



Full wwPDB EM Validation Report ⓘ

Nov 12, 2022 – 02:21 PM EST

PDB ID : 6PSV
EMDB ID : EMD-20465
Title : Escherichia coli RNA polymerase promoter unwinding intermediate (TpreR_{Po})
with TraR and rpsT P2 promoter
Authors : Chen, J.; Chiu, C.E.; Campbell, E.A.; Darst, S.A.
Deposited on : 2019-07-13
Resolution : 3.50 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

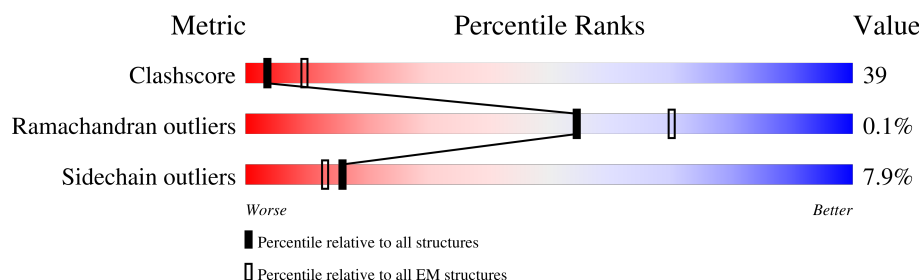
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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 | N | 72 | |
| 2 | G | 329 | |
| 2 | H | 329 | |
| 2 | M | 329 | |
| 3 | I | 1342 | |
| 4 | J | 1430 | |
| 5 | K | 91 | |
| 6 | L | 616 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--------------------------------------------------------------------------------|
| 7 | O | 85 | <div><div><div></div><div></div><div></div></div><div>7%15%49%35%</div></div> |
| 8 | P | 85 | <div><div><div></div><div></div><div></div></div><div>12%13%46%41%</div></div> |

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 32487 atoms, of which 156 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 Protein TraR.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1 | N | 72 | Total | C | N | O | S | 0 | 0 |
| | | | 571 | 353 | 105 | 108 | 5 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2 | G | 228 | Total | C | N | O | S | 0 | 0 |
| | | | 1761 | 1099 | 312 | 344 | 6 | | |
| 2 | H | 219 | Total | C | N | O | S | 0 | 0 |
| | | | 1664 | 1040 | 291 | 327 | 6 | | |
| 2 | M | 73 | Total | C | N | O | S | 0 | 0 |
| | | | 572 | 362 | 100 | 108 | 2 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 3 | I | 1340 | Total | C | N | O | S | 0 | 0 |
| | | | 10564 | 6628 | 1838 | 2055 | 43 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 4 | J | 1345 | Total | C | N | O | S | 0 | 0 |
| | | | 10466 | 6577 | 1867 | 1972 | 50 | | |

There are 24 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| J | 1 | VAL | - | expression tag | UNP P0A8T7 |
| J | 1408 | LEU | - | expression tag | UNP P0A8T7 |
| J | 1409 | GLU | - | expression tag | UNP P0A8T7 |
| J | 1410 | LEU | - | expression tag | UNP P0A8T7 |
| J | 1411 | GLU | - | expression tag | UNP P0A8T7 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| J | 1412 | VAL | - | expression tag | UNP P0A8T7 |
| J | 1413 | LEU | - | expression tag | UNP P0A8T7 |
| J | 1414 | PHE | - | expression tag | UNP P0A8T7 |
| J | 1415 | GLN | - | expression tag | UNP P0A8T7 |
| J | 1416 | GLY | - | expression tag | UNP P0A8T7 |
| J | 1417 | PRO | - | expression tag | UNP P0A8T7 |
| J | 1418 | SER | - | expression tag | UNP P0A8T7 |
| J | 1419 | SER | - | expression tag | UNP P0A8T7 |
| J | 1420 | GLY | - | expression tag | UNP P0A8T7 |
| J | 1421 | HIS | - | expression tag | UNP P0A8T7 |
| J | 1422 | HIS | - | expression tag | UNP P0A8T7 |
| J | 1423 | HIS | - | expression tag | UNP P0A8T7 |
| J | 1424 | HIS | - | expression tag | UNP P0A8T7 |
| J | 1425 | HIS | - | expression tag | UNP P0A8T7 |
| J | 1426 | HIS | - | expression tag | UNP P0A8T7 |
| J | 1427 | HIS | - | expression tag | UNP P0A8T7 |
| J | 1428 | HIS | - | expression tag | UNP P0A8T7 |
| J | 1429 | HIS | - | expression tag | UNP P0A8T7 |
| J | 1430 | HIS | - | expression tag | UNP P0A8T7 |

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit omega.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5 | K | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 627 | 382 | 118 | 126 | 1 | | |

- Molecule 6 is a protein called RNA polymerase sigma factor RpoD.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6 | L | 474 | Total | C | N | O | S | 0 | 0 |
| | | | 3846 | 2409 | 685 | 729 | 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 7 is a DNA chain called DNA (85-MER).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 7 | O | 55 | Total | C | N | O | P | 0 | 0 |
| | | | 1128 | 539 | 211 | 323 | 55 | | |

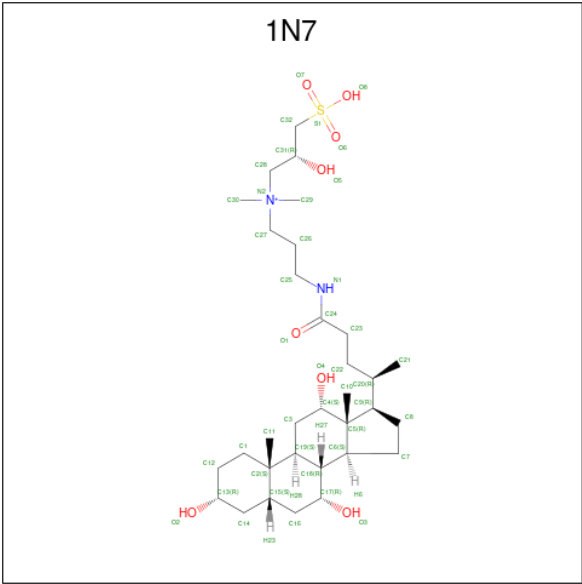
- Molecule 8 is a DNA chain called DNA (85-MER).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 8 | P | 50 | Total | C | N | O | P | 0 | 0 |
| | | | 1020 | 491 | 169 | 310 | 50 | | |

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 9 | N | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 9 | J | 2 | Total | Zn | 0 |
| | | | 2 | 2 | |

- Molecule 10 is CHAPSO (three-letter code: 1N7) (formula: C₃₂H₅₉N₂O₈S).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 10 | N | 1 | Total | C | H | O | 0 |
| | | | 66 | 24 | 39 | 3 | |
| 10 | I | 1 | Total | C | H | O | 0 |
| | | | 66 | 24 | 39 | 3 | |
| 10 | J | 1 | Total | C | H | O | 0 |
| | | | 66 | 24 | 39 | 3 | |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 10 | L | 1 | Total | C | H | O | 0 |
| | | | 66 | 24 | 39 | 3 | |

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

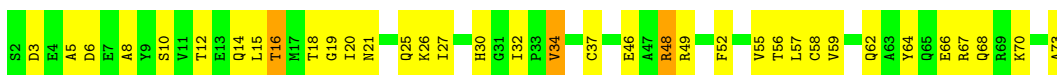
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 11 | J | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

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.

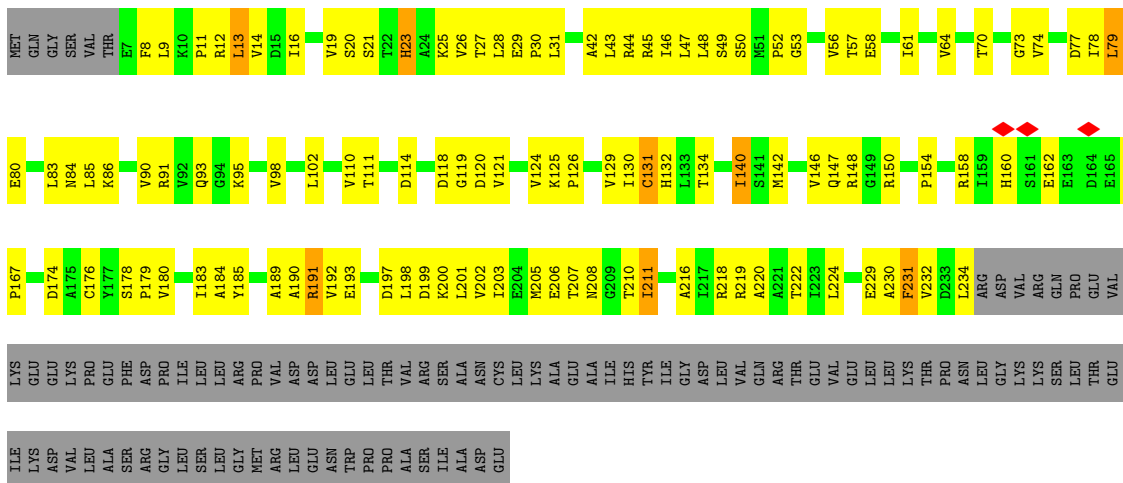
• Molecule 1: Protein TraR

Chain N: 




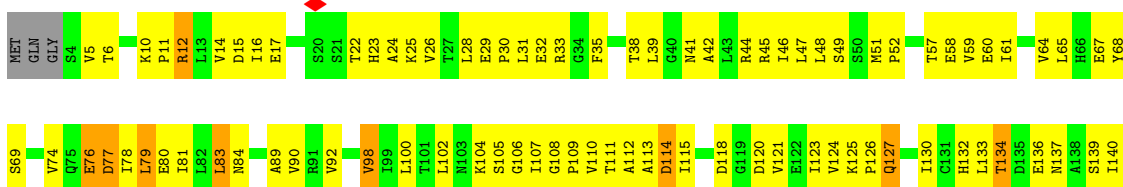
• Molecule 2: DNA-directed RNA polymerase subunit alpha

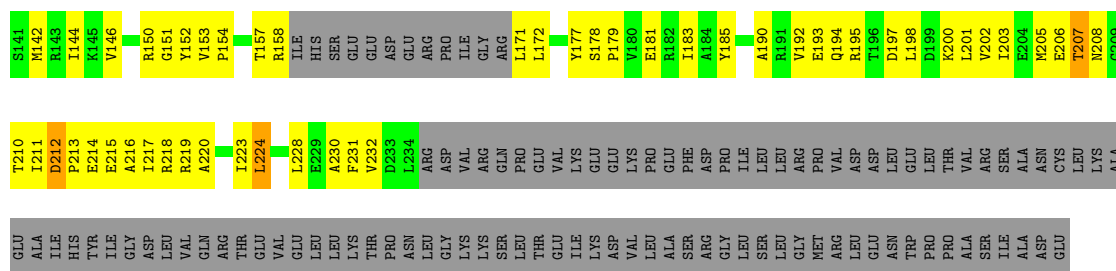
Chain G: 



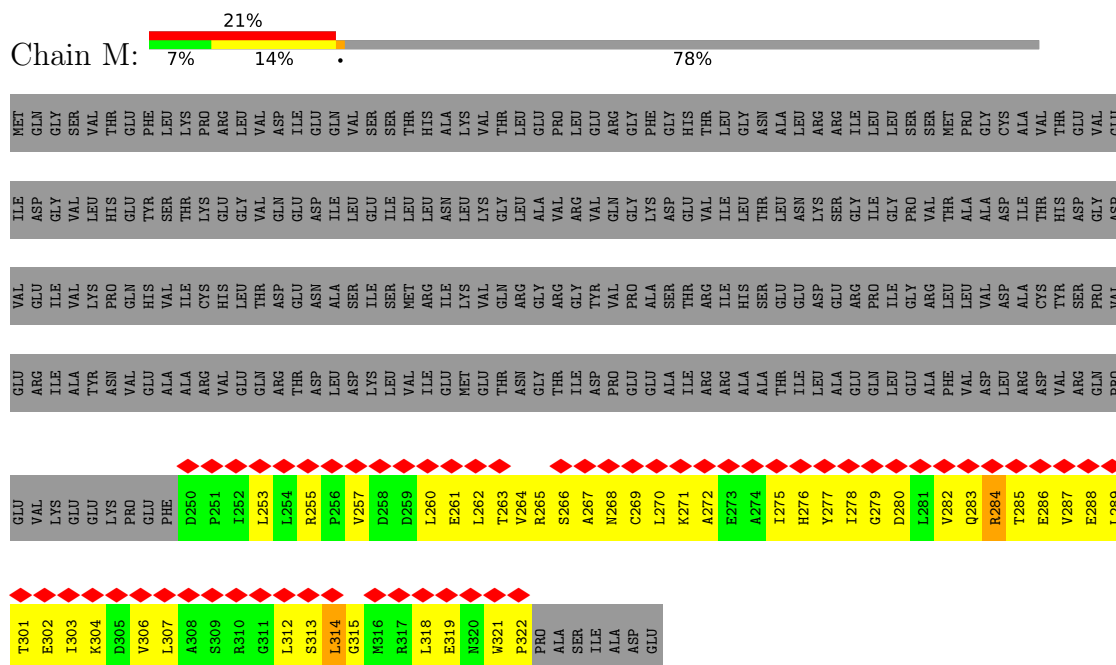
• Molecule 2: DNA-directed RNA polymerase subunit alpha

Chain H: 

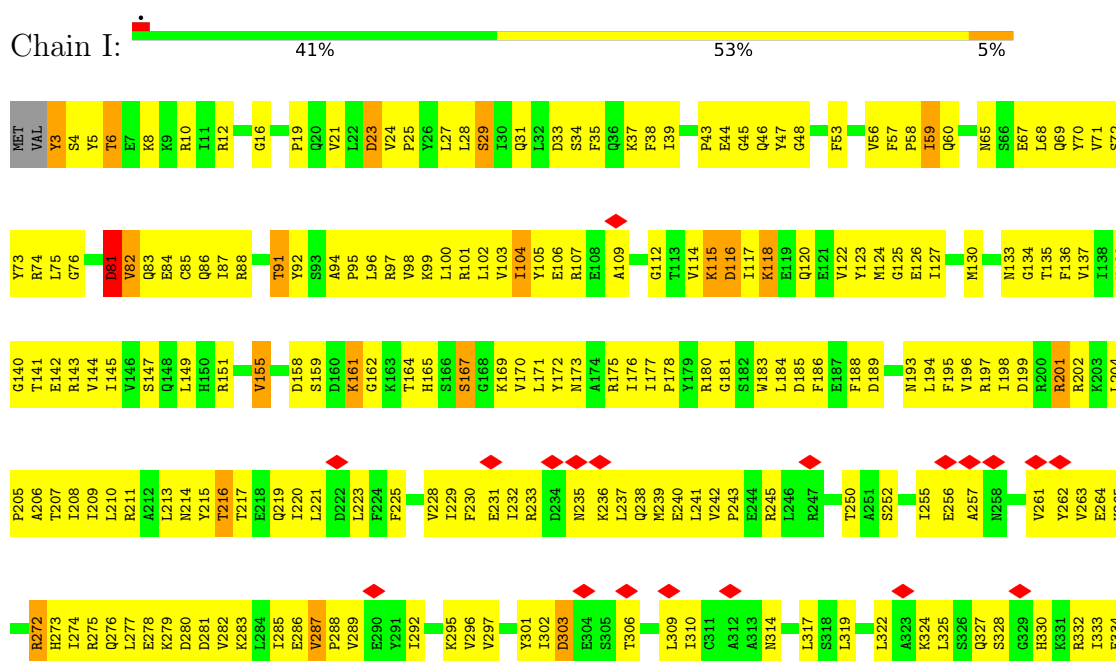


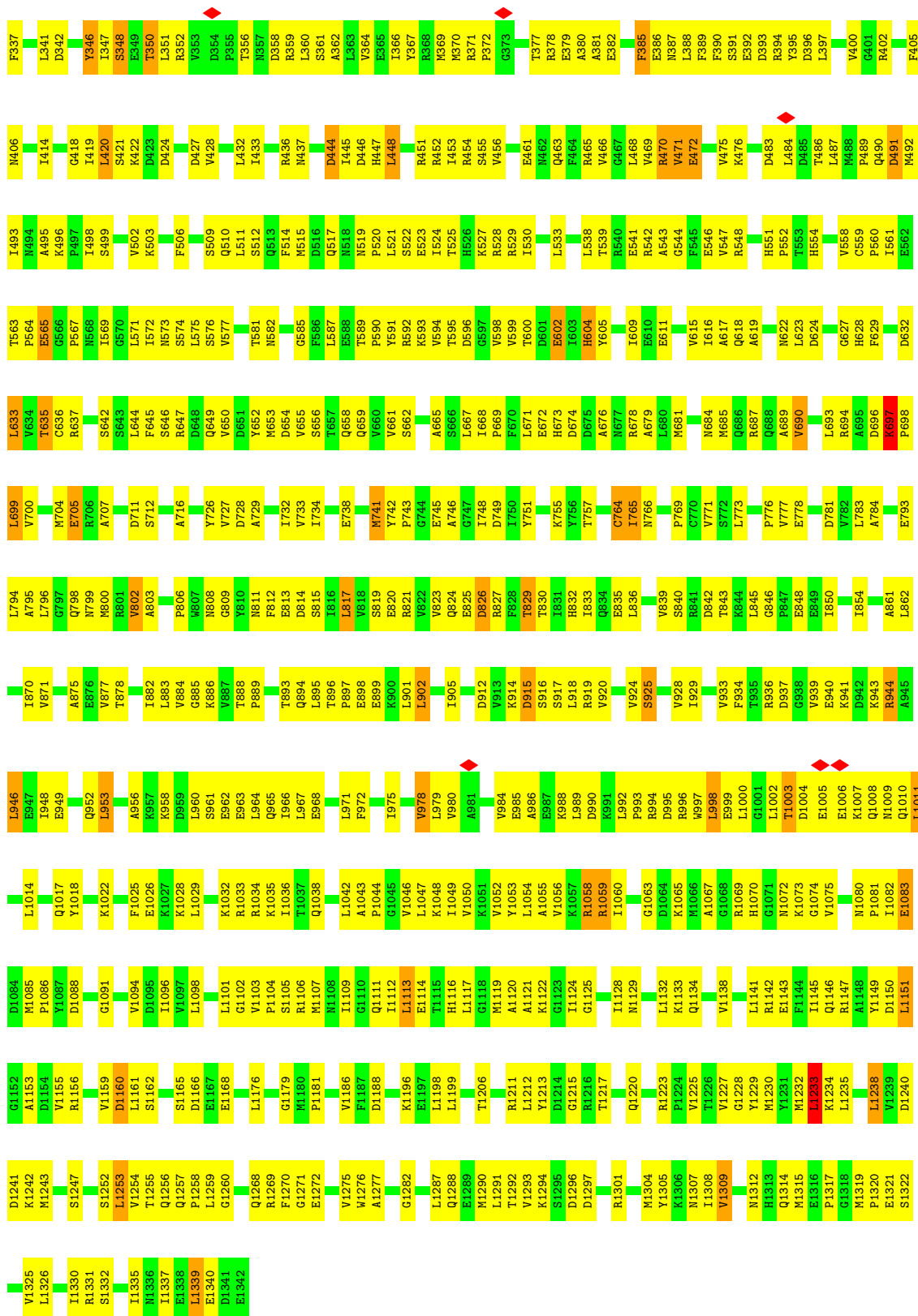


• Molecule 2: DNA-directed RNA polymerase subunit alpha



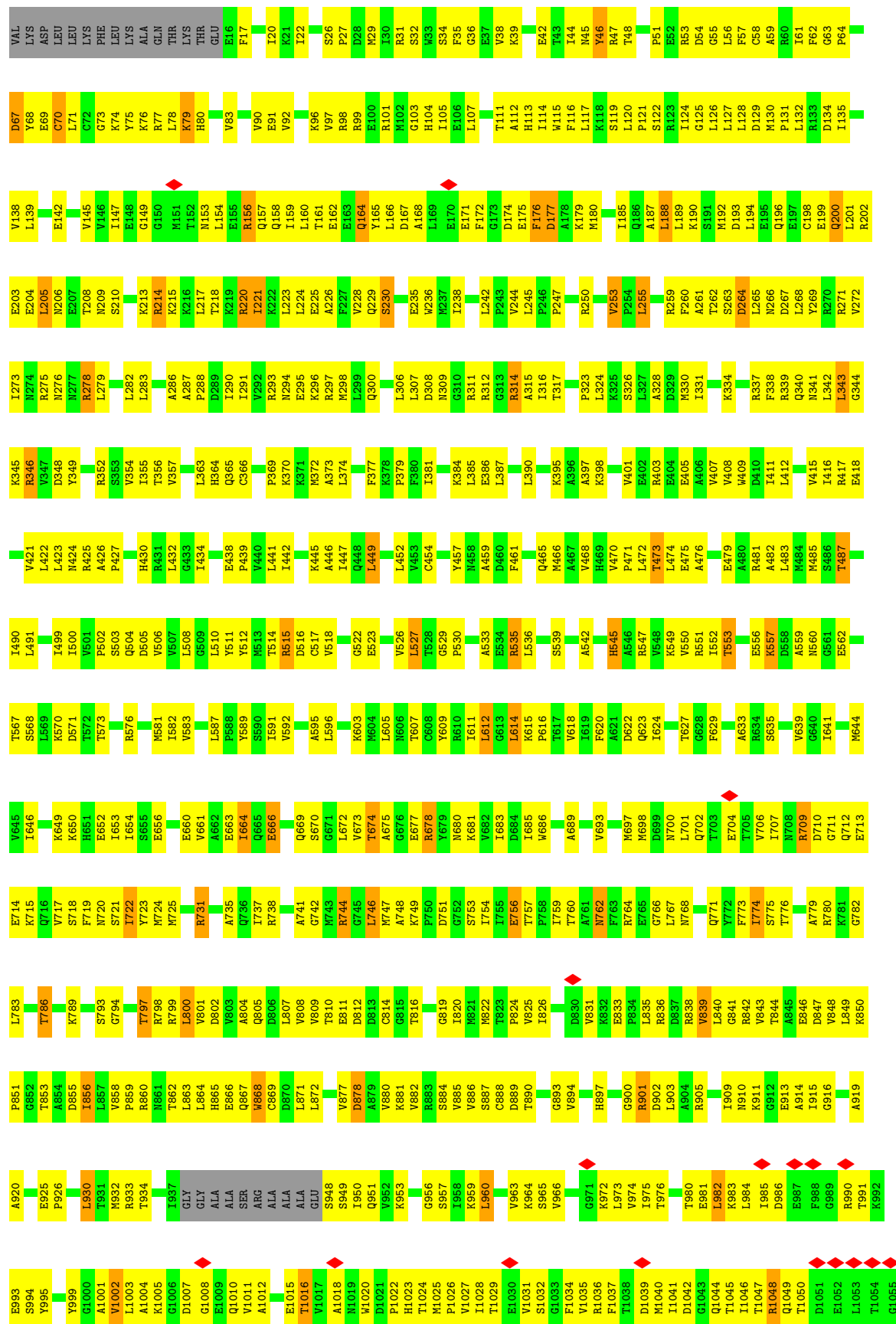
• Molecule 3: DNA-directed RNA polymerase subunit beta

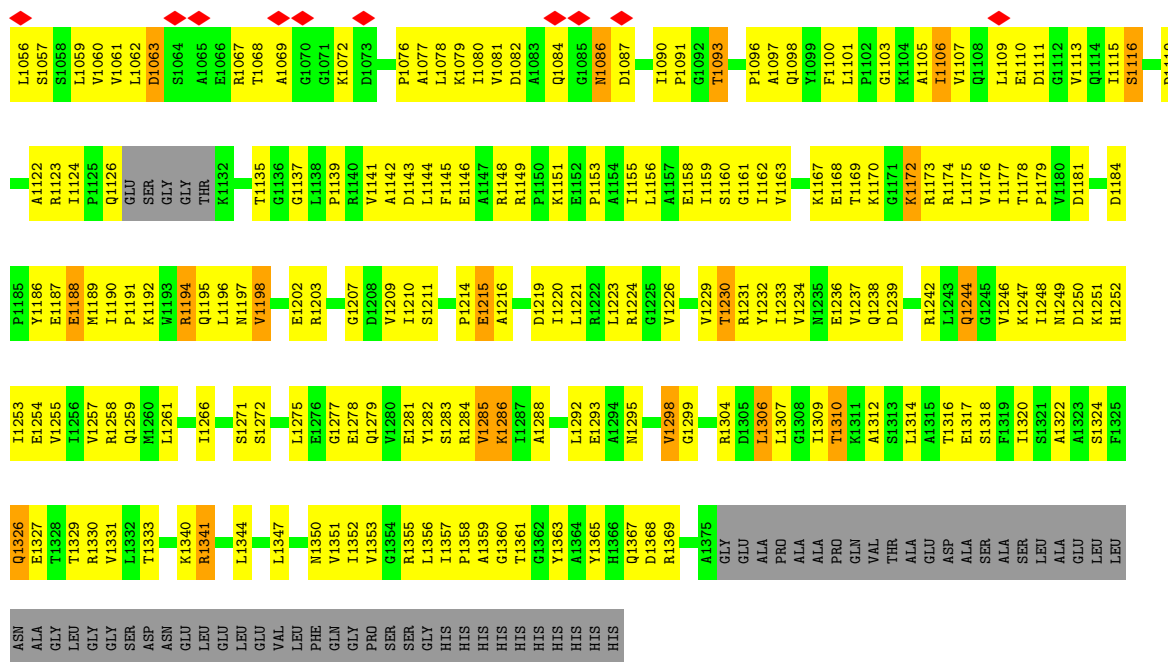




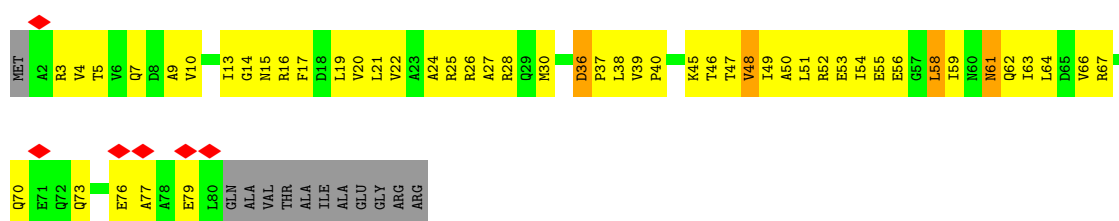
- Molecule 4: DNA-directed RNA polymerase subunit beta'



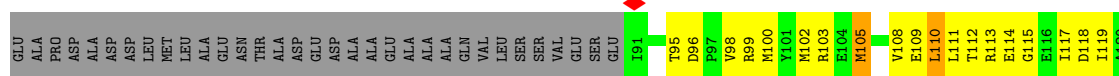
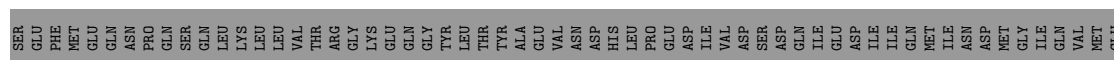


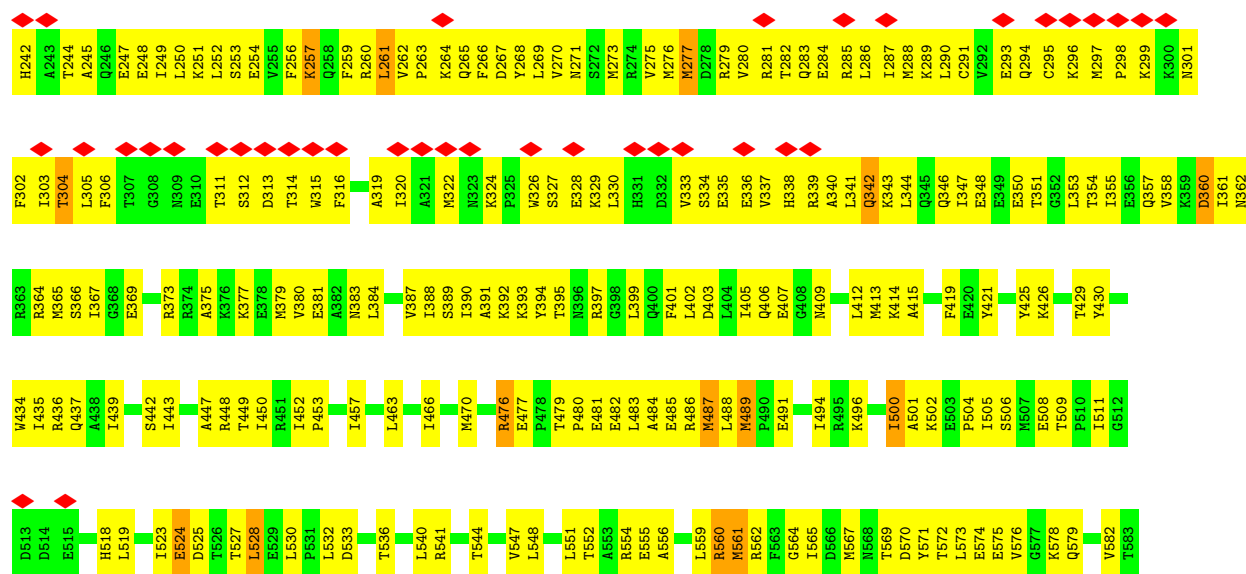


• Molecule 5: DNA-directed RNA polymerase subunit omega

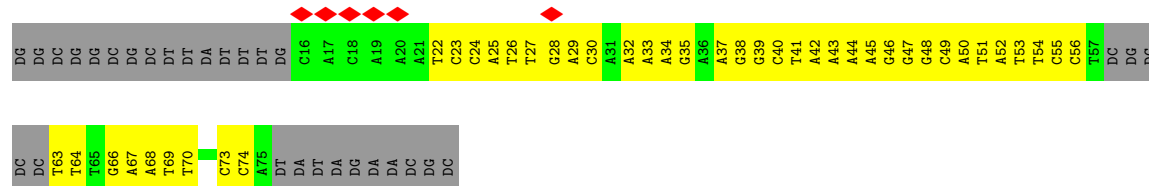
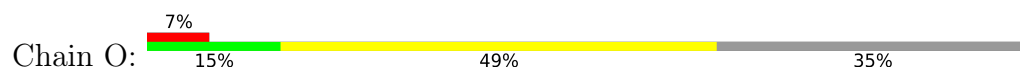


• Molecule 6: RNA polymerase sigma factor RpoD

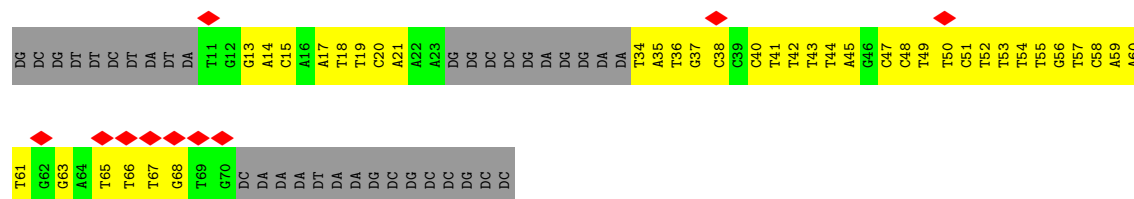
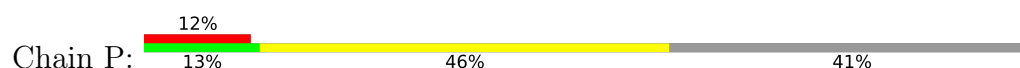




• Molecule 7: DNA (85-MER)



• Molecule 8: DNA (85-MER)



4 Experimental information

| Property | Value | Source |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 81732 | 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 ($e^-/\text{\AA}^2$) | 80 | 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 | 0.226 | Depositor |
| Minimum map value | -0.146 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.007 | Depositor |
| Recommended contour level | 0.02 | Depositor |
| Map size (\AA) | 332.8, 332.8, 332.8 | wwPDB |
| Map dimensions | 256, 256, 256 | wwPDB |
| Map angles ($^\circ$) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (\AA) | 1.3, 1.3, 1.3 | Depositor |

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, 1N7

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 | N | 0.46 | 0/581 | 0.52 | 0/785 |
| 2 | G | 0.51 | 0/1783 | 0.57 | 0/2417 |
| 2 | H | 0.45 | 0/1683 | 0.59 | 0/2285 |
| 2 | M | 0.27 | 0/579 | 0.50 | 0/784 |
| 3 | I | 0.53 | 0/10733 | 0.57 | 2/14482 (0.0%) |
| 4 | J | 0.50 | 0/10625 | 0.57 | 2/14345 (0.0%) |
| 5 | K | 0.38 | 0/629 | 0.52 | 0/847 |
| 6 | L | 0.32 | 0/3898 | 0.50 | 0/5242 |
| 7 | O | 0.63 | 0/1266 | 0.95 | 0/1948 |
| 8 | P | 0.62 | 0/1138 | 1.03 | 0/1752 |
| All | All | 0.50 | 0/32915 | 0.61 | 4/44887 (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 | H | 0 | 1 |
| 3 | I | 0 | 1 |
| 4 | J | 0 | 1 |
| 6 | L | 0 | 2 |
| All | All | 0 | 5 |

There are no bond length outliers.

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 4 | J | 1215 | GLU | C-N-CA | -5.46 | 108.06 | 121.70 |
| 3 | I | 1233 | LEU | CA-CB-CG | 5.20 | 127.26 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3 | I | 633 | LEU | CA-CB-CG | 5.14 | 127.12 | 115.30 |
| 4 | J | 39 | LYS | C-N-CA | -5.05 | 109.07 | 121.70 |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 2 | H | 12 | ARG | Peptide |
| 3 | I | 81 | ASP | Peptide |
| 4 | J | 177 | ASP | Peptide |
| 6 | L | 110 | LEU | Peptide |
| 6 | L | 500 | ILE | Peptide |

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | N | 571 | 0 | 558 | 43 | 0 |
| 2 | G | 1761 | 0 | 1787 | 123 | 0 |
| 2 | H | 1664 | 0 | 1672 | 142 | 0 |
| 2 | M | 572 | 0 | 602 | 66 | 0 |
| 3 | I | 10564 | 0 | 10571 | 835 | 0 |
| 4 | J | 10466 | 0 | 10689 | 914 | 0 |
| 5 | K | 627 | 0 | 634 | 62 | 0 |
| 6 | L | 3846 | 0 | 3896 | 403 | 0 |
| 7 | O | 1128 | 0 | 621 | 76 | 0 |
| 8 | P | 1020 | 0 | 573 | 61 | 0 |
| 9 | J | 2 | 0 | 0 | 0 | 0 |
| 9 | N | 1 | 0 | 0 | 0 | 0 |
| 10 | I | 27 | 39 | 38 | 6 | 0 |
| 10 | J | 27 | 39 | 37 | 3 | 0 |
| 10 | L | 27 | 39 | 37 | 3 | 0 |
| 10 | N | 27 | 39 | 38 | 4 | 0 |
| 11 | J | 1 | 0 | 0 | 0 | 0 |
| All | All | 32331 | 156 | 31753 | 2518 | 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 39.

All (2518) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:L:701:1N7:C19 | 10:L:701:1N7:C3 | 1.84 | 1.55 |
| 10:N:102:1N7:C19 | 10:N:102:1N7:C3 | 1.82 | 1.55 |
| 10:I:1401:1N7:C3 | 10:I:1401:1N7:C19 | 1.83 | 1.53 |
| 10:J:1504:1N7:C19 | 10:J:1504:1N7:C3 | 1.84 | 1.51 |
| 6:L:95:THR:HA | 6:L:100:MET:HE3 | 1.34 | 1.06 |
| 3:I:103:VAL:HB | 3:I:114:VAL:HG11 | 1.42 | 1.00 |
| 3:I:176:ILE:HD11 | 3:I:428:VAL:HG21 | 1.42 | 1.00 |
| 6:L:140:ALA:HB1 | 6:L:269:LEU:HD13 | 1.43 | 0.99 |
| 2:M:275:ILE:HG22 | 2:M:280:ASP:HB3 | 1.42 | 0.99 |
| 4:J:1215:GLU:HG3 | 4:J:1220:ILE:HD11 | 1.45 | 0.98 |
| 6:L:547:VAL:HG11 | 6:L:607:LEU:HD21 | 1.46 | 0.97 |
| 6:L:287:ILE:HG12 | 6:L:337:VAL:HG13 | 1.47 | 0.96 |
| 6:L:119:ILE:HG23 | 6:L:375:ALA:HB1 | 1.47 | 0.95 |
| 3:I:255:ILE:HG22 | 3:I:262:TYR:HB2 | 1.47 | 0.95 |
| 6:L:280:VAL:HG22 | 6:L:347:ILE:HD13 | 1.47 | 0.94 |
| 2:H:104:LYS:HD2 | 2:H:110:VAL:HG22 | 1.47 | 0.94 |
| 4:J:1190:ILE:HG21 | 4:J:1196:LEU:HD11 | 1.50 | 0.94 |
| 2:M:300:LEU:HA | 2:M:303:ILE:HD12 | 1.49 | 0.93 |
| 3:I:322:LEU:HD12 | 3:I:325:LEU:HD11 | 1.50 | 0.93 |
| 4:J:417:ARG:HB3 | 5:K:45:LYS:HE2 | 1.47 | 0.93 |
| 2:H:46:ILE:HD11 | 2:H:224:LEU:HD13 | 1.51 | 0.92 |
| 3:I:12:ARG:HG3 | 3:I:1181:PRO:HB2 | 1.50 | 0.92 |
| 3:I:839:VAL:HG12 | 3:I:1049:ILE:HG12 | 1.52 | 0.92 |
| 4:J:925:GLU:HG3 | 4:J:926:PRO:HD3 | 1.52 | 0.92 |
| 8:P:41:DT:H1' | 8:P:42:DT:H5' | 1.51 | 0.91 |
| 4:J:201:LEU:HD22 | 4:J:217:LEU:HD21 | 1.52 | 0.91 |
| 6:L:287:ILE:HA | 6:L:337:VAL:HG22 | 1.53 | 0.91 |
| 4:J:559:ALA:HB3 | 4:J:562:GLU:HB2 | 1.50 | 0.91 |
| 3:I:633:LEU:HD13 | 3:I:644:LEU:HD12 | 1.49 | 0.90 |
| 3:I:289:VAL:HG21 | 3:I:322:LEU:HD22 | 1.52 | 0.90 |
| 4:J:130:MET:HE3 | 4:J:159:ILE:HD11 | 1.54 | 0.90 |
| 4:J:661:VAL:HG23 | 4:J:685:ILE:HD11 | 1.54 | 0.90 |
| 4:J:701:LEU:HD21 | 4:J:723:TYR:HB2 | 1.52 | 0.90 |
| 3:I:155:VAL:HG23 | 3:I:176:ILE:HG12 | 1.54 | 0.89 |
| 3:I:1212:LEU:HD22 | 3:I:1225:VAL:HG21 | 1.53 | 0.89 |
| 4:J:1109:LEU:HD11 | 4:J:1113:VAL:HG11 | 1.54 | 0.89 |
| 4:J:930:LEU:HD22 | 4:J:1244:GLN:HG3 | 1.52 | 0.89 |
| 4:J:279:LEU:HD11 | 4:J:296:LYS:HG2 | 1.54 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:953:LEU:HD21 | 3:I:1033:ARG:HG2 | 1.54 | 0.89 |
| 4:J:1172:LYS:HB3 | 4:J:1191:PRO:HA | 1.53 | 0.88 |
| 3:I:1287:LEU:HD23 | 4:J:1357:ILE:HD11 | 1.55 | 0.88 |
| 4:J:338:PHE:HA | 4:J:342:LEU:HD12 | 1.55 | 0.87 |
| 4:J:814:CYS:HB2 | 4:J:889:ASP:HB3 | 1.56 | 0.87 |
| 3:I:221:LEU:HD21 | 3:I:351:LEU:HD11 | 1.57 | 0.87 |
| 3:I:590:PRO:HB2 | 3:I:655:VAL:HG11 | 1.54 | 0.86 |
| 4:J:79:LYS:HG3 | 6:L:569:THR:HB | 1.58 | 0.86 |
| 2:H:23:HIS:HB2 | 2:H:206:GLU:HG2 | 1.58 | 0.86 |
| 6:L:140:ALA:HA | 6:L:269:LEU:HD22 | 1.58 | 0.86 |
| 4:J:975:ILE:HD13 | 4:J:980:THR:HG21 | 1.57 | 0.85 |
| 4:J:1090:ILE:HG12 | 4:J:1097:ALA:HB2 | 1.58 | 0.85 |
| 8:P:68:DG:H5'' | 2:M:294:ASN:HA | 1.57 | 0.85 |
| 4:J:253:VAL:HG23 | 4:J:261:ALA:HB3 | 1.58 | 0.85 |
| 2:H:98:VAL:HG12 | 2:H:146:VAL:HG22 | 1.56 | 0.85 |
| 8:P:40:DC:H1' | 8:P:41:DT:H5' | 1.58 | 0.85 |
| 4:J:973:LEU:HD22 | 4:J:1003:LEU:HD12 | 1.59 | 0.85 |
| 3:I:232:ILE:HG13 | 3:I:333:ILE:HD11 | 1.59 | 0.85 |
| 4:J:1144:LEU:HD11 | 4:J:1236:GLU:HG2 | 1.59 | 0.85 |
| 7:O:23:DC:O2 | 8:P:63:DG:N2 | 2.11 | 0.84 |
| 4:J:1060:VAL:HG22 | 4:J:1106:ILE:HG12 | 1.59 | 0.84 |
| 4:J:972:LYS:HD3 | 4:J:1002:VAL:HB | 1.58 | 0.84 |
| 7:O:42:DA:H1' | 7:O:43:DA:H5' | 1.58 | 0.84 |
| 1:N:52:PHE:HB2 | 1:N:55:VAL:HG13 | 1.60 | 0.84 |
| 3:I:29:SER:O | 3:I:33:ASP:HB2 | 1.78 | 0.83 |
| 4:J:205:LEU:HD12 | 4:J:214:ARG:HB2 | 1.61 | 0.83 |
| 4:J:117:LEU:HD11 | 4:J:139:LEU:HD11 | 1.61 | 0.83 |
| 3:I:109:ALA:HB1 | 3:I:112:GLY:HA3 | 1.59 | 0.82 |
| 4:J:1161:GLY:HA3 | 4:J:1179:PRO:HA | 1.59 | 0.82 |
| 2:H:78:ILE:HA | 2:H:81:ILE:HD12 | 1.60 | 0.82 |
| 3:I:699:LEU:HB2 | 3:I:799:ASN:HD22 | 1.44 | 0.82 |
| 2:M:304:LYS:HD2 | 2:M:314:LEU:HD11 | 1.60 | 0.82 |
| 6:L:302:PHE:O | 6:L:306:PHE:N | 2.11 | 0.82 |
| 2:H:102:LEU:HD13 | 2:H:115:ILE:HG12 | 1.59 | 0.81 |
| 6:L:426:LYS:HG2 | 7:O:52:DA:H3' | 1.60 | 0.81 |
| 4:J:831:VAL:HG12 | 4:J:833:GLU:H | 1.43 | 0.81 |
| 4:J:1078:LEU:HG | 4:J:1101:LEU:HD11 | 1.60 | 0.81 |
| 3:I:229:ILE:HD12 | 3:I:334:GLU:HG2 | 1.63 | 0.81 |
| 4:J:697:MET:HE1 | 4:J:741:ALA:HB3 | 1.61 | 0.81 |
| 5:K:26:ARG:HD3 | 5:K:64:LEU:HD21 | 1.63 | 0.81 |
| 4:J:1176:VAL:HG22 | 4:J:1187:GLU:HA | 1.62 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:L:437:GLN:HB2 | 7:O:49:DC:H41 | 1.45 | 0.81 |
| 6:L:231:THR:HG23 | 6:L:248:GLU:HB3 | 1.63 | 0.81 |
| 4:J:1025:MET:HB2 | 4:J:1124:ILE:HB | 1.61 | 0.81 |
| 4:J:1024:THR:HG23 | 4:J:1123:ARG:HA | 1.62 | 0.80 |
| 3:I:28:LEU:HD21 | 3:I:524:ILE:HD13 | 1.63 | 0.80 |
| 4:J:515:ARG:HH21 | 4:J:717:VAL:HB | 1.46 | 0.80 |
| 4:J:957:SER:HA | 4:J:1010:GLN:HA | 1.63 | 0.80 |
| 2:G:179:PRO:HG3 | 2:G:211:ILE:HG13 | 1.63 | 0.80 |
| 3:I:829:THR:HB | 3:I:1059:ARG:HA | 1.62 | 0.80 |
| 4:J:1107:VAL:HG12 | 4:J:1122:ALA:HB2 | 1.60 | 0.80 |
| 6:L:330:LEU:HD23 | 6:L:333:VAL:HG11 | 1.64 | 0.80 |
| 4:J:553:THR:HB | 4:J:567:THR:HG22 | 1.64 | 0.80 |
| 4:J:158:GLN:HG2 | 4:J:160:LEU:HD21 | 1.64 | 0.79 |
| 4:J:262:THR:HG23 | 4:J:266:ASN:HD22 | 1.46 | 0.79 |
| 6:L:110:LEU:HB2 | 6:L:111:LEU:HD13 | 1.62 | 0.79 |
| 4:J:1069:ALA:HA | 4:J:1072:LYS:HB3 | 1.65 | 0.79 |
| 6:L:262:VAL:HG12 | 6:L:264:LYS:H | 1.48 | 0.79 |
| 2:H:201:LEU:HD21 | 2:H:203:ILE:HD11 | 1.65 | 0.79 |
| 2:M:279:GLY:HA2 | 2:M:282:VAL:HG22 | 1.63 | 0.79 |
| 4:J:1239:ASP:OD1 | 4:J:1242:ARG:NH2 | 2.14 | 0.79 |
| 4:J:69:GLU:HG3 | 4:J:76:LYS:HG2 | 1.65 | 0.79 |
| 4:J:426:ALA:HB3 | 4:J:427:PRO:HD3 | 1.65 | 0.79 |
| 4:J:452:LEU:HD13 | 4:J:500:ILE:HG22 | 1.64 | 0.78 |
| 3:I:871:VAL:O | 3:I:944:ARG:NH2 | 2.17 | 0.78 |
| 3:I:301:TYR:OH | 3:I:332:ARG:O | 2.02 | 0.78 |
| 3:I:528:ARG:NH2 | 3:I:576:SER:O | 2.16 | 0.78 |
| 6:L:285:ARG:HA | 6:L:289:LYS:HD3 | 1.64 | 0.78 |
| 3:I:453:ILE:HD12 | 3:I:530:ILE:HD12 | 1.65 | 0.78 |
| 6:L:114:GLU:HA | 6:L:117:ILE:HD12 | 1.64 | 0.78 |
| 4:J:1023:HIS:HA | 4:J:1126:GLN:HE21 | 1.49 | 0.77 |
| 2:G:93:GLN:HB3 | 2:G:120:ASP:HB3 | 1.66 | 0.77 |
| 3:I:88:ARG:NH2 | 3:I:1035:LYS:O | 2.17 | 0.77 |
| 3:I:561:ILE:HD11 | 3:I:665:ALA:HB1 | 1.66 | 0.77 |
| 3:I:716:ALA:HB3 | 3:I:784:ALA:HB3 | 1.66 | 0.77 |
| 3:I:1294:LYS:NZ | 4:J:470:VAL:O | 2.17 | 0.77 |
| 3:I:1151:LEU:HD12 | 3:I:1198:LEU:HD12 | 1.65 | 0.77 |
| 4:J:311:ARG:HH22 | 4:J:1329:THR:HG21 | 1.46 | 0.77 |
| 5:K:22:VAL:HG22 | 5:K:61:ASN:HB2 | 1.65 | 0.77 |
| 2:M:284:ARG:HB3 | 2:M:288:GLU:HG2 | 1.64 | 0.77 |
| 7:O:46:DG:H2'' | 7:O:47:DG:H5' | 1.67 | 0.77 |
| 2:M:257:VAL:HG11 | 2:M:270:LEU:HD23 | 1.65 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:453:ILE:HG13 | 3:I:587:LEU:HG | 1.66 | 0.76 |
| 4:J:1169:THR:H | 4:J:1173:ARG:HA | 1.50 | 0.76 |
| 4:J:950:ILE:HD13 | 4:J:995:TYR:HB3 | 1.66 | 0.76 |
| 6:L:291:CYS:O | 6:L:297:MET:N | 2.19 | 0.76 |
| 3:I:565:GLU:HA | 3:I:569:ILE:HD11 | 1.65 | 0.76 |
| 6:L:291:CYS:HA | 6:L:295:CYS:HB3 | 1.67 | 0.76 |
| 4:J:218:THR:HA | 4:J:221:ILE:HG22 | 1.68 | 0.76 |
| 3:I:180:ARG:NH2 | 3:I:392:GLU:O | 2.17 | 0.75 |
| 6:L:394:TYR:OH | 6:L:436:ARG:NH1 | 2.20 | 0.75 |
| 3:I:297:VAL:HA | 3:I:335:THR:HA | 1.68 | 0.75 |
| 4:J:1059:LEU:HD11 | 4:J:1110:GLU:HG2 | 1.68 | 0.75 |
| 4:J:1275:LEU:HD12 | 4:J:1277:GLY:H | 1.50 | 0.75 |
| 3:I:611:GLU:OE2 | 3:I:637:ARG:NH2 | 2.20 | 0.75 |
| 3:I:1269:ARG:NH1 | 4:J:344:GLY:O | 2.20 | 0.75 |
| 4:J:115:TRP:O | 4:J:119:SER:OG | 2.05 | 0.74 |
| 2:M:282:VAL:HG11 | 2:M:312:LEU:HD12 | 1.68 | 0.74 |
| 2:G:110:VAL:HG11 | 2:G:140:ILE:HD11 | 1.69 | 0.74 |
| 2:H:80:GLU:OE2 | 4:J:551:ARG:NH2 | 2.20 | 0.74 |
| 2:H:193:GLU:OE1 | 2:H:193:GLU:N | 2.21 | 0.74 |
| 3:I:1065:LYS:HE2 | 3:I:1235:LEU:HD12 | 1.68 | 0.74 |
| 4:J:909:ILE:HD11 | 4:J:913:GLU:HB3 | 1.70 | 0.74 |
| 7:O:23:DC:N3 | 8:P:63:DG:N1 | 2.35 | 0.74 |
| 3:I:56:VAL:HG11 | 3:I:468:LEU:HD13 | 1.70 | 0.74 |
| 6:L:379:MET:O | 6:L:383:ASN:ND2 | 2.20 | 0.74 |
| 3:I:211:ARG:NH1 | 3:I:215:TYR:O | 2.20 | 0.73 |
| 4:J:697:MET:HE3 | 4:J:738:ARG:HA | 1.70 | 0.73 |
| 4:J:1059:LEU:HB2 | 4:J:1107:VAL:HG22 | 1.68 | 0.73 |
| 6:L:330:LEU:HA | 6:L:333:VAL:HG12 | 1.69 | 0.73 |
| 4:J:298:MET:HE1 | 6:L:402:LEU:HB3 | 1.69 | 0.73 |
| 4:J:799:ARG:NH2 | 4:J:1146:GLU:OE2 | 2.21 | 0.73 |
| 8:P:14:DA:H2'' | 8:P:15:DC:H5' | 1.70 | 0.73 |
| 4:J:317:THR:HG22 | 4:J:323:PRO:HA | 1.70 | 0.73 |
| 4:J:518:VAL:HG11 | 4:J:707:ILE:HD13 | 1.68 | 0.73 |
| 6:L:316:PHE:HE2 | 6:L:334:SER:HA | 1.52 | 0.73 |
| 4:J:308:ASP:HB3 | 4:J:328:ALA:HB3 | 1.70 | 0.73 |
| 3:I:1002:LEU:HD12 | 3:I:1003:THR:H | 1.53 | 0.73 |
| 4:J:278:ARG:NH1 | 6:L:403:ASP:OD1 | 2.16 | 0.73 |
| 2:G:102:LEU:HD11 | 2:G:110:VAL:HG21 | 1.70 | 0.72 |
| 4:J:926:PRO:HB3 | 4:J:1246:VAL:HG11 | 1.69 | 0.72 |
| 3:I:812:PHE:O | 4:J:504:GLN:NE2 | 2.22 | 0.72 |
| 3:I:1196:LYS:HG3 | 3:I:1206:THR:HG23 | 1.71 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:1036:ARG:HH21 | 4:J:1081:VAL:HG11 | 1.55 | 0.72 |
| 2:M:255:ARG:HB2 | 2:M:278:ILE:HG13 | 1.72 | 0.72 |
| 3:I:794:LEU:HD21 | 3:I:796:LEU:HD21 | 1.72 | 0.72 |
| 6:L:377:LYS:O | 6:L:381:GLU:HG2 | 1.90 | 0.72 |
| 3:I:595:THR:HG22 | 3:I:596:ASP:H | 1.55 | 0.72 |
| 3:I:12:ARG:NH2 | 3:I:793:GLU:OE1 | 2.22 | 0.72 |
| 4:J:1158:GLU:HG3 | 4:J:1186:TYR:OH | 1.90 | 0.72 |
| 3:I:896:THR:HG22 | 3:I:897:PRO:HD2 | 1.71 | 0.71 |
| 3:I:1116:HIS:HE1 | 4:J:641:ILE:H | 1.38 | 0.71 |
| 3:I:444:ASP:N | 3:I:444:ASP:OD1 | 2.19 | 0.71 |
| 3:I:1176:LEU:HD22 | 3:I:1181:PRO:HD3 | 1.73 | 0.71 |
| 3:I:943:LYS:HA | 3:I:946:LEU:HD23 | 1.73 | 0.71 |
| 4:J:405:GLU:O | 4:J:408:VAL:HG12 | 1.90 | 0.71 |
| 4:J:957:SER:OG | 4:J:1008:GLY:O | 2.09 | 0.71 |
| 10:N:102:1N7:C3 | 10:N:102:1N7:C18 | 2.66 | 0.71 |
| 2:G:160:HIS:N | 2:G:162:GLU:OE1 | 2.24 | 0.71 |
| 4:J:1158:GLU:HA | 4:J:1223:LEU:HD11 | 1.71 | 0.71 |
| 6:L:562:ARG:HG3 | 6:L:576:VAL:HG21 | 1.73 | 0.71 |
| 3:I:1143:GLU:OE2 | 3:I:1147:ARG:NH1 | 2.22 | 0.71 |
| 6:L:573:LEU:HD22 | 8:P:55:DT:H3' | 1.72 | 0.71 |
| 2:G:29:GLU:HB3 | 2:G:30:PRO:HD3 | 1.72 | 0.70 |
| 2:H:67:GLU:HG2 | 2:H:68:TYR:HD1 | 1.53 | 0.70 |
| 3:I:1142:ARG:NH2 | 3:I:1161:LEU:O | 2.24 | 0.70 |
| 4:J:825:VAL:HG12 | 4:J:833:GLU:HB2 | 1.73 | 0.70 |
| 2:H:16:ILE:HG13 | 2:H:26:VAL:HG22 | 1.73 | 0.70 |
| 4:J:644:MET:HG2 | 4:J:722:ILE:HD12 | 1.74 | 0.70 |
| 4:J:981:GLU:OE1 | 4:J:983:LYS:NZ | 2.22 | 0.70 |
| 2:M:263:THR:OG1 | 2:M:302:GLU:OE2 | 2.06 | 0.70 |
| 5:K:76:GLU:HA | 5:K:79:GLU:HB2 | 1.74 | 0.70 |
| 3:I:593:LYS:O | 3:I:600:THR:OG1 | 2.08 | 0.70 |
| 8:P:56:DG:H2'' | 8:P:57:DT:H71 | 1.71 | 0.70 |
| 2:G:20:SER:OG | 2:G:21:SER:N | 2.23 | 0.70 |
| 4:J:147:ILE:HG22 | 4:J:188:LEU:HG | 1.72 | 0.70 |
| 1:N:48:ARG:NH2 | 1:N:62:GLN:OE1 | 2.24 | 0.70 |
| 4:J:139:LEU:HD21 | 4:J:185:ILE:HG13 | 1.74 | 0.70 |
| 2:H:212:ASP:N | 2:H:212:ASP:OD1 | 2.23 | 0.70 |
| 4:J:198:CYS:HB2 | 4:J:221:ILE:HD11 | 1.73 | 0.70 |
| 4:J:482:ALA:O | 5:K:16:ARG:NH1 | 2.24 | 0.70 |
| 3:I:124:MET:HB2 | 3:I:498:ILE:HD12 | 1.73 | 0.69 |
| 4:J:661:VAL:CG2 | 4:J:685:ILE:HD11 | 2.22 | 0.69 |
| 6:L:391:ALA:HB3 | 6:L:405:ILE:HD13 | 1.73 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:N:62:GLN:O | 1:N:66:GLU:HG2 | 1.92 | 0.69 |
| 1:N:6:ASP:OD2 | 3:I:1106:ARG:NH1 | 2.24 | 0.69 |
| 3:I:1104:PRO:HG2 | 4:J:725:MET:HE3 | 1.74 | 0.69 |
| 4:J:819:GLY:HA3 | 4:J:882:VAL:O | 1.93 | 0.69 |
| 6:L:220:LYS:NZ | 6:L:223:GLU:OE1 | 2.24 | 0.69 |
| 6:L:305:LEU:HD21 | 6:L:319:ALA:HB2 | 1.74 | 0.69 |
| 6:L:344:LEU:HA | 6:L:347:ILE:HD12 | 1.72 | 0.69 |
| 6:L:479:THR:HG23 | 6:L:482:GLU:H | 1.57 | 0.69 |
| 3:I:346:TYR:O | 3:I:350:THR:OG1 | 2.10 | 0.69 |
| 3:I:745:GLU:HG3 | 3:I:1017:GLN:HB3 | 1.74 | 0.69 |
| 4:J:878:ASP:OD2 | 4:J:878:ASP:N | 2.26 | 0.69 |
| 6:L:606:VAL:HG23 | 6:L:607:LEU:HD22 | 1.74 | 0.69 |
| 3:I:27:LEU:O | 3:I:528:ARG:NH1 | 2.25 | 0.69 |
| 3:I:905:ILE:HG12 | 6:L:598:LEU:HD12 | 1.73 | 0.69 |
| 4:J:490:ILE:HD11 | 4:J:614:LEU:HD12 | 1.75 | 0.69 |
| 7:O:55:DC:H6 | 7:O:55:DC:H5' | 1.56 | 0.69 |
| 3:I:241:LEU:N | 3:I:283:LYS:O | 2.23 | 0.69 |
| 3:I:560:PRO:O | 4:J:780:ARG:NH2 | 2.24 | 0.69 |
| 4:J:128:LEU:HD11 | 4:J:189:LEU:HD21 | 1.73 | 0.69 |
| 6:L:96:ASP:O | 6:L:100:MET:HG2 | 1.92 | 0.69 |
| 10:L:701:1N7:C3 | 10:L:701:1N7:C18 | 2.66 | 0.69 |
| 1:N:6:ASP:OD1 | 3:I:678:ARG:NH2 | 2.26 | 0.69 |
| 3:I:979:LEU:HD11 | 3:I:1011:LEU:HD11 | 1.75 | 0.69 |
| 2:G:192:VAL:HB | 2:G:198:LEU:HD12 | 1.73 | 0.68 |
| 3:I:886:LYS:NZ | 3:I:916:SER:O | 2.25 | 0.68 |
| 3:I:1006:GLU:OE2 | 3:I:1009:ASN:ND2 | 2.26 | 0.68 |
| 6:L:285:ARG:HG3 | 6:L:289:LYS:HE2 | 1.73 | 0.68 |
| 3:I:314:ASN:O | 3:I:352:ARG:NH1 | 2.23 | 0.68 |
| 3:I:548:ARG:NH2 | 3:I:567:PRO:O | 2.26 | 0.68 |
| 4:J:884:SER:HB2 | 4:J:886:VAL:HG12 | 1.75 | 0.68 |
| 4:J:964:LYS:O | 4:J:976:THR:OG1 | 2.10 | 0.68 |
| 3:I:3:TYR:O | 3:I:8:LYS:NZ | 2.25 | 0.68 |
| 4:J:154:LEU:HD12 | 4:J:176:PHE:CZ | 2.29 | 0.68 |
| 4:J:475:GLU:HG2 | 5:K:24:ALA:HB1 | 1.74 | 0.68 |
| 4:J:559:ALA:CB | 4:J:562:GLU:HB2 | 2.23 | 0.68 |
| 6:L:297:MET:HE1 | 6:L:302:PHE:HA | 1.76 | 0.68 |
| 2:G:224:LEU:HD23 | 2:H:228:LEU:HD11 | 1.76 | 0.68 |
| 4:J:518:VAL:HG11 | 4:J:707:ILE:CD1 | 2.24 | 0.68 |
| 6:L:547:VAL:CG1 | 6:L:607:LEU:HD21 | 2.24 | 0.68 |
| 3:I:1105:SER:HB2 | 4:J:731:ARG:HG3 | 1.74 | 0.68 |
| 3:I:741:MET:HG2 | 3:I:746:ALA:HB1 | 1.75 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:381:ILE:HD11 | 4:J:412:LEU:HD13 | 1.74 | 0.68 |
| 4:J:1020:TRP:HE1 | 4:J:1022:PRO:HB3 | 1.58 | 0.68 |
| 6:L:586:ARG:HE | 7:O:25:DA:H5'' | 1.59 | 0.68 |
| 3:I:395:TYR:CE2 | 3:I:420:LEU:HD22 | 2.29 | 0.68 |
| 3:I:1109:ILE:HG12 | 4:J:644:MET:HE1 | 1.74 | 0.68 |
| 4:J:17:PHE:HZ | 4:J:1353:VAL:HG21 | 1.59 | 0.68 |
| 3:I:120:GLN:HG2 | 3:I:490:GLN:HE22 | 1.58 | 0.67 |
| 4:J:1069:ALA:HB1 | 4:J:1072:LYS:HD3 | 1.75 | 0.67 |
| 7:O:73:DC:H2'' | 7:O:74:DC:H5'' | 1.74 | 0.67 |
| 3:I:989:LEU:HD13 | 3:I:1000:LEU:HD11 | 1.75 | 0.67 |
| 4:J:510:LEU:O | 4:J:514:THR:HG22 | 1.94 | 0.67 |
| 4:J:974:VAL:HA | 4:J:1001:ALA:O | 1.94 | 0.67 |
| 6:L:130:VAL:O | 6:L:134:VAL:HG23 | 1.93 | 0.67 |
| 6:L:291:CYS:HA | 6:L:295:CYS:CB | 2.24 | 0.67 |
| 10:I:1401:1N7:C3 | 10:I:1401:1N7:C18 | 2.67 | 0.67 |
| 4:J:47:ARG:NH2 | 7:O:44:DA:OP1 | 2.22 | 0.67 |
| 2:G:192:VAL:CB | 2:G:198:LEU:HD12 | 2.25 | 0.67 |
| 3:I:65:ASN:O | 3:I:105:TYR:N | 2.25 | 0.67 |
| 4:J:825:VAL:CG1 | 4:J:833:GLU:HB2 | 2.24 | 0.67 |
| 3:I:96:LEU:HD23 | 3:I:124:MET:HG3 | 1.75 | 0.67 |
| 3:I:233:ARG:O | 3:I:238:GLN:NE2 | 2.27 | 0.67 |
| 3:I:560:PRO:HB3 | 4:J:776:THR:HG21 | 1.75 | 0.67 |
| 3:I:180:ARG:O | 3:I:396:ASP:N | 2.18 | 0.67 |
| 7:O:26:DT:H2' | 7:O:27:DT:H71 | 1.77 | 0.67 |
| 3:I:57:PHE:HD2 | 3:I:70:TYR:HB2 | 1.60 | 0.67 |
| 3:I:870:ILE:HD13 | 3:I:1050:VAL:HG11 | 1.77 | 0.67 |
| 4:J:965:SER:OG | 4:J:966:VAL:N | 2.24 | 0.67 |
| 2:G:84:ASN:ND2 | 2:G:130:ILE:O | 2.23 | 0.67 |
| 6:L:126:GLY:O | 6:L:130:VAL:HG23 | 1.95 | 0.67 |
| 3:I:68:LEU:HD23 | 3:I:475:VAL:HG11 | 1.77 | 0.67 |
| 4:J:888:CYS:SG | 4:J:889:ASP:N | 2.65 | 0.67 |
| 4:J:975:ILE:HG21 | 4:J:980:THR:HG21 | 1.76 | 0.67 |
| 4:J:985:ILE:HD13 | 4:J:991:THR:HA | 1.77 | 0.67 |
| 3:I:175:ARG:HG2 | 3:I:177:ILE:HG13 | 1.77 | 0.66 |
| 3:I:324:LYS:O | 3:I:327:GLN:NE2 | 2.23 | 0.66 |
| 4:J:527:LEU:HD23 | 4:J:533:ALA:HB2 | 1.77 | 0.66 |
| 2:M:275:ILE:CG2 | 2:M:280:ASP:HB3 | 2.21 | 0.66 |
| 6:L:148:TYR:HA | 6:L:161:LEU:HD11 | 1.76 | 0.66 |
| 10:N:102:1N7:C3 | 10:N:102:1N7:C2 | 2.70 | 0.66 |
| 3:I:243:PRO:HB3 | 3:I:277:LEU:HD23 | 1.76 | 0.66 |
| 3:I:301:TYR:O | 3:I:310:ILE:HB | 1.95 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:964:LEU:HG | 3:I:968:GLU:OE2 | 1.95 | 0.66 |
| 4:J:168:ALA:HA | 4:J:171:GLU:HB3 | 1.76 | 0.66 |
| 3:I:1103:VAL:HG11 | 3:I:1112:ILE:HG13 | 1.78 | 0.66 |
| 3:I:1276:TRP:HH2 | 4:J:798:ARG:HG2 | 1.60 | 0.66 |
| 4:J:185:ILE:O | 4:J:189:LEU:HG | 1.95 | 0.66 |
| 3:I:1314:GLN:OE1 | 5:K:28:ARG:NH2 | 2.28 | 0.66 |
| 3:I:23:ASP:OD1 | 3:I:23:ASP:N | 2.28 | 0.66 |
| 3:I:257:ALA:HB3 | 3:I:282:VAL:HG21 | 1.78 | 0.66 |
| 3:I:933:VAL:HG23 | 3:I:1050:VAL:HG22 | 1.75 | 0.66 |
| 4:J:768:ASN:OD1 | 4:J:768:ASN:N | 2.29 | 0.66 |
| 3:I:1010:GLN:O | 3:I:1014:LEU:HG | 1.96 | 0.66 |
| 6:L:135:ALA:HB1 | 6:L:253:SER:HA | 1.77 | 0.66 |
| 7:O:33:DA:H2' | 7:O:33:DA:OP2 | 1.95 | 0.66 |
| 4:J:265:LEU:HD11 | 4:J:330:MET:SD | 2.35 | 0.66 |
| 4:J:842:ARG:NH2 | 4:J:1254:GLU:OE1 | 2.29 | 0.66 |
| 6:L:162:ILE:HG23 | 6:L:260:ARG:O | 1.95 | 0.66 |
| 4:J:1059:LEU:HD13 | 4:J:1107:VAL:HG23 | 1.76 | 0.65 |
| 3:I:69:GLN:HE21 | 3:I:101:ARG:HD2 | 1.61 | 0.65 |
| 3:I:875:ALA:O | 3:I:877:VAL:HG13 | 1.96 | 0.65 |
| 3:I:902:LEU:HD21 | 6:L:611:LEU:HG | 1.78 | 0.65 |
| 4:J:154:LEU:HD12 | 4:J:176:PHE:HZ | 1.59 | 0.65 |
| 4:J:614:LEU:HD22 | 5:K:7:GLN:HG3 | 1.77 | 0.65 |
| 4:J:1050:THR:HG23 | 4:J:1057:SER:HA | 1.77 | 0.65 |
| 3:I:726:TYR:CE2 | 3:I:728:ASP:HB2 | 2.31 | 0.65 |
| 6:L:234:THR:OG1 | 6:L:248:GLU:OE1 | 2.15 | 0.65 |
| 4:J:514:THR:OG1 | 4:J:576:ARG:HG3 | 1.95 | 0.65 |
| 2:G:98:VAL:HG11 | 2:G:121:VAL:CG2 | 2.27 | 0.65 |
| 2:H:125:LYS:NZ | 2:H:127:GLN:OE1 | 2.29 | 0.65 |
| 3:I:1340:GLU:HG2 | 4:J:1341:ARG:NH2 | 2.12 | 0.65 |
| 4:J:1077:ALA:HB2 | 4:J:1100:PHE:HA | 1.77 | 0.65 |
| 5:K:59:ILE:O | 5:K:63:ILE:HB | 1.97 | 0.65 |
| 6:L:387:VAL:HG11 | 6:L:409:ASN:OD1 | 1.97 | 0.65 |
| 6:L:572:THR:O | 6:L:576:VAL:HG23 | 1.97 | 0.65 |
| 4:J:128:LEU:HD21 | 4:J:189:LEU:HD23 | 1.78 | 0.65 |
| 4:J:603:LYS:O | 4:J:607:THR:HG23 | 1.96 | 0.65 |
| 2:M:253:LEU:HD11 | 2:M:282:VAL:HG21 | 1.79 | 0.65 |
| 3:I:177:ILE:HG12 | 3:I:183:TRP:HE3 | 1.60 | 0.65 |
| 3:I:693:LEU:HB2 | 3:I:829:THR:O | 1.97 | 0.64 |
| 3:I:1305:TYR:O | 3:I:1309:VAL:HG13 | 1.97 | 0.64 |
| 4:J:511:TYR:HE2 | 4:J:724:MET:HG2 | 1.60 | 0.64 |
| 8:P:43:DT:H2'' | 8:P:44:DT:H71 | 1.79 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:N:14:GLN:O | 1:N:18:THR:HG22 | 1.97 | 0.64 |
| 3:I:561:ILE:HD11 | 3:I:665:ALA:CB | 2.27 | 0.64 |
| 3:I:885:GLY:HA2 | 3:I:917:SER:HB3 | 1.78 | 0.64 |
| 7:O:56:DC:H6 | 7:O:56:DC:H5' | 1.61 | 0.64 |
| 3:I:325:LEU:HA | 3:I:328:SER:HB2 | 1.80 | 0.64 |
| 3:I:884:VAL:HG23 | 3:I:918:LEU:HD23 | 1.77 | 0.64 |
| 4:J:1232:TYR:HD2 | 4:J:1233:ILE:HD12 | 1.62 | 0.64 |
| 6:L:289:LYS:O | 6:L:293:GLU:HB3 | 1.98 | 0.64 |
| 3:I:241:LEU:HB3 | 3:I:283:LYS:HA | 1.80 | 0.64 |
| 3:I:1085:MET:HE2 | 3:I:1085:MET:HA | 1.79 | 0.64 |
| 4:J:430:HIS:HB3 | 4:J:925:GLU:HG2 | 1.80 | 0.64 |
| 6:L:216:LEU:O | 6:L:220:LYS:HG2 | 1.98 | 0.64 |
| 2:H:92:VAL:HG23 | 2:H:121:VAL:HG12 | 1.80 | 0.64 |
| 2:H:105:SER:OG | 2:H:106:GLY:N | 2.30 | 0.64 |
| 3:I:245:ARG:HB3 | 3:I:337:PHE:CZ | 2.32 | 0.64 |
| 3:I:1042:LEU:HB3 | 3:I:1046:VAL:HG13 | 1.78 | 0.64 |
| 6:L:291:CYS:O | 6:L:296:LYS:N | 2.30 | 0.64 |
| 2:M:302:GLU:O | 2:M:306:VAL:HG23 | 1.98 | 0.64 |
| 3:I:391:SER:CB | 3:I:394:ARG:HB2 | 2.28 | 0.64 |
| 4:J:425:ARG:HG2 | 4:J:426:ALA:H | 1.61 | 0.64 |
| 6:L:295:CYS:SG | 6:L:329:LYS:HB2 | 2.38 | 0.64 |
| 3:I:81:ASP:OD1 | 3:I:84:GLU:HB2 | 1.98 | 0.64 |
| 3:I:130:MET:SD | 3:I:134:GLY:HA2 | 2.38 | 0.64 |
| 3:I:400:VAL:HG21 | 3:I:452:ARG:HD2 | 1.79 | 0.64 |
| 8:P:60:DA:H2'' | 8:P:61:DT:H5' | 1.80 | 0.64 |
| 1:N:64:TYR:HD1 | 3:I:341:LEU:HD22 | 1.62 | 0.64 |
| 3:I:894:GLN:HG2 | 4:J:77:ARG:HH22 | 1.63 | 0.64 |
| 3:I:956:ALA:HB1 | 3:I:1032:LYS:HG2 | 1.79 | 0.64 |
| 4:J:910:ASN:OD1 | 5:K:15:ASN:HA | 1.97 | 0.64 |
| 6:L:286:LEU:HD11 | 6:L:336:GLU:HB3 | 1.78 | 0.64 |
| 1:N:46:GLU:HG2 | 1:N:49:ARG:HH22 | 1.63 | 0.64 |
| 1:N:52:PHE:HB2 | 1:N:55:VAL:CG1 | 2.27 | 0.64 |
| 2:G:211:ILE:HG23 | 2:G:216:ALA:HB2 | 1.80 | 0.64 |
| 3:I:390:PHE:HA | 3:I:419:ILE:CD1 | 2.27 | 0.64 |
| 3:I:565:GLU:HA | 3:I:569:ILE:CD1 | 2.28 | 0.64 |
| 4:J:848:VAL:HB | 4:J:858:VAL:HG22 | 1.79 | 0.64 |
| 6:L:141:ILE:HD12 | 6:L:256:PHE:CD1 | 2.31 | 0.64 |
| 6:L:147:GLN:HB3 | 6:L:161:LEU:HD21 | 1.79 | 0.64 |
| 6:L:282:THR:HG23 | 6:L:285:ARG:HH21 | 1.63 | 0.64 |
| 3:I:387:ASN:HA | 3:I:391:SER:OG | 1.98 | 0.63 |
| 3:I:733:VAL:HG13 | 3:I:748:ILE:HD13 | 1.80 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:1141:VAL:HG22 | 4:J:1237:VAL:HG23 | 1.80 | 0.63 |
| 2:H:12:ARG:HA | 2:H:14:VAL:H | 1.64 | 0.63 |
| 4:J:398:LYS:HD2 | 6:L:532:LEU:CD2 | 2.28 | 0.63 |
| 4:J:847:ASP:HB3 | 4:J:856:ILE:CG2 | 2.28 | 0.63 |
| 6:L:165:PHE:HB2 | 6:L:167:ASP:OD1 | 1.97 | 0.63 |
| 4:J:17:PHE:CZ | 4:J:1353:VAL:HG21 | 2.33 | 0.63 |
| 4:J:797:THR:O | 4:J:801:VAL:HG13 | 1.98 | 0.63 |
| 6:L:224:LEU:HD13 | 6:L:256:PHE:HE1 | 1.63 | 0.63 |
| 6:L:303:ILE:HA | 6:L:306:PHE:HB3 | 1.80 | 0.63 |
| 3:I:979:LEU:HD23 | 3:I:1000:LEU:HD12 | 1.80 | 0.63 |
| 3:I:1026:GLU:HA | 3:I:1029:LEU:HD23 | 1.80 | 0.63 |
| 10:L:701:1N7:C3 | 10:L:701:1N7:C2 | 2.73 | 0.63 |
| 4:J:709:ARG:HB3 | 4:J:711:GLY:HA3 | 1.80 | 0.63 |
| 4:J:948:SER:O | 4:J:948:SER:OG | 2.17 | 0.63 |
| 6:L:344:LEU:HD11 | 6:L:355:ILE:HG13 | 1.81 | 0.63 |
| 1:N:48:ARG:HH12 | 1:N:59:VAL:HA | 1.61 | 0.63 |
| 2:G:208:ASN:OD1 | 2:G:210:THR:HG23 | 1.99 | 0.63 |
| 6:L:573:LEU:HB2 | 6:L:587:ILE:HD11 | 1.81 | 0.63 |
| 3:I:391:SER:O | 3:I:395:TYR:N | 2.31 | 0.63 |
| 4:J:291:ILE:HD11 | 6:L:380:VAL:HG11 | 1.81 | 0.63 |
| 4:J:573:THR:OG1 | 4:J:576:ARG:HD2 | 1.99 | 0.63 |
| 4:J:949:SER:OG | 4:J:1018:ALA:O | 2.16 | 0.63 |
| 6:L:552:THR:OG1 | 6:L:597:LYS:NZ | 2.26 | 0.63 |
| 3:I:225:PHE:HB2 | 3:I:336:LEU:HD22 | 1.81 | 0.63 |
| 3:I:742:TYR:HB3 | 3:I:743:PRO:HD2 | 1.80 | 0.63 |
| 4:J:314:ARG:HD2 | 4:J:315:ALA:H | 1.63 | 0.63 |
| 4:J:844:THR:OG1 | 4:J:860:ARG:O | 2.11 | 0.63 |
| 3:I:929:ILE:HD13 | 3:I:1055:ALA:HB2 | 1.80 | 0.62 |
| 4:J:1357:ILE:HG22 | 4:J:1359:ALA:H | 1.64 | 0.62 |
| 6:L:146:GLU:O | 6:L:150:ARG:HG3 | 1.99 | 0.62 |
| 2:G:184:ALA:HB2 | 3:I:1091:GLY:HA3 | 1.81 | 0.62 |
| 3:I:994:ARG:HA | 3:I:997:TRP:CD2 | 2.34 | 0.62 |
| 4:J:202:ARG:HA | 4:J:205:LEU:HD23 | 1.80 | 0.62 |
| 4:J:550:VAL:HG23 | 4:J:552:ILE:HG23 | 1.79 | 0.62 |
| 3:I:5:TYR:HA | 3:I:8:LYS:HE2 | 1.80 | 0.62 |
| 10:I:1401:1N7:C3 | 10:I:1401:1N7:C2 | 2.72 | 0.62 |
| 4:J:56:LEU:O | 4:J:250:ARG:NH2 | 2.28 | 0.62 |
| 4:J:129:ASP:HB2 | 4:J:220:ARG:HH21 | 1.63 | 0.62 |
| 4:J:710:ASP:N | 4:J:711:GLY:HA3 | 2.13 | 0.62 |
| 4:J:847:ASP:HB3 | 4:J:856:ILE:HG21 | 1.80 | 0.62 |
| 4:J:1173:ARG:NH1 | 4:J:1192:LYS:HE2 | 2.15 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:L:548:LEU:HD12 | 6:L:560:ARG:HE | 1.64 | 0.62 |
| 3:I:225:PHE:CE2 | 3:I:347:ILE:HB | 2.33 | 0.62 |
| 3:I:362:ALA:O | 3:I:366:ILE:HG13 | 1.99 | 0.62 |
| 4:J:180:MET:HE1 | 4:J:293:ARG:HE | 1.64 | 0.62 |
| 4:J:826:ILE:HG12 | 4:J:831:VAL:HG22 | 1.81 | 0.62 |
| 1:N:27:ILE:HD11 | 4:J:680:ASN:HB3 | 1.80 | 0.62 |
| 3:I:525:THR:O | 3:I:529:ARG:HG3 | 1.98 | 0.62 |
| 3:I:667:LEU:HD23 | 3:I:704:MET:HB3 | 1.82 | 0.62 |
| 3:I:707:ALA:O | 3:I:711:ASP:HB2 | 1.99 | 0.62 |
| 4:J:418:GLU:HG3 | 5:K:48:VAL:HG21 | 1.81 | 0.62 |
| 4:J:782:GLY:O | 4:J:786:THR:HG23 | 1.99 | 0.62 |
| 2:G:70:THR:HG23 | 3:I:729:ALA:HB3 | 1.82 | 0.62 |
| 2:H:64:VAL:CG1 | 2:H:69:SER:HB2 | 2.30 | 0.62 |
| 3:I:59:ILE:HG21 | 3:I:472:GLU:HB2 | 1.82 | 0.62 |
| 3:I:591:TYR:HB3 | 3:I:652:TYR:HB3 | 1.80 | 0.62 |
| 3:I:1138:VAL:O | 3:I:1142:ARG:HG3 | 1.99 | 0.62 |
| 4:J:689:ALA:O | 4:J:693:VAL:HG23 | 2.00 | 0.62 |
| 6:L:315:TRP:CZ2 | 6:L:341:LEU:HD11 | 2.34 | 0.62 |
| 2:G:57:THR:HG22 | 2:G:58:GLU:HG3 | 1.81 | 0.62 |
| 3:I:453:ILE:HD11 | 3:I:587:LEU:HD11 | 1.81 | 0.62 |
| 4:J:215:LYS:O | 4:J:218:THR:HG22 | 1.98 | 0.62 |
| 4:J:288:PRO:HD2 | 4:J:291:ILE:HD12 | 1.81 | 0.62 |
| 5:K:54:ILE:HD13 | 5:K:59:ILE:HB | 1.82 | 0.62 |
| 3:I:575:LEU:HD12 | 3:I:587:LEU:HD21 | 1.80 | 0.62 |
| 4:J:117:LEU:HD11 | 4:J:139:LEU:CD1 | 2.29 | 0.62 |
| 4:J:412:LEU:O | 4:J:415:VAL:HG22 | 1.99 | 0.62 |
| 4:J:508:LEU:HD13 | 4:J:725:MET:HG2 | 1.82 | 0.62 |
| 6:L:301:ASN:O | 6:L:304:THR:HG22 | 2.00 | 0.62 |
| 3:I:1242:LYS:HD2 | 4:J:465:GLN:HE22 | 1.64 | 0.62 |
| 4:J:652:GLU:O | 4:J:656:GLU:HG3 | 2.00 | 0.62 |
| 4:J:742:GLY:O | 4:J:762:ASN:HB3 | 1.98 | 0.62 |
| 3:I:257:ALA:HB2 | 3:I:285:ILE:HG22 | 1.81 | 0.62 |
| 3:I:1111:GLN:HG3 | 3:I:1230:MET:HE1 | 1.81 | 0.62 |
| 3:I:1125:GLY:HA3 | 3:I:1179:GLY:H | 1.65 | 0.62 |
| 3:I:1304:MET:SD | 3:I:1315:MET:HB3 | 2.39 | 0.62 |
| 4:J:681:LYS:O | 4:J:685:ILE:HG23 | 2.00 | 0.62 |
| 4:J:1037:PHE:HZ | 4:J:1110:GLU:HA | 1.64 | 0.62 |
| 1:N:56:THR:O | 1:N:57:LEU:HD23 | 2.00 | 0.61 |
| 2:H:228:LEU:O | 2:H:232:VAL:HG23 | 2.00 | 0.61 |
| 3:I:67:GLU:O | 3:I:103:VAL:HG22 | 2.00 | 0.61 |
| 3:I:1042:LEU:HB3 | 3:I:1046:VAL:CG1 | 2.30 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:1173:ARG:HG3 | 4:J:1192:LYS:HD3 | 1.82 | 0.61 |
| 5:K:58:LEU:O | 5:K:59:ILE:HD13 | 2.00 | 0.61 |
| 6:L:114:GLU:HA | 6:L:117:ILE:CD1 | 2.28 | 0.61 |
| 2:G:98:VAL:HG11 | 2:G:121:VAL:HG21 | 1.82 | 0.61 |
| 2:H:76:GLU:OE1 | 2:H:132:HIS:N | 2.27 | 0.61 |
| 3:I:1104:PRO:HG2 | 4:J:725:MET:CE | 2.29 | 0.61 |
| 4:J:1047:THR:HG23 | 4:J:1049:GLN:HB2 | 1.81 | 0.61 |
| 4:J:1060:VAL:CG2 | 4:J:1106:ILE:HG12 | 2.30 | 0.61 |
| 6:L:366:SER:O | 6:L:369:GLU:HG3 | 2.00 | 0.61 |
| 6:L:530:LEU:O | 6:L:533:ASP:N | 2.31 | 0.61 |
| 3:I:229:ILE:CD1 | 3:I:334:GLU:HG2 | 2.29 | 0.61 |
| 3:I:391:SER:HB2 | 3:I:394:ARG:HB2 | 1.82 | 0.61 |
| 4:J:46:TYR:HD1 | 6:L:500:ILE:HD12 | 1.63 | 0.61 |
| 4:J:424:ASN:HB2 | 4:J:434:ILE:HG12 | 1.83 | 0.61 |
| 3:I:232:ILE:HG13 | 3:I:333:ILE:CD1 | 2.29 | 0.61 |
| 4:J:474:LEU:HD23 | 5:K:28:ARG:HG2 | 1.82 | 0.61 |
| 6:L:389:SER:OG | 7:O:54:DT:H4' | 2.00 | 0.61 |
| 2:G:183:ILE:CD1 | 2:G:205:MET:HB2 | 2.31 | 0.61 |
| 4:J:411:ILE:O | 4:J:415:VAL:HG13 | 2.00 | 0.61 |
| 4:J:1238:GLN:HB3 | 4:J:1242:ARG:HH12 | 1.65 | 0.61 |
| 2:G:86:LYS:NZ | 3:I:826:ASP:OD2 | 2.33 | 0.61 |
| 2:H:30:PRO:HG3 | 2:H:192:VAL:HG11 | 1.81 | 0.61 |
| 4:J:397:ALA:O | 4:J:401:VAL:HG13 | 2.00 | 0.61 |
| 4:J:697:MET:CE | 4:J:741:ALA:HB3 | 2.31 | 0.61 |
| 6:L:290:LEU:O | 6:L:294:GLN:HB3 | 2.00 | 0.61 |
| 4:J:225:GLU:O | 4:J:229:GLN:HG2 | 2.01 | 0.61 |
| 4:J:1059:LEU:HB2 | 4:J:1107:VAL:CG2 | 2.30 | 0.61 |
| 6:L:261:LEU:HB2 | 6:L:266:PHE:HD1 | 1.64 | 0.61 |
| 3:I:102:LEU:HB3 | 3:I:489:PRO:HG3 | 1.82 | 0.61 |
| 4:J:1209:VAL:O | 4:J:1210:ILE:HD13 | 2.00 | 0.61 |
| 6:L:108:VAL:HG13 | 6:L:109:GLU:O | 2.00 | 0.61 |
| 8:P:44:DT:H2'' | 8:P:45:DA:C8 | 2.34 | 0.61 |
| 1:N:20:ILE:HG12 | 4:J:754:ILE:HD13 | 1.83 | 0.61 |
| 3:I:136:PHE:CD2 | 3:I:145:ILE:HD13 | 2.36 | 0.61 |
| 4:J:985:ILE:HD11 | 4:J:991:THR:HG22 | 1.82 | 0.61 |
| 4:J:1005:LYS:HE2 | 4:J:1011:VAL:HG22 | 1.83 | 0.61 |
| 6:L:102:MET:HE2 | 6:L:388:ILE:HD13 | 1.83 | 0.61 |
| 6:L:316:PHE:CD1 | 6:L:337:VAL:HG11 | 2.35 | 0.61 |
| 6:L:425:TYR:OH | 7:O:50:DA:O3' | 2.12 | 0.61 |
| 1:N:48:ARG:NH2 | 4:J:677:GLU:OE1 | 2.34 | 0.61 |
| 3:I:122:VAL:HG21 | 3:I:493:ILE:CG2 | 2.31 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:235:ASN:OD1 | 3:I:238:GLN:NE2 | 2.25 | 0.61 |
| 4:J:1105:ALA:HA | 4:J:1123:ARG:O | 2.01 | 0.61 |
| 4:J:1368:ASP:OD1 | 4:J:1369:ARG:N | 2.34 | 0.61 |
| 6:L:150:ARG:NE | 6:L:155:GLU:OE1 | 2.34 | 0.61 |
| 3:I:994:ARG:HG2 | 3:I:997:TRP:CH2 | 2.36 | 0.60 |
| 4:J:615:LYS:HE3 | 5:K:4:VAL:HG21 | 1.83 | 0.60 |
| 4:J:1155:ILE:HG12 | 4:J:1190:ILE:CD1 | 2.31 | 0.60 |
| 6:L:162:ILE:HG22 | 6:L:164:GLY:N | 2.16 | 0.60 |
| 7:O:40:DC:H1' | 7:O:41:DT:H5' | 1.83 | 0.60 |
| 3:I:24:VAL:HG12 | 3:I:25:PRO:HD2 | 1.82 | 0.60 |
| 3:I:71:VAL:HB | 3:I:99:LYS:O | 2.02 | 0.60 |
| 3:I:250:THR:HA | 3:I:268:ARG:HA | 1.81 | 0.60 |
| 3:I:214:ASN:HD21 | 3:I:359:ARG:HD2 | 1.66 | 0.60 |
| 4:J:1044:GLN:O | 4:J:1067:ARG:HD3 | 2.01 | 0.60 |
| 6:L:249:ILE:HG22 | 6:L:250:LEU:HD22 | 1.82 | 0.60 |
| 4:J:51:PRO:HB2 | 4:J:57:PHE:O | 2.02 | 0.60 |
| 4:J:83:VAL:O | 4:J:92:VAL:HG12 | 2.01 | 0.60 |
| 4:J:210:SER:O | 4:J:214:ARG:NH1 | 2.35 | 0.60 |
| 6:L:286:LEU:O | 6:L:290:LEU:HD13 | 2.01 | 0.60 |
| 6:L:347:ILE:HA | 6:L:350:GLU:OE1 | 2.01 | 0.60 |
| 2:M:279:GLY:O | 2:M:283:GLN:HG3 | 2.01 | 0.60 |
| 3:I:75:LEU:HD12 | 3:I:94:ALA:HB3 | 1.83 | 0.60 |
| 3:I:1305:TYR:CE1 | 4:J:379:PRO:HG3 | 2.36 | 0.60 |
| 4:J:69:GLU:OE2 | 4:J:76:LYS:NZ | 2.34 | 0.60 |
| 4:J:70:CYS:SG | 4:J:73:GLY:N | 2.73 | 0.60 |
| 4:J:196:GLN:HA | 4:J:199:GLU:OE1 | 2.01 | 0.60 |
| 4:J:807:LEU:HD12 | 4:J:1259:GLN:OE1 | 2.01 | 0.60 |
| 4:J:1082:ASP:OD1 | 4:J:1086:ASN:N | 2.29 | 0.60 |
| 3:I:123:TYR:OH | 3:I:126:GLU:OE2 | 2.16 | 0.60 |
| 3:I:1101:LEU:HD13 | 4:J:504:GLN:HB2 | 1.83 | 0.60 |
| 4:J:885:VAL:HG23 | 4:J:894:VAL:HG21 | 1.83 | 0.60 |
| 6:L:383:ASN:HB2 | 6:L:412:LEU:HD21 | 1.84 | 0.60 |
| 6:L:452:ILE:HG13 | 6:L:457:ILE:HG13 | 1.84 | 0.60 |
| 3:I:104:ILE:HG13 | 3:I:115:LYS:HG3 | 1.82 | 0.60 |
| 3:I:213:LEU:HD11 | 3:I:422:LYS:HG3 | 1.84 | 0.60 |
| 3:I:738:GLU:HA | 3:I:741:MET:HE2 | 1.84 | 0.60 |
| 3:I:1007:LYS:HA | 3:I:1010:GLN:HE21 | 1.65 | 0.60 |
| 3:I:1339:LEU:HG | 4:J:17:PHE:CD2 | 2.37 | 0.60 |
| 4:J:514:THR:HG21 | 4:J:596:LEU:HB2 | 1.84 | 0.60 |
| 4:J:1047:THR:HG22 | 4:J:1060:VAL:O | 2.02 | 0.60 |
| 6:L:330:LEU:HD23 | 6:L:333:VAL:CG1 | 2.31 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:M:303:ILE:O | 2:M:307:LEU:HD13 | 2.01 | 0.60 |
| 1:N:12:THR:O | 1:N:16:THR:HG23 | 2.01 | 0.60 |
| 3:I:105:TYR:HA | 3:I:114:VAL:HA | 1.82 | 0.60 |
| 3:I:936:ARG:HG2 | 3:I:937:ASP:H | 1.65 | 0.60 |
| 3:I:1297:ASP:O | 3:I:1301:ARG:HB2 | 2.01 | 0.60 |
| 4:J:142:GLU:OE2 | 6:L:103:ARG:NH2 | 2.35 | 0.60 |
| 4:J:515:ARG:NH2 | 4:J:717:VAL:HB | 2.16 | 0.60 |
| 4:J:810:THR:CG2 | 4:J:893:GLY:HA3 | 2.32 | 0.60 |
| 4:J:950:ILE:HD13 | 4:J:995:TYR:CB | 2.31 | 0.60 |
| 4:J:1155:ILE:CD1 | 4:J:1210:ILE:HB | 2.32 | 0.60 |
| 3:I:1005:GLU:OE1 | 3:I:1005:GLU:N | 2.32 | 0.60 |
| 3:I:1109:ILE:O | 3:I:1113:LEU:HD12 | 2.01 | 0.60 |
| 4:J:385:LEU:CD2 | 4:J:411:ILE:HG13 | 2.30 | 0.60 |
| 6:L:141:ILE:HG23 | 6:L:144:LEU:HD23 | 1.84 | 0.60 |
| 6:L:227:GLN:HG2 | 6:L:252:LEU:HA | 1.83 | 0.60 |
| 2:H:35:PHE:HA | 2:H:38:THR:CG2 | 2.32 | 0.60 |
| 3:I:139:ASN:O | 3:I:141:THR:HG23 | 2.01 | 0.60 |
| 3:I:277:LEU:O | 3:I:281:ASP:HA | 2.02 | 0.60 |
| 3:I:390:PHE:HA | 3:I:419:ILE:HD11 | 1.83 | 0.60 |
| 3:I:524:ILE:HD11 | 3:I:712:SER:HB3 | 1.83 | 0.60 |
| 3:I:1070:HIS:NE2 | 3:I:1114:GLU:OE1 | 2.23 | 0.60 |
| 3:I:1326:LEU:O | 3:I:1330:ILE:HG13 | 2.02 | 0.60 |
| 4:J:308:ASP:HB3 | 4:J:328:ALA:CB | 2.31 | 0.60 |
| 4:J:530:PRO:HB2 | 4:J:581:MET:CE | 2.32 | 0.60 |
| 4:J:670:SER:OG | 4:J:672:LEU:HD13 | 2.02 | 0.60 |
| 4:J:963:VAL:HG22 | 4:J:980:THR:OG1 | 2.02 | 0.60 |
| 6:L:102:MET:HE1 | 6:L:388:ILE:HG21 | 1.83 | 0.60 |
| 6:L:118:ASP:O | 6:L:122:ARG:HG3 | 2.01 | 0.60 |
| 6:L:231:THR:HG23 | 6:L:248:GLU:CB | 2.32 | 0.60 |
| 2:H:118:ASP:HB3 | 2:H:121:VAL:HG22 | 1.83 | 0.59 |
| 4:J:309:ASN:HD21 | 4:J:324:LEU:HB2 | 1.67 | 0.59 |
| 4:J:1175:LEU:O | 4:J:1188:GLU:N | 2.35 | 0.59 |
| 3:I:1234:LYS:HE2 | 3:I:1238:LEU:HD11 | 1.84 | 0.59 |
| 4:J:71:LEU:H | 4:J:90:VAL:HG21 | 1.66 | 0.59 |
| 4:J:168:ALA:O | 4:J:172:PHE:N | 2.31 | 0.59 |
| 4:J:824:PRO:HB2 | 4:J:831:VAL:HG11 | 1.83 | 0.59 |
| 3:I:98:VAL:HG21 | 3:I:124:MET:HE3 | 1.84 | 0.59 |
| 4:J:1173:ARG:NH2 | 4:J:1196:LEU:HG | 2.17 | 0.59 |
| 4:J:1221:LEU:CD2 | 4:J:1306:LEU:HB2 | 2.31 | 0.59 |
| 1:N:64:TYR:O | 1:N:68:GLN:HG2 | 2.02 | 0.59 |
| 3:I:242:VAL:HB | 3:I:245:ARG:HG3 | 1.85 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:J:843:VAL:HG23 | 4:J:863:LEU:HD12 | 1.83 | 0.59 |
| 2:M:283:GLN:O | 2:M:315:GLY:HA2 | 2.02 | 0.59 |
| 2:M:298:LYS:O | 2:M:301:THR:HG22 | 2.02 | 0.59 |
| 3:I:1103:VAL:HG11 | 3:I:1112:ILE:CD1 | 2.32 | 0.59 |
| 4:J:262:THR:HG22 | 4:J:263:SER:O | 2.03 | 0.59 |
| 4:J:553:THR:CB | 4:J:567:THR:HG22 | 2.32 | 0.59 |
| 4:J:844:THR:HG23 | 4:J:864:LEU:HD21 | 1.83 | 0.59 |
| 6:L:335:GLU:HG3 | 6:L:336:GLU:OE1 | 2.03 | 0.59 |
| 7:O:73:DC:H2'' | 7:O:74:DC:C5' | 2.31 | 0.59 |
| 2:M:268:ASN:O | 2:M:271:LYS:HB3 | 2.02 | 0.59 |
| 2:H:208:ASN:OD1 | 2:H:210:THR:HG23 | 2.03 | 0.59 |
| 6:L:277:MET:HG3 | 6:L:281:ARG:HH12 | 1.67 | 0.59 |
| 2:M:255:ARG:HB2 | 2:M:278:ILE:CD1 | 2.33 | 0.59 |
| 2:H:83:LEU:HD11 | 4:J:526:VAL:HB | 1.84 | 0.59 |
| 2:H:190:ALA:O | 2:H:198:LEU:HB2 | 2.02 | 0.59 |
| 3:I:395:TYR:HE2 | 3:I:420:LEU:HD22 | 1.67 | 0.59 |
| 4:J:422:LEU:CD1 | 4:J:471:PRO:HG3 | 2.33 | 0.59 |
| 4:J:663:GLU:O | 4:J:666:GLU:HG3 | 2.03 | 0.59 |
| 3:I:241:LEU:HD21 | 3:I:277:LEU:HD11 | 1.85 | 0.59 |
| 3:I:257:ALA:CB | 3:I:282:VAL:HG21 | 2.33 | 0.59 |
| 3:I:896:THR:CG2 | 3:I:897:PRO:HD2 | 2.33 | 0.59 |
| 3:I:1247:SER:O | 4:J:348:ASP:HB3 | 2.03 | 0.59 |
| 4:J:850:LYS:HD2 | 4:J:851:PRO:HD2 | 1.85 | 0.59 |
| 2:G:154:PRO:O | 2:G:158:ARG:HG3 | 2.02 | 0.59 |
| 3:I:1259:LEU:HD11 | 6:L:524:GLU:HB3 | 1.85 | 0.59 |
| 4:J:224:LEU:O | 4:J:228:VAL:HG12 | 2.03 | 0.59 |
| 4:J:260:PHE:O | 6:L:505:ILE:N | 2.35 | 0.59 |
| 2:G:57:THR:HG22 | 2:G:58:GLU:CG | 2.33 | 0.59 |
| 2:H:24:ALA:HB2 | 2:H:213:PRO:HG2 | 1.84 | 0.59 |
| 3:I:940:GLU:OE1 | 3:I:940:GLU:N | 2.35 | 0.59 |
| 3:I:960:LEU:HB3 | 3:I:1025:PHE:HD1 | 1.68 | 0.59 |
| 4:J:438:GLU:HG3 | 4:J:485:MET:CE | 2.33 | 0.59 |
| 4:J:1350:ASN:HD22 | 4:J:1358:PRO:HD3 | 1.68 | 0.59 |
| 4:J:306:LEU:HD22 | 4:J:306:LEU:O | 2.02 | 0.58 |
| 4:J:822:MET:CE | 4:J:838:ARG:HB3 | 2.33 | 0.58 |
| 4:J:1036:ARG:HA | 4:J:1111:ASP:OD2 | 2.03 | 0.58 |
| 6:L:127:ILE:O | 6:L:131:GLN:HG3 | 2.01 | 0.58 |
| 2:G:134:THR:HG21 | 3:I:727:VAL:O | 2.02 | 0.58 |
| 2:H:74:VAL:HG22 | 2:H:133:LEU:CD2 | 2.33 | 0.58 |
| 4:J:1046:ILE:HA | 4:J:1061:VAL:HA | 1.86 | 0.58 |
| 4:J:1046:ILE:HA | 4:J:1062:LEU:H | 1.67 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:K:53:GLU:HB3 | 5:K:59:ILE:HG12 | 1.85 | 0.58 |
| 2:M:304:LYS:HD2 | 2:M:314:LEU:CD1 | 2.32 | 0.58 |
| 3:I:646:SER:H | 3:I:649:GLN:HE21 | 1.49 | 0.58 |
| 3:I:823:VAL:HG22 | 3:I:1060:ILE:CG2 | 2.33 | 0.58 |
| 4:J:290:ILE:HD13 | 6:L:381:GLU:OE1 | 2.03 | 0.58 |
| 4:J:1175:LEU:HD23 | 4:J:1190:ILE:HG13 | 1.86 | 0.58 |
| 6:L:137:TYR:CD2 | 6:L:140:ALA:HB2 | 2.38 | 0.58 |
| 8:P:47:DC:H2'' | 8:P:48:DC:C6 | 2.38 | 0.58 |
| 3:I:525:THR:HG21 | 3:I:687:ARG:HD3 | 1.85 | 0.58 |
| 3:I:745:GLU:HB2 | 3:I:1017:GLN:CG | 2.33 | 0.58 |
| 4:J:1047:THR:CG2 | 4:J:1060:VAL:HB | 2.32 | 0.58 |
| 6:L:273:MET:HB3 | 6:L:362:ASN:HD21 | 1.67 | 0.58 |
| 2:G:102:LEU:HD11 | 2:G:110:VAL:CG2 | 2.34 | 0.58 |
| 2:H:32:GLU:HB3 | 2:H:35:PHE:HD2 | 1.67 | 0.58 |
| 3:I:1120:ALA:HB2 | 3:I:1199:LEU:HD12 | 1.84 | 0.58 |
| 6:L:117:ILE:HG23 | 6:L:421:TYR:CD2 | 2.39 | 0.58 |
| 6:L:470:MET:HG2 | 6:L:486:ARG:HD2 | 1.85 | 0.58 |
| 8:P:66:DT:H2' | 8:P:67:DT:H71 | 1.84 | 0.58 |
| 3:I:245:ARG:HD2 | 3:I:337:PHE:CE2 | 2.39 | 0.58 |
| 4:J:1049:GLN:HG2 | 4:J:1050:THR:H | 1.69 | 0.58 |
| 4:J:1174:ARG:HG2 | 4:J:1189:MET:CE | 2.33 | 0.58 |
| 6:L:227:GLN:OE1 | 6:L:251:LYS:HB3 | 2.04 | 0.58 |
| 6:L:484:ALA:HB2 | 6:L:494:ILE:HD13 | 1.84 | 0.58 |
| 6:L:561:MET:HA | 6:L:567:MET:HE1 | 1.85 | 0.58 |
| 6:L:585:GLU:HG2 | 7:O:27:DT:O4 | 2.03 | 0.58 |
| 3:I:106:GLU:OE2 | 3:I:115:LYS:HB3 | 2.03 | 0.58 |
| 3:I:1111:GLN:HG3 | 3:I:1230:MET:CE | 2.34 | 0.58 |
| 4:J:79:LYS:HG3 | 6:L:569:THR:CB | 2.32 | 0.58 |
| 2:H:35:PHE:HA | 2:H:38:THR:HG22 | 1.86 | 0.58 |
| 2:H:215:GLU:OE1 | 2:H:218:ARG:NH2 | 2.30 | 0.58 |
| 3:I:676:ALA:HB3 | 4:J:779:ALA:CB | 2.33 | 0.58 |
| 3:I:685:MET:SD | 3:I:1073:LYS:HG2 | 2.44 | 0.58 |
| 3:I:843:THR:OG1 | 3:I:846:GLY:O | 2.20 | 0.58 |
| 3:I:948:ILE:O | 3:I:952:GLN:HG3 | 2.03 | 0.58 |
| 4:J:814:CYS:CB | 4:J:889:ASP:HB3 | 2.31 | 0.58 |
| 6:L:487:MET:O | 6:L:488:LEU:HD23 | 2.04 | 0.58 |
| 8:P:34:DT:H2'' | 8:P:35:DA:C5 | 2.39 | 0.58 |
| 3:I:348:SER:HA | 3:I:351:LEU:HD12 | 1.85 | 0.58 |
| 3:I:369:MET:HE3 | 3:I:370:MET:HG2 | 1.85 | 0.58 |
| 3:I:590:PRO:HG3 | 3:I:605:TYR:HE1 | 1.69 | 0.58 |
| 3:I:697:LYS:HA | 3:I:795:ALA:HB2 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:398:LYS:HD2 | 6:L:532:LEU:HD21 | 1.84 | 0.58 |
| 4:J:1026:PRO:HB2 | 4:J:1028:ILE:HG23 | 1.84 | 0.58 |
| 6:L:117:ILE:O | 6:L:121:LYS:HG3 | 2.04 | 0.58 |
| 6:L:276:MET:HE1 | 6:L:279:ARG:HH21 | 1.68 | 0.58 |
| 6:L:496:LYS:O | 6:L:500:ILE:HG12 | 2.04 | 0.58 |
| 6:L:552:THR:HB | 6:L:555:GLU:HB3 | 1.86 | 0.58 |
| 1:N:8:ALA:HB2 | 4:J:783:LEU:HD12 | 1.84 | 0.58 |
| 3:I:72:SER:OG | 3:I:73:TYR:N | 2.37 | 0.58 |
| 3:I:220:ILE:HG22 | 3:I:221:LEU:HD23 | 1.85 | 0.58 |
| 4:J:131:PRO:HG2 | 4:J:134:ASP:OD2 | 2.04 | 0.58 |
| 4:J:311:ARG:NH2 | 4:J:1329:THR:HG21 | 2.18 | 0.58 |
| 4:J:527:LEU:HD22 | 4:J:550:VAL:HG12 | 1.85 | 0.58 |
| 3:I:888:THR:HG23 | 3:I:916:SER:HB2 | 1.84 | 0.57 |
| 4:J:846:GLU:HG2 | 4:J:881:LYS:HB3 | 1.86 | 0.57 |
| 5:K:10:VAL:CG2 | 5:K:16:ARG:HG3 | 2.33 | 0.57 |
| 3:I:175:ARG:HD2 | 3:I:177:ILE:HD11 | 1.84 | 0.57 |
| 3:I:189:ASP:OD1 | 3:I:193:ASN:N | 2.36 | 0.57 |
| 3:I:256:GLU:HB3 | 3:I:261:VAL:HA | 1.86 | 0.57 |
| 3:I:1213:TYR:CE1 | 3:I:1220:GLN:HB2 | 2.39 | 0.57 |
| 4:J:697:MET:CE | 4:J:738:ARG:HA | 2.33 | 0.57 |
| 10:J:1504:1N7:C3 | 10:J:1504:1N7:C2 | 2.76 | 0.57 |
| 6:L:137:TYR:CZ | 6:L:139:GLU:HB3 | 2.39 | 0.57 |
| 6:L:341:LEU:HD23 | 6:L:344:LEU:HD22 | 1.85 | 0.57 |
| 6:L:606:VAL:O | 6:L:609:SER:OG | 2.08 | 0.57 |
| 2:H:134:THR:HG23 | 2:H:136:GLU:HB2 | 1.86 | 0.57 |
| 3:I:28:LEU:HD22 | 3:I:527:LYS:HD2 | 1.85 | 0.57 |
| 3:I:463:GLN:O | 3:I:466:VAL:HG12 | 2.04 | 0.57 |
| 3:I:964:LEU:HD22 | 3:I:1025:PHE:HB3 | 1.86 | 0.57 |
| 3:I:1120:ALA:HB1 | 3:I:1198:LEU:HD23 | 1.86 | 0.57 |
| 4:J:824:PRO:HB2 | 4:J:831:VAL:CG1 | 2.34 | 0.57 |
| 4:J:1040:MET:HE3 | 4:J:1046:ILE:HD13 | 1.86 | 0.57 |
| 4:J:1162:ILE:HG13 | 4:J:1202:GLU:O | 2.03 | 0.57 |
| 2:M:255:ARG:HB2 | 2:M:278:ILE:CG1 | 2.34 | 0.57 |
| 2:H:14:VAL:HG22 | 2:H:28:LEU:HD12 | 1.85 | 0.57 |
| 3:I:263:VAL:HG12 | 3:I:264:GLU:H | 1.68 | 0.57 |
| 3:I:924:VAL:HG23 | 3:I:1056:VAL:HG21 | 1.86 | 0.57 |
| 4:J:26:SER:HB3 | 4:J:236:TRP:CZ2 | 2.40 | 0.57 |
| 4:J:334:LYS:O | 4:J:340:GLN:HB2 | 2.03 | 0.57 |
| 6:L:288:MET:HA | 6:L:291:CYS:SG | 2.45 | 0.57 |
| 6:L:390:ILE:HG21 | 6:L:435:ILE:HG22 | 1.84 | 0.57 |
| 7:O:29:DA:H2'' | 7:O:30:DC:C5' | 2.35 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:O:69:DT:H6 | 7:O:69:DT:H5' | 1.69 | 0.57 |
| 2:M:298:LYS:HA | 2:M:301:THR:HG22 | 1.84 | 0.57 |
| 2:G:211:ILE:CG2 | 2:G:216:ALA:HB2 | 2.34 | 0.57 |
| 3:I:599:VAL:HG21 | 3:I:623:LEU:HD21 | 1.85 | 0.57 |
| 5:K:45:LYS:O | 5:K:49:ILE:HG12 | 2.04 | 0.57 |
| 6:L:426:LYS:CB | 7:O:52:DA:H5'' | 2.34 | 0.57 |
| 1:N:30:HIS:CD2 | 1:N:32:ILE:HG13 | 2.38 | 0.57 |
| 4:J:132:LEU:HA | 4:J:135:ILE:HD13 | 1.87 | 0.57 |
| 4:J:153:ASN:ND2 | 4:J:171:GLU:OE2 | 2.37 | 0.57 |
| 6:L:102:MET:CE | 6:L:388:ILE:HD13 | 2.35 | 0.57 |
| 6:L:244:THR:HA | 6:L:247:GLU:OE1 | 2.05 | 0.57 |
| 2:M:279:GLY:HA2 | 2:M:282:VAL:CG2 | 2.35 | 0.57 |
| 2:H:102:LEU:HB3 | 2:H:142:MET:HG2 | 1.85 | 0.57 |
| 2:H:185:TYR:HA | 2:H:202:VAL:O | 2.04 | 0.57 |
| 3:I:558:VAL:HG13 | 3:I:573:ASN:HB3 | 1.86 | 0.57 |
| 3:I:617:ALA:HA | 3:I:636:CYS:SG | 2.45 | 0.57 |
| 4:J:514:THR:CG2 | 4:J:596:LEU:HB2 | 2.35 | 0.57 |
| 4:J:999:TYR:OH | 4:J:1028:ILE:HG12 | 2.04 | 0.57 |
| 4:J:1031:VAL:HG23 | 4:J:1080:ILE:HG21 | 1.85 | 0.57 |
| 4:J:1307:LEU:HD22 | 4:J:1312:ALA:HA | 1.85 | 0.57 |
| 4:J:1327:GLU:O | 4:J:1331:VAL:HG23 | 2.04 | 0.57 |
| 3:I:196:VAL:HG23 | 3:I:206:ALA:HA | 1.87 | 0.57 |
| 4:J:128:LEU:HD23 | 4:J:192:MET:CE | 2.35 | 0.57 |
| 4:J:271:ARG:NH1 | 4:J:316:ILE:HG21 | 2.20 | 0.57 |
| 4:J:1161:GLY:CA | 4:J:1179:PRO:HA | 2.32 | 0.57 |
| 6:L:98:VAL:CA | 6:L:402:LEU:HD11 | 2.34 | 0.57 |
| 7:O:37:DA:H2'' | 7:O:38:DG:C8 | 2.39 | 0.57 |
| 2:G:197:ASP:O | 2:G:198:LEU:HD23 | 2.05 | 0.57 |
| 3:I:122:VAL:HG21 | 3:I:493:ILE:HG21 | 1.86 | 0.57 |
| 4:J:430:HIS:CD2 | 4:J:432:LEU:HD12 | 2.40 | 0.57 |
| 4:J:552:ILE:HD11 | 4:J:570:LYS:HZ3 | 1.70 | 0.57 |
| 4:J:1238:GLN:HB3 | 4:J:1242:ARG:NH1 | 2.19 | 0.57 |
| 6:L:165:PHE:CD1 | 6:L:259:PHE:HA | 2.40 | 0.57 |
| 2:G:52:PRO:HG2 | 2:G:219:ARG:HE | 1.70 | 0.57 |
| 3:I:1287:LEU:CD2 | 4:J:1357:ILE:HD11 | 2.32 | 0.57 |
| 4:J:198:CYS:CB | 4:J:221:ILE:HD11 | 2.34 | 0.57 |
| 6:L:285:ARG:O | 6:L:289:LYS:HB2 | 2.04 | 0.57 |
| 6:L:560:ARG:HG3 | 6:L:565:ILE:CG2 | 2.35 | 0.57 |
| 3:I:901:LEU:HD13 | 6:L:565:ILE:HD11 | 1.87 | 0.56 |
| 3:I:960:LEU:HB3 | 3:I:1025:PHE:CD1 | 2.40 | 0.56 |
| 4:J:385:LEU:HD21 | 4:J:411:ILE:HG13 | 1.85 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:1179:PRO:HD2 | 4:J:1184:ASP:HA | 1.87 | 0.56 |
| 7:O:25:DA:C2' | 7:O:26:DT:H5'' | 2.35 | 0.56 |
| 1:N:27:ILE:HD11 | 4:J:680:ASN:CB | 2.36 | 0.56 |
| 3:I:57:PHE:HE2 | 3:I:100:LEU:HD21 | 1.68 | 0.56 |
| 3:I:979:LEU:HD11 | 3:I:1011:LEU:CD1 | 2.35 | 0.56 |
| 6:L:213:ASP:HB2 | 6:L:214:PRO:HD2 | 1.86 | 0.56 |
| 6:L:288:MET:HB3 | 6:L:302:PHE:CZ | 2.40 | 0.56 |
| 3:I:56:VAL:HG13 | 3:I:57:PHE:CD1 | 2.39 | 0.56 |
| 3:I:359:ARG:HH22 | 3:I:382:GLU:HG2 | 1.70 | 0.56 |
| 4:J:20:ILE:HD13 | 4:J:1320:ILE:HD12 | 1.86 | 0.56 |
| 4:J:54:ASP:HB2 | 4:J:61:ILE:HD11 | 1.87 | 0.56 |
| 4:J:384:LYS:HG2 | 4:J:411:ILE:HG23 | 1.87 | 0.56 |
| 4:J:502:PRO:HB3 | 4:J:506:VAL:HB | 1.86 | 0.56 |
| 4:J:984:LEU:CB | 4:J:993:GLU:HB2 | 2.35 | 0.56 |
| 4:J:1031:VAL:CG2 | 4:J:1080:ILE:HG21 | 2.35 | 0.56 |
| 4:J:1162:ILE:HA | 4:J:1203:ARG:HA | 1.87 | 0.56 |
| 4:J:1226:VAL:HA | 4:J:1229:VAL:HG12 | 1.87 | 0.56 |
| 4:J:1322:ALA:HB3 | 4:J:1331:VAL:HG11 | 1.87 | 0.56 |
| 6:L:285:ARG:HG3 | 6:L:289:LYS:CE | 2.35 | 0.56 |
| 8:P:66:DT:C2' | 8:P:67:DT:H71 | 2.35 | 0.56 |
| 2:G:11:PRO:O | 2:G:30:PRO:HD2 | 2.05 | 0.56 |
| 2:G:180:VAL:HG12 | 2:G:207:THR:HG22 | 1.87 | 0.56 |
| 3:I:850:ILE:HD13 | 3:I:886:LYS:HB2 | 1.87 | 0.56 |
| 3:I:1112:ILE:HD11 | 4:J:639:VAL:HG13 | 1.87 | 0.56 |
| 4:J:202:ARG:HA | 4:J:205:LEU:CD2 | 2.36 | 0.56 |
| 4:J:202:ARG:O | 4:J:205:LEU:HD23 | 2.05 | 0.56 |
| 4:J:288:PRO:HG2 | 4:J:291:ILE:HG13 | 1.86 | 0.56 |
| 5:K:52:ARG:O | 5:K:56:GLU:HG2 | 2.05 | 0.56 |
| 6:L:585:GLU:OE1 | 6:L:588:ARG:HD2 | 2.06 | 0.56 |
| 3:I:302:ILE:HG22 | 3:I:309:LEU:HA | 1.87 | 0.56 |
| 4:J:134:ASP:HB3 | 4:J:159:ILE:HD11 | 1.88 | 0.56 |
| 4:J:1168:GLU:HG3 | 4:J:1173:ARG:CG | 2.36 | 0.56 |
| 7:O:46:DG:C2' | 7:O:47:DG:H5' | 2.34 | 0.56 |
| 2:M:278:ILE:O | 2:M:282:VAL:HG13 | 2.05 | 0.56 |
| 2:H:45:ARG:O | 2:H:49:SER:OG | 2.21 | 0.56 |
| 4:J:759:ILE:HD11 | 4:J:774:ILE:CG2 | 2.35 | 0.56 |
| 4:J:1189:MET:O | 4:J:1191:PRO:HD3 | 2.06 | 0.56 |
| 6:L:339:ARG:O | 6:L:342:GLN:HG3 | 2.06 | 0.56 |
| 6:L:572:THR:HB | 8:P:55:DT:H5'' | 1.87 | 0.56 |
| 6:L:573:LEU:HG | 6:L:584:ARG:HG2 | 1.87 | 0.56 |
| 4:J:1298:VAL:HG13 | 4:J:1299:GLY:O | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:1359:ALA:O | 4:J:1363:TYR:HB2 | 2.06 | 0.56 |
| 2:G:130:ILE:HG22 | 2:G:131:CYS:SG | 2.46 | 0.56 |
| 3:I:81:ASP:O | 3:I:83:GLN:N | 2.39 | 0.56 |
| 3:I:370:MET:CE | 3:I:388:LEU:HD11 | 2.36 | 0.56 |
| 4:J:707:ILE:CD1 | 4:J:714:GLU:HB3 | 2.36 | 0.56 |
| 4:J:1063:ASP:OD2 | 4:J:1103:GLY:HA3 | 2.05 | 0.56 |
| 6:L:295:CYS:O | 6:L:326:TRP:HB2 | 2.05 | 0.56 |
| 2:H:219:ARG:O | 2:H:223:ILE:HG13 | 2.06 | 0.56 |
| 3:I:210:LEU:CD2 | 3:I:220:ILE:HG12 | 2.36 | 0.56 |
| 3:I:689:ALA:HB2 | 3:I:1233:LEU:HB3 | 1.88 | 0.56 |
| 3:I:1296:ASP:OD1 | 3:I:1321:GLU:HB3 | 2.06 | 0.56 |
| 4:J:121:PRO:HB2 | 4:J:126:LEU:CD2 | 2.36 | 0.56 |
| 4:J:683:ILE:HD11 | 4:J:756:GLU:HA | 1.88 | 0.56 |
| 6:L:573:LEU:HG | 6:L:584:ARG:HB3 | 1.88 | 0.56 |
| 3:I:1141:LEU:O | 3:I:1145:ILE:HG12 | 2.06 | 0.56 |
| 6:L:384:LEU:O | 6:L:387:VAL:HG12 | 2.06 | 0.56 |
| 4:J:317:THR:HG22 | 4:J:323:PRO:CA | 2.35 | 0.55 |
| 4:J:700:ASN:O | 4:J:704:GLU:HB2 | 2.05 | 0.55 |
| 8:P:52:DT:H2'' | 8:P:53:DT:C5 | 2.41 | 0.55 |
| 1:N:3:ASP:O | 1:N:6:ASP:N | 2.35 | 0.55 |
| 3:I:369:MET:CE | 3:I:370:MET:HG2 | 2.36 | 0.55 |
| 3:I:468:LEU:O | 3:I:471:VAL:HG12 | 2.05 | 0.55 |
| 4:J:1175:LEU:CD2 | 4:J:1190:ILE:HG13 | 2.37 | 0.55 |
| 6:L:547:VAL:HG23 | 6:L:548:LEU:HD23 | 1.88 | 0.55 |
| 2:H:98:VAL:HG21 | 2:H:121:VAL:HG11 | 1.87 | 0.55 |
| 3:I:44:GLU:N | 3:I:44:GLU:OE2 | 2.39 | 0.55 |
| 3:I:377:THR:HB | 3:I:380:ALA:HB3 | 1.89 | 0.55 |
| 3:I:988:LYS:O | 3:I:992:LEU:HD22 | 2.06 | 0.55 |
| 4:J:722:ILE:HG23 | 4:J:737:ILE:HD12 | 1.89 | 0.55 |
| 6:L:397:ARG:HB2 | 6:L:443:ILE:HD13 | 1.89 | 0.55 |
| 6:L:604:SER:HA | 6:L:607:LEU:HD23 | 1.89 | 0.55 |
| 8:P:34:DT:H2'' | 8:P:35:DA:N7 | 2.20 | 0.55 |
| 1:N:46:GLU:HA | 1:N:49:ARG:NH2 | 2.21 | 0.55 |
| 2:H:33:ARG:NH1 | 3:I:1081:PRO:HG3 | 2.21 | 0.55 |
| 3:I:194:LEU:HD12 | 3:I:206:ALA:CB | 2.36 | 0.55 |
| 3:I:845:LEU:HD21 | 3:I:889:PRO:O | 2.06 | 0.55 |
| 3:I:1260:GLY:HA2 | 4:J:346:ARG:NH1 | 2.20 | 0.55 |
| 4:J:42:GLU:O | 4:J:55:GLY:HA3 | 2.06 | 0.55 |
| 4:J:556:GLU:OE1 | 4:J:556:GLU:N | 2.39 | 0.55 |
| 4:J:1035:VAL:HG23 | 4:J:1113:VAL:O | 2.07 | 0.55 |
| 4:J:1145:PHE:O | 4:J:1309:ILE:HG23 | 2.06 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:1167:LYS:HD3 | 4:J:1170:LYS:HD2 | 1.87 | 0.55 |
| 6:L:110:LEU:CB | 6:L:111:LEU:HD13 | 2.34 | 0.55 |
| 6:L:225:ARG:O | 6:L:229:VAL:HG22 | 2.06 | 0.55 |
| 6:L:313:ASP:OD1 | 6:L:316:PHE:HB3 | 2.07 | 0.55 |
| 7:O:33:DA:H2'' | 7:O:34:DA:C8 | 2.41 | 0.55 |
| 7:O:49:DC:H2'' | 7:O:50:DA:OP1 | 2.05 | 0.55 |
| 8:P:41:DT:C1' | 8:P:42:DT:H5' | 2.31 | 0.55 |
| 3:I:214:ASN:ND2 | 3:I:359:ARG:HD2 | 2.21 | 0.55 |
| 3:I:689:ALA:CB | 3:I:1233:LEU:HB3 | 2.37 | 0.55 |
| 4:J:511:TYR:CE2 | 4:J:724:MET:HG2 | 2.40 | 0.55 |
| 8:P:20:DC:H2'' | 8:P:21:DA:C8 | 2.42 | 0.55 |
| 3:I:201:ARG:NH2 | 3:I:370:MET:O | 2.40 | 0.55 |
| 3:I:633:LEU:HD13 | 3:I:644:LEU:CD1 | 2.32 | 0.55 |
| 3:I:806:PRO:O | 4:J:633:ALA:HA | 2.07 | 0.55 |
| 6:L:429:THR:HA | 7:O:53:DT:C7 | 2.37 | 0.55 |
| 3:I:367:TYR:CZ | 3:I:371:ARG:HG3 | 2.41 | 0.55 |
| 3:I:802:VAL:HG21 | 3:I:1098:LEU:HD12 | 1.88 | 0.55 |
| 4:J:35:PHE:CE2 | 4:J:101:ARG:HG2 | 2.42 | 0.55 |
| 4:J:759:ILE:HD11 | 4:J:774:ILE:HG21 | 1.89 | 0.55 |
| 4:J:973:LEU:HD22 | 4:J:1003:LEU:CD1 | 2.34 | 0.55 |
| 4:J:1155:ILE:HD13 | 4:J:1210:ILE:HB | 1.87 | 0.55 |
| 2:G:47:LEU:CD2 | 2:G:220:ALA:HB2 | 2.37 | 0.55 |
| 2:H:98:VAL:HG21 | 2:H:121:VAL:CG1 | 2.37 | 0.55 |
| 3:I:67:GLU:HB3 | 3:I:103:VAL:CG2 | 2.36 | 0.55 |
| 3:I:1138:VAL:HA | 3:I:1141:LEU:HB2 | 1.87 | 0.55 |
| 4:J:1046:ILE:C | 4:J:1062:LEU:HG | 2.26 | 0.55 |
| 4:J:1170:LYS:N | 4:J:1172:LYS:O | 2.39 | 0.55 |
| 4:J:1197:ASN:OD1 | 4:J:1211:SER:HA | 2.06 | 0.55 |
| 2:M:257:VAL:HG11 | 2:M:270:LEU:CD2 | 2.36 | 0.55 |
| 2:H:79:LEU:HD23 | 2:H:80:GLU:H | 1.72 | 0.55 |
| 3:I:16:GLY:HA2 | 3:I:1188:ASP:O | 2.07 | 0.55 |
| 3:I:671:LEU:O | 3:I:674:ASP:HB2 | 2.06 | 0.55 |
| 3:I:975:ILE:O | 3:I:978:VAL:HG12 | 2.07 | 0.55 |
| 4:J:1190:ILE:CG2 | 4:J:1196:LEU:HD21 | 2.37 | 0.55 |
| 8:P:50:DT:H2'' | 8:P:51:DC:C5 | 2.42 | 0.55 |
| 3:I:5:TYR:HA | 3:I:8:LYS:CE | 2.37 | 0.55 |
| 3:I:102:LEU:CB | 3:I:489:PRO:HG3 | 2.36 | 0.55 |
| 3:I:207:THR:HG21 | 3:I:351:LEU:HD23 | 1.88 | 0.55 |
| 3:I:995:ASP:O | 3:I:998:LEU:HD22 | 2.06 | 0.55 |
| 4:J:850:LYS:CD | 4:J:851:PRO:HD2 | 2.36 | 0.55 |
| 4:J:1141:VAL:HG22 | 4:J:1237:VAL:CG2 | 2.37 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:L:544:THR:O | 6:L:548:LEU:HG | 2.07 | 0.55 |
| 3:I:356:THR:HG21 | 3:I:361:SER:OG | 2.06 | 0.54 |
| 3:I:658:GLN:NE2 | 3:I:704:MET:SD | 2.80 | 0.54 |
| 4:J:316:ILE:O | 4:J:324:LEU:HD13 | 2.07 | 0.54 |
| 4:J:407:VAL:O | 4:J:411:ILE:HG12 | 2.07 | 0.54 |
| 4:J:1079:LYS:HA | 4:J:1098:GLN:CB | 2.37 | 0.54 |
| 3:I:21:VAL:HG11 | 3:I:592:ARG:CZ | 2.38 | 0.54 |
| 3:I:558:VAL:CG1 | 3:I:573:ASN:HB3 | 2.37 | 0.54 |
| 3:I:669:PRO:HG3 | 3:I:1069:ARG:NH2 | 2.23 | 0.54 |
| 3:I:673:HIS:CD2 | 4:J:766:GLY:HA2 | 2.42 | 0.54 |
| 3:I:1086:PRO:HD2 | 3:I:1094:VAL:CG2 | 2.37 | 0.54 |
| 4:J:298:MET:CE | 6:L:402:LEU:HB3 | 2.35 | 0.54 |
| 4:J:1042:ASP:HA | 4:J:1046:ILE:O | 2.07 | 0.54 |
| 6:L:290:LEU:HD23 | 6:L:294:GLN:OE1 | 2.07 | 0.54 |
| 2:H:181:GLU:HA | 4:J:535:ARG:NH1 | 2.22 | 0.54 |
| 3:I:297:VAL:HA | 3:I:335:THR:HG22 | 1.88 | 0.54 |
| 4:J:1048:ARG:NE | 4:J:1048:ARG:HA | 2.22 | 0.54 |
| 4:J:1271:SER:OG | 4:J:1298:VAL:HG12 | 2.07 | 0.54 |
| 4:J:64:PRO:HG3 | 4:J:91:GLU:O | 2.07 | 0.54 |
| 4:J:98:ARG:O | 4:J:247:PRO:HD2 | 2.07 | 0.54 |
| 4:J:128:LEU:HA | 4:J:192:MET:HE1 | 1.89 | 0.54 |
| 4:J:773:PHE:O | 4:J:776:THR:HG22 | 2.07 | 0.54 |
| 10:J:1504:1N7:H31 | 10:J:1504:1N7:H5 | 1.90 | 0.54 |
| 6:L:311:THR:HG21 | 6:L:348:GLU:OE2 | 2.06 | 0.54 |
| 6:L:429:THR:HA | 7:O:53:DT:H72 | 1.90 | 0.54 |
| 3:I:870:ILE:HD13 | 3:I:1050:VAL:CG1 | 2.38 | 0.54 |
| 4:J:664:ILE:CD1 | 4:J:681:LYS:HG2 | 2.38 | 0.54 |
| 4:J:1146:GLU:OE1 | 4:J:1310:THR:HG22 | 2.08 | 0.54 |
| 6:L:226:ALA:O | 6:L:230:VAL:HG12 | 2.06 | 0.54 |
| 6:L:399:LEU:HD13 | 6:L:443:ILE:HG12 | 1.89 | 0.54 |
| 7:O:66:DG:H2'' | 7:O:67:DA:C5' | 2.38 | 0.54 |
| 2:H:42:ALA:HB1 | 2:H:224:LEU:HD21 | 1.90 | 0.54 |
| 3:I:195:PHE:C | 3:I:206:ALA:HB2 | 2.28 | 0.54 |
| 3:I:221:LEU:HD22 | 3:I:225:PHE:CE2 | 2.43 | 0.54 |
| 3:I:496:LYS:HE3 | 8:P:34:DT:H5'' | 1.90 | 0.54 |
| 3:I:633:LEU:HA | 3:I:645:PHE:O | 2.08 | 0.54 |
| 4:J:38:VAL:HG13 | 4:J:55:GLY:O | 2.08 | 0.54 |
| 4:J:1153:PRO:HA | 4:J:1214:PRO:O | 2.08 | 0.54 |
| 7:O:56:DC:H5' | 7:O:56:DC:C6 | 2.41 | 0.54 |
| 3:I:1234:LYS:HE2 | 3:I:1238:LEU:CD1 | 2.38 | 0.54 |
| 4:J:153:ASN:O | 4:J:154:LEU:HD23 | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:205:LEU:HD12 | 4:J:214:ARG:CB | 2.36 | 0.54 |
| 4:J:953:LYS:HB2 | 4:J:993:GLU:OE2 | 2.07 | 0.54 |
| 4:J:1107:VAL:HA | 4:J:1122:ALA:HB2 | 1.90 | 0.54 |
| 1:N:20:ILE:HG12 | 4:J:754:ILE:CD1 | 2.37 | 0.54 |
| 3:I:176:ILE:HD13 | 3:I:405:PHE:HE1 | 1.72 | 0.54 |
| 3:I:194:LEU:HD12 | 3:I:206:ALA:HB3 | 1.89 | 0.54 |
| 3:I:581:THR:HG22 | 3:I:585:GLY:HA2 | 1.90 | 0.54 |
| 3:I:941:LYS:NZ | 3:I:949:GLU:OE1 | 2.24 | 0.54 |
| 3:I:1276:TRP:CE2 | 4:J:801:VAL:HG21 | 2.43 | 0.54 |
| 4:J:810:THR:HG21 | 4:J:893:GLY:HA3 | 1.90 | 0.54 |
| 4:J:1047:THR:CG2 | 4:J:1049:GLN:HB2 | 2.38 | 0.54 |
| 6:L:165:PHE:CE1 | 6:L:259:PHE:HA | 2.42 | 0.54 |
| 2:H:64:VAL:HG11 | 2:H:78:ILE:HD12 | 1.89 | 0.54 |
| 3:I:1260:GLY:HA2 | 4:J:346:ARG:HH12 | 1.71 | 0.54 |
| 4:J:147:ILE:HD11 | 4:J:179:LYS:NZ | 2.22 | 0.54 |
| 4:J:473:THR:CG2 | 4:J:476:ALA:H | 2.21 | 0.54 |
| 4:J:582:ILE:HD13 | 4:J:623:GLN:O | 2.08 | 0.54 |
| 4:J:826:ILE:CG1 | 4:J:831:VAL:HG22 | 2.38 | 0.54 |
| 4:J:1036:ARG:NH2 | 4:J:1081:VAL:HG11 | 2.23 | 0.54 |
| 4:J:1168:GLU:HG3 | 4:J:1173:ARG:HG2 | 1.90 | 0.54 |
| 5:K:22:VAL:CG2 | 5:K:61:ASN:HB2 | 2.37 | 0.54 |
| 5:K:50:ALA:O | 5:K:54:ILE:HG12 | 2.08 | 0.54 |
| 6:L:312:SER:O | 6:L:315:TRP:NE1 | 2.41 | 0.54 |
| 2:M:255:ARG:O | 2:M:278:ILE:N | 2.40 | 0.54 |
| 1:N:20:ILE:N | 4:J:754:ILE:HD11 | 2.22 | 0.54 |
| 2:H:205:MET:HE1 | 2:H:217:ILE:HG13 | 1.88 | 0.54 |
| 3:I:236:LYS:NZ | 3:I:288:PRO:HB3 | 2.22 | 0.54 |
| 3:I:347:ILE:H | 3:I:347:ILE:HD12 | 1.73 | 0.54 |
| 4:J:812:ASP:O | 4:J:897:HIS:ND1 | 2.32 | 0.54 |
| 4:J:1179:PRO:CD | 4:J:1184:ASP:HA | 2.38 | 0.54 |
| 4:J:1357:ILE:HG22 | 4:J:1359:ALA:N | 2.23 | 0.54 |
| 6:L:150:ARG:HB3 | 6:L:155:GLU:OE1 | 2.08 | 0.54 |
| 2:H:74:VAL:HG22 | 2:H:133:LEU:HD23 | 1.88 | 0.53 |
| 3:I:727:VAL:HG21 | 3:I:771:VAL:O | 2.07 | 0.53 |
| 3:I:798:GLN:OE1 | 3:I:827:ARG:HD2 | 2.08 | 0.53 |
| 3:I:1124:ILE:O | 3:I:1128:ILE:HG13 | 2.07 | 0.53 |
| 4:J:822:MET:HE2 | 4:J:838:ARG:HB3 | 1.90 | 0.53 |
| 4:J:887:SER:O | 4:J:887:SER:OG | 2.23 | 0.53 |
| 6:L:415:ALA:HB2 | 6:L:434:TRP:HB2 | 1.90 | 0.53 |
| 6:L:425:TYR:CE2 | 6:L:429:THR:HB | 2.44 | 0.53 |
| 2:G:150:ARG:NH2 | 2:H:32:GLU:OE2 | 2.41 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:109:PRO:HB3 | 2:H:132:HIS:CD2 | 2.44 | 0.53 |
| 3:I:221:LEU:HD11 | 3:I:314:ASN:HB3 | 1.89 | 0.53 |
| 3:I:242:VAL:HG11 | 3:I:245:ARG:CZ | 2.38 | 0.53 |
| 3:I:533:LEU:HD21 | 3:I:571:LEU:HD13 | 1.90 | 0.53 |
| 3:I:619:ALA:HB2 | 3:I:654:ASP:HB2 | 1.91 | 0.53 |
| 3:I:1102:GLY:O | 3:I:1106:ARG:HB2 | 2.08 | 0.53 |
| 3:I:1321:GLU:OE2 | 4:J:99:ARG:NH2 | 2.42 | 0.53 |
| 6:L:584:ARG:HD3 | 6:L:584:ARG:H | 1.73 | 0.53 |
| 7:O:67:DA:H2'' | 7:O:68:DA:C8 | 2.43 | 0.53 |
| 2:H:29:GLU:OE1 | 2:H:200:LYS:HD2 | 2.08 | 0.53 |
| 3:I:56:VAL:CG1 | 3:I:468:LEU:HD13 | 2.38 | 0.53 |
| 3:I:289:VAL:HG21 | 3:I:322:LEU:CD2 | 2.32 | 0.53 |
| 3:I:359:ARG:O | 3:I:362:ALA:HB3 | 2.08 | 0.53 |
| 3:I:542:ARG:HH21 | 7:O:63:DT:C5' | 2.21 | 0.53 |
| 4:J:1197:ASN:HB2 | 4:J:1210:ILE:O | 2.08 | 0.53 |
| 5:K:27:ALA:HA | 5:K:46:THR:HG22 | 1.90 | 0.53 |
| 6:L:227:GLN:O | 6:L:231:THR:OG1 | 2.11 | 0.53 |
| 6:L:291:CYS:CA | 6:L:295:CYS:HB3 | 2.38 | 0.53 |
| 6:L:573:LEU:HD23 | 6:L:574:GLU:H | 1.73 | 0.53 |
| 2:H:14:VAL:HG22 | 2:H:28:LEU:CD1 | 2.38 | 0.53 |
| 3:I:829:THR:CB | 3:I:1059:ARG:HA | 2.36 | 0.53 |
| 3:I:1103:VAL:HG11 | 3:I:1112:ILE:CG1 | 2.38 | 0.53 |
| 4:J:308:ASP:HA | 4:J:326:SER:OG | 2.08 | 0.53 |
| 4:J:311:ARG:NH2 | 8:P:21:DA:OP1 | 2.41 | 0.53 |
| 6:L:285:ARG:CA | 6:L:289:LYS:HD3 | 2.35 | 0.53 |
| 6:L:287:ILE:HG23 | 6:L:337:VAL:HG13 | 1.89 | 0.53 |
| 2:M:304:LYS:CD | 2:M:314:LEU:HD11 | 2.37 | 0.53 |
| 2:G:79:LEU:CD1 | 3:I:693:LEU:HD11 | 2.38 | 0.53 |
| 2:G:179:PRO:HG3 | 2:G:211:ILE:CG1 | 2.38 | 0.53 |
| 2:H:205:MET:CE | 2:H:217:ILE:HG13 | 2.39 | 0.53 |
| 3:I:104:ILE:HG12 | 3:I:116:ASP:O | 2.08 | 0.53 |
| 3:I:158:ASP:OD1 | 3:I:159:SER:N | 2.41 | 0.53 |
| 3:I:1340:GLU:HG2 | 4:J:1341:ARG:HH22 | 1.72 | 0.53 |
| 4:J:259:ARG:CZ | 6:L:505:ILE:HD11 | 2.39 | 0.53 |
| 4:J:801:VAL:HG12 | 4:J:920:ALA:CB | 2.38 | 0.53 |
| 4:J:1025:MET:HG2 | 4:J:1124:ILE:O | 2.08 | 0.53 |
| 6:L:141:ILE:HD12 | 6:L:256:PHE:CE1 | 2.43 | 0.53 |
| 6:L:312:SER:OG | 6:L:314:THR:HG22 | 2.09 | 0.53 |
| 6:L:453:PRO:HG2 | 7:O:44:DA:OP2 | 2.08 | 0.53 |
| 2:G:95:LYS:HE2 | 2:G:120:ASP:OD2 | 2.09 | 0.53 |
| 2:H:79:LEU:HD23 | 2:H:80:GLU:N | 2.24 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:302:ILE:CG2 | 3:I:309:LEU:HD12 | 2.38 | 0.53 |
| 4:J:218:THR:HA | 4:J:221:ILE:CG2 | 2.38 | 0.53 |
| 3:I:897:PRO:HB3 | 6:L:564:GLY:HA3 | 1.89 | 0.53 |
| 3:I:992:LEU:O | 3:I:997:TRP:NE1 | 2.39 | 0.53 |
| 3:I:1075:VAL:HG12 | 4:J:461:PHE:O | 2.09 | 0.53 |
| 4:J:275:ARG:HD3 | 4:J:298:MET:HG2 | 1.91 | 0.53 |
| 4:J:972:LYS:HZ2 | 4:J:1004:ALA:HA | 1.74 | 0.53 |
| 3:I:76:GLY:HA3 | 3:I:95:PRO:HD2 | 1.90 | 0.53 |
| 3:I:230:PHE:HZ | 3:I:295:LYS:HE3 | 1.74 | 0.53 |
| 3:I:1043:ALA:HB1 | 3:I:1044:PRO:HD2 | 1.91 | 0.53 |
| 3:I:1082:ILE:H | 3:I:1082:ILE:HD12 | 1.73 | 0.53 |
| 3:I:1213:TYR:CD1 | 3:I:1220:GLN:HB2 | 2.43 | 0.53 |
| 4:J:719:PHE:HA | 4:J:724:MET:HE2 | 1.90 | 0.53 |
| 6:L:113:ARG:CD | 6:L:426:LYS:HE2 | 2.38 | 0.53 |
| 2:M:321:TRP:CD2 | 2:M:322:PRO:HA | 2.43 | 0.53 |
| 3:I:145:ILE:HA | 3:I:511:LEU:O | 2.09 | 0.53 |
| 3:I:963:GLU:O | 3:I:967:LEU:HG | 2.08 | 0.53 |
| 4:J:282:LEU:HD12 | 4:J:295:GLU:HG2 | 1.91 | 0.53 |
| 4:J:286:ALA:HB1 | 6:L:373:ARG:NH1 | 2.24 | 0.53 |
| 4:J:866:GLU:N | 4:J:866:GLU:OE1 | 2.42 | 0.53 |
| 4:J:960:LEU:HB2 | 4:J:963:VAL:HG21 | 1.89 | 0.53 |
| 6:L:216:LEU:HA | 6:L:219:GLU:HG2 | 1.91 | 0.53 |
| 6:L:476:ARG:HG3 | 6:L:477:GLU:H | 1.73 | 0.53 |
| 2:G:42:ALA:O | 2:G:46:ILE:HG12 | 2.09 | 0.53 |
| 3:I:965:GLN:HA | 3:I:968:GLU:CD | 2.29 | 0.53 |
| 3:I:1212:LEU:HD22 | 3:I:1225:VAL:CG2 | 2.34 | 0.53 |
| 3:I:1238:LEU:H | 3:I:1238:LEU:HD22 | 1.74 | 0.53 |
| 4:J:111:THR:HG21 | 4:J:300:GLN:HA | 1.91 | 0.53 |
| 4:J:591:ILE:HG22 | 4:J:592:VAL:HG13 | 1.91 | 0.53 |
| 4:J:793:SER:O | 4:J:797:THR:HG22 | 2.09 | 0.53 |
| 6:L:98:VAL:N | 6:L:402:LEU:HD11 | 2.24 | 0.53 |
| 6:L:353:LEU:HD22 | 6:L:357:GLN:OE1 | 2.09 | 0.53 |
| 6:L:560:ARG:HG3 | 6:L:565:ILE:HG21 | 1.90 | 0.53 |
| 3:I:623:LEU:HD11 | 3:I:653:MET:HE3 | 1.90 | 0.52 |
| 4:J:384:LYS:HE3 | 4:J:415:VAL:HG12 | 1.90 | 0.52 |
| 4:J:551:ARG:HA | 4:J:568:SER:O | 2.09 | 0.52 |
| 4:J:902:ASP:HB3 | 4:J:905:ARG:O | 2.09 | 0.52 |
| 5:K:36:ASP:OD1 | 5:K:36:ASP:N | 2.42 | 0.52 |
| 6:L:126:GLY:O | 6:L:129:GLN:NE2 | 2.26 | 0.52 |
| 8:P:18:DT:H2' | 8:P:19:DT:H72 | 1.91 | 0.52 |
| 2:M:280:ASP:O | 2:M:284:ARG:NH1 | 2.42 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:G:183:ILE:HD13 | 2:G:205:MET:HB2 | 1.91 | 0.52 |
| 2:H:31:LEU:HD11 | 2:H:39:LEU:HD12 | 1.91 | 0.52 |
| 3:I:172:TYR:O | 3:I:432:LEU:HD11 | 2.09 | 0.52 |
| 3:I:225:PHE:CZ | 3:I:347:ILE:HB | 2.45 | 0.52 |
| 3:I:230:PHE:HA | 3:I:239:MET:HA | 1.90 | 0.52 |
| 3:I:420:LEU:HD23 | 3:I:420:LEU:O | 2.09 | 0.52 |
| 3:I:602:GLU:O | 3:I:602:GLU:HG3 | 2.08 | 0.52 |
| 3:I:964:LEU:HD22 | 3:I:1025:PHE:CB | 2.40 | 0.52 |
| 4:J:614:LEU:HD23 | 5:K:5:THR:HG21 | 1.91 | 0.52 |
| 4:J:833:GLU:OE2 | 4:J:1242:ARG:HD3 | 2.10 | 0.52 |
| 4:J:848:VAL:HB | 4:J:858:VAL:CG2 | 2.39 | 0.52 |
| 6:L:233:ASP:N | 6:L:233:ASP:OD1 | 2.41 | 0.52 |
| 6:L:561:MET:HA | 6:L:567:MET:CE | 2.38 | 0.52 |
| 3:I:19:PRO:HA | 3:I:1156:ARG:HD2 | 1.90 | 0.52 |
| 3:I:101:ARG:HA | 3:I:118:LYS:O | 2.09 | 0.52 |
| 3:I:738:GLU:HA | 3:I:741:MET:CE | 2.40 | 0.52 |
| 4:J:287:ALA:HB1 | 4:J:288:PRO:HD2 | 1.91 | 0.52 |
| 4:J:516:ASP:HB3 | 4:J:573:THR:HG21 | 1.90 | 0.52 |
| 4:J:706:VAL:HG12 | 4:J:715:LYS:HG3 | 1.90 | 0.52 |
| 4:J:1047:THR:HB | 4:J:1062:LEU:CD2 | 2.39 | 0.52 |
| 4:J:1173:ARG:HB2 | 4:J:1192:LYS:HD2 | 1.92 | 0.52 |
| 2:H:15:ASP:O | 2:H:26:VAL:HG13 | 2.08 | 0.52 |
| 3:I:165:HIS:ND1 | 3:I:167:SER:HB3 | 2.25 | 0.52 |
| 3:I:177:ILE:HG12 | 3:I:183:TRP:CE3 | 2.44 | 0.52 |
| 4:J:844:THR:OG1 | 4:J:862:THR:OG1 | 2.28 | 0.52 |
| 4:J:1144:LEU:HD11 | 4:J:1236:GLU:CG | 2.37 | 0.52 |
| 4:J:1178:THR:HG22 | 4:J:1184:ASP:HB2 | 1.91 | 0.52 |
| 1:N:37:CYS:HB2 | 1:N:58:CYS:HB3 | 1.91 | 0.52 |
| 2:G:85:LEU:CD2 | 2:G:130:ILE:HD13 | 2.40 | 0.52 |
| 4:J:512:TYR:CE2 | 4:J:635:SER:HB2 | 2.44 | 0.52 |
| 4:J:675:ALA:O | 4:J:678:ARG:HG3 | 2.08 | 0.52 |
| 4:J:850:LYS:O | 4:J:853:THR:N | 2.33 | 0.52 |
| 4:J:885:VAL:HG23 | 4:J:894:VAL:CG2 | 2.38 | 0.52 |
| 4:J:1027:VAL:HG21 | 4:J:1122:ALA:HB3 | 1.92 | 0.52 |
| 4:J:1041:ILE:HD12 | 4:J:1045:THR:OG1 | 2.09 | 0.52 |
| 4:J:1162:ILE:O | 4:J:1178:THR:N | 2.34 | 0.52 |
| 4:J:1281:GLU:OE1 | 4:J:1283:SER:HB2 | 2.09 | 0.52 |
| 5:K:62:GLN:O | 5:K:66:VAL:HG23 | 2.10 | 0.52 |
| 6:L:123:ILE:O | 6:L:127:ILE:HD12 | 2.09 | 0.52 |
| 6:L:151:VAL:HG13 | 6:L:156:ALA:O | 2.10 | 0.52 |
| 7:O:39:DG:H2'' | 7:O:40:DC:H5' | 1.89 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:17:GLU:HB2 | 2:H:25:LYS:O | 2.10 | 0.52 |
| 3:I:211:ARG:HH12 | 3:I:216:THR:HA | 1.75 | 0.52 |
| 3:I:637:ARG:HA | 3:I:642:SER:HA | 1.90 | 0.52 |
| 3:I:1212:LEU:HD11 | 3:I:1227:VAL:HG21 | 1.91 | 0.52 |
| 4:J:473:THR:HG22 | 4:J:476:ALA:H | 1.74 | 0.52 |
| 4:J:1232:TYR:CD2 | 4:J:1233:ILE:HD12 | 2.45 | 0.52 |
| 6:L:354:THR:O | 6:L:358:VAL:HG23 | 2.10 | 0.52 |
| 6:L:508:GLU:HA | 6:L:518:HIS:HB3 | 1.91 | 0.52 |
| 3:I:155:VAL:HG23 | 3:I:176:ILE:CG1 | 2.34 | 0.52 |
| 4:J:116:PHE:O | 4:J:124:ILE:HG13 | 2.10 | 0.52 |
| 4:J:975:ILE:HD13 | 4:J:980:THR:CG2 | 2.35 | 0.52 |
| 4:J:1155:ILE:HD12 | 4:J:1155:ILE:O | 2.09 | 0.52 |
| 4:J:1284:ARG:HH12 | 4:J:1288:ALA:HB2 | 1.75 | 0.52 |
| 4:J:1363:TYR:O | 4:J:1367:GLN:HG2 | 2.08 | 0.52 |
| 2:G:45:ARG:NH2 | 3:I:1215:GLY:O | 2.43 | 0.52 |
| 3:I:569:ILE:CD1 | 4:J:783:LEU:HD23 | 2.40 | 0.52 |
| 3:I:893:THR:O | 3:I:894:GLN:HB2 | 2.10 | 0.52 |
| 3:I:1254:VAL:HG13 | 3:I:1255:THR:HG23 | 1.92 | 0.52 |
| 3:I:1297:ASP:OD2 | 3:I:1319:MET:N | 2.43 | 0.52 |
| 4:J:516:ASP:N | 4:J:516:ASP:OD1 | 2.43 | 0.52 |
| 4:J:799:ARG:HA | 4:J:802:ASP:OD1 | 2.08 | 0.52 |
| 4:J:810:THR:O | 4:J:810:THR:OG1 | 2.27 | 0.52 |
| 4:J:1090:ILE:HG22 | 4:J:1091:PRO:HD2 | 1.91 | 0.52 |
| 6:L:343:LYS:O | 6:L:347:ILE:HG13 | 2.10 | 0.52 |
| 8:P:18:DT:C6 | 8:P:19:DT:H72 | 2.45 | 0.52 |
| 2:G:12:ARG:HG2 | 2:H:230:ALA:CB | 2.40 | 0.52 |
| 2:G:16:ILE:HG22 | 2:G:26:VAL:HG13 | 1.91 | 0.52 |
| 2:G:229:GLU:HA | 2:G:232:VAL:HG12 | 1.92 | 0.52 |
| 3:I:840:SER:OG | 3:I:848:GLU:O | 2.26 | 0.52 |
| 4:J:131:PRO:O | 4:J:135:ILE:HD12 | 2.09 | 0.52 |
| 4:J:1063:ASP:O | 4:J:1067:ARG:HB3 | 2.10 | 0.52 |
| 6:L:130:VAL:HG13 | 6:L:365:MET:CG | 2.40 | 0.52 |
| 6:L:585:GLU:O | 6:L:589:GLN:HB2 | 2.09 | 0.52 |
| 1:N:73:ALA:HB3 | 3:I:169:LYS:HG3 | 1.91 | 0.52 |
| 3:I:43:PRO:HB2 | 3:I:44:GLU:OE2 | 2.10 | 0.52 |
| 3:I:58:PRO:HB2 | 3:I:67:GLU:OE2 | 2.09 | 0.52 |
| 3:I:593:LYS:HD3 | 3:I:604:HIS:CE1 | 2.45 | 0.52 |
| 3:I:820:GLU:O | 3:I:824:GLN:HG3 | 2.10 | 0.52 |
| 3:I:961:SER:O | 3:I:965:GLN:HG2 | 2.10 | 0.52 |
| 4:J:511:TYR:HA | 4:J:595:ALA:O | 2.10 | 0.52 |
| 4:J:859:PRO:HG2 | 4:J:862:THR:CG2 | 2.40 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:L:313:ASP:CG | 6:L:316:PHE:HB3 | 2.30 | 0.52 |
| 2:H:44:ARG:HH11 | 2:H:185:TYR:HE1 | 1.57 | 0.51 |
| 3:I:172:TYR:CD2 | 3:I:436:ARG:HD3 | 2.45 | 0.51 |
| 3:I:241:LEU:HD22 | 3:I:285:ILE:CG2 | 2.40 | 0.51 |
| 3:I:519:ASN:OD1 | 3:I:796:LEU:HD22 | 2.10 | 0.51 |
| 3:I:980:VAL:HA | 3:I:984:VAL:HB | 1.92 | 0.51 |
| 3:I:1088:ASP:OD1 | 3:I:1088:ASP:N | 2.39 | 0.51 |
| 3:I:1257:GLN:NE2 | 3:I:1296:ASP:OD2 | 2.35 | 0.51 |
| 4:J:1059:LEU:HD11 | 4:J:1110:GLU:CG | 2.39 | 0.51 |
| 6:L:551:LEU:HB2 | 6:L:556:ALA:HB2 | 1.91 | 0.51 |
| 6:L:554:ARG:NH2 | 6:L:582:VAL:HG11 | 2.25 | 0.51 |
| 6:L:605:GLU:OE1 | 6:L:606:VAL:HG13 | 2.09 | 0.51 |
| 2:H:60:GLU:OE2 | 2:H:65:LEU:HD21 | 2.11 | 0.51 |
| 3:I:228:VAL:O | 3:I:334:GLU:HA | 2.10 | 0.51 |
| 3:I:757:THR:HG22 | 3:I:765:ILE:HG12 | 1.91 | 0.51 |
| 3:I:836:LEU:CD1 | 3:I:1054:LEU:HD13 | 2.40 | 0.51 |
| 3:I:898:GLU:OE2 | 6:L:541:ARG:HG2 | 2.11 | 0.51 |
| 4:J:836:ARG:HA | 4:J:869:CYS:SG | 2.49 | 0.51 |
| 6:L:470:MET:CG | 6:L:486:ARG:HD2 | 2.39 | 0.51 |
| 1:N:16:THR:O | 1:N:20:ILE:HG13 | 2.09 | 0.51 |
| 3:I:202:ARG:HD2 | 8:P:18:DT:OP1 | 2.10 | 0.51 |
| 3:I:596:ASP:OD1 | 3:I:596:ASP:N | 2.42 | 0.51 |
| 3:I:966:ILE:HG12 | 10:I:1401:1N7:C16 | 2.41 | 0.51 |
| 3:I:979:LEU:CD2 | 3:I:1000:LEU:HD12 | 2.40 | 0.51 |
| 3:I:1075:VAL:HG21 | 4:J:354:VAL:HG11 | 1.92 | 0.51 |
| 3:I:1211:ARG:HG3 | 3:I:1211:ARG:O | 2.11 | 0.51 |
| 4:J:114:ILE:HG21 | 4:J:308:ASP:OD1 | 2.09 | 0.51 |
| 4:J:268:LEU:O | 4:J:272:VAL:HG23 | 2.10 | 0.51 |
| 4:J:1184:ASP:OD1 | 4:J:1184:ASP:N | 2.32 | 0.51 |
| 4:J:1266:ILE:CD1 | 4:J:1285:VAL:HG21 | 2.41 | 0.51 |
| 6:L:143:TYR:HD2 | 6:L:269:LEU:HD21 | 1.74 | 0.51 |
| 6:L:148:TYR:HE1 | 6:L:158:LEU:HD23 | 1.75 | 0.51 |
| 6:L:335:GLU:O | 6:L:339:ARG:HG3 | 2.10 | 0.51 |
| 2:G:180:VAL:HG12 | 2:G:207:THR:CG2 | 2.40 | 0.51 |
| 2:H:107:ILE:HG13 | 2:H:108:GLY:N | 2.26 | 0.51 |
| 3:I:175:ARG:HG3 | 3:I:184:LEU:O | 2.10 | 0.51 |
| 3:I:188:PHE:HA | 3:I:194:LEU:HA | 1.93 | 0.51 |
| 3:I:421:SER:OG | 3:I:422:LYS:N | 2.43 | 0.51 |
| 3:I:817:LEU:HD13 | 3:I:1085:MET:HE3 | 1.91 | 0.51 |
| 3:I:1102:GLY:O | 3:I:1106:ARG:HD3 | 2.11 | 0.51 |
| 3:I:1291:LEU:CD2 | 4:J:1351:VAL:HG13 | 2.40 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:1155:ILE:CD1 | 4:J:1211:SER:H | 2.23 | 0.51 |
| 6:L:271:ASN:O | 6:L:275:VAL:HG12 | 2.10 | 0.51 |
| 2:G:53:GLY:O | 2:G:148:ARG:HA | 2.11 | 0.51 |
| 3:I:115:LYS:HG3 | 3:I:116:ASP:H | 1.76 | 0.51 |
| 3:I:239:MET:HG2 | 3:I:240:GLU:O | 2.10 | 0.51 |
| 3:I:1254:VAL:O | 4:J:99:ARG:NH2 | 2.34 | 0.51 |
| 4:J:164:GLN:O | 4:J:167:ASP:HB3 | 2.10 | 0.51 |
| 4:J:512:TYR:CD2 | 4:J:635:SER:HB2 | 2.46 | 0.51 |
| 4:J:706:VAL:CG1 | 4:J:715:LYS:HG3 | 2.41 | 0.51 |
| 4:J:1040:MET:SD | 4:J:1078:LEU:HD23 | 2.51 | 0.51 |
| 6:L:311:THR:HA | 6:L:344:LEU:HD21 | 1.92 | 0.51 |
| 6:L:360:ASP:O | 6:L:364:ARG:HG2 | 2.11 | 0.51 |
| 6:L:392:LYS:O | 6:L:395:THR:HG23 | 2.11 | 0.51 |
| 2:G:12:ARG:HB3 | 2:G:12:ARG:NH1 | 2.25 | 0.51 |
| 2:G:210:THR:OG1 | 2:G:211:ILE:N | 2.43 | 0.51 |
| 2:G:222:THR:HB | 2:H:232:VAL:HG13 | 1.92 | 0.51 |
| 3:I:115:LYS:NZ | 3:I:484:LEU:HB3 | 2.26 | 0.51 |
| 3:I:385:PHE:CE1 | 3:I:386:GLU:HG2 | 2.46 | 0.51 |
| 3:I:1018:TYR:CZ | 3:I:1022:LYS:HE3 | 2.45 | 0.51 |
| 3:I:1120:ALA:HB2 | 3:I:1199:LEU:CD1 | 2.41 | 0.51 |
| 4:J:62:PHE:CD1 | 4:J:247:PRO:HD3 | 2.46 | 0.51 |
| 4:J:807:LEU:HD23 | 4:J:808:VAL:N | 2.25 | 0.51 |
| 4:J:1056:LEU:HD23 | 4:J:1057:SER:O | 2.09 | 0.51 |
| 5:K:39:VAL:HG23 | 5:K:40:PRO:HD2 | 1.92 | 0.51 |
| 6:L:348:GLU:OE2 | 6:L:354:THR:HA | 2.10 | 0.51 |
| 2:G:8:PHE:O | 2:G:9:LEU:HD23 | 2.11 | 0.51 |
| 3:I:519:ASN:O | 3:I:523:GLU:HG3 | 2.11 | 0.51 |
| 3:I:565:GLU:HA | 3:I:569:ILE:CG1 | 2.41 | 0.51 |
| 3:I:1308:ILE:HD11 | 4:J:472:LEU:HB3 | 1.92 | 0.51 |
| 3:I:1308:ILE:HG21 | 4:J:379:PRO:HB2 | 1.92 | 0.51 |
| 4:J:158:GLN:O | 4:J:160:LEU:HG | 2.10 | 0.51 |
| 4:J:681:LYS:HE3 | 4:J:685:ILE:CG2 | 2.41 | 0.51 |
| 4:J:1090:ILE:HB | 4:J:1093:THR:OG1 | 2.11 | 0.51 |
| 2:H:52:PRO:HG3 | 2:H:150:ARG:HD3 | 1.91 | 0.51 |
| 3:I:53:PHE:CD1 | 3:I:468:LEU:HD11 | 2.46 | 0.51 |
| 3:I:324:LYS:HA | 3:I:327:GLN:CG | 2.41 | 0.51 |
| 3:I:854:ILE:HD11 | 3:I:885:GLY:CA | 2.40 | 0.51 |
| 3:I:1101:LEU:CD1 | 4:J:504:GLN:HB2 | 2.40 | 0.51 |
| 4:J:147:ILE:HD13 | 4:J:187:ALA:HB1 | 1.93 | 0.51 |
| 4:J:615:LYS:HB3 | 4:J:616:PRO:HD3 | 1.92 | 0.51 |
| 4:J:794:GLY:HA2 | 4:J:797:THR:CG2 | 2.40 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:934:THR:HA | 4:J:1137:GLY:HA3 | 1.93 | 0.51 |
| 7:O:40:DC:H1' | 7:O:41:DT:C5' | 2.41 | 0.51 |
| 8:P:57:DT:H1' | 8:P:58:DC:H5'' | 1.93 | 0.51 |
| 2:G:8:PHE:HE2 | 2:H:223:ILE:HD13 | 1.75 | 0.51 |
| 2:H:136:GLU:HG2 | 2:H:137:ASN:H | 1.76 | 0.51 |
| 3:I:84:GLU:OE1 | 3:I:88:ARG:HG3 | 2.10 | 0.51 |
| 3:I:301:TYR:HB3 | 3:I:330:HIS:CD2 | 2.46 | 0.51 |
| 4:J:490:ILE:O | 4:J:491:LEU:HD23 | 2.10 | 0.51 |
| 4:J:826:ILE:HG13 | 4:J:831:VAL:HG13 | 1.93 | 0.51 |
| 6:L:388:ILE:HA | 6:L:405:ILE:HD12 | 1.92 | 0.51 |
| 3:I:178:PRO:HB3 | 3:I:397:LEU:HD12 | 1.93 | 0.51 |
| 3:I:276:GLN:HA | 3:I:279:LYS:HE3 | 1.92 | 0.51 |
| 3:I:389:PHE:O | 3:I:419:ILE:HD11 | 2.11 | 0.51 |
| 3:I:667:LEU:CD2 | 3:I:704:MET:HB3 | 2.41 | 0.51 |
| 3:I:1321:GLU:O | 3:I:1325:VAL:HG23 | 2.11 | 0.51 |
| 4:J:267:ASP:OD2 | 4:J:324:LEU:HD21 | 2.11 | 0.51 |
| 4:J:482:ALA:O | 4:J:483:LEU:HD23 | 2.11 | 0.51 |
| 6:L:115:GLY:HA2 | 6:L:118:ASP:OD2 | 2.11 | 0.51 |
| 6:L:216:LEU:O | 6:L:219:GLU:HG2 | 2.11 | 0.51 |
| 7:O:66:DG:H2'' | 7:O:67:DA:H5' | 1.92 | 0.51 |
| 2:H:112:ALA:O | 2:H:115:ILE:HG13 | 2.10 | 0.50 |
| 3:I:242:VAL:HG11 | 3:I:245:ARG:NE | 2.26 | 0.50 |
| 3:I:257:ALA:HB2 | 3:I:285:ILE:CG2 | 2.41 | 0.50 |
| 3:I:559:CYS:CB | 3:I:662:SER:HB3 | 2.41 | 0.50 |
| 4:J:128:LEU:HD11 | 4:J:189:LEU:CD2 | 2.41 | 0.50 |
| 4:J:279:LEU:HD23 | 4:J:283:LEU:HG | 1.91 | 0.50 |
| 4:J:1174:ARG:HG2 | 4:J:1189:MET:HE1 | 1.94 | 0.50 |
| 4:J:1257:VAL:HG13 | 4:J:1261:LEU:HD21 | 1.93 | 0.50 |
| 6:L:256:PHE:HA | 6:L:259:PHE:CD2 | 2.46 | 0.50 |
| 2:H:89:ALA:O | 2:H:124:VAL:HG23 | 2.10 | 0.50 |
| 3:I:31:GLN:HG3 | 3:I:527:LYS:HB3 | 1.93 | 0.50 |
| 3:I:195:PHE:CA | 3:I:206:ALA:HB2 | 2.41 | 0.50 |
| 3:I:483:ASP:HB2 | 3:I:486:THR:OG1 | 2.12 | 0.50 |
| 3:I:598:VAL:HA | 3:I:627:GLY:O | 2.10 | 0.50 |
| 3:I:1337:ILE:HB | 4:J:22:ILE:HG13 | 1.93 | 0.50 |
| 4:J:370:LYS:HA | 4:J:441:LEU:HD12 | 1.93 | 0.50 |
| 4:J:1040:MET:HE3 | 4:J:1046:ILE:HG21 | 1.93 | 0.50 |
| 6:L:573:LEU:HG | 6:L:584:ARG:CB | 2.41 | 0.50 |
| 2:M:266:SER:OG | 2:M:303:ILE:HD11 | 2.11 | 0.50 |
| 3:I:98:VAL:HG21 | 3:I:124:MET:CE | 2.41 | 0.50 |
| 3:I:448:LEU:HD12 | 3:I:554:HIS:ND1 | 2.27 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:1002:LEU:HD12 | 3:I:1003:THR:N | 2.22 | 0.50 |
| 3:I:1122:LYS:HA | 3:I:1179:GLY:HA2 | 1.92 | 0.50 |
| 3:I:1153:ALA:O | 3:I:1155:VAL:HG13 | 2.11 | 0.50 |
| 3:I:1291:LEU:HD21 | 4:J:1351:VAL:HG13 | 1.93 | 0.50 |
| 4:J:201:LEU:CD2 | 4:J:217:LEU:HD21 | 2.34 | 0.50 |
| 4:J:449:LEU:HD13 | 4:J:466:MET:SD | 2.52 | 0.50 |
| 4:J:709:ARG:HH11 | 4:J:710:ASP:H | 1.57 | 0.50 |
| 4:J:1307:LEU:CD2 | 4:J:1312:ALA:HA | 2.40 | 0.50 |
| 7:O:55:DC:H5' | 7:O:55:DC:C6 | 2.43 | 0.50 |
| 3:I:230:PHE:CZ | 3:I:295:LYS:HE3 | 2.45 | 0.50 |
| 3:I:264:GLU:OE2 | 3:I:265:LYS:HB3 | 2.11 | 0.50 |
| 3:I:272:ARG:O | 3:I:276:GLN:HG3 | 2.11 | 0.50 |
| 3:I:509:SER:OG | 3:I:510:GLN:N | 2.45 | 0.50 |
| 3:I:741:MET:HG2 | 3:I:746:ALA:CB | 2.40 | 0.50 |
| 3:I:832:HIS:ND1 | 3:I:1058:ARG:HD2 | 2.26 | 0.50 |
| 3:I:1096:ILE:HD12 | 3:I:1232:MET:SD | 2.51 | 0.50 |
| 4:J:516:ASP:HA | 4:J:545:HIS:HB2 | 1.93 | 0.50 |
| 4:J:583:VAL:HG13 | 4:J:587:LEU:HD22 | 1.92 | 0.50 |
| 3:I:962:GLU:O | 3:I:966:ILE:HG13 | 2.10 | 0.50 |
| 4:J:1061:VAL:HB | 4:J:1103:GLY:HA2 | 1.94 | 0.50 |
| 6:L:575:GLU:O | 6:L:578:LYS:HG2 | 2.11 | 0.50 |
| 2:H:30:PRO:HG2 | 2:H:192:VAL:HG21 | 1.93 | 0.50 |
| 3:I:207:THR:HG21 | 3:I:351:LEU:CD2 | 2.41 | 0.50 |
| 3:I:402:ARG:NE | 3:I:406:ASN:OD1 | 2.45 | 0.50 |
| 4:J:707:ILE:HD11 | 4:J:714:GLU:HB3 | 1.93 | 0.50 |
| 4:J:986:ASP:OD1 | 4:J:986:ASP:N | 2.42 | 0.50 |
| 4:J:1040:MET:CE | 4:J:1046:ILE:HD13 | 2.41 | 0.50 |
| 4:J:1063:ASP:O | 4:J:1067:ARG:N | 2.43 | 0.50 |
| 4:J:1079:LYS:HD3 | 4:J:1087:ASP:OD1 | 2.12 | 0.50 |
| 4:J:1178:THR:CG2 | 4:J:1184:ASP:HB2 | 2.42 | 0.50 |
| 6:L:346:GLN:O | 6:L:350:GLU:HG3 | 2.11 | 0.50 |
| 7:O:51:DT:H2' | 7:O:52:DA:C8 | 2.47 | 0.50 |
| 2:H:22:THR:O | 2:H:213:PRO:HG3 | 2.11 | 0.50 |
| 2:H:105:SER:HB2 | 2:H:139:SER:HB2 | 1.93 | 0.50 |
| 4:J:438:GLU:HG3 | 4:J:485:MET:HE3 | 1.94 | 0.50 |
| 4:J:475:GLU:O | 4:J:479:GLU:HG3 | 2.12 | 0.50 |
| 4:J:848:VAL:CG2 | 4:J:880:VAL:HG13 | 2.42 | 0.50 |
| 4:J:910:ASN:HB3 | 5:K:15:ASN:OD1 | 2.11 | 0.50 |
| 4:J:984:LEU:HB2 | 4:J:993:GLU:HB2 | 1.93 | 0.50 |
| 4:J:1024:THR:CG2 | 4:J:1123:ARG:HA | 2.38 | 0.50 |
| 5:K:53:GLU:HB3 | 5:K:59:ILE:CG1 | 2.42 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 7:O:28:DG:H2'' | 7:O:29:DA:C5' | 2.41 | 0.50 |
| 2:H:16:ILE:CG1 | 2:H:26:VAL:HG22 | 2.42 | 0.50 |
| 2:H:64:VAL:HG13 | 2:H:69:SER:HB2 | 1.94 | 0.50 |
| 3:I:310:ILE:O | 3:I:324:LYS:NZ | 2.41 | 0.50 |
| 3:I:461:GLU:OE2 | 3:I:465:ARG:NH2 | 2.43 | 0.50 |
| 4:J:260:PHE:HB2 | 6:L:504:PRO:HB3 | 1.93 | 0.50 |
| 4:J:491:LEU:HD11 | 4:J:609:TYR:CE2 | 2.47 | 0.50 |
| 4:J:808:VAL:HG22 | 4:J:914:ALA:HA | 1.93 | 0.50 |
| 4:J:839:VAL:CG2 | 4:J:882:VAL:HG11 | 2.41 | 0.50 |
| 4:J:1173:ARG:HH22 | 4:J:1196:LEU:HG | 1.77 | 0.50 |
| 6:L:136:GLU:HB3 | 6:L:361:ILE:HD13 | 1.93 | 0.50 |
| 6:L:262:VAL:HG13 | 6:L:263:PRO:HD2 | 1.93 | 0.50 |
| 6:L:290:LEU:C | 6:L:294:GLN:HB3 | 2.32 | 0.50 |
| 7:O:69:DT:H2' | 7:O:70:DT:H71 | 1.92 | 0.50 |
| 1:N:64:TYR:CD1 | 3:I:341:LEU:HD22 | 2.47 | 0.50 |
| 2:H:59:VAL:O | 2:H:171:LEU:HB2 | 2.11 | 0.50 |
| 3:I:74:ARG:NH1 | 3:I:97:ARG:HG3 | 2.27 | 0.50 |
| 3:I:905:ILE:CD1 | 6:L:595:LEU:HB2 | 2.42 | 0.50 |
| 3:I:953:LEU:HD21 | 3:I:1033:ARG:CG | 2.34 | 0.50 |
| 4:J:112:ALA:HA | 4:J:238:ILE:HD13 | 1.93 | 0.50 |
| 4:J:1047:THR:HG22 | 4:J:1060:VAL:HB | 1.92 | 0.50 |
| 6:L:227:GLN:NE2 | 6:L:231:THR:OG1 | 2.45 | 0.50 |
| 6:L:548:LEU:HD13 | 6:L:560:ARG:HD2 | 1.94 | 0.50 |
| 3:I:104:ILE:HD11 | 3:I:116:ASP:CB | 2.41 | 0.49 |
| 3:I:499:SER:O | 3:I:503:LYS:HG3 | 2.12 | 0.49 |
| 3:I:808:ASN:H | 4:J:633:ALA:HB2 | 1.77 | 0.49 |
| 3:I:1282:GLY:HA3 | 5:K:17:PHE:CE1 | 2.47 | 0.49 |
| 4:J:264:ASP:OD1 | 4:J:264:ASP:N | 2.44 | 0.49 |
| 4:J:957:SER:N | 4:J:985:ILE:O | 2.30 | 0.49 |
| 4:J:1059:LEU:O | 4:J:1106:ILE:HA | 2.12 | 0.49 |
| 5:K:4:VAL:HG23 | 5:K:5:THR:OG1 | 2.11 | 0.49 |
| 6:L:311:THR:HA | 6:L:344:LEU:CD2 | 2.42 | 0.49 |
| 6:L:584:ARG:O | 6:L:587:ILE:HG13 | 2.12 | 0.49 |
| 8:P:52:DT:H2'' | 8:P:53:DT:C7 | 2.42 | 0.49 |
| 2:G:12:ARG:HB3 | 2:G:12:ARG:CZ | 2.41 | 0.49 |
| 3:I:109:ALA:HB1 | 3:I:112:GLY:CA | 2.35 | 0.49 |
| 4:J:483:LEU:CD2 | 5:K:16:ARG:HD3 | 2.42 | 0.49 |
| 4:J:1327:GLU:HB2 | 8:P:21:DA:H4' | 1.93 | 0.49 |
| 1:N:19:GLY:C | 4:J:754:ILE:HD11 | 2.32 | 0.49 |
| 3:I:241:LEU:HD23 | 3:I:282:VAL:O | 2.12 | 0.49 |
| 4:J:653:ILE:HG21 | 4:J:693:VAL:CG2 | 2.42 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:J:824:PRO:HG2 | 4:J:826:ILE:HD11 | 1.93 | 0.49 |
| 4:J:833:GLU:CD | 4:J:1242:ARG:HD3 | 2.33 | 0.49 |
| 5:K:79:GLU:HG2 | 5:K:79:GLU:O | 2.12 | 0.49 |
| 6:L:291:CYS:HA | 6:L:295:CYS:H | 1.76 | 0.49 |
| 6:L:425:TYR:HH | 7:O:50:DA:C3' | 2.22 | 0.49 |
| 7:O:35:DG:N2 | 8:P:52:DT:O2 | 2.45 | 0.49 |
| 3:I:360:LEU:O | 3:I:364:VAL:HG23 | 2.12 | 0.49 |
| 3:I:905:ILE:HD11 | 6:L:595:LEU:HB2 | 1.94 | 0.49 |
| 3:I:936:ARG:HB3 | 3:I:939:VAL:CG2 | 2.43 | 0.49 |
| 3:I:1112:ILE:CD1 | 4:J:639:VAL:HG13 | 2.41 | 0.49 |
| 4:J:111:THR:CG2 | 4:J:300:GLN:HA | 2.42 | 0.49 |
| 4:J:204:GLU:O | 4:J:208:THR:OG1 | 2.20 | 0.49 |
| 5:K:3:ARG:NE | 5:K:5:THR:O | 2.39 | 0.49 |
| 5:K:30:MET:SD | 5:K:37:PRO:HB3 | 2.52 | 0.49 |
| 3:I:829:THR:O | 3:I:829:THR:OG1 | 2.29 | 0.49 |
| 3:I:1271:GLY:O | 3:I:1275:VAL:HG23 | 2.13 | 0.49 |
| 3:I:1307:ASN:HB3 | 3:I:1312:ASN:O | 2.12 | 0.49 |
| 4:J:128:LEU:HD23 | 4:J:192:MET:HE3 | 1.94 | 0.49 |
| 4:J:287:ALA:HB2 | 6:L:413:MET:HE1 | 1.94 | 0.49 |
| 4:J:421:VAL:HG13 | 4:J:439:PRO:HG3 | 1.92 | 0.49 |
| 4:J:515:ARG:O | 4:J:545:HIS:HB3 | 2.13 | 0.49 |
| 4:J:712:GLN:HG2 | 4:J:713:GLU:N | 2.28 | 0.49 |
| 6:L:162:ILE:N | 6:L:262:VAL:HG23 | 2.27 | 0.49 |
| 6:L:284:GLU:HG3 | 6:L:306:PHE:CE1 | 2.48 | 0.49 |
| 6:L:305:LEU:O | 6:L:315:TRP:HB2 | 2.12 | 0.49 |
| 2:G:11:PRO:HG3 | 2:G:31:LEU:HD21 | 1.94 | 0.49 |
| 3:I:147:SER:HB2 | 3:I:530:ILE:HD13 | 1.94 | 0.49 |
| 3:I:732:ILE:HD11 | 3:I:769:PRO:HB3 | 1.93 | 0.49 |
| 3:I:814:ASP:O | 3:I:1074:GLY:HA2 | 2.12 | 0.49 |
| 3:I:885:GLY:HA2 | 3:I:917:SER:CB | 2.41 | 0.49 |
| 4:J:1172:LYS:HG2 | 4:J:1191:PRO:HG3 | 1.94 | 0.49 |
| 5:K:59:ILE:HG23 | 5:K:64:LEU:HD11 | 1.95 | 0.49 |
| 6:L:162:ILE:CA | 6:L:262:VAL:HG23 | 2.43 | 0.49 |
| 6:L:242:HIS:N | 6:L:245:ALA:HB2 | 2.27 | 0.49 |
| 6:L:479:THR:HG22 | 6:L:482:GLU:OE1 | 2.12 | 0.49 |
| 2:G:189:ALA:HB1 | 2:G:191:ARG:HH12 | 1.77 | 0.49 |
| 3:I:1075:VAL:CG1 | 4:J:461:PHE:HB3 | 2.43 | 0.49 |
| 4:J:255:LEU:HD21 | 6:L:523:ILE:CD1 | 2.43 | 0.49 |
| 4:J:982:LEU:O | 4:J:994:SER:HA | 2.12 | 0.49 |
| 5:K:10:VAL:HG21 | 5:K:16:ARG:HG3 | 1.93 | 0.49 |
| 6:L:489:MET:HB2 | 6:L:494:ILE:HD11 | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:262:LEU:HD21 | 2:M:303:ILE:HA | 1.95 | 0.49 |
| 2:G:85:LEU:HD23 | 2:G:130:ILE:HD13 | 1.94 | 0.49 |
| 3:I:196:VAL:HG21 | 3:I:209:ILE:HD11 | 1.95 | 0.49 |
| 3:I:491:ASP:OD1 | 3:I:491:ASP:N | 2.44 | 0.49 |
| 4:J:206:ASN:O | 4:J:209:ASN:ND2 | 2.45 | 0.49 |
| 5:K:16:ARG:O | 5:K:16:ARG:HG2 | 2.12 | 0.49 |
| 6:L:113:ARG:CZ | 6:L:426:LYS:HD3 | 2.43 | 0.49 |
| 6:L:480:PRO:HA | 6:L:483:LEU:HB2 | 1.94 | 0.49 |
| 2:G:102:LEU:HD21 | 2:G:114:ASP:HB2 | 1.95 | 0.49 |
| 3:I:367:TYR:CE2 | 3:I:371:ARG:HG3 | 2.48 | 0.49 |
| 3:I:581:THR:CG2 | 3:I:585:GLY:HA2 | 2.42 | 0.49 |
| 3:I:671:LEU:HD11 | 3:I:679:ALA:HB1 | 1.94 | 0.49 |
| 3:I:998:LEU:HD23 | 3:I:999:GLU:N | 2.28 | 0.49 |
| 3:I:1026:GLU:OE1 | 3:I:1029:LEU:HD21 | 2.13 | 0.49 |
| 2:M:257:VAL:HG13 | 2:M:276:HIS:O | 2.13 | 0.49 |
| 2:M:298:LYS:CA | 2:M:301:THR:HG22 | 2.42 | 0.49 |
| 2:H:61:ILE:HG12 | 2:H:142:MET:HB3 | 1.94 | 0.49 |
| 3:I:158:ASP:HB3 | 3:I:173:ASN:OD1 | 2.13 | 0.49 |
| 3:I:965:GLN:HA | 3:I:968:GLU:OE1 | 2.13 | 0.49 |
| 4:J:34:SER:OG | 4:J:35:PHE:N | 2.45 | 0.49 |
| 4:J:646:ILE:HD12 | 4:J:762:ASN:HD21 | 1.78 | 0.49 |
| 4:J:925:GLU:CG | 4:J:926:PRO:HD3 | 2.32 | 0.49 |
| 6:L:213:ASP:O | 6:L:216:LEU:HG | 2.12 | 0.49 |
| 6:L:276:MET:O | 6:L:280:VAL:HG23 | 2.13 | 0.49 |
| 3:I:471:VAL:HG21 | 3:I:493:ILE:HG13 | 1.95 | 0.48 |
| 3:I:894:GLN:HG2 | 4:J:77:ARG:NH2 | 2.25 | 0.48 |
| 4:J:75:TYR:HB3 | 4:J:80:HIS:HD2 | 1.78 | 0.48 |
| 4:J:646:ILE:HD12 | 4:J:762:ASN:ND2 | 2.28 | 0.48 |
| 4:J:709:ARG:C | 4:J:711:GLY:HA3 | 2.33 | 0.48 |
| 4:J:800:LEU:CD1 | 4:J:1309:ILE:HD12 | 2.43 | 0.48 |
| 4:J:965:SER:HB2 | 4:J:975:ILE:HA | 1.95 | 0.48 |
| 4:J:1177:ILE:HD12 | 4:J:1186:TYR:CD2 | 2.48 | 0.48 |
| 4:J:1215:GLU:CG | 4:J:1220:ILE:HD11 | 2.32 | 0.48 |
| 6:L:162:ILE:HG13 | 6:L:165:PHE:CZ | 2.48 | 0.48 |
| 6:L:391:ALA:CB | 6:L:405:ILE:HD13 | 2.43 | 0.48 |
| 2:G:190:ALA:HB2 | 2:G:200:LYS:CB | 2.43 | 0.48 |
| 4:J:129:ASP:HB2 | 4:J:220:ARG:NH2 | 2.28 | 0.48 |
| 4:J:171:GLU:HG2 | 4:J:172:PHE:CD1 | 2.47 | 0.48 |
| 4:J:253:VAL:HG21 | 6:L:523:ILE:HG21 | 1.95 | 0.48 |
| 4:J:416:ILE:HG13 | 4:J:441:LEU:HD21 | 1.94 | 0.48 |
| 4:J:438:GLU:HG3 | 4:J:485:MET:HE1 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:L:448:ARG:HH22 | 6:L:501:ALA:HA | 1.78 | 0.48 |
| 6:L:587:ILE:HD12 | 6:L:588:ARG:N | 2.28 | 0.48 |
| 7:O:23:DC:OP1 | 2:M:264:VAL:HG21 | 2.14 | 0.48 |
| 3:I:751:TYR:CE2 | 3:I:783:LEU:HD12 | 2.48 | 0.48 |
| 3:I:1043:ALA:O | 3:I:1046:VAL:HG12 | 2.14 | 0.48 |
| 3:I:1291:LEU:O | 4:J:345:LYS:HE3 | 2.12 | 0.48 |
| 4:J:218:THR:CA | 4:J:221:ILE:HG22 | 2.41 | 0.48 |
| 4:J:888:CYS:HB3 | 4:J:1258:ARG:NH1 | 2.28 | 0.48 |
| 4:J:1142:ALA:O | 4:J:1146:GLU:HG2 | 2.13 | 0.48 |
| 4:J:1330:ARG:HA | 4:J:1333:THR:HG22 | 1.95 | 0.48 |
| 6:L:491:GLU:H | 6:L:494:ILE:HD12 | 1.78 | 0.48 |
| 6:L:502:LYS:HD3 | 6:L:502:LYS:HA | 1.56 | 0.48 |
| 6:L:595:LEU:O | 6:L:599:ARG:HG2 | 2.13 | 0.48 |
| 1:N:26:LYS:O | 1:N:27:ILE:HD13 | 2.13 | 0.48 |
| 2:H:41:ASN:OD1 | 3:I:1217:THR:HG23 | 2.14 | 0.48 |
| 3:I:37:LYS:HE2 | 3:I:37:LYS:HA | 1.94 | 0.48 |
| 3:I:188:PHE:CE1 | 3:I:194:LEU:HB3 | 2.48 | 0.48 |
| 3:I:220:ILE:HG22 | 3:I:221:LEU:CD2 | 2.43 | 0.48 |
| 3:I:576:SER:OG | 3:I:577:VAL:N | 2.45 | 0.48 |
| 3:I:799:ASN:OD1 | 3:I:799:ASN:N | 2.43 | 0.48 |
| 3:I:901:LEU:CD1 | 6:L:565:ILE:HD11 | 2.44 | 0.48 |
| 4:J:56:LEU:HB3 | 4:J:250:ARG:HH12 | 1.79 | 0.48 |
| 4:J:975:ILE:HG21 | 4:J:980:THR:CG2 | 2.43 | 0.48 |
| 4:J:1246:VAL:HG12 | 4:J:1247:LYS:H | 1.78 | 0.48 |
| 5:K:66:VAL:O | 5:K:70:GLN:HG3 | 2.14 | 0.48 |
| 6:L:248:GLU:HA | 6:L:251:LYS:HE2 | 1.94 | 0.48 |
| 2:G:13:LEU:HA | 2:G:28:LEU:HA | 1.95 | 0.48 |
| 2:H:92:VAL:HA | 2:H:121:VAL:HA | 1.94 | 0.48 |
| 2:H:158:ARG:HE | 2:H:172:LEU:CD1 | 2.25 | 0.48 |
| 3:I:162:GLY:H | 3:I:170:VAL:HG12 | 1.78 | 0.48 |
| 3:I:221:LEU:CD1 | 3:I:314:ASN:HB3 | 2.43 | 0.48 |
| 3:I:395:TYR:CD2 | 3:I:419:ILE:HG13 | 2.49 | 0.48 |
| 3:I:594:VAL:HG22 | 3:I:599:VAL:HG22 | 1.94 | 0.48 |
| 3:I:685:MET:SD | 3:I:1073:LYS:HE2 | 2.54 | 0.48 |
| 3:I:971:LEU:CD2 | 3:I:1018:TYR:HB2 | 2.43 | 0.48 |
| 3:I:985:GLU:O | 3:I:989:LEU:HB2 | 2.13 | 0.48 |
| 3:I:1086:PRO:HD2 | 3:I:1094:VAL:HG22 | 1.96 | 0.48 |
| 4:J:56:LEU:CD2 | 4:J:269:TYR:HB3 | 2.43 | 0.48 |
| 4:J:59:ALA:HA | 4:J:63:GLY:O | 2.12 | 0.48 |
| 4:J:134:ASP:O | 4:J:138:VAL:HG12 | 2.13 | 0.48 |
| 4:J:145:VAL:HG22 | 4:J:159:ILE:HA | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:J:253:VAL:CG2 | 4:J:261:ALA:HB3 | 2.38 | 0.48 |
| 4:J:395:LYS:HD3 | 6:L:536:THR:HG21 | 1.96 | 0.48 |
| 6:L:162:ILE:HG13 | 6:L:165:PHE:CE2 | 2.49 | 0.48 |
| 3:I:301:TYR:OH | 3:I:333:ILE:HA | 2.13 | 0.48 |
| 3:I:896:THR:HG22 | 3:I:897:PRO:CD | 2.42 | 0.48 |
| 3:I:902:LEU:HD21 | 6:L:611:LEU:CG | 2.44 | 0.48 |
| 4:J:1035:VAL:HG21 | 4:J:1109:LEU:CD2 | 2.43 | 0.48 |
| 5:K:9:ALA:HB1 | 5:K:19:LEU:HD13 | 1.95 | 0.48 |
| 3:I:83:GLN:O | 3:I:87:ILE:HG13 | 2.12 | 0.48 |
| 3:I:255:ILE:CG2 | 3:I:262:TYR:HB2 | 2.31 | 0.48 |
| 3:I:402:ARG:HG3 | 3:I:406:ASN:HD21 | 1.79 | 0.48 |
| 3:I:861:ALA:C | 3:I:862:LEU:HD23 | 2.34 | 0.48 |
| 3:I:1288:GLN:NE2 | 3:I:1317:PRO:HG3 | 2.28 | 0.48 |
| 4:J:27:PRO:O | 4:J:31:ARG:HG3 | 2.13 | 0.48 |
| 4:J:121:PRO:HB2 | 4:J:126:LEU:HD21 | 1.96 | 0.48 |
| 4:J:226:ALA:O | 4:J:230:SER:OG | 2.29 | 0.48 |
| 4:J:259:ARG:HB3 | 6:L:505:ILE:CD1 | 2.43 | 0.48 |
| 4:J:841:GLY:HA3 | 4:J:901:ARG:HG2 | 1.96 | 0.48 |
| 4:J:1079:LYS:HA | 4:J:1098:GLN:HB2 | 1.96 | 0.48 |
| 4:J:1178:THR:HB | 4:J:1184:ASP:HB2 | 1.94 | 0.48 |
| 6:L:141:ILE:HG21 | 6:L:256:PHE:CE1 | 2.49 | 0.48 |
| 8:P:35:DA:H2" | 8:P:36:DT:C4 | 2.48 | 0.48 |
| 1:N:16:THR:HG22 | 4:J:748:ALA:HB3 | 1.96 | 0.48 |
| 2:G:49:SER:OG | 2:G:50:SER:N | 2.46 | 0.48 |
| 2:G:70:THR:CG2 | 3:I:729:ALA:HB3 | 2.44 | 0.48 |
| 2:H:14:VAL:HG13 | 2:H:28:LEU:CD1 | 2.44 | 0.48 |
| 4:J:75:TYR:HB3 | 4:J:80:HIS:CD2 | 2.49 | 0.48 |
| 4:J:174:ASP:HB3 | 4:J:175:GLU:OE2 | 2.12 | 0.48 |
| 4:J:235:GLU:OE1 | 4:J:235:GLU:N | 2.39 | 0.48 |
| 4:J:294:ASN:HD22 | 6:L:406:GLN:HE21 | 1.61 | 0.48 |
| 4:J:1077:ALA:CB | 4:J:1100:PHE:HA | 2.43 | 0.48 |
| 5:K:26:ARG:HH21 | 5:K:38:LEU:HD13 | 1.79 | 0.48 |
| 6:L:297:MET:CE | 6:L:305:LEU:HD22 | 2.44 | 0.48 |
| 6:L:419:PHE:HB2 | 6:L:430:TYR:CD2 | 2.49 | 0.48 |
| 2:M:257:VAL:HA | 2:M:260:LEU:CD1 | 2.43 | 0.48 |
| 1:N:67:ARG:O | 1:N:70:LYS:HB3 | 2.14 | 0.48 |
| 2:G:29:GLU:HB3 | 2:G:30:PRO:CD | 2.43 | 0.48 |
| 2:G:190:ALA:HB2 | 2:G:200:LYS:HB3 | 1.96 | 0.48 |
| 3:I:196:VAL:HG23 | 3:I:206:ALA:CB | 2.44 | 0.48 |
| 3:I:391:SER:HB3 | 3:I:394:ARG:HB2 | 1.94 | 0.48 |
| 3:I:757:THR:O | 3:I:765:ILE:HG23 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:1326:LEU:HD22 | 4:J:342:LEU:HD11 | 1.96 | 0.48 |
| 4:J:97:VAL:CG2 | 4:J:101:ARG:HE | 2.27 | 0.48 |
| 4:J:849:LEU:HD13 | 4:J:856:ILE:HA | 1.95 | 0.48 |
| 4:J:893:GLY:O | 4:J:894:VAL:HG23 | 2.13 | 0.48 |
| 6:L:118:ASP:O | 6:L:121:LYS:HB2 | 2.14 | 0.48 |
| 6:L:302:PHE:CE2 | 6:L:306:PHE:HB2 | 2.49 | 0.48 |
| 6:L:327:SER:HA | 6:L:330:LEU:HD12 | 1.95 | 0.48 |
| 7:O:27:DT:H2'' | 7:O:28:DG:H8 | 1.79 | 0.48 |
| 3:I:229:ILE:HG21 | 3:I:240:GLU:OE2 | 2.13 | 0.48 |
| 3:I:341:LEU:HG | 3:I:342:ASP:OD1 | 2.14 | 0.48 |
| 3:I:1129:ASN:O | 3:I:1133:LYS:HB2 | 2.13 | 0.48 |
| 4:J:103:GLY:CA | 4:J:244:VAL:HG22 | 2.44 | 0.48 |
| 4:J:373:ALA:HB3 | 4:J:441:LEU:HD11 | 1.95 | 0.48 |
| 4:J:1306:LEU:C | 4:J:1307:LEU:HD12 | 2.34 | 0.48 |
| 5:K:10:VAL:HG22 | 5:K:16:ARG:HG3 | 1.95 | 0.48 |
| 6:L:117:ILE:HG22 | 6:L:121:LYS:NZ | 2.29 | 0.48 |
| 6:L:141:ILE:HD12 | 6:L:256:PHE:CG | 2.48 | 0.48 |
| 3:I:45:GLY:HA3 | 3:I:46:GLN:HA | 1.58 | 0.47 |
| 3:I:229:ILE:HB | 3:I:240:GLU:CG | 2.44 | 0.47 |
| 3:I:877:VAL:CG2 | 3:I:920:VAL:HG21 | 2.44 | 0.47 |
| 3:I:882:ILE:H | 3:I:882:ILE:HD12 | 1.78 | 0.47 |
| 3:I:1098:LEU:HD23 | 3:I:1098:LEU:HA | 1.47 | 0.47 |
| 3:I:1119:MET:HB2 | 3:I:1228:GLY:CA | 2.44 | 0.47 |
| 4:J:122:SER:OG | 4:J:125:GLY:HA3 | 2.14 | 0.47 |
| 4:J:913:GLU:O | 4:J:915:ILE:HG23 | 2.14 | 0.47 |
| 6:L:252:LEU:HG | 6:L:256:PHE:CE2 | 2.49 | 0.47 |
| 3:I:287:VAL:HG23 | 3:I:292:ILE:HD11 | 1.96 | 0.47 |
| 3:I:342:ASP:O | 3:I:437:ASN:ND2 | 2.47 | 0.47 |
| 3:I:824:GLN:NE2 | 3:I:1082:ILE:HD11 | 2.30 | 0.47 |
| 3:I:972:PHE:CD1 | 3:I:975:ILE:HD12 | 2.49 | 0.47 |
| 3:I:1272:GLU:OE1 | 4:J:798:ARG:NH1 | 2.46 | 0.47 |
| 4:J:135:ILE:HA | 4:J:138:VAL:HG12 | 1.96 | 0.47 |
| 4:J:867:GLN:HG2 | 4:J:868:TRP:N | 2.29 | 0.47 |
| 6:L:266:PHE:O | 6:L:270:VAL:HG23 | 2.14 | 0.47 |
| 8:P:59:DA:H2'' | 8:P:60:DA:O5' | 2.15 | 0.47 |
| 2:H:16:ILE:HG12 | 2:H:17:GLU:H | 1.78 | 0.47 |
| 2:H:65:LEU:O | 2:H:65:LEU:HD22 | 2.14 | 0.47 |
| 2:H:213:PRO:O | 2:H:216:ALA:N | 2.47 | 0.47 |
| 3:I:181:GLY:HA3 | 3:I:395:TYR:CD1 | 2.50 | 0.47 |
| 3:I:517:GLN:O | 3:I:517:GLN:HG2 | 2.15 | 0.47 |
| 3:I:519:ASN:HB3 | 3:I:522:SER:H | 1.78 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:519:ASN:HD21 | 3:I:796:LEU:HD13 | 1.79 | 0.47 |
| 3:I:764:CYS:HB2 | 3:I:833:ILE:HD11 | 1.97 | 0.47 |
| 3:I:1124:ILE:HD11 | 3:I:1198:LEU:HG | 1.95 | 0.47 |
| 4:J:44:ILE:HG13 | 6:L:450:ILE:HG22 | 1.96 | 0.47 |
| 4:J:71:LEU:N | 4:J:90:VAL:HG21 | 2.27 | 0.47 |
| 4:J:278:ARG:NE | 6:L:407:GLU:OE2 | 2.46 | 0.47 |
| 4:J:425:ARG:HD3 | 4:J:459:ALA:HB2 | 1.97 | 0.47 |
| 4:J:653:ILE:HG21 | 4:J:693:VAL:HG22 | 1.96 | 0.47 |
| 4:J:1011:VAL:HG12 | 4:J:1012:ALA:O | 2.14 | 0.47 |
| 5:K:10:VAL:HG13 | 5:K:16:ARG:HB2 | 1.96 | 0.47 |
| 6:L:294:GLN:O | 6:L:329:LYS:HE2 | 2.14 | 0.47 |
| 8:P:51:DC:H2'' | 8:P:52:DT:C6 | 2.49 | 0.47 |
| 2:H:105:SER:HB2 | 2:H:139:SER:CB | 2.43 | 0.47 |
| 3:I:28:LEU:HD21 | 3:I:524:ILE:CD1 | 2.41 | 0.47 |
| 3:I:195:PHE:HA | 3:I:206:ALA:HB2 | 1.97 | 0.47 |
| 3:I:524:ILE:HD11 | 3:I:712:SER:CB | 2.44 | 0.47 |
| 3:I:985:GLU:O | 3:I:989:LEU:N | 2.48 | 0.47 |
| 4:J:105:ILE:HD12 | 4:J:242:LEU:HD22 | 1.95 | 0.47 |
| 4:J:147:ILE:HG13 | 4:J:177:ASP:OD1 | 2.13 | 0.47 |
| 4:J:609:TYR:HE1 | 4:J:614:LEU:HD12 | 1.79 | 0.47 |
| 4:J:1207:GLY:HA2 | 4:J:1223:LEU:HB3 | 1.96 | 0.47 |
| 6:L:279:ARG:O | 6:L:283:GLN:HG2 | 2.14 | 0.47 |
| 7:O:63:DT:H2'' | 7:O:64:DT:C6 | 2.49 | 0.47 |
| 2:M:298:LYS:HA | 2:M:301:THR:CG2 | 2.45 | 0.47 |
| 1:N:8:ALA:CB | 4:J:783:LEU:HD12 | 2.45 | 0.47 |
| 1:N:15:LEU:HD23 | 1:N:15:LEU:O | 2.13 | 0.47 |
| 2:G:218:ARG:O | 2:G:222:THR:HG22 | 2.14 | 0.47 |
| 3:I:12:ARG:HH22 | 3:I:698:PRO:HD2 | 1.80 | 0.47 |
| 3:I:256:GLU:CB | 3:I:261:VAL:HA | 2.43 | 0.47 |
| 3:I:367:TYR:CD1 | 3:I:381:ALA:HA | 2.50 | 0.47 |
| 4:J:1156:LEU:HD11 | 4:J:1224:ARG:HH21 | 1.80 | 0.47 |
| 4:J:1356:LEU:HD12 | 4:J:1365:TYR:CD2 | 2.49 | 0.47 |
| 6:L:593:LYS:O | 6:L:596:ARG:HB2 | 2.13 | 0.47 |
| 7:O:29:DA:H2'' | 7:O:30:DC:O4' | 2.14 | 0.47 |
| 8:P:19:DT:H2'' | 8:P:20:DC:C6 | 2.50 | 0.47 |
| 2:G:23:HIS:CB | 2:G:206:GLU:HA | 2.45 | 0.47 |
| 3:I:44:GLU:O | 3:I:46:GLN:NE2 | 2.47 | 0.47 |
| 3:I:96:LEU:HD23 | 3:I:124:MET:O | 2.13 | 0.47 |
| 3:I:105:TYR:HB3 | 3:I:109:ALA:O | 2.14 | 0.47 |
| 3:I:269:ILE:H | 3:I:269:ILE:HD12 | 1.79 | 0.47 |
| 3:I:444:ASP:O | 3:I:447:HIS:HB2 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:632:ASP:HA | 3:I:647:ARG:HE | 1.80 | 0.47 |
| 3:I:809:GLY:O | 4:J:357:VAL:HG11 | 2.15 | 0.47 |
| 3:I:958:LYS:O | 3:I:961:SER:OG | 2.22 | 0.47 |
| 3:I:1101:LEU:HD23 | 4:J:725:MET:SD | 2.55 | 0.47 |
| 3:I:1101:LEU:O | 4:J:731:ARG:HG2 | 2.14 | 0.47 |
| 3:I:1103:VAL:HG11 | 3:I:1112:ILE:HD11 | 1.97 | 0.47 |
| 3:I:1223:ARG:NH2 | 4:J:721:SER:OG | 2.26 | 0.47 |
| 3:I:1331:ARG:HA | 3:I:1335:ILE:O | 2.15 | 0.47 |
| 4:J:364:HIS:HB3 | 4:J:487:THR:CG2 | 2.45 | 0.47 |
| 4:J:820:ILE:HD11 | 4:J:822:MET:SD | 2.54 | 0.47 |
| 4:J:949:SER:OG | 4:J:950:ILE:N | 2.45 | 0.47 |
| 4:J:1226:VAL:O | 4:J:1230:THR:HG22 | 2.14 | 0.47 |
| 4:J:1237:VAL:CG1 | 4:J:1253:ILE:HD13 | 2.45 | 0.47 |
| 6:L:119:ILE:HB | 6:L:379:MET:CE | 2.45 | 0.47 |
| 6:L:344:LEU:HG | 6:L:355:ILE:HD11 | 1.95 | 0.47 |
| 6:L:391:ALA:HB2 | 6:L:439:ILE:HD11 | 1.97 | 0.47 |
| 2:G:61:ILE:HG12 | 2:G:142:MET:HB3 | 1.96 | 0.47 |
| 3:I:216:THR:CG2 | 3:I:219:GLN:H | 2.27 | 0.47 |
| 3:I:237:LEU:HD11 | 3:I:322:LEU:CD1 | 2.44 | 0.47 |
| 3:I:272:ARG:HA | 3:I:275:ARG:HG3 | 1.97 | 0.47 |
| 3:I:378:ARG:HG3 | 3:I:379:GLU:N | 2.30 | 0.47 |
| 3:I:593:LYS:HD2 | 3:I:652:TYR:HE1 | 1.80 | 0.47 |
| 3:I:803:ALA:HB2 | 3:I:1094:VAL:HG11 | 1.97 | 0.47 |
| 3:I:1004:ASP:OD1 | 3:I:1004:ASP:N | 2.42 | 0.47 |
| 4:J:198:CYS:O | 4:J:202:ARG:HG2 | 2.14 | 0.47 |
| 4:J:949:SER:HA | 4:J:1020:TRP:CH2 | 2.50 | 0.47 |
| 6:L:130:VAL:HG13 | 6:L:365:MET:HG2 | 1.96 | 0.47 |
| 6:L:212:ILE:N | 6:L:216:LEU:HD21 | 2.30 | 0.47 |
| 6:L:290:LEU:CA | 6:L:294:GLN:HB3 | 2.44 | 0.47 |
| 6:L:324:LYS:H | 6:L:327:SER:CB | 2.28 | 0.47 |
| 6:L:327:SER:HA | 6:L:330:LEU:CD1 | 2.45 | 0.47 |
| 6:L:344:LEU:HG | 6:L:355:ILE:CD1 | 2.44 | 0.47 |
| 6:L:409:ASN:O | 6:L:413:MET:HG3 | 2.14 | 0.47 |
| 6:L:573:LEU:HB3 | 8:P:56:DG:OP2 | 2.15 | 0.47 |
| 7:O:32:DA:H2" | 7:O:33:DA:H8 | 1.80 | 0.47 |
| 2:M:284:ARG:CB | 2:M:288:GLU:HG2 | 2.40 | 0.47 |
| 2:M:300:LEU:HD13 | 2:M:300:LEU:O | 2.13 | 0.47 |
| 1:N:20:ILE:HD13 | 4:J:746:LEU:HD13 | 1.97 | 0.47 |
| 3:I:734:ILE:O | 3:I:734:ILE:HG13 | 2.14 | 0.47 |
| 3:I:912:ASP:OD1 | 3:I:912:ASP:N | 2.45 | 0.47 |
| 4:J:53:ARG:HA | 4:J:54:ASP:HA | 1.54 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:1107:VAL:HA | 4:J:1122:ALA:CB | 2.45 | 0.47 |
| 4:J:1221:LEU:HD23 | 4:J:1306:LEU:HB2 | 1.97 | 0.47 |
| 3:I:1160:ASP:OD1 | 3:I:1162:SER:HB3 | 2.15 | 0.47 |
| 4:J:1159:ILE:HD12 | 4:J:1160:SER:H | 1.79 | 0.47 |
| 8:P:68:DG:OP1 | 2:M:295:LEU:N | 2.47 | 0.47 |
| 2:G:90:VAL:HG11 | 2:G:146:VAL:HG21 | 1.97 | 0.47 |
| 2:G:111:THR:HA | 2:G:129:VAL:HA | 1.96 | 0.47 |
| 3:I:6:THR:HB | 3:I:781:ASP:OD1 | 2.15 | 0.47 |
| 3:I:24:VAL:HG11 | 3:I:704:MET:CE | 2.45 | 0.47 |
| 3:I:319:LEU:O | 3:I:322:LEU:HB3 | 2.14 | 0.47 |
| 3:I:629:PHE:CE2 | 3:I:650:VAL:HG21 | 2.50 | 0.47 |
| 3:I:1151:LEU:HD22 | 3:I:1151:LEU:HA | 1.68 | 0.47 |
| 5:K:14:GLY:O | 5:K:15:ASN:HB3 | 2.15 | 0.47 |
| 6:L:137:TYR:HD2 | 6:L:140:ALA:HB2 | 1.78 | 0.47 |
| 6:L:484:ALA:CB | 6:L:494:ILE:HD13 | 2.45 | 0.47 |
| 2:M:298:LYS:O | 2:M:302:GLU:HG3 | 2.15 | 0.47 |
| 3:I:125:GLY:H | 3:I:495:ALA:HB1 | 1.79 | 0.46 |
| 3:I:878:THR:HG22 | 3:I:925:SER:HB3 | 1.96 | 0.46 |
| 4:J:20:ILE:HD13 | 4:J:1320:ILE:CD1 | 2.45 | 0.46 |
| 4:J:872:LEU:HD11 | 4:J:877:VAL:HB | 1.98 | 0.46 |
| 4:J:948:SER:OG | 4:J:1022:PRO:HG3 | 2.15 | 0.46 |
| 4:J:982:LEU:O | 4:J:982:LEU:HD23 | 2.15 | 0.46 |
| 4:J:1158:GLU:HG3 | 4:J:1186:TYR:CZ | 2.50 | 0.46 |
| 4:J:1251:LYS:O | 4:J:1255:VAL:HG12 | 2.14 | 0.46 |
| 6:L:157:ARG:N | 6:L:160:ASP:OD2 | 2.48 | 0.46 |
| 2:H:41:ASN:O | 2:H:45:ARG:HG3 | 2.15 | 0.46 |
| 3:I:272:ARG:HA | 3:I:275:ARG:CG | 2.44 | 0.46 |
| 3:I:530:ILE:HG13 | 3:I:575:LEU:HB2 | 1.97 | 0.46 |
| 3:I:996:ARG:HD3 | 3:I:996:ARG:HA | 1.67 | 0.46 |
| 3:I:1276:TRP:CZ2 | 4:J:801:VAL:HG21 | 2.51 | 0.46 |
| 4:J:271:ARG:O | 4:J:275:ARG:HG3 | 2.15 | 0.46 |
| 4:J:909:ILE:HD11 | 4:J:913:GLU:CB | 2.43 | 0.46 |
| 4:J:1060:VAL:HG23 | 4:J:1106:ILE:HG23 | 1.97 | 0.46 |
| 4:J:1194:ARG:HG2 | 4:J:1195:GLN:N | 2.29 | 0.46 |
| 6:L:316:PHE:CE2 | 6:L:334:SER:HA | 2.41 | 0.46 |
| 6:L:506:SER:O | 6:L:509:THR:HG22 | 2.16 | 0.46 |
| 7:O:39:DG:H2'' | 7:O:40:DC:C5' | 2.46 | 0.46 |
| 1:N:52:PHE:HE2 | 4:J:673:VAL:HG12 | 1.81 | 0.46 |
| 3:I:178:PRO:HG3 | 3:I:395:TYR:CE1 | 2.51 | 0.46 |
| 3:I:391:SER:O | 3:I:394:ARG:N | 2.48 | 0.46 |
| 3:I:727:VAL:O | 3:I:727:VAL:HG13 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:105:ILE:HD12 | 4:J:242:LEU:CD2 | 2.45 | 0.46 |
| 4:J:132:LEU:HA | 4:J:135:ILE:CD1 | 2.45 | 0.46 |
| 4:J:220:ARG:NH1 | 4:J:224:LEU:HD11 | 2.30 | 0.46 |
| 4:J:841:GLY:O | 4:J:901:ARG:HB3 | 2.15 | 0.46 |
| 4:J:850:LYS:HG3 | 4:J:851:PRO:N | 2.30 | 0.46 |
| 4:J:1045:THR:O | 4:J:1061:VAL:HG13 | 2.15 | 0.46 |
| 4:J:1209:VAL:HB | 4:J:1211:SER:O | 2.14 | 0.46 |
| 4:J:1327:GLU:OE2 | 4:J:1330:ARG:HB2 | 2.14 | 0.46 |
| 5:K:27:ALA:O | 5:K:46:THR:HG21 | 2.14 | 0.46 |
| 6:L:112:THR:O | 6:L:115:GLY:N | 2.47 | 0.46 |
| 6:L:151:VAL:HG11 | 6:L:158:LEU:HA | 1.97 | 0.46 |
| 6:L:248:GLU:HG3 | 6:L:251:LYS:HZ1 | 1.80 | 0.46 |
| 1:N:5:ALA:HB2 | 3:I:681:MET:SD | 2.55 | 0.46 |
| 2:G:124:VAL:HG13 | 2:G:125:LYS:H | 1.80 | 0.46 |
| 3:I:164:THR:HG21 | 3:I:171:LEU:HG | 1.96 | 0.46 |
| 3:I:1026:GLU:O | 3:I:1029:LEU:HG | 2.15 | 0.46 |
| 3:I:1282:GLY:CA | 4:J:1360:GLY:HA3 | 2.46 | 0.46 |
| 4:J:268:LEU:HD21 | 4:J:324:LEU:HD22 | 1.97 | 0.46 |
| 4:J:314:ARG:HD3 | 4:J:314:ARG:HA | 1.70 | 0.46 |
| 4:J:395:LYS:HD3 | 6:L:536:THR:CG2 | 2.45 | 0.46 |
| 4:J:570:LYS:HG3 | 4:J:589:TYR:CD2 | 2.50 | 0.46 |
| 4:J:702:GLN:O | 4:J:718:SER:HB3 | 2.16 | 0.46 |
| 4:J:984:LEU:HB3 | 4:J:993:GLU:HB2 | 1.96 | 0.46 |
| 4:J:1035:VAL:HG21 | 4:J:1109:LEU:HD23 | 1.98 | 0.46 |
| 6:L:290:LEU:HA | 6:L:294:GLN:HB3 | 1.98 | 0.46 |
| 6:L:452:ILE:HD11 | 6:L:457:ILE:HG12 | 1.98 | 0.46 |
| 6:L:551:LEU:HD13 | 6:L:555:GLU:OE2 | 2.16 | 0.46 |
| 7:O:47:DG:H2'' | 7:O:48:DG:OP2 | 2.16 | 0.46 |
| 8:P:37:DG:H1' | 8:P:38:DC:H5' | 1.97 | 0.46 |
| 2:H:102:LEU:HD21 | 2:H:130:ILE:HD13 | 1.97 | 0.46 |
| 2:H:113:ALA:HB2 | 2:H:126:PRO:HB3 | 1.96 | 0.46 |
| 3:I:278:GLU:O | 3:I:281:ASP:HB3 | 2.15 | 0.46 |
| 3:I:289:VAL:CG2 | 3:I:322:LEU:HD22 | 2.35 | 0.46 |
| 3:I:322:LEU:HA | 3:I:325:LEU:HG | 1.97 | 0.46 |
| 3:I:656:SER:O | 3:I:659:GLN:HB2 | 2.16 | 0.46 |
| 3:I:1028:LYS:HB2 | 3:I:1028:LYS:HE3 | 1.60 | 0.46 |
| 4:J:825:VAL:O | 4:J:825:VAL:HG13 | 2.15 | 0.46 |
| 4:J:1284:ARG:NH1 | 4:J:1288:ALA:HB2 | 2.30 | 0.46 |
| 6:L:265:GLN:HA | 6:L:268:TYR:CB | 2.45 | 0.46 |
| 6:L:286:LEU:HD23 | 6:L:340:ALA:HB2 | 1.98 | 0.46 |
| 2:M:269:CYS:SG | 2:M:295:LEU:HD12 | 2.55 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:299:SER:O | 2:M:302:GLU:HB2 | 2.15 | 0.46 |
| 3:I:105:TYR:CD1 | 3:I:114:VAL:HG13 | 2.50 | 0.46 |
| 3:I:229:ILE:HB | 3:I:240:GLU:HG3 | 1.98 | 0.46 |
| 3:I:453:ILE:CD1 | 3:I:530:ILE:HD12 | 2.40 | 0.46 |
| 3:I:468:LEU:HD23 | 3:I:468:LEU:HA | 1.48 | 0.46 |
| 3:I:559:CYS:SG | 3:I:662:SER:HB3 | 2.55 | 0.46 |
| 4:J:44:ILE:CG1 | 6:L:450:ILE:HG22 | 2.45 | 0.46 |
| 4:J:1162:ILE:HG13 | 4:J:1202:GLU:C | 2.36 | 0.46 |
| 6:L:311:THR:HG22 | 6:L:344:LEU:HD21 | 1.98 | 0.46 |
| 8:P:37:DG:H2'' | 8:P:38:DC:H5' | 1.96 | 0.46 |
| 2:M:286:GLU:OE2 | 2:M:314:LEU:HD13 | 2.16 | 0.46 |
| 2:G:13:LEU:HB3 | 2:H:231:PHE:HE1 | 1.81 | 0.46 |
| 2:H:194:GLN:HA | 2:H:195:ARG:C | 2.35 | 0.46 |
| 3:I:149:LEU:HA | 3:I:452:ARG:O | 2.15 | 0.46 |
| 3:I:198:ILE:HG22 | 3:I:199:ASP:H | 1.79 | 0.46 |
| 3:I:243:PRO:CB | 3:I:277:LEU:HD23 | 2.44 | 0.46 |
| 3:I:422:LYS:HZ2 | 3:I:422:LYS:HG2 | 1.65 | 0.46 |
| 3:I:544:GLY:O | 3:I:548:ARG:HD2 | 2.15 | 0.46 |
| 3:I:564:PRO:O | 3:I:569:ILE:HG12 | 2.15 | 0.46 |
| 3:I:681:MET:CE | 3:I:1073:LYS:HE3 | 2.45 | 0.46 |
| 6:L:328:GLU:N | 6:L:328:GLU:OE1 | 2.49 | 0.46 |
| 6:L:334:SER:O | 6:L:338:HIS:HB2 | 2.16 | 0.46 |
| 6:L:574:GLU:HA | 6:L:584:ARG:HG2 | 1.98 | 0.46 |
| 8:P:17:DA:C8 | 8:P:18:DT:H72 | 2.50 | 0.46 |
| 8:P:53:DT:H2'' | 8:P:54:DT:OP2 | 2.16 | 0.46 |
| 3:I:346:TYR:CD2 | 3:I:433:ILE:HG23 | 2.51 | 0.46 |
| 3:I:395:TYR:HD2 | 3:I:419:ILE:HG13 | 1.80 | 0.46 |
| 3:I:673:HIS:ND1 | 3:I:1113:LEU:HD13 | 2.30 | 0.46 |
| 4:J:161:THR:HG22 | 4:J:162:GLU:H | 1.80 | 0.46 |
| 4:J:422:LEU:HD11 | 4:J:471:PRO:HG3 | 1.97 | 0.46 |
| 6:L:299:LYS:O | 6:L:303:ILE:HG22 | 2.14 | 0.46 |
| 6:L:481:GLU:O | 6:L:485:GLU:HG2 | 2.15 | 0.46 |
| 7:O:27:DT:H2'' | 7:O:28:DG:C8 | 2.51 | 0.46 |
| 2:M:264:VAL:HA | 2:M:267:ALA:HB3 | 1.98 | 0.46 |
| 3:I:161:LYS:HA | 3:I:170:VAL:CG1 | 2.46 | 0.46 |
| 3:I:1105:SER:CB | 4:J:731:ARG:HG3 | 2.42 | 0.46 |
| 4:J:46:TYR:CD1 | 6:L:500:ILE:HD12 | 2.49 | 0.46 |
| 4:J:801:VAL:HG12 | 4:J:920:ALA:HB1 | 1.97 | 0.46 |
| 4:J:835:LEU:HD13 | 4:J:835:LEU:O | 2.16 | 0.46 |
| 4:J:1037:PHE:CZ | 4:J:1110:GLU:HA | 2.48 | 0.46 |
| 4:J:1069:ALA:O | 4:J:1072:LYS:HD3 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:1176:VAL:HA | 4:J:1186:TYR:O | 2.15 | 0.46 |
| 4:J:1293:GLU:OE1 | 4:J:1298:VAL:HA | 2.16 | 0.46 |
| 6:L:140:ALA:CA | 6:L:269:LEU:HD22 | 2.40 | 0.46 |
| 6:L:283:GLN:HB3 | 6:L:340:ALA:HB1 | 1.98 | 0.46 |
| 6:L:525:ASP:OD2 | 6:L:527:THR:OG1 | 2.18 | 0.46 |
| 2:H:105:SER:HB2 | 2:H:139:SER:OG | 2.15 | 0.46 |
| 3:I:225:PHE:HB2 | 3:I:336:LEU:CD2 | 2.45 | 0.46 |
| 4:J:147:ILE:HD13 | 4:J:187:ALA:CB | 2.45 | 0.46 |
| 4:J:149:GLY:HA2 | 4:J:177:ASP:OD2 | 2.16 | 0.46 |
| 4:J:660:GLU:O | 4:J:663:GLU:HG3 | 2.16 | 0.46 |
| 4:J:822:MET:HE3 | 4:J:838:ARG:HE | 1.80 | 0.46 |
| 5:K:25:ARG:NH1 | 5:K:64:LEU:HD13 | 2.31 | 0.46 |
| 6:L:141:ILE:HA | 6:L:144:LEU:HB3 | 1.97 | 0.46 |
| 6:L:391:ALA:HB3 | 6:L:405:ILE:CD1 | 2.42 | 0.46 |
| 2:G:28:LEU:HG | 2:H:231:PHE:HZ | 1.81 | 0.45 |
| 2:G:47:LEU:O | 2:G:180:VAL:HG21 | 2.16 | 0.45 |
| 2:G:110:VAL:CG1 | 2:G:131:CYS:HB2 | 2.46 | 0.45 |
| 2:G:150:ARG:HD3 | 2:H:5:VAL:O | 2.17 | 0.45 |
| 3:I:60:GLN:O | 3:I:476:LYS:HG2 | 2.16 | 0.45 |
| 3:I:178:PRO:HG3 | 3:I:395:TYR:HE1 | 1.81 | 0.45 |
| 3:I:303:ASP:HB3 | 3:I:306:THR:HG23 | 1.99 | 0.45 |
| 4:J:54:ASP:OD1 | 4:J:54:ASP:N | 2.49 | 0.45 |
| 4:J:74:LYS:HG3 | 4:J:75:TYR:CE1 | 2.51 | 0.45 |
| 4:J:356:THR:HG23 | 4:J:446:ALA:HB1 | 1.98 | 0.45 |
| 4:J:385:LEU:HD23 | 4:J:411:ILE:HG13 | 1.97 | 0.45 |
| 4:J:390:LEU:CD2 | 4:J:407:VAL:HB | 2.46 | 0.45 |
| 4:J:515:ARG:NH2 | 4:J:717:VAL:O | 2.49 | 0.45 |
| 4:J:800:LEU:HD12 | 4:J:800:LEU:HA | 1.65 | 0.45 |
| 4:J:836:ARG:O | 4:J:840:LEU:HB2 | 2.16 | 0.45 |
| 4:J:1047:THR:HG21 | 4:J:1060:VAL:HB | 1.97 | 0.45 |
| 7:O:33:DA:H2'' | 7:O:34:DA:N7 | 2.31 | 0.45 |
| 8:P:57:DT:H2'' | 8:P:58:DC:C5' | 2.46 | 0.45 |
| 3:I:58:PRO:HB3 | 3:I:69:GLN:HB3 | 1.97 | 0.45 |
| 3:I:990:ASP:N | 3:I:990:ASP:OD1 | 2.50 | 0.45 |
| 4:J:1047:THR:HB | 4:J:1062:LEU:HD23 | 1.97 | 0.45 |
| 2:G:52:PRO:HG2 | 2:G:219:ARG:NE | 2.31 | 0.45 |
| 2:H:46:ILE:CD1 | 2:H:224:LEU:HD22 | 2.47 | 0.45 |
| 2:H:197:ASP:O | 2:H:198:LEU:HD13 | 2.16 | 0.45 |
| 3:I:1151:LEU:HD11 | 3:I:1198:LEU:HA | 1.97 | 0.45 |
| 4:J:193:ASP:OD1 | 4:J:194:LEU:N | 2.49 | 0.45 |
| 4:J:218:THR:O | 4:J:221:ILE:HG22 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:J:349:TYR:CD2 | 4:J:472:LEU:HD11 | 2.51 | 0.45 |
| 4:J:1139:PRO:O | 4:J:1143:ASP:N | 2.35 | 0.45 |
| 4:J:1275:LEU:HG | 4:J:1278:GLU:HB2 | 1.97 | 0.45 |
| 6:L:236:LYS:HD2 | 6:L:236:LYS:HA | 1.78 | 0.45 |
| 7:O:23:DC:H2" | 7:O:24:DC:C6 | 2.51 | 0.45 |
| 2:G:31:LEU:HD23 | 2:G:31:LEU:HA | 1.78 | 0.45 |
| 2:G:47:LEU:HD21 | 2:G:220:ALA:HB2 | 1.97 | 0.45 |
| 2:H:133:LEU:HD23 | 2:H:133:LEU:HA | 1.80 | 0.45 |
| 3:I:29:SER:O | 3:I:33:ASP:CB | 2.59 | 0.45 |
| 3:I:161:LYS:HA | 3:I:170:VAL:HG12 | 1.99 | 0.45 |
| 3:I:223:LEU:HD12 | 3:I:223:LEU:HA | 1.62 | 0.45 |
| 3:I:1165:SER:OG | 3:I:1166:ASP:N | 2.50 | 0.45 |
| 4:J:74:LYS:HG3 | 4:J:75:TYR:CD1 | 2.51 | 0.45 |
| 4:J:121:PRO:HB2 | 4:J:126:LEU:HD23 | 1.97 | 0.45 |
| 4:J:135:ILE:O | 4:J:139:LEU:HG | 2.15 | 0.45 |
| 4:J:1039:ASP:O | 4:J:1076:PRO:HA | 2.15 | 0.45 |
| 4:J:1292:LEU:O | 4:J:1295:ASN:N | 2.50 | 0.45 |
| 7:O:45:DA:H2" | 7:O:46:DG:H5" | 1.98 | 0.45 |
| 2:G:190:ALA:HB2 | 2:G:200:LYS:HE3 | 1.99 | 0.45 |
| 3:I:24:VAL:CG1 | 3:I:25:PRO:HD2 | 2.46 | 0.45 |
| 3:I:243:PRO:HA | 3:I:277:LEU:HD23 | 1.98 | 0.45 |
| 3:I:543:ALA:HA | 3:I:544:GLY:HA3 | 1.69 | 0.45 |
| 3:I:778:GLU:O | 3:I:781:ASP:HB3 | 2.16 | 0.45 |
| 3:I:854:ILE:HD11 | 3:I:885:GLY:HA3 | 1.98 | 0.45 |
| 3:I:966:ILE:HG12 | 10:I:1401:1N7:H26 | 1.99 | 0.45 |
| 4:J:309:ASN:ND2 | 4:J:324:LEU:HB2 | 2.30 | 0.45 |
| 4:J:1010:GLN:O | 4:J:1010:GLN:HG3 | 2.16 | 0.45 |
| 4:J:1178:THR:CB | 4:J:1184:ASP:HB2 | 2.46 | 0.45 |
| 4:J:1257:VAL:O | 4:J:1261:LEU:HG | 2.16 | 0.45 |
| 6:L:261:LEU:HB3 | 6:L:266:PHE:HB2 | 1.98 | 0.45 |
| 3:I:668:ILE:HD12 | 3:I:671:LEU:HD13 | 1.98 | 0.45 |
| 3:I:689:ALA:HB3 | 3:I:796:LEU:HB3 | 1.99 | 0.45 |
| 3:I:1291:LEU:HB2 | 4:J:345:LYS:HE3 | 1.99 | 0.45 |
| 4:J:156:ARG:HG3 | 4:J:157:GLN:N | 2.30 | 0.45 |
| 4:J:514:THR:HG21 | 4:J:596:LEU:CG | 2.47 | 0.45 |
| 4:J:718:SER:OG | 4:J:720:ASN:HB2 | 2.16 | 0.45 |
| 4:J:749:LYS:HE3 | 4:J:753:SER:OG | 2.17 | 0.45 |
| 4:J:800:LEU:HD13 | 4:J:1309:ILE:HD12 | 1.97 | 0.45 |
| 4:J:985:ILE:HD13 | 4:J:991:THR:CA | 2.46 | 0.45 |
| 6:L:113:ARG:HD2 | 6:L:426:LYS:HE2 | 1.98 | 0.45 |
| 7:O:32:DA:H2" | 7:O:33:DA:C8 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 8:P:52:DT:H2'' | 8:P:53:DT:H71 | 1.99 | 0.45 |
| 2:G:13:LEU:HB3 | 2:H:231:PHE:CE1 | 2.51 | 0.45 |
| 3:I:57:PHE:CD2 | 3:I:70:TYR:HB2 | 2.48 | 0.45 |
| 3:I:185:ASP:HB2 | 3:I:197:ARG:O | 2.17 | 0.45 |
| 3:I:755:LYS:HA | 3:I:755:LYS:CE | 2.47 | 0.45 |
| 3:I:996:ARG:HA | 3:I:998:LEU:HD22 | 1.99 | 0.45 |
| 3:I:1242:LYS:HD2 | 4:J:465:GLN:NE2 | 2.31 | 0.45 |
| 4:J:46:TYR:CE2 | 6:L:453:PRO:HD3 | 2.52 | 0.45 |
| 4:J:560:ASN:OD1 | 4:J:560:ASN:N | 2.50 | 0.45 |
| 7:O:25:DA:H2' | 7:O:26:DT:C6 | 2.52 | 0.45 |
| 8:P:48:DC:H2'' | 8:P:49:DT:C6 | 2.51 | 0.45 |
| 2:G:91:ARG:NH1 | 2:G:210:THR:O | 2.50 | 0.45 |
| 2:G:118:ASP:OD2 | 2:G:119:GLY:N | 2.44 | 0.45 |
| 2:H:11:PRO:HB2 | 2:H:28:LEU:HD11 | 1.98 | 0.45 |
| 3:I:575:LEU:CD1 | 3:I:587:LEU:HD21 | 2.46 | 0.45 |
| 3:I:577:VAL:HG23 | 3:I:661:VAL:O | 2.17 | 0.45 |
| 3:I:672:GLU:HG2 | 3:I:673:HIS:CD2 | 2.51 | 0.45 |
| 4:J:120:LEU:HG | 4:J:1330:ARG:HG3 | 1.98 | 0.45 |
| 4:J:291:ILE:HG22 | 6:L:406:GLN:HE22 | 1.82 | 0.45 |
| 4:J:697:MET:HE2 | 4:J:742:GLY:H | 1.81 | 0.45 |
| 4:J:911:LYS:HG3 | 4:J:911:LYS:O | 2.15 | 0.45 |
| 4:J:993:GLU:HB3 | 4:J:995:TYR:CE2 | 2.52 | 0.45 |
| 4:J:1029:THR:HG21 | 4:J:1115:ILE:CD1 | 2.47 | 0.45 |
| 6:L:99:ARG:O | 6:L:103:ARG:HG3 | 2.17 | 0.45 |
| 6:L:298:PRO:HB2 | 6:L:301:ASN:OD1 | 2.17 | 0.45 |
| 2:G:64:VAL:HG22 | 2:G:78:ILE:CD1 | 2.47 | 0.45 |
| 2:G:192:VAL:HG22 | 2:G:193:GLU:H | 1.82 | 0.45 |
| 2:H:78:ILE:HA | 2:H:81:ILE:CD1 | 2.40 | 0.45 |
| 3:I:175:ARG:HE | 3:I:175:ARG:HB2 | 1.50 | 0.45 |
| 3:I:241:LEU:HD22 | 3:I:285:ILE:HG23 | 1.97 | 0.45 |
| 3:I:360:LEU:HD21 | 3:I:378:ARG:HD3 | 1.99 | 0.45 |
| 3:I:506:PHE:O | 3:I:512:SER:OG | 2.26 | 0.45 |
| 3:I:565:GLU:H | 3:I:565:GLU:HG3 | 1.57 | 0.45 |
| 3:I:590:PRO:HB2 | 3:I:655:VAL:CG1 | 2.36 | 0.45 |
| 3:I:830:THR:HG23 | 3:I:832:HIS:HE1 | 1.82 | 0.45 |
| 3:I:884:VAL:CG2 | 3:I:918:LEU:HD23 | 2.43 | 0.45 |
| 3:I:986:ALA:HA | 3:I:989:LEU:HB2 | 1.99 | 0.45 |
| 4:J:522:GLY:HA3 | 4:J:542:ALA:HA | 1.99 | 0.45 |
| 4:J:549:LYS:HG3 | 4:J:571:ASP:OD1 | 2.17 | 0.45 |
| 4:J:709:ARG:HD3 | 4:J:710:ASP:H | 1.80 | 0.45 |
| 6:L:265:GLN:HA | 6:L:268:TYR:HB2 | 1.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:L:322:MET:CG | 6:L:324:LYS:HG2 | 2.47 | 0.45 |
| 6:L:574:GLU:HG2 | 6:L:584:ARG:CD | 2.47 | 0.45 |
| 2:M:269:CYS:O | 2:M:272:ALA:HB3 | 2.17 | 0.45 |
| 2:G:45:ARG:HG2 | 2:H:38:THR:HB | 1.98 | 0.45 |
| 2:G:79:LEU:HD11 | 3:I:693:LEU:HD11 | 1.98 | 0.45 |
| 2:H:11:PRO:HB2 | 2:H:14:VAL:HG22 | 1.98 | 0.45 |
| 3:I:529:ARG:NH1 | 3:I:574:SER:OG | 2.49 | 0.45 |
| 3:I:835:GLU:OE2 | 3:I:1053:TYR:OH | 2.26 | 0.45 |
| 4:J:69:GLU:N | 4:J:92:VAL:HG23 | 2.32 | 0.45 |
| 4:J:97:VAL:HG21 | 4:J:101:ARG:HE | 1.81 | 0.45 |
| 4:J:514:THR:O | 4:J:514:THR:HG23 | 2.17 | 0.45 |
| 4:J:985:ILE:HG23 | 4:J:990:ARG:O | 2.16 | 0.45 |
| 4:J:1069:ALA:CB | 4:J:1072:LYS:HD3 | 2.43 | 0.45 |
| 6:L:392:LYS:HD2 | 7:O:56:DC:O5' | 2.16 | 0.45 |
| 6:L:544:THR:HA | 6:L:547:VAL:HG22 | 1.99 | 0.45 |
| 2:G:166:ARG:N | 2:G:167:PRO:HD2 | 2.32 | 0.44 |
| 2:H:84:ASN:ND2 | 4:J:551:ARG:HH12 | 2.15 | 0.44 |
| 3:I:28:LEU:HD13 | 3:I:133:ASN:O | 2.17 | 0.44 |
| 3:I:231:GLU:N | 3:I:238:GLN:O | 2.23 | 0.44 |
| 3:I:815:SER:OG | 4:J:357:VAL:HG23 | 2.17 | 0.44 |
| 3:I:995:ASP:OD1 | 3:I:995:ASP:N | 2.48 | 0.44 |
| 3:I:1072:ASN:OD1 | 3:I:1072:ASN:N | 2.50 | 0.44 |
| 4:J:36:GLY:HA3 | 4:J:61:ILE:HG23 | 1.99 | 0.44 |
| 4:J:487:THR:HG22 | 4:J:618:VAL:CG1 | 2.48 | 0.44 |
| 4:J:611:ILE:HG22 | 4:J:612:LEU:CD1 | 2.47 | 0.44 |
| 4:J:1198:VAL:HB | 4:J:1210:ILE:HG23 | 1.97 | 0.44 |
| 5:K:13:ILE:HD12 | 5:K:54:ILE:HD12 | 1.99 | 0.44 |
| 6:L:98:VAL:HA | 6:L:402:LEU:HD11 | 1.99 | 0.44 |
| 7:O:29:DA:H2' | 7:O:30:DC:C6 | 2.52 | 0.44 |
| 8:P:37:DG:C2' | 8:P:38:DC:H5' | 2.46 | 0.44 |
| 8:P:48:DC:OP2 | 8:P:48:DC:H2' | 2.17 | 0.44 |
| 2:M:265:ARG:HH21 | 2:M:294:ASN:HB2 | 1.82 | 0.44 |
| 3:I:120:GLN:CG | 3:I:490:GLN:HE22 | 2.27 | 0.44 |
| 3:I:188:PHE:CD1 | 3:I:194:LEU:HB3 | 2.53 | 0.44 |
| 3:I:237:LEU:HD11 | 3:I:322:LEU:HD11 | 1.98 | 0.44 |
| 3:I:448:LEU:HD12 | 3:I:554:HIS:CE1 | 2.52 | 0.44 |
| 3:I:633:LEU:HD22 | 3:I:644:LEU:HB3 | 1.99 | 0.44 |
| 3:I:975:ILE:HG12 | 3:I:1014:LEU:HD12 | 1.99 | 0.44 |
| 3:I:993:PRO:HB2 | 3:I:995:ASP:OD1 | 2.17 | 0.44 |
| 3:I:1048:LYS:HB2 | 3:I:1048:LYS:HE3 | 1.53 | 0.44 |
| 3:I:1146:GLN:NE2 | 3:I:1150:ASP:OD1 | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:I:1308:ILE:CG2 | 4:J:379:PRO:HB2 | 2.48 | 0.44 |
| 4:J:523:GLU:OE1 | 4:J:547:ARG:HB2 | 2.17 | 0.44 |
| 4:J:1282:TYR:O | 4:J:1286:LYS:HB2 | 2.17 | 0.44 |
| 4:J:1307:LEU:CB | 4:J:1312:ALA:HB2 | 2.47 | 0.44 |
| 4:J:1347:LEU:O | 4:J:1351:VAL:HG23 | 2.18 | 0.44 |
| 5:K:51:LEU:HA | 5:K:51:LEU:HD13 | 1.67 | 0.44 |
| 5:K:76:GLU:O | 5:K:79:GLU:HB3 | 2.15 | 0.44 |
| 6:L:607:LEU:HD22 | 6:L:607:LEU:H | 1.82 | 0.44 |
| 7:O:41:DT:H2'' | 7:O:42:DA:OP2 | 2.17 | 0.44 |
| 8:P:68:DG:OP1 | 8:P:68:DG:H3' | 2.18 | 0.44 |
| 2:G:231:PHE:HZ | 2:H:201:LEU:CD2 | 2.30 | 0.44 |
| 2:H:32:GLU:HB3 | 2:H:35:PHE:CD2 | 2.50 | 0.44 |
| 2:H:211:ILE:HD11 | 2:H:215:GLU:CB | 2.48 | 0.44 |
| 3:I:230:PHE:CZ | 3:I:295:LYS:HG3 | 2.53 | 0.44 |
| 3:I:1277:ALA:HB3 | 4:J:434:ILE:HD12 | 1.99 | 0.44 |
| 4:J:201:LEU:HD23 | 4:J:201:LEU:HA | 1.65 | 0.44 |
| 6:L:167:ASP:HB2 | 6:L:212:ILE:N | 2.33 | 0.44 |
| 6:L:519:LEU:O | 6:L:519:LEU:HD23 | 2.18 | 0.44 |
| 6:L:540:LEU:HD23 | 6:L:610:PHE:CD2 | 2.52 | 0.44 |
| 2:G:124:VAL:O | 2:G:126:PRO:HD3 | 2.17 | 0.44 |
| 2:H:32:GLU:HG3 | 2:H:33:ARG:N | 2.32 | 0.44 |
| 2:H:47:LEU:CD2 | 2:H:220:ALA:HB2 | 2.47 | 0.44 |
| 3:I:217:THR:O | 3:I:221:LEU:HG | 2.17 | 0.44 |
| 3:I:221:LEU:HB3 | 3:I:336:LEU:CD2 | 2.47 | 0.44 |
| 3:I:985:GLU:HG2 | 3:I:988:LYS:HE2 | 2.00 | 0.44 |
| 4:J:514:THR:HG21 | 4:J:596:LEU:HD12 | 2.00 | 0.44 |
| 4:J:620:PHE:O | 4:J:624:ILE:HB | 2.18 | 0.44 |
| 4:J:1096:PRO:HB2 | 4:J:1098:GLN:OE1 | 2.18 | 0.44 |
| 4:J:1163:VAL:HA | 4:J:1177:ILE:HA | 1.97 | 0.44 |
| 4:J:1317:GLU:HG2 | 4:J:1318:SER:N | 2.32 | 0.44 |
| 6:L:254:GLU:O | 6:L:257:LYS:HB3 | 2.18 | 0.44 |
| 7:O:45:DA:H2'' | 7:O:46:DG:C5' | 2.48 | 0.44 |
| 2:G:79:LEU:O | 2:G:79:LEU:HD22 | 2.17 | 0.44 |
| 2:H:102:LEU:HB3 | 2:H:142:MET:CG | 2.47 | 0.44 |
| 3:I:252:SER:O | 3:I:252:SER:OG | 2.30 | 0.44 |
| 3:I:529:ARG:HD3 | 3:I:572:ILE:HG22 | 2.00 | 0.44 |
| 4:J:165:TYR:CD2 | 4:J:166:LEU:HD22 | 2.52 | 0.44 |
| 4:J:253:VAL:HG21 | 6:L:523:ILE:HD12 | 1.99 | 0.44 |
| 4:J:356:THR:HG23 | 4:J:446:ALA:CB | 2.47 | 0.44 |
| 4:J:557:LYS:HA | 4:J:562:GLU:O | 2.17 | 0.44 |
| 4:J:801:VAL:O | 4:J:805:GLN:HB2 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:J:1286:LYS:HE3 | 4:J:1286:LYS:HB3 | 1.89 | 0.44 |
| 5:K:59:ILE:CG2 | 5:K:64:LEU:HD11 | 2.47 | 0.44 |
| 6:L:148:TYR:CA | 6:L:161:LEU:HD11 | 2.44 | 0.44 |
| 6:L:231:THR:CG2 | 6:L:248:GLU:HB3 | 2.41 | 0.44 |
| 8:P:57:DT:H2" | 8:P:58:DC:H5" | 1.98 | 0.44 |
| 2:G:43:LEU:O | 2:G:47:LEU:HG | 2.17 | 0.44 |
| 2:G:47:LEU:HD23 | 2:G:220:ALA:HB2 | 1.99 | 0.44 |
| 2:G:48:LEU:HD23 | 2:G:48:LEU:HA | 1.70 | 0.44 |
| 2:G:83:LEU:HD23 | 3:I:694:ARG:CZ | 2.47 | 0.44 |
| 2:G:176:CYS:O | 2:G:178:SER:N | 2.51 | 0.44 |
| 3:I:58:PRO:HB3 | 3:I:69:GLN:HA | 1.99 | 0.44 |
| 3:I:106:GLU:HB2 | 3:I:109:ALA:HB3 | 2.00 | 0.44 |
| 3:I:269:ILE:HG23 | 3:I:273:HIS:HB2 | 2.00 | 0.44 |
| 3:I:283:LYS:O | 3:I:283:LYS:HG2 | 2.17 | 0.44 |
| 3:I:529:ARG:HG2 | 3:I:529:ARG:HH11 | 1.81 | 0.44 |
| 3:I:966:ILE:HG12 | 10:I:1401:1N7:H25 | 1.98 | 0.44 |
| 3:I:1035:LYS:HB2 | 3:I:1035:LYS:HE3 | 1.74 | 0.44 |
| 3:I:1103:VAL:HB | 3:I:1104:PRO:HD3 | 1.99 | 0.44 |
| 3:I:1119:MET:HB2 | 3:I:1228:GLY:HA2 | 2.00 | 0.44 |
| 3:I:1165:SER:O | 3:I:1168:GLU:HB2 | 2.18 | 0.44 |
| 3:I:1255:THR:O | 3:I:1257:GLN:N | 2.50 | 0.44 |
| 4:J:168:ALA:HA | 4:J:171:GLU:OE1 | 2.18 | 0.44 |
| 4:J:200:GLN:HG3 | 4:J:201:LEU:N | 2.33 | 0.44 |
| 4:J:338:PHE:CE1 | 4:J:1352:ILE:HD13 | 2.53 | 0.44 |
| 4:J:902:ASP:O | 4:J:903:LEU:HG | 2.17 | 0.44 |
| 4:J:919:ALA:HA | 4:J:1252:HIS:HD1 | 1.82 | 0.44 |
| 6:L:367:ILE:HD12 | 6:L:367:ILE:HA | 1.78 | 0.44 |
| 6:L:559:LEU:HD12 | 6:L:559:LEU:HA | 1.76 | 0.44 |
| 7:O:32:DA:H2" | 7:O:33:DA:OP2 | 2.17 | 0.44 |
| 8:P:66:DT:H2" | 8:P:67:DT:C6 | 2.53 | 0.44 |
| 2:H:31:LEU:HD12 | 2:H:35:PHE:HB3 | 2.00 | 0.44 |
| 2:H:207:THR:OG1 | 2:H:208:ASN:N | 2.50 | 0.44 |
| 3:I:563:THR:OG1 | 3:I:564:PRO:HD2 | 2.18 | 0.44 |
| 3:I:645:PHE:HB3 | 3:I:649:GLN:HG3 | 1.99 | 0.44 |
| 3:I:700:VAL:CG2 | 3:I:1117:LEU:HD23 | 2.48 | 0.44 |
| 3:I:817:LEU:HD23 | 3:I:817:LEU:HA | 1.65 | 0.44 |
| 3:I:894:GLN:HG3 | 3:I:895:LEU:H | 1.82 | 0.44 |
| 4:J:836:ARG:NH1 | 4:J:840:LEU:HD22 | 2.33 | 0.44 |
| 4:J:963:VAL:CG1 | 4:J:975:ILE:HG12 | 2.48 | 0.44 |
| 4:J:1011:VAL:CG1 | 4:J:1015:GLU:HB2 | 2.48 | 0.44 |
| 6:L:399:LEU:CD1 | 6:L:447:ALA:HB2 | 2.48 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:L:551:LEU:HB3 | 6:L:555:GLU:OE1 | 2.17 | 0.44 |
| 6:L:573:LEU:HG | 6:L:584:ARG:CG | 2.47 | 0.44 |
| 7:O:24:DC:H2'' | 7:O:25:DA:O4' | 2.18 | 0.44 |
| 2:G:14:VAL:HG22 | 2:G:27:THR:HB | 2.00 | 0.44 |
| 2:H:104:LYS:HG3 | 2:H:114:ASP:HB3 | 1.99 | 0.44 |
| 3:I:91:THR:HA | 3:I:137:VAL:O | 2.18 | 0.44 |
| 3:I:262:TYR:OH | 3:I:280:ASP:OD1 | 2.30 | 0.44 |
| 3:I:681:MET:HE3 | 3:I:1073:LYS:HE3 | 1.99 | 0.44 |
| 3:I:745:GLU:HB2 | 3:I:1017:GLN:HG3 | 2.00 | 0.44 |
| 3:I:820:GLU:O | 3:I:820:GLU:HG2 | 2.18 | 0.44 |
| 3:I:877:VAL:HG23 | 3:I:920:VAL:HG21 | 2.00 | 0.44 |
| 4:J:34:SER:OG | 4:J:36:GLY:O | 2.34 | 0.44 |
| 4:J:166:LEU:HA | 4:J:166:LEU:HD13 | 1.83 | 0.44 |
| 4:J:217:LEU:O | 4:J:217:LEU:HD13 | 2.18 | 0.44 |
| 4:J:900:GLY:HA3 | 4:J:1251:LYS:HE3 | 2.00 | 0.44 |
| 4:J:981:GLU:HG2 | 4:J:982:LEU:N | 2.33 | 0.44 |
| 6:L:399:LEU:HD23 | 6:L:403:ASP:HB3 | 2.00 | 0.44 |
| 6:L:453:PRO:HG2 | 7:O:44:DA:P | 2.57 | 0.44 |
| 6:L:574:GLU:HA | 6:L:584:ARG:CG | 2.48 | 0.44 |
| 2:G:31:LEU:HB2 | 2:G:199:ASP:O | 2.17 | 0.44 |
| 2:G:192:VAL:CG2 | 2:G:198:LEU:HD12 | 2.48 | 0.44 |
| 2:H:205:MET:HE3 | 2:H:213:PRO:HB3 | 2.00 | 0.44 |
| 3:I:144:VAL:HG21 | 3:I:527:LYS:HG2 | 2.00 | 0.44 |
| 3:I:622:ASN:C | 3:I:623:LEU:HD12 | 2.38 | 0.44 |
| 4:J:865:HIS:O | 4:J:869:CYS:HB2 | 2.18 | 0.44 |
| 5:K:48:VAL:O | 5:K:52:ARG:HG3 | 2.17 | 0.44 |
| 3:I:10:ARG:HD2 | 3:I:1181:PRO:CG | 2.48 | 0.43 |
| 3:I:1124:ILE:HD12 | 3:I:1198:LEU:HD21 | 2.00 | 0.43 |
| 4:J:104:HIS:HA | 4:J:242:LEU:O | 2.17 | 0.43 |
| 4:J:288:PRO:HB3 | 6:L:377:LYS:HB2 | 1.99 | 0.43 |
| 6:L:110:LEU:O | 6:L:110:LEU:HD12 | 2.17 | 0.43 |
| 6:L:330:LEU:HA | 6:L:333:VAL:CG1 | 2.44 | 0.43 |
| 6:L:415:ALA:HB2 | 6:L:434:TRP:CB | 2.48 | 0.43 |
| 2:M:277:TYR:HB2 | 2:M:280:ASP:CG | 2.38 | 0.43 |
| 2:M:282:VAL:HB | 2:M:313:SER:O | 2.18 | 0.43 |
| 2:G:23:HIS:HB2 | 2:G:206:GLU:HA | 1.99 | 0.43 |
| 3:I:228:VAL:C | 3:I:229:ILE:HD13 | 2.38 | 0.43 |
| 3:I:466:VAL:O | 3:I:469:VAL:HG22 | 2.18 | 0.43 |
| 3:I:1258:PRO:HG3 | 4:J:348:ASP:OD1 | 2.17 | 0.43 |
| 4:J:530:PRO:HB2 | 4:J:581:MET:HE2 | 1.98 | 0.43 |
| 4:J:905:ARG:N | 4:J:905:ARG:HD2 | 2.34 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:1115:ILE:HG21 | 4:J:1119:ASP:OD2 | 2.18 | 0.43 |
| 4:J:1145:PHE:HB3 | 4:J:1309:ILE:HD13 | 1.99 | 0.43 |
| 7:O:22:DT:H6 | 7:O:22:DT:H5' | 1.84 | 0.43 |
| 8:P:67:DT:H4' | 2:M:265:ARG:CZ | 2.49 | 0.43 |
| 2:M:255:ARG:O | 2:M:278:ILE:HG13 | 2.17 | 0.43 |
| 2:G:45:ARG:HD3 | 3:I:1083:GLU:CB | 2.48 | 0.43 |
| 3:I:250:THR:HG22 | 3:I:268:ARG:CB | 2.47 | 0.43 |
| 3:I:699:LEU:CB | 3:I:799:ASN:HD22 | 2.23 | 0.43 |
| 4:J:536:LEU:HD12 | 4:J:536:LEU:HA | 1.73 | 0.43 |
| 4:J:666:GLU:O | 4:J:669:GLN:HB2 | 2.18 | 0.43 |
| 4:J:697:MET:SD | 4:J:698:MET:HE2 | 2.59 | 0.43 |
| 4:J:965:SER:OG | 4:J:973:LEU:HG | 2.18 | 0.43 |
| 4:J:1078:LEU:CG | 4:J:1101:LEU:HD11 | 2.41 | 0.43 |
| 6:L:287:ILE:HD11 | 6:L:340:ALA:HB3 | 2.00 | 0.43 |
| 2:H:64:VAL:HG11 | 2:H:69:SER:HB2 | 1.99 | 0.43 |
| 2:H:65:LEU:O | 2:H:65:LEU:HD13 | 2.19 | 0.43 |
| 3:I:34:SER:OG | 3:I:455:SER:HB2 | 2.18 | 0.43 |
| 3:I:261:VAL:HG23 | 3:I:261:VAL:O | 2.18 | 0.43 |
| 3:I:528:ARG:NH2 | 3:I:575:LEU:HD23 | 2.34 | 0.43 |
| 3:I:1034:ARG:O | 3:I:1038:GLN:HB3 | 2.19 | 0.43 |
| 4:J:203:GLU:OE2 | 4:J:203:GLU:HA | 2.18 | 0.43 |
| 4:J:210:SER:HB2 | 4:J:213:LYS:CG | 2.49 | 0.43 |
| 4:J:421:VAL:HG13 | 4:J:439:PRO:CG | 2.48 | 0.43 |
| 4:J:623:GLN:O | 4:J:627:THR:HG22 | 2.18 | 0.43 |
| 4:J:1173:ARG:HD2 | 4:J:1174:ARG:O | 2.17 | 0.43 |
| 5:K:73:GLN:O | 5:K:77:ALA:N | 2.51 | 0.43 |
| 6:L:261:LEU:CB | 6:L:266:PHE:HB2 | 2.48 | 0.43 |
| 6:L:287:ILE:HG23 | 6:L:337:VAL:CG1 | 2.49 | 0.43 |
| 6:L:293:GLU:O | 6:L:293:GLU:HG2 | 2.19 | 0.43 |
| 6:L:571:TYR:HB2 | 6:L:576:VAL:HG22 | 2.00 | 0.43 |
| 2:G:49:SER:OG | 2:G:50:SER:OG | 2.14 | 0.43 |
| 3:I:196:VAL:HG21 | 3:I:209:ILE:CD1 | 2.48 | 0.43 |
| 3:I:615:VAL:HG13 | 3:I:615:VAL:O | 2.18 | 0.43 |
| 4:J:128:LEU:HD23 | 4:J:192:MET:HE1 | 2.00 | 0.43 |
| 4:J:644:MET:HE3 | 4:J:764:ARG:HB2 | 1.99 | 0.43 |
| 4:J:1109:LEU:HD11 | 4:J:1113:VAL:CG1 | 2.36 | 0.43 |
| 6:L:393:LYS:HA | 6:L:393:LYS:HD3 | 1.89 | 0.43 |
| 6:L:452:ILE:CG1 | 6:L:457:ILE:HG13 | 2.49 | 0.43 |
| 6:L:509:THR:HG23 | 6:L:509:THR:O | 2.19 | 0.43 |
| 6:L:593:LYS:HA | 6:L:596:ARG:HB2 | 1.99 | 0.43 |
| 2:M:300:LEU:HA | 2:M:303:ILE:CD1 | 2.34 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:154:PRO:HA | 2:G:174:ASP:HB3 | 1.99 | 0.43 |
| 2:H:51:MET:HB3 | 2:H:178:SER:HB2 | 1.99 | 0.43 |
| 2:H:109:PRO:HB3 | 2:H:132:HIS:HD2 | 1.83 | 0.43 |
| 2:H:140:ILE:HD12 | 2:H:140:ILE:HA | 1.79 | 0.43 |
| 2:H:192:VAL:HG23 | 2:H:192:VAL:O | 2.19 | 0.43 |
| 3:I:233:ARG:HB2 | 3:I:238:GLN:CD | 2.39 | 0.43 |
| 3:I:255:ILE:O | 3:I:262:TYR:N | 2.51 | 0.43 |
| 3:I:325:LEU:O | 3:I:328:SER:HB3 | 2.18 | 0.43 |
| 3:I:594:VAL:HG12 | 3:I:595:THR:O | 2.18 | 0.43 |
| 3:I:616:ILE:O | 3:I:636:CYS:HB3 | 2.17 | 0.43 |
| 3:I:883:LEU:HD11 | 3:I:920:VAL:HG22 | 2.01 | 0.43 |
| 3:I:1106:ARG:NH1 | 4:J:731:ARG:HH12 | 2.16 | 0.43 |
| 4:J:57:PHE:HZ | 4:J:266:ASN:HD21 | 1.67 | 0.43 |
| 4:J:294:ASN:ND2 | 6:L:406:GLN:HE21 | 2.16 | 0.43 |
| 4:J:819:GLY:CA | 4:J:882:VAL:O | 2.64 | 0.43 |
| 4:J:836:ARG:HH12 | 4:J:840:LEU:HD22 | 1.83 | 0.43 |
| 4:J:1149:ARG:HG2 | 4:J:1216:ALA:CB | 2.48 | 0.43 |
| 4:J:1219:ASP:O | 4:J:1223:LEU:HB2 | 2.19 | 0.43 |
| 6:L:102:MET:O | 6:L:105:MET:HG3 | 2.18 | 0.43 |
| 6:L:151:VAL:HG22 | 6:L:156:ALA:HB3 | 1.99 | 0.43 |
| 6:L:267:ASP:HA | 6:L:270:VAL:HB | 1.99 | 0.43 |
| 6:L:573:LEU:HD22 | 8:P:56:DG:OP2 | 2.18 | 0.43 |
| 8:P:67:DT:H2' | 8:P:68:DG:OP2 | 2.18 | 0.43 |
| 2:G:80:GLU:O | 2:G:80:GLU:HG2 | 2.18 | 0.43 |
| 3:I:205:PRO:O | 3:I:208:ILE:HG23 | 2.18 | 0.43 |
| 3:I:830:THR:HG23 | 3:I:832:HIS:CE1 | 2.53 | 0.43 |
| 3:I:1006:GLU:HA | 3:I:1009:ASN:HB3 | 1.99 | 0.43 |
| 3:I:1067:ALA:HB2 | 3:I:1073:LYS:HA | 2.01 | 0.43 |
| 3:I:1292:THR:HG22 | 3:I:1297:ASP:HB2 | 2.01 | 0.43 |
| 4:J:67:ASP:OD1 | 4:J:67:ASP:N | 2.45 | 0.43 |
| 4:J:418:GLU:HG3 | 5:K:48:VAL:CG2 | 2.49 | 0.43 |
| 4:J:438:GLU:OE2 | 4:J:481:ARG:NH2 | 2.43 | 0.43 |
| 6:L:280:VAL:HG11 | 6:L:355:ILE:CG2 | 2.49 | 0.43 |
| 8:P:56:DG:C2' | 8:P:57:DT:H71 | 2.43 | 0.43 |
| 8:P:60:DA:H2' | 8:P:61:DT:C5' | 2.48 | 0.43 |
| 2:H:78:ILE:HG12 | 2:H:81:ILE:HD12 | 2.01 | 0.43 |
| 2:H:134:THR:CG2 | 2:H:136:GLU:HB2 | 2.49 | 0.43 |
| 3:I:324:LYS:HA | 3:I:327:GLN:HG3 | 1.99 | 0.43 |
| 3:I:928:VAL:HG13 | 3:I:1052:VAL:HG13 | 2.01 | 0.43 |
| 4:J:68:TYR:C | 4:J:92:VAL:HG23 | 2.39 | 0.43 |
| 4:J:210:SER:OG | 4:J:213:LYS:HD2 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:759:ILE:HG23 | 4:J:771:GLN:HB3 | 2.00 | 0.43 |
| 4:J:847:ASP:HB3 | 4:J:856:ILE:HG23 | 1.99 | 0.43 |
| 6:L:143:TYR:CD2 | 6:L:269:LEU:HD21 | 2.53 | 0.43 |
| 6:L:569:THR:HG22 | 6:L:570:ASP:H | 1.84 | 0.43 |
| 3:I:43:PRO:C | 3:I:46:GLN:HE22 | 2.21 | 0.43 |
| 3:I:161:LYS:HD3 | 3:I:161:LYS:H | 1.83 | 0.43 |
| 3:I:624:ASP:OD1 | 3:I:628:HIS:HB2 | 2.18 | 0.43 |
| 3:I:646:SER:H | 3:I:649:GLN:NE2 | 2.15 | 0.43 |
| 3:I:934:PHE:O | 3:I:1049:ILE:N | 2.47 | 0.43 |
| 3:I:1075:VAL:HG12 | 4:J:461:PHE:HB3 | 2.01 | 0.43 |
| 7:O:69:DT:H2'' | 7:O:70:DT:O5' | 2.19 | 0.43 |
| 2:G:73:GLY:O | 2:G:134:THR:N | 2.44 | 0.43 |
| 2:G:79:LEU:HD23 | 2:G:79:LEU:HA | 1.75 | 0.43 |
| 3:I:104:ILE:HD11 | 3:I:116:ASP:HB2 | 2.00 | 0.43 |
| 3:I:136:PHE:HD2 | 3:I:145:ILE:HD13 | 1.83 | 0.43 |
| 3:I:184:LEU:HG | 3:I:185:ASP:N | 2.34 | 0.43 |
| 3:I:1002:LEU:HD21 | 3:I:1007:LYS:HB3 | 2.00 | 0.43 |
| 4:J:22:ILE:HG22 | 4:J:1340:LYS:O | 2.19 | 0.43 |
| 4:J:365:GLN:HA | 4:J:438:GLU:H | 1.84 | 0.43 |
| 4:J:1361:THR:HG21 | 5:K:20:VAL:HG11 | 2.01 | 0.43 |
| 6:L:414:LYS:HE3 | 6:L:434:TRP:CZ3 | 2.54 | 0.43 |
| 8:P:17:DA:H2'' | 8:P:18:DT:O5' | 2.19 | 0.43 |
| 2:M:285:THR:HG22 | 2:M:286:GLU:H | 1.83 | 0.43 |
| 3:I:658:GLN:HG2 | 3:I:658:GLN:O | 2.19 | 0.42 |
| 4:J:45:ASN:HB3 | 4:J:48:THR:O | 2.18 | 0.42 |
| 4:J:190:LYS:HE3 | 4:J:190:LYS:HB3 | 1.83 | 0.42 |
| 4:J:831:VAL:HG12 | 4:J:833:GLU:N | 2.23 | 0.42 |
| 4:J:859:PRO:HG2 | 4:J:862:THR:HG21 | 2.00 | 0.42 |
| 4:J:972:LYS:CD | 4:J:1002:VAL:HB | 2.39 | 0.42 |
| 4:J:1316:THR:HG22 | 4:J:1318:SER:H | 1.84 | 0.42 |
| 2:G:25:LYS:HA | 2:G:203:ILE:O | 2.19 | 0.42 |
| 2:G:201:LEU:HD12 | 2:G:202:VAL:N | 2.34 | 0.42 |
| 3:I:35:PHE:CD2 | 3:I:130:MET:HB3 | 2.54 | 0.42 |
| 3:I:181:GLY:CA | 3:I:395:TYR:HA | 2.49 | 0.42 |
| 3:I:741:MET:CG | 3:I:746:ALA:HB1 | 2.46 | 0.42 |
| 3:I:777:VAL:HG11 | 3:I:783:LEU:CD2 | 2.49 | 0.42 |
| 3:I:812:PHE:CE2 | 3:I:813:GLU:HG2 | 2.53 | 0.42 |
| 3:I:823:VAL:HG22 | 3:I:1060:ILE:HG21 | 2.00 | 0.42 |
| 3:I:1149:TYR:CD2 | 3:I:1159:VAL:HG11 | 2.54 | 0.42 |
| 4:J:260:PHE:CB | 6:L:504:PRO:HB3 | 2.49 | 0.42 |
| 4:J:343:LEU:HD11 | 4:J:1352:ILE:HG12 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:649:LYS:O | 4:J:653:ILE:HB | 2.19 | 0.42 |
| 6:L:276:MET:SD | 6:L:279:ARG:NH2 | 2.92 | 0.42 |
| 8:P:20:DC:H2" | 8:P:21:DA:H8 | 1.83 | 0.42 |
| 2:M:261:GLU:OE2 | 2:M:261:GLU:HA | 2.19 | 0.42 |
| 3:I:232:ILE:HG12 | 3:I:237:LEU:HD13 | 2.02 | 0.42 |
| 3:I:1058:ARG:HE | 3:I:1058:ARG:HB3 | 1.44 | 0.42 |
| 3:I:1122:LYS:HG2 | 3:I:1229:TYR:CZ | 2.54 | 0.42 |
| 4:J:54:ASP:HB2 | 4:J:61:ILE:CD1 | 2.49 | 0.42 |
| 4:J:363:LEU:HD12 | 4:J:363:LEU:O | 2.19 | 0.42 |
| 4:J:369:PRO:HG2 | 4:J:372:MET:HB2 | 2.01 | 0.42 |
| 4:J:529:GLY:HA2 | 4:J:551:ARG:O | 2.19 | 0.42 |
| 4:J:612:LEU:HA | 4:J:612:LEU:HD12 | 1.83 | 0.42 |
| 4:J:660:GLU:OE2 | 4:J:685:ILE:HB | 2.19 | 0.42 |
| 4:J:674:THR:OG1 | 4:J:675:ALA:N | 2.52 | 0.42 |
| 4:J:1036:ARG:HE | 4:J:1081:VAL:HG21 | 1.84 | 0.42 |
| 4:J:1037:PHE:HB3 | 4:J:1040:MET:SD | 2.59 | 0.42 |
| 4:J:1163:VAL:CG2 | 4:J:1175:LEU:HD11 | 2.49 | 0.42 |
| 6:L:584:ARG:HA | 6:L:587:ILE:HG13 | 2.00 | 0.42 |
| 1:N:49:ARG:CZ | 1:N:49:ARG:HB3 | 2.49 | 0.42 |
| 2:G:224:LEU:HD23 | 2:H:228:LEU:CD1 | 2.48 | 0.42 |
| 2:H:49:SER:O | 2:H:151:GLY:HA3 | 2.19 | 0.42 |
| 3:I:346:TYR:CE1 | 3:I:436:ARG:HG3 | 2.55 | 0.42 |
| 3:I:826:ASP:OD1 | 3:I:829:THR:HG21 | 2.19 | 0.42 |
| 3:I:854:ILE:CG2 | 3:I:915:ASP:HB2 | 2.50 | 0.42 |
| 3:I:1332:SER:CB | 4:J:245:LEU:HD13 | 2.50 | 0.42 |
| 4:J:374:LEU:O | 4:J:374:LEU:HG | 2.19 | 0.42 |
| 4:J:474:LEU:CD1 | 5:K:47:THR:HG22 | 2.49 | 0.42 |
| 4:J:766:GLY:O | 4:J:767:LEU:HD12 | 2.18 | 0.42 |
| 4:J:814:CYS:SG | 4:J:816:THR:HG22 | 2.60 | 0.42 |
| 4:J:1067:ARG:HG3 | 4:J:1068:THR:O | 2.20 | 0.42 |
| 4:J:1163:VAL:HG22 | 4:J:1175:LEU:HD11 | 2.00 | 0.42 |
| 4:J:1248:ILE:HG22 | 4:J:1249:ASN:N | 2.34 | 0.42 |
| 6:L:226:ALA:HA | 6:L:229:VAL:HG22 | 2.00 | 0.42 |
| 6:L:463:LEU:HA | 6:L:463:LEU:HD23 | 1.58 | 0.42 |
| 3:I:211:ARG:HH11 | 3:I:220:ILE:HD12 | 1.85 | 0.42 |
| 3:I:216:THR:HG22 | 3:I:219:GLN:HB2 | 2.02 | 0.42 |
| 3:I:359:ARG:HH22 | 3:I:382:GLU:CG | 2.31 | 0.42 |
| 3:I:397:LEU:N | 3:I:418:GLY:O | 2.53 | 0.42 |
| 3:I:470:ARG:HD3 | 3:I:470:ARG:HA | 1.65 | 0.42 |
| 3:I:757:THR:CG2 | 3:I:765:ILE:HG12 | 2.49 | 0.42 |
| 3:I:1141:LEU:HD12 | 3:I:1141:LEU:HA | 1.61 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:I:1256:GLN:OE1 | 6:L:528:LEU:HD23 | 2.19 | 0.42 |
| 4:J:418:GLU:HB2 | 5:K:45:LYS:CG | 2.49 | 0.42 |
| 4:J:454:CYS:HG | 4:J:461:PHE:HZ | 1.64 | 0.42 |
| 4:J:500:ILE:HG22 | 4:J:500:ILE:O | 2.19 | 0.42 |
| 4:J:822:MET:HE2 | 4:J:838:ARG:O | 2.20 | 0.42 |
| 4:J:1025:MET:SD | 4:J:1126:GLN:HG2 | 2.59 | 0.42 |
| 4:J:1032:SER:CB | 4:J:1116:SER:HA | 2.49 | 0.42 |
| 6:L:582:VAL:CG2 | 6:L:586:ARG:HB3 | 2.49 | 0.42 |
| 2:H:151:GLY:O | 2:H:177:TYR:HB2 | 2.20 | 0.42 |
| 2:H:152:TYR:HE2 | 2:H:154:PRO:HG3 | 1.84 | 0.42 |
| 3:I:5:TYR:CD2 | 3:I:776:PRO:HG2 | 2.54 | 0.42 |
| 3:I:127:ILE:O | 3:I:127:ILE:HG13 | 2.19 | 0.42 |
| 3:I:241:LEU:HD13 | 3:I:285:ILE:HG12 | 2.02 | 0.42 |
| 3:I:794:LEU:CD2 | 3:I:796:LEU:HD21 | 2.46 | 0.42 |
| 4:J:370:LYS:HZ3 | 4:J:441:LEU:HB3 | 1.84 | 0.42 |
| 4:J:475:GLU:H | 4:J:475:GLU:HG3 | 1.64 | 0.42 |
| 4:J:804:ALA:O | 4:J:916:GLY:HA3 | 2.20 | 0.42 |
| 4:J:999:TYR:CD2 | 4:J:1026:PRO:HG2 | 2.54 | 0.42 |
| 4:J:1281:GLU:HG2 | 4:J:1283:SER:H | 1.84 | 0.42 |
| 4:J:1347:LEU:HG | 4:J:1357:ILE:HG23 | 2.02 | 0.42 |
| 6:L:138:PRO:HG2 | 6:L:351:THR:O | 2.19 | 0.42 |
| 6:L:157:ARG:HG2 | 6:L:158:LEU:N | 2.35 | 0.42 |
| 7:O:22:DT:H2'' | 7:O:23:DC:OP2 | 2.19 | 0.42 |
| 7:O:74:DC:H5' | 7:O:74:DC:H6 | 1.85 | 0.42 |
| 2:M:253:LEU:CD1 | 2:M:282:VAL:HG21 | 2.49 | 0.42 |
| 2:M:300:LEU:HD22 | 2:M:303:ILE:HB | 2.01 | 0.42 |
| 1:N:21:ASN:O | 1:N:25:GLN:HG3 | 2.20 | 0.42 |
| 2:G:224:LEU:CD2 | 2:H:228:LEU:HD11 | 2.46 | 0.42 |
| 2:H:74:VAL:HG22 | 2:H:133:LEU:HD21 | 2.02 | 0.42 |
| 3:I:76:GLY:N | 3:I:95:PRO:O | 2.44 | 0.42 |
| 3:I:82:VAL:HG22 | 3:I:92:TYR:CD2 | 2.54 | 0.42 |
| 3:I:99:LYS:HE2 | 3:I:99:LYS:HB2 | 1.82 | 0.42 |
| 3:I:117:ILE:C | 3:I:118:LYS:HG3 | 2.40 | 0.42 |
| 3:I:811:ASN:HA | 3:I:815:SER:HB2 | 2.00 | 0.42 |
| 3:I:1002:LEU:HG | 3:I:1007:LYS:HB2 | 2.01 | 0.42 |
| 3:I:1080:ASN:OD1 | 3:I:1081:PRO:HD2 | 2.19 | 0.42 |
| 4:J:130:MET:O | 4:J:135:ILE:HD11 | 2.19 | 0.42 |
| 4:J:255:LEU:HA | 4:J:255:LEU:HD22 | 1.82 | 0.42 |
| 4:J:551:ARG:O | 4:J:551:ARG:HG2 | 2.19 | 0.42 |
| 4:J:698:MET:O | 4:J:702:GLN:HG2 | 2.19 | 0.42 |
| 4:J:1181:ASP:N | 4:J:1181:ASP:OD1 | 2.51 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:1306:LEU:HG | 4:J:1307:LEU:N | 2.34 | 0.42 |
| 4:J:1314:LEU:HD21 | 4:J:1326:GLN:CB | 2.50 | 0.42 |
| 6:L:126:GLY:O | 6:L:129:GLN:HG3 | 2.20 | 0.42 |
| 6:L:253:SER:O | 6:L:256:PHE:HB2 | 2.19 | 0.42 |
| 1:N:48:ARG:HG2 | 4:J:672:LEU:O | 2.19 | 0.42 |
| 2:G:57:THR:CB | 2:G:147:GLN:HE21 | 2.32 | 0.42 |
| 2:G:229:GLU:O | 2:G:232:VAL:HG12 | 2.19 | 0.42 |
| 2:H:120:ASP:OD1 | 2:H:121:VAL:HG13 | 2.19 | 0.42 |
| 2:H:200:LYS:HG2 | 2:H:200:LYS:O | 2.19 | 0.42 |
| 3:I:245:ARG:HB3 | 3:I:337:PHE:CE2 | 2.55 | 0.42 |
| 3:I:817:LEU:HD13 | 3:I:1085:MET:CE | 2.50 | 0.42 |
| 3:I:914:LYS:HE2 | 3:I:914:LYS:HB3 | 1.62 | 0.42 |
| 3:I:1243:MET:CE | 4:J:445:LYS:HD3 | 2.50 | 0.42 |
| 3:I:1253:LEU:HA | 3:I:1253:LEU:HD23 | 1.65 | 0.42 |
| 3:I:1320:PRO:HB2 | 4:J:345:LYS:NZ | 2.34 | 0.42 |
| 4:J:650:LYS:O | 4:J:654:ILE:HG23 | 2.20 | 0.42 |
| 4:J:1048:ARG:HH22 | 4:J:1057:SER:CB | 2.33 | 0.42 |
| 4:J:1347:LEU:HG | 4:J:1357:ILE:CG2 | 2.50 | 0.42 |
| 6:L:280:VAL:HG11 | 6:L:355:ILE:HG23 | 2.02 | 0.42 |
| 6:L:344:LEU:CD1 | 6:L:355:ILE:HG13 | 2.49 | 0.42 |
| 6:L:390:ILE:HD12 | 6:L:435:ILE:HG21 | 2.01 | 0.42 |
| 7:O:29:DA:H2' | 7:O:30:DC:H6 | 1.85 | 0.42 |
| 2:M:275:ILE:HG22 | 2:M:280:ASP:CB | 2.31 | 0.42 |
| 2:M:318:LEU:HG | 2:M:319:GLU:H | 1.85 | 0.42 |
| 2:H:11:PRO:HB2 | 2:H:28:LEU:CD1 | 2.50 | 0.42 |
| 2:H:23:HIS:CB | 2:H:206:GLU:HG2 | 2.39 | 0.42 |
| 3:I:213:LEU:HD21 | 3:I:422:LYS:O | 2.20 | 0.42 |
| 3:I:371:ARG:HD2 | 3:I:371:ARG:HA | 1.80 | 0.42 |
| 3:I:1268:GLN:NE2 | 4:J:352:ARG:HE | 2.18 | 0.42 |
| 4:J:500:ILE:HG23 | 4:J:500:ILE:HD12 | 1.77 | 0.42 |
| 4:J:1155:ILE:HD11 | 4:J:1211:SER:H | 1.84 | 0.42 |
| 4:J:1322:ALA:CB | 4:J:1331:VAL:HG11 | 2.48 | 0.42 |
| 5:K:21:LEU:HD23 | 5:K:21:LEU:HA | 1.82 | 0.42 |
| 6:L:129:GLN:NE2 | 6:L:130:VAL:HG23 | 2.34 | 0.42 |
| 6:L:336:GLU:O | 6:L:339:ARG:HB2 | 2.20 | 0.42 |
| 6:L:401:PHE:CZ | 6:L:405:ILE:HD11 | 2.54 | 0.42 |
| 2:G:185:TYR:HB2 | 2:G:201:LEU:HD11 | 2.02 | 0.42 |
| 2:G:191:ARG:H | 2:G:191:ARG:HD2 | 1.84 | 0.42 |
| 3:I:269:ILE:HG22 | 3:I:274:ILE:HD11 | 2.02 | 0.42 |
| 3:I:551:HIS:ND1 | 3:I:552:PRO:HD2 | 2.34 | 0.42 |
| 4:J:412:LEU:O | 4:J:416:ILE:HG12 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:J:499:ILE:HA | 4:J:499:ILE:HD12 | 1.83 | 0.42 |
| 4:J:505:ASP:HB2 | 4:J:629:PHE:HE1 | 1.85 | 0.42 |
| 4:J:622:ASP:OD2 | 4:J:622:ASP:N | 2.51 | 0.42 |
| 4:J:686:TRP:CE3 | 4:J:686:TRP:HA | 2.54 | 0.42 |
| 4:J:932:MET:HG2 | 4:J:933:ARG:HG3 | 2.02 | 0.42 |
| 8:P:19:DT:H2'' | 8:P:20:DC:H6 | 1.85 | 0.42 |
| 2:G:27:THR:CG2 | 2:G:200:LYS:HG3 | 2.50 | 0.41 |
| 2:G:102:LEU:HB3 | 2:G:142:MET:HG3 | 2.01 | 0.41 |
| 2:G:222:THR:CB | 2:H:232:VAL:HG13 | 2.50 | 0.41 |
| 2:H:211:ILE:HD11 | 2:H:215:GLU:HG3 | 2.02 | 0.41 |
| 3:I:38:PHE:HA | 3:I:48:GLY:HA2 | 2.00 | 0.41 |
| 3:I:104:ILE:C | 3:I:114:VAL:HG12 | 2.41 | 0.41 |
| 3:I:184:LEU:HD21 | 3:I:186:PHE:HE2 | 1.84 | 0.41 |
| 3:I:402:ARG:NH2 | 3:I:424:ASP:OD1 | 2.52 | 0.41 |
| 3:I:813:GLU:HB2 | 4:J:461:PHE:HD2 | 1.85 | 0.41 |
| 3:I:1063:GLY:HA2 | 3:I:1075:VAL:CG2 | 2.50 | 0.41 |
| 4:J:809:VAL:HG23 | 4:J:915:ILE:HG23 | 2.02 | 0.41 |
| 4:J:824:PRO:CB | 4:J:831:VAL:HG11 | 2.50 | 0.41 |
| 6:L:140:ALA:CB | 6:L:269:LEU:HD13 | 2.31 | 0.41 |
| 6:L:261:LEU:HB2 | 6:L:266:PHE:CD1 | 2.49 | 0.41 |
| 6:L:344:LEU:O | 6:L:347:ILE:HB | 2.20 | 0.41 |
| 6:L:602:SER:O | 6:L:603:ARG:HD2 | 2.20 | 0.41 |
| 7:O:34:DA:H1' | 7:O:35:DG:C8 | 2.56 | 0.41 |
| 2:M:287:VAL:HA | 2:M:290:LEU:HB3 | 2.02 | 0.41 |
| 2:G:154:PRO:C | 2:G:158:ARG:HG3 | 2.41 | 0.41 |
| 3:I:115:LYS:HZ2 | 3:I:484:LEU:HB3 | 1.84 | 0.41 |
| 3:I:136:PHE:CE2 | 3:I:145:ILE:HD13 | 2.55 | 0.41 |
| 3:I:274:ILE:H | 3:I:274:ILE:HD12 | 1.85 | 0.41 |
| 3:I:346:TYR:CE2 | 3:I:433:ILE:HG23 | 2.55 | 0.41 |
| 3:I:360:LEU:HA | 3:I:360:LEU:HD23 | 1.66 | 0.41 |
| 3:I:432:LEU:HA | 3:I:432:LEU:HD12 | 1.74 | 0.41 |
| 3:I:848:GLU:OE1 | 3:I:888:THR:HG22 | 2.19 | 0.41 |
| 3:I:1290:MET:HG3 | 3:I:1294:LYS:HE2 | 2.02 | 0.41 |
| 4:J:69:GLU:CG | 4:J:76:LYS:HG2 | 2.44 | 0.41 |
| 4:J:127:LEU:O | 4:J:127:LEU:HD12 | 2.20 | 0.41 |
| 4:J:210:SER:HB2 | 4:J:213:LYS:HB2 | 2.02 | 0.41 |
| 4:J:255:LEU:HD21 | 6:L:523:ILE:HD11 | 2.02 | 0.41 |
| 4:J:409:TRP:HA | 4:J:409:TRP:CE3 | 2.55 | 0.41 |
| 4:J:709:ARG:NH1 | 4:J:710:ASP:HB3 | 2.34 | 0.41 |
| 4:J:843:VAL:HG22 | 4:J:863:LEU:HA | 2.01 | 0.41 |
| 4:J:985:ILE:CD1 | 4:J:991:THR:HG22 | 2.48 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:1007:ASP:N | 4:J:1007:ASP:OD2 | 2.50 | 0.41 |
| 4:J:1082:ASP:OD2 | 4:J:1084:GLN:HB2 | 2.20 | 0.41 |
| 6:L:491:GLU:HG2 | 6:L:491:GLU:O | 2.20 | 0.41 |
| 2:G:192:VAL:HG21 | 2:G:198:LEU:HD12 | 2.03 | 0.41 |
| 3:I:238:GLN:HA | 3:I:286:GLU:HA | 2.01 | 0.41 |
| 3:I:241:LEU:HD23 | 3:I:282:VAL:HG23 | 2.02 | 0.41 |
| 3:I:358:ASP:OD1 | 3:I:358:ASP:N | 2.52 | 0.41 |
| 3:I:623:LEU:HD11 | 3:I:653:MET:CE | 2.49 | 0.41 |
| 3:I:840:SER:O | 3:I:1047:LEU:HB2 | 2.20 | 0.41 |
| 3:I:898:GLU:OE2 | 6:L:541:ARG:HA | 2.21 | 0.41 |
| 4:J:113:HIS:HB3 | 4:J:116:PHE:HD2 | 1.85 | 0.41 |
| 4:J:193:ASP:OD2 | 4:J:196:GLN:HG2 | 2.20 | 0.41 |
| 4:J:902:ASP:C | 4:J:903:LEU:HG | 2.41 | 0.41 |
| 4:J:959:LYS:HD2 | 4:J:959:LYS:HA | 1.76 | 0.41 |
| 4:J:1170:LYS:CD | 4:J:1174:ARG:HH21 | 2.33 | 0.41 |
| 4:J:1178:THR:HG22 | 4:J:1184:ASP:O | 2.21 | 0.41 |
| 4:J:1230:THR:HG23 | 4:J:1231:ARG:H | 1.85 | 0.41 |
| 6:L:142:THR:O | 6:L:146:GLU:HG2 | 2.20 | 0.41 |
| 2:M:321:TRP:CE3 | 2:M:322:PRO:HA | 2.56 | 0.41 |
| 1:N:14:GLN:HB2 | 10:N:102:1N7:C21 | 2.50 | 0.41 |
| 2:H:14:VAL:HG13 | 2:H:28:LEU:HD13 | 2.01 | 0.41 |
| 2:H:77:ASP:HB3 | 2:H:79:LEU:CD2 | 2.51 | 0.41 |
| 2:H:195:ARG:NH1 | 2:H:198:LEU:HD11 | 2.35 | 0.41 |
| 3:I:59:ILE:HD12 | 3:I:475:VAL:HB | 2.02 | 0.41 |
| 3:I:204:LEU:HD11 | 3:I:369:MET:HE2 | 2.01 | 0.41 |
| 3:I:369:MET:SD | 3:I:370:MET:HG2 | 2.60 | 0.41 |
| 3:I:520:PRO:HB2 | 3:I:794:LEU:HD13 | 2.02 | 0.41 |
| 4:J:269:TYR:O | 4:J:273:ILE:HG13 | 2.21 | 0.41 |
| 4:J:447:ILE:HD11 | 4:J:468:VAL:CG2 | 2.50 | 0.41 |
| 4:J:502:PRO:HB3 | 4:J:506:VAL:CB | 2.50 | 0.41 |
| 2:H:153:VAL:HA | 2:H:154:PRO:HD3 | 1.91 | 0.41 |
| 3:I:10:ARG:HG3 | 3:I:1176:LEU:CD2 | 2.51 | 0.41 |
| 3:I:229:ILE:HG23 | 3:I:334:GLU:HG2 | 2.03 | 0.41 |
| 3:I:288:PRO:O | 3:I:292:ILE:HG13 | 2.19 | 0.41 |
| 3:I:546:GLU:O | 3:I:546:GLU:HG2 | 2.20 | 0.41 |
| 3:I:672:GLU:OE1 | 3:I:672:GLU:N | 2.40 | 0.41 |
| 3:I:1290:MET:HA | 3:I:1294:LYS:HG3 | 2.03 | 0.41 |
| 4:J:26:SER:O | 4:J:29:MET:HB3 | 2.20 | 0.41 |
| 4:J:73:GLY:CA | 4:J:76:LYS:HE2 | 2.50 | 0.41 |
| 4:J:107:LEU:HA | 4:J:276:ASN:HD21 | 1.85 | 0.41 |
| 4:J:474:LEU:HD11 | 5:K:47:THR:HG22 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:811:GLU:HG3 | 4:J:812:ASP:H | 1.85 | 0.41 |
| 4:J:990:ARG:HA | 4:J:990:ARG:HD2 | 1.88 | 0.41 |
| 4:J:1250:ASP:O | 4:J:1254:GLU:HG3 | 2.21 | 0.41 |
| 5:K:39:VAL:CG2 | 5:K:40:PRO:HD2 | 2.51 | 0.41 |
| 6:L:119:ILE:CG2 | 6:L:375:ALA:HB1 | 2.35 | 0.41 |
| 6:L:316:PHE:HZ | 6:L:333:VAL:HG13 | 1.86 | 0.41 |
| 2:M:264:VAL:HG12 | 2:M:268:ASN:ND2 | 2.36 | 0.41 |
| 2:M:270:LEU:HD21 | 2:M:275:ILE:O | 2.20 | 0.41 |
| 2:G:134:THR:HG22 | 3:I:773:LEU:HD12 | 2.01 | 0.41 |
| 2:H:44:ARG:O | 2:H:48:LEU:HB2 | 2.21 | 0.41 |
| 3:I:147:SER:HB3 | 3:I:454:ARG:O | 2.20 | 0.41 |
| 3:I:169:LYS:HD3 | 3:I:436:ARG:NH2 | 2.35 | 0.41 |
| 3:I:229:ILE:HG23 | 3:I:334:GLU:CG | 2.50 | 0.41 |
| 3:I:446:ASP:HA | 3:I:451:ARG:HD2 | 2.03 | 0.41 |
| 3:I:905:ILE:HD12 | 3:I:905:ILE:HA | 1.90 | 0.41 |
| 4:J:180:MET:HE2 | 4:J:180:MET:HB2 | 1.82 | 0.41 |
| 4:J:198:CYS:HA | 4:J:221:ILE:CD1 | 2.50 | 0.41 |
| 4:J:282:LEU:HD23 | 4:J:282:LEU:HA | 1.86 | 0.41 |
| 4:J:387:LEU:HA | 4:J:387:LEU:HD23 | 1.86 | 0.41 |
| 4:J:423:LEU:HD23 | 4:J:449:LEU:HD12 | 2.02 | 0.41 |
| 4:J:438:GLU:HA | 4:J:439:PRO:HD3 | 1.93 | 0.41 |
| 4:J:683:ILE:HD13 | 4:J:683:ILE:HA | 1.88 | 0.41 |
| 4:J:735:ALA:O | 4:J:738:ARG:HB3 | 2.19 | 0.41 |
| 4:J:1107:VAL:CG1 | 4:J:1122:ALA:HB2 | 2.40 | 0.41 |
| 4:J:1145:PHE:HB3 | 4:J:1309:ILE:HG21 | 2.01 | 0.41 |
| 4:J:1155:ILE:HG12 | 4:J:1190:ILE:HD11 | 2.02 | 0.41 |
| 4:J:1230:THR:HG23 | 4:J:1231:ARG:N | 2.36 | 0.41 |
| 6:L:586:ARG:NE | 7:O:25:DA:H5" | 2.31 | 0.41 |
| 1:N:5:ALA:HB3 | 3:I:678:ARG:CZ | 2.51 | 0.41 |
| 3:I:27:LEU:HG | 3:I:711:ASP:OD2 | 2.20 | 0.41 |
| 3:I:135:THR:HG21 | 3:I:515:MET:SD | 2.61 | 0.41 |
| 3:I:151:ARG:CZ | 3:I:445:ILE:HG21 | 2.50 | 0.41 |
| 3:I:414:ILE:H | 3:I:414:ILE:HG12 | 1.70 | 0.41 |
| 3:I:452:ARG:HH11 | 3:I:452:ARG:HD3 | 1.74 | 0.41 |
| 3:I:699:LEU:HD13 | 3:I:1121:ALA:HB3 | 2.02 | 0.41 |
| 3:I:1063:GLY:O | 3:I:1075:VAL:HG23 | 2.21 | 0.41 |
| 4:J:744:ARG:HE | 4:J:744:ARG:HB2 | 1.48 | 0.41 |
| 4:J:956:GLY:HA2 | 4:J:986:ASP:HA | 2.03 | 0.41 |
| 4:J:1168:GLU:HA | 4:J:1173:ARG:HG2 | 2.02 | 0.41 |
| 6:L:571:TYR:HB3 | 6:L:575:GLU:HB3 | 2.01 | 0.41 |
| 7:O:23:DC:N4 | 8:P:63:DG:O6 | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:N:34:VAL:HG21 | 1:N:56:THR:HA | 2.03 | 0.41 |
| 2:G:230:ALA:CB | 2:H:11:PRO:HD2 | 2.51 | 0.41 |
| 3:I:75:LEU:HD11 | 3:I:127:ILE:HD11 | 2.03 | 0.41 |
| 3:I:86:GLN:HA | 3:I:140:GLY:HA2 | 2.02 | 0.41 |
| 3:I:126:GLU:O | 3:I:126:GLU:HG2 | 2.21 | 0.41 |
| 3:I:296:VAL:O | 3:I:336:LEU:N | 2.47 | 0.41 |
| 3:I:803:ALA:HB2 | 3:I:1227:VAL:HG13 | 2.03 | 0.41 |
| 3:I:899:GLU:HA | 3:I:899:GLU:OE2 | 2.20 | 0.41 |
| 4:J:747:MET:HG2 | 4:J:759:ILE:HG12 | 2.03 | 0.41 |
| 4:J:901:ARG:HG3 | 4:J:902:ASP:O | 2.21 | 0.41 |
| 6:L:136:GLU:OE1 | 6:L:361:ILE:HG12 | 2.20 | 0.41 |
| 6:L:265:GLN:O | 6:L:268:TYR:HB3 | 2.21 | 0.41 |
| 6:L:347:ILE:O | 6:L:350:GLU:HB2 | 2.20 | 0.41 |
| 6:L:470:MET:HG2 | 6:L:486:ARG:HH11 | 1.86 | 0.41 |
| 7:O:25:DA:H2' | 7:O:26:DT:H6 | 1.85 | 0.41 |
| 7:O:46:DG:H8 | 7:O:46:DG:H5' | 1.86 | 0.41 |
| 2:G:8:PHE:C | 2:G:9:LEU:HD23 | 2.40 | 0.41 |
| 2:G:74:VAL:HA | 2:G:132:HIS:O | 2.21 | 0.41 |
| 2:G:198:LEU:HD23 | 2:G:198:LEU:HA | 1.76 | 0.41 |
| 2:H:16:ILE:HD11 | 2:H:214:GLU:HB3 | 2.01 | 0.41 |
| 2:H:157:THR:HG22 | 2:H:157:THR:O | 2.21 | 0.41 |
| 2:H:178:SER:HA | 2:H:179:PRO:HD3 | 1.88 | 0.41 |
| 3:I:100:LEU:HD23 | 3:I:100:LEU:HA | 1.73 | 0.41 |
| 3:I:201:ARG:HH12 | 3:I:372:PRO:HG3 | 1.84 | 0.41 |
| 3:I:379:GLU:OE1 | 3:I:382:GLU:HB3 | 2.21 | 0.41 |
| 3:I:696:ASP:O | 3:I:697:LYS:HB3 | 2.21 | 0.41 |
| 3:I:1293:VAL:HG11 | 3:I:1304:MET:HG2 | 2.03 | 0.41 |
| 3:I:1326:LEU:HD11 | 4:J:331:ILE:HG23 | 2.01 | 0.41 |
| 4:J:159:ILE:O | 4:J:160:LEU:HD23 | 2.21 | 0.41 |
| 4:J:180:MET:CE | 4:J:293:ARG:HE | 2.31 | 0.41 |
| 4:J:198:CYS:CA | 4:J:221:ILE:HD11 | 2.51 | 0.41 |
| 4:J:307:LEU:HD23 | 4:J:307:LEU:HA | 1.83 | 0.41 |
| 4:J:334:LYS:HE2 | 4:J:339:ARG:HH21 | 1.85 | 0.41 |
| 4:J:338:PHE:O | 4:J:343:LEU:HD22 | 2.20 | 0.41 |
| 4:J:364:HIS:CD2 | 5:K:4:VAL:HG12 | 2.56 | 0.41 |
| 4:J:490:ILE:HD11 | 4:J:609:TYR:CE1 | 2.56 | 0.41 |
| 4:J:504:GLN:OE1 | 4:J:731:ARG:NH2 | 2.54 | 0.41 |
| 4:J:649:LYS:O | 4:J:653:ILE:HD13 | 2.20 | 0.41 |
| 4:J:919:ALA:HB2 | 4:J:1255:VAL:HG11 | 2.02 | 0.41 |
| 4:J:953:LYS:HD3 | 4:J:995:TYR:OH | 2.21 | 0.41 |
| 4:J:1049:GLN:HG2 | 4:J:1050:THR:N | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:1059:LEU:CD1 | 4:J:1110:GLU:HG2 | 2.44 | 0.41 |
| 4:J:1176:VAL:HG13 | 4:J:1186:TYR:O | 2.20 | 0.41 |
| 5:K:9:ALA:HB2 | 5:K:55:GLU:OE1 | 2.21 | 0.41 |
| 5:K:26:ARG:NH2 | 5:K:53:GLU:OE2 | 2.53 | 0.41 |
| 6:L:122:ARG:HG3 | 6:L:122:ARG:H | 1.64 | 0.41 |
| 6:L:311:THR:HG22 | 6:L:355:ILE:HG12 | 2.03 | 0.41 |
| 6:L:426:LYS:HB2 | 7:O:52:DA:H5" | 2.03 | 0.41 |
| 6:L:483:LEU:HD23 | 6:L:483:LEU:HA | 1.76 | 0.41 |
| 6:L:571:TYR:HB2 | 6:L:576:VAL:CG2 | 2.51 | 0.41 |
| 6:L:578:LYS:HG3 | 6:L:579:GLN:N | 2.35 | 0.41 |
| 7:O:25:DA:C8 | 7:O:26:DT:H72 | 2.56 | 0.41 |
| 7:O:51:DT:H2" | 7:O:52:DA:OP1 | 2.18 | 0.41 |
| 2:M:270:LEU:HD12 | 2:M:270:LEU:HA | 1.71 | 0.41 |
| 2:M:289:LEU:O | 2:M:295:LEU:HD22 | 2.21 | 0.41 |
| 2:H:57:THR:HG22 | 2:H:58:GLU:HG2 | 2.03 | 0.41 |
| 3:I:198:ILE:HG22 | 3:I:199:ASP:N | 2.35 | 0.41 |
| 3:I:237:LEU:HD23 | 3:I:289:VAL:HB | 2.03 | 0.41 |
| 3:I:678:ARG:NH2 | 3:I:1106:ARG:HG3 | 2.35 | 0.41 |
| 3:I:821:ARG:HD2 | 3:I:825:GLU:OE2 | 2.21 | 0.41 |
| 3:I:1134:GLN:HE21 | 3:I:1134:GLN:HB3 | 1.60 | 0.41 |
| 4:J:1190:ILE:HG21 | 4:J:1196:LEU:HD21 | 2.03 | 0.41 |
| 5:K:13:ILE:CD1 | 5:K:54:ILE:HD12 | 2.50 | 0.41 |
| 6:L:147:GLN:HA | 6:L:150:ARG:HD3 | 2.03 | 0.41 |
| 6:L:257:LYS:O | 6:L:257:LYS:HG2 | 2.21 | 0.41 |
| 2:G:234:LEU:HD23 | 2:G:234:LEU:HA | 1.82 | 0.40 |
| 2:H:10:LYS:HB3 | 2:H:11:PRO:HD2 | 2.03 | 0.40 |
| 2:H:90:VAL:HG22 | 2:H:123:ILE:HD13 | 2.03 | 0.40 |
| 3:I:370:MET:HE1 | 3:I:388:LEU:HD11 | 2.03 | 0.40 |
| 3:I:593:LYS:HD2 | 3:I:652:TYR:CE1 | 2.55 | 0.40 |
| 3:I:678:ARG:HA | 3:I:678:ARG:HD3 | 1.61 | 0.40 |
| 3:I:755:LYS:HA | 3:I:755:LYS:HE3 | 2.03 | 0.40 |
| 3:I:960:LEU:HD21 | 3:I:1028:LYS:HB3 | 2.03 | 0.40 |
| 3:I:1109:ILE:HG12 | 4:J:644:MET:CE | 2.47 | 0.40 |
| 3:I:1322:SER:OG | 4:J:342:LEU:HD23 | 2.20 | 0.40 |
| 4:J:262:THR:CG2 | 4:J:266:ASN:HB2 | 2.51 | 0.40 |
| 4:J:355:ILE:HG21 | 4:J:466:MET:HB2 | 2.03 | 0.40 |
| 4:J:369:PRO:HA | 4:J:442:ILE:O | 2.22 | 0.40 |
| 4:J:1314:LEU:HD21 | 4:J:1326:GLN:HB2 | 2.03 | 0.40 |
| 6:L:324:LYS:H | 6:L:327:SER:HB2 | 1.86 | 0.40 |
| 6:L:380:VAL:O | 6:L:384:LEU:HG | 2.21 | 0.40 |
| 6:L:390:ILE:HG21 | 6:L:435:ILE:CG2 | 2.51 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:L:511:ILE:HG23 | 6:L:511:ILE:O | 2.21 | 0.40 |
| 6:L:555:GLU:OE1 | 6:L:556:ALA:N | 2.54 | 0.40 |
| 8:P:13:DG:H2" | 8:P:14:DA:OP2 | 2.21 | 0.40 |
| 8:P:57:DT:C2' | 8:P:58:DC:H5" | 2.50 | 0.40 |
| 8:P:65:DT:C6 | 8:P:66:DT:H72 | 2.56 | 0.40 |
| 2:G:183:ILE:HD12 | 2:G:205:MET:HB2 | 2.03 | 0.40 |
| 2:H:100:LEU:HB2 | 2:H:144:ILE:HG23 | 2.03 | 0.40 |
| 3:I:322:LEU:O | 3:I:325:LEU:HG | 2.20 | 0.40 |
| 3:I:705:GLU:H | 3:I:705:GLU:HG2 | 1.48 | 0.40 |
| 3:I:1256:GLN:HB3 | 3:I:1301:ARG:HH12 | 1.86 | 0.40 |
| 4:J:96:LYS:HE3 | 4:J:96:LYS:HB2 | 1.76 | 0.40 |
| 4:J:126:LEU:HD12 | 4:J:223:LEU:HD23 | 2.03 | 0.40 |
| 4:J:135:ILE:HD12 | 4:J:135:ILE:H | 1.86 | 0.40 |
| 4:J:449:LEU:HD11 | 4:J:457:TYR:HE2 | 1.86 | 0.40 |
| 4:J:490:ILE:HD11 | 4:J:609:TYR:HE1 | 1.86 | 0.40 |
| 4:J:1047:THR:N | 4:J:1060:VAL:O | 2.34 | 0.40 |
| 4:J:1172:LYS:HB3 | 4:J:1191:PRO:CA | 2.36 | 0.40 |
| 6:L:141:ILE:HA | 6:L:144:LEU:CB | 2.51 | 0.40 |
| 6:L:288:MET:HB3 | 6:L:302:PHE:CE2 | 2.56 | 0.40 |
| 8:P:60:DA:C8 | 8:P:61:DT:H72 | 2.56 | 0.40 |
| 2:M:253:LEU:HB3 | 2:M:321:TRP:CZ2 | 2.57 | 0.40 |
| 2:M:265:ARG:HE | 2:M:294:ASN:HD22 | 1.69 | 0.40 |
| 3:I:136:PHE:CZ | 3:I:456:VAL:HG21 | 2.56 | 0.40 |
| 3:I:230:PHE:CE1 | 3:I:292:ILE:HG23 | 2.56 | 0.40 |
| 3:I:590:PRO:HG3 | 3:I:605:TYR:CE1 | 2.52 | 0.40 |
| 3:I:593:LYS:HD3 | 3:I:604:HIS:NE2 | 2.37 | 0.40 |
| 3:I:986:ALA:HA | 3:I:989:LEU:CB | 2.52 | 0.40 |
| 4:J:330:MET:O | 4:J:337:ARG:HG2 | 2.21 | 0.40 |
| 4:J:373:ALA:O | 4:J:377:PHE:HD2 | 2.04 | 0.40 |
| 4:J:510:LEU:HD21 | 4:J:624:ILE:HG12 | 2.03 | 0.40 |
| 4:J:557:LYS:HB3 | 4:J:557:LYS:HE2 | 1.71 | 0.40 |
| 4:J:1173:ARG:HD2 | 4:J:1174:ARG:N | 2.36 | 0.40 |
| 6:L:320:ILE:HG12 | 6:L:330:LEU:HB3 | 2.03 | 0.40 |
| 1:N:52:PHE:CZ | 4:J:677:GLU:HG2 | 2.56 | 0.40 |
| 2:H:48:LEU:HD13 | 2:H:183:ILE:HD13 | 2.04 | 0.40 |
| 2:H:172:LEU:HD13 | 2:H:172:LEU:HA | 1.98 | 0.40 |
| 3:I:135:THR:OG1 | 3:I:142:GLU:OE2 | 2.40 | 0.40 |
| 3:I:317:LEU:HD23 | 3:I:317:LEU:HA | 1.84 | 0.40 |
| 3:I:324:LYS:O | 3:I:327:GLN:HG3 | 2.21 | 0.40 |
| 3:I:541:GLU:HG3 | 3:I:542:ARG:N | 2.37 | 0.40 |
| 3:I:565:GLU:HA | 3:I:569:ILE:HG12 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:I:618:GLN:HB2 | 3:I:635:THR:O | 2.21 | 0.40 |
| 4:J:160:LEU:HD22 | 4:J:164:GLN:CD | 2.42 | 0.40 |
| 4:J:326:SER:O | 4:J:330:MET:HG3 | 2.22 | 0.40 |
| 4:J:490:ILE:CD1 | 4:J:614:LEU:HD12 | 2.49 | 0.40 |
| 4:J:951:GLN:OE1 | 4:J:1016:THR:HB | 2.22 | 0.40 |
| 4:J:1034:PHE:O | 4:J:1080:ILE:HD12 | 2.21 | 0.40 |
| 4:J:1151:LYS:HA | 4:J:1151:LYS:HD3 | 1.75 | 0.40 |
| 2:M:255:ARG:HB2 | 2:M:278:ILE:HD11 | 2.02 | 0.40 |
| 2:G:57:THR:HG22 | 2:G:58:GLU:HG2 | 2.04 | 0.40 |
| 2:G:77:ASP:N | 2:G:77:ASP:OD1 | 2.54 | 0.40 |
| 3:I:180:ARG:NH2 | 3:I:393:ASP:HA | 2.36 | 0.40 |
| 3:I:528:ARG:HH11 | 3:I:528:ARG:HG2 | 1.86 | 0.40 |
| 3:I:596:ASP:OD1 | 3:I:598:VAL:HG23 | 2.21 | 0.40 |
| 3:I:690:VAL:HG11 | 3:I:830:THR:HG21 | 2.03 | 0.40 |
| 3:I:1252:SER:OG | 3:I:1253:LEU:N | 2.54 | 0.40 |
| 4:J:314:ARG:HD2 | 4:J:315:ALA:N | 2.32 | 0.40 |
| 4:J:1230:THR:O | 4:J:1234:VAL:HG23 | 2.21 | 0.40 |
| 6:L:95:THR:O | 6:L:95:THR:HG23 | 2.22 | 0.40 |
| 6:L:450:ILE:HG13 | 6:L:450:ILE:O | 2.21 | 0.40 |
| 7:O:66:DG:H2' | 7:O:67:DA:C8 | 2.57 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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 | N | 70/72 (97%) | 66 (94%) | 4 (6%) | 0 | 100 | 100 |
| 2 | G | 226/329 (69%) | 192 (85%) | 34 (15%) | 0 | 100 | 100 |
| 2 | H | 215/329 (65%) | 185 (86%) | 30 (14%) | 0 | 100 | 100 |
| 2 | M | 71/329 (22%) | 68 (96%) | 3 (4%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|------------------|------------|-----------|----------|-------------|-----|
| 3 | I | 1338/1342 (100%) | 1164 (87%) | 170 (13%) | 4 (0%) | 41 | 75 |
| 4 | J | 1339/1430 (94%) | 1202 (90%) | 137 (10%) | 0 | 100 | 100 |
| 5 | K | 77/91 (85%) | 66 (86%) | 10 (13%) | 1 (1%) | 12 | 48 |
| 6 | L | 468/616 (76%) | 433 (92%) | 35 (8%) | 0 | 100 | 100 |
| All | All | 3804/4538 (84%) | 3376 (89%) | 423 (11%) | 5 (0%) | 54 | 84 |

All (5) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | I | 82 | VAL |
| 5 | K | 61 | ASN |
| 3 | I | 81 | ASP |
| 3 | I | 1059 | ARG |
| 3 | 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 | N | 61/61 (100%) | 57 (93%) | 4 (7%) | 16 | 49 |
| 2 | G | 194/286 (68%) | 183 (94%) | 11 (6%) | 20 | 53 |
| 2 | H | 181/286 (63%) | 168 (93%) | 13 (7%) | 14 | 45 |
| 2 | M | 65/286 (23%) | 62 (95%) | 3 (5%) | 27 | 61 |
| 3 | I | 1154/1157 (100%) | 1057 (92%) | 97 (8%) | 11 | 40 |
| 4 | J | 1128/1189 (95%) | 1023 (91%) | 105 (9%) | 9 | 35 |
| 5 | K | 67/75 (89%) | 63 (94%) | 4 (6%) | 19 | 52 |
| 6 | L | 418/543 (77%) | 396 (95%) | 22 (5%) | 22 | 55 |
| All | All | 3268/3883 (84%) | 3009 (92%) | 259 (8%) | 16 | 41 |

All (259) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | N | 10 | SER |
| 1 | N | 16 | THR |
| 1 | N | 34 | VAL |
| 1 | N | 48 | ARG |
| 2 | G | 13 | LEU |
| 2 | G | 19 | VAL |
| 2 | G | 23 | HIS |
| 2 | G | 44 | ARG |
| 2 | G | 56 | VAL |
| 2 | G | 79 | LEU |
| 2 | G | 131 | CYS |
| 2 | G | 140 | ILE |
| 2 | G | 191 | ARG |
| 2 | G | 211 | ILE |
| 2 | G | 231 | PHE |
| 2 | H | 6 | THR |
| 2 | H | 76 | GLU |
| 2 | H | 77 | ASP |
| 2 | H | 79 | LEU |
| 2 | H | 83 | LEU |
| 2 | H | 98 | VAL |
| 2 | H | 111 | THR |
| 2 | H | 114 | ASP |
| 2 | H | 127 | GLN |
| 2 | H | 134 | THR |
| 2 | H | 207 | THR |
| 2 | H | 212 | ASP |
| 2 | H | 224 | LEU |
| 3 | I | 3 | TYR |
| 3 | I | 4 | SER |
| 3 | I | 6 | THR |
| 3 | I | 23 | ASP |
| 3 | I | 29 | SER |
| 3 | I | 39 | ILE |
| 3 | I | 47 | TYR |
| 3 | I | 59 | ILE |
| 3 | I | 85 | CYS |
| 3 | I | 91 | THR |
| 3 | I | 104 | ILE |
| 3 | I | 107 | ARG |
| 3 | I | 115 | LYS |
| 3 | I | 116 | ASP |
| 3 | I | 118 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | I | 143 | ARG |
| 3 | I | 155 | VAL |
| 3 | I | 161 | LYS |
| 3 | I | 167 | SER |
| 3 | I | 201 | ARG |
| 3 | I | 216 | THR |
| 3 | I | 272 | ARG |
| 3 | I | 287 | VAL |
| 3 | I | 303 | ASP |
| 3 | I | 346 | TYR |
| 3 | I | 348 | SER |
| 3 | I | 350 | THR |
| 3 | I | 385 | PHE |
| 3 | I | 420 | LEU |
| 3 | I | 427 | ASP |
| 3 | I | 444 | ASP |
| 3 | I | 448 | LEU |
| 3 | I | 470 | ARG |
| 3 | I | 471 | VAL |
| 3 | I | 472 | GLU |
| 3 | I | 487 | LEU |
| 3 | I | 491 | ASP |
| 3 | I | 492 | MET |
| 3 | I | 502 | VAL |
| 3 | I | 514 | PHE |
| 3 | I | 521 | LEU |
| 3 | I | 538 | LEU |
| 3 | I | 539 | THR |
| 3 | I | 547 | VAL |
| 3 | I | 565 | GLU |
| 3 | I | 582 | ASN |
| 3 | I | 589 | THR |
| 3 | I | 602 | GLU |
| 3 | I | 604 | HIS |
| 3 | I | 609 | ILE |
| 3 | I | 635 | THR |
| 3 | I | 684 | ASN |
| 3 | I | 690 | VAL |
| 3 | I | 697 | LYS |
| 3 | I | 699 | LEU |
| 3 | I | 705 | GLU |
| 3 | I | 741 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | I | 749 | ASP |
| 3 | I | 764 | CYS |
| 3 | I | 765 | ILE |
| 3 | I | 766 | ASN |
| 3 | I | 800 | MET |
| 3 | I | 802 | VAL |
| 3 | I | 817 | LEU |
| 3 | I | 819 | SER |
| 3 | I | 826 | ASP |
| 3 | I | 829 | THR |
| 3 | I | 842 | ASP |
| 3 | I | 902 | LEU |
| 3 | I | 915 | ASP |
| 3 | I | 919 | ARG |
| 3 | I | 925 | SER |
| 3 | I | 944 | ARG |
| 3 | I | 946 | LEU |
| 3 | I | 953 | LEU |
| 3 | I | 978 | VAL |
| 3 | I | 998 | LEU |
| 3 | I | 1003 | THR |
| 3 | I | 1008 | GLN |
| 3 | I | 1011 | LEU |
| 3 | I | 1036 | ILE |
| 3 | I | 1058 | ARG |
| 3 | I | 1083 | GLU |
| 3 | I | 1107 | MET |
| 3 | I | 1113 | LEU |
| 3 | I | 1132 | LEU |
| 3 | I | 1151 | LEU |
| 3 | I | 1160 | ASP |
| 3 | I | 1186 | VAL |
| 3 | I | 1233 | LEU |
| 3 | I | 1238 | LEU |
| 3 | I | 1240 | ASP |
| 3 | I | 1241 | ASP |
| 3 | I | 1253 | LEU |
| 3 | I | 1270 | PHE |
| 3 | I | 1309 | VAL |
| 3 | I | 1339 | LEU |
| 4 | J | 32 | SER |
| 4 | J | 46 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | J | 58 | CYS |
| 4 | J | 67 | ASP |
| 4 | J | 70 | CYS |
| 4 | J | 78 | LEU |
| 4 | J | 79 | LYS |
| 4 | J | 156 | ARG |
| 4 | J | 164 | GLN |
| 4 | J | 176 | PHE |
| 4 | J | 188 | LEU |
| 4 | J | 200 | GLN |
| 4 | J | 205 | LEU |
| 4 | J | 214 | ARG |
| 4 | J | 220 | ARG |
| 4 | J | 221 | ILE |
| 4 | J | 230 | SER |
| 4 | J | 253 | VAL |
| 4 | J | 255 | LEU |
| 4 | J | 264 | ASP |
| 4 | J | 278 | ARG |
| 4 | J | 297 | ARG |
| 4 | J | 312 | ARG |
| 4 | J | 314 | ARG |
| 4 | J | 341 | ASN |
| 4 | J | 343 | LEU |
| 4 | J | 346 | ARG |
| 4 | J | 366 | CYS |
| 4 | J | 386 | GLU |
| 4 | J | 403 | ARG |
| 4 | J | 449 | LEU |
| 4 | J | 473 | THR |
| 4 | J | 487 | THR |
| 4 | J | 503 | SER |
| 4 | J | 515 | ARG |
| 4 | J | 517 | CYS |
| 4 | J | 527 | LEU |
| 4 | J | 535 | ARG |
| 4 | J | 539 | SER |
| 4 | J | 545 | HIS |
| 4 | J | 553 | THR |
| 4 | J | 557 | LYS |
| 4 | J | 605 | LEU |
| 4 | J | 612 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 4 | J | 614 | LEU |
| 4 | J | 664 | ILE |
| 4 | J | 666 | GLU |
| 4 | J | 674 | THR |
| 4 | J | 678 | ARG |
| 4 | J | 709 | ARG |
| 4 | J | 722 | ILE |
| 4 | J | 731 | ARG |
| 4 | J | 744 | ARG |
| 4 | J | 746 | LEU |
| 4 | J | 751 | ASP |
| 4 | J | 756 | GLU |
| 4 | J | 757 | THR |
| 4 | J | 760 | THR |
| 4 | J | 762 | ASN |
| 4 | J | 774 | ILE |
| 4 | J | 775 | SER |
| 4 | J | 786 | THR |
| 4 | J | 789 | LYS |
| 4 | J | 797 | THR |
| 4 | J | 800 | LEU |
| 4 | J | 839 | VAL |
| 4 | J | 855 | ASP |
| 4 | J | 856 | ILE |
| 4 | J | 868 | TRP |
| 4 | J | 871 | LEU |
| 4 | J | 878 | ASP |
| 4 | J | 890 | THR |
| 4 | J | 901 | ARG |
| 4 | J | 930 | LEU |
| 4 | J | 960 | LEU |
| 4 | J | 982 | LEU |
| 4 | J | 1002 | VAL |
| 4 | J | 1016 | THR |
| 4 | J | 1048 | ARG |
| 4 | J | 1063 | ASP |
| 4 | J | 1086 | ASN |
| 4 | J | 1093 | THR |
| 4 | J | 1106 | ILE |
| 4 | J | 1116 | SER |
| 4 | J | 1135 | THR |
| 4 | J | 1148 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 4 | J | 1172 | LYS |
| 4 | J | 1188 | GLU |
| 4 | J | 1194 | ARG |
| 4 | J | 1198 | VAL |
| 4 | J | 1230 | THR |
| 4 | J | 1244 | GLN |
| 4 | J | 1272 | SER |
| 4 | J | 1279 | GLN |
| 4 | J | 1285 | VAL |
| 4 | J | 1286 | LYS |
| 4 | J | 1298 | VAL |
| 4 | J | 1304 | ARG |
| 4 | J | 1306 | LEU |
| 4 | J | 1310 | THR |
| 4 | J | 1324 | SER |
| 4 | J | 1326 | GLN |
| 4 | J | 1341 | ARG |
| 4 | J | 1344 | LEU |
| 4 | J | 1355 | ARG |
| 5 | K | 36 | ASP |
| 5 | K | 48 | VAL |
| 5 | K | 58 | LEU |
| 5 | K | 67 | ARG |
| 6 | L | 105 | MET |
| 6 | L | 132 | CYS |
| 6 | L | 233 | ASP |
| 6 | L | 257 | LYS |
| 6 | L | 261 | LEU |
| 6 | L | 277 | MET |
| 6 | L | 304 | THR |
| 6 | L | 342 | GLN |
| 6 | L | 360 | ASP |
| 6 | L | 442 | SER |
| 6 | L | 449 | THR |
| 6 | L | 466 | ILE |
| 6 | L | 476 | ARG |
| 6 | L | 487 | MET |
| 6 | L | 489 | MET |
| 6 | L | 524 | GLU |
| 6 | L | 528 | LEU |
| 6 | L | 560 | ARG |
| 6 | L | 561 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | L | 584 | ARG |
| 6 | L | 588 | ARG |
| 6 | L | 590 | ILE |
| 2 | M | 284 | ARG |
| 2 | M | 299 | SER |
| 2 | M | 314 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | N | 30 | HIS |
| 2 | G | 132 | HIS |
| 2 | G | 137 | ASN |
| 2 | H | 84 | ASN |
| 2 | H | 128 | HIS |
| 2 | H | 227 | GLN |
| 3 | I | 46 | GLN |
| 3 | I | 65 | ASN |
| 3 | I | 69 | GLN |
| 3 | I | 214 | ASN |
| 3 | I | 314 | ASN |
| 3 | I | 463 | GLN |
| 3 | I | 618 | GLN |
| 3 | I | 620 | ASN |
| 3 | I | 622 | ASN |
| 3 | I | 649 | GLN |
| 3 | I | 659 | GLN |
| 3 | I | 677 | ASN |
| 3 | I | 824 | GLN |
| 3 | I | 856 | ASN |
| 3 | I | 1010 | GLN |
| 3 | I | 1116 | HIS |
| 3 | I | 1134 | GLN |
| 3 | I | 1244 | HIS |
| 3 | I | 1257 | GLN |
| 3 | I | 1268 | GLN |
| 4 | J | 45 | ASN |
| 4 | J | 80 | HIS |
| 4 | J | 157 | GLN |
| 4 | J | 164 | GLN |
| 4 | J | 266 | ASN |
| 4 | J | 341 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 4 | J | 488 | ASN |
| 4 | J | 680 | ASN |
| 4 | J | 1023 | HIS |
| 4 | J | 1049 | GLN |
| 4 | J | 1114 | GLN |
| 4 | J | 1126 | GLN |
| 4 | J | 1249 | ASN |
| 4 | J | 1295 | ASN |
| 4 | J | 1366 | HIS |
| 6 | L | 246 | GLN |
| 6 | L | 362 | ASN |
| 6 | L | 406 | GLN |
| 6 | L | 464 | ASN |
| 6 | L | 600 | HIS |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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 |
| 10 | 1N7 | J | 1504 | - | 30,30,46 | 5.06 | 16 (53%) | 47,48,72 | 2.15 | 13 (27%) |
| 10 | 1N7 | L | 701 | - | 30,30,46 | 5.10 | 15 (50%) | 47,48,72 | 2.34 | 18 (38%) |
| 10 | 1N7 | N | 102 | - | 30,30,46 | 4.87 | 14 (46%) | 47,48,72 | 2.41 | 18 (38%) |
| 10 | 1N7 | I | 1401 | - | 30,30,46 | 4.97 | 15 (50%) | 47,48,72 | 2.57 | 21 (44%) |

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 |
|-----|------|-------|------|------|---------|-----------|---------|
| 10 | 1N7 | J | 1504 | - | - | 3/7/72/92 | 0/4/4/4 |
| 10 | 1N7 | L | 701 | - | - | 4/7/72/92 | 0/4/4/4 |
| 10 | 1N7 | N | 102 | - | - | 2/7/72/92 | 0/4/4/4 |
| 10 | 1N7 | I | 1401 | - | - | 2/7/72/92 | 0/4/4/4 |

All (60) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10 | L | 701 | 1N7 | C3-C19 | 18.34 | 1.84 | 1.53 |
| 10 | J | 1504 | 1N7 | C3-C19 | 18.28 | 1.84 | 1.53 |
| 10 | I | 1401 | 1N7 | C3-C19 | 17.85 | 1.83 | 1.53 |
| 10 | N | 102 | 1N7 | C3-C19 | 17.29 | 1.82 | 1.53 |
| 10 | L | 701 | 1N7 | C3-C4 | 12.03 | 1.73 | 1.53 |
| 10 | I | 1401 | 1N7 | C3-C4 | 12.02 | 1.73 | 1.53 |
| 10 | J | 1504 | 1N7 | C3-C4 | 11.65 | 1.72 | 1.53 |
| 10 | N | 102 | 1N7 | C3-C4 | 11.43 | 1.72 | 1.53 |
| 10 | L | 701 | 1N7 | C5-C4 | -9.36 | 1.39 | 1.54 |
| 10 | I | 1401 | 1N7 | C5-C4 | -9.04 | 1.40 | 1.54 |
| 10 | N | 102 | 1N7 | C5-C4 | -8.89 | 1.40 | 1.54 |
| 10 | J | 1504 | 1N7 | C5-C4 | -8.78 | 1.40 | 1.54 |
| 10 | I | 1401 | 1N7 | C2-C19 | -7.47 | 1.42 | 1.56 |
| 10 | N | 102 | 1N7 | C2-C19 | -7.23 | 1.42 | 1.56 |
| 10 | L | 701 | 1N7 | C2-C19 | -7.11 | 1.43 | 1.56 |
| 10 | J | 1504 | 1N7 | C2-C19 | -7.01 | 1.43 | 1.56 |
| 10 | L | 701 | 1N7 | C8-C7 | 5.98 | 1.70 | 1.54 |
| 10 | N | 102 | 1N7 | C8-C7 | 5.60 | 1.69 | 1.54 |
| 10 | J | 1504 | 1N7 | C8-C7 | 5.60 | 1.69 | 1.54 |
| 10 | I | 1401 | 1N7 | C8-C7 | 5.54 | 1.69 | 1.54 |
| 10 | N | 102 | 1N7 | C5-C9 | 4.89 | 1.63 | 1.55 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 10 | J | 1504 | 1N7 | C2-C15 | 4.47 | 1.62 | 1.55 |
| 10 | L | 701 | 1N7 | O4-C4 | -4.35 | 1.36 | 1.43 |
| 10 | L | 701 | 1N7 | C7-C6 | 4.22 | 1.63 | 1.54 |
| 10 | J | 1504 | 1N7 | O4-C4 | -4.11 | 1.36 | 1.43 |
| 10 | I | 1401 | 1N7 | C5-C9 | 4.05 | 1.62 | 1.55 |
| 10 | N | 102 | 1N7 | O4-C4 | -3.95 | 1.37 | 1.43 |
| 10 | J | 1504 | 1N7 | C5-C9 | 3.87 | 1.62 | 1.55 |
| 10 | J | 1504 | 1N7 | C18-C6 | -3.80 | 1.46 | 1.53 |
| 10 | L | 701 | 1N7 | C5-C6 | -3.69 | 1.49 | 1.55 |
| 10 | L | 701 | 1N7 | C5-C9 | 3.62 | 1.61 | 1.55 |
| 10 | I | 1401 | 1N7 | O4-C4 | -3.59 | 1.37 | 1.43 |
| 10 | L | 701 | 1N7 | C14-C15 | -3.57 | 1.48 | 1.53 |
| 10 | I | 1401 | 1N7 | C14-C15 | -3.44 | 1.48 | 1.53 |
| 10 | N | 102 | 1N7 | C2-C15 | 3.39 | 1.60 | 1.55 |
| 10 | J | 1504 | 1N7 | C5-C6 | -3.28 | 1.49 | 1.55 |
| 10 | I | 1401 | 1N7 | C18-C6 | -3.28 | 1.47 | 1.53 |
| 10 | L | 701 | 1N7 | C2-C15 | 3.19 | 1.60 | 1.55 |
| 10 | I | 1401 | 1N7 | C5-C6 | -3.14 | 1.50 | 1.55 |
| 10 | I | 1401 | 1N7 | C2-C15 | 3.10 | 1.60 | 1.55 |
| 10 | N | 102 | 1N7 | C18-C6 | -3.05 | 1.47 | 1.53 |
| 10 | I | 1401 | 1N7 | C7-C6 | 3.04 | 1.60 | 1.54 |
| 10 | J | 1504 | 1N7 | C7-C6 | 3.04 | 1.60 | 1.54 |
| 10 | N | 102 | 1N7 | C5-C6 | -2.95 | 1.50 | 1.55 |
| 10 | N | 102 | 1N7 | C14-C15 | -2.85 | 1.49 | 1.53 |
| 10 | N | 102 | 1N7 | C7-C6 | 2.73 | 1.60 | 1.54 |
| 10 | J | 1504 | 1N7 | C14-C15 | -2.63 | 1.49 | 1.53 |
| 10 | J | 1504 | 1N7 | C14-C13 | 2.55 | 1.56 | 1.51 |
| 10 | J | 1504 | 1N7 | C10-C5 | 2.48 | 1.58 | 1.54 |
| 10 | I | 1401 | 1N7 | O2-C13 | -2.48 | 1.36 | 1.43 |
| 10 | L | 701 | 1N7 | C18-C6 | -2.47 | 1.49 | 1.53 |
| 10 | N | 102 | 1N7 | O2-C13 | -2.36 | 1.36 | 1.43 |
| 10 | L | 701 | 1N7 | O2-C13 | -2.32 | 1.36 | 1.43 |
| 10 | N | 102 | 1N7 | C10-C5 | 2.23 | 1.58 | 1.54 |
| 10 | J | 1504 | 1N7 | O2-C13 | -2.22 | 1.36 | 1.43 |
| 10 | L | 701 | 1N7 | C12-C13 | 2.19 | 1.56 | 1.51 |
| 10 | J | 1504 | 1N7 | C11-C2 | 2.15 | 1.58 | 1.54 |
| 10 | L | 701 | 1N7 | C14-C13 | 2.08 | 1.55 | 1.51 |
| 10 | I | 1401 | 1N7 | C1-C2 | 2.07 | 1.57 | 1.54 |
| 10 | I | 1401 | 1N7 | C10-C5 | 2.05 | 1.57 | 1.54 |

All (70) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 10 | J | 1504 | 1N7 | C7-C6-C18 | -7.63 | 107.66 | 118.33 |
| 10 | I | 1401 | 1N7 | C9-C5-C4 | -5.72 | 112.44 | 117.67 |
| 10 | I | 1401 | 1N7 | C7-C6-C18 | -5.68 | 110.39 | 118.33 |
| 10 | N | 102 | 1N7 | C9-C5-C4 | -5.43 | 112.71 | 117.67 |
| 10 | L | 701 | 1N7 | C9-C5-C4 | -5.38 | 112.75 | 117.67 |
| 10 | J | 1504 | 1N7 | C16-C15-C14 | -5.37 | 105.01 | 111.19 |
| 10 | L | 701 | 1N7 | C21-C20-C9 | -5.07 | 105.16 | 112.92 |
| 10 | L | 701 | 1N7 | C2-C19-C18 | 5.05 | 117.24 | 111.82 |
| 10 | N | 102 | 1N7 | C19-C3-C4 | -4.97 | 107.74 | 114.30 |
| 10 | N | 102 | 1N7 | C21-C20-C22 | -4.96 | 102.58 | 110.36 |
| 10 | N | 102 | 1N7 | C7-C6-C18 | -4.69 | 111.78 | 118.33 |
| 10 | L | 701 | 1N7 | C6-C5-C4 | 4.67 | 111.75 | 107.40 |
| 10 | I | 1401 | 1N7 | C5-C6-C18 | 4.57 | 120.58 | 114.74 |
| 10 | N | 102 | 1N7 | C9-C5-C6 | 4.53 | 104.66 | 100.09 |
| 10 | I | 1401 | 1N7 | C19-C18-C17 | -4.36 | 106.66 | 111.88 |
| 10 | I | 1401 | 1N7 | C19-C3-C4 | -4.32 | 108.60 | 114.30 |
| 10 | L | 701 | 1N7 | C3-C19-C18 | -4.17 | 104.77 | 110.88 |
| 10 | N | 102 | 1N7 | C5-C6-C18 | 4.12 | 120.00 | 114.74 |
| 10 | N | 102 | 1N7 | C2-C19-C18 | 4.05 | 116.16 | 111.82 |
| 10 | I | 1401 | 1N7 | C14-C13-C12 | -4.03 | 105.74 | 110.55 |
| 10 | N | 102 | 1N7 | C3-C19-C18 | -3.98 | 105.06 | 110.88 |
| 10 | J | 1504 | 1N7 | C9-C5-C6 | 3.80 | 103.92 | 100.09 |
| 10 | L | 701 | 1N7 | C19-C18-C17 | -3.77 | 107.36 | 111.88 |
| 10 | J | 1504 | 1N7 | C7-C6-C5 | 3.76 | 107.24 | 103.55 |
| 10 | I | 1401 | 1N7 | C3-C19-C18 | -3.71 | 105.44 | 110.88 |
| 10 | I | 1401 | 1N7 | C16-C15-C2 | -3.67 | 108.76 | 112.66 |
| 10 | I | 1401 | 1N7 | C9-C5-C6 | 3.66 | 103.78 | 100.09 |
| 10 | L | 701 | 1N7 | C22-C20-C9 | 3.63 | 117.78 | 110.28 |
| 10 | I | 1401 | 1N7 | C2-C19-C18 | 3.57 | 115.65 | 111.82 |
| 10 | I | 1401 | 1N7 | C15-C14-C13 | -3.56 | 107.53 | 112.76 |
| 10 | L | 701 | 1N7 | C15-C14-C13 | -3.53 | 107.58 | 112.76 |
| 10 | I | 1401 | 1N7 | C8-C7-C6 | -3.50 | 98.20 | 105.13 |
| 10 | J | 1504 | 1N7 | C9-C5-C4 | -3.42 | 114.54 | 117.67 |
| 10 | N | 102 | 1N7 | C14-C13-C12 | -3.41 | 106.48 | 110.55 |
| 10 | I | 1401 | 1N7 | C6-C5-C4 | 3.39 | 110.56 | 107.40 |
| 10 | N | 102 | 1N7 | C16-C15-C2 | -3.31 | 109.14 | 112.66 |
| 10 | I | 1401 | 1N7 | C14-C15-C2 | 3.12 | 115.97 | 112.66 |
| 10 | L | 701 | 1N7 | C19-C2-C15 | 3.11 | 112.95 | 108.58 |
| 10 | N | 102 | 1N7 | C8-C9-C20 | -3.06 | 107.41 | 112.15 |
| 10 | J | 1504 | 1N7 | C5-C6-C18 | 3.06 | 118.64 | 114.74 |
| 10 | I | 1401 | 1N7 | C19-C2-C15 | 2.98 | 112.77 | 108.58 |
| 10 | L | 701 | 1N7 | C11-C2-C19 | 2.98 | 115.29 | 111.18 |
| 10 | N | 102 | 1N7 | C11-C2-C1 | -2.97 | 103.47 | 108.26 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 10 | I | 1401 | 1N7 | C11-C2-C15 | -2.97 | 105.33 | 110.36 |
| 10 | I | 1401 | 1N7 | C3-C4-C5 | -2.87 | 108.30 | 111.24 |
| 10 | J | 1504 | 1N7 | C10-C5-C6 | 2.86 | 115.68 | 111.21 |
| 10 | I | 1401 | 1N7 | C1-C12-C13 | -2.83 | 106.84 | 110.47 |
| 10 | L | 701 | 1N7 | C11-C2-C15 | -2.82 | 105.58 | 110.36 |
| 10 | I | 1401 | 1N7 | C8-C9-C20 | -2.68 | 107.99 | 112.15 |
| 10 | N | 102 | 1N7 | C8-C7-C6 | -2.68 | 99.82 | 105.13 |
| 10 | N | 102 | 1N7 | C1-C12-C13 | -2.65 | 107.06 | 110.47 |
| 10 | N | 102 | 1N7 | C6-C5-C4 | 2.61 | 109.83 | 107.40 |
| 10 | L | 701 | 1N7 | C7-C6-C18 | -2.58 | 114.72 | 118.33 |
| 10 | J | 1504 | 1N7 | C11-C2-C1 | -2.58 | 104.11 | 108.26 |
| 10 | L | 701 | 1N7 | C10-C5-C4 | -2.57 | 106.45 | 109.07 |
| 10 | J | 1504 | 1N7 | C8-C9-C20 | -2.54 | 108.21 | 112.15 |
| 10 | L | 701 | 1N7 | C14-C15-C2 | -2.50 | 110.00 | 112.66 |
| 10 | J | 1504 | 1N7 | C10-C5-C9 | -2.41 | 107.43 | 111.21 |
| 10 | L | 701 | 1N7 | C21-C20-C22 | -2.36 | 106.66 | 110.36 |
| 10 | L | 701 | 1N7 | C7-C8-C9 | -2.35 | 100.47 | 105.13 |
| 10 | J | 1504 | 1N7 | C11-C2-C19 | 2.31 | 114.36 | 111.18 |
| 10 | I | 1401 | 1N7 | C21-C20-C22 | -2.29 | 106.77 | 110.36 |
| 10 | L | 701 | 1N7 | C5-C6-C18 | 2.29 | 117.66 | 114.74 |
| 10 | J | 1504 | 1N7 | C19-C18-C17 | -2.28 | 109.15 | 111.88 |
| 10 | I | 1401 | 1N7 | C11-C2-C1 | -2.20 | 104.71 | 108.26 |
| 10 | N | 102 | 1N7 | C22-C20-C9 | 2.15 | 114.73 | 110.28 |
| 10 | L | 701 | 1N7 | C11-C2-C1 | -2.12 | 104.84 | 108.26 |
| 10 | N | 102 | 1N7 | C15-C14-C13 | -2.04 | 109.75 | 112.76 |
| 10 | N | 102 | 1N7 | C3-C4-C5 | -2.04 | 109.15 | 111.24 |
| 10 | J | 1504 | 1N7 | C1-C12-C13 | 2.01 | 113.05 | 110.47 |

There are no chirality outliers.

All (11) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 10 | L | 701 | 1N7 | C22-C20-C9-C5 |
| 10 | N | 102 | 1N7 | C21-C20-C22-C23 |
| 10 | J | 1504 | 1N7 | C9-C20-C22-C23 |
| 10 | L | 701 | 1N7 | C21-C20-C9-C8 |
| 10 | L | 701 | 1N7 | C21-C20-C9-C5 |
| 10 | J | 1504 | 1N7 | C21-C20-C22-C23 |
| 10 | N | 102 | 1N7 | C9-C20-C22-C23 |
| 10 | I | 1401 | 1N7 | C9-C20-C22-C23 |
| 10 | I | 1401 | 1N7 | C21-C20-C22-C23 |
| 10 | L | 701 | 1N7 | C22-C20-C9-C8 |

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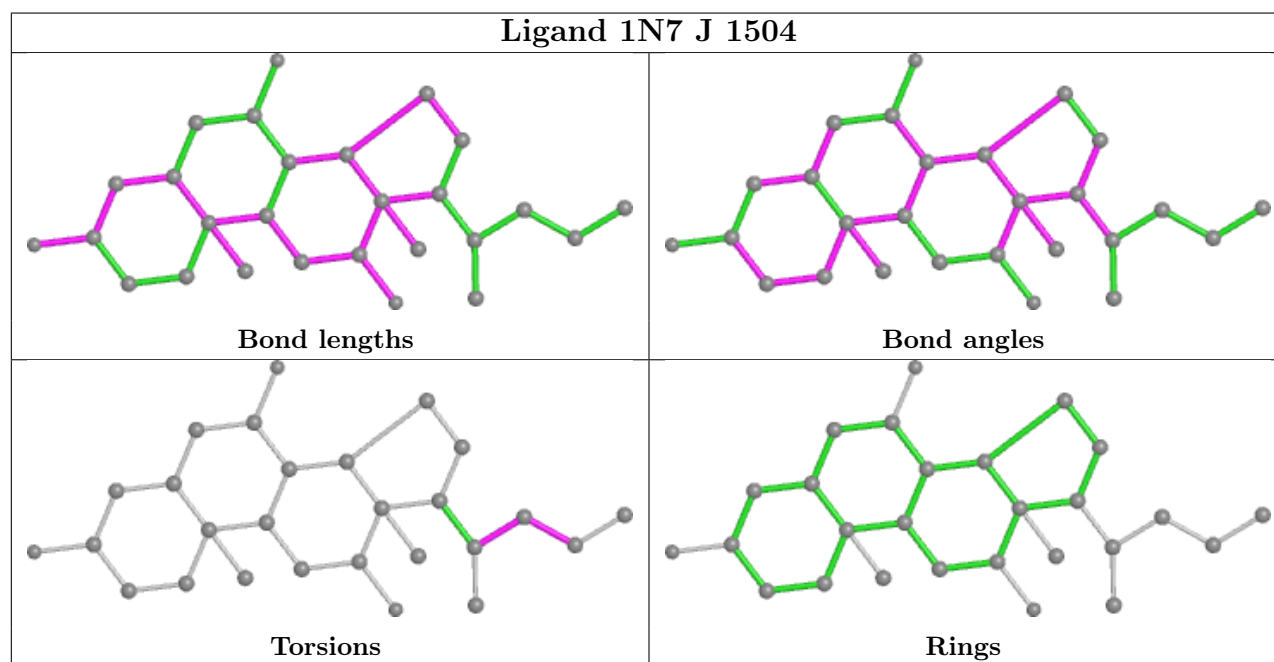
| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 10 | J | 1504 | 1N7 | C20-C22-C23-C24 |

There are no ring outliers.

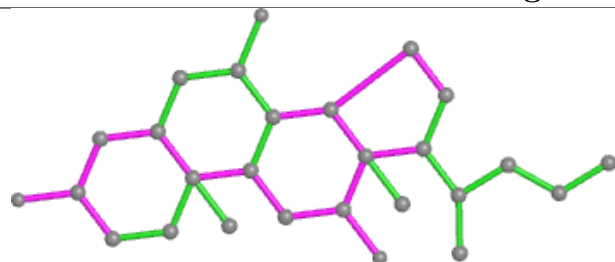
4 monomers are involved in 16 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 10 | J | 1504 | 1N7 | 3 | 0 |
| 10 | L | 701 | 1N7 | 3 | 0 |
| 10 | N | 102 | 1N7 | 4 | 0 |
| 10 | I | 1401 | 1N7 | 6 | 0 |

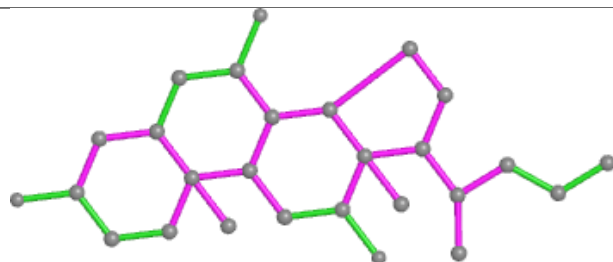
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



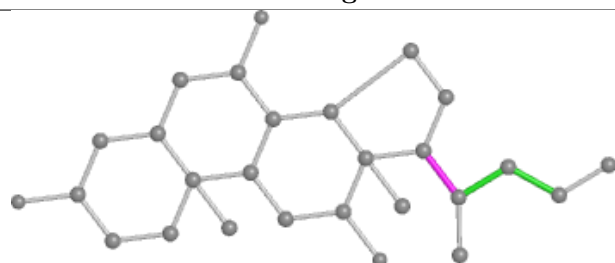
Ligand 1N7 L 701



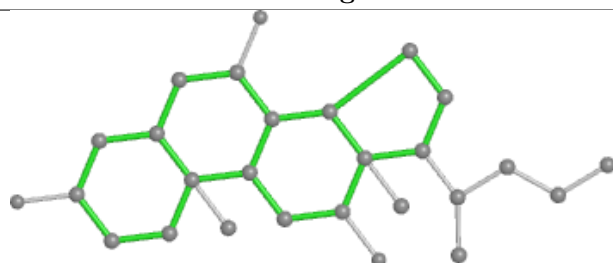
Bond lengths



Bond angles

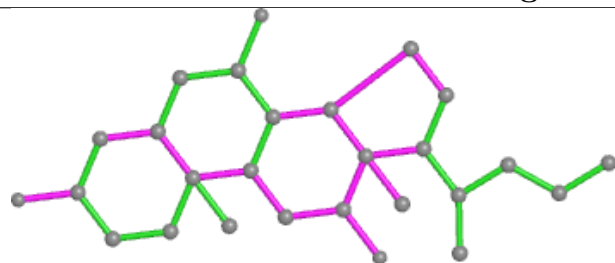


Torsions

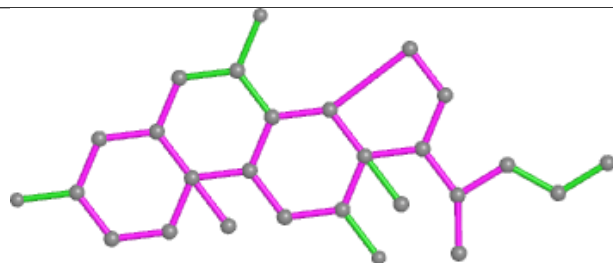


Rings

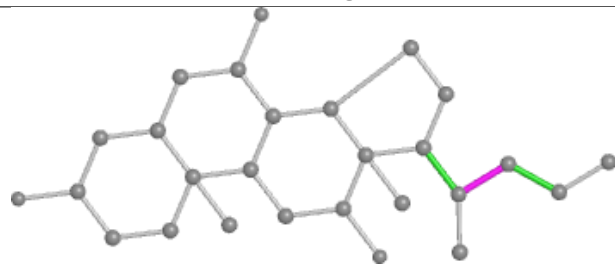
Ligand 1N7 N 102



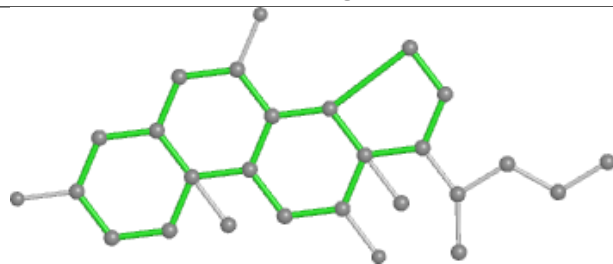
Bond lengths



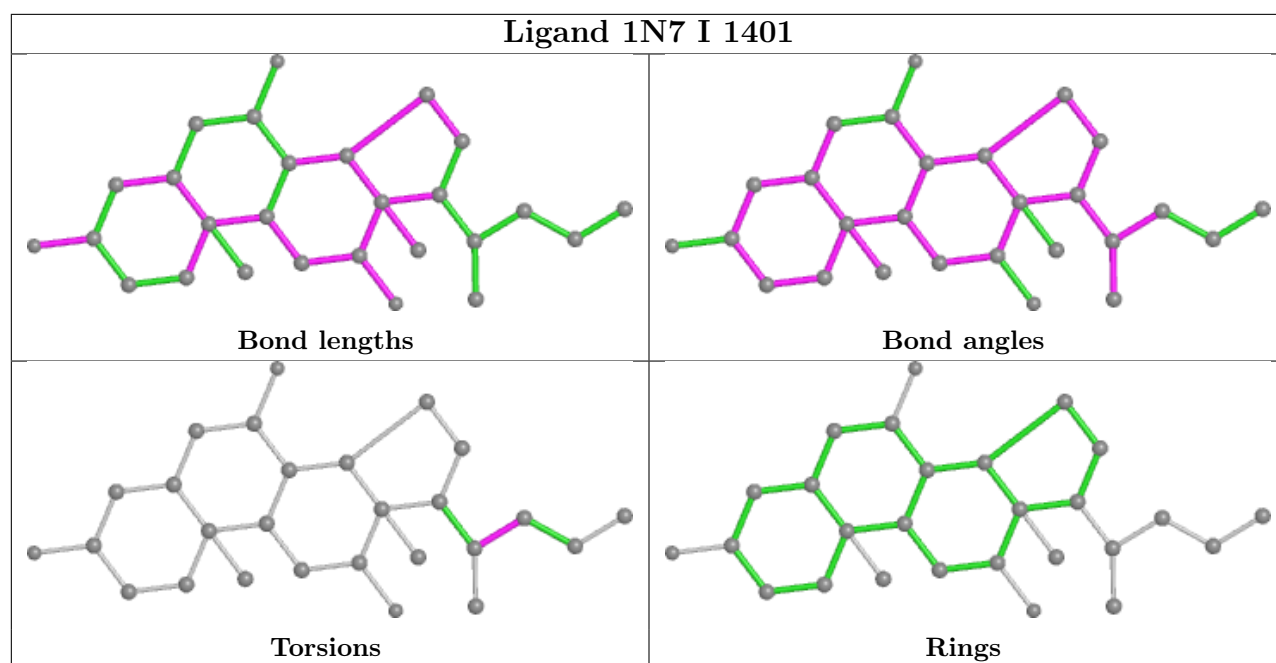
Bond angles



Torsions



Rings



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.

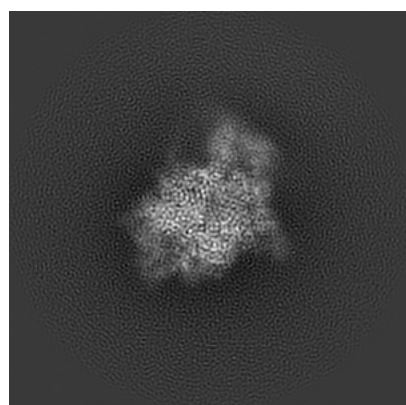
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20465. These allow visual inspection of the internal detail of the map and identification of artifacts.

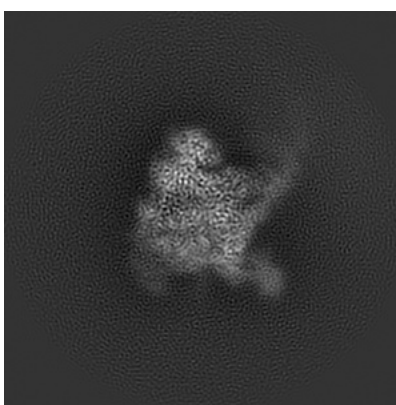
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

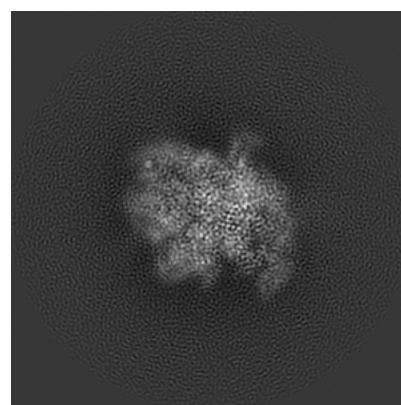
6.1.1 Primary map



X



Y

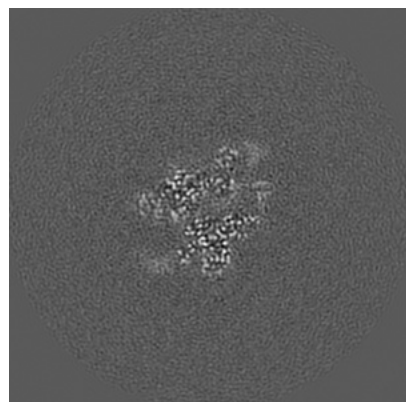


Z

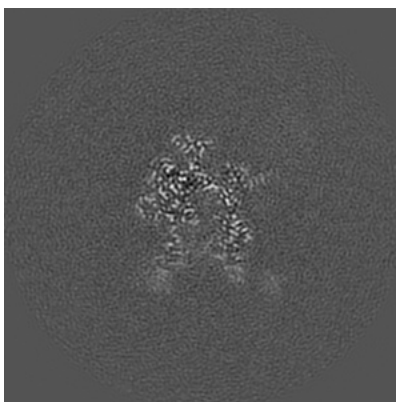
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

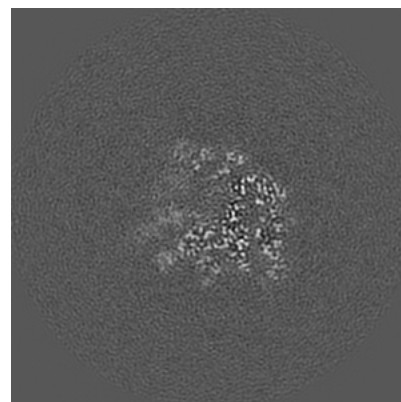
6.2.1 Primary map



X Index: 128



Y Index: 128

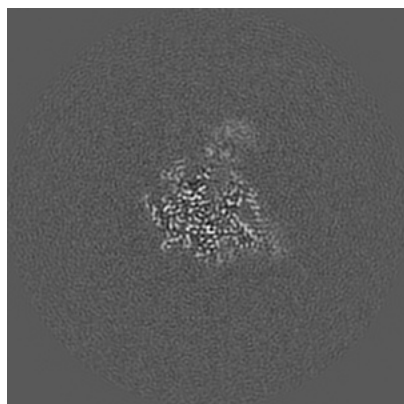


Z Index: 128

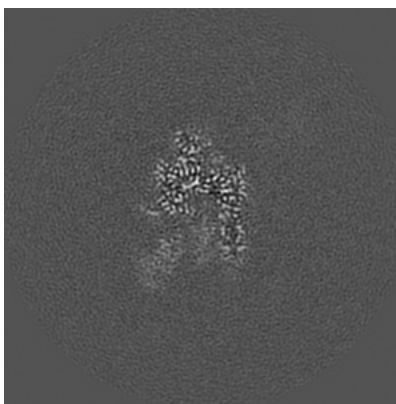
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

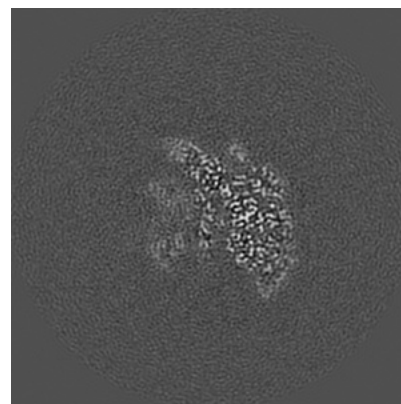
6.3.1 Primary map



X Index: 146



Y Index: 123

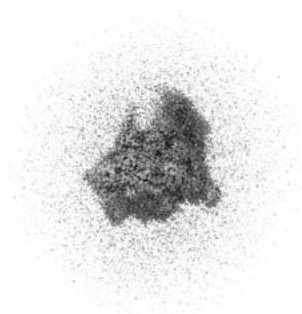


Z Index: 120

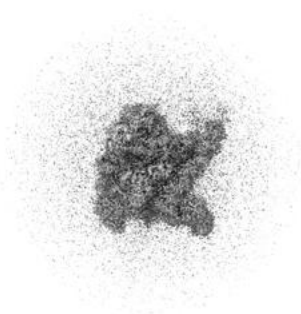
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

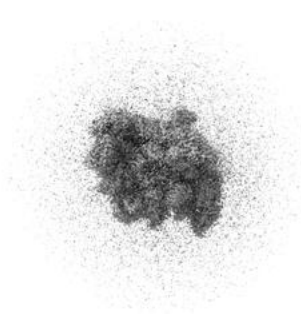
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

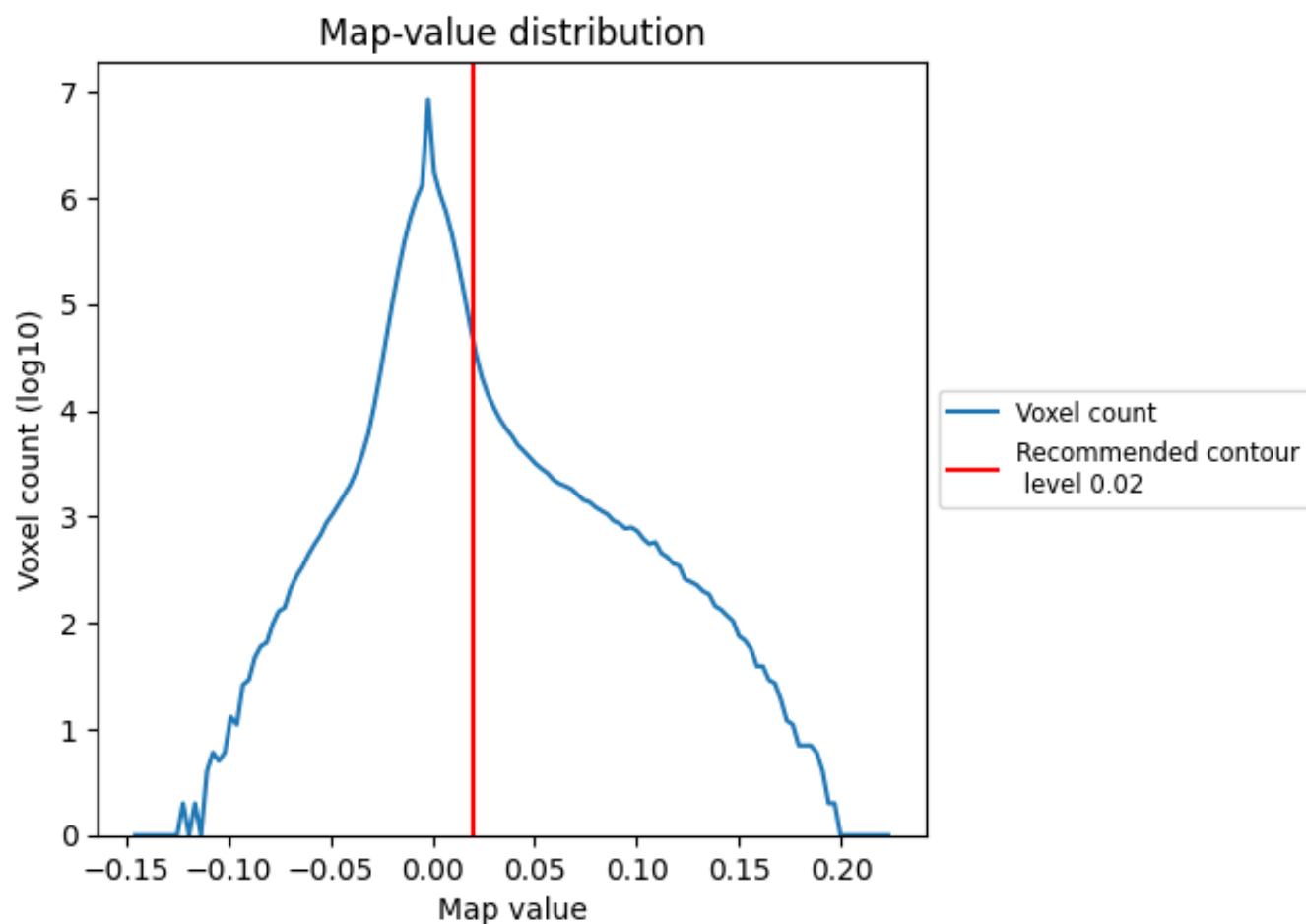
6.5 Mask visualisation

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

7 Map analysis [i](#)

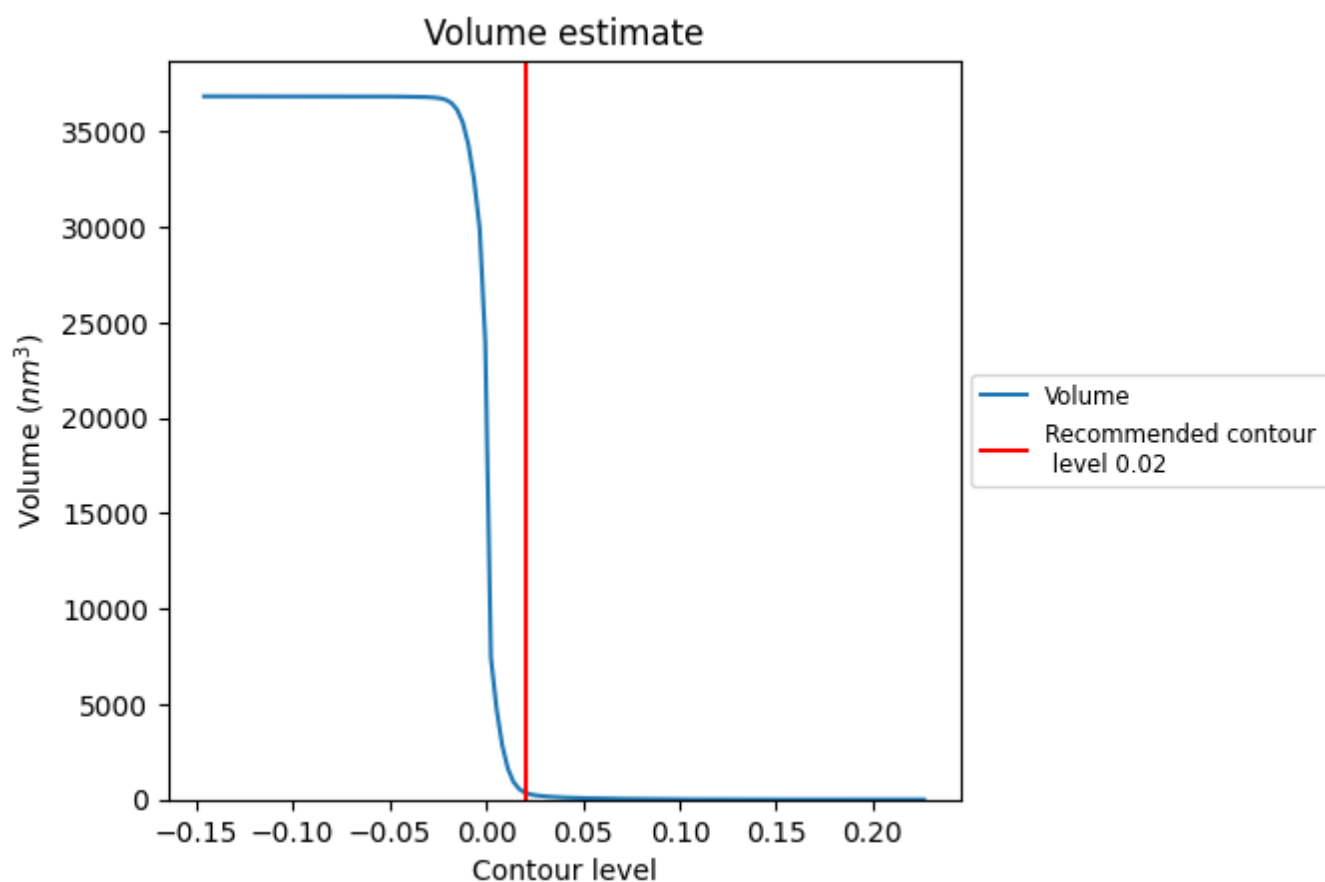
This section contains the results of statistical analysis of the map.

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.

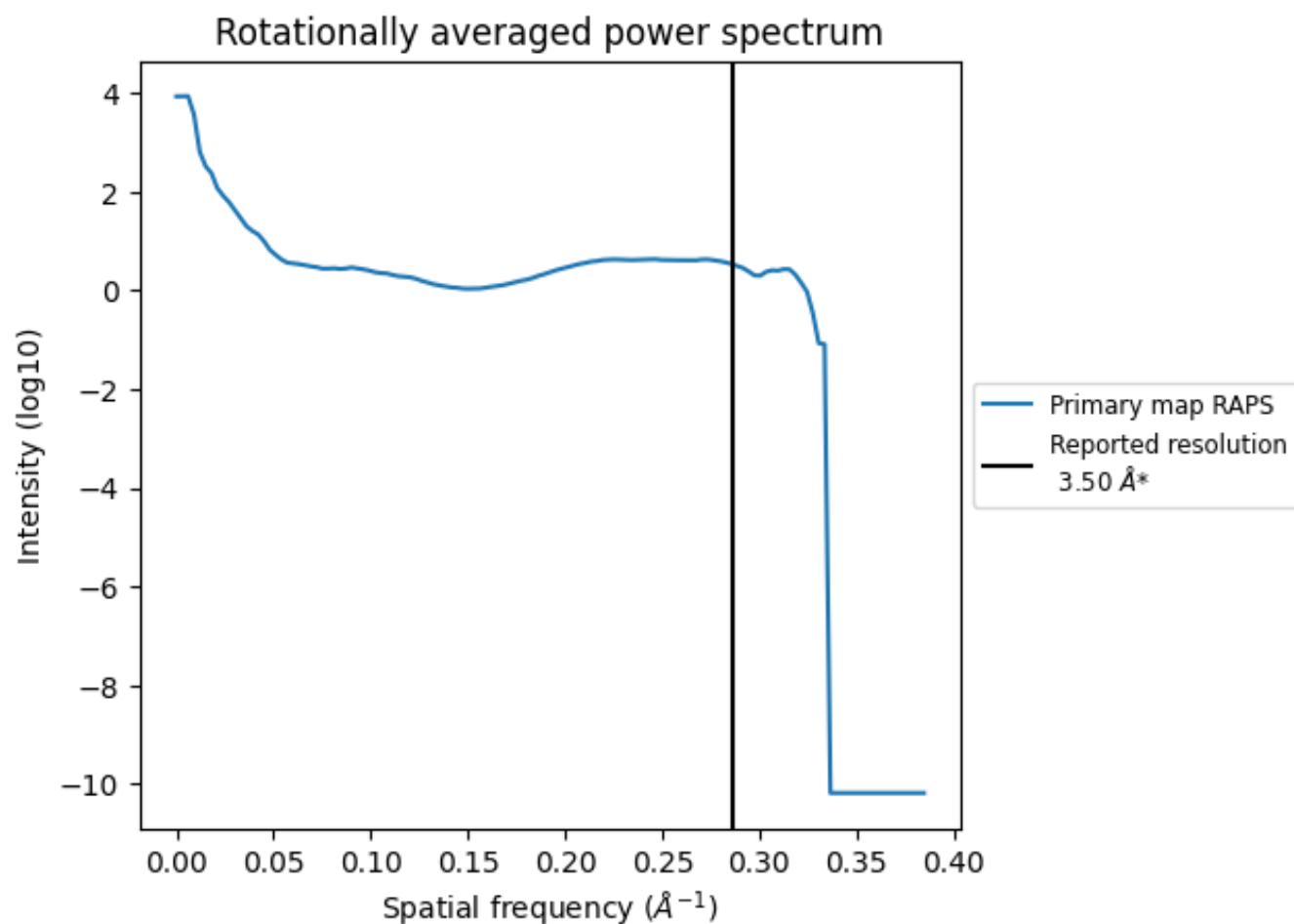
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 368 nm^3 ; this corresponds to an approximate mass of 332 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 ⓘ

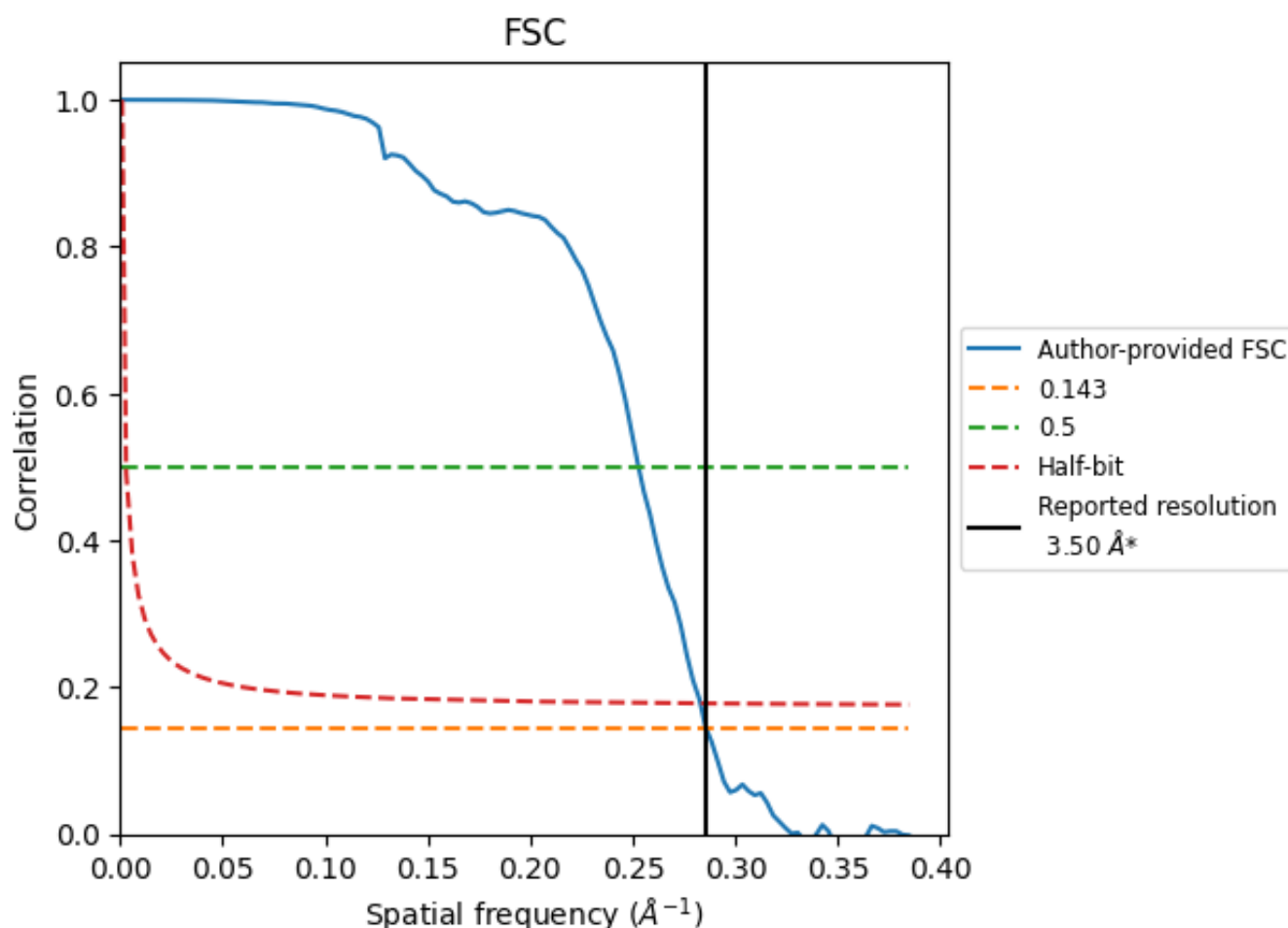


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

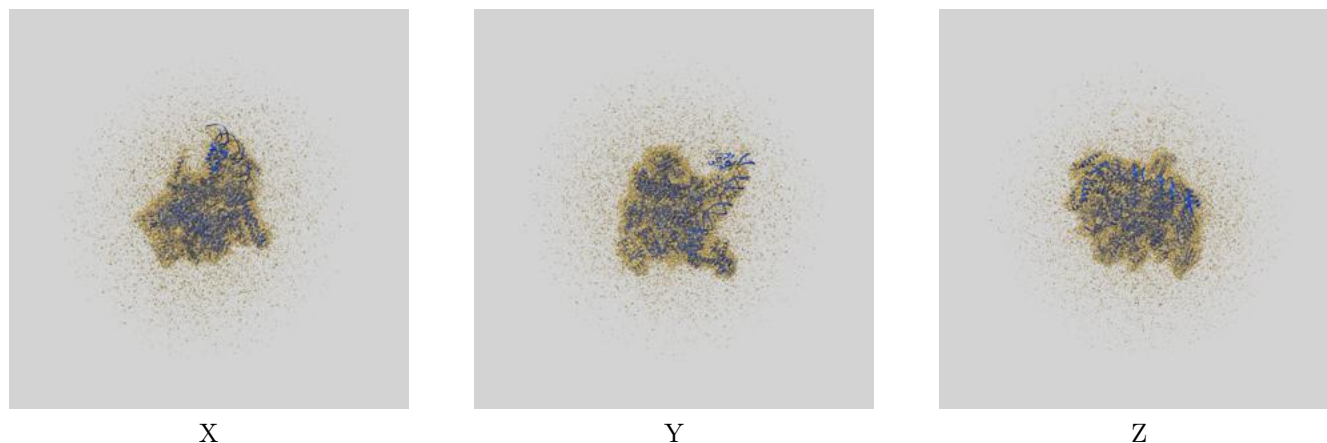
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.50 | - | - |
| Author-provided FSC curve | 3.50 | 3.96 | 3.53 |
| Unmasked-calculated* | - | - | - |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

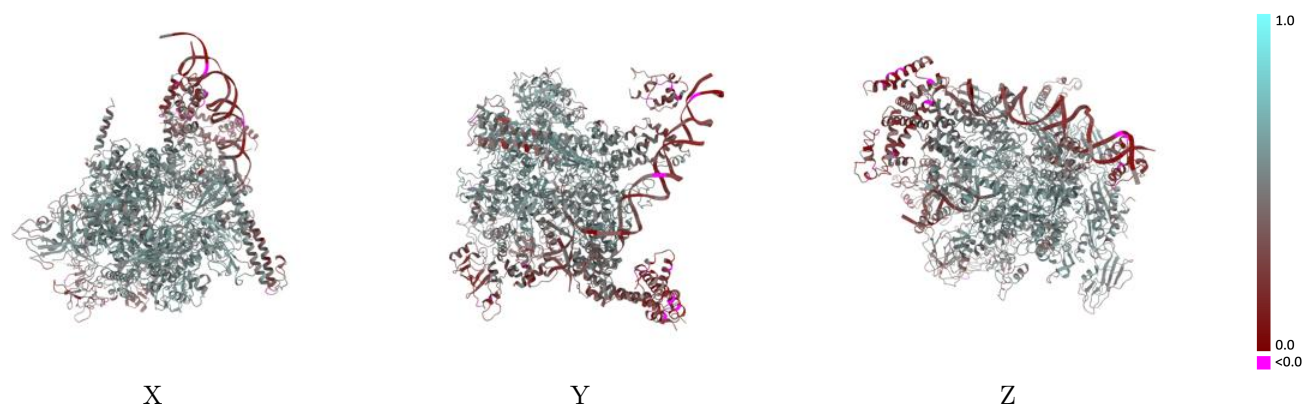
This section contains information regarding the fit between EMDB map EMD-20465 and PDB model 6PSV. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



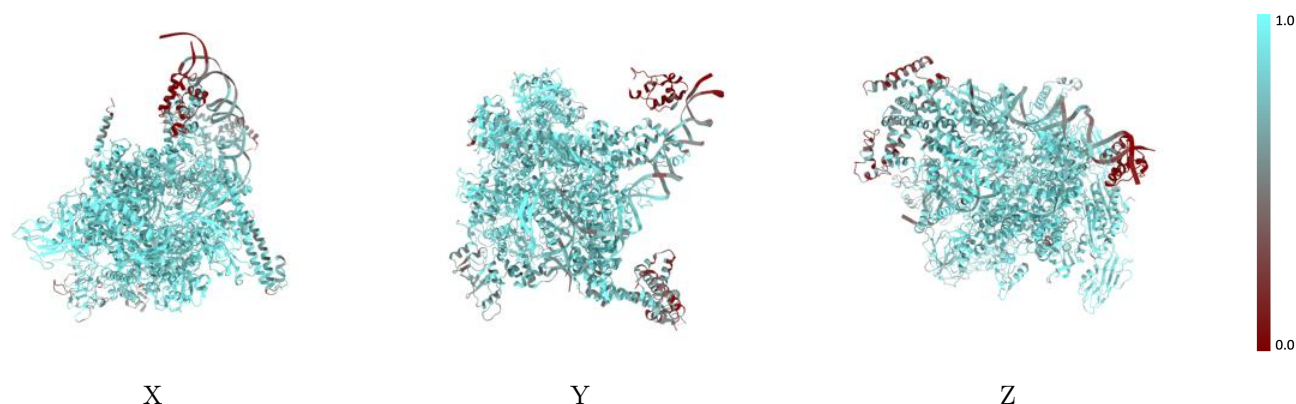
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



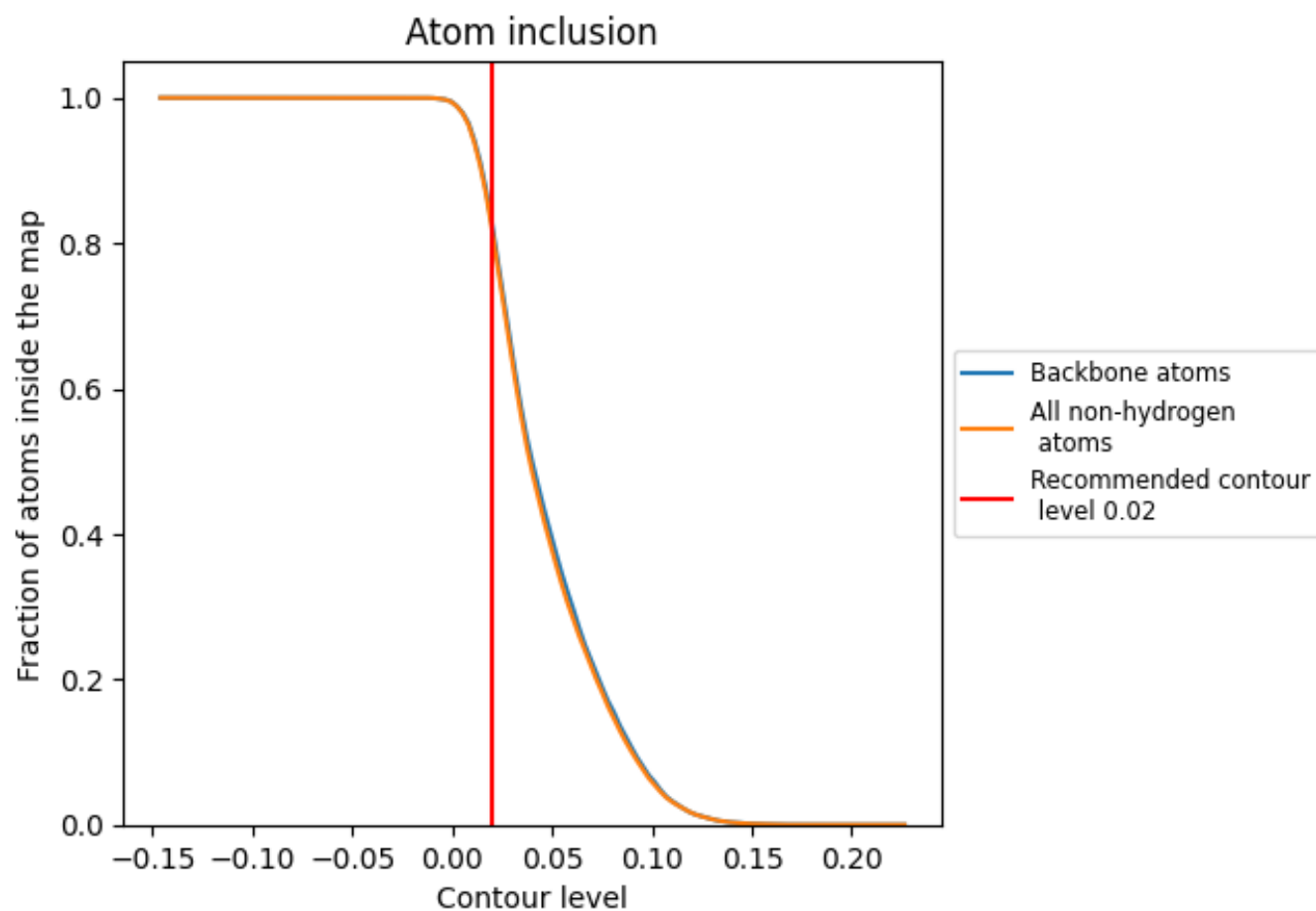
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion ⓘ



At the recommended contour level, 83% of all backbone atoms, 82% 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 (0.02) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--------------------|--------------------|
| All | <div></div> 0.8187 | <div></div> 0.4680 |
| G | <div></div> 0.8980 | <div></div> 0.5330 |
| H | <div></div> 0.8990 | <div></div> 0.5120 |
| I | <div></div> 0.8715 | <div></div> 0.5020 |
| J | <div></div> 0.8745 | <div></div> 0.5050 |
| K | <div></div> 0.7692 | <div></div> 0.5000 |
| L | <div></div> 0.7031 | <div></div> 0.3630 |
| M | <div></div> 0.0893 | <div></div> 0.2660 |
| N | <div></div> 0.8765 | <div></div> 0.5060 |
| O | <div></div> 0.6303 | <div></div> 0.2580 |
| P | <div></div> 0.5794 | <div></div> 0.2620 |

1.0

0.0

<0.0