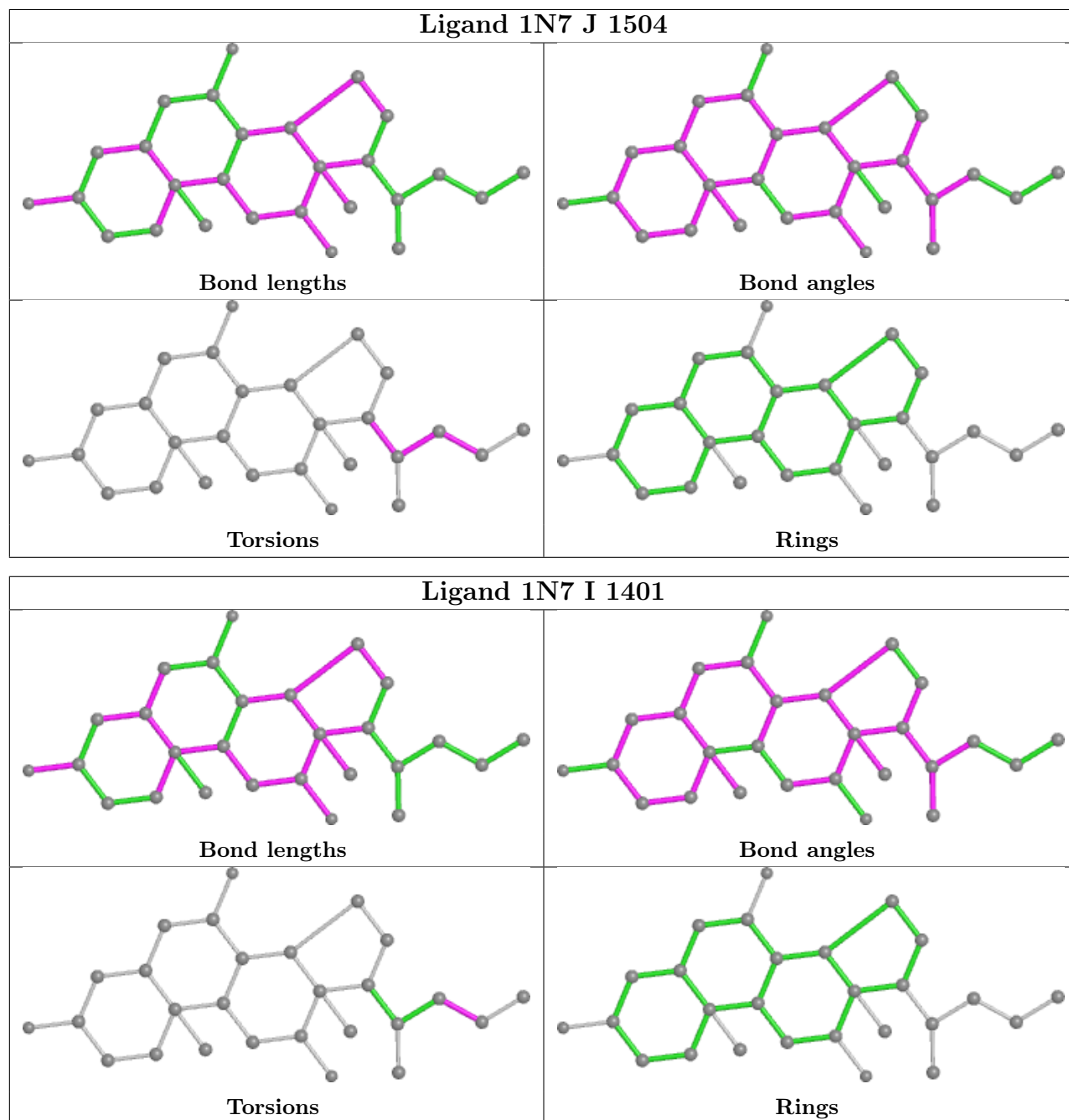
There are no ring outliers.

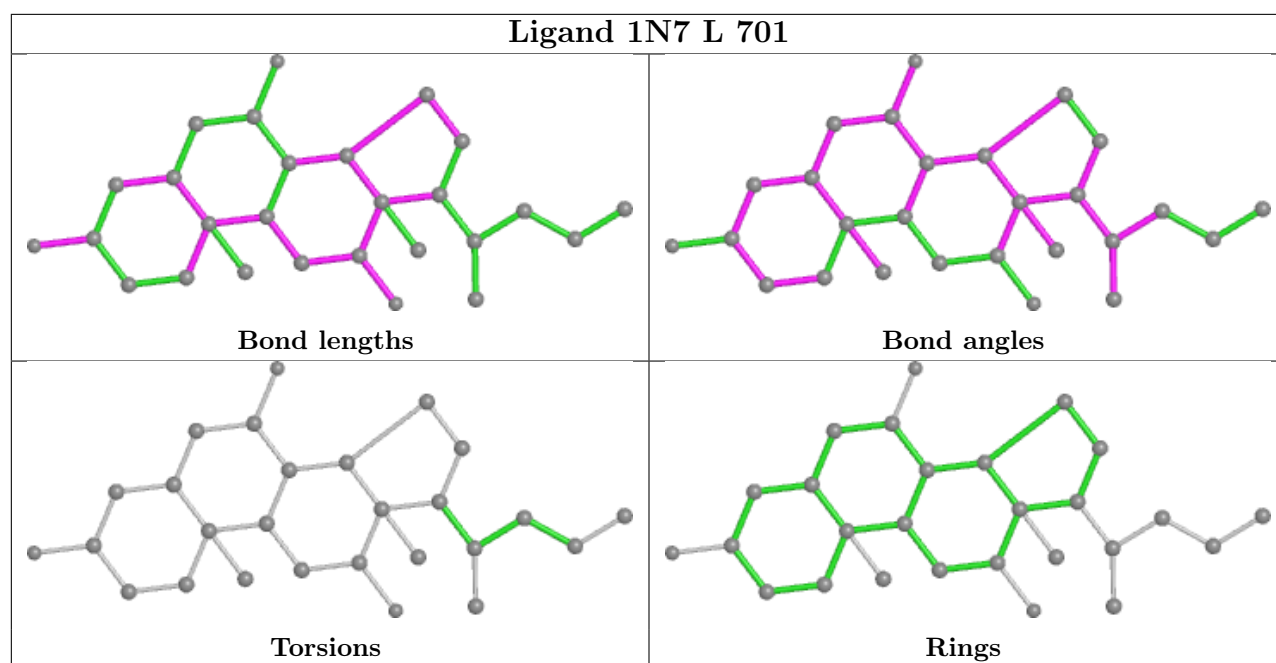
3 monomers are involved in 14 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 8 | J | 1504 | 1N7 | 4 | 0 |
| 8 | I | 1401 | 1N7 | 6 | 0 |
| 8 | L | 701 | 1N7 | 4 | 0 |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

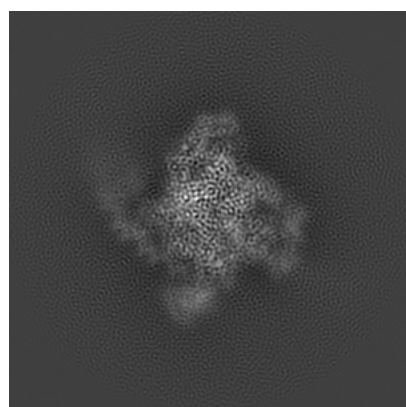
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20203. These allow visual inspection of the internal detail of the map and identification of artifacts.

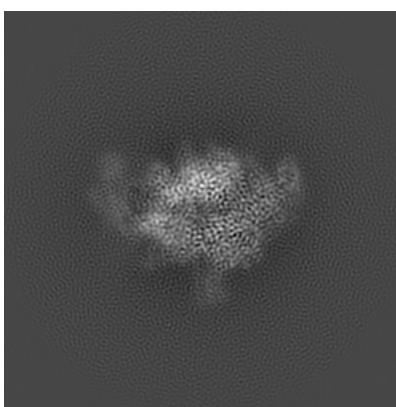
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

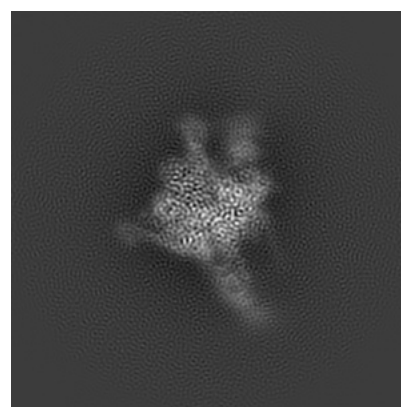
6.1.1 Primary map



X



Y

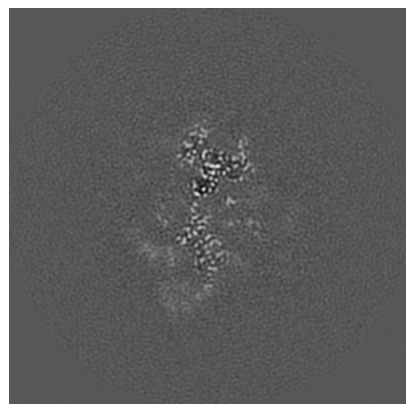


Z

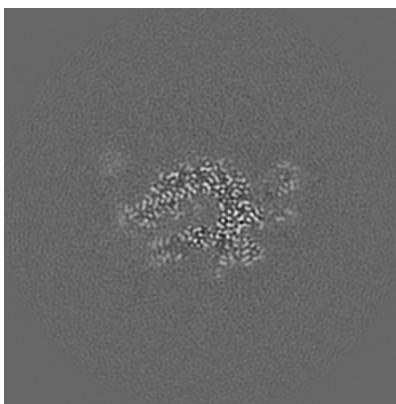
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

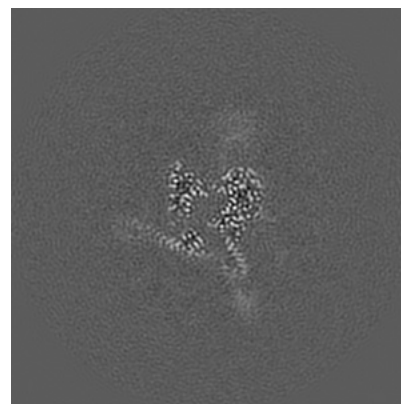
6.2.1 Primary map



X Index: 128



Y Index: 128

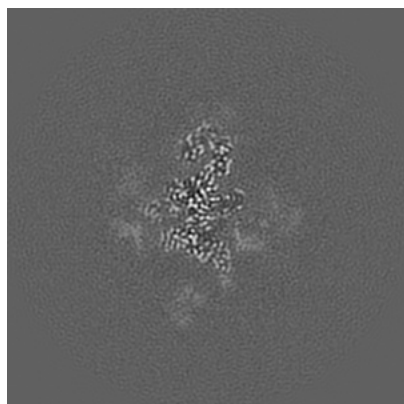


Z Index: 128

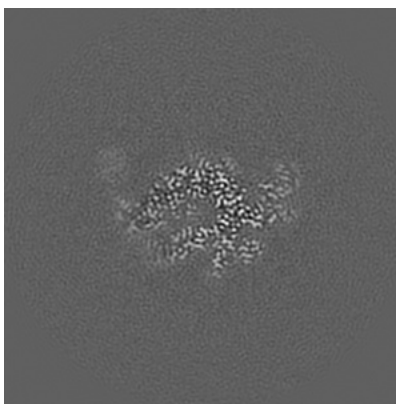
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

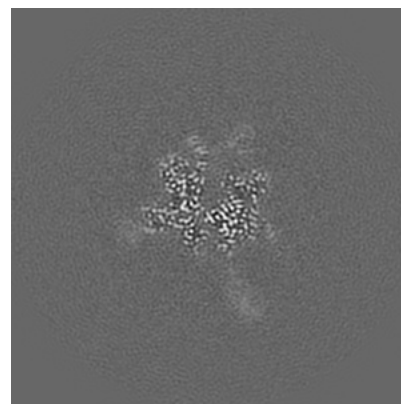
6.3.1 Primary map



X Index: 138



Y Index: 126

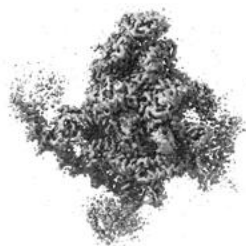


Z Index: 136

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

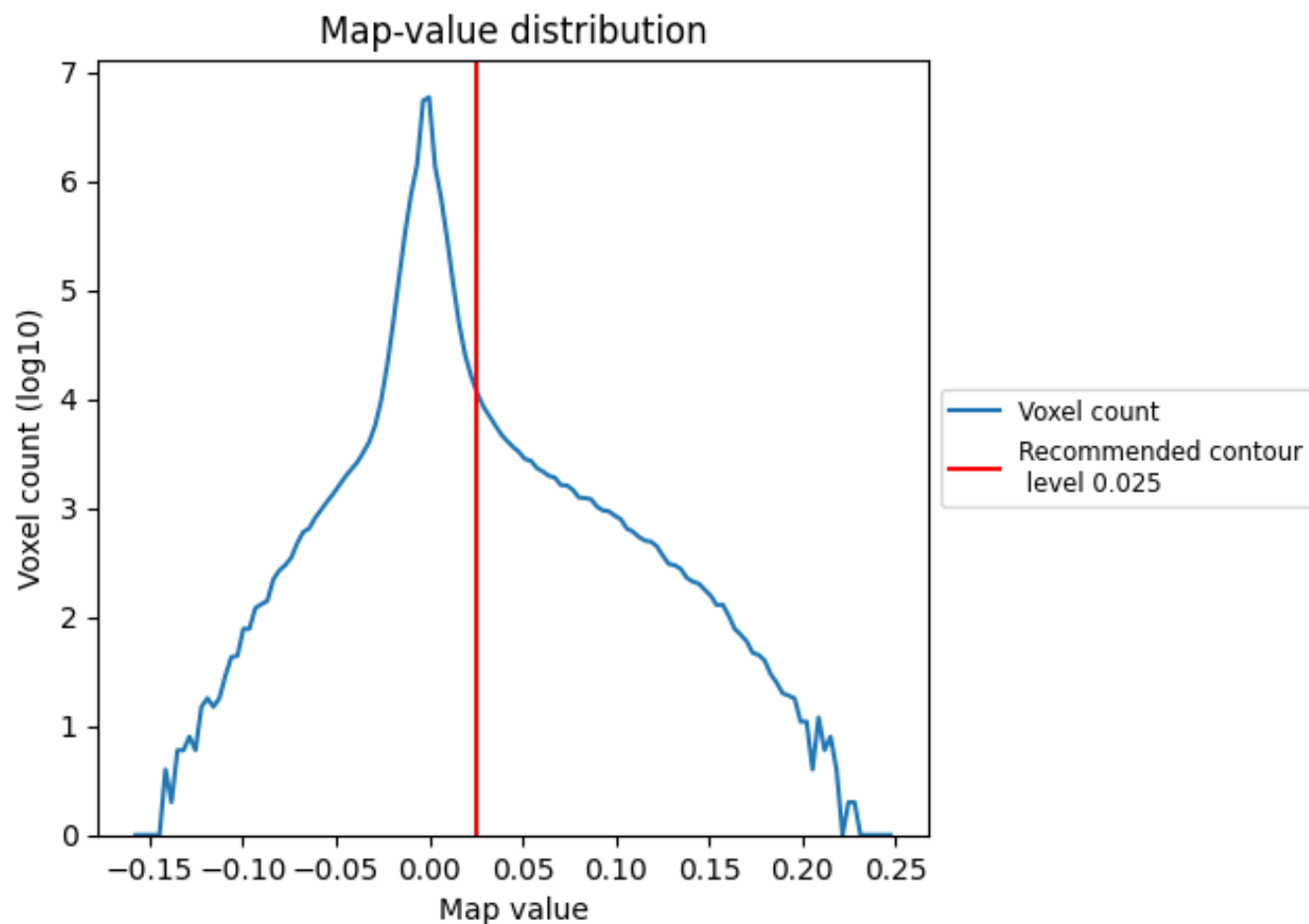
6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

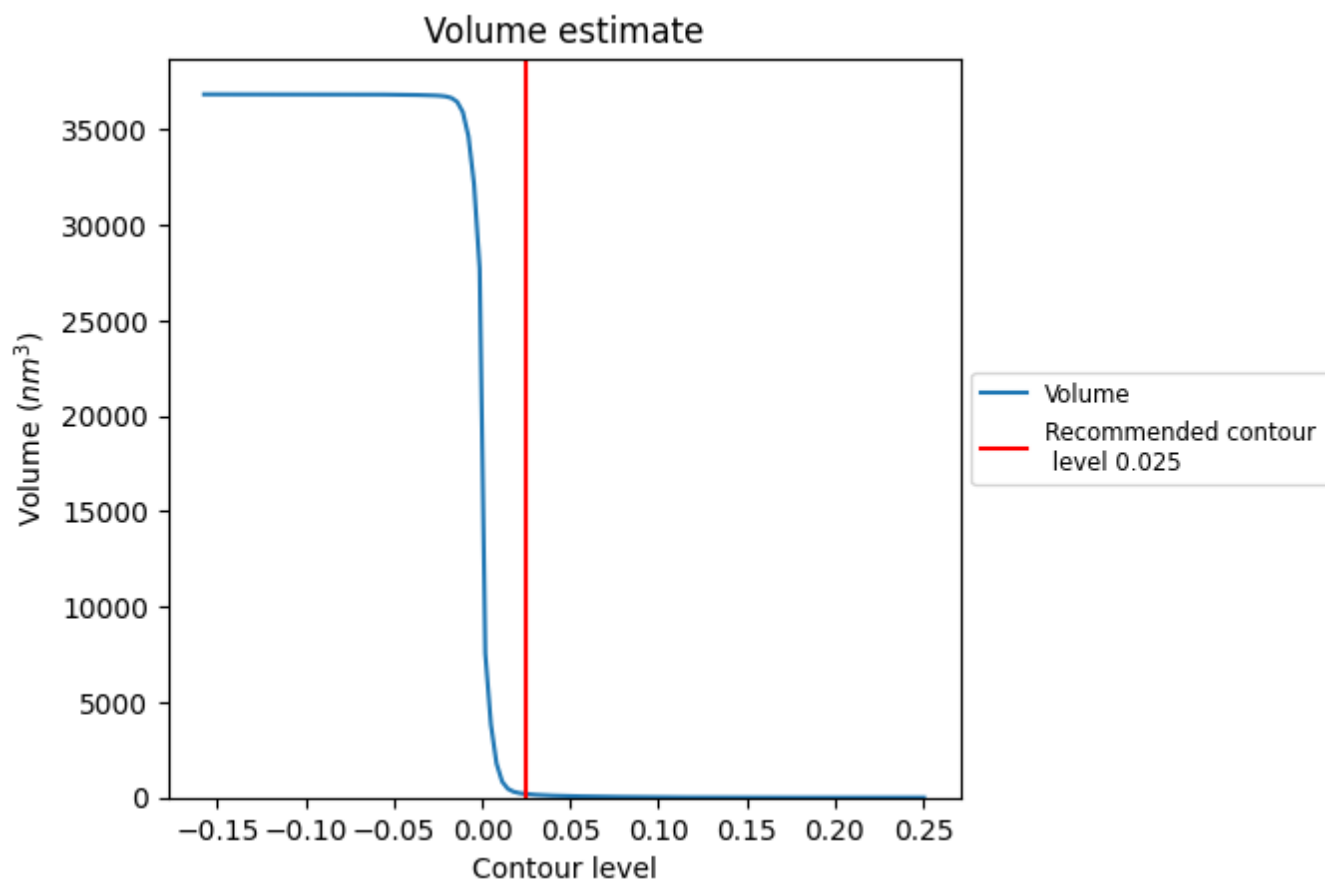
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

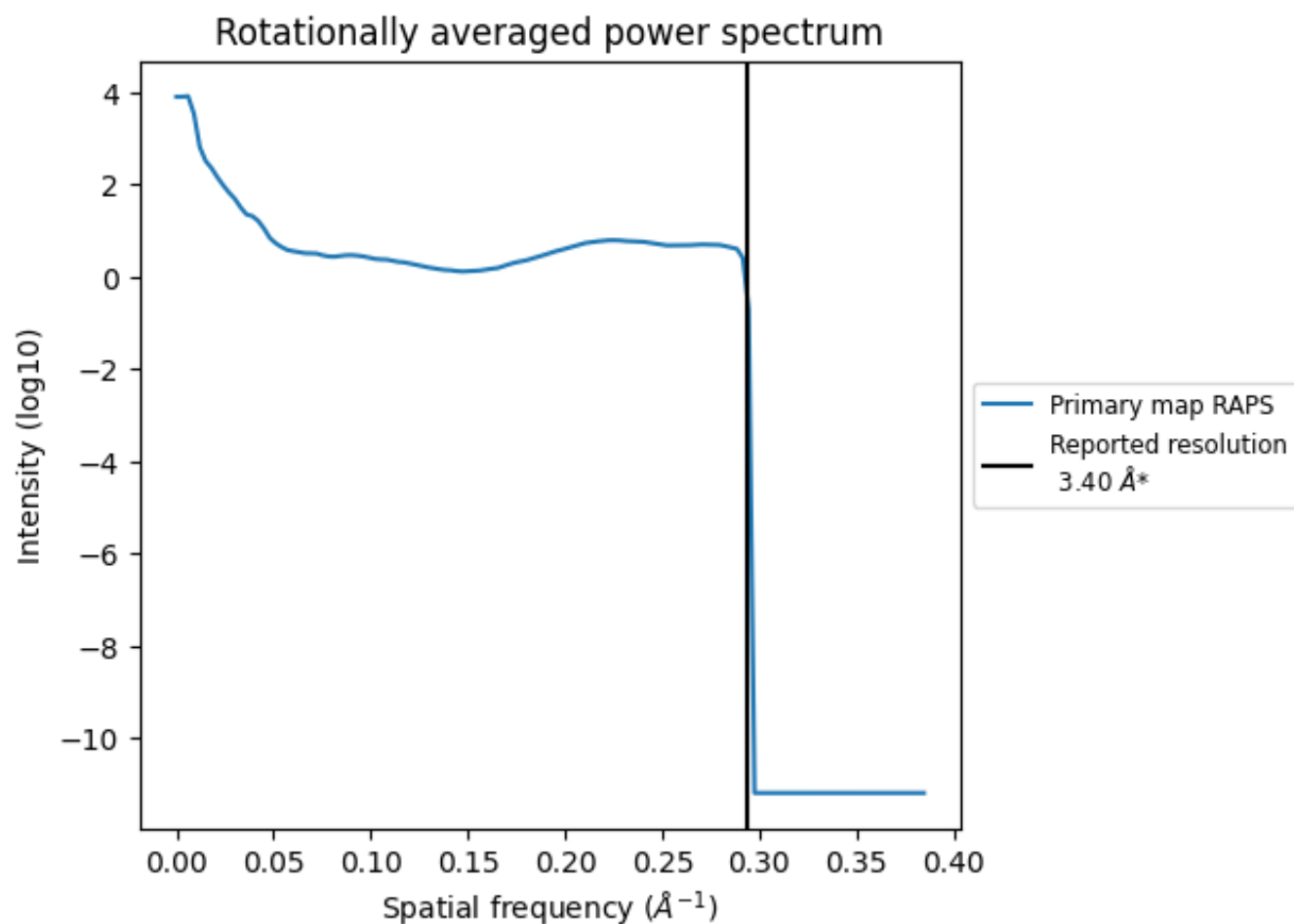
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 187 nm³; this corresponds to an approximate mass of 169 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

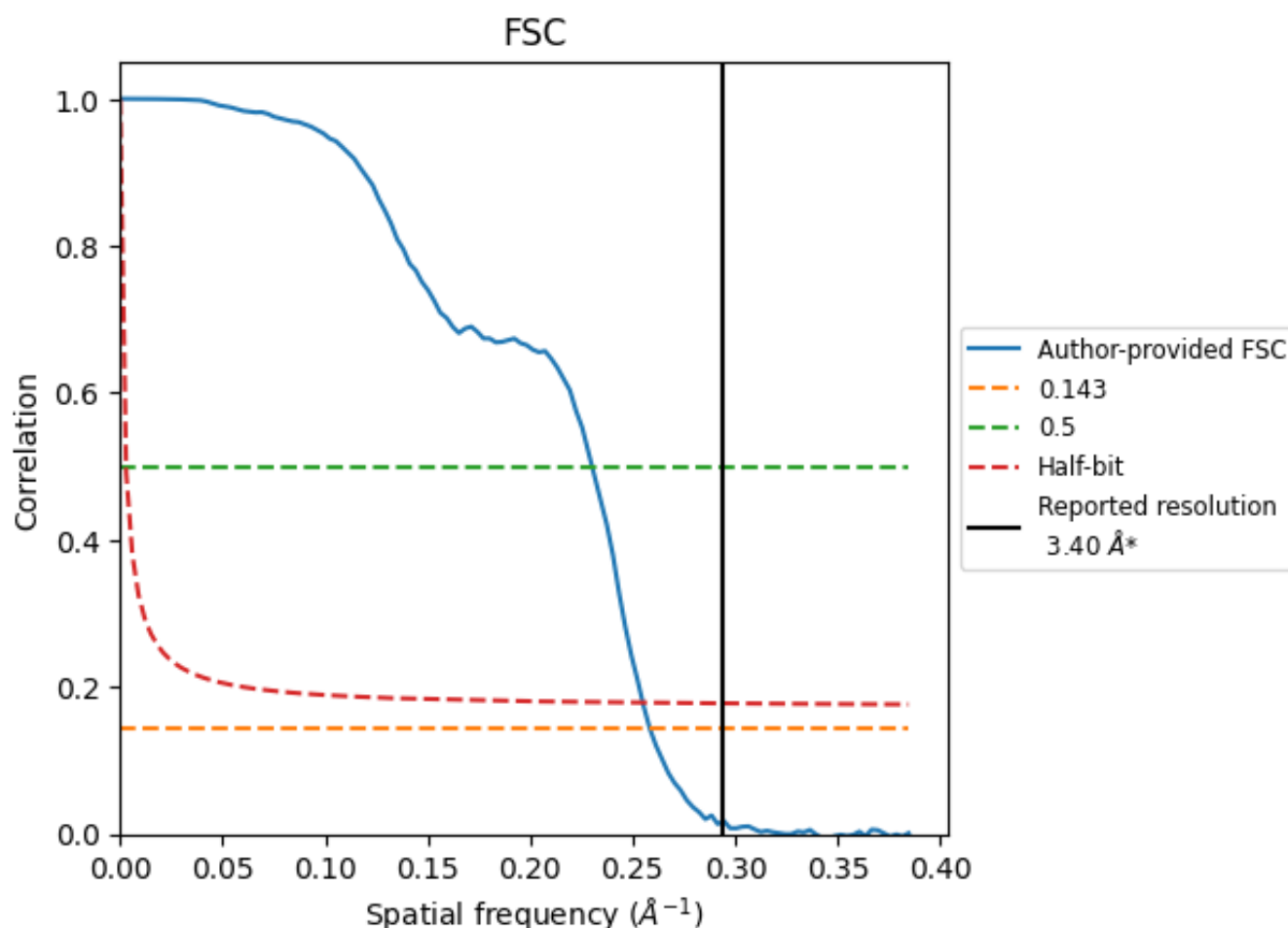


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

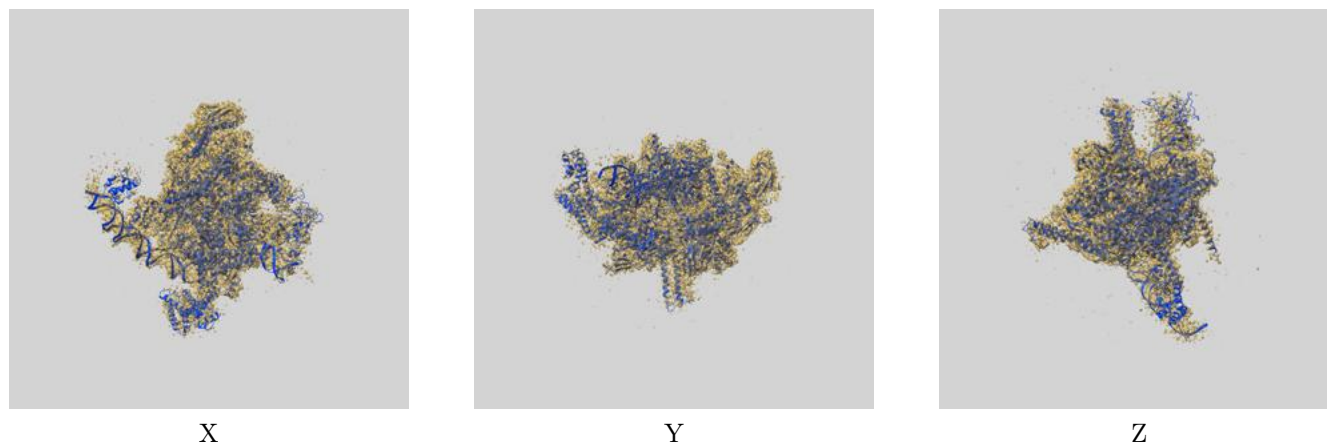
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.40 | - | - |
| Author-provided FSC curve | 3.87 | 4.34 | 3.92 |
| Unmasked-calculated* | - | - | - |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.87 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

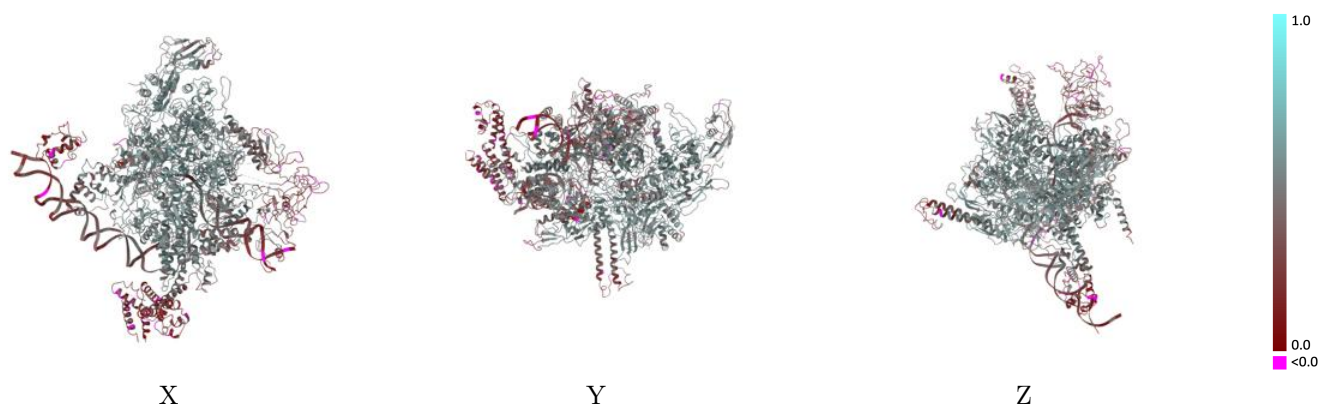
This section contains information regarding the fit between EMDB map EMD-20203 and PDB model 6OUL. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



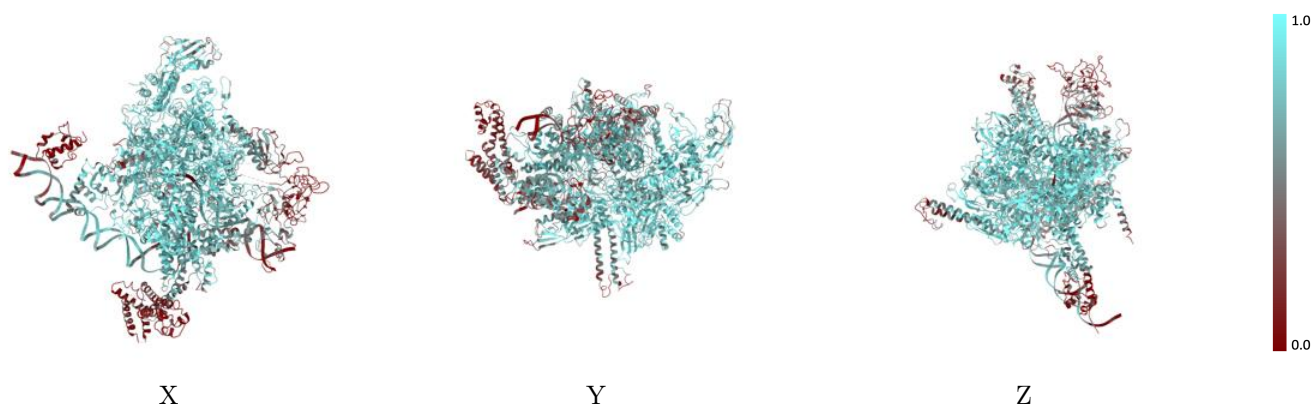
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



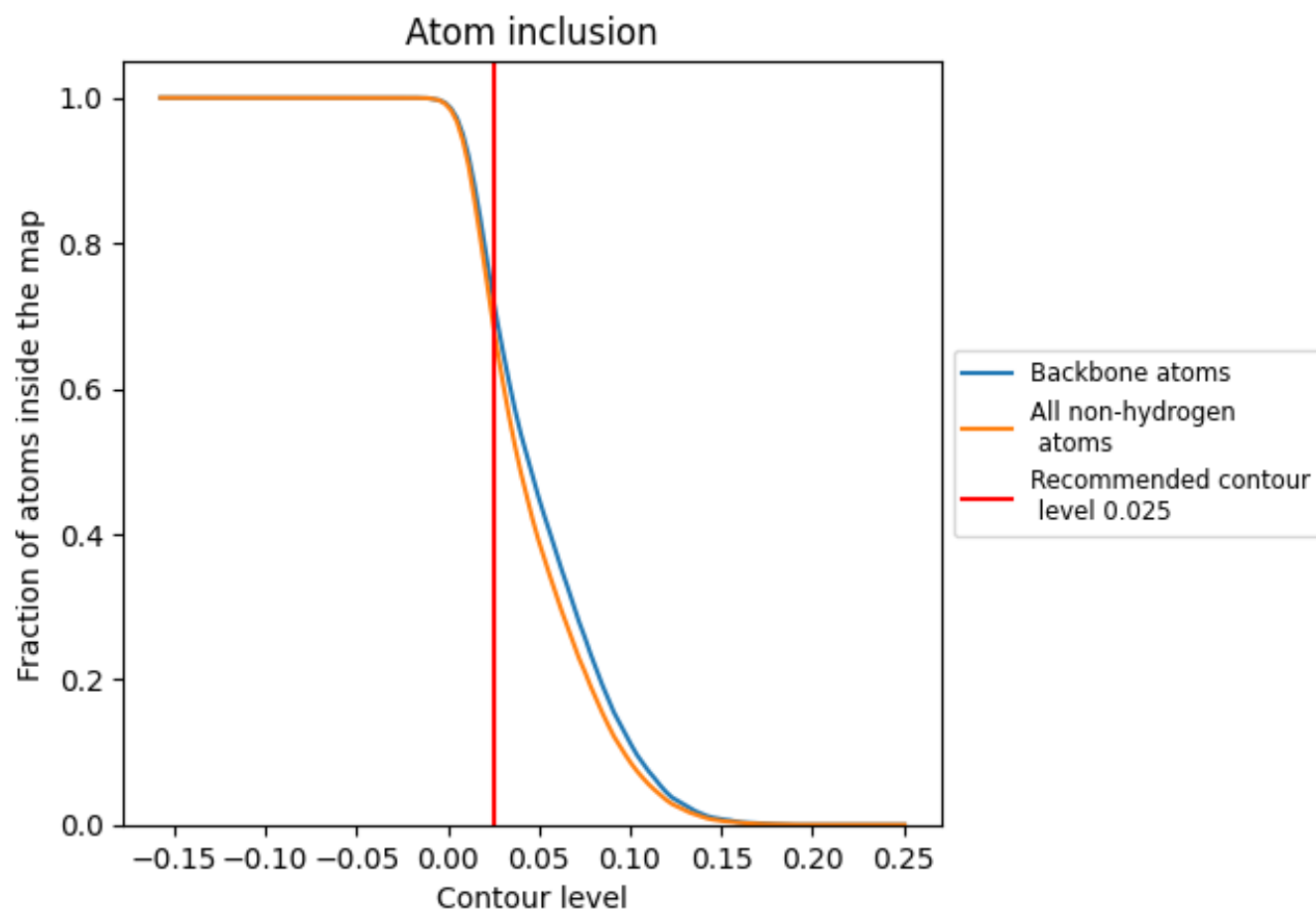
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--------------------|--------------------|
| All | <div></div> 0.6864 | <div></div> 0.4600 |
| G | <div></div> 0.7842 | <div></div> 0.5150 |
| H | <div></div> 0.7483 | <div></div> 0.4900 |
| I | <div></div> 0.7638 | <div></div> 0.4990 |
| J | <div></div> 0.7242 | <div></div> 0.4850 |
| K | <div></div> 0.6792 | <div></div> 0.4830 |
| L | <div></div> 0.5052 | <div></div> 0.3730 |
| P | <div></div> 0.5539 | <div></div> 0.3180 |
| Q | <div></div> 0.5381 | <div></div> 0.2950 |
| R | <div></div> 0.0768 | <div></div> 0.2020 |

1.0

0.0

<0.0