



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:30 am GMT

PDB ID : 3VXU
Title : The complex between T36-5 TCR and HLA-A24 bound to HIV-1 Nef134-10(2F) peptide
Authors : Shimizu, A.; Fukai, S.; Yamagata, A.; Iwamoto, A.
Deposited on : 2012-09-20
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

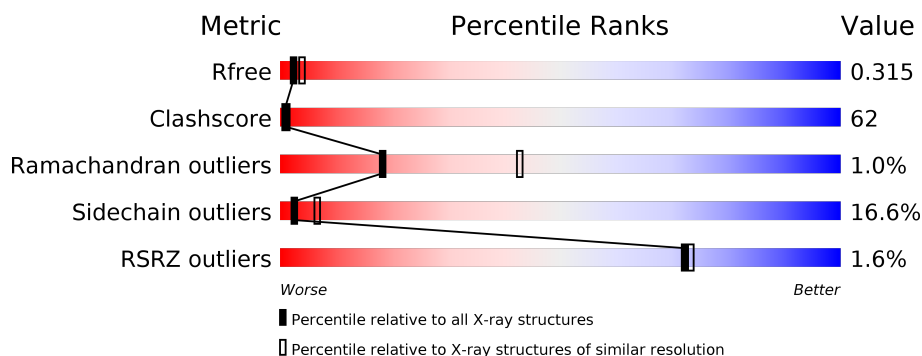
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 100719 | 2259 (2.70-2.70) |
| Clashscore | 112137 | 2590 (2.70-2.70) |
| Ramachandran outliers | 110173 | 2550 (2.70-2.70) |
| Sidechain outliers | 110143 | 2550 (2.70-2.70) |
| RSRZ outliers | 101464 | 2275 (2.70-2.70) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | A | 275 | <div> <div>3%</div> <div>28% 60% 11%</div> </div> |
| 1 | F | 275 | <div> <div>%</div> <div>35% 55% 11%</div> </div> |
| 2 | B | 100 | <div> <div>2%</div> <div>38% 48% 13%</div> </div> |
| 2 | G | 100 | <div> <div>5%</div> <div>45% 42% 12%</div> </div> |
| 3 | C | 10 | <div> <div>10% 90%</div> </div> |
| 3 | H | 10 | <div> <div>100%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 4 | D | 205 | <div><div><div></div><div></div><div></div></div><div>%31%54%12%•</div></div> |
| 4 | I | 205 | <div><div><div></div><div></div><div></div></div><div>2%29%54%14%•</div></div> |
| 5 | E | 242 | <div><div><div></div><div></div><div></div></div><div>28%60%12%</div></div> |
| 5 | J | 242 | <div><div><div></div><div></div><div></div></div><div>31%59%10%</div></div> |

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13256 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called HLA class I histocompatibility antigen, A-24 alpha chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 274 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2222 | 1382 | 403 | 427 | 10 | | | |
| 1 | F | 274 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2222 | 1382 | 403 | 427 | 10 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | 0 | MET | - | EXPRESSION TAG | UNP P05534 |
| F | 0 | MET | - | EXPRESSION TAG | UNP P05534 |

- Molecule 2 is a protein called Beta-2-microglobulin.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2 | B | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 829 | 528 | 140 | 158 | 3 | | | |
| 2 | G | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 829 | 528 | 140 | 158 | 3 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| B | 0 | MET | - | EXPRESSION TAG | UNP P61769 |
| G | 0 | MET | - | EXPRESSION TAG | UNP P61769 |

- Molecule 3 is a protein called 10-mer peptide from Protein Nef.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 3 | C | 10 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 91 | 64 | 14 | 12 | 1 | | | |
| 3 | H | 10 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 91 | 64 | 14 | 12 | 1 | | | |

- Molecule 4 is a protein called T36-5 TCR alpha chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4 | D | 199 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1553 | 968 | 257 | 321 | 7 | | | |
| 4 | I | 199 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1553 | 968 | 257 | 321 | 7 | | | |

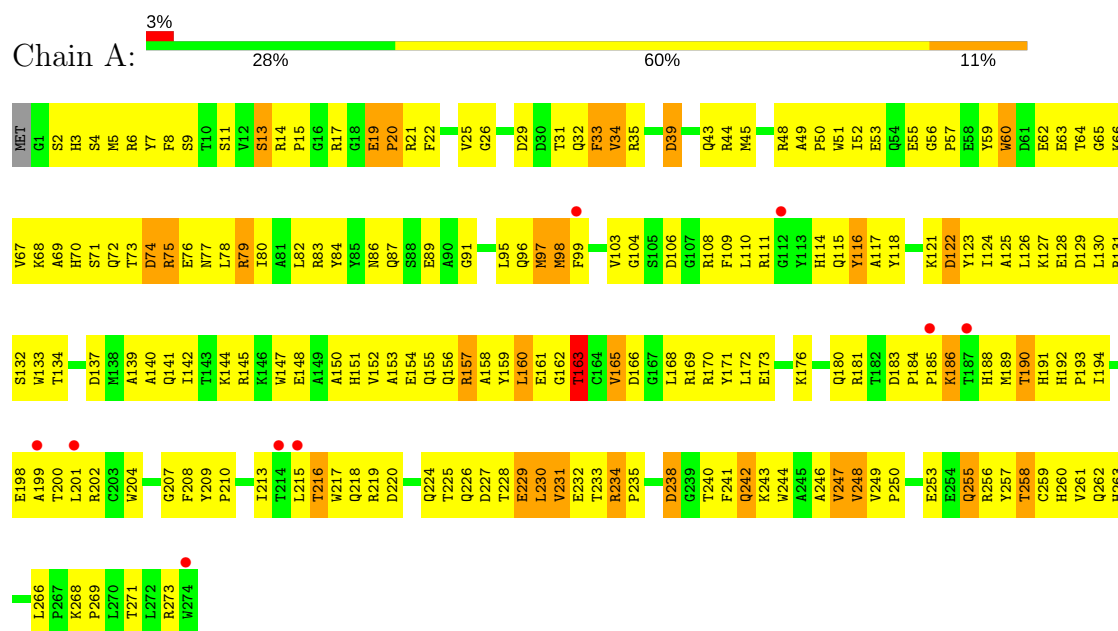
- Molecule 5 is a protein called T36-5 TCR beta chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5 | E | 241 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1933 | 1217 | 336 | 372 | 8 | | | |
| 5 | J | 241 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1933 | 1217 | 336 | 372 | 8 | | | |

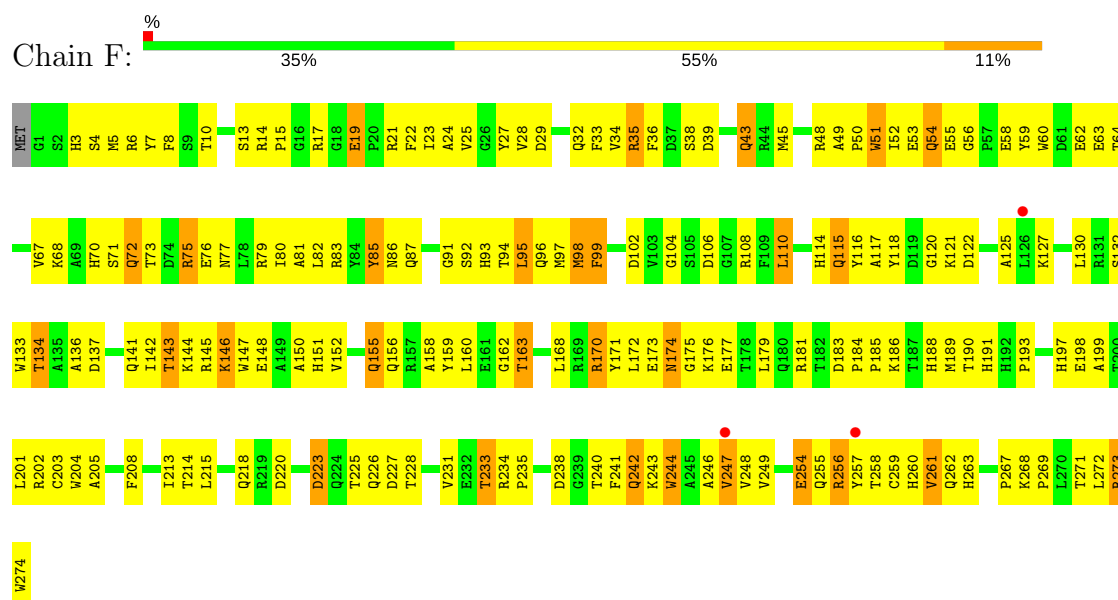
3 Residue-property plots

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

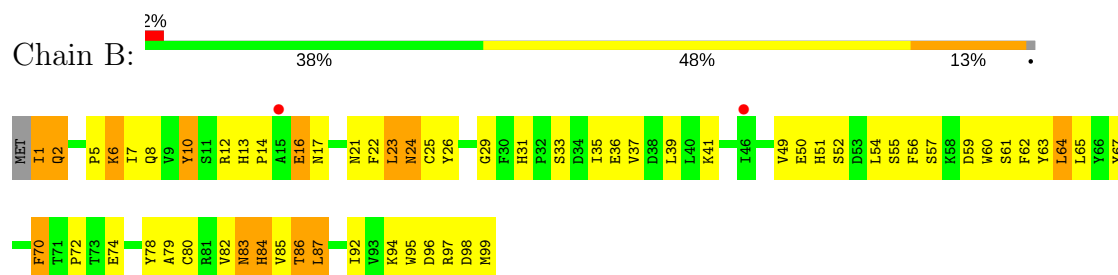
- Molecule 1: HLA class I histocompatibility antigen, A-24 alpha chain



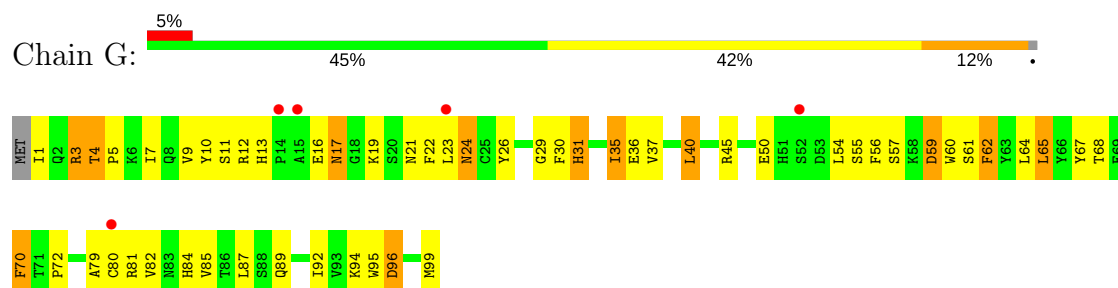
- Molecule 1: HLA class I histocompatibility antigen, A-24 alpha chain



- Molecule 2: Beta-2-microglobulin



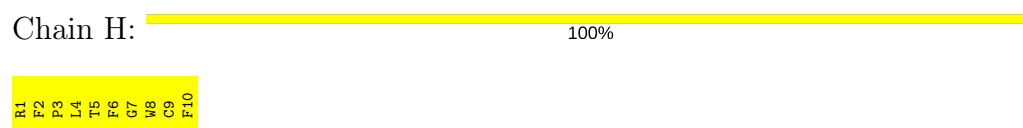
- Molecule 2: Beta-2-microglobulin



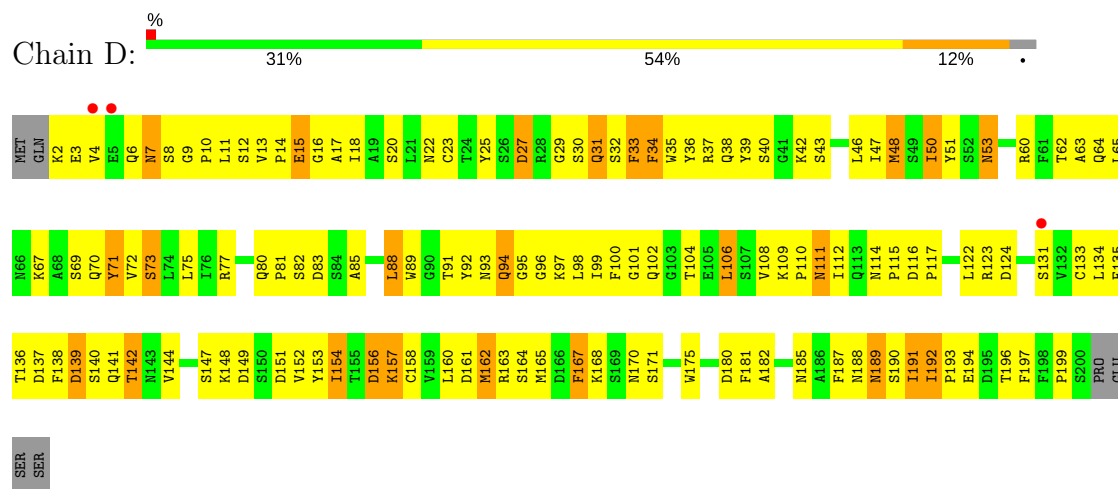
- Molecule 3: 10-mer peptide from Protein Nef



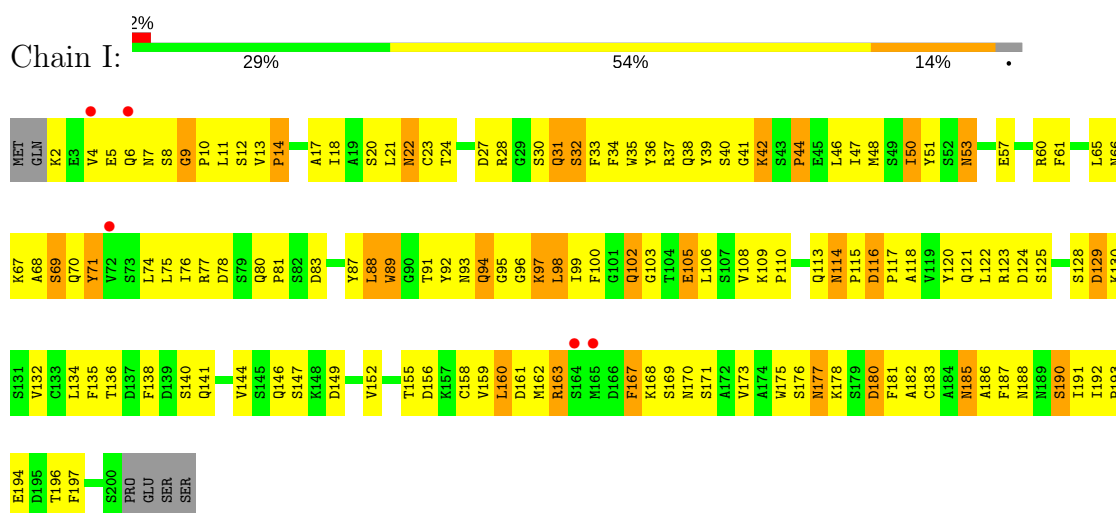
- Molecule 3: 10-mer peptide from Protein Nef



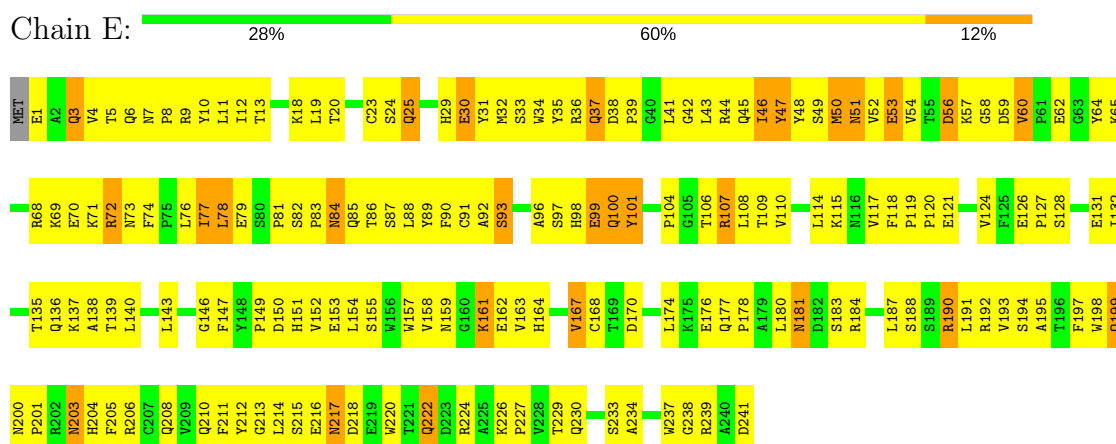
- Molecule 4: T36-5 TCR alpha chain



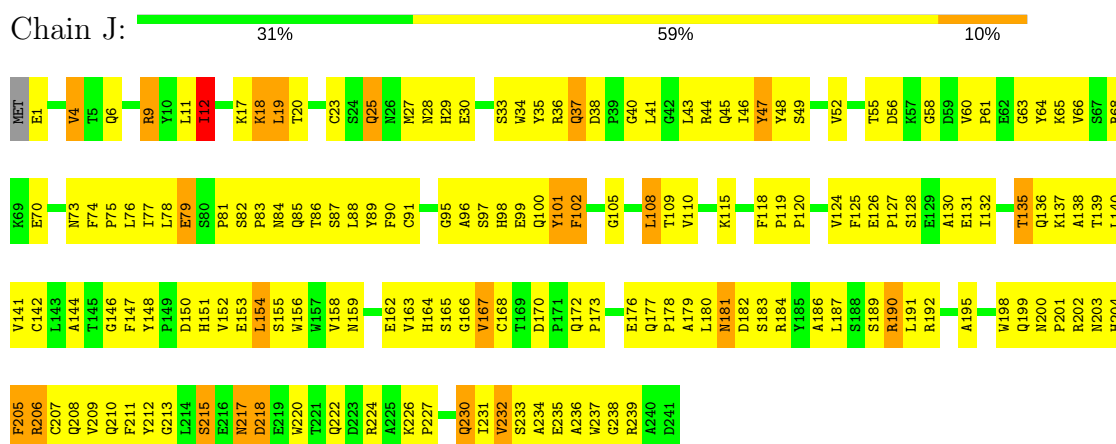
- Molecule 4: T36-5 TCR alpha chain



• Molecule 5: T36-5 TCR beta chain



• Molecule 5: T36-5 TCR beta chain



4 Data and refinement statistics

| Property | Value | Source |
|---|--|------------------|
| Space group | P 32 | Depositor |
| Cell constants a, b, c, α , β , γ | 73.16Å 73.16Å 415.66Å 90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 32.35 – 2.70 32.35 – 2.60 | Depositor EDS |
| % Data completeness (in resolution range) | 92.2 (32.35-2.70) 95.9 (32.35-2.60) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | 0.08 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.36 (at 2.61Å) | Xtriage |
| Refinement program | CNS 1.3 | Depositor |
| R, R_{free} | 0.272 , 0.323 0.267 , 0.315 | Depositor DCC |
| R_{free} test set | 3144 reflections (5.02%) | DCC |
| Wilson B-factor (Å ²) | 38.6 | Xtriage |
| Anisotropy | 0.111 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.21 , -40.9 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$ | Xtriage |
| Estimated twinning fraction | 0.069 for -h,-k,l 0.499 for h,-h-k,-l 0.069 for -k,-h,-l | Xtriage |
| Reported twinning fraction | 0.500 for h,k,l 0.500 for h,-h-k,-l | Depositor |
| Outliers | 0 of 73574 reflections | Xtriage |
| F_o, F_c correlation | 0.88 | EDS |
| Total number of atoms | 13256 | wwPDB-VP |
| Average B, all atoms (Å ²) | 67.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | A | 0.53 | 0/2282 | 0.70 | 0/3092 |
| 1 | F | 0.55 | 0/2282 | 0.74 | 1/3092 (0.0%) |
| 2 | B | 0.54 | 0/852 | 0.71 | 0/1152 |
| 2 | G | 0.60 | 0/852 | 0.71 | 0/1152 |
| 3 | C | 0.65 | 0/96 | 0.83 | 0/128 |
| 3 | H | 0.65 | 0/96 | 0.71 | 0/128 |
| 4 | D | 0.58 | 0/1587 | 0.80 | 0/2149 |
| 4 | I | 0.59 | 0/1587 | 0.80 | 0/2149 |
| 5 | E | 0.54 | 0/1986 | 0.71 | 0/2705 |
| 5 | J | 0.52 | 0/1986 | 0.74 | 1/2705 (0.0%) |
| All | All | 0.55 | 0/13606 | 0.74 | 2/18452 (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 |
|-----|-------|---------------------|---------------------|
| 5 | J | 0 | 2 |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 5 | J | 12 | ILE | CB-CA-C | -5.57 | 100.45 | 111.60 |
| 1 | F | 95 | LEU | CA-CB-CG | -5.03 | 103.74 | 115.30 |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 5 | J | 101 | TYR | Sidechain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 5 | J | 47 | TYR | Sidechain |

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 2222 | 0 | 2082 | 315 | 0 |
| 1 | F | 2222 | 0 | 2082 | 278 | 0 |
| 2 | B | 829 | 0 | 794 | 92 | 0 |
| 2 | G | 829 | 0 | 794 | 92 | 0 |
| 3 | C | 91 | 0 | 85 | 24 | 0 |
| 3 | H | 91 | 0 | 85 | 31 | 0 |
| 4 | D | 1553 | 0 | 1461 | 212 | 0 |
| 4 | I | 1553 | 0 | 1461 | 233 | 0 |
| 5 | E | 1933 | 0 | 1845 | 267 | 0 |
| 5 | J | 1933 | 0 | 1845 | 282 | 0 |
| All | All | 13256 | 0 | 12534 | 1612 | 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 62.

All (1612) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:69:ALA:HA | 5:E:51:ASN:HB2 | 1.20 | 1.19 |
| 5:J:177:GLN:HB3 | 5:J:180:LEU:HD13 | 1.19 | 1.19 |
| 5:J:35:TYR:HB3 | 5:J:43:LEU:HD11 | 1.24 | 1.16 |
| 1:A:4:SER:HB2 | 1:A:6:ARG:HH12 | 1.08 | 1.14 |
| 4:D:114:ASN:HA | 1:F:108:ARG:HH22 | 0.98 | 1.11 |
| 4:D:114:ASN:HA | 1:F:108:ARG:NH2 | 1.66 | 1.10 |
| 4:D:3:GLU:HG3 | 4:D:4:VAL:H | 1.09 | 1.10 |
| 1:A:68:LYS:HZ1 | 5:E:53:GLU:HB3 | 1.07 | 1.09 |
| 5:E:107:ARG:HB3 | 5:E:107:ARG:HH11 | 1.16 | 1.08 |
| 4:D:114:ASN:CA | 1:F:108:ARG:HH22 | 1.68 | 1.05 |
| 1:F:45:MET:H | 1:F:64:THR:HG22 | 1.22 | 1.04 |
| 5:J:181:ASN:ND2 | 5:J:181:ASN:H | 1.52 | 1.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:4:SER:HB2 | 1:A:6:ARG:NH1 | 1.72 | 1.03 |
| 4:I:94:GLN:HB3 | 4:I:97:LYS:HD3 | 1.42 | 1.02 |
| 5:J:206:ARG:HH22 | 5:J:208:GLN:HB2 | 1.24 | 1.02 |
| 4:D:18:ILE:HG12 | 4:D:77:ARG:HA | 1.42 | 1.01 |
| 4:I:66:ASN:HB3 | 4:I:71:TYR:CE2 | 1.97 | 1.00 |
| 5:J:52:VAL:HA | 5:J:68:ARG:HG3 | 1.44 | 0.99 |
| 1:A:69:ALA:CA | 5:E:51:ASN:HB2 | 1.93 | 0.99 |
| 1:F:23:ILE:HD13 | 2:G:54:LEU:HB3 | 1.42 | 0.99 |
| 4:I:161:ASP:HB2 | 4:I:168:LYS:HE2 | 1.40 | 0.99 |
| 5:E:86:THR:HG23 | 5:E:109:THR:HA | 1.41 | 0.98 |
| 1:F:10:THR:HB | 1:F:23:ILE:HG22 | 1.44 | 0.98 |
| 1:A:144:LYS:O | 1:A:148:GLU:HG3 | 1.62 | 0.98 |
| 1:A:115:GLN:HG2 | 1:A:125:ALA:HB1 | 1.42 | 0.98 |
| 5:E:92:ALA:HB1 | 5:E:100:GLN:HG2 | 1.44 | 0.98 |
| 1:F:159:TYR:HD2 | 1:F:160:LEU:HD23 | 1.26 | 0.97 |
| 1:A:69:ALA:HA | 5:E:51:ASN:CB | 1.95 | 0.97 |
| 1:F:49:ALA:O | 1:F:52:ILE:HG22 | 1.64 | 0.96 |
| 5:J:181:ASN:H | 5:J:181:ASN:HD22 | 1.07 | 0.96 |
| 1:A:200:THR:HG21 | 1:A:202:ARG:HH12 | 1.27 | 0.96 |
| 1:F:33:PHE:HD2 | 1:F:34:VAL:HG13 | 1.31 | 0.95 |
| 4:D:14:PRO:HB2 | 4:I:71:TYR:CZ | 2.01 | 0.95 |
| 4:I:167:PHE:HZ | 5:J:192:ARG:HH11 | 1.03 | 0.95 |
| 1:F:156:GLN:HA | 1:F:156:GLN:NE2 | 1.81 | 0.95 |
| 5:E:177:GLN:HB3 | 5:E:180:LEU:HD13 | 1.45 | 0.95 |
| 4:I:185:ASN:HA | 4:I:188:ASN:ND2 | 1.81 | 0.95 |
| 1:A:243:LYS:HD3 | 1:A:244:TRP:N | 1.82 | 0.94 |
| 1:A:76:GLU:HA | 1:A:79:ARG:HD3 | 1.49 | 0.94 |
| 1:A:216:THR:HG23 | 1:A:260:HIS:HB2 | 1.51 | 0.93 |
| 5:J:36:ARG:HH12 | 5:J:85:GLN:HA | 1.32 | 0.93 |
| 1:A:45:MET:HG3 | 1:A:67:VAL:HG11 | 1.47 | 0.93 |
| 4:I:10:PRO:HB3 | 4:I:105:GLU:HG2 | 1.47 | 0.93 |
| 4:D:3:GLU:HG3 | 4:D:4:VAL:N | 1.82 | 0.92 |
| 5:J:154:LEU:HD21 | 5:J:207:CYS:SG | 2.10 | 0.92 |
| 4:I:161:ASP:HB2 | 4:I:168:LYS:CE | 1.99 | 0.91 |
| 1:A:156:GLN:O | 1:A:160:LEU:HG | 1.69 | 0.91 |
| 1:F:234:ARG:HG3 | 1:F:242:GLN:HG3 | 1.53 | 0.91 |
| 2:G:12:ARG:HG2 | 2:G:21:ASN:HD21 | 1.36 | 0.90 |
| 1:F:156:GLN:HA | 1:F:156:GLN:HE21 | 1.35 | 0.90 |
| 2:G:24:ASN:HD22 | 2:G:24:ASN:H | 1.18 | 0.89 |
| 5:J:230:GLN:HE22 | 5:J:232:VAL:HG13 | 1.38 | 0.89 |
| 1:A:62:GLU:OE1 | 4:D:95:GLY:HA3 | 1.72 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:37:VAL:HG22 | 2:G:82:VAL:HG22 | 1.53 | 0.89 |
| 1:A:35:ARG:HH12 | 1:A:48:ARG:NE | 1.70 | 0.89 |
| 5:J:206:ARG:NH1 | 5:J:233:SER:HB3 | 1.87 | 0.88 |
| 4:I:66:ASN:HB3 | 4:I:71:TYR:HE2 | 1.36 | 0.88 |
| 5:E:212:TYR:HA | 5:E:229:THR:HG23 | 1.56 | 0.88 |
| 1:F:156:GLN:O | 1:F:160:LEU:HG | 1.74 | 0.88 |
| 1:A:213:ILE:HG13 | 1:A:262:GLN:O | 1.74 | 0.87 |
| 1:F:70:HIS:HD1 | 3:H:2:PHE:HZ | 1.23 | 0.87 |
| 5:J:180:LEU:N | 5:J:180:LEU:HD12 | 1.89 | 0.87 |
| 1:F:234:ARG:CG | 1:F:242:GLN:HG3 | 2.04 | 0.87 |
| 4:I:159:VAL:HG12 | 4:I:168:LYS:NZ | 1.88 | 0.87 |
| 1:F:233:THR:HG23 | 1:F:243:LYS:HB2 | 1.57 | 0.86 |
| 1:A:185:PRO:HB3 | 1:A:208:PHE:HB3 | 1.55 | 0.86 |
| 5:J:66:VAL:HG12 | 5:J:75:PRO:O | 1.75 | 0.86 |
| 2:G:12:ARG:HD2 | 2:G:22:PHE:HB2 | 1.58 | 0.86 |
| 1:F:106:ASP:OD2 | 1:F:108:ARG:HB2 | 1.75 | 0.86 |
| 5:E:64:TYR:O | 5:E:65:LYS:HD2 | 1.75 | 0.86 |
| 1:A:145:ARG:HA | 1:A:148:GLU:OE2 | 1.77 | 0.85 |
| 4:I:159:VAL:HG12 | 4:I:168:LYS:HZ2 | 1.42 | 0.85 |
| 1:A:249:VAL:HG13 | 1:A:257:TYR:HE2 | 1.41 | 0.85 |
| 4:D:97:LYS:HB2 | 5:E:45:GLN:OE1 | 1.77 | 0.85 |
| 1:A:25:VAL:HB | 1:A:32:GLN:HE22 | 1.41 | 0.85 |
| 4:I:88:LEU:N | 4:I:88:LEU:HD23 | 1.91 | 0.85 |
| 5:J:173:PRO:HA | 5:J:187:LEU:HD13 | 1.59 | 0.85 |
| 5:J:159:ASN:HD21 | 5:J:204:HIS:H | 1.22 | 0.84 |
| 1:A:63:GLU:OE1 | 3:C:1:ARG:HG3 | 1.76 | 0.84 |
| 5:J:35:TYR:CB | 5:J:43:LEU:HD11 | 2.07 | 0.84 |
| 5:E:107:ARG:HB3 | 5:E:107:ARG:NH1 | 1.92 | 0.84 |
| 5:E:19:LEU:HD12 | 5:E:78:LEU:HD13 | 1.59 | 0.84 |
| 5:E:46:ILE:N | 5:E:46:ILE:HD12 | 1.90 | 0.84 |
| 5:J:142:CYS:HB2 | 5:J:156:TRP:CH2 | 2.13 | 0.83 |
| 1:F:19:GLU:HG3 | 1:F:75:ARG:HE | 1.42 | 0.83 |
| 5:E:135:THR:HG22 | 5:E:137:LYS:HG3 | 1.59 | 0.83 |
| 5:J:36:ARG:NH1 | 5:J:85:GLN:HA | 1.92 | 0.83 |
| 1:A:69:ALA:HB2 | 5:E:50:MET:HB2 | 1.61 | 0.83 |
| 1:F:268:LYS:HD2 | 1:F:269:PRO:HD2 | 1.61 | 0.83 |
| 1:A:68:LYS:NZ | 5:E:53:GLU:HB3 | 1.92 | 0.82 |
| 5:E:36:ARG:HH21 | 5:E:87:SER:HB2 | 1.43 | 0.82 |
| 5:J:159:ASN:ND2 | 5:J:204:HIS:H | 1.77 | 0.82 |
| 1:F:45:MET:H | 1:F:64:THR:CG2 | 1.92 | 0.82 |
| 4:I:120:TYR:CE1 | 5:J:131:GLU:HA | 2.14 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:4:SER:CB | 1:A:6:ARG:HH12 | 1.89 | 0.81 |
| 5:E:88:LEU:HD13 | 5:E:107:ARG:HG2 | 1.62 | 0.81 |
| 4:D:114:ASN:HB3 | 1:F:108:ARG:HH12 | 1.45 | 0.81 |
| 2:G:24:ASN:N | 2:G:24:ASN:HD22 | 1.72 | 0.81 |
| 4:I:158:CYS:HB3 | 5:J:190:ARG:NH1 | 1.95 | 0.81 |
| 1:A:215:LEU:HD12 | 1:A:243:LYS:HD2 | 1.62 | 0.81 |
| 2:G:56:PHE:HB2 | 2:G:61:SER:O | 1.81 | 0.81 |
| 2:G:24:ASN:N | 2:G:24:ASN:ND2 | 2.25 | 0.81 |
| 4:I:61:PHE:C | 4:I:77:ARG:HH22 | 1.83 | 0.81 |
| 1:A:152:VAL:HG12 | 1:A:156:GLN:HE21 | 1.45 | 0.81 |
| 4:D:3:GLU:CG | 4:D:4:VAL:H | 1.90 | 0.81 |
| 4:I:144:VAL:HG21 | 4:I:156:ASP:HA | 1.63 | 0.81 |
| 1:A:249:VAL:HG13 | 1:A:257:TYR:CE2 | 2.15 | 0.81 |
| 2:B:51:HIS:HD2 | 2:B:64:LEU:HD21 | 1.45 | 0.81 |
| 4:I:78:ASP:OD1 | 4:I:78:ASP:O | 1.99 | 0.81 |
| 5:E:190:ARG:N | 5:E:190:ARG:HD2 | 1.95 | 0.80 |
| 5:E:137:LYS:HB2 | 5:E:192:ARG:CZ | 2.11 | 0.80 |
| 1:A:165:VAL:O | 1:A:169:ARG:HG3 | 1.81 | 0.80 |
| 4:I:160:LEU:HD11 | 4:I:167:PHE:HE2 | 1.46 | 0.80 |
| 5:J:38:ASP:H | 5:J:44:ARG:NH2 | 1.79 | 0.80 |
| 1:A:200:THR:HG21 | 1:A:202:ARG:NH1 | 1.97 | 0.80 |
| 5:E:19:LEU:CD1 | 5:E:78:LEU:HD13 | 2.11 | 0.80 |
| 1:F:259:CYS:SG | 1:F:272:LEU:HD13 | 2.22 | 0.80 |
| 1:F:75:ARG:HH11 | 1:F:75:ARG:HG2 | 1.46 | 0.80 |
| 5:J:177:GLN:HB3 | 5:J:180:LEU:CD1 | 2.09 | 0.80 |
| 1:F:202:ARG:NH1 | 1:F:246:ALA:HB2 | 1.95 | 0.80 |
| 5:E:170:ASP:HB2 | 5:E:187:LEU:HD11 | 1.62 | 0.79 |
| 1:F:115:GLN:HG3 | 2:G:60:TRP:CH2 | 2.16 | 0.79 |
| 5:E:199:GLN:O | 5:E:201:PRO:HD3 | 1.82 | 0.79 |
| 2:G:13:HIS:HB2 | 2:G:21:ASN:ND2 | 1.97 | 0.79 |
| 5:E:83:PRO:HA | 5:E:110:VAL:HB | 1.63 | 0.79 |
| 1:A:141:GLN:O | 1:A:145:ARG:HG3 | 1.82 | 0.79 |
| 4:I:155:THR:HG22 | 4:I:173:VAL:H | 1.46 | 0.79 |
| 2:G:12:ARG:HG2 | 2:G:21:ASN:ND2 | 1.97 | 0.79 |
| 1:A:152:VAL:CG1 | 1:A:156:GLN:HE21 | 1.96 | 0.78 |
| 1:A:19:GLU:OE2 | 1:A:19:GLU:HA | 1.82 | 0.78 |
| 1:F:75:ARG:HG2 | 1:F:75:ARG:NH1 | 1.99 | 0.78 |
| 1:F:58:GLU:O | 1:F:62:GLU:HG3 | 1.84 | 0.78 |
| 1:A:57:PRO:HA | 1:A:60:TRP:HD1 | 1.48 | 0.78 |
| 2:B:21:ASN:CG | 2:B:22:PHE:H | 1.88 | 0.77 |
| 2:B:56:PHE:HB3 | 2:B:62:PHE:CD2 | 2.18 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:31:GLN:HB3 | 4:D:67:LYS:NZ | 2.00 | 0.77 |
| 5:J:12:ILE:HD12 | 5:J:12:ILE:H | 1.49 | 0.77 |
| 4:D:153:TYR:HB2 | 4:D:175:TRP:CZ2 | 2.20 | 0.77 |
| 4:I:66:ASN:CB | 4:I:71:TYR:HE2 | 1.96 | 0.77 |
| 5:J:86:THR:HG23 | 5:J:109:THR:HA | 1.65 | 0.77 |
| 4:D:31:GLN:HA | 4:D:67:LYS:HE2 | 1.65 | 0.77 |
| 5:E:159:ASN:HD21 | 5:E:204:HIS:H | 1.33 | 0.77 |
| 5:E:52:VAL:HA | 5:E:68:ARG:CG | 2.14 | 0.77 |
| 1:A:26:GLY:HA3 | 1:A:33:PHE:CE1 | 2.20 | 0.76 |
| 4:I:123:ARG:HB3 | 5:J:126:GLU:HB2 | 1.68 | 0.76 |
| 5:J:154:LEU:HD23 | 5:J:208:GLN:O | 1.86 | 0.76 |
| 2:B:56:PHE:HB2 | 2:B:61:SER:O | 1.84 | 0.76 |
| 5:E:154:LEU:HD23 | 5:E:155:SER:N | 2.00 | 0.76 |
| 4:I:47:ILE:HD12 | 4:I:48:MET:N | 2.00 | 0.76 |
| 5:J:181:ASN:N | 5:J:181:ASN:HD22 | 1.83 | 0.76 |
| 1:A:243:LYS:HD3 | 1:A:244:TRP:H | 1.50 | 0.76 |
| 4:I:159:VAL:HG22 | 4:I:170:ASN:OD1 | 1.86 | 0.76 |
| 5:J:64:TYR:O | 5:J:65:LYS:HD2 | 1.85 | 0.76 |
| 1:F:45:MET:N | 1:F:64:THR:HG22 | 1.98 | 0.76 |
| 1:F:25:VAL:HB | 1:F:32:GLN:NE2 | 2.00 | 0.76 |
| 4:I:120:TYR:CZ | 5:J:131:GLU:HA | 2.20 | 0.76 |
| 4:I:46:LEU:HD22 | 5:J:99:GLU:HB3 | 1.67 | 0.75 |
| 1:F:8:PHE:HD2 | 1:F:25:VAL:HG23 | 1.50 | 0.75 |
| 1:F:45:MET:HG3 | 1:F:60:TRP:HZ3 | 1.49 | 0.75 |
| 1:A:108:ARG:NH2 | 4:I:114:ASN:HB2 | 2.01 | 0.75 |
| 1:A:33:PHE:CD1 | 1:A:34:VAL:N | 2.55 | 0.75 |
| 4:I:122:LEU:HB3 | 5:J:125:PHE:HB3 | 1.68 | 0.75 |
| 1:A:35:ARG:NH1 | 1:A:48:ARG:NE | 2.34 | 0.75 |
| 5:E:159:ASN:ND2 | 5:E:204:HIS:H | 1.84 | 0.75 |
| 3:C:7:GLY:H | 5:E:30:GLU:HG3 | 1.51 | 0.75 |
| 5:J:63:GLY:O | 5:J:78:LEU:HD12 | 1.87 | 0.75 |
| 2:B:10:TYR:O | 2:B:24:ASN:ND2 | 2.20 | 0.74 |
| 5:E:52:VAL:HA | 5:E:68:ARG:HG2 | 1.69 | 0.74 |
| 1:A:215:LEU:CD1 | 1:A:243:LYS:HD2 | 2.18 | 0.74 |
| 4:D:71:TYR:HD2 | 4:D:71:TYR:O | 1.70 | 0.74 |
| 1:F:59:TYR:O | 1:F:63:GLU:HG2 | 1.87 | 0.74 |
| 5:J:85:GLN:O | 5:J:108:LEU:HD11 | 1.87 | 0.74 |
| 1:A:115:GLN:HG2 | 1:A:125:ALA:CB | 2.18 | 0.74 |
| 4:D:29:GLY:O | 4:D:31:GLN:HG3 | 1.87 | 0.74 |
| 5:J:35:TYR:HB3 | 5:J:43:LEU:CD1 | 2.14 | 0.74 |
| 5:J:181:ASN:ND2 | 5:J:181:ASN:N | 2.33 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:45:MET:CG | 1:A:67:VAL:HG11 | 2.17 | 0.73 |
| 5:E:100:GLN:C | 5:E:101:TYR:HD2 | 1.92 | 0.73 |
| 1:A:80:ILE:HG23 | 1:A:83:ARG:NH2 | 2.02 | 0.73 |
| 1:A:258:THR:HB | 1:A:260:HIS:CE1 | 2.22 | 0.73 |
| 4:D:50:ILE:HD11 | 4:D:65:LEU:HB3 | 1.71 | 0.73 |
| 1:F:22:PHE:CD2 | 1:F:71:SER:HB3 | 2.22 | 0.73 |
| 1:F:156:GLN:HE21 | 1:F:156:GLN:CA | 2.01 | 0.73 |
| 5:E:161:LYS:NZ | 5:E:161:LYS:HB2 | 2.04 | 0.73 |
| 5:E:119:PRO:HD3 | 5:E:227:PRO:HB3 | 1.69 | 0.73 |
| 1:F:121:LYS:HE2 | 2:G:1:ILE:HG12 | 1.70 | 0.73 |
| 4:I:160:LEU:HD12 | 4:I:160:LEU:C | 2.08 | 0.73 |
| 5:J:205:PHE:HE2 | 5:J:238:GLY:N | 1.86 | 0.72 |
| 5:J:9:ARG:HB3 | 5:J:9:ARG:HH11 | 1.53 | 0.72 |
| 1:A:213:ILE:HB | 1:A:263:HIS:HD2 | 1.54 | 0.72 |
| 2:B:35:ILE:HD12 | 2:B:84:HIS:HD2 | 1.54 | 0.72 |
| 1:A:157:ARG:HA | 1:A:160:LEU:CD1 | 2.19 | 0.72 |
| 1:A:137:ASP:O | 1:A:141:GLN:HG3 | 1.90 | 0.72 |
| 5:E:158:VAL:HG23 | 5:E:163:VAL:HG21 | 1.70 | 0.72 |
| 4:I:50:ILE:C | 4:I:50:ILE:HD12 | 2.10 | 0.72 |
| 1:F:159:TYR:CD2 | 1:F:160:LEU:HD23 | 2.18 | 0.72 |
| 1:F:4:SER:HB2 | 1:F:102:ASP:OD1 | 1.89 | 0.72 |
| 4:D:22:ASN:HD22 | 4:D:71:TYR:HE1 | 1.38 | 0.72 |
| 5:E:19:LEU:HD11 | 5:E:78:LEU:HD22 | 1.71 | 0.71 |
| 5:J:77:ILE:N | 5:J:77:ILE:HD12 | 2.04 | 0.71 |
| 1:A:258:THR:HG22 | 1:A:271:THR:HG23 | 1.70 | 0.71 |
| 1:F:173:GLU:OE2 | 1:F:176:LYS:NZ | 2.22 | 0.71 |
| 1:F:272:LEU:HD12 | 1:F:272:LEU:N | 2.05 | 0.71 |
| 2:G:84:HIS:ND1 | 2:G:85:VAL:N | 2.39 | 0.71 |
| 4:I:160:LEU:HD12 | 4:I:160:LEU:O | 1.90 | 0.71 |
| 1:A:75:ARG:HD3 | 1:A:79:ARG:HD2 | 1.72 | 0.71 |
| 4:D:94:GLN:CB | 4:D:97:LYS:HE2 | 2.20 | 0.71 |
| 4:D:122:LEU:HG | 5:E:126:GLU:O | 1.90 | 0.71 |
| 2:G:31:HIS:HE1 | 2:G:60:TRP:O | 1.72 | 0.71 |
| 5:E:49:SER:OG | 5:E:68:ARG:HD3 | 1.89 | 0.71 |
| 1:F:51:TRP:CZ2 | 1:F:179:LEU:HD21 | 2.26 | 0.71 |
| 4:I:160:LEU:HD13 | 4:I:162:MET:HE3 | 1.71 | 0.71 |
| 1:A:216:THR:CG2 | 1:A:260:HIS:HB2 | 2.19 | 0.71 |
| 4:I:149:ASP:HB3 | 4:I:152:VAL:CG1 | 2.21 | 0.71 |
| 1:A:63:GLU:OE2 | 1:A:63:GLU:HA | 1.90 | 0.71 |
| 2:G:81:ARG:HA | 2:G:92:ILE:HG12 | 1.72 | 0.71 |
| 1:A:253:GLU:O | 1:A:257:TYR:CE2 | 2.44 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:4:LEU:HD21 | 4:D:96:GLY:HA2 | 1.72 | 0.70 |
| 4:I:18:ILE:HG12 | 4:I:77:ARG:HA | 1.73 | 0.70 |
| 4:D:64:GLN:OE1 | 4:I:17:ALA:HA | 1.92 | 0.70 |
| 4:D:62:THR:HG22 | 4:D:75:LEU:HD13 | 1.74 | 0.70 |
| 1:A:190:THR:HG21 | 2:B:98:ASP:OD1 | 1.92 | 0.70 |
| 4:D:167:PHE:HD2 | 4:D:168:LYS:N | 1.89 | 0.70 |
| 4:D:71:TYR:C | 4:D:71:TYR:CD2 | 2.64 | 0.70 |
| 1:F:51:TRP:CE2 | 1:F:179:LEU:HD11 | 2.27 | 0.70 |
| 1:F:28:VAL:HG23 | 1:F:33:PHE:CD1 | 2.26 | 0.70 |
| 5:E:5:THR:HB | 5:E:24:SER:OG | 1.92 | 0.70 |
| 4:I:100:PHE:CE2 | 5:J:43:LEU:HD23 | 2.27 | 0.70 |
| 4:I:178:LYS:HE3 | 4:I:180:ASP:HB2 | 1.72 | 0.70 |
| 5:J:102:PHE:N | 5:J:102:PHE:CD2 | 2.59 | 0.70 |
| 5:J:200:ASN:HD21 | 5:J:202:ARG:HB3 | 1.55 | 0.70 |
| 4:D:71:TYR:CE2 | 4:D:73:SER:HB3 | 2.27 | 0.70 |
| 1:A:57:PRO:HA | 1:A:60:TRP:CD1 | 2.26 | 0.70 |
| 1:F:19:GLU:HG3 | 1:F:75:ARG:NE | 2.07 | 0.70 |
| 5:J:119:PRO:HD3 | 5:J:227:PRO:HB3 | 1.71 | 0.70 |
| 4:D:185:ASN:HA | 4:D:188:ASN:ND2 | 2.06 | 0.69 |
| 4:D:94:GLN:HB3 | 4:D:97:LYS:NZ | 2.06 | 0.69 |
| 5:E:77:ILE:N | 5:E:77:ILE:HD12 | 2.07 | 0.69 |
| 2:B:29:GLY:HA2 | 2:B:61:SER:HB2 | 1.74 | 0.69 |
| 1:F:185:PRO:HB3 | 1:F:208:PHE:HB3 | 1.74 | 0.69 |
| 1:F:35:ARG:HH11 | 1:F:35:ARG:HG2 | 1.58 | 0.69 |
| 1:A:200:THR:CG2 | 1:A:202:ARG:HH12 | 2.02 | 0.69 |
| 1:A:33:PHE:HD1 | 1:A:34:VAL:H | 1.40 | 0.69 |
| 3:H:4:LEU:HD22 | 3:H:6:PHE:CE2 | 2.28 | 0.69 |
| 5:J:108:LEU:C | 5:J:108:LEU:HD12 | 2.12 | 0.69 |
| 1:A:231:VAL:O | 1:A:243:LYS:HE3 | 1.92 | 0.69 |
| 1:A:26:GLY:HA3 | 1:A:33:PHE:HE1 | 1.57 | 0.69 |
| 5:E:132:ILE:HG23 | 5:E:195:ALA:CB | 2.23 | 0.69 |
| 4:I:185:ASN:HA | 4:I:188:ASN:HD21 | 1.58 | 0.69 |
| 5:E:132:ILE:HG23 | 5:E:195:ALA:HB1 | 1.74 | 0.69 |
| 1:F:202:ARG:HD3 | 1:F:244:TRP:CD1 | 2.28 | 0.69 |
| 1:F:28:VAL:HG23 | 1:F:33:PHE:HD1 | 1.57 | 0.69 |
| 3:H:4:LEU:HD22 | 3:H:6:PHE:HE2 | 1.57 | 0.69 |
| 4:D:148:LYS:HD3 | 4:D:189:ASN:OD1 | 1.93 | 0.69 |
| 5:E:118:PHE:HB3 | 5:E:184:ARG:HH21 | 1.57 | 0.69 |
| 1:F:108:ARG:HH11 | 1:F:108:ARG:HG3 | 1.57 | 0.69 |
| 4:I:97:LYS:HE3 | 5:J:48:TYR:HE2 | 1.57 | 0.69 |
| 1:A:209:TYR:HD1 | 1:A:241:PHE:HE1 | 1.41 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:68:LYS:HZ1 | 5:E:53:GLU:CB | 1.97 | 0.69 |
| 5:E:37:GLN:CG | 5:E:43:LEU:HD12 | 2.23 | 0.68 |
| 5:E:78:LEU:N | 5:E:78:LEU:HD12 | 2.08 | 0.68 |
| 2:G:7:ILE:N | 2:G:7:ILE:HD12 | 2.09 | 0.68 |
| 4:I:34:PHE:HZ | 5:J:98:HIS:HB2 | 1.59 | 0.68 |
| 2:B:23:LEU:HD21 | 2:B:39:LEU:HD22 | 1.74 | 0.68 |
| 1:A:156:GLN:O | 1:A:160:LEU:CG | 2.41 | 0.68 |
| 2:B:95:TRP:CZ2 | 2:B:97:ARG:HG2 | 2.29 | 0.68 |
| 1:F:51:TRP:CZ2 | 1:F:179:LEU:HD11 | 2.28 | 0.68 |
| 2:G:13:HIS:H | 2:G:21:ASN:HD21 | 1.42 | 0.68 |
| 5:J:127:PRO:HD3 | 5:J:140:LEU:CD2 | 2.23 | 0.68 |
| 4:I:35:TRP:HB3 | 4:I:47:ILE:HD11 | 1.76 | 0.68 |
| 5:J:18:LYS:HG3 | 5:J:79:GLU:OE1 | 1.94 | 0.68 |
| 4:D:33:PHE:O | 4:D:50:ILE:HG23 | 1.93 | 0.68 |
| 2:G:12:ARG:HG3 | 2:G:13:HIS:HD2 | 1.58 | 0.68 |
| 1:A:235:PRO:HG2 | 2:B:65:LEU:HD13 | 1.76 | 0.67 |
| 1:A:75:ARG:NH1 | 1:A:79:ARG:HE | 1.93 | 0.67 |
| 4:I:46:LEU:HD21 | 5:J:99:GLU:OE2 | 1.95 | 0.67 |
| 1:F:14:ARG:HB3 | 1:F:17:ARG:HB2 | 1.77 | 0.67 |
| 1:F:25:VAL:HB | 1:F:32:GLN:HE21 | 1.57 | 0.67 |
| 2:G:29:GLY:HA2 | 2:G:61:SER:HB2 | 1.75 | 0.67 |
| 1:A:49:ALA:O | 1:A:52:ILE:HG22 | 1.93 | 0.67 |
| 1:F:19:GLU:CD | 1:F:75:ARG:HH21 | 1.97 | 0.67 |
| 1:F:96:GLN:OE1 | 2:G:60:TRP:HB3 | 1.95 | 0.67 |
| 4:D:12:SER:HA | 4:D:109:LYS:HZ3 | 1.60 | 0.67 |
| 4:D:144:VAL:HG21 | 4:D:156:ASP:HA | 1.76 | 0.67 |
| 1:F:27:TYR:CZ | 1:F:32:GLN:HB2 | 2.29 | 0.67 |
| 4:I:20:SER:C | 4:I:21:LEU:HD23 | 2.15 | 0.67 |
| 5:J:87:SER:OG | 5:J:88:LEU:N | 2.25 | 0.67 |
| 5:J:199:GLN:O | 5:J:201:PRO:HD3 | 1.94 | 0.67 |
| 1:A:69:ALA:O | 5:E:51:ASN:ND2 | 2.28 | 0.67 |
| 4:D:14:PRO:HD2 | 4:I:71:TYR:CE1 | 2.29 | 0.67 |
| 5:J:179:ALA:C | 5:J:180:LEU:HD12 | 2.15 | 0.67 |
| 5:E:167:VAL:HG12 | 5:E:191:LEU:HD13 | 1.76 | 0.67 |
| 1:F:127:LYS:HE2 | 1:F:134:THR:HB | 1.76 | 0.67 |
| 1:F:146:LYS:NZ | 1:F:146:LYS:HB3 | 2.10 | 0.67 |
| 5:J:12:ILE:HD12 | 5:J:12:ILE:N | 2.09 | 0.67 |
| 1:A:186:LYS:NZ | 1:A:186:LYS:HB2 | 2.10 | 0.67 |
| 4:D:191:ILE:H | 4:D:191:ILE:HD12 | 1.60 | 0.67 |
| 1:F:181:ARG:HG2 | 1:F:181:ARG:HH11 | 1.60 | 0.67 |
| 4:I:162:MET:HE3 | 5:J:166:GLY:HA2 | 1.76 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:226:GLN:OE1 | 1:A:226:GLN:HA | 1.95 | 0.67 |
| 4:D:112:ILE:HG13 | 4:D:170:ASN:HD21 | 1.58 | 0.67 |
| 4:D:91:THR:HG23 | 4:D:91:THR:O | 1.95 | 0.67 |
| 1:F:146:LYS:CB | 1:F:146:LYS:NZ | 2.58 | 0.66 |
| 4:D:89:TRP:HZ3 | 4:D:91:THR:CG2 | 2.09 | 0.66 |
| 4:I:159:VAL:CG1 | 4:I:168:LYS:HZ2 | 2.07 | 0.66 |
| 4:D:18:ILE:CD1 | 4:D:77:ARG:HG2 | 2.25 | 0.66 |
| 5:E:137:LYS:HB2 | 5:E:192:ARG:NH2 | 2.10 | 0.66 |
| 4:D:2:LYS:NZ | 5:E:43:LEU:N | 2.44 | 0.66 |
| 1:F:234:ARG:HE | 1:F:242:GLN:CD | 1.98 | 0.66 |
| 5:J:135:THR:O | 5:J:137:LYS:NZ | 2.29 | 0.66 |
| 4:I:162:MET:CE | 5:J:192:ARG:HB3 | 2.25 | 0.66 |
| 4:I:66:ASN:HB3 | 4:I:71:TYR:CD2 | 2.31 | 0.66 |
| 1:A:142:ILE:HA | 1:A:145:ARG:HH11 | 1.60 | 0.66 |
| 1:A:117:ALA:HB2 | 2:B:60:TRP:CE2 | 2.31 | 0.66 |
| 2:B:96:ASP:HB3 | 2:B:99:MET:HA | 1.77 | 0.66 |
| 1:F:193:PRO:HA | 1:F:199:ALA:HA | 1.76 | 0.66 |
| 1:F:228:THR:HG22 | 1:F:247:VAL:HG12 | 1.78 | 0.66 |
| 5:J:144:ALA:C | 5:J:147:PHE:HE2 | 1.98 | 0.66 |
| 5:E:9:ARG:NH1 | 5:E:104:PRO:HB2 | 2.11 | 0.66 |
| 5:J:120:PRO:HG2 | 5:J:232:VAL:HG21 | 1.77 | 0.66 |
| 4:D:83:ASP:O | 4:D:106:LEU:HD23 | 1.96 | 0.66 |
| 1:F:97:MET:HB2 | 1:F:116:TYR:CE1 | 2.31 | 0.66 |
| 1:F:70:HIS:HD2 | 1:F:73:THR:HB | 1.58 | 0.66 |
| 4:I:60:ARG:NH2 | 4:I:80:GLN:HG2 | 2.10 | 0.66 |
| 3:H:3:PRO:HG2 | 3:H:5:THR:CG2 | 2.25 | 0.66 |
| 1:F:76:GLU:HA | 1:F:76:GLU:OE2 | 1.96 | 0.66 |
| 4:D:94:GLN:HG3 | 4:D:97:LYS:HE2 | 1.78 | 0.65 |
| 5:E:64:TYR:C | 5:E:65:LYS:HD2 | 2.14 | 0.65 |
| 4:I:20:SER:O | 4:I:21:LEU:HD23 | 1.96 | 0.65 |
| 5:J:79:GLU:HA | 5:J:79:GLU:OE1 | 1.95 | 0.65 |
| 1:F:231:VAL:HG13 | 1:F:244:TRP:CZ3 | 2.31 | 0.65 |
| 5:J:127:PRO:HD3 | 5:J:140:LEU:HD21 | 1.78 | 0.65 |
| 1:F:213:ILE:HG13 | 1:F:262:GLN:O | 1.97 | 0.65 |
| 4:D:167:PHE:CE1 | 5:E:137:LYS:HE3 | 2.32 | 0.65 |
| 1:F:202:ARG:HH12 | 1:F:246:ALA:HB2 | 1.59 | 0.65 |
| 4:D:142:THR:HG21 | 4:D:193:PRO:HD3 | 1.79 | 0.65 |
| 1:A:258:THR:HG22 | 1:A:271:THR:CG2 | 2.27 | 0.65 |
| 5:E:32:MET:HE1 | 5:E:71:LYS:O | 1.96 | 0.65 |
| 5:E:46:ILE:N | 5:E:46:ILE:CD1 | 2.59 | 0.65 |
| 4:I:124:ASP:HA | 5:J:125:PHE:CZ | 2.31 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:33:PHE:HD1 | 1:A:34:VAL:N | 1.94 | 0.65 |
| 1:A:68:LYS:HG2 | 5:E:54:VAL:HG22 | 1.79 | 0.65 |
| 1:A:76:GLU:O | 1:A:80:ILE:HG13 | 1.97 | 0.65 |
| 5:E:101:TYR:CD2 | 5:E:101:TYR:N | 2.65 | 0.65 |
| 5:E:23:CYS:HB2 | 5:E:34:TRP:CZ2 | 2.31 | 0.65 |
| 4:I:136:THR:HG21 | 5:J:192:ARG:HH22 | 1.61 | 0.65 |
| 4:I:38:GLN:HE22 | 5:J:37:GLN:NE2 | 1.95 | 0.65 |
| 1:A:154:GLU:HB2 | 4:D:51:TYR:HB2 | 1.78 | 0.64 |
| 5:J:220:TRP:HH2 | 5:J:224:ARG:HH21 | 1.42 | 0.64 |
| 4:D:114:ASN:CB | 1:F:108:ARG:HH12 | 2.11 | 0.64 |
| 5:E:146:GLY:O | 5:E:184:ARG:NH2 | 2.30 | 0.64 |
| 5:J:180:LEU:CD1 | 5:J:180:LEU:N | 2.59 | 0.64 |
| 2:G:45:ARG:HE | 2:G:81:ARG:HH22 | 1.45 | 0.64 |
| 2:B:24:ASN:N | 2:B:24:ASN:ND2 | 2.44 | 0.64 |
| 4:D:64:GLN:NE2 | 4:I:18:ILE:HD12 | 2.11 | 0.64 |
| 1:A:127:LYS:HD3 | 1:A:132:SER:OG | 1.98 | 0.64 |
| 4:D:31:GLN:HA | 4:D:67:LYS:CE | 2.28 | 0.64 |
| 4:D:2:LYS:HZ1 | 5:E:43:LEU:H | 1.44 | 0.64 |
| 4:D:191:ILE:HD12 | 4:D:191:ILE:N | 2.13 | 0.64 |
| 1:A:235:PRO:CG | 2:B:65:LEU:HD13 | 2.28 | 0.64 |
| 1:A:242:GLN:OE1 | 2:B:10:TYR:HE2 | 1.81 | 0.64 |
| 1:A:69:ALA:CB | 5:E:51:ASN:HB2 | 2.28 | 0.64 |
| 1:A:75:ARG:O | 1:A:75:ARG:HD3 | 1.98 | 0.64 |
| 4:D:92:TYR:HE2 | 5:E:98:HIS:HB3 | 1.63 | 0.64 |
| 1:A:13:SER:OG | 1:A:15:PRO:HD3 | 1.97 | 0.63 |
| 1:A:229:GLU:OE2 | 1:A:230:LEU:N | 2.31 | 0.63 |
| 5:E:48:TYR:CE2 | 5:E:56:ASP:HB2 | 2.33 | 0.63 |
| 1:A:21:ARG:CZ | 1:A:39:ASP:HB2 | 2.28 | 0.63 |
| 1:A:56:GLY:O | 1:A:59:TYR:HB3 | 1.98 | 0.63 |
| 1:F:159:TYR:O | 1:F:163:THR:OG1 | 2.15 | 0.63 |
| 2:G:21:ASN:CG | 2:G:22:PHE:H | 2.01 | 0.63 |
| 5:J:159:ASN:HD21 | 5:J:204:HIS:N | 1.94 | 0.63 |
| 1:A:158:ALA:HB1 | 4:D:67:LYS:HZ1 | 1.63 | 0.63 |
| 1:A:126:LEU:HD13 | 1:A:133:TRP:CZ3 | 2.34 | 0.63 |
| 1:A:228:THR:HG22 | 1:A:247:VAL:HG12 | 1.79 | 0.63 |
| 5:E:194:SER:OG | 5:E:197:PHE:HB2 | 1.98 | 0.63 |
| 2:B:10:TYR:OH | 2:B:26:TYR:HB2 | 1.99 | 0.63 |
| 5:J:206:ARG:HG3 | 5:J:235:GLU:HB3 | 1.80 | 0.63 |
| 4:D:191:ILE:CD1 | 4:D:191:ILE:H | 2.10 | 0.63 |
| 5:E:164:HIS:O | 5:E:167:VAL:HG13 | 1.98 | 0.63 |
| 4:D:92:TYR:CE2 | 5:E:98:HIS:HB3 | 2.33 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:J:154:LEU:HG | 5:J:209:VAL:HG22 | 1.81 | 0.63 |
| 1:A:68:LYS:CG | 5:E:54:VAL:HG22 | 2.29 | 0.63 |
| 1:F:146:LYS:CB | 1:F:146:LYS:HZ2 | 2.12 | 0.63 |
| 4:I:167:PHE:HZ | 5:J:192:ARG:NH1 | 1.85 | 0.63 |
| 1:A:162:GLY:O | 1:A:165:VAL:HG23 | 1.99 | 0.63 |
| 4:D:80:GLN:HB2 | 4:D:83:ASP:OD2 | 1.98 | 0.63 |
| 1:F:202:ARG:HG3 | 1:F:202:ARG:HH11 | 1.63 | 0.63 |
| 4:I:136:THR:HG21 | 5:J:192:ARG:NH2 | 2.14 | 0.63 |
| 2:G:12:ARG:HG2 | 2:G:13:HIS:N | 2.14 | 0.63 |
| 5:J:177:GLN:HG3 | 5:J:180:LEU:HD22 | 1.81 | 0.63 |
| 4:I:97:LYS:HB3 | 5:J:48:TYR:CE2 | 2.34 | 0.63 |
| 1:A:108:ARG:O | 1:A:110:LEU:HD13 | 1.99 | 0.62 |
| 4:D:185:ASN:HA | 4:D:188:ASN:HD21 | 1.64 | 0.62 |
| 4:I:60:ARG:HH21 | 4:I:80:GLN:HG2 | 1.62 | 0.62 |
| 2:B:35:ILE:HD11 | 2:B:82:VAL:HG13 | 1.80 | 0.62 |
| 3:C:4:LEU:HB3 | 3:C:6:PHE:CE2 | 2.33 | 0.62 |
| 4:I:92:TYR:HA | 4:I:97:LYS:O | 1.98 | 0.62 |
| 1:A:111:ARG:NH2 | 1:A:128:GLU:HA | 2.14 | 0.62 |
| 1:A:79:ARG:HH11 | 1:A:79:ARG:HB2 | 1.65 | 0.62 |
| 4:D:147:SER:OG | 4:D:152:VAL:HG13 | 1.99 | 0.62 |
| 4:D:48:MET:HE3 | 4:D:63:ALA:N | 2.15 | 0.62 |
| 1:F:127:LYS:CE | 1:F:134:THR:HB | 2.30 | 0.62 |
| 4:D:182:ALA:HB3 | 4:D:185:ASN:HD21 | 1.63 | 0.62 |
| 4:D:31:GLN:HB3 | 4:D:67:LYS:HZ3 | 1.63 | 0.62 |
| 4:I:50:ILE:HD12 | 4:I:51:TYR:N | 2.14 | 0.62 |
| 5:J:36:ARG:HG3 | 5:J:87:SER:OG | 2.00 | 0.62 |
| 5:E:239:ARG:HH11 | 5:E:239:ARG:HG3 | 1.64 | 0.62 |
| 1:F:150:ALA:O | 1:F:151:HIS:HB2 | 1.99 | 0.62 |
| 1:F:158:ALA:CB | 4:I:31:GLN:HB2 | 2.29 | 0.62 |
| 5:E:150:ASP:OD1 | 5:E:150:ASP:O | 2.17 | 0.62 |
| 1:A:65:GLY:O | 5:E:54:VAL:HG11 | 2.00 | 0.62 |
| 4:I:138:PHE:CZ | 4:I:170:ASN:HB3 | 2.35 | 0.62 |
| 2:B:2:GLN:HG3 | 2:B:31:HIS:O | 1.99 | 0.62 |
| 2:B:33:SER:HB2 | 2:B:54:LEU:HD11 | 1.81 | 0.62 |
| 1:F:175:GLY:O | 1:F:179:LEU:HG | 1.99 | 0.62 |
| 4:I:34:PHE:CZ | 5:J:98:HIS:HB2 | 2.34 | 0.62 |
| 4:D:108:VAL:HG12 | 4:D:108:VAL:O | 1.97 | 0.62 |
| 5:E:4:VAL:HG13 | 5:E:23:CYS:SG | 2.40 | 0.62 |
| 1:F:115:GLN:HG3 | 2:G:60:TRP:HH2 | 1.63 | 0.62 |
| 1:F:33:PHE:CD2 | 1:F:34:VAL:HG13 | 2.24 | 0.62 |
| 5:J:177:GLN:CB | 5:J:180:LEU:HD13 | 2.12 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:111:ARG:NH1 | 1:A:128:GLU:OE1 | 2.33 | 0.62 |
| 1:A:99:PHE:CD1 | 1:A:114:HIS:HD2 | 2.18 | 0.62 |
| 5:E:128:SER:O | 5:E:132:ILE:HD12 | 1.99 | 0.62 |
| 5:E:48:TYR:HE1 | 5:E:50:MET:HE2 | 1.65 | 0.62 |
| 1:F:234:ARG:HG2 | 1:F:242:GLN:HG3 | 1.82 | 0.62 |
| 2:G:57:SER:O | 2:G:59:ASP:O | 2.18 | 0.62 |
| 4:I:88:LEU:HB3 | 4:I:103:GLY:HA2 | 1.81 | 0.62 |
| 5:J:102:PHE:HD2 | 5:J:102:PHE:N | 1.97 | 0.62 |
| 1:A:193:PRO:HA | 1:A:199:ALA:HA | 1.81 | 0.61 |
| 4:D:88:LEU:N | 4:D:88:LEU:HD23 | 2.15 | 0.61 |
| 3:H:6:PHE:CZ | 5:J:98:HIS:HD2 | 2.18 | 0.61 |
| 1:A:80:ILE:HG23 | 1:A:83:ARG:HH22 | 1.62 | 0.61 |
| 1:F:146:LYS:HB2 | 1:F:146:LYS:HZ2 | 1.65 | 0.61 |
| 1:A:111:ARG:HD3 | 1:A:128:GLU:OE2 | 1.99 | 0.61 |
| 1:A:7:TYR:CE2 | 3:C:2:PHE:HA | 2.35 | 0.61 |
| 1:A:155:GLN:OE1 | 3:C:8:TRP:HZ2 | 1.83 | 0.61 |
| 5:E:168:CYS:O | 5:E:190:ARG:HD2 | 2.00 | 0.61 |
| 1:F:51:TRP:HZ2 | 1:F:179:LEU:HD21 | 1.65 | 0.61 |
| 2:G:17:ASN:HA | 2:G:72:PRO:O | 1.99 | 0.61 |
| 3:H:3:PRO:HG2 | 3:H:5:THR:HG22 | 1.81 | 0.61 |
| 4:I:38:GLN:HB2 | 4:I:44:PRO:HG3 | 1.82 | 0.61 |
| 4:D:112:ILE:CD1 | 4:D:170:ASN:HD21 | 2.14 | 0.61 |
| 5:E:52:VAL:HA | 5:E:68:ARG:HG3 | 1.82 | 0.61 |
| 1:F:158:ALA:HB3 | 4:I:31:GLN:HB2 | 1.83 | 0.61 |
| 1:A:34:VAL:HG21 | 1:A:45:MET:CE | 2.30 | 0.61 |
| 4:D:92:TYR:HA | 4:D:97:LYS:O | 2.00 | 0.61 |
| 1:F:168:LEU:O | 1:F:172:LEU:HG | 2.01 | 0.61 |
| 1:F:63:GLU:O | 1:F:67:VAL:HG12 | 2.00 | 0.61 |
| 4:I:129:ASP:OD1 | 4:I:130:LYS:HG3 | 2.01 | 0.61 |
| 2:B:51:HIS:CD2 | 2:B:64:LEU:HD21 | 2.33 | 0.61 |
| 5:E:52:VAL:HG13 | 5:E:68:ARG:O | 1.99 | 0.61 |
| 1:F:75:ARG:HH11 | 1:F:75:ARG:CG | 2.11 | 0.61 |
| 5:J:4:VAL:HG21 | 5:J:102:PHE:C | 2.21 | 0.61 |
| 1:A:26:GLY:O | 1:A:32:GLN:OE1 | 2.18 | 0.61 |
| 1:F:191:HIS:HE1 | 1:F:193:PRO:HG3 | 1.65 | 0.61 |
| 5:E:32:MET:SD | 5:E:68:ARG:CZ | 2.89 | 0.61 |
| 4:D:135:PHE:HB2 | 4:D:187:PHE:CE2 | 2.35 | 0.60 |
| 1:F:99:PHE:HE2 | 1:F:159:TYR:CE2 | 2.19 | 0.60 |
| 5:J:163:VAL:O | 5:J:164:HIS:ND1 | 2.34 | 0.60 |
| 1:F:233:THR:HG23 | 1:F:243:LYS:HD2 | 1.83 | 0.60 |
| 5:J:230:GLN:HE22 | 5:J:232:VAL:CG1 | 2.10 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:133:TRP:CZ2 | 1:A:152:VAL:HB | 2.36 | 0.60 |
| 2:B:33:SER:HB3 | 2:B:62:PHE:CD1 | 2.36 | 0.60 |
| 2:B:23:LEU:HD11 | 2:B:39:LEU:HD22 | 1.83 | 0.60 |
| 4:D:18:ILE:HD11 | 4:D:77:ARG:HG2 | 1.83 | 0.60 |
| 5:E:19:LEU:HD12 | 5:E:19:LEU:C | 2.22 | 0.60 |
| 1:F:267:PRO:HG2 | 1:F:268:LYS:H | 1.65 | 0.60 |
| 2:G:12:ARG:CD | 2:G:22:PHE:HB2 | 2.31 | 0.60 |
| 4:I:81:PRO:HA | 4:I:108:VAL:HB | 1.83 | 0.60 |
| 4:I:41:GLY:C | 4:I:42:LYS:HE2 | 2.21 | 0.60 |
| 4:D:154:ILE:HD11 | 4:D:187:PHE:CD1 | 2.35 | 0.60 |
| 2:G:80:CYS:O | 2:G:92:ILE:HA | 2.02 | 0.60 |
| 4:I:149:ASP:HB3 | 4:I:152:VAL:HG11 | 1.81 | 0.60 |
| 4:I:91:THR:OG1 | 4:I:93:ASN:ND2 | 2.34 | 0.60 |
| 5:J:38:ASP:H | 5:J:44:ARG:HH22 | 1.47 | 0.60 |
| 1:A:192:HIS:HD2 | 1:A:202:ARG:HH21 | 1.50 | 0.60 |
| 5:E:190:ARG:H | 5:E:190:ARG:HD2 | 1.63 | 0.60 |
| 1:F:144:LYS:O | 1:F:148:GLU:HG3 | 2.01 | 0.60 |
| 1:A:250:PRO:O | 1:A:253:GLU:HB2 | 2.01 | 0.60 |
| 1:F:155:GLN:HE22 | 5:J:98:HIS:CE1 | 2.19 | 0.60 |
| 1:F:70:HIS:O | 1:F:73:THR:HB | 2.02 | 0.60 |
| 1:A:238:ASP:OD2 | 2:B:12:ARG:HD3 | 2.01 | 0.60 |
| 1:F:249:VAL:HG22 | 1:F:257:TYR:CE1 | 2.37 | 0.60 |
| 1:F:260:HIS:CE1 | 1:F:271:THR:HG23 | 2.37 | 0.60 |
| 5:J:12:ILE:HD11 | 5:J:213:GLY:O | 2.01 | 0.60 |
| 1:A:127:LYS:HB2 | 1:A:129:ASP:OD1 | 2.01 | 0.60 |
| 1:A:99:PHE:HD1 | 1:A:114:HIS:HD2 | 1.49 | 0.60 |
| 4:D:60:ARG:HH22 | 4:D:83:ASP:CG | 2.04 | 0.60 |
| 4:I:158:CYS:HB3 | 5:J:190:ARG:HH12 | 1.66 | 0.60 |
| 2:B:7:ILE:N | 2:B:7:ILE:HD12 | 2.16 | 0.60 |
| 5:E:206:ARG:NH1 | 5:E:208:GLN:OE1 | 2.35 | 0.60 |
| 1:F:43:GLN:HA | 1:F:43:GLN:HE21 | 1.67 | 0.60 |
| 1:A:189:MET:SD | 1:A:201:LEU:HD22 | 2.42 | 0.60 |
| 1:A:261:VAL:HG12 | 1:A:266:LEU:HD11 | 1.83 | 0.60 |
| 1:F:81:ALA:HB1 | 1:F:118:TYR:CE2 | 2.37 | 0.60 |
| 1:F:70:HIS:HE1 | 1:F:97:MET:SD | 2.25 | 0.60 |
| 4:I:190:SER:O | 4:I:192:ILE:HG23 | 2.02 | 0.60 |
| 5:E:49:SER:CB | 5:E:68:ARG:HD3 | 2.32 | 0.59 |
| 2:G:45:ARG:HB2 | 2:G:81:ARG:HH22 | 1.66 | 0.59 |
| 1:A:33:PHE:CD1 | 1:A:34:VAL:HG13 | 2.37 | 0.59 |
| 2:B:24:ASN:H | 2:B:24:ASN:ND2 | 1.99 | 0.59 |
| 4:D:71:TYR:C | 4:D:71:TYR:HD2 | 2.04 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:117:ALA:HB2 | 2:G:60:TRP:CD2 | 2.37 | 0.59 |
| 5:J:200:ASN:ND2 | 5:J:202:ARG:HB3 | 2.16 | 0.59 |
| 1:A:104:GLY:N | 1:A:110:LEU:HD13 | 2.18 | 0.59 |
| 5:E:82:SER:HB2 | 5:E:85:GLN:HG3 | 1.84 | 0.59 |
| 1:A:25:VAL:HB | 1:A:32:GLN:NE2 | 2.13 | 0.59 |
| 4:D:94:GLN:HB3 | 4:D:97:LYS:CE | 2.32 | 0.59 |
| 5:J:230:GLN:NE2 | 5:J:232:VAL:HG22 | 2.17 | 0.59 |
| 2:B:17:ASN:HA | 2:B:72:PRO:O | 2.02 | 0.59 |
| 5:E:82:SER:O | 5:E:110:VAL:HG21 | 2.02 | 0.59 |
| 5:E:39:PRO:O | 5:E:41:LEU:HD22 | 2.03 | 0.59 |
| 1:F:259:CYS:HB3 | 1:F:272:LEU:HB2 | 1.83 | 0.59 |
| 2:G:21:ASN:HB3 | 2:G:70:PHE:CE1 | 2.38 | 0.59 |
| 1:F:152:VAL:HA | 1:F:155:GLN:HG3 | 1.84 | 0.59 |
| 1:F:36:PHE:HB2 | 1:F:45:MET:CE | 2.33 | 0.59 |
| 4:I:13:VAL:HG13 | 4:I:14:PRO:HD2 | 1.85 | 0.59 |
| 4:I:6:GLN:NE2 | 4:I:102:GLN:HB2 | 2.18 | 0.59 |
| 4:I:93:ASN:O | 4:I:95:GLY:N | 2.35 | 0.59 |
| 5:J:41:LEU:HB3 | 5:J:44:ARG:CZ | 2.32 | 0.59 |
| 3:C:5:THR:HA | 3:C:8:TRP:CZ3 | 2.36 | 0.59 |
| 2:B:39:LEU:HD12 | 2:B:49:VAL:CG2 | 2.33 | 0.59 |
| 4:D:14:PRO:HB2 | 4:I:71:TYR:OH | 2.02 | 0.59 |
| 5:E:11:LEU:CD2 | 5:E:19:LEU:HD22 | 2.32 | 0.59 |
| 1:F:273:ARG:HH11 | 1:F:273:ARG:HG3 | 1.68 | 0.59 |
| 2:B:21:ASN:ND2 | 2:B:22:PHE:H | 2.01 | 0.59 |
| 4:D:89:TRP:HZ3 | 4:D:91:THR:HG21 | 1.67 | 0.59 |
| 1:A:152:VAL:CG1 | 1:A:156:GLN:NE2 | 2.66 | 0.58 |
| 1:F:268:LYS:HD2 | 1:F:269:PRO:CD | 2.31 | 0.58 |
| 5:J:230:GLN:HE21 | 5:J:232:VAL:HG22 | 1.67 | 0.58 |
| 4:D:152:VAL:HG13 | 4:D:152:VAL:O | 2.03 | 0.58 |
| 4:D:148:LYS:CD | 4:D:189:ASN:OD1 | 2.51 | 0.58 |
| 5:E:198:TRP:CZ2 | 5:E:239:ARG:HB3 | 2.38 | 0.58 |
| 1:F:181:ARG:NH1 | 1:F:181:ARG:HG2 | 2.18 | 0.58 |
| 5:J:138:ALA:O | 5:J:192:ARG:HA | 2.02 | 0.58 |
| 5:E:154:LEU:HD23 | 5:E:154:LEU:C | 2.23 | 0.58 |
| 5:E:138:ALA:O | 5:E:192:ARG:HA | 2.03 | 0.58 |
| 1:F:54:GLN:OE1 | 1:F:174:ASN:ND2 | 2.36 | 0.58 |
| 4:I:161:ASP:CB | 4:I:168:LYS:HE2 | 2.26 | 0.58 |
| 4:I:74:LEU:HG | 4:I:75:LEU:N | 2.18 | 0.58 |
| 1:A:242:GLN:HE22 | 2:B:10:TYR:HD2 | 1.51 | 0.58 |
| 5:E:217:ASN:HD22 | 5:E:217:ASN:N | 1.99 | 0.58 |
| 5:J:132:ILE:HG23 | 5:J:195:ALA:HB1 | 1.86 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:J:6:GLN:OE1 | 5:J:91:CYS:N | 2.35 | 0.58 |
| 1:F:244:TRP:C | 1:F:244:TRP:HE3 | 2.07 | 0.58 |
| 1:F:5:MET:O | 1:F:6:ARG:HD3 | 2.03 | 0.58 |
| 2:G:23:LEU:HG | 2:G:70:PHE:CE1 | 2.39 | 0.58 |
| 4:I:155:THR:CG2 | 4:I:173:VAL:H | 2.16 | 0.58 |
| 1:A:98:MET:O | 1:A:114:HIS:HA | 2.03 | 0.58 |
| 1:A:231:VAL:O | 1:A:243:LYS:CE | 2.52 | 0.58 |
| 5:E:101:TYR:HD2 | 5:E:101:TYR:N | 2.01 | 0.58 |
| 4:I:163:ARG:HG2 | 5:J:165:SER:OG | 2.03 | 0.58 |
| 4:I:93:ASN:C | 4:I:95:GLY:H | 2.07 | 0.58 |
| 5:J:132:ILE:HD12 | 5:J:132:ILE:N | 2.18 | 0.58 |
| 4:D:94:GLN:HB2 | 4:D:97:LYS:HG3 | 1.85 | 0.58 |
| 1:A:157:ARG:HA | 1:A:160:LEU:HD12 | 1.86 | 0.58 |
| 2:B:24:ASN:HD22 | 2:B:24:ASN:H | 1.52 | 0.58 |
| 2:B:57:SER:O | 2:B:59:ASP:O | 2.22 | 0.58 |
| 5:E:20:THR:O | 5:E:20:THR:HG23 | 2.04 | 0.58 |
| 1:A:5:MET:SD | 1:A:171:TYR:HE2 | 2.27 | 0.58 |
| 2:B:1:ILE:HD12 | 2:B:1:ILE:O | 2.03 | 0.58 |
| 4:D:93:ASN:O | 4:D:95:GLY:N | 2.36 | 0.58 |
| 1:F:142:ILE:O | 1:F:146:LYS:HG3 | 2.04 | 0.58 |
| 2:G:11:SER:HB2 | 2:G:21:ASN:OD1 | 2.03 | 0.58 |
| 4:I:121:GLN:HB2 | 4:I:183:CYS:SG | 2.43 | 0.58 |
| 5:J:126:GLU:HA | 5:J:140:LEU:HD23 | 1.84 | 0.58 |
| 3:H:2:PHE:CG | 3:H:3:PRO:HD2 | 2.39 | 0.57 |
| 1:A:6:ARG:HG2 | 1:A:6:ARG:HH11 | 1.70 | 0.57 |
| 5:E:37:GLN:HG3 | 5:E:43:LEU:CD1 | 2.34 | 0.57 |
| 1:F:233:THR:OG1 | 1:F:243:LYS:HD2 | 2.04 | 0.57 |
| 4:I:162:MET:HE1 | 5:J:192:ARG:HB3 | 1.86 | 0.57 |
| 1:A:117:ALA:HB2 | 2:B:60:TRP:CD2 | 2.39 | 0.57 |
| 1:A:255:GLN:O | 1:A:273:ARG:HD3 | 2.03 | 0.57 |
| 4:D:31:GLN:HB3 | 4:D:67:LYS:HZ1 | 1.67 | 0.57 |
| 2:B:83:ASN:HD22 | 2:B:84:HIS:N | 2.02 | 0.57 |
| 4:D:149:ASP:HB3 | 4:D:152:VAL:CG1 | 2.35 | 0.57 |
| 5:E:118:PHE:CE1 | 5:E:224:ARG:CZ | 2.87 | 0.57 |
| 4:I:94:GLN:HB2 | 4:I:99:ILE:HD11 | 1.87 | 0.57 |
| 5:J:108:LEU:HD12 | 5:J:108:LEU:O | 2.05 | 0.57 |
| 1:A:227:ASP:O | 1:A:248:VAL:HG23 | 2.03 | 0.57 |
| 4:I:11:LEU:HD12 | 4:I:12:SER:H | 1.69 | 0.57 |
| 4:I:182:ALA:O | 4:I:185:ASN:ND2 | 2.37 | 0.57 |
| 4:I:97:LYS:HE3 | 5:J:48:TYR:CE2 | 2.38 | 0.57 |
| 1:A:200:THR:CG2 | 1:A:202:ARG:NH1 | 2.65 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:131:SER:HB2 | 4:D:181:PHE:CE2 | 2.40 | 0.57 |
| 4:D:158:CYS:HB3 | 5:E:190:ARG:NH1 | 2.19 | 0.57 |
| 5:E:118:PHE:HE1 | 5:E:224:ARG:CZ | 2.17 | 0.57 |
| 5:J:135:THR:O | 5:J:136:GLN:HB2 | 2.04 | 0.57 |
| 5:J:206:ARG:HH11 | 5:J:233:SER:HB3 | 1.70 | 0.57 |
| 2:B:23:LEU:HD11 | 2:B:39:LEU:CD2 | 2.34 | 0.57 |
| 5:E:37:GLN:HG2 | 5:E:42:GLY:C | 2.26 | 0.57 |
| 4:I:122:LEU:CD1 | 5:J:141:VAL:HB | 2.33 | 0.57 |
| 3:H:3:PRO:O | 3:H:5:THR:HG23 | 2.04 | 0.57 |
| 4:I:50:ILE:O | 4:I:50:ILE:HG13 | 2.04 | 0.57 |
| 5:J:9:ARG:HH11 | 5:J:9:ARG:CB | 2.18 | 0.57 |
| 4:D:158:CYS:CB | 5:E:190:ARG:NH1 | 2.68 | 0.57 |
| 5:E:135:THR:HG21 | 5:E:192:ARG:NH1 | 2.20 | 0.57 |
| 5:E:23:CYS:HB2 | 5:E:34:TRP:HZ2 | 1.70 | 0.57 |
| 1:A:68:LYS:HE3 | 5:E:53:GLU:O | 2.05 | 0.57 |
| 1:F:130:LEU:HD13 | 1:F:160:LEU:HD12 | 1.87 | 0.57 |
| 4:I:11:LEU:HD12 | 4:I:12:SER:N | 2.19 | 0.57 |
| 4:D:123:ARG:HB3 | 5:E:126:GLU:HB2 | 1.87 | 0.56 |
| 4:I:78:ASP:OD1 | 4:I:80:GLN:NE2 | 2.38 | 0.56 |
| 1:F:156:GLN:OE1 | 3:H:8:TRP:HH2 | 1.88 | 0.56 |
| 4:I:53:ASN:C | 4:I:53:ASN:HD22 | 2.09 | 0.56 |
| 5:J:206:ARG:NH1 | 5:J:233:SER:CB | 2.64 | 0.56 |
| 1:A:147:TRP:CE3 | 1:A:152:VAL:HG11 | 2.40 | 0.56 |
| 1:A:33:PHE:CE1 | 1:A:34:VAL:HG22 | 2.40 | 0.56 |
| 1:A:35:ARG:HH12 | 1:A:48:ARG:CZ | 2.18 | 0.56 |
| 1:F:143:THR:HA | 1:F:146:LYS:HD3 | 1.88 | 0.56 |
| 4:I:177:ASN:HD22 | 4:I:178:LYS:N | 2.03 | 0.56 |
| 4:I:22:ASN:N | 4:I:22:ASN:OD1 | 2.38 | 0.56 |
| 5:J:154:LEU:CD2 | 5:J:155:SER:H | 2.18 | 0.56 |
| 5:J:170:ASP:OD1 | 5:J:190:ARG:NH2 | 2.39 | 0.56 |
| 1:A:103:VAL:C | 1:A:110:LEU:HD22 | 2.26 | 0.56 |
| 2:B:56:PHE:C | 2:B:63:TYR:CE2 | 2.79 | 0.56 |
| 4:D:48:MET:HE3 | 4:D:63:ALA:H | 1.69 | 0.56 |
| 4:D:94:GLN:CG | 4:D:97:LYS:HE2 | 2.34 | 0.56 |
| 5:E:30:GLU:O | 5:E:68:ARG:NH2 | 2.38 | 0.56 |
| 1:A:234:ARG:HG3 | 1:A:242:GLN:HG3 | 1.87 | 0.56 |
| 1:F:120:GLY:HA3 | 2:G:31:HIS:NE2 | 2.20 | 0.56 |
| 4:I:122:LEU:HD12 | 4:I:132:VAL:HB | 1.87 | 0.56 |
| 1:A:209:TYR:HD1 | 1:A:241:PHE:CE1 | 2.22 | 0.56 |
| 2:B:57:SER:N | 2:B:63:TYR:HE2 | 2.02 | 0.56 |
| 4:D:167:PHE:HD2 | 4:D:168:LYS:H | 1.52 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:7:TYR:HE2 | 3:H:2:PHE:N | 2.04 | 0.56 |
| 4:I:35:TRP:CB | 4:I:47:ILE:HD11 | 2.35 | 0.56 |
| 5:J:230:GLN:NE2 | 5:J:232:VAL:HG13 | 2.16 | 0.56 |
| 1:F:254:GLU:OE2 | 1:F:274:TRP:HD1 | 1.89 | 0.56 |
| 4:I:149:ASP:HB3 | 4:I:152:VAL:HG12 | 1.86 | 0.56 |
| 4:I:176:SER:HB3 | 4:I:181:PHE:CG | 2.41 | 0.56 |
| 1:A:108:ARG:HH22 | 4:I:114:ASN:HB2 | 1.70 | 0.56 |
| 1:F:141:GLN:O | 1:F:145:ARG:HG3 | 2.04 | 0.56 |
| 1:F:33:PHE:CE2 | 1:F:34:VAL:HG22 | 2.40 | 0.56 |
| 1:F:117:ALA:HB2 | 2:G:60:TRP:CE2 | 2.40 | 0.56 |
| 1:F:244:TRP:HE1 | 2:G:99:MET:CG | 2.18 | 0.56 |
| 4:I:167:PHE:C | 4:I:167:PHE:CD2 | 2.79 | 0.56 |
| 4:D:89:TRP:CZ2 | 4:D:101:GLY:HA3 | 2.40 | 0.56 |
| 4:D:197:PHE:CZ | 4:D:199:PRO:HA | 2.40 | 0.56 |
| 1:F:233:THR:HG23 | 1:F:243:LYS:CB | 2.34 | 0.56 |
| 4:D:93:ASN:C | 4:D:95:GLY:H | 2.10 | 0.56 |
| 5:E:180:LEU:HD12 | 5:E:180:LEU:N | 2.21 | 0.56 |
| 5:E:143:LEU:HD12 | 5:E:188:SER:HB3 | 1.87 | 0.56 |
| 2:G:5:PRO:HD3 | 2:G:84:HIS:HD2 | 1.71 | 0.56 |
| 5:J:120:PRO:HB3 | 5:J:147:PHE:CD2 | 2.41 | 0.56 |
| 5:J:127:PRO:HD2 | 5:J:198:TRP:CZ2 | 2.41 | 0.56 |
| 4:I:38:GLN:HE22 | 5:J:37:GLN:HE21 | 1.52 | 0.56 |
| 5:J:38:ASP:HB2 | 5:J:44:ARG:HH22 | 1.71 | 0.56 |
| 5:J:49:SER:OG | 5:J:68:ARG:HG2 | 2.06 | 0.56 |
| 1:A:235:PRO:HG2 | 2:B:65:LEU:CD1 | 2.35 | 0.56 |
| 2:B:80:CYS:O | 2:B:92:ILE:HA | 2.06 | 0.56 |
| 1:F:249:VAL:HG22 | 1:F:257:TYR:CD1 | 2.40 | 0.56 |
| 5:J:64:TYR:HB3 | 5:J:76:LEU:HD11 | 1.88 | 0.56 |
| 1:A:202:ARG:HG3 | 1:A:246:ALA:HB2 | 1.88 | 0.55 |
| 5:E:48:TYR:CZ | 5:E:56:ASP:HB2 | 2.42 | 0.55 |
| 1:F:14:ARG:CZ | 1:F:21:ARG:HB2 | 2.37 | 0.55 |
| 5:J:211:PHE:CE2 | 5:J:213:GLY:HA3 | 2.41 | 0.55 |
| 1:A:14:ARG:NH2 | 1:A:19:GLU:O | 2.37 | 0.55 |
| 1:A:97:MET:CE | 1:A:99:PHE:HB2 | 2.36 | 0.55 |
| 4:D:91:THR:HG23 | 4:D:93:ASN:ND2 | 2.21 | 0.55 |
| 1:F:244:TRP:HE1 | 2:G:99:MET:HG3 | 1.72 | 0.55 |
| 4:I:77:ARG:HG3 | 4:I:77:ARG:HH11 | 1.71 | 0.55 |
| 4:I:123:ARG:HD3 | 5:J:126:GLU:OE2 | 2.06 | 0.55 |
| 2:B:10:TYR:N | 2:B:10:TYR:CD1 | 2.75 | 0.55 |
| 1:A:96:GLN:OE1 | 2:B:60:TRP:HB3 | 2.06 | 0.55 |
| 5:E:118:PHE:HB3 | 5:E:184:ARG:NH2 | 2.21 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:132:ILE:HG21 | 5:E:199:GLN:HE22 | 1.72 | 0.55 |
| 1:F:227:ASP:O | 1:F:248:VAL:HG23 | 2.07 | 0.55 |
| 5:J:200:ASN:O | 5:J:238:GLY:HA3 | 2.06 | 0.55 |
| 5:J:36:ARG:NE | 5:J:87:SER:CB | 2.70 | 0.55 |
| 4:D:38:GLN:NE2 | 4:D:42:LYS:O | 2.39 | 0.55 |
| 1:F:115:GLN:CG | 2:G:60:TRP:HH2 | 2.19 | 0.55 |
| 1:F:218:GLN:HB2 | 1:F:258:THR:OG1 | 2.07 | 0.55 |
| 4:I:160:LEU:HB3 | 5:J:168:CYS:HB2 | 1.89 | 0.55 |
| 1:A:55:GLU:O | 1:A:60:TRP:CZ2 | 2.60 | 0.55 |
| 4:I:50:ILE:CD1 | 4:I:65:LEU:HD22 | 2.36 | 0.55 |
| 1:A:123:TYR:CZ | 1:A:140:ALA:HA | 2.41 | 0.55 |
| 4:D:112:ILE:CG1 | 4:D:170:ASN:HD21 | 2.18 | 0.55 |
| 1:F:19:GLU:CG | 1:F:75:ARG:HE | 2.15 | 0.55 |
| 1:A:156:GLN:O | 1:A:160:LEU:CD2 | 2.54 | 0.55 |
| 4:D:39:TYR:CE1 | 4:D:85:ALA:HB2 | 2.41 | 0.55 |
| 5:J:126:GLU:HA | 5:J:140:LEU:CD2 | 2.36 | 0.55 |
| 5:J:205:PHE:HD2 | 5:J:236:ALA:O | 1.88 | 0.55 |
| 5:J:27:MET:O | 5:J:28:ASN:HB3 | 2.07 | 0.55 |
| 1:A:224:GLN:O | 1:A:228:THR:HG21 | 2.06 | 0.55 |
| 2:B:21:ASN:CG | 2:B:22:PHE:N | 2.59 | 0.55 |
| 5:E:124:VAL:HG23 | 5:E:234:ALA:HB3 | 1.88 | 0.55 |
| 5:E:77:ILE:C | 5:E:78:LEU:HD12 | 2.27 | 0.55 |
| 4:D:167:PHE:CD1 | 5:E:137:LYS:HE3 | 2.41 | 0.55 |
| 1:F:168:LEU:O | 1:F:168:LEU:HD12 | 2.06 | 0.55 |
| 1:F:215:LEU:HD21 | 1:F:261:VAL:HG13 | 1.88 | 0.55 |
| 1:F:259:CYS:O | 1:F:272:LEU:HD12 | 2.07 | 0.55 |
| 2:G:5:PRO:HD3 | 2:G:84:HIS:CD2 | 2.42 | 0.55 |
| 4:I:30:SER:HA | 4:I:93:ASN:OD1 | 2.07 | 0.55 |
| 4:I:50:ILE:HD13 | 4:I:65:LEU:HD22 | 1.89 | 0.55 |
| 1:A:83:ARG:NH1 | 1:A:84:TYR:CE1 | 2.74 | 0.54 |
| 2:B:23:LEU:HD12 | 2:B:24:ASN:N | 2.22 | 0.54 |
| 4:D:27:ASP:O | 4:D:30:SER:OG | 2.14 | 0.54 |
| 5:E:127:PRO:HG3 | 5:E:139:THR:O | 2.07 | 0.54 |
| 5:E:170:ASP:HB2 | 5:E:187:LEU:CD1 | 2.35 | 0.54 |
| 5:E:131:GLU:HG2 | 5:E:137:LYS:O | 2.07 | 0.54 |
| 4:D:2:LYS:NZ | 5:E:43:LEU:H | 2.04 | 0.54 |
| 2:G:10:TYR:CD1 | 2:G:10:TYR:N | 2.75 | 0.54 |
| 1:A:231:VAL:O | 1:A:243:LYS:NZ | 2.40 | 0.54 |
| 5:E:49:SER:HB3 | 5:E:68:ARG:HH11 | 1.72 | 0.54 |
| 1:F:115:GLN:HG3 | 2:G:60:TRP:CZ2 | 2.42 | 0.54 |
| 4:I:36:TYR:OH | 5:J:100:GLN:HB2 | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:152:VAL:HG12 | 1:A:156:GLN:NE2 | 2.20 | 0.54 |
| 2:G:79:ALA:HB2 | 2:G:94:LYS:HA | 1.89 | 0.54 |
| 1:A:157:ARG:HA | 1:A:160:LEU:HD11 | 1.88 | 0.54 |
| 4:I:159:VAL:HG12 | 4:I:168:LYS:HZ1 | 1.70 | 0.54 |
| 5:J:172:GLN:OE1 | 5:J:173:PRO:HD2 | 2.06 | 0.54 |
| 5:J:25:GLN:NE2 | 5:J:29:HIS:H | 2.05 | 0.54 |
| 5:E:211:PHE:HD2 | 5:E:230:GLN:HG2 | 1.73 | 0.54 |
| 1:F:35:ARG:C | 1:F:35:ARG:HD2 | 2.28 | 0.54 |
| 2:G:31:HIS:CE1 | 2:G:60:TRP:O | 2.59 | 0.54 |
| 4:I:185:ASN:HD22 | 4:I:186:ALA:N | 2.05 | 0.54 |
| 3:C:4:LEU:HB3 | 3:C:6:PHE:HE2 | 1.71 | 0.54 |
| 1:F:45:MET:HG3 | 1:F:60:TRP:CZ3 | 2.38 | 0.54 |
| 4:I:160:LEU:HD11 | 4:I:167:PHE:CE2 | 2.35 | 0.54 |
| 4:I:122:LEU:HD11 | 5:J:141:VAL:HB | 1.90 | 0.54 |
| 5:J:38:ASP:N | 5:J:44:ARG:HH22 | 2.05 | 0.54 |
| 1:A:108:ARG:NH2 | 4:I:114:ASN:CB | 2.70 | 0.54 |
| 2:B:56:PHE:CB | 2:B:61:SER:O | 2.56 | 0.54 |
| 4:D:133:CYS:SG | 4:D:181:PHE:CE1 | 3.01 | 0.54 |
| 4:D:23:CYS:HB2 | 4:D:72:VAL:CG1 | 2.38 | 0.54 |
| 5:E:118:PHE:CE1 | 5:E:224:ARG:NH2 | 2.75 | 0.54 |
| 4:I:191:ILE:O | 4:I:191:ILE:HG13 | 2.08 | 0.54 |
| 5:J:153:GLU:HG2 | 5:J:212:TYR:HE2 | 1.73 | 0.54 |
| 5:J:41:LEU:CB | 5:J:44:ARG:CZ | 2.86 | 0.54 |
| 5:J:49:SER:OG | 5:J:68:ARG:NH1 | 2.40 | 0.54 |
| 4:D:149:ASP:HB3 | 4:D:152:VAL:HG11 | 1.90 | 0.54 |
| 5:E:168:CYS:O | 5:E:190:ARG:CD | 2.56 | 0.54 |
| 1:F:235:PRO:HG2 | 2:G:65:LEU:HD13 | 1.89 | 0.54 |
| 2:G:45:ARG:HH21 | 2:G:81:ARG:HH12 | 1.55 | 0.54 |
| 4:I:32:SER:HG | 4:I:51:TYR:HE1 | 1.55 | 0.54 |
| 1:A:83:ARG:HH11 | 1:A:83:ARG:HG2 | 1.72 | 0.54 |
| 4:D:187:PHE:O | 4:D:190:SER:OG | 2.26 | 0.54 |
| 4:D:50:ILE:HD11 | 4:D:65:LEU:CB | 2.38 | 0.54 |
| 1:A:68:LYS:CE | 5:E:53:GLU:O | 2.56 | 0.53 |
| 2:B:35:ILE:HG12 | 2:B:37:VAL:HG23 | 1.89 | 0.53 |
| 4:I:178:LYS:HG2 | 4:I:180:ASP:HB2 | 1.88 | 0.53 |
| 1:A:75:ARG:HH11 | 1:A:79:ARG:HE | 1.56 | 0.53 |
| 4:D:89:TRP:CE2 | 4:D:101:GLY:HA3 | 2.44 | 0.53 |
| 1:F:191:HIS:HB3 | 1:F:274:TRP:CH2 | 2.43 | 0.53 |
| 4:I:162:MET:HE2 | 5:J:192:ARG:HB3 | 1.87 | 0.53 |
| 4:I:80:GLN:HB2 | 4:I:83:ASP:OD2 | 2.07 | 0.53 |
| 3:C:3:PRO:HG2 | 3:C:5:THR:HG23 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:I:178:LYS:HG2 | 4:I:180:ASP:H | 1.73 | 0.53 |
| 5:J:38:ASP:N | 5:J:44:ARG:NH2 | 2.53 | 0.53 |
| 1:A:26:GLY:CA | 1:A:33:PHE:CE1 | 2.89 | 0.53 |
| 4:D:123:ARG:NH1 | 5:E:239:ARG:NE | 2.57 | 0.53 |
| 1:A:154:GLU:HG3 | 4:D:51:TYR:CD2 | 2.43 | 0.53 |
| 4:D:94:GLN:HB3 | 4:D:97:LYS:HE2 | 1.88 | 0.53 |
| 1:A:215:LEU:HD12 | 1:A:243:LYS:CD | 2.37 | 0.53 |
| 5:E:117:VAL:HG12 | 5:E:227:PRO:HB2 | 1.89 | 0.53 |
| 5:E:35:TYR:HA | 5:E:46:ILE:CD1 | 2.37 | 0.53 |
| 1:F:99:PHE:CE2 | 3:H:3:PRO:HG3 | 2.43 | 0.53 |
| 1:A:123:TYR:CD2 | 1:A:124:ILE:HG22 | 2.44 | 0.53 |
| 1:A:176:LYS:HD2 | 1:A:180:GLN:NE2 | 2.23 | 0.53 |
| 2:B:39:LEU:HD12 | 2:B:49:VAL:HG21 | 1.91 | 0.53 |
| 2:B:41:LYS:HA | 2:B:78:TYR:HD2 | 1.74 | 0.53 |
| 4:D:111:ASN:OD1 | 4:I:68:ALA:HB3 | 2.09 | 0.53 |
| 4:D:62:THR:O | 4:D:75:LEU:HD12 | 2.09 | 0.53 |
| 5:E:11:LEU:HD23 | 5:E:19:LEU:HD22 | 1.91 | 0.53 |
| 4:I:66:ASN:OD1 | 4:I:69:SER:N | 2.31 | 0.53 |
| 1:A:208:PHE:CE2 | 1:A:241:PHE:HB2 | 2.44 | 0.53 |
| 2:B:56:PHE:CD2 | 2:B:62:PHE:CE2 | 2.97 | 0.53 |
| 5:E:167:VAL:HA | 5:E:190:ARG:O | 2.09 | 0.53 |
| 5:E:32:MET:SD | 5:E:71:LYS:O | 2.66 | 0.53 |
| 4:I:178:LYS:HE3 | 4:I:180:ASP:CB | 2.37 | 0.53 |
| 5:E:220:TRP:CH2 | 5:E:222:GLN:HG3 | 2.43 | 0.53 |
| 5:E:97:SER:OG | 5:E:98:HIS:N | 2.33 | 0.53 |
| 1:F:226:GLN:O | 1:F:227:ASP:HB2 | 2.08 | 0.53 |
| 5:J:132:ILE:HG23 | 5:J:195:ALA:CB | 2.38 | 0.53 |
| 5:J:47:TYR:CD1 | 5:J:66:VAL:HG22 | 2.43 | 0.53 |
| 5:E:37:GLN:HB2 | 5:E:43:LEU:HD12 | 1.90 | 0.53 |
| 1:F:98:MET:O | 1:F:114:HIS:HA | 2.08 | 0.53 |
| 5:J:64:TYR:CD1 | 5:J:78:LEU:HD13 | 2.44 | 0.53 |
| 1:A:242:GLN:OE1 | 2:B:10:TYR:CE2 | 2.61 | 0.53 |
| 4:D:88:LEU:H | 4:D:88:LEU:HD23 | 1.73 | 0.53 |
| 4:D:96:GLY:HA3 | 5:E:50:MET:CE | 2.39 | 0.53 |
| 1:F:70:HIS:ND1 | 3:H:2:PHE:HZ | 2.01 | 0.53 |
| 4:I:50:ILE:C | 4:I:50:ILE:CD1 | 2.72 | 0.52 |
| 4:D:182:ALA:HB3 | 4:D:185:ASN:ND2 | 2.25 | 0.52 |
| 4:D:114:ASN:CB | 1:F:108:ARG:HH22 | 2.20 | 0.52 |
| 1:F:35:ARG:HD2 | 1:F:36:PHE:N | 2.24 | 0.52 |
| 1:F:96:GLN:NE2 | 2:G:56:PHE:CD2 | 2.77 | 0.52 |
| 3:H:9:CYS:SG | 5:J:30:GLU:OE1 | 2.67 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:J:25:GLN:NE2 | 5:J:29:HIS:HB2 | 2.25 | 0.52 |
| 4:I:46:LEU:HD11 | 5:J:99:GLU:HG2 | 1.92 | 0.52 |
| 1:A:15:PRO:HG2 | 1:A:91:GLY:O | 2.09 | 0.52 |
| 1:A:8:PHE:HB2 | 1:A:25:VAL:HG22 | 1.92 | 0.52 |
| 4:D:123:ARG:CZ | 5:E:239:ARG:CZ | 2.87 | 0.52 |
| 4:D:72:VAL:O | 4:D:72:VAL:HG13 | 2.08 | 0.52 |
| 4:D:94:GLN:HB2 | 4:D:99:ILE:HD11 | 1.92 | 0.52 |
| 1:F:231:VAL:HG22 | 1:F:244:TRP:O | 2.09 | 0.52 |
| 4:I:132:VAL:HG23 | 5:J:125:PHE:CE1 | 2.44 | 0.52 |
| 4:I:88:LEU:N | 4:I:88:LEU:CD2 | 2.63 | 0.52 |
| 4:I:120:TYR:CE1 | 5:J:131:GLU:CA | 2.90 | 0.52 |
| 1:A:130:LEU:CB | 1:A:157:ARG:HG3 | 2.39 | 0.52 |
| 4:D:69:SER:O | 4:D:70:GLN:HB2 | 2.10 | 0.52 |
| 5:E:132:ILE:HD12 | 5:E:132:ILE:H | 1.73 | 0.52 |
| 1:A:66:LYS:HG3 | 5:E:50:MET:CE | 2.40 | 0.52 |
| 5:J:41:LEU:HB3 | 5:J:44:ARG:NH1 | 2.24 | 0.52 |
| 1:A:55:GLU:CB | 1:A:59:TYR:CD2 | 2.93 | 0.52 |
| 4:D:153:TYR:HB2 | 4:D:175:TRP:CE2 | 2.45 | 0.52 |
| 1:F:155:GLN:O | 4:I:31:GLN:NE2 | 2.42 | 0.52 |
| 1:F:190:THR:O | 1:F:201:LEU:HD23 | 2.09 | 0.52 |
| 1:F:72:GLN:O | 1:F:72:GLN:OE1 | 2.28 | 0.52 |
| 5:J:167:VAL:HA | 5:J:190:ARG:O | 2.09 | 0.52 |
| 5:J:200:ASN:HD22 | 5:J:203:ASN:CG | 2.13 | 0.52 |
| 1:A:133:TRP:HZ2 | 1:A:152:VAL:HB | 1.74 | 0.52 |
| 3:C:6:PHE:CD1 | 5:E:31:TYR:HB2 | 2.45 | 0.52 |
| 5:E:37:GLN:CB | 5:E:43:LEU:HD12 | 2.39 | 0.52 |
| 2:G:96:ASP:HB3 | 2:G:99:MET:HA | 1.91 | 0.52 |
| 2:B:55:SER:OG | 2:B:63:TYR:CE1 | 2.62 | 0.52 |
| 5:E:135:THR:HG22 | 5:E:137:LYS:CG | 2.35 | 0.52 |
| 5:E:135:THR:HG21 | 5:E:192:ARG:HH12 | 1.74 | 0.52 |
| 2:G:1:ILE:O | 2:G:1:ILE:HD12 | 2.10 | 0.52 |
| 4:I:35:TRP:HB2 | 4:I:48:MET:HB3 | 1.91 | 0.52 |
| 1:A:123:TYR:HD2 | 1:A:124:ILE:HG22 | 1.75 | 0.52 |
| 1:A:130:LEU:HB3 | 1:A:157:ARG:HG3 | 1.91 | 0.52 |
| 4:D:39:TYR:OH | 4:D:82:SER:O | 2.18 | 0.52 |
| 5:E:9:ARG:HH12 | 5:E:104:PRO:C | 2.12 | 0.52 |
| 5:J:83:PRO:HA | 5:J:110:VAL:HB | 1.92 | 0.52 |
| 1:A:160:LEU:O | 1:A:165:VAL:HG22 | 2.09 | 0.52 |
| 5:E:37:GLN:HG2 | 5:E:42:GLY:O | 2.10 | 0.52 |
| 1:F:95:LEU:HD12 | 1:F:117:ALA:O | 2.10 | 0.52 |
| 4:I:53:ASN:ND2 | 4:I:65:LEU:O | 2.43 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 5:J:206:ARG:HB3 | 5:J:206:ARG:CZ | 2.39 | 0.52 |
| 5:J:41:LEU:CB | 5:J:44:ARG:NH1 | 2.72 | 0.52 |
| 2:B:57:SER:N | 2:B:63:TYR:CE2 | 2.78 | 0.52 |
| 4:D:53:ASN:HD21 | 4:D:67:LYS:HB2 | 1.74 | 0.52 |
| 2:G:13:HIS:N | 2:G:21:ASN:HD21 | 2.08 | 0.52 |
| 2:G:19:LYS:O | 2:G:72:PRO:HD2 | 2.09 | 0.52 |
| 5:J:70:GLU:HG3 | 5:J:73:ASN:H | 1.74 | 0.51 |
| 1:A:209:TYR:CD1 | 1:A:210:PRO:HA | 2.44 | 0.51 |
| 1:A:242:GLN:NE2 | 2:B:10:TYR:CD2 | 2.78 | 0.51 |
| 4:D:3:GLU:HG3 | 4:D:4:VAL:HG12 | 1.91 | 0.51 |
| 5:E:161:LYS:HB2 | 5:E:161:LYS:HZ2 | 1.75 | 0.51 |
| 4:I:149:ASP:O | 4:I:152:VAL:CG1 | 2.58 | 0.51 |
| 4:I:33:PHE:O | 4:I:50:ILE:HG23 | 2.10 | 0.51 |
| 1:F:104:GLY:N | 1:F:110:LEU:HD23 | 2.24 | 0.51 |
| 4:I:124:ASP:HA | 5:J:125:PHE:CE1 | 2.45 | 0.51 |
| 5:E:37:GLN:HG3 | 5:E:43:LEU:HD12 | 1.90 | 0.51 |
| 1:F:5:MET:SD | 1:F:171:TYR:HE2 | 2.33 | 0.51 |
| 2:G:1:ILE:HD12 | 2:G:1:ILE:C | 2.31 | 0.51 |
| 1:F:159:TYR:CZ | 3:H:3:PRO:HB3 | 2.46 | 0.51 |
| 5:E:158:VAL:CG2 | 5:E:163:VAL:HG21 | 2.38 | 0.51 |
| 5:J:19:LEU:H | 5:J:19:LEU:HD12 | 1.76 | 0.51 |
| 5:J:220:TRP:HH2 | 5:J:224:ARG:NH2 | 2.08 | 0.51 |
| 4:D:157:LYS:H | 4:D:157:LYS:CD | 2.23 | 0.51 |
| 5:E:136:GLN:HA | 5:E:136:GLN:OE1 | 2.10 | 0.51 |
| 5:E:153:GLU:HB2 | 5:E:210:GLN:HB3 | 1.92 | 0.51 |
| 5:J:131:GLU:HG2 | 5:J:137:LYS:O | 2.10 | 0.51 |
| 5:J:25:GLN:OE1 | 5:J:27:MET:N | 2.43 | 0.51 |
| 1:F:261:VAL:CG2 | 1:F:272:LEU:HD11 | 2.41 | 0.51 |
| 4:I:14:PRO:HA | 4:I:109:LYS:HB2 | 1.93 | 0.51 |
| 5:J:49:SER:CB | 5:J:68:ARG:HH11 | 2.24 | 0.51 |
| 4:D:131:SER:HB2 | 4:D:181:PHE:HE2 | 1.76 | 0.51 |
| 5:E:45:GLN:C | 5:E:46:ILE:HD12 | 2.31 | 0.51 |
| 1:F:191:HIS:CE1 | 1:F:193:PRO:HG3 | 2.45 | 0.51 |
| 2:G:4:THR:OG1 | 2:G:5:PRO:HD2 | 2.10 | 0.51 |
| 1:F:70:HIS:HB2 | 3:H:2:PHE:HE2 | 1.76 | 0.51 |
| 4:I:77:ARG:O | 4:I:78:ASP:HB3 | 2.11 | 0.51 |
| 5:E:12:ILE:HD11 | 5:E:213:GLY:HA2 | 1.93 | 0.51 |
| 5:E:200:ASN:O | 5:E:238:GLY:HA3 | 2.11 | 0.51 |
| 5:J:206:ARG:HG2 | 5:J:206:ARG:HH11 | 1.75 | 0.51 |
| 1:A:99:PHE:HD1 | 1:A:114:HIS:CD2 | 2.28 | 0.50 |
| 5:E:187:LEU:HG | 5:E:188:SER:N | 2.26 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:47:TYR:CZ | 5:E:57:LYS:HB3 | 2.45 | 0.50 |
| 5:E:62:GLU:HA | 5:E:62:GLU:OE1 | 2.11 | 0.50 |
| 2:G:23:LEU:HG | 2:G:70:PHE:CZ | 2.46 | 0.50 |
| 4:I:173:VAL:HG12 | 4:I:175:TRP:CE3 | 2.45 | 0.50 |
| 5:J:40:GLY:C | 5:J:41:LEU:HD22 | 2.32 | 0.50 |
| 1:A:22:PHE:CE1 | 1:A:71:SER:HA | 2.46 | 0.50 |
| 5:E:4:VAL:HG11 | 5:E:91:CYS:O | 2.11 | 0.50 |
| 5:E:78:LEU:N | 5:E:78:LEU:CD1 | 2.73 | 0.50 |
| 1:F:27:TYR:CE2 | 1:F:32:GLN:N | 2.79 | 0.50 |
| 1:F:80:ILE:HG23 | 1:F:83:ARG:NH2 | 2.26 | 0.50 |
| 4:I:160:LEU:CD1 | 4:I:160:LEU:C | 2.79 | 0.50 |
| 5:J:144:ALA:O | 5:J:147:PHE:HE2 | 1.95 | 0.50 |
| 5:J:77:ILE:N | 5:J:77:ILE:CD1 | 2.71 | 0.50 |
| 5:J:36:ARG:HE | 5:J:87:SER:CB | 2.25 | 0.50 |
| 4:D:37:ARG:HB2 | 4:D:47:ILE:HD13 | 1.93 | 0.50 |
| 4:I:50:ILE:O | 4:I:50:ILE:CG1 | 2.59 | 0.50 |
| 5:J:23:CYS:HB2 | 5:J:34:TRP:CZ2 | 2.46 | 0.50 |
| 5:J:47:TYR:CD1 | 5:J:66:VAL:CG2 | 2.95 | 0.50 |
| 5:E:46:ILE:HG23 | 5:E:60:VAL:O | 2.11 | 0.50 |
| 2:G:40:LEU:HD21 | 2:G:81:ARG:HE | 1.76 | 0.50 |
| 1:A:75:ARG:CD | 1:A:79:ARG:HD2 | 2.42 | 0.50 |
| 4:D:147:SER:CB | 4:D:152:VAL:HG13 | 2.41 | 0.50 |
| 5:E:208:GLN:HG2 | 5:E:233:SER:OG | 2.10 | 0.50 |
| 5:E:96:ALA:O | 5:E:97:SER:HB3 | 2.10 | 0.50 |
| 1:F:10:THR:HB | 1:F:23:ILE:CG2 | 2.31 | 0.50 |
| 1:F:7:TYR:HE2 | 3:H:2:PHE:CA | 2.25 | 0.50 |
| 4:I:176:SER:HB3 | 4:I:181:PHE:CD2 | 2.46 | 0.50 |
| 4:I:65:LEU:HD21 | 4:I:67:LYS:HG3 | 1.93 | 0.50 |
| 5:E:211:PHE:HB3 | 5:E:230:GLN:O | 2.11 | 0.50 |
| 5:E:77:ILE:H | 5:E:77:ILE:HD12 | 1.77 | 0.50 |
| 1:F:244:TRP:C | 1:F:244:TRP:CE3 | 2.85 | 0.50 |
| 2:G:40:LEU:HD21 | 2:G:81:ARG:NE | 2.27 | 0.50 |
| 2:B:84:HIS:HB3 | 2:B:86:THR:HG23 | 1.92 | 0.50 |
| 4:D:185:ASN:CA | 4:D:188:ASN:ND2 | 2.75 | 0.50 |
| 5:J:128:SER:OG | 5:J:130:ALA:HB3 | 2.12 | 0.50 |
| 5:J:139:THR:OG1 | 5:J:192:ARG:HB2 | 2.12 | 0.50 |
| 5:J:70:GLU:CD | 5:J:73:ASN:HD22 | 2.15 | 0.50 |
| 4:D:39:TYR:CD1 | 4:D:85:ALA:HB2 | 2.46 | 0.50 |
| 1:F:220:ASP:OD2 | 1:F:256:ARG:HD3 | 2.11 | 0.50 |
| 4:I:30:SER:O | 4:I:67:LYS:NZ | 2.41 | 0.50 |
| 4:I:33:PHE:H | 4:I:50:ILE:HG13 | 1.76 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:J:173:PRO:CA | 5:J:187:LEU:HD13 | 2.36 | 0.50 |
| 1:A:45:MET:SD | 1:A:63:GLU:HB3 | 2.52 | 0.50 |
| 1:F:99:PHE:HZ | 1:F:156:GLN:CD | 2.15 | 0.50 |
| 4:I:88:LEU:HB3 | 4:I:103:GLY:CA | 2.41 | 0.50 |
| 5:J:164:HIS:O | 5:J:167:VAL:HG13 | 2.12 | 0.50 |
| 5:J:200:ASN:HB3 | 5:J:203:ASN:OD1 | 2.12 | 0.50 |
| 1:A:68:LYS:HD3 | 5:E:54:VAL:HA | 1.93 | 0.49 |
| 2:B:79:ALA:HB2 | 2:B:94:LYS:HA | 1.94 | 0.49 |
| 3:C:2:PHE:CG | 3:C:3:PRO:HD2 | 2.46 | 0.49 |
| 4:I:152:VAL:HG13 | 4:I:152:VAL:O | 2.11 | 0.49 |
| 5:J:176:GLU:O | 5:J:178:PRO:HD3 | 2.12 | 0.49 |
| 5:J:96:ALA:O | 5:J:97:SER:OG | 2.29 | 0.49 |
| 1:A:152:VAL:HG13 | 1:A:156:GLN:HE21 | 1.77 | 0.49 |
| 1:A:159:TYR:CE2 | 1:A:163:THR:HB | 2.46 | 0.49 |
| 1:A:3:HIS:HB3 | 1:A:29:ASP:OD2 | 2.12 | 0.49 |
| 1:A:75:ARG:C | 1:A:75:ARG:HD3 | 2.32 | 0.49 |
| 1:A:156:GLN:NE2 | 3:C:8:TRP:CH2 | 2.79 | 0.49 |
| 5:E:132:ILE:CG2 | 5:E:195:ALA:HB1 | 2.40 | 0.49 |
| 5:E:140:LEU:HD12 | 5:E:140:LEU:N | 2.27 | 0.49 |
| 2:G:23:LEU:HD21 | 2:G:95:TRP:CE3 | 2.47 | 0.49 |
| 5:J:36:ARG:HE | 5:J:87:SER:HB2 | 1.77 | 0.49 |
| 1:A:2:SER:O | 1:A:3:HIS:ND1 | 2.45 | 0.49 |
| 2:B:41:LYS:HG3 | 2:B:78:TYR:HE2 | 1.77 | 0.49 |
| 4:D:12:SER:HB2 | 4:D:109:LYS:CE | 2.41 | 0.49 |
| 1:F:147:TRP:CD1 | 1:F:147:TRP:N | 2.74 | 0.49 |
| 1:A:130:LEU:HD13 | 1:A:160:LEU:HD12 | 1.92 | 0.49 |
| 5:E:157:TRP:CE3 | 5:E:162:GLU:N | 2.80 | 0.49 |
| 5:J:156:TRP:NE1 | 5:J:189:SER:OG | 2.44 | 0.49 |
| 1:A:104:GLY:H | 1:A:110:LEU:HD13 | 1.75 | 0.49 |
| 1:A:9:SER:OG | 1:A:97:MET:HB3 | 2.12 | 0.49 |
| 4:I:136:THR:CG2 | 5:J:192:ARG:HH22 | 2.25 | 0.49 |
| 4:D:139:ASP:O | 4:D:142:THR:OG1 | 2.30 | 0.49 |
| 4:D:149:ASP:O | 4:D:152:VAL:HG12 | 2.13 | 0.49 |
| 4:D:133:CYS:SG | 4:D:181:PHE:CZ | 3.06 | 0.49 |
| 5:E:132:ILE:N | 5:E:132:ILE:HD12 | 2.27 | 0.49 |
| 5:E:36:ARG:NE | 5:E:38:ASP:OD2 | 2.46 | 0.49 |
| 5:E:72:ARG:HB2 | 5:E:73:ASN:HD22 | 1.76 | 0.49 |
| 1:F:143:THR:HG23 | 1:F:146:LYS:HD3 | 1.93 | 0.49 |
| 4:I:134:LEU:HD21 | 5:J:139:THR:HG21 | 1.94 | 0.49 |
| 4:I:161:ASP:HB2 | 4:I:168:LYS:NZ | 2.28 | 0.49 |
| 5:J:90:PHE:CE1 | 5:J:105:GLY:HA3 | 2.48 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:141:GLN:OE1 | 4:D:141:GLN:HA | 2.13 | 0.49 |
| 4:I:177:ASN:HD22 | 4:I:177:ASN:C | 2.16 | 0.49 |
| 5:J:147:PHE:CZ | 5:J:186:ALA:HA | 2.47 | 0.49 |
| 1:A:111:ARG:CZ | 1:A:128:GLU:HA | 2.43 | 0.49 |
| 1:A:55:GLU:OE2 | 1:A:170:ARG:NH2 | 2.46 | 0.49 |
| 2:B:92:ILE:N | 2:B:92:ILE:HD12 | 2.28 | 0.49 |
| 1:F:51:TRP:HE1 | 1:F:179:LEU:HD21 | 1.78 | 0.49 |
| 4:I:47:ILE:HD12 | 4:I:47:ILE:C | 2.33 | 0.49 |
| 4:I:91:THR:O | 4:I:91:THR:HG23 | 2.13 | 0.49 |
| 4:I:171:SER:OG | 5:J:190:ARG:NH1 | 2.46 | 0.49 |
| 5:J:97:SER:O | 5:J:98:HIS:ND1 | 2.46 | 0.49 |
| 4:D:89:TRP:CZ3 | 4:D:91:THR:HG22 | 2.48 | 0.49 |
| 5:E:107:ARG:NH1 | 5:E:151:HIS:NE2 | 2.60 | 0.49 |
| 5:E:32:MET:SD | 5:E:68:ARG:NH2 | 2.85 | 0.49 |
| 1:F:272:LEU:H | 1:F:272:LEU:HD12 | 1.77 | 0.49 |
| 1:F:35:ARG:NH1 | 1:F:35:ARG:HG2 | 2.26 | 0.49 |
| 1:F:143:THR:HG23 | 3:H:10:PHE:HA | 1.95 | 0.49 |
| 3:H:4:LEU:HD21 | 4:I:96:GLY:HA2 | 1.95 | 0.49 |
| 1:A:26:GLY:O | 1:A:33:PHE:CD1 | 2.66 | 0.48 |
| 4:D:192:ILE:HG13 | 4:D:193:PRO:N | 2.28 | 0.48 |
| 5:E:51:ASN:O | 5:E:68:ARG:HG2 | 2.13 | 0.48 |
| 2:G:54:LEU:HD12 | 2:G:55:SER:N | 2.27 | 0.48 |
| 4:I:4:VAL:HG22 | 4:I:5:GLU:CD | 2.33 | 0.48 |
| 5:J:158:VAL:HG12 | 5:J:158:VAL:O | 2.13 | 0.48 |
| 2:G:12:ARG:HG2 | 2:G:13:HIS:H | 1.78 | 0.48 |
| 4:I:147:SER:OG | 4:I:152:VAL:O | 2.21 | 0.48 |
| 1:A:106:ASP:OD1 | 1:A:108:ARG:HB2 | 2.13 | 0.48 |
| 2:B:7:ILE:C | 2:B:8:GLN:HE21 | 2.17 | 0.48 |
| 1:F:202:ARG:HD3 | 1:F:244:TRP:NE1 | 2.28 | 0.48 |
| 1:F:51:TRP:CE2 | 1:F:179:LEU:HD21 | 2.48 | 0.48 |
| 4:I:47:ILE:HD12 | 4:I:48:MET:CB | 2.43 | 0.48 |
| 4:I:122:LEU:HD11 | 5:J:141:VAL:CG2 | 2.42 | 0.48 |
| 5:J:78:LEU:HD11 | 5:J:85:GLN:NE2 | 2.28 | 0.48 |
| 4:D:30:SER:C | 4:D:31:GLN:HG3 | 2.32 | 0.48 |
| 5:E:7:ASN:OD1 | 5:E:8:PRO:HA | 2.13 | 0.48 |
| 4:D:36:TYR:CD1 | 4:D:46:LEU:HA | 2.49 | 0.48 |
| 5:E:143:LEU:CD1 | 5:E:188:SER:HB3 | 2.43 | 0.48 |
| 2:G:10:TYR:O | 2:G:24:ASN:ND2 | 2.46 | 0.48 |
| 2:G:81:ARG:CA | 2:G:92:ILE:HG12 | 2.41 | 0.48 |
| 1:A:35:ARG:NH1 | 1:A:48:ARG:CD | 2.77 | 0.48 |
| 1:A:55:GLU:HB2 | 1:A:59:TYR:CD2 | 2.49 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:83:ASN:HD22 | 2:B:83:ASN:C | 2.15 | 0.48 |
| 4:D:134:LEU:HD11 | 4:D:171:SER:HB2 | 1.96 | 0.48 |
| 4:D:192:ILE:HD11 | 4:D:196:THR:HB | 1.96 | 0.48 |
| 1:A:66:LYS:HG3 | 5:E:50:MET:HE1 | 1.95 | 0.48 |
| 1:F:242:GLN:O | 1:F:243:LYS:HB2 | 2.14 | 0.48 |
| 3:H:8:TRP:CD1 | 3:H:8:TRP:N | 2.78 | 0.48 |
| 4:I:167:PHE:CZ | 4:I:169:SER:HB3 | 2.49 | 0.48 |
| 4:I:46:LEU:CD2 | 5:J:99:GLU:HB3 | 2.40 | 0.48 |
| 1:F:108:ARG:NH1 | 1:F:108:ARG:HG3 | 2.27 | 0.48 |
| 1:F:213:ILE:HG13 | 1:F:263:HIS:HB2 | 1.94 | 0.48 |
| 2:G:30:PHE:O | 2:G:62:PHE:HD1 | 1.96 | 0.48 |
| 4:I:162:MET:HG3 | 5:J:166:GLY:HA2 | 1.96 | 0.48 |
| 4:I:160:LEU:C | 4:I:168:LYS:HZ3 | 2.17 | 0.48 |
| 4:I:77:ARG:HG3 | 4:I:77:ARG:NH1 | 2.28 | 0.48 |
| 4:I:36:TYR:CE1 | 5:J:102:PHE:CE2 | 3.02 | 0.48 |
| 5:J:177:GLN:HB2 | 5:J:183:SER:HB2 | 1.95 | 0.48 |
| 1:A:73:THR:HG23 | 5:E:30:GLU:OE1 | 2.12 | 0.48 |
| 2:G:3:ARG:HD2 | 2:G:29:GLY:O | 2.13 | 0.48 |
| 5:E:152:VAL:HA | 5:E:210:GLN:O | 2.14 | 0.48 |
| 1:F:231:VAL:CG2 | 1:F:244:TRP:H | 2.27 | 0.48 |
| 5:J:205:PHE:HE2 | 5:J:237:TRP:C | 2.16 | 0.48 |
| 4:D:192:ILE:HD11 | 4:D:196:THR:HG21 | 1.96 | 0.48 |
| 5:E:237:TRP:N | 5:E:237:TRP:CD1 | 2.82 | 0.48 |
| 5:E:19:LEU:HD11 | 5:E:78:LEU:HD13 | 1.92 | 0.48 |
| 5:J:125:PHE:O | 5:J:140:LEU:HD23 | 2.14 | 0.48 |
| 5:J:205:PHE:CE2 | 5:J:238:GLY:N | 2.75 | 0.48 |
| 5:J:35:TYR:CD1 | 5:J:45:GLN:HA | 2.48 | 0.48 |
| 1:A:242:GLN:O | 1:A:243:LYS:HB2 | 2.13 | 0.47 |
| 2:B:22:PHE:C | 2:B:70:PHE:HE1 | 2.17 | 0.47 |
| 5:E:92:ALA:HB1 | 5:E:100:GLN:CG | 2.30 | 0.47 |
| 1:F:133:TRP:HB2 | 1:F:144:LYS:HG3 | 1.95 | 0.47 |
| 2:B:26:TYR:HD1 | 2:B:64:LEU:O | 1.97 | 0.47 |
| 4:D:192:ILE:CD1 | 4:D:196:THR:HG21 | 2.44 | 0.47 |
| 4:I:114:ASN:HD22 | 4:I:114:ASN:C | 2.18 | 0.47 |
| 1:A:72:GLN:HB2 | 5:E:51:ASN:CG | 2.35 | 0.47 |
| 2:B:41:LYS:HA | 2:B:78:TYR:CD2 | 2.49 | 0.47 |
| 4:D:164:SER:OG | 4:D:165:MET:HG2 | 2.15 | 0.47 |
| 5:E:49:SER:HB2 | 5:E:74:PHE:CE1 | 2.49 | 0.47 |
| 1:F:15:PRO:HG2 | 1:F:91:GLY:O | 2.14 | 0.47 |
| 1:F:51:TRP:CD1 | 1:F:175:GLY:CA | 2.97 | 0.47 |
| 4:I:99:ILE:HD12 | 4:I:99:ILE:N | 2.30 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:J:108:LEU:C | 5:J:108:LEU:CD1 | 2.82 | 0.47 |
| 4:I:132:VAL:HG23 | 5:J:125:PHE:CD1 | 2.49 | 0.47 |
| 5:J:162:GLU:CG | 5:J:164:HIS:CE1 | 2.98 | 0.47 |
| 4:I:92:TYR:OH | 5:J:98:HIS:O | 2.32 | 0.47 |
| 1:A:139:ALA:HA | 1:A:142:ILE:CD1 | 2.44 | 0.47 |
| 5:E:84:ASN:N | 5:E:84:ASN:HD22 | 2.12 | 0.47 |
| 5:J:218:ASP:N | 5:J:218:ASP:OD1 | 2.47 | 0.47 |
| 1:A:194:ILE:HD11 | 1:A:198:GLU:HB3 | 1.96 | 0.47 |
| 1:A:229:GLU:O | 1:A:230:LEU:HD12 | 2.14 | 0.47 |
| 1:A:209:TYR:CD1 | 1:A:241:PHE:HE1 | 2.27 | 0.47 |
| 4:D:114:ASN:OD1 | 1:F:108:ARG:NH1 | 2.47 | 0.47 |
| 4:D:48:MET:CE | 4:D:63:ALA:N | 2.77 | 0.47 |
| 4:D:94:GLN:CB | 4:D:97:LYS:CE | 2.89 | 0.47 |
| 5:E:32:MET:CE | 5:E:71:LYS:O | 2.62 | 0.47 |
| 1:F:202:ARG:NH1 | 1:F:244:TRP:CZ3 | 2.82 | 0.47 |
| 2:G:13:HIS:HB2 | 2:G:21:ASN:HD21 | 1.76 | 0.47 |
| 1:A:87:GLN:NE2 | 1:A:118:TYR:OH | 2.47 | 0.47 |
| 1:A:200:THR:HG21 | 1:A:202:ARG:HH22 | 1.79 | 0.47 |
| 4:D:81:PRO:HA | 4:D:108:VAL:CG1 | 2.44 | 0.47 |
| 4:D:35:TRP:O | 4:D:46:LEU:HD12 | 2.15 | 0.47 |
| 5:E:36:ARG:HB2 | 5:E:89:TYR:CE1 | 2.49 | 0.47 |
| 1:F:99:PHE:HZ | 1:F:156:GLN:OE1 | 1.98 | 0.47 |
| 1:F:168:LEU:HD11 | 1:F:172:LEU:HD21 | 1.96 | 0.47 |
| 3:H:2:PHE:CD1 | 3:H:3:PRO:HD2 | 2.50 | 0.47 |
| 5:J:86:THR:HA | 5:J:108:LEU:HD12 | 1.96 | 0.47 |
| 5:J:204:HIS:NE2 | 5:J:235:GLU:HB2 | 2.30 | 0.47 |
| 1:A:185:PRO:HG3 | 1:A:213:ILE:HD12 | 1.95 | 0.47 |
| 4:D:80:GLN:C | 4:D:108:VAL:HG11 | 2.35 | 0.47 |
| 4:D:123:ARG:NH1 | 5:E:239:ARG:CZ | 2.78 | 0.47 |
| 5:E:177:GLN:O | 5:E:183:SER:HB2 | 2.14 | 0.47 |
| 5:E:31:TYR:C | 5:E:32:MET:HG3 | 2.34 | 0.47 |
| 1:F:233:THR:CG2 | 1:F:243:LYS:HD2 | 2.44 | 0.47 |
| 4:I:135:PHE:CE1 | 4:I:138:PHE:HB3 | 2.49 | 0.47 |
| 4:I:162:MET:HG3 | 5:J:166:GLY:CA | 2.45 | 0.47 |
| 5:J:49:SER:HB3 | 5:J:68:ARG:NH1 | 2.29 | 0.47 |
| 5:J:76:LEU:C | 5:J:77:ILE:HD12 | 2.34 | 0.47 |
| 5:J:97:SER:OG | 5:J:98:HIS:N | 2.47 | 0.47 |
| 1:A:258:THR:CG2 | 1:A:271:THR:CG2 | 2.93 | 0.47 |
| 1:A:26:GLY:CA | 1:A:33:PHE:HE1 | 2.25 | 0.47 |
| 4:D:13:VAL:O | 4:D:108:VAL:HA | 2.15 | 0.47 |
| 5:E:86:THR:CG2 | 5:E:109:THR:HA | 2.29 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:150:ALA:HB3 | 1:F:152:VAL:HG23 | 1.95 | 0.47 |
| 1:F:51:TRP:CZ2 | 1:F:179:LEU:CD2 | 2.98 | 0.47 |
| 4:I:110:PRO:HD2 | 4:I:140:SER:OG | 2.14 | 0.47 |
| 4:I:50:ILE:HD12 | 4:I:51:TYR:CA | 2.44 | 0.47 |
| 5:J:18:LYS:HB2 | 5:J:79:GLU:O | 2.15 | 0.47 |
| 2:B:12:ARG:H | 2:B:21:ASN:HD21 | 1.63 | 0.47 |
| 4:D:12:SER:HA | 4:D:109:LYS:NZ | 2.27 | 0.47 |
| 4:D:162:MET:CE | 5:E:192:ARG:HG2 | 2.45 | 0.47 |
| 5:E:19:LEU:HD11 | 5:E:78:LEU:CD2 | 2.42 | 0.47 |
| 5:E:199:GLN:HA | 5:E:239:ARG:O | 2.14 | 0.47 |
| 1:F:33:PHE:CD2 | 1:F:34:VAL:HG22 | 2.50 | 0.47 |
| 4:I:135:PHE:CZ | 4:I:138:PHE:HB3 | 2.50 | 0.47 |
| 4:I:4:VAL:HG13 | 4:I:5:GLU:HG2 | 1.96 | 0.47 |
| 1:A:130:LEU:HB3 | 1:A:157:ARG:CG | 2.45 | 0.47 |
| 1:A:49:ALA:HB1 | 1:A:51:TRP:CE2 | 2.50 | 0.47 |
| 4:D:154:ILE:HD11 | 4:D:187:PHE:HD1 | 1.77 | 0.47 |
| 5:E:11:LEU:O | 5:E:108:LEU:HD12 | 2.15 | 0.47 |
| 4:D:25:TYR:CD2 | 4:D:33:PHE:CE1 | 3.03 | 0.47 |
| 4:D:36:TYR:CE1 | 4:D:46:LEU:HB2 | 2.50 | 0.47 |
| 1:F:202:ARG:NH1 | 1:F:202:ARG:HG3 | 2.27 | 0.47 |
| 1:F:203:CYS:SG | 1:F:272:LEU:HD22 | 2.55 | 0.47 |
| 1:F:4:SER:OG | 1:F:6:ARG:NE | 2.47 | 0.47 |
| 2:G:12:ARG:CG | 2:G:13:HIS:N | 2.78 | 0.47 |
| 4:I:6:GLN:HE21 | 4:I:102:GLN:HB2 | 1.77 | 0.47 |
| 5:J:9:ARG:HH11 | 5:J:9:ARG:CG | 2.28 | 0.47 |
| 1:A:83:ARG:HH12 | 1:A:84:TYR:HE1 | 1.56 | 0.46 |
| 2:B:50:GLU:HB3 | 2:B:67:TYR:CE1 | 2.50 | 0.46 |
| 5:E:128:SER:O | 5:E:132:ILE:CD1 | 2.63 | 0.46 |
| 1:F:162:GLY:O | 1:F:163:THR:C | 2.53 | 0.46 |
| 5:J:86:THR:HA | 5:J:108:LEU:CD1 | 2.45 | 0.46 |
| 1:A:159:TYR:CD1 | 4:D:31:GLN:NE2 | 2.83 | 0.46 |
| 1:A:234:ARG:NH2 | 2:B:10:TYR:CB | 2.78 | 0.46 |
| 2:B:23:LEU:O | 2:B:67:TYR:HA | 2.15 | 0.46 |
| 1:F:51:TRP:NE1 | 1:F:179:LEU:HD21 | 2.29 | 0.46 |
| 1:A:129:ASP:OD2 | 1:A:131:ARG:HB2 | 2.15 | 0.46 |
| 1:A:13:SER:HA | 1:A:20:PRO:HG3 | 1.97 | 0.46 |
| 2:B:8:GLN:O | 2:B:25:CYS:HA | 2.16 | 0.46 |
| 1:F:244:TRP:O | 1:F:244:TRP:HE3 | 1.97 | 0.46 |
| 5:J:215:SER:C | 5:J:217:ASN:H | 2.18 | 0.46 |
| 5:J:25:GLN:OE1 | 5:J:28:ASN:N | 2.49 | 0.46 |
| 4:D:34:PHE:CD2 | 4:D:34:PHE:N | 2.83 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:48:MET:HG2 | 4:D:63:ALA:HB2 | 1.97 | 0.46 |
| 1:F:7:TYR:CD2 | 3:H:2:PHE:HD1 | 2.33 | 0.46 |
| 4:I:9:GLY:HA2 | 4:I:10:PRO:HD3 | 1.68 | 0.46 |
| 4:I:118:ALA:HB2 | 4:I:197:PHE:HB3 | 1.97 | 0.46 |
| 4:I:92:TYR:CE2 | 5:J:98:HIS:HB3 | 2.51 | 0.46 |
| 4:D:36:TYR:HD1 | 4:D:46:LEU:N | 2.14 | 0.46 |
| 4:D:23:CYS:HB2 | 4:D:72:VAL:HG12 | 1.98 | 0.46 |
| 5:E:115:LYS:NZ | 5:E:118:PHE:HZ | 2.13 | 0.46 |
| 5:E:135:THR:O | 5:E:136:GLN:HB2 | 2.15 | 0.46 |
| 5:E:31:TYR:CD2 | 5:E:100:GLN:NE2 | 2.84 | 0.46 |
| 1:F:51:TRP:HZ2 | 1:F:179:LEU:CD2 | 2.26 | 0.46 |
| 1:F:158:ALA:HB1 | 4:I:31:GLN:HB2 | 1.98 | 0.46 |
| 5:J:154:LEU:CD2 | 5:J:209:VAL:HG22 | 2.46 | 0.46 |
| 1:A:33:PHE:CG | 1:A:34:VAL:HG13 | 2.50 | 0.46 |
| 4:D:89:TRP:CZ3 | 4:D:91:THR:CG2 | 2.94 | 0.46 |
| 5:E:52:VAL:O | 5:E:54:VAL:HG23 | 2.16 | 0.46 |
| 5:E:6:GLN:NE2 | 5:E:34:TRP:CZ3 | 2.84 | 0.46 |
| 5:E:32:MET:HG2 | 5:E:93:SER:OG | 2.15 | 0.46 |
| 4:I:123:ARG:CB | 5:J:126:GLU:HB2 | 2.41 | 0.46 |
| 1:A:55:GLU:O | 1:A:60:TRP:HZ2 | 1.98 | 0.46 |
| 2:B:52:SER:O | 2:B:64:LEU:HD21 | 2.16 | 0.46 |
| 5:E:107:ARG:CZ | 5:E:150:ASP:OD1 | 2.64 | 0.46 |
| 5:E:25:GLN:HB3 | 5:E:25:GLN:HE21 | 1.53 | 0.46 |
| 1:F:122:ASP:O | 1:F:136:ALA:CB | 2.64 | 0.46 |
| 2:G:56:PHE:CB | 2:G:61:SER:O | 2.58 | 0.46 |
| 5:J:19:LEU:N | 5:J:19:LEU:HD12 | 2.30 | 0.46 |
| 5:J:60:VAL:HG23 | 5:J:60:VAL:O | 2.16 | 0.46 |
| 1:A:4:SER:N | 1:A:29:ASP:OD1 | 2.49 | 0.46 |
| 4:D:14:PRO:HB2 | 4:I:71:TYR:CE1 | 2.48 | 0.46 |
| 4:D:133:CYS:SG | 4:D:181:PHE:HE1 | 2.39 | 0.46 |
| 4:D:96:GLY:HA3 | 5:E:50:MET:HE1 | 1.96 | 0.46 |
| 5:E:32:MET:HB2 | 5:E:68:ARG:NH1 | 2.31 | 0.46 |
| 1:F:51:TRP:CD1 | 1:F:175:GLY:HA3 | 2.51 | 0.46 |
| 1:F:76:GLU:O | 1:F:80:ILE:HG13 | 2.15 | 0.46 |
| 4:I:192:ILE:HG13 | 4:I:193:PRO:O | 2.16 | 0.46 |
| 5:J:49:SER:CB | 5:J:68:ARG:NH1 | 2.79 | 0.46 |
| 2:B:83:ASN:ND2 | 2:B:83:ASN:C | 2.68 | 0.46 |
| 4:D:114:ASN:HB3 | 1:F:108:ARG:NH1 | 2.23 | 0.46 |
| 4:D:187:PHE:HB3 | 4:D:190:SER:OG | 2.16 | 0.46 |
| 5:E:117:VAL:HG12 | 5:E:227:PRO:CB | 2.46 | 0.46 |
| 5:E:53:GLU:OE1 | 5:E:69:LYS:HA | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:F:13:SER:O | 1:F:92:SER:HB2 | 2.16 | 0.46 |
| 4:I:160:LEU:CD1 | 4:I:162:MET:HE3 | 2.42 | 0.46 |
| 4:I:28:ARG:HA | 4:I:70:GLN:NE2 | 2.30 | 0.46 |
| 5:J:124:VAL:HG23 | 5:J:234:ALA:HB3 | 1.98 | 0.46 |
| 3:H:6:PHE:CZ | 5:J:98:HIS:CD2 | 3.02 | 0.46 |
| 4:D:156:ASP:OD2 | 4:D:157:LYS:HD3 | 2.15 | 0.46 |
| 1:F:120:GLY:CA | 2:G:31:HIS:NE2 | 2.79 | 0.46 |
| 1:F:93:HIS:HB3 | 1:F:118:TYR:CE1 | 2.51 | 0.46 |
| 4:D:189:ASN:HD22 | 4:D:189:ASN:HA | 1.66 | 0.45 |
| 4:D:88:LEU:N | 4:D:88:LEU:CD2 | 2.78 | 0.45 |
| 5:E:36:ARG:NH2 | 5:E:87:SER:HB2 | 2.23 | 0.45 |
| 1:F:35:ARG:O | 1:F:45:MET:SD | 2.74 | 0.45 |
| 4:I:69:SER:O | 4:I:70:GLN:HB2 | 2.16 | 0.45 |
| 5:J:218:ASP:O | 5:J:226:LYS:NZ | 2.42 | 0.45 |
| 1:A:152:VAL:HG13 | 1:A:156:GLN:NE2 | 2.30 | 0.45 |
| 1:A:190:THR:HG21 | 2:B:98:ASP:CG | 2.36 | 0.45 |
| 4:D:192:ILE:HD11 | 4:D:196:THR:CB | 2.46 | 0.45 |
| 1:F:98:MET:HB3 | 1:F:115:GLN:HG2 | 1.98 | 0.45 |
| 5:J:154:LEU:HD22 | 5:J:155:SER:H | 1.81 | 0.45 |
| 4:I:159:VAL:N | 5:J:168:CYS:SG | 2.88 | 0.45 |
| 5:J:199:GLN:HA | 5:J:239:ARG:O | 2.15 | 0.45 |
| 1:A:185:PRO:HG3 | 1:A:213:ILE:CD1 | 2.46 | 0.45 |
| 1:A:219:ARG:HG3 | 1:A:257:TYR:CE1 | 2.52 | 0.45 |
| 2:B:5:PRO:O | 2:B:7:ILE:HD12 | 2.17 | 0.45 |
| 1:F:240:THR:C | 1:F:241:PHE:CD1 | 2.90 | 0.45 |
| 2:G:37:VAL:HG13 | 2:G:80:CYS:SG | 2.56 | 0.45 |
| 4:I:135:PHE:HB2 | 4:I:187:PHE:CE2 | 2.51 | 0.45 |
| 1:A:51:TRP:CZ3 | 1:A:52:ILE:HD13 | 2.52 | 0.45 |
| 1:A:53:GLU:HA | 1:A:60:TRP:HH2 | 1.81 | 0.45 |
| 3:C:3:PRO:HG2 | 3:C:5:THR:CG2 | 2.46 | 0.45 |
| 1:F:50:PRO:HA | 1:F:53:GLU:OE1 | 2.15 | 0.45 |
| 2:G:62:PHE:N | 2:G:62:PHE:CD1 | 2.84 | 0.45 |
| 2:G:23:LEU:O | 2:G:67:TYR:HA | 2.17 | 0.45 |
| 2:G:81:ARG:CB | 2:G:92:ILE:HG12 | 2.47 | 0.45 |
| 5:J:154:LEU:HD22 | 5:J:155:SER:N | 2.31 | 0.45 |
| 5:J:82:SER:HB2 | 5:J:84:ASN:OD1 | 2.16 | 0.45 |
| 5:J:97:SER:C | 5:J:98:HIS:ND1 | 2.70 | 0.45 |
| 2:B:23:LEU:HG | 2:B:23:LEU:O | 2.17 | 0.45 |
| 4:D:91:THR:CG2 | 4:D:91:THR:O | 2.63 | 0.45 |
| 5:E:72:ARG:H | 5:E:72:ARG:HD2 | 1.81 | 0.45 |
| 5:E:79:GLU:C | 5:E:81:PRO:HD3 | 2.37 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:202:ARG:HD2 | 1:F:204:TRP:CE2 | 2.51 | 0.45 |
| 1:F:43:GLN:HE21 | 1:F:43:GLN:CA | 2.28 | 0.45 |
| 2:G:45:ARG:HB2 | 2:G:81:ARG:NH2 | 2.30 | 0.45 |
| 2:G:40:LEU:HD11 | 2:G:81:ARG:HB2 | 1.99 | 0.45 |
| 5:E:108:LEU:HD12 | 5:E:109:THR:H | 1.82 | 0.45 |
| 5:E:49:SER:CB | 5:E:74:PHE:CE1 | 3.00 | 0.45 |
| 1:F:117:ALA:CB | 2:G:60:TRP:CD2 | 2.99 | 0.45 |
| 1:F:99:PHE:CE2 | 1:F:159:TYR:CE2 | 3.03 | 0.45 |
| 1:F:256:ARG:HG2 | 1:F:256:ARG:HH11 | 1.82 | 0.45 |
| 4:I:160:LEU:C | 4:I:168:LYS:NZ | 2.70 | 0.45 |
| 4:I:33:PHE:HB2 | 4:I:50:ILE:HG12 | 1.99 | 0.45 |
| 5:J:210:GLN:HE21 | 5:J:231:ILE:HG12 | 1.81 | 0.45 |
| 1:A:145:ARG:O | 1:A:148:GLU:HB2 | 2.17 | 0.45 |
| 1:A:186:LYS:HB2 | 1:A:186:LYS:HZ3 | 1.80 | 0.45 |
| 5:E:88:LEU:CD1 | 5:E:107:ARG:HG2 | 2.41 | 0.45 |
| 5:J:11:LEU:HD12 | 5:J:12:ILE:H | 1.80 | 0.45 |
| 1:A:188:HIS:CE1 | 1:A:204:TRP:CB | 3.00 | 0.45 |
| 1:A:43:GLN:NE2 | 1:A:43:GLN:HA | 2.32 | 0.45 |
| 5:E:124:VAL:HG23 | 5:E:234:ALA:CB | 2.46 | 0.45 |
| 3:C:7:GLY:N | 5:E:30:GLU:HG3 | 2.25 | 0.45 |
| 5:J:20:THR:OG1 | 5:J:77:ILE:HG13 | 2.17 | 0.45 |
| 5:J:210:GLN:NE2 | 5:J:231:ILE:CG1 | 2.80 | 0.45 |
| 5:J:52:VAL:HG13 | 5:J:68:ARG:O | 2.17 | 0.45 |
| 4:D:154:ILE:O | 4:D:154:ILE:HG22 | 2.17 | 0.45 |
| 4:D:89:TRP:HZ3 | 4:D:91:THR:HG22 | 1.77 | 0.45 |
| 1:F:99:PHE:CE1 | 1:F:114:HIS:CG | 3.04 | 0.45 |
| 1:A:200:THR:HG21 | 1:A:202:ARG:CZ | 2.47 | 0.44 |
| 4:D:139:ASP:C | 4:D:141:GLN:H | 2.20 | 0.44 |
| 5:E:127:PRO:HG3 | 5:E:139:THR:C | 2.38 | 0.44 |
| 5:E:215:SER:C | 5:E:217:ASN:H | 2.20 | 0.44 |
| 5:E:38:ASP:OD2 | 5:E:44:ARG:NH2 | 2.44 | 0.44 |
| 1:F:70:HIS:HD2 | 1:F:73:THR:CB | 2.27 | 0.44 |
| 2:G:21:ASN:CG | 2:G:22:PHE:N | 2.69 | 0.44 |
| 4:I:102:GLN:OE1 | 4:I:102:GLN:C | 2.56 | 0.44 |
| 4:I:116:ASP:N | 4:I:117:PRO:HD3 | 2.32 | 0.44 |
| 4:I:21:LEU:N | 4:I:21:LEU:HD23 | 2.32 | 0.44 |
| 5:J:154:LEU:HD23 | 5:J:155:SER:H | 1.81 | 0.44 |
| 5:J:210:GLN:HG2 | 5:J:212:TYR:CE2 | 2.52 | 0.44 |
| 1:A:97:MET:HE2 | 1:A:99:PHE:HB2 | 1.99 | 0.44 |
| 4:D:12:SER:CB | 4:D:109:LYS:HZ1 | 2.30 | 0.44 |
| 4:D:17:ALA:HB2 | 4:I:71:TYR:OH | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:272:LEU:CD1 | 1:F:272:LEU:N | 2.74 | 0.44 |
| 1:F:56:GLY:O | 1:F:59:TYR:HB3 | 2.17 | 0.44 |
| 1:F:82:LEU:HD23 | 1:F:87:GLN:HB2 | 2.00 | 0.44 |
| 4:I:161:ASP:HB2 | 4:I:168:LYS:HG2 | 2.00 | 0.44 |
| 4:I:23:CYS:HB3 | 4:I:89:TRP:CZ2 | 2.52 | 0.44 |
| 3:H:7:GLY:HA2 | 5:J:30:GLU:CG | 2.48 | 0.44 |
| 1:A:57:PRO:CA | 1:A:60:TRP:HD1 | 2.26 | 0.44 |
| 4:D:136:THR:OG1 | 4:D:137:ASP:N | 2.50 | 0.44 |
| 4:D:15:GLU:HG3 | 4:D:16:GLY:N | 2.33 | 0.44 |
| 1:F:202:ARG:HD3 | 1:F:244:TRP:CG | 2.52 | 0.44 |
| 4:I:87:TYR:C | 4:I:88:LEU:HD23 | 2.37 | 0.44 |
| 1:A:208:PHE:CZ | 1:A:241:PHE:HB2 | 2.52 | 0.44 |
| 1:A:68:LYS:HB3 | 5:E:54:VAL:HG22 | 1.99 | 0.44 |
| 1:A:75:ARG:NH1 | 1:A:79:ARG:NE | 2.62 | 0.44 |
| 4:D:192:ILE:HD11 | 4:D:196:THR:CG2 | 2.47 | 0.44 |
| 5:E:159:ASN:OD1 | 5:E:203:ASN:ND2 | 2.50 | 0.44 |
| 5:E:218:ASP:O | 5:E:226:LYS:NZ | 2.43 | 0.44 |
| 3:C:4:LEU:O | 5:E:98:HIS:NE2 | 2.50 | 0.44 |
| 1:F:146:LYS:HB3 | 1:F:146:LYS:HZ3 | 1.82 | 0.44 |
| 4:I:182:ALA:H | 4:I:185:ASN:HD21 | 1.66 | 0.44 |
| 5:J:18:LYS:HG2 | 5:J:19:LEU:N | 2.32 | 0.44 |
| 1:A:234:ARG:O | 1:A:242:GLN:HG3 | 2.17 | 0.44 |
| 1:A:249:VAL:CG1 | 1:A:257:TYR:CE2 | 2.95 | 0.44 |
| 1:A:63:GLU:O | 1:A:67:VAL:HG12 | 2.17 | 0.44 |
| 2:B:14:PRO:O | 2:B:16:GLU:HG2 | 2.18 | 0.44 |
| 2:B:56:PHE:HD2 | 2:B:62:PHE:CE2 | 2.36 | 0.44 |
| 4:D:75:LEU:N | 4:D:75:LEU:HD12 | 2.32 | 0.44 |
| 4:D:158:CYS:HB2 | 5:E:190:ARG:NH1 | 2.32 | 0.44 |
| 5:E:85:GLN:O | 5:E:89:TYR:OH | 2.23 | 0.44 |
| 1:F:189:MET:HB2 | 1:F:189:MET:HE2 | 1.82 | 0.44 |
| 1:F:51:TRP:CZ2 | 1:F:179:LEU:CD1 | 3.00 | 0.44 |
| 4:I:93:ASN:C | 4:I:95:GLY:N | 2.70 | 0.44 |
| 5:J:152:VAL:HG12 | 5:J:210:GLN:O | 2.17 | 0.44 |
| 5:J:36:ARG:NH2 | 5:J:84:ASN:O | 2.46 | 0.44 |
| 1:A:66:LYS:HB2 | 1:A:66:LYS:HE3 | 1.74 | 0.44 |
| 5:E:203:ASN:HB3 | 5:E:205:PHE:CZ | 2.53 | 0.44 |
| 1:F:204:TRP:HH2 | 2:G:99:MET:CE | 2.31 | 0.44 |
| 1:F:260:HIS:CE1 | 1:F:271:THR:CG2 | 3.00 | 0.44 |
| 4:I:185:ASN:HD22 | 4:I:185:ASN:C | 2.20 | 0.44 |
| 5:J:162:GLU:CG | 5:J:164:HIS:HE1 | 2.30 | 0.44 |
| 1:A:200:THR:CG2 | 1:A:202:ARG:HH22 | 2.31 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:138:PHE:O | 4:D:170:ASN:ND2 | 2.51 | 0.44 |
| 3:C:4:LEU:CD2 | 4:D:96:GLY:HA2 | 2.46 | 0.44 |
| 5:E:8:PRO:O | 5:E:106:THR:HG23 | 2.17 | 0.44 |
| 1:F:156:GLN:OE1 | 3:H:8:TRP:CH2 | 2.70 | 0.44 |
| 1:F:99:PHE:CE2 | 3:H:3:PRO:HB3 | 2.53 | 0.44 |
| 4:I:38:GLN:CG | 4:I:44:PRO:HG3 | 2.48 | 0.44 |
| 1:A:111:ARG:NH2 | 1:A:128:GLU:CA | 2.79 | 0.44 |
| 1:A:202:ARG:HH11 | 1:A:246:ALA:HB2 | 1.83 | 0.44 |
| 1:A:219:ARG:HG3 | 1:A:257:TYR:HE1 | 1.83 | 0.44 |
| 1:A:68:LYS:NZ | 5:E:53:GLU:O | 2.51 | 0.44 |
| 1:F:144:LYS:O | 1:F:148:GLU:CG | 2.65 | 0.44 |
| 1:F:67:VAL:HG13 | 1:F:68:LYS:N | 2.33 | 0.44 |
| 5:J:154:LEU:CD2 | 5:J:155:SER:N | 2.81 | 0.44 |
| 1:A:207:GLY:HA2 | 1:A:240:THR:HB | 2.00 | 0.44 |
| 2:B:23:LEU:N | 2:B:70:PHE:CE1 | 2.85 | 0.44 |
| 3:C:4:LEU:HD22 | 3:C:6:PHE:HE2 | 1.83 | 0.44 |
| 4:D:115:PRO:HD2 | 1:F:108:ARG:NH2 | 2.32 | 0.44 |
| 5:E:70:GLU:HB3 | 5:E:72:ARG:HD2 | 2.00 | 0.44 |
| 1:F:106:ASP:CG | 1:F:108:ARG:HB2 | 2.38 | 0.44 |
| 1:F:202:ARG:HD3 | 1:F:244:TRP:CE2 | 2.52 | 0.44 |
| 1:F:244:TRP:CE3 | 1:F:244:TRP:O | 2.71 | 0.44 |
| 1:F:51:TRP:C | 1:F:51:TRP:HE3 | 2.22 | 0.44 |
| 5:J:148:TYR:HB2 | 5:J:184:ARG:HG3 | 2.00 | 0.44 |
| 1:A:126:LEU:HD13 | 1:A:133:TRP:CE3 | 2.52 | 0.43 |
| 5:E:86:THR:O | 5:E:87:SER:HB2 | 2.18 | 0.43 |
| 1:A:109:PHE:O | 1:A:110:LEU:HD12 | 2.17 | 0.43 |
| 1:A:121:LYS:HD3 | 1:A:122:ASP:H | 1.84 | 0.43 |
| 1:A:11:SER:OG | 1:A:78:LEU:HD11 | 2.18 | 0.43 |
| 4:D:11:LEU:HG | 4:D:12:SER:N | 2.31 | 0.43 |
| 1:A:159:TYR:CD1 | 4:D:31:GLN:OE1 | 2.70 | 0.43 |
| 1:A:65:GLY:HA2 | 5:E:54:VAL:CG1 | 2.48 | 0.43 |
| 1:F:106:ASP:OD2 | 1:F:108:ARG:CB | 2.58 | 0.43 |
| 2:G:22:PHE:HD2 | 2:G:67:TYR:HD2 | 1.64 | 0.43 |
| 2:G:54:LEU:HA | 2:G:64:LEU:HD21 | 2.00 | 0.43 |
| 4:I:4:VAL:HG22 | 4:I:5:GLU:N | 2.33 | 0.43 |
| 5:J:41:LEU:N | 5:J:41:LEU:HD22 | 2.33 | 0.43 |
| 5:E:181:ASN:N | 5:E:181:ASN:OD1 | 2.51 | 0.43 |
| 1:A:150:ALA:HB1 | 5:E:96:ALA:HB1 | 1.99 | 0.43 |
| 1:F:8:PHE:CD2 | 1:F:25:VAL:HG23 | 2.40 | 0.43 |
| 4:I:37:ARG:CZ | 4:I:39:TYR:OH | 2.66 | 0.43 |
| 4:I:87:TYR:CE2 | 4:I:106:LEU:HB3 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:I:88:LEU:HD12 | 4:I:100:PHE:CD1 | 2.53 | 0.43 |
| 1:A:170:ARG:HH11 | 1:A:170:ARG:HG3 | 1.84 | 0.43 |
| 1:A:50:PRO:HA | 1:A:53:GLU:OE2 | 2.19 | 0.43 |
| 4:D:53:ASN:HA | 4:D:65:LEU:HD23 | 1.99 | 0.43 |
| 4:I:109:LYS:HD2 | 4:I:140:SER:OG | 2.18 | 0.43 |
| 4:I:38:GLN:CB | 4:I:44:PRO:HG3 | 2.48 | 0.43 |
| 5:J:43:LEU:HD12 | 5:J:44:ARG:N | 2.32 | 0.43 |
| 1:A:19:GLU:CA | 1:A:19:GLU:OE2 | 2.54 | 0.43 |
| 1:A:268:LYS:HG3 | 1:A:269:PRO:HD2 | 2.01 | 0.43 |
| 3:C:4:LEU:CD2 | 3:C:6:PHE:HE2 | 2.30 | 0.43 |
| 1:F:231:VAL:HG13 | 1:F:244:TRP:CH2 | 2.54 | 0.43 |
| 1:F:22:PHE:CE2 | 1:F:71:SER:HB3 | 2.52 | 0.43 |
| 4:I:160:LEU:O | 4:I:168:LYS:HA | 2.19 | 0.43 |
| 5:J:150:ASP:C | 5:J:151:HIS:HD2 | 2.22 | 0.43 |
| 4:D:110:PRO:HG2 | 4:D:112:ILE:HD11 | 2.00 | 0.43 |
| 4:D:157:LYS:CD | 4:D:157:LYS:N | 2.82 | 0.43 |
| 4:I:124:ASP:OD2 | 5:J:125:PHE:CZ | 2.72 | 0.43 |
| 1:A:133:TRP:HB2 | 1:A:144:LYS:HG3 | 2.00 | 0.43 |
| 5:E:6:GLN:OE1 | 5:E:91:CYS:N | 2.46 | 0.43 |
| 1:A:208:PHE:HZ | 1:A:233:THR:HG23 | 1.84 | 0.43 |
| 1:A:33:PHE:CD1 | 1:A:33:PHE:C | 2.91 | 0.43 |
| 1:A:48:ARG:HA | 1:A:48:ARG:HD2 | 1.63 | 0.43 |
| 1:A:44:ARG:HA | 1:A:64:THR:HG23 | 2.00 | 0.43 |
| 2:B:56:PHE:CD2 | 2:B:62:PHE:HE2 | 2.36 | 0.43 |
| 1:A:147:TRP:CZ2 | 3:C:8:TRP:HB3 | 2.54 | 0.43 |
| 4:D:81:PRO:N | 4:D:108:VAL:HG11 | 2.34 | 0.43 |
| 4:D:161:ASP:OD2 | 4:D:163:ARG:HG2 | 2.19 | 0.43 |
| 5:E:9:ARG:HB3 | 5:E:10:TYR:CD2 | 2.54 | 0.43 |
| 1:F:205:ALA:O | 1:F:208:PHE:HE1 | 2.02 | 0.43 |
| 5:J:152:VAL:HA | 5:J:210:GLN:O | 2.19 | 0.43 |
| 5:J:46:ILE:O | 5:J:58:GLY:N | 2.41 | 0.43 |
| 1:A:162:GLY:O | 1:A:163:THR:C | 2.57 | 0.43 |
| 1:A:191:HIS:CE1 | 1:A:193:PRO:HG3 | 2.54 | 0.43 |
| 1:A:82:LEU:HD22 | 1:A:87:GLN:HB2 | 2.01 | 0.43 |
| 4:D:116:ASP:N | 4:D:117:PRO:HD3 | 2.33 | 0.43 |
| 4:D:194:GLU:HA | 4:D:194:GLU:OE1 | 2.19 | 0.43 |
| 1:A:158:ALA:HB1 | 4:D:31:GLN:CB | 2.49 | 0.43 |
| 5:E:176:GLU:O | 5:E:178:PRO:HD3 | 2.18 | 0.43 |
| 1:F:201:LEU:HD23 | 1:F:201:LEU:HA | 1.94 | 0.43 |
| 1:F:234:ARG:HG3 | 1:F:242:GLN:CG | 2.38 | 0.43 |
| 5:J:127:PRO:HD2 | 5:J:198:TRP:CE2 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:J:38:ASP:CB | 5:J:44:ARG:HH22 | 2.30 | 0.43 |
| 1:A:130:LEU:O | 1:A:157:ARG:HG3 | 2.18 | 0.43 |
| 1:A:44:ARG:HG2 | 1:A:64:THR:HG21 | 2.01 | 0.43 |
| 2:B:23:LEU:HD21 | 2:B:39:LEU:HD13 | 2.01 | 0.43 |
| 4:D:111:ASN:HA | 4:D:111:ASN:HD22 | 1.48 | 0.43 |
| 5:E:132:ILE:HG23 | 5:E:195:ALA:HB2 | 1.99 | 0.43 |
| 5:E:19:LEU:HD12 | 5:E:19:LEU:O | 2.19 | 0.43 |
| 1:F:104:GLY:CA | 1:F:110:LEU:HD23 | 2.49 | 0.43 |
| 1:F:99:PHE:HE1 | 1:F:114:HIS:CG | 2.37 | 0.43 |
| 1:F:218:GLN:OE1 | 1:F:223:ASP:N | 2.52 | 0.43 |
| 1:F:7:TYR:HE1 | 1:F:33:PHE:CZ | 2.36 | 0.43 |
| 2:G:9:VAL:HA | 2:G:24:ASN:O | 2.18 | 0.43 |
| 4:I:36:TYR:CD1 | 4:I:46:LEU:N | 2.87 | 0.43 |
| 4:I:94:GLN:CB | 4:I:97:LYS:HD3 | 2.30 | 0.43 |
| 5:J:203:ASN:O | 5:J:205:PHE:CE2 | 2.72 | 0.43 |
| 1:A:11:SER:HA | 1:A:21:ARG:O | 2.19 | 0.42 |
| 1:A:111:ARG:HD3 | 1:A:128:GLU:CD | 2.39 | 0.42 |
| 1:A:200:THR:HG21 | 1:A:202:ARG:NH2 | 2.34 | 0.42 |
| 1:A:98:MET:SD | 1:A:99:PHE:N | 2.91 | 0.42 |
| 4:I:193:PRO:HB2 | 4:I:196:THR:OG1 | 2.19 | 0.42 |
| 4:I:42:LYS:N | 4:I:42:LYS:HE2 | 2.34 | 0.42 |
| 1:A:150:ALA:HB3 | 1:A:152:VAL:HG23 | 2.01 | 0.42 |
| 4:D:112:ILE:HD13 | 4:D:112:ILE:N | 2.34 | 0.42 |
| 4:D:30:SER:HB3 | 4:D:33:PHE:CE2 | 2.54 | 0.42 |
| 4:D:32:SER:C | 4:D:33:PHE:HD2 | 2.22 | 0.42 |
| 4:D:43:SER:HA | 5:E:90:PHE:CZ | 2.55 | 0.42 |
| 5:E:79:GLU:O | 5:E:81:PRO:HD3 | 2.18 | 0.42 |
| 1:F:185:PRO:HB3 | 1:F:208:PHE:CD1 | 2.54 | 0.42 |
| 1:F:33:PHE:C | 1:F:48:ARG:HB2 | 2.40 | 0.42 |
| 2:G:12:ARG:HD2 | 2:G:22:PHE:CB | 2.39 | 0.42 |
| 5:J:132:ILE:N | 5:J:132:ILE:CD1 | 2.82 | 0.42 |
| 5:J:64:TYR:CD1 | 5:J:78:LEU:CD1 | 3.02 | 0.42 |
| 1:A:108:ARG:O | 1:A:110:LEU:CD1 | 2.64 | 0.42 |
| 1:A:161:GLU:O | 1:A:165:VAL:HG21 | 2.20 | 0.42 |
| 1:A:188:HIS:CE1 | 1:A:204:TRP:HB2 | 2.54 | 0.42 |
| 1:A:213:ILE:CD1 | 1:A:263:HIS:HB2 | 2.49 | 0.42 |
| 1:A:268:LYS:HA | 1:A:268:LYS:HD2 | 1.85 | 0.42 |
| 2:B:23:LEU:CD2 | 2:B:39:LEU:HD13 | 2.50 | 0.42 |
| 4:D:12:SER:CB | 4:D:109:LYS:NZ | 2.82 | 0.42 |
| 5:E:114:LEU:HD13 | 5:E:214:LEU:HD21 | 2.02 | 0.42 |
| 5:E:86:THR:OG1 | 5:E:110:VAL:HG23 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:125:ALA:O | 1:F:134:THR:CG2 | 2.68 | 0.42 |
| 1:F:137:ASP:OD1 | 1:F:137:ASP:C | 2.56 | 0.42 |
| 1:F:159:TYR:OH | 3:H:1:ARG:O | 2.31 | 0.42 |
| 4:I:185:ASN:ND2 | 4:I:185:ASN:C | 2.70 | 0.42 |
| 4:I:35:TRP:O | 4:I:47:ILE:HG13 | 2.18 | 0.42 |
| 5:J:146:GLY:HA2 | 5:J:176:GLU:OE2 | 2.20 | 0.42 |
| 5:J:79:GLU:C | 5:J:81:PRO:HD3 | 2.40 | 0.42 |
| 1:A:220:ASP:OD1 | 1:A:256:ARG:HD3 | 2.19 | 0.42 |
| 1:A:235:PRO:HG2 | 2:B:65:LEU:HD22 | 2.01 | 0.42 |
| 4:D:25:TYR:CE2 | 4:D:33:PHE:CZ | 3.07 | 0.42 |
| 1:A:157:ARG:CZ | 1:A:161:GLU:OE1 | 2.67 | 0.42 |
| 1:A:183:ASP:HA | 1:A:184:PRO:HD3 | 1.79 | 0.42 |
| 1:A:44:ARG:HA | 1:A:64:THR:CG2 | 2.50 | 0.42 |
| 2:B:41:LYS:HG3 | 2:B:78:TYR:CE2 | 2.55 | 0.42 |
| 1:F:127:LYS:HE3 | 1:F:133:TRP:O | 2.19 | 0.42 |
| 4:I:163:ARG:H | 4:I:163:ARG:HG2 | 1.42 | 0.42 |
| 4:I:14:PRO:HG2 | 4:I:17:ALA:CB | 2.49 | 0.42 |
| 4:I:36:TYR:CE1 | 5:J:102:PHE:HE2 | 2.35 | 0.42 |
| 4:I:124:ASP:OD2 | 5:J:125:PHE:HZ | 2.02 | 0.42 |
| 5:J:177:GLN:O | 5:J:183:SER:HB2 | 2.20 | 0.42 |
| 1:A:63:GLU:OE2 | 1:A:63:GLU:CA | 2.64 | 0.42 |
| 4:D:37:ARG:CB | 4:D:47:ILE:HD13 | 2.49 | 0.42 |
| 5:E:154:LEU:HD23 | 5:E:155:SER:CA | 2.48 | 0.42 |
| 5:E:64:TYR:CD1 | 5:E:76:LEU:HD21 | 2.55 | 0.42 |
| 1:F:34:VAL:CG1 | 1:F:60:TRP:HH2 | 2.33 | 0.42 |
| 5:J:131:GLU:O | 5:J:135:THR:OG1 | 2.19 | 0.42 |
| 1:A:51:TRP:HZ3 | 1:A:52:ILE:HD13 | 1.85 | 0.42 |
| 1:A:98:MET:C | 1:A:98:MET:SD | 2.98 | 0.42 |
| 4:D:122:LEU:HD12 | 5:E:128:SER:N | 2.35 | 0.42 |
| 1:F:8:PHE:O | 1:F:24:ALA:HA | 2.20 | 0.42 |
| 4:I:185:ASN:N | 4:I:185:ASN:HD22 | 2.16 | 0.42 |
| 4:I:89:TRP:CD1 | 4:I:89:TRP:N | 2.88 | 0.42 |
| 5:J:68:ARG:HG2 | 5:J:68:ARG:HH11 | 1.84 | 0.42 |
| 1:A:244:TRP:HE1 | 2:B:99:MET:HG3 | 1.84 | 0.42 |
| 2:B:35:ILE:HD11 | 2:B:82:VAL:CG1 | 2.48 | 0.42 |
| 4:D:60:ARG:NH2 | 4:D:83:ASP:OD2 | 2.42 | 0.42 |
| 5:E:239:ARG:NH1 | 5:E:239:ARG:HG3 | 2.33 | 0.42 |
| 4:D:2:LYS:NZ | 5:E:42:GLY:HA3 | 2.35 | 0.42 |
| 1:F:115:GLN:HE21 | 1:F:115:GLN:HB3 | 1.55 | 0.42 |
| 1:F:202:ARG:NH1 | 1:F:244:TRP:CH2 | 2.88 | 0.42 |
| 1:F:22:PHE:CD2 | 1:F:71:SER:CB | 3.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:10:TYR:OH | 2:G:26:TYR:HB2 | 2.20 | 0.42 |
| 2:G:35:ILE:HD11 | 2:G:84:HIS:CD2 | 2.55 | 0.42 |
| 1:A:134:THR:HG23 | 1:A:134:THR:O | 2.20 | 0.42 |
| 1:A:123:TYR:CE1 | 1:A:140:ALA:HA | 2.55 | 0.42 |
| 2:B:33:SER:HB3 | 2:B:62:PHE:CE1 | 2.55 | 0.42 |
| 2:B:22:PHE:C | 2:B:70:PHE:CE1 | 2.93 | 0.42 |
| 4:D:34:PHE:HB3 | 4:D:46:LEU:CD1 | 2.50 | 0.42 |
| 4:D:122:LEU:HG | 5:E:127:PRO:HA | 2.01 | 0.42 |
| 5:E:20:THR:O | 5:E:20:THR:CG2 | 2.67 | 0.42 |
| 1:F:191:HIS:HB2 | 1:F:274:TRP:CZ3 | 2.55 | 0.42 |
| 1:F:71:SER:O | 1:F:75:ARG:HB2 | 2.20 | 0.42 |
| 1:F:96:GLN:HB3 | 2:G:56:PHE:CE2 | 2.55 | 0.42 |
| 2:G:35:ILE:HD11 | 2:G:84:HIS:CG | 2.55 | 0.42 |
| 5:J:89:TYR:CE2 | 5:J:108:LEU:HG | 2.55 | 0.42 |
| 5:J:25:GLN:HE22 | 5:J:29:HIS:N | 2.17 | 0.42 |
| 5:J:36:ARG:NH2 | 5:J:86:THR:O | 2.53 | 0.42 |
| 1:A:123:TYR:CE2 | 3:C:10:PHE:CE2 | 3.08 | 0.42 |
| 3:C:5:THR:HG22 | 3:C:8:TRP:HZ3 | 1.84 | 0.42 |
| 4:D:94:GLN:HB2 | 4:D:97:LYS:CG | 2.48 | 0.42 |
| 1:A:150:ALA:CB | 5:E:96:ALA:HB1 | 2.50 | 0.42 |
| 1:F:82:LEU:HD21 | 1:F:93:HIS:CE1 | 2.55 | 0.42 |
| 4:I:47:ILE:HD12 | 4:I:48:MET:HB2 | 2.01 | 0.42 |
| 5:J:172:GLN:HA | 5:J:173:PRO:HD3 | 1.94 | 0.42 |
| 1:A:217:TRP:CD1 | 1:A:247:VAL:HG13 | 2.54 | 0.41 |
| 5:E:3:GLN:N | 5:E:3:GLN:OE1 | 2.53 | 0.41 |
| 1:F:77:ASN:HA | 1:F:80:ILE:HD12 | 2.02 | 0.41 |
| 1:F:8:PHE:HE2 | 1:F:27:TYR:CD1 | 2.38 | 0.41 |
| 4:I:98:LEU:HD12 | 5:J:35:TYR:OH | 2.19 | 0.41 |
| 1:A:52:ILE:HA | 1:A:52:ILE:HD12 | 1.88 | 0.41 |
| 1:A:232:GLU:CD | 2:B:6:LYS:HE2 | 2.40 | 0.41 |
| 4:D:93:ASN:C | 4:D:95:GLY:N | 2.73 | 0.41 |
| 5:E:46:ILE:O | 5:E:58:GLY:N | 2.45 | 0.41 |
| 1:F:85:TYR:HB3 | 1:F:87:GLN:HG3 | 2.01 | 0.41 |
| 4:I:160:LEU:O | 4:I:168:LYS:NZ | 2.52 | 0.41 |
| 5:J:120:PRO:HG2 | 5:J:232:VAL:CG2 | 2.49 | 0.41 |
| 5:J:176:GLU:C | 5:J:178:PRO:HD3 | 2.39 | 0.41 |
| 5:J:29:HIS:CD2 | 5:J:95:GLY:HA3 | 2.55 | 0.41 |
| 1:A:173:GLU:OE1 | 1:A:176:LYS:HD3 | 2.21 | 0.41 |
| 1:A:244:TRP:C | 1:A:244:TRP:CE3 | 2.93 | 0.41 |
| 1:A:213:ILE:CG1 | 1:A:262:GLN:O | 2.59 | 0.41 |
| 1:A:74:ASP:HB3 | 1:A:95:LEU:HD23 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:7:ILE:C | 2:B:8:GLN:NE2 | 2.73 | 0.41 |
| 5:E:87:SER:OG | 5:E:88:LEU:N | 2.52 | 0.41 |
| 1:F:23:ILE:O | 1:F:23:ILE:CG2 | 2.68 | 0.41 |
| 1:F:3:HIS:HB3 | 1:F:29:ASP:OD2 | 2.19 | 0.41 |
| 2:G:12:ARG:NH1 | 2:G:22:PHE:CD1 | 2.88 | 0.41 |
| 5:J:25:GLN:NE2 | 5:J:29:HIS:N | 2.68 | 0.41 |
| 1:A:14:ARG:HB3 | 1:A:17:ARG:HB2 | 2.01 | 0.41 |
| 1:A:255:GLN:HB3 | 1:A:255:GLN:HE21 | 1.71 | 0.41 |
| 1:A:70:HIS:HA | 1:A:73:THR:OG1 | 2.21 | 0.41 |
| 5:E:11:LEU:HD21 | 5:E:19:LEU:HD22 | 2.02 | 0.41 |
| 5:E:7:ASN:HA | 5:E:8:PRO:HA | 1.64 | 0.41 |
| 1:F:156:GLN:O | 1:F:159:TYR:HB3 | 2.20 | 0.41 |
| 1:F:204:TRP:HH2 | 2:G:99:MET:HE2 | 1.85 | 0.41 |
| 1:F:33:PHE:O | 1:F:48:ARG:N | 2.47 | 0.41 |
| 4:I:114:ASN:HA | 4:I:115:PRO:HD2 | 1.94 | 0.41 |
| 4:I:13:VAL:O | 4:I:108:VAL:HA | 2.21 | 0.41 |
| 5:J:132:ILE:CG2 | 5:J:195:ALA:HB1 | 2.49 | 0.41 |
| 5:J:19:LEU:HD11 | 5:J:78:LEU:HB3 | 2.02 | 0.41 |
| 5:E:220:TRP:NE1 | 5:E:226:LYS:HA | 2.36 | 0.41 |
| 5:E:82:SER:HB2 | 5:E:85:GLN:CG | 2.50 | 0.41 |
| 1:F:241:PHE:CD1 | 1:F:241:PHE:N | 2.88 | 0.41 |
| 5:J:144:ALA:O | 5:J:147:PHE:CE2 | 2.73 | 0.41 |
| 5:J:191:LEU:HD12 | 5:J:192:ARG:N | 2.35 | 0.41 |
| 5:J:204:HIS:HD2 | 5:J:236:ALA:O | 2.03 | 0.41 |
| 1:A:133:TRP:CZ2 | 1:A:153:ALA:N | 2.88 | 0.41 |
| 1:A:158:ALA:HB1 | 4:D:31:GLN:HB2 | 2.03 | 0.41 |
| 2:B:23:LEU:C | 2:B:23:LEU:HD12 | 2.41 | 0.41 |
| 3:C:2:PHE:CD2 | 3:C:3:PRO:O | 2.74 | 0.41 |
| 4:D:14:PRO:HD2 | 4:I:71:TYR:HE1 | 1.82 | 0.41 |
| 5:E:118:PHE:O | 5:E:147:PHE:HA | 2.21 | 0.41 |
| 5:E:193:VAL:HG23 | 5:E:194:SER:O | 2.20 | 0.41 |
| 5:E:25:GLN:OE1 | 5:E:29:HIS:HB2 | 2.19 | 0.41 |
| 5:E:77:ILE:CD1 | 5:E:77:ILE:N | 2.77 | 0.41 |
| 1:A:218:GLN:HB2 | 1:A:260:HIS:NE2 | 2.36 | 0.41 |
| 1:A:259:CYS:O | 1:A:271:THR:HA | 2.19 | 0.41 |
| 1:A:95:LEU:HD11 | 1:A:116:TYR:CD1 | 2.54 | 0.41 |
| 1:A:99:PHE:CE2 | 3:C:3:PRO:HG3 | 2.55 | 0.41 |
| 2:B:84:HIS:CB | 2:B:87:LEU:HD12 | 2.51 | 0.41 |
| 4:D:138:PHE:HE2 | 4:D:171:SER:HA | 1.85 | 0.41 |
| 5:E:161:LYS:HZ3 | 5:E:161:LYS:HB2 | 1.83 | 0.41 |
| 1:F:80:ILE:CD1 | 3:H:10:PHE:H | 2.33 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:I:141:GLN:HA | 4:I:141:GLN:OE1 | 2.21 | 0.41 |
| 1:A:5:MET:SD | 1:A:171:TYR:CE2 | 3.10 | 0.41 |
| 1:A:87:GLN:OE1 | 1:A:118:TYR:OH | 2.31 | 0.41 |
| 2:B:35:ILE:HD12 | 2:B:84:HIS:CD2 | 2.44 | 0.41 |
| 4:D:50:ILE:CD1 | 4:D:65:LEU:HB3 | 2.46 | 0.41 |
| 4:D:99:ILE:N | 4:D:99:ILE:HD12 | 2.36 | 0.41 |
| 4:D:123:ARG:NH1 | 5:E:239:ARG:HD3 | 2.35 | 0.41 |
| 5:J:163:VAL:C | 5:J:164:HIS:ND1 | 2.74 | 0.41 |
| 5:J:36:ARG:NE | 5:J:87:SER:HB3 | 2.34 | 0.41 |
| 5:J:41:LEU:HB2 | 5:J:44:ARG:NH2 | 2.36 | 0.41 |
| 5:J:47:TYR:CE2 | 5:J:61:PRO:HB2 | 2.56 | 0.41 |
| 1:A:95:LEU:HD11 | 1:A:116:TYR:CE1 | 2.55 | 0.41 |
| 1:A:217:TRP:CH2 | 1:A:259:CYS:HB2 | 2.55 | 0.41 |
| 1:F:127:LYS:HG3 | 1:F:134:THR:HG22 | 2.02 | 0.41 |
| 5:E:117:VAL:HG12 | 5:E:227:PRO:CG | 2.51 | 0.41 |
| 1:A:68:LYS:CB | 5:E:54:VAL:HG22 | 2.51 | 0.41 |
| 5:E:97:SER:O | 5:E:98:HIS:ND1 | 2.54 | 0.41 |
| 1:F:34:VAL:HG12 | 1:F:60:TRP:HH2 | 1.86 | 0.41 |
| 1:F:55:GLU:OE1 | 1:F:55:GLU:HA | 2.21 | 0.41 |
| 2:G:30:PHE:O | 2:G:62:PHE:CD1 | 2.73 | 0.41 |
| 2:G:4:THR:OG1 | 2:G:87:LEU:HD21 | 2.20 | 0.41 |
| 1:F:70:HIS:ND1 | 3:H:2:PHE:CZ | 2.70 | 0.41 |
| 4:I:18:ILE:HA | 4:I:76:ILE:O | 2.20 | 0.41 |
| 1:A:124:ILE:HD11 | 1:A:144:LYS:HB2 | 2.03 | 0.41 |
| 1:A:5:MET:HB2 | 1:A:168:LEU:HD13 | 2.03 | 0.41 |
| 1:A:74:ASP:HA | 1:A:77:ASN:ND2 | 2.35 | 0.41 |
| 5:E:187:LEU:HG | 5:E:188:SER:H | 1.85 | 0.41 |
| 5:E:9:ARG:NH1 | 5:E:104:PRO:CB | 2.81 | 0.41 |
| 1:F:183:ASP:HA | 1:F:184:PRO:HD3 | 1.79 | 0.41 |
| 1:F:51:TRP:CD1 | 1:F:175:GLY:HA2 | 2.56 | 0.41 |
| 1:F:80:ILE:HD13 | 3:H:10:PHE:H | 1.85 | 0.41 |
| 4:I:134:LEU:CD2 | 5:J:139:THR:HG21 | 2.51 | 0.41 |
| 5:J:150:ASP:C | 5:J:151:HIS:CD2 | 2.95 | 0.41 |
| 5:J:49:SER:HB3 | 5:J:68:ARG:HH11 | 1.86 | 0.41 |
| 1:A:151:HIS:O | 1:A:154:GLU:HG2 | 2.20 | 0.40 |
| 5:E:217:ASN:ND2 | 5:E:217:ASN:N | 2.68 | 0.40 |
| 5:E:25:GLN:OE1 | 5:E:29:HIS:N | 2.31 | 0.40 |
| 5:E:57:LYS:H | 5:E:57:LYS:HG2 | 1.55 | 0.40 |
| 1:F:143:THR:HA | 1:F:146:LYS:CD | 2.51 | 0.40 |
| 4:I:114:ASN:ND2 | 4:I:114:ASN:C | 2.74 | 0.40 |
| 5:J:118:PHE:O | 5:J:147:PHE:HA | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:J:154:LEU:CG | 5:J:209:VAL:HG22 | 2.49 | 0.40 |
| 1:A:34:VAL:HG21 | 1:A:45:MET:HE1 | 2.03 | 0.40 |
| 4:D:9:GLY:HA2 | 4:D:10:PRO:HD3 | 1.73 | 0.40 |
| 5:E:159:ASN:HD22 | 5:E:204:HIS:HB3 | 1.87 | 0.40 |
| 5:E:30:GLU:HB3 | 5:E:51:ASN:ND2 | 2.36 | 0.40 |
| 5:E:97:SER:HB3 | 5:E:99:GLU:OE1 | 2.21 | 0.40 |
| 1:F:55:GLU:OE2 | 1:F:170:ARG:NE | 2.54 | 0.40 |
| 1:F:197:HIS:CE1 | 1:F:198:GLU:HG3 | 2.56 | 0.40 |
| 4:I:28:ARG:HA | 4:I:70:GLN:HE21 | 1.84 | 0.40 |
| 4:I:125:SER:N | 5:J:125:PHE:CE2 | 2.89 | 0.40 |
| 5:J:41:LEU:HB2 | 5:J:44:ARG:CZ | 2.51 | 0.40 |
| 5:J:43:LEU:HD12 | 5:J:44:ARG:H | 1.86 | 0.40 |
| 1:A:185:PRO:CB | 1:A:208:PHE:HB3 | 2.38 | 0.40 |
| 1:A:234:ARG:NH2 | 2:B:10:TYR:CG | 2.89 | 0.40 |
| 1:A:33:PHE:C | 1:A:48:ARG:HB2 | 2.42 | 0.40 |
| 4:D:160:LEU:HD12 | 4:D:160:LEU:O | 2.21 | 0.40 |
| 1:F:267:PRO:CG | 1:F:268:LYS:H | 2.33 | 0.40 |
| 2:G:12:ARG:HD2 | 2:G:22:PHE:N | 2.37 | 0.40 |
| 1:F:115:GLN:CG | 2:G:60:TRP:CH2 | 2.93 | 0.40 |
| 4:I:170:ASN:O | 4:I:171:SER:HB3 | 2.21 | 0.40 |
| 4:I:94:GLN:HB3 | 4:I:97:LYS:CD | 2.30 | 0.40 |
| 5:J:159:ASN:ND2 | 5:J:204:HIS:N | 2.56 | 0.40 |
| 5:J:206:ARG:NH2 | 5:J:208:GLN:HE21 | 2.20 | 0.40 |
| 5:J:205:PHE:CD2 | 5:J:236:ALA:O | 2.70 | 0.40 |
| 5:J:47:TYR:HE2 | 5:J:61:PRO:HB2 | 1.86 | 0.40 |
| 5:J:33:SER:HA | 5:J:74:PHE:HE2 | 1.86 | 0.40 |
| 5:J:9:ARG:NH1 | 5:J:9:ARG:CG | 2.83 | 0.40 |
| 1:A:181:ARG:HG2 | 1:A:181:ARG:HH11 | 1.86 | 0.40 |
| 1:A:191:HIS:HE1 | 1:A:193:PRO:HG3 | 1.86 | 0.40 |
| 1:A:31:THR:OG1 | 1:A:209:TYR:OH | 2.36 | 0.40 |
| 2:B:12:ARG:N | 2:B:21:ASN:HD21 | 2.18 | 0.40 |
| 1:F:228:THR:HG22 | 1:F:247:VAL:CG1 | 2.46 | 0.40 |
| 2:G:16:GLU:OE2 | 2:G:19:LYS:NZ | 2.47 | 0.40 |
| 5:J:206:ARG:HH11 | 5:J:206:ARG:CG | 2.34 | 0.40 |
| 1:A:234:ARG:CZ | 2:B:10:TYR:CG | 3.04 | 0.40 |
| 1:A:99:PHE:CD2 | 3:C:3:PRO:HG3 | 2.57 | 0.40 |
| 5:E:99:GLU:H | 5:E:99:GLU:HG2 | 1.59 | 0.40 |
| 1:F:7:TYR:HE2 | 3:H:2:PHE:HA | 1.86 | 0.40 |
| 1:F:80:ILE:HG21 | 3:H:10:PHE:HB2 | 2.04 | 0.40 |
| 2:G:95:TRP:CD1 | 2:G:95:TRP:C | 2.92 | 0.40 |
| 4:I:122:LEU:HD11 | 5:J:141:VAL:CB | 2.50 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|---------------|--------------------------|-------------------|
| 5:J:156:TRP:HZ2 | 5:J:189:SER:O | 2.05 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1 | A | 272/275 (99%) | 259 (95%) | 12 (4%) | 1 (0%) | 38 | 66 |
| 1 | F | 272/275 (99%) | 257 (94%) | 14 (5%) | 1 (0%) | 38 | 66 |
| 2 | B | 97/100 (97%) | 93 (96%) | 4 (4%) | 0 | 100 | 100 |
| 2 | G | 97/100 (97%) | 93 (96%) | 4 (4%) | 0 | 100 | 100 |
| 3 | C | 8/10 (80%) | 8 (100%) | 0 | 0 | 100 | 100 |
| 3 | H | 8/10 (80%) | 8 (100%) | 0 | 0 | 100 | 100 |
| 4 | D | 197/205 (96%) | 167 (85%) | 24 (12%) | 6 (3%) | 5 | 12 |
| 4 | I | 197/205 (96%) | 169 (86%) | 22 (11%) | 6 (3%) | 5 | 12 |
| 5 | E | 239/242 (99%) | 223 (93%) | 15 (6%) | 1 (0%) | 38 | 66 |
| 5 | J | 239/242 (99%) | 220 (92%) | 18 (8%) | 1 (0%) | 38 | 66 |
| All | All | 1626/1664 (98%) | 1497 (92%) | 113 (7%) | 16 (1%) | 18 | 43 |

All (16) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | D | 94 | GLN |
| 4 | D | 8 | SER |
| 4 | D | 40 | SER |
| 4 | I | 7 | ASN |
| 4 | I | 40 | SER |
| 4 | I | 94 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | D | 7 | ASN |
| 4 | I | 8 | SER |
| 1 | F | 163 | THR |
| 1 | A | 163 | THR |
| 4 | D | 27 | ASP |
| 4 | D | 53 | ASN |
| 5 | E | 222 | GLN |
| 4 | I | 27 | ASP |
| 5 | J | 222 | GLN |
| 4 | I | 9 | GLY |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|-----|
| 1 | A | 230/231 (100%) | 194 (84%) | 36 (16%) | 3 | 8 |
| 1 | F | 230/231 (100%) | 190 (83%) | 40 (17%) | 2 | 5 |
| 2 | B | 94/95 (99%) | 77 (82%) | 17 (18%) | 2 | 5 |
| 2 | G | 94/95 (99%) | 78 (83%) | 16 (17%) | 2 | 6 |
| 3 | C | 9/9 (100%) | 9 (100%) | 0 | 100 | 100 |
| 3 | H | 9/9 (100%) | 9 (100%) | 0 | 100 | 100 |
| 4 | D | 177/183 (97%) | 145 (82%) | 32 (18%) | 2 | 5 |
| 4 | I | 177/183 (97%) | 144 (81%) | 33 (19%) | 2 | 5 |
| 5 | E | 214/215 (100%) | 176 (82%) | 38 (18%) | 2 | 5 |
| 5 | J | 214/215 (100%) | 185 (86%) | 29 (14%) | 4 | 10 |
| All | All | 1448/1466 (99%) | 1207 (83%) | 241 (17%) | 2 | 6 |

All (241) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 13 | SER |
| 1 | A | 19 | GLU |
| 1 | A | 20 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 33 | PHE |
| 1 | A | 34 | VAL |
| 1 | A | 39 | ASP |
| 1 | A | 60 | TRP |
| 1 | A | 74 | ASP |
| 1 | A | 75 | ARG |
| 1 | A | 79 | ARG |
| 1 | A | 86 | ASN |
| 1 | A | 89 | GLU |
| 1 | A | 97 | MET |
| 1 | A | 98 | MET |
| 1 | A | 116 | TYR |
| 1 | A | 122 | ASP |
| 1 | A | 157 | ARG |
| 1 | A | 160 | LEU |
| 1 | A | 163 | THR |
| 1 | A | 165 | VAL |
| 1 | A | 166 | ASP |
| 1 | A | 172 | LEU |
| 1 | A | 186 | LYS |
| 1 | A | 190 | THR |
| 1 | A | 216 | THR |
| 1 | A | 225 | THR |
| 1 | A | 229 | GLU |
| 1 | A | 230 | LEU |
| 1 | A | 231 | VAL |
| 1 | A | 234 | ARG |
| 1 | A | 238 | ASP |
| 1 | A | 242 | GLN |
| 1 | A | 247 | VAL |
| 1 | A | 248 | VAL |
| 1 | A | 255 | GLN |
| 1 | A | 258 | THR |
| 2 | B | 1 | ILE |
| 2 | B | 2 | GLN |
| 2 | B | 6 | LYS |
| 2 | B | 10 | TYR |
| 2 | B | 13 | HIS |
| 2 | B | 16 | GLU |
| 2 | B | 23 | LEU |
| 2 | B | 24 | ASN |
| 2 | B | 36 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 64 | LEU |
| 2 | B | 70 | PHE |
| 2 | B | 74 | GLU |
| 2 | B | 83 | ASN |
| 2 | B | 84 | HIS |
| 2 | B | 85 | VAL |
| 2 | B | 86 | THR |
| 2 | B | 87 | LEU |
| 4 | D | 6 | GLN |
| 4 | D | 7 | ASN |
| 4 | D | 15 | GLU |
| 4 | D | 20 | SER |
| 4 | D | 31 | GLN |
| 4 | D | 33 | PHE |
| 4 | D | 34 | PHE |
| 4 | D | 48 | MET |
| 4 | D | 50 | ILE |
| 4 | D | 71 | TYR |
| 4 | D | 73 | SER |
| 4 | D | 88 | LEU |
| 4 | D | 98 | LEU |
| 4 | D | 100 | PHE |
| 4 | D | 102 | GLN |
| 4 | D | 104 | THR |
| 4 | D | 106 | LEU |
| 4 | D | 111 | ASN |
| 4 | D | 124 | ASP |
| 4 | D | 139 | ASP |
| 4 | D | 140 | SER |
| 4 | D | 142 | THR |
| 4 | D | 151 | ASP |
| 4 | D | 154 | ILE |
| 4 | D | 156 | ASP |
| 4 | D | 157 | LYS |
| 4 | D | 162 | MET |
| 4 | D | 167 | PHE |
| 4 | D | 180 | ASP |
| 4 | D | 189 | ASN |
| 4 | D | 191 | ILE |
| 4 | D | 192 | ILE |
| 5 | E | 1 | GLU |
| 5 | E | 3 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | E | 13 | THR |
| 5 | E | 18 | LYS |
| 5 | E | 25 | GLN |
| 5 | E | 30 | GLU |
| 5 | E | 33 | SER |
| 5 | E | 37 | GLN |
| 5 | E | 46 | ILE |
| 5 | E | 47 | TYR |
| 5 | E | 50 | MET |
| 5 | E | 51 | ASN |
| 5 | E | 53 | GLU |
| 5 | E | 56 | ASP |
| 5 | E | 59 | ASP |
| 5 | E | 60 | VAL |
| 5 | E | 72 | ARG |
| 5 | E | 77 | ILE |
| 5 | E | 78 | LEU |
| 5 | E | 84 | ASN |
| 5 | E | 93 | SER |
| 5 | E | 99 | GLU |
| 5 | E | 100 | GLN |
| 5 | E | 101 | TYR |
| 5 | E | 107 | ARG |
| 5 | E | 120 | PRO |
| 5 | E | 121 | GLU |
| 5 | E | 149 | PRO |
| 5 | E | 161 | LYS |
| 5 | E | 167 | VAL |
| 5 | E | 174 | LEU |
| 5 | E | 181 | ASN |
| 5 | E | 190 | ARG |
| 5 | E | 199 | GLN |
| 5 | E | 203 | ASN |
| 5 | E | 216 | GLU |
| 5 | E | 217 | ASN |
| 5 | E | 241 | ASP |
| 1 | F | 19 | GLU |
| 1 | F | 35 | ARG |
| 1 | F | 38 | SER |
| 1 | F | 39 | ASP |
| 1 | F | 43 | GLN |
| 1 | F | 51 | TRP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 54 | GLN |
| 1 | F | 72 | GLN |
| 1 | F | 75 | ARG |
| 1 | F | 79 | ARG |
| 1 | F | 85 | TYR |
| 1 | F | 86 | ASN |
| 1 | F | 94 | THR |
| 1 | F | 98 | MET |
| 1 | F | 99 | PHE |
| 1 | F | 110 | LEU |
| 1 | F | 115 | GLN |
| 1 | F | 132 | SER |
| 1 | F | 134 | THR |
| 1 | F | 143 | THR |
| 1 | F | 146 | LYS |
| 1 | F | 155 | GLN |
| 1 | F | 170 | ARG |
| 1 | F | 174 | ASN |
| 1 | F | 177 | GLU |
| 1 | F | 186 | LYS |
| 1 | F | 188 | HIS |
| 1 | F | 214 | THR |
| 1 | F | 223 | ASP |
| 1 | F | 225 | THR |
| 1 | F | 233 | THR |
| 1 | F | 238 | ASP |
| 1 | F | 242 | GLN |
| 1 | F | 244 | TRP |
| 1 | F | 247 | VAL |
| 1 | F | 254 | GLU |
| 1 | F | 255 | GLN |
| 1 | F | 256 | ARG |
| 1 | F | 261 | VAL |
| 1 | F | 273 | ARG |
| 2 | G | 3 | ARG |
| 2 | G | 4 | THR |
| 2 | G | 17 | ASN |
| 2 | G | 24 | ASN |
| 2 | G | 31 | HIS |
| 2 | G | 35 | ILE |
| 2 | G | 36 | GLU |
| 2 | G | 40 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | G | 50 | GLU |
| 2 | G | 59 | ASP |
| 2 | G | 62 | PHE |
| 2 | G | 65 | LEU |
| 2 | G | 68 | THR |
| 2 | G | 70 | PHE |
| 2 | G | 89 | GLN |
| 2 | G | 96 | ASP |
| 4 | I | 2 | LYS |
| 4 | I | 14 | PRO |
| 4 | I | 22 | ASN |
| 4 | I | 24 | THR |
| 4 | I | 31 | GLN |
| 4 | I | 32 | SER |
| 4 | I | 42 | LYS |
| 4 | I | 44 | PRO |
| 4 | I | 50 | ILE |
| 4 | I | 53 | ASN |
| 4 | I | 57 | GLU |
| 4 | I | 69 | SER |
| 4 | I | 71 | TYR |
| 4 | I | 88 | LEU |
| 4 | I | 89 | TRP |
| 4 | I | 97 | LYS |
| 4 | I | 98 | LEU |
| 4 | I | 102 | GLN |
| 4 | I | 105 | GLU |
| 4 | I | 113 | GLN |
| 4 | I | 114 | ASN |
| 4 | I | 116 | ASP |
| 4 | I | 128 | SER |
| 4 | I | 129 | ASP |
| 4 | I | 146 | GLN |
| 4 | I | 160 | LEU |
| 4 | I | 163 | ARG |
| 4 | I | 167 | PHE |
| 4 | I | 177 | ASN |
| 4 | I | 180 | ASP |
| 4 | I | 185 | ASN |
| 4 | I | 190 | SER |
| 4 | I | 194 | GLU |
| 5 | J | 1 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | J | 4 | VAL |
| 5 | J | 9 | ARG |
| 5 | J | 12 | ILE |
| 5 | J | 17 | LYS |
| 5 | J | 18 | LYS |
| 5 | J | 19 | LEU |
| 5 | J | 25 | GLN |
| 5 | J | 37 | GLN |
| 5 | J | 55 | THR |
| 5 | J | 56 | ASP |
| 5 | J | 79 | GLU |
| 5 | J | 101 | TYR |
| 5 | J | 102 | PHE |
| 5 | J | 108 | LEU |
| 5 | J | 115 | LYS |
| 5 | J | 135 | THR |
| 5 | J | 154 | LEU |
| 5 | J | 167 | VAL |
| 5 | J | 181 | ASN |
| 5 | J | 182 | ASP |
| 5 | J | 190 | ARG |
| 5 | J | 205 | PHE |
| 5 | J | 206 | ARG |
| 5 | J | 215 | SER |
| 5 | J | 217 | ASN |
| 5 | J | 218 | ASP |
| 5 | J | 230 | GLN |
| 5 | J | 232 | VAL |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 32 | GLN |
| 1 | A | 43 | GLN |
| 1 | A | 77 | ASN |
| 1 | A | 86 | ASN |
| 1 | A | 114 | HIS |
| 1 | A | 141 | GLN |
| 1 | A | 155 | GLN |
| 1 | A | 156 | GLN |
| 1 | A | 180 | GLN |
| 1 | A | 188 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 192 | HIS |
| 1 | A | 218 | GLN |
| 1 | A | 255 | GLN |
| 2 | B | 8 | GLN |
| 2 | B | 24 | ASN |
| 2 | B | 51 | HIS |
| 2 | B | 83 | ASN |
| 2 | B | 84 | HIS |
| 4 | D | 6 | GLN |
| 4 | D | 64 | GLN |
| 4 | D | 170 | ASN |
| 4 | D | 185 | ASN |
| 4 | D | 188 | ASN |
| 5 | E | 51 | ASN |
| 5 | E | 73 | ASN |
| 5 | E | 84 | ASN |
| 5 | E | 159 | ASN |
| 5 | E | 199 | GLN |
| 5 | E | 203 | ASN |
| 5 | E | 208 | GLN |
| 5 | E | 217 | ASN |
| 1 | F | 32 | GLN |
| 1 | F | 43 | GLN |
| 1 | F | 86 | ASN |
| 1 | F | 115 | GLN |
| 1 | F | 141 | GLN |
| 1 | F | 155 | GLN |
| 1 | F | 156 | GLN |
| 1 | F | 174 | ASN |
| 1 | F | 188 | HIS |
| 1 | F | 191 | HIS |
| 1 | F | 255 | GLN |
| 1 | F | 260 | HIS |
| 2 | G | 2 | GLN |
| 2 | G | 13 | HIS |
| 2 | G | 21 | ASN |
| 2 | G | 24 | ASN |
| 2 | G | 31 | HIS |
| 4 | I | 6 | GLN |
| 4 | I | 53 | ASN |
| 4 | I | 64 | GLN |
| 4 | I | 70 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | I | 80 | GLN |
| 4 | I | 93 | ASN |
| 4 | I | 113 | GLN |
| 4 | I | 114 | ASN |
| 4 | I | 177 | ASN |
| 4 | I | 185 | ASN |
| 4 | I | 188 | ASN |
| 4 | I | 189 | ASN |
| 5 | J | 37 | GLN |
| 5 | J | 98 | HIS |
| 5 | J | 151 | HIS |
| 5 | J | 159 | ASN |
| 5 | J | 181 | ASN |
| 5 | J | 200 | ASN |
| 5 | J | 208 | GLN |
| 5 | J | 210 | GLN |
| 5 | J | 217 | ASN |
| 5 | J | 230 | GLN |

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | A | 274/275 (99%) | 0.02 | 9 (3%) 47 46 | 36, 69, 105, 120 | 0 |
| 1 | F | 274/275 (99%) | -0.16 | 3 (1%) 80 81 | 33, 67, 86, 91 | 0 |
| 2 | B | 99/100 (99%) | 0.02 | 2 (2%) 65 66 | 53, 68, 93, 97 | 0 |
| 2 | G | 99/100 (99%) | 0.25 | 5 (5%) 29 27 | 49, 79, 96, 101 | 0 |
| 3 | C | 10/10 (100%) | -0.46 | 0 100 100 | 44, 48, 56, 57 | 0 |
| 3 | H | 10/10 (100%) | -0.16 | 0 100 100 | 34, 40, 59, 64 | 0 |
| 4 | D | 199/205 (97%) | 0.06 | 3 (1%) 74 75 | 32, 61, 97, 115 | 0 |
| 4 | I | 199/205 (97%) | 0.09 | 5 (2%) 58 58 | 20, 64, 102, 119 | 0 |
| 5 | E | 241/242 (99%) | -0.27 | 0 100 100 | 35, 64, 81, 92 | 0 |
| 5 | J | 241/242 (99%) | -0.25 | 0 100 100 | 29, 62, 84, 94 | 0 |
| All | All | 1646/1664 (98%) | -0.07 | 27 (1%) 72 73 | 20, 66, 96, 120 | 0 |

All (27) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4 | I | 164 | SER | 5.2 |
| 4 | D | 131 | SER | 4.8 |
| 4 | I | 165 | MET | 4.5 |
| 1 | A | 199 | ALA | 4.4 |
| 1 | A | 215 | LEU | 3.9 |
| 1 | A | 185 | PRO | 3.8 |
| 4 | D | 4 | VAL | 3.7 |
| 1 | A | 201 | LEU | 3.3 |
| 4 | D | 5 | GLU | 3.2 |
| 1 | A | 214 | THR | 3.0 |
| 4 | I | 4 | VAL | 2.8 |
| 1 | F | 257 | TYR | 2.7 |
| 1 | A | 112 | GLY | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 99 | PHE | 2.7 |
| 2 | B | 15 | ALA | 2.6 |
| 2 | G | 23 | LEU | 2.6 |
| 1 | A | 274 | TRP | 2.5 |
| 2 | G | 15 | ALA | 2.4 |
| 2 | G | 80 | CYS | 2.4 |
| 1 | F | 247 | VAL | 2.3 |
| 1 | F | 126 | LEU | 2.2 |
| 2 | G | 52 | SER | 2.2 |
| 4 | I | 6 | GLN | 2.1 |
| 2 | G | 14 | PRO | 2.1 |
| 1 | A | 187 | THR | 2.0 |
| 4 | I | 72 | VAL | 2.0 |
| 2 | B | 46 | ILE | 2.0 |

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.