

Full wwPDB X-ray Structure Validation Report (i)

Aug 15, 2023 – 01:00 AM EDT

| PDB ID | : | 1QZX |
|--------------|---|---|
| Title | : | Crystal structure of the complete core of archaeal SRP and implications for |
| | | inter-domain communication |
| Authors | : | Rosendal, K.R.; Wild, K.; Montoya, G.; Sinning, I. |
| Deposited on | : | 2003-09-18 |
| Resolution | : | 4.00 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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

| MolProbity | : | 4.02b-467 |
|--------------------------------|---|--|
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.35 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.35 |

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 4.00 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.



| Motria | Whole archive | Similar resolution | | |
|-----------------------|----------------------|---|--|--|
| | $(\# {\rm Entries})$ | $(\# { m Entries}, { m resolution} { m range}({ m \AA}))$ | | |
| R _{free} | 130704 | 1087 (4.30-3.70) | | |
| Clashscore | 141614 | 1148 (4.30-3.70) | | |
| Ramachandran outliers | 138981 | 1108 (4.30-3.70) | | |
| Sidechain outliers | 138945 | 1099 (4.30-3.70) | | |

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

| Mol | Chain | Length | | Quality of chain | |
|-----|-------|--------|-----|------------------|--------|
| 1 | А | 440 | 21% | 63% | 11% •• |
| 1 | В | 440 | 22% | 62% | 11% •• |



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2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6698 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.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace | |
|-----|-------|----------|-------|------|-----|-----|--------------|---------|-------|---|
| 1 | Δ | 495 | Total | С | Ν | 0 | \mathbf{S} | 0 | 0 | 0 |
| | 1 A | 420 | 3349 | 2142 | 565 | 628 | 14 | 0 | 0 | 0 |
| 1 | р | 495 | Total | С | Ν | 0 | S | 0 | 0 | 0 |
| I D | 420 | 3349 | 2142 | 565 | 628 | 14 | 0 | 0 | U | |

• Molecule 1 is a protein called Signal recognition 54 kDa protein.

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| А | -7 | MET | - | expression tag | UNP Q97ZE7 |
| A | -6 | GLY | - | expression tag | UNP Q97ZE7 |
| А | -5 | HIS | - | expression tag | UNP Q97ZE7 |
| A | -4 | HIS | - | expression tag | UNP Q97ZE7 |
| A | -3 | HIS | - | expression tag | UNP Q97ZE7 |
| A | -2 | HIS | - | expression tag | UNP Q97ZE7 |
| A | -1 | HIS | - | expression tag | UNP Q97ZE7 |
| A | 0 | HIS | - | expression tag | UNP Q97ZE7 |
| В | -7 | MET | - | expression tag | UNP Q97ZE7 |
| В | -6 | GLY | - | expression tag | UNP Q97ZE7 |
| В | -5 | HIS | - | expression tag | UNP Q97ZE7 |
| В | -4 | HIS | - | expression tag | UNP Q97ZE7 |
| В | -3 | HIS | - | expression tag | UNP Q97ZE7 |
| В | -2 | HIS | - | expression tag | UNP Q97ZE7 |
| В | -1 | HIS | - | expression tag | UNP Q97ZE7 |
| B | 0 | HIS | _ | expression tag | UNP Q97ZE7 |

There are 16 discrepancies between the modelled and reference sequences:



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: Signal recognition 54 kDa protein

 \bullet Molecule 1: Signal recognition 54 kDa protein









4 Data and refinement statistics (i)

| Property | Value | Source |
|--|---|-----------|
| Space group | I 4 | Depositor |
| Cell constants | 197.91Å 197.91 Å 64.31 Å | Deresiter |
| a, b, c, α , β , γ | 90.00° 90.00° 90.00° | Depositor |
| $\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$ | 40.00 - 4.00 | Depositor |
| Resolution (A) | 38.81 - 4.00 | EDS |
| % Data completeness | 89.0 (40.00-4.00) | Depositor |
| (in resolution range) | 97.9(38.81-4.00) | EDS |
| R _{merge} | (Not available) | Depositor |
| R _{sym} | 0.08 | Depositor |
| $< I/\sigma(I) > 1$ | 2.70 (at 3.99Å) | Xtriage |
| Refinement program | CNS 1.1 | Depositor |
| D D | 0.313 , 0.383 | Depositor |
| Λ, Λ_{free} | 0.404 , 0.403 | DCC |
| R_{free} test set | 725 reflections (6.88%) | wwPDB-VP |
| Wilson B-factor $(Å^2)$ | 171.1 | Xtriage |
| Anisotropy | 0.085 | Xtriage |
| Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$ | 0.34, 26.6 | EDS |
| L-test for twinning ² | $< L > = 0.45, < L^2 > = 0.28$ | Xtriage |
| Estimated twinning fraction | 0.428 for -k,-h,-l | Xtriage |
| F_o, F_c correlation | 0.82 | EDS |
| Total number of atoms | 6698 | wwPDB-VP |
| Average B, all atoms $(Å^2)$ | 84.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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).

| Mal | Chain | Bo | nd lengths | Bond angles | | |
|-----|-------|------|----------------|-------------|---------------|--|
| | | RMSZ | # Z > 5 | RMSZ | # Z > 5 | |
| 1 | А | 0.71 | 5/3399~(0.1%) | 0.88 | 4/4569~(0.1%) | |
| 1 | В | 0.71 | 5/3399~(0.1%) | 0.88 | 4/4569~(0.1%) | |
| All | All | 0.71 | 10/6798~(0.1%) | 0.88 | 8/9138~(0.1%) | |

All (10) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | $\operatorname{Observed}(\operatorname{\AA})$ | $\operatorname{Ideal}(\operatorname{\AA})$ |
|-----|-------|-----|------|---------|-------|---|--|
| 1 | А | 361 | THR | CB-CG2 | -6.78 | 1.29 | 1.52 |
| 1 | В | 361 | THR | CB-CG2 | -6.78 | 1.29 | 1.52 |
| 1 | В | 227 | TYR | CD2-CE2 | -5.99 | 1.30 | 1.39 |
| 1 | А | 227 | TYR | CD2-CE2 | -5.96 | 1.30 | 1.39 |
| 1 | А | 361 | THR | CA-CB | 5.92 | 1.68 | 1.53 |
| 1 | В | 361 | THR | CA-CB | 5.91 | 1.68 | 1.53 |
| 1 | В | 360 | PRO | N-CD | 5.33 | 1.55 | 1.47 |
| 1 | А | 360 | PRO | N-CD | 5.33 | 1.55 | 1.47 |
| 1 | А | 360 | PRO | C-N | -5.15 | 1.22 | 1.34 |
| 1 | В | 360 | PRO | C-N | -5.13 | 1.22 | 1.34 |

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|-----|------|----------|-------|------------------|---------------|
| 1 | А | 292 | LEU | CA-CB-CG | -5.79 | 101.99 | 115.30 |
| 1 | В | 292 | LEU | CA-CB-CG | -5.77 | 102.03 | 115.30 |
| 1 | В | 361 | THR | N-CA-CB | 5.21 | 120.20 | 110.30 |
| 1 | А | 361 | THR | N-CA-CB | 5.20 | 120.19 | 110.30 |
| 1 | В | 332 | VAL | N-CA-C | -5.16 | 97.06 | 111.00 |
| 1 | А | 332 | VAL | N-CA-C | -5.16 | 97.07 | 111.00 |
| 1 | В | 359 | LEU | CB-CA-C | 5.02 | 119.74 | 110.20 |
| 1 | A | 359 | LEU | CB-CA-C | 5.02 | 119.74 | 110.20 |

There are no chirality outliers.

There are no planarity outliers.



5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | А | 3349 | 0 | 3486 | 713 | 43 |
| 1 | В | 3349 | 0 | 3486 | 708 | 43 |
| All | All | 6698 | 0 | 6972 | 1324 | 43 |

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 97.

All (1324) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom 1 | Atom 2 | Interatomic | Clash |
|------------------|------------------|--------------|-------------|
| Atom-1 | Atom-2 | distance (Å) | overlap (Å) |
| 1:B:362:PRO:HD3 | 1:B:367:LEU:CD2 | 1.43 | 1.47 |
| 1:B:190:HIS:CD2 | 1:B:197:LYS:HD2 | 1.49 | 1.45 |
| 1:A:190:HIS:CD2 | 1:A:197:LYS:HD2 | 1.49 | 1.44 |
| 1:A:362:PRO:HD3 | 1:A:367:LEU:CD2 | 1.43 | 1.43 |
| 1:B:359:LEU:CG | 1:B:360:PRO:HD3 | 1.49 | 1.42 |
| 1:A:359:LEU:CG | 1:A:360:PRO:HD3 | 1.49 | 1.39 |
| 1:A:362:PRO:CD | 1:A:367:LEU:HD21 | 1.54 | 1.38 |
| 1:B:362:PRO:CD | 1:B:367:LEU:HD21 | 1.54 | 1.38 |
| 1:A:361:THR:HA | 1:A:367:LEU:CD1 | 1.54 | 1.36 |
| 1:A:385:THR:HG21 | 1:B:382:ASN:O | 1.25 | 1.35 |
| 1:A:382:ASN:O | 1:B:385:THR:HG21 | 1.27 | 1.34 |
| 1:B:361:THR:HA | 1:B:367:LEU:CD1 | 1.54 | 1.34 |
| 1:A:361:THR:CA | 1:A:367:LEU:HD11 | 1.62 | 1.28 |
| 1:B:361:THR:CA | 1:B:367:LEU:HD11 | 1.62 | 1.27 |
| 1:A:164:ILE:CD1 | 1:A:208:VAL:HG21 | 1.66 | 1.24 |
| 1:B:164:ILE:CD1 | 1:B:208:VAL:HG21 | 1.66 | 1.24 |
| 1:B:92:PRO:HB2 | 1:B:97:PHE:CE2 | 1.75 | 1.21 |
| 1:B:359:LEU:CD1 | 1:B:360:PRO:HD3 | 1.70 | 1.20 |
| 1:A:92:PRO:HB2 | 1:A:97:PHE:CE2 | 1.75 | 1.20 |
| 1:A:359:LEU:CD1 | 1:A:360:PRO:HD3 | 1.70 | 1.20 |
| 1:A:2:LEU:HD22 | 1:A:291:ILE:HG21 | 1.23 | 1.17 |
| 1:B:356:GLY:O | 1:B:357:ILE:HG13 | 1.47 | 1.14 |
| 1:B:164:ILE:HD11 | 1:B:208:VAL:HG21 | 1.20 | 1.13 |
| 1:A:190:HIS:CD2 | 1:A:197:LYS:CD | 2.31 | 1.13 |
| 1:B:359:LEU:HG | 1:B:360:PRO:HD3 | 1.15 | 1.13 |



| | louis page | Interatomic | Clash |
|------------------|------------------|--------------|-------------|
| Atom-1 | Atom-2 | distance (Å) | overlap (Å) |
| 1:A:359:LEU:HG | 1:A:360:PRO:HD3 | 1.15 | 1.13 |
| 1:B:190:HIS:CD2 | 1:B:197:LYS:CD | 2.31 | 1.13 |
| 1:B:194:GLU:HB3 | 1:B:197:LYS:CE | 1.80 | 1.11 |
| 1:A:129:LEU:HD13 | 1:A:143:LEU:HD21 | 1.29 | 1.11 |
| 1:A:194:GLU:HB3 | 1:A:197:LYS:CE | 1.80 | 1.11 |
| 1:B:2:LEU:HD22 | 1:B:291:ILE:HG21 | 1.23 | 1.11 |
| 1:B:17:THR:HG22 | 1:B:18:PRO:CD | 1.81 | 1.10 |
| 1:A:17:THR:HG22 | 1:A:18:PRO:CD | 1.82 | 1.10 |
| 1:A:356:GLY:O | 1:A:357:ILE:HG13 | 1.47 | 1.10 |
| 1:A:194:GLU:HB3 | 1:A:197:LYS:HE3 | 1.16 | 1.10 |
| 1:A:164:ILE:HD11 | 1:A:208:VAL:CG2 | 1.82 | 1.09 |
| 1:B:164:ILE:HD11 | 1:B:208:VAL:CG2 | 1.82 | 1.08 |
| 1:B:129:LEU:HD13 | 1:B:143:LEU:HD21 | 1.29 | 1.08 |
| 1:A:164:ILE:HD11 | 1:A:208:VAL:HG21 | 1.20 | 1.07 |
| 1:B:359:LEU:HG | 1:B:360:PRO:CD | 1.84 | 1.07 |
| 1:A:17:THR:CG2 | 1:A:18:PRO:HD2 | 1.83 | 1.07 |
| 1:A:359:LEU:HG | 1:A:360:PRO:CD | 1.84 | 1.07 |
| 1:A:126:LYS:HE3 | 1:B:364:GLU:OE2 | 1.54 | 1.07 |
| 1:B:17:THR:CG2 | 1:B:18:PRO:HD2 | 1.83 | 1.07 |
| 1:B:190:HIS:CG | 1:B:197:LYS:HD2 | 1.88 | 1.07 |
| 1:B:194:GLU:HB3 | 1:B:197:LYS:HE3 | 1.16 | 1.07 |
| 1:A:122:LYS:O | 1:B:359:LEU:HD13 | 1.55 | 1.06 |
| 1:A:190:HIS:CG | 1:A:197:LYS:HD2 | 1.88 | 1.06 |
| 1:B:409:LEU:HD13 | 1:B:413:GLU:OE1 | 1.56 | 1.06 |
| 1:B:157:GLU:HB3 | 1:B:160:ASN:ND2 | 1.70 | 1.06 |
| 1:A:364:GLU:OE2 | 1:B:126:LYS:HE3 | 1.56 | 1.05 |
| 1:A:157:GLU:HB3 | 1:A:160:ASN:ND2 | 1.69 | 1.05 |
| 1:A:409:LEU:HD13 | 1:A:413:GLU:OE1 | 1.56 | 1.05 |
| 1:B:378:LEU:HA | 1:B:381:LEU:HD12 | 1.39 | 1.05 |
| 1:A:348:VAL:O | 1:A:352:ILE:HG13 | 1.56 | 1.05 |
| 1:A:378:LEU:HA | 1:A:381:LEU:HD12 | 1.39 | 1.04 |
| 1:A:359:LEU:HD13 | 1:B:122:LYS:O | 1.57 | 1.04 |
| 1:B:194:GLU:CB | 1:B:197:LYS:HE3 | 1.87 | 1.04 |
| 1:B:348:VAL:O | 1:B:352:ILE:HG13 | 1.56 | 1.04 |
| 1:A:329:LEU:HD22 | 1:A:392:PRO:HB3 | 1.40 | 1.03 |
| 1:A:385:THR:HG21 | 1:B:382:ASN:C | 1.79 | 1.03 |
| 1:A:194:GLU:CB | 1:A:197:LYS:HE3 | 1.87 | 1.03 |
| 1:A:359:LEU:CG | 1:A:360:PRO:CD | 2.36 | 1.03 |
| 1:B:157:GLU:HB3 | 1:B:160:ASN:HD22 | 1.18 | 1.03 |
| 1:A:382:ASN:C | 1:B:385:THR:HG21 | 1.79 | 1.02 |
| 1:B:303:LYS:O | 1:B:307:LEU:HG | 1.59 | 1.02 |



| | | Interatomic | Clash |
|------------------|------------------|-------------------------|-------------|
| Atom-1 | Atom-2 | distance (\AA) | overlap (Å) |
| 1:B:61:PRO:HD2 | 1:B:64:LEU:HD12 | 1.40 | 1.02 |
| 1:B:359:LEU:CG | 1:B:360:PRO:CD | 2.36 | 1.02 |
| 1:A:303:LYS:O | 1:A:307:LEU:HG | 1.59 | 1.02 |
| 1:A:157:GLU:HB3 | 1:A:160:ASN:HD22 | 1.18 | 1.01 |
| 1:B:361:THR:HG23 | 1:B:362:PRO:HD2 | 1.40 | 1.01 |
| 1:B:383:SER:HB3 | 1:B:403:ILE:HG23 | 1.41 | 1.01 |
| 1:A:383:SER:HB3 | 1:A:403:ILE:HG23 | 1.41 | 1.00 |
| 1:A:402:ARG:HD3 | 1:B:402:ARG:HD3 | 1.37 | 1.00 |
| 1:B:378:LEU:HA | 1:B:381:LEU:CD1 | 1.91 | 1.00 |
| 1:A:378:LEU:HA | 1:A:381:LEU:CD1 | 1.91 | 0.99 |
| 1:A:359:LEU:HD12 | 1:A:360:PRO:HD3 | 1.42 | 0.99 |
| 1:A:361:THR:HG23 | 1:A:362:PRO:HD2 | 1.40 | 0.99 |
| 1:A:61:PRO:HD2 | 1:A:64:LEU:HD12 | 1.40 | 0.99 |
| 1:B:329:LEU:HD22 | 1:B:392:PRO:HB3 | 1.40 | 0.99 |
| 1:B:359:LEU:HD12 | 1:B:360:PRO:HD3 | 1.42 | 0.98 |
| 1:A:384:MET:O | 1:B:385:THR:HA | 1.64 | 0.97 |
| 1:A:385:THR:HA | 1:B:384:MET:O | 1.64 | 0.97 |
| 1:A:385:THR:CG2 | 1:B:382:ASN:O | 2.11 | 0.97 |
| 1:A:382:ASN:O | 1:B:385:THR:CG2 | 2.12 | 0.97 |
| 1:A:1:MET:SD | 1:A:37:SER:CB | 2.55 | 0.95 |
| 1:B:164:ILE:CG1 | 1:B:208:VAL:HG21 | 1.97 | 0.95 |
| 1:B:1:MET:SD | 1:B:37:SER:CB | 2.55 | 0.95 |
| 1:A:164:ILE:CG1 | 1:A:208:VAL:HG21 | 1.97 | 0.95 |
| 1:A:301:LEU:HG | 1:A:305:LYS:HD2 | 1.49 | 0.95 |
| 1:A:397:LYS:HA | 1:A:400:MET:HE3 | 1.49 | 0.94 |
| 1:A:335:GLN:O | 1:A:339:LEU:HD22 | 1.66 | 0.94 |
| 1:B:75:TYR:CD2 | 1:B:297:ILE:HG23 | 2.02 | 0.94 |
| 1:B:94:LYS:N | 1:B:97:PHE:CZ | 2.36 | 0.94 |
| 1:A:75:TYR:CD2 | 1:A:297:ILE:HG23 | 2.02 | 0.94 |
| 1:A:72:SER:HB2 | 1:A:300:ILE:HD11 | 1.48 | 0.94 |
| 1:B:301:LEU:HG | 1:B:305:LYS:HD2 | 1.49 | 0.94 |
| 1:A:94:LYS:N | 1:A:97:PHE:CZ | 2.36 | 0.93 |
| 1:A:15:GLY:HA2 | 1:A:67:LYS:NZ | 1.83 | 0.93 |
| 1:B:72:SER:HB2 | 1:B:300:ILE:HD11 | 1.48 | 0.93 |
| 1:B:335:GLN:O | 1:B:339:LEU:HD22 | 1.66 | 0.93 |
| 1:B:15:GLY:HA2 | 1:B:67:LYS:NZ | 1.83 | 0.93 |
| 1:B:200:GLU:CD | 1:B:201:GLU:N | 2.23 | 0.93 |
| 1:B:397:LYS:HA | 1:B:400:MET:HE3 | 1.49 | 0.92 |
| 1:B:197:LYS:O | 1:B:200:GLU:OE1 | 1.87 | 0.92 |
| 1:A:200:GLU:CD | 1:A:201:GLU:N | 2.23 | 0.92 |
| 1:B:157:GLU:CB | 1:B:160:ASN:HD22 | 1.82 | 0.92 |



| | | Interatomic | Clash |
|------------------|------------------|--------------|-------------|
| Atom-1 | Atom-2 | distance (Å) | overlap (Å) |
| 1:A:197:LYS:O | 1:A:200:GLU:OE1 | 1.87 | 0.92 |
| 1:B:15:GLY:HA2 | 1:B:67:LYS:HZ3 | 1.34 | 0.92 |
| 1:B:297:ILE:O | 1:B:300:ILE:HB | 1.69 | 0.92 |
| 1:A:327:LEU:HD12 | 1:A:391:ASN:OD1 | 1.70 | 0.91 |
| 1:A:297:ILE:O | 1:A:300:ILE:HB | 1.69 | 0.91 |
| 1:B:221:SER:HA | 1:B:250:THR:HG21 | 1.53 | 0.91 |
| 1:A:221:SER:HA | 1:A:250:THR:HG21 | 1.53 | 0.91 |
| 1:A:349:LEU:HA | 1:A:352:ILE:HB | 1.53 | 0.91 |
| 1:B:327:LEU:HD12 | 1:B:391:ASN:OD1 | 1.70 | 0.91 |
| 1:B:295:GLY:HA2 | 1:B:298:GLU:HB2 | 1.52 | 0.91 |
| 1:A:157:GLU:CB | 1:A:160:ASN:HD22 | 1.82 | 0.91 |
| 1:B:317:MET:SD | 1:B:328:THR:OG1 | 2.29 | 0.91 |
| 1:B:362:PRO:CD | 1:B:367:LEU:CD2 | 2.27 | 0.91 |
| 1:A:331:ASP:O | 1:A:332:VAL:HG23 | 1.71 | 0.90 |
| 1:A:301:LEU:HD11 | 1:A:305:LYS:HE3 | 1.51 | 0.90 |
| 1:A:317:MET:SD | 1:A:328:THR:OG1 | 2.29 | 0.90 |
| 1:B:301:LEU:HD11 | 1:B:305:LYS:HE3 | 1.51 | 0.90 |
| 1:A:281:THR:HG21 | 1:B:315:LYS:NZ | 1.86 | 0.90 |
| 1:A:295:GLY:HA2 | 1:A:298:GLU:HB2 | 1.52 | 0.90 |
| 1:B:361:THR:OG1 | 1:B:367:LEU:HG | 1.70 | 0.90 |
| 1:B:331:ASP:O | 1:B:332:VAL:HG23 | 1.71 | 0.90 |
| 1:B:349:LEU:HA | 1:B:352:ILE:HB | 1.53 | 0.90 |
| 1:A:85:ASP:CG | 1:A:285:LYS:HD3 | 1.92 | 0.90 |
| 1:A:2:LEU:HD22 | 1:A:291:ILE:HD13 | 1.51 | 0.89 |
| 1:B:2:LEU:HD22 | 1:B:291:ILE:HD13 | 1.51 | 0.89 |
| 1:B:85:ASP:CG | 1:B:285:LYS:HD3 | 1.92 | 0.89 |
| 1:A:361:THR:OG1 | 1:A:367:LEU:HG | 1.70 | 0.89 |
| 1:A:315:LYS:NZ | 1:B:281:THR:HG21 | 1.87 | 0.89 |
| 1:A:362:PRO:CD | 1:A:367:LEU:CD2 | 2.27 | 0.89 |
| 1:A:329:LEU:CD2 | 1:A:392:PRO:HB3 | 2.03 | 0.89 |
| 1:B:329:LEU:CD2 | 1:B:392:PRO:HB3 | 2.03 | 0.89 |
| 1:B:17:THR:HG22 | 1:B:18:PRO:HD2 | 0.92 | 0.88 |
| 1:B:1:MET:SD | 1:B:37:SER:HB3 | 2.15 | 0.87 |
| 1:B:118:TYR:HE2 | 1:B:277:ASP:HB3 | 1.40 | 0.87 |
| 1:A:167:ALA:HB1 | 1:A:209:LEU:HD11 | 1.57 | 0.87 |
| 1:A:118:TYR:HE2 | 1:A:277:ASP:HB3 | 1.40 | 0.87 |
| 1:A:150:ILE:HG13 | 1:A:152:VAL:HG23 | 1.56 | 0.87 |
| 1:A:359:LEU:CB | 1:A:360:PRO:CD | 2.53 | 0.87 |
| 1:B:167:ALA:HB1 | 1:B:209:LEU:HD11 | 1.57 | 0.87 |
| 1:A:86:LYS:HE2 | 1:A:266:THR:HG23 | 1.56 | 0.86 |
| 1:B:359:LEU:CB | 1:B:360:PRO:CD | 2.53 | 0.86 |



| | A L O | Interatomic | Clash |
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| Atom-1 | Atom-2 | distance (\AA) | overlap (Å) |
| 1:B:216:LEU:HB3 | 1:B:242:VAL:HG22 | 1.56 | 0.86 |
| 1:A:2:LEU:CD2 | 1:A:291:ILE:HG21 | 2.06 | 0.86 |
| 1:A:383:SER:CB | 1:A:403:ILE:HG23 | 2.06 | 0.86 |
| 1:B:150:ILE:HG13 | 1:B:152:VAL:HG23 | 1.56 | 0.86 |
| 1:A:216:LEU:HB3 | 1:A:242:VAL:HG22 | 1.56 | 0.86 |
| 1:A:359:LEU:HD12 | 1:A:360:PRO:CD | 2.06 | 0.86 |
| 1:B:2:LEU:HD22 | 1:B:291:ILE:CG2 | 2.05 | 0.85 |
| 1:B:86:LYS:HE2 | 1:B:266:THR:HG23 | 1.56 | 0.85 |
| 1:B:383:SER:CB | 1:B:403:ILE:HG23 | 2.06 | 0.85 |
| 1:B:359:LEU:HD12 | 1:B:360:PRO:CD | 2.06 | 0.85 |
| 1:A:1:MET:SD | 1:A:37:SER:HB3 | 2.15 | 0.85 |
| 1:A:402:ARG:CZ | 1:B:402:ARG:HG2 | 2.07 | 0.85 |
| 1:B:381:LEU:N | 1:B:381:LEU:HD23 | 1.92 | 0.85 |
| 1:B:422:ASN:O | 1:B:426:ARG:HG3 | 1.77 | 0.84 |
| 1:A:2:LEU:HD22 | 1:A:291:ILE:CG2 | 2.05 | 0.84 |
| 1:A:95:LEU:HD23 | 1:A:97:PHE:CE1 | 2.12 | 0.84 |
| 1:A:402:ARG:HG2 | 1:B:402:ARG:CZ | 2.07 | 0.84 |
| 1:B:372:GLU:O | 1:B:374:ILE:N | 2.10 | 0.84 |
| 1:A:123:ARG:CZ | 1:B:318:GLU:OE1 | 2.26 | 0.84 |
| 1:A:381:LEU:N | 1:A:381:LEU:HD23 | 1.92 | 0.84 |
| 1:A:422:ASN:O | 1:A:426:ARG:HG3 | 1.77 | 0.84 |
| 1:B:95:LEU:HD23 | 1:B:97:PHE:CE1 | 2.12 | 0.84 |
| 1:B:417:LEU:HB3 | 1:B:421:TYR:HE1 | 1.41 | 0.84 |
| 1:A:310:TYR:OH | 1:A:355:LEU:HD23 | 1.78 | 0.84 |
| 1:A:69:TRP:O | 1:A:73:ILE:HG13 | 1.78 | 0.84 |
| 1:A:417:LEU:HB3 | 1:A:421:TYR:HE1 | 1.41 | 0.84 |
| 1:A:17:THR:HG22 | 1:A:18:PRO:HD2 | 0.92 | 0.83 |
| 1:A:200:GLU:OE2 | 1:A:201:GLU:HA | 1.78 | 0.83 |
| 1:A:164:ILE:HG23 | 1:A:165:GLU:N | 1.94 | 0.83 |
| 1:A:372:GLU:O | 1:A:374:ILE:N | 2.10 | 0.83 |
| 1:B:69:TRP:O | 1:B:73:ILE:HG13 | 1.78 | 0.83 |
| 1:B:164:ILE:HG23 | 1:B:165:GLU:N | 1.94 | 0.83 |
| 1:B:2:LEU:CD2 | 1:B:291:ILE:HG21 | 2.06 | 0.83 |
| 1:A:372:GLU:C | 1:A:374:ILE:H | 1.78 | 0.83 |
| 1:B:310:TYR:OH | 1:B:355:LEU:HD23 | 1.78 | 0.83 |
| 1:A:92:PRO:HB2 | 1:A:97:PHE:CZ | 2.14 | 0.82 |
| 1:A:318:GLU:OE1 | 1:B:123:ARG:CZ | 2.26 | 0.82 |
| 1:B:92:PRO:HB2 | 1:B:97:PHE:CZ | 2.14 | 0.82 |
| 1:B:418:LEU:HA | 1:B:421:TYR:HD1 | 1.44 | 0.82 |
| 1:A:418:LEU:HA | 1:A:421:TYR:HD1 | 1.43 | 0.82 |
| 1:A:313:ILE:HD11 | 1:A:331:ASP:OD1 | 1.80 | 0.82 |



| | | Interatomic | Clash |
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| Atom-1 | Atom-2 | distance (Å) | overlap (Å) |
| 1:B:200:GLU:OE2 | 1:B:201:GLU:HA | 1.78 | 0.81 |
| 1:B:380:ALA:HA | 1:B:383:SER:HB2 | 1.61 | 0.81 |
| 1:A:55:LEU:HD13 | 1:A:55:LEU:O | 1.80 | 0.81 |
| 1:B:164:ILE:CD1 | 1:B:208:VAL:CG2 | 2.51 | 0.81 |
| 1:A:15:GLY:HA2 | 1:A:67:LYS:HZ3 | 1.40 | 0.81 |
| 1:A:2:LEU:CD2 | 1:A:291:ILE:HD13 | 2.11 | 0.81 |
| 1:B:55:LEU:HD13 | 1:B:55:LEU:O | 1.80 | 0.81 |
| 1:B:100:MET:HE3 | 1:B:205:MET:O | 1.80 | 0.81 |
| 1:A:380:ALA:HA | 1:A:383:SER:HB2 | 1.61 | 0.81 |
| 1:B:2:LEU:CD2 | 1:B:291:ILE:HD13 | 2.11 | 0.81 |
| 1:B:75:TYR:HD2 | 1:B:297:ILE:HG23 | 1.45 | 0.81 |
| 1:A:378:LEU:O | 1:A:381:LEU:HG | 1.81 | 0.80 |
| 1:A:176:LYS:O | 1:A:178:LYS:N | 2.14 | 0.80 |
| 1:B:176:LYS:O | 1:B:178:LYS:N | 2.15 | 0.80 |
| 1:A:6:ARG:HG3 | 1:A:292:LEU:HD23 | 1.62 | 0.80 |
| 1:B:372:GLU:C | 1:B:374:ILE:H | 1.78 | 0.80 |
| 1:B:313:ILE:HD11 | 1:B:331:ASP:OD1 | 1.80 | 0.80 |
| 1:B:359:LEU:CB | 1:B:360:PRO:HD3 | 2.11 | 0.80 |
| 1:A:75:TYR:HD2 | 1:A:297:ILE:HG23 | 1.45 | 0.80 |
| 1:B:378:LEU:O | 1:B:381:LEU:HG | 1.81 | 0.80 |
| 1:B:394:ILE:HG22 | 1:B:399:ARG:NH1 | 1.96 | 0.80 |
| 1:B:6:ARG:HG3 | 1:B:292:LEU:HD23 | 1.62 | 0.80 |
| 1:B:346:SER:O | 1:B:348:VAL:N | 2.15 | 0.80 |
| 1:A:359:LEU:CB | 1:A:360:PRO:HD3 | 2.11 | 0.80 |
| 1:A:346:SER:O | 1:A:348:VAL:N | 2.15 | 0.80 |
| 1:A:129:LEU:CD1 | 1:A:143:LEU:HD21 | 2.11 | 0.80 |
| 1:A:163:PRO:HG2 | 1:A:164:ILE:H | 1.47 | 0.79 |
| 1:B:199:LEU:HD23 | 1:B:202:MET:SD | 2.23 | 0.79 |
| 1:B:94:LYS:N | 1:B:97:PHE:HZ | 1.81 | 0.79 |
| 1:A:417:LEU:HB3 | 1:A:421:TYR:CE1 | 2.18 | 0.79 |
| 1:A:199:LEU:HD23 | 1:A:202:MET:SD | 2.23 | 0.78 |
| 1:B:272:THR:HG21 | 1:B:280:GLU:OE2 | 1.82 | 0.78 |
| 1:B:417:LEU:HB3 | 1:B:421:TYR:CE1 | 2.18 | 0.78 |
| 1:A:172:ASP:O | 1:A:176:LYS:HG3 | 1.83 | 0.78 |
| 1:A:272:THR:HG21 | 1:A:280:GLU:OE2 | 1.82 | 0.78 |
| 1:B:172:ASP:O | 1:B:176:LYS:HG3 | 1.83 | 0.78 |
| 1:A:94:LYS:N | 1:A:97:PHE:HZ | 1.81 | 0.78 |
| 1:A:100:MET:HE3 | 1:A:205:MET:O | 1.83 | 0.78 |
| 1:A:394:ILE:HG22 | 1:A:399:ARG:NH1 | 1.96 | 0.78 |
| 1:B:129:LEU:CD1 | 1:B:143:LEU:HD21 | 2.11 | 0.78 |
| 1:A:124:GLY:HA3 | 1:B:359:LEU:CA | 2.14 | 0.78 |



| | | Interatomic | Clash |
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| Atom-1 | Atom-2 | distance $(Å)$ | overlap (Å) |
| 1:A:234:HIS:CE1 | 1:A:265:ALA:CB | 2.67 | 0.78 |
| 1:B:82:PHE:C | 1:B:261:VAL:HG21 | 2.04 | 0.78 |
| 1:B:163:PRO:HG2 | 1:B:164:ILE:H | 1.47 | 0.78 |
| 1:A:402:ARG:HD3 | 1:B:402:ARG:CD | 2.14 | 0.78 |
| 1:A:384:MET:HE2 | 1:A:389:LEU:HD23 | 1.66 | 0.77 |
| 1:B:234:HIS:CE1 | 1:B:265:ALA:CB | 2.67 | 0.77 |
| 1:A:82:PHE:C | 1:A:261:VAL:HG21 | 2.04 | 0.77 |
| 1:A:299:SER:O | 1:A:303:LYS:HG2 | 1.85 | 0.77 |
| 1:A:222:ILE:HG21 | 1:A:226:ALA:HB2 | 1.68 | 0.76 |
| 1:A:396:ASP:O | 1:A:400:MET:HG3 | 1.86 | 0.76 |
| 1:B:299:SER:O | 1:B:303:LYS:HG2 | 1.85 | 0.76 |
| 1:B:222:ILE:HG21 | 1:B:226:ALA:HB2 | 1.67 | 0.76 |
| 1:A:402:ARG:CD | 1:B:402:ARG:HD3 | 2.14 | 0.76 |
| 1:B:194:GLU:HB3 | 1:B:197:LYS:CD | 2.16 | 0.76 |
| 1:A:87:GLU:HG3 | 1:B:315:LYS:HZ1 | 1.50 | 0.76 |
| 1:B:396:ASP:O | 1:B:400:MET:HG3 | 1.86 | 0.76 |
| 1:A:124:GLY:HA3 | 1:B:359:LEU:HA | 1.68 | 0.76 |
| 1:A:361:THR:OG1 | 1:A:367:LEU:CG | 2.34 | 0.76 |
| 1:A:383:SER:O | 1:A:403:ILE:HG12 | 1.85 | 0.76 |
| 1:B:383:SER:O | 1:B:403:ILE:HG12 | 1.85 | 0.76 |
| 1:A:194:GLU:HB3 | 1:A:197:LYS:CD | 2.16 | 0.76 |
| 1:A:359:LEU:CA | 1:B:124:GLY:HA3 | 2.16 | 0.76 |
| 1:B:200:GLU:OE2 | 1:B:201:GLU:CA | 2.33 | 0.75 |
| 1:A:200:GLU:OE2 | 1:A:201:GLU:CA | 2.34 | 0.75 |
| 1:B:234:HIS:CE1 | 1:B:265:ALA:HB1 | 2.22 | 0.75 |
| 1:A:356:GLY:O | 1:A:357:ILE:CG1 | 2.32 | 0.75 |
| 1:A:234:HIS:CE1 | 1:A:265:ALA:HB1 | 2.22 | 0.75 |
| 1:A:329:LEU:CD1 | 1:A:421:TYR:HB3 | 2.17 | 0.75 |
| 1:A:402:ARG:HG2 | 1:B:402:ARG:NH2 | 2.02 | 0.75 |
| 1:B:361:THR:OG1 | 1:B:367:LEU:CG | 2.34 | 0.75 |
| 1:A:122:LYS:O | 1:B:359:LEU:CD1 | 2.33 | 0.74 |
| 1:B:92:PRO:HB2 | 1:B:97:PHE:CD2 | 2.22 | 0.74 |
| 1:B:222:ILE:CG2 | 1:B:226:ALA:HB2 | 2.17 | 0.74 |
| 1:B:335:GLN:HB3 | 1:B:355:LEU:HD22 | 1.70 | 0.74 |
| 1:A:335:GLN:HB3 | 1:A:355:LEU:HD22 | 1.70 | 0.74 |
| 1:A:359:LEU:HA | 1:B:124:GLY:HA3 | 1.68 | 0.74 |
| 1:A:382:ASN:CA | 1:B:385:THR:HG21 | 2.18 | 0.74 |
| 1:B:118:TYR:CE2 | 1:B:277:ASP:HB3 | 2.22 | 0.74 |
| 1:A:349:LEU:HD22 | 1:A:371:GLU:HG2 | 1.70 | 0.74 |
| 1:A:402:ARG:NH2 | 1:B:402:ARG:HG2 | 2.03 | 0.74 |
| 1:B:329:LEU:HD22 | 1:B:392:PRO:CB | 2.17 | 0.74 |



| | | Interatomic | Clash |
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| Atom-1 | Atom-2 | distance (Å) | overlap (Å) |
| 1:B:329:LEU:CD1 | 1:B:421:TYR:HB3 | 2.17 | 0.74 |
| 1:B:378:LEU:O | 1:B:380:ALA:O | 2.06 | 0.74 |
| 1:A:164:ILE:HG23 | 1:A:165:GLU:H | 1.50 | 0.74 |
| 1:A:118:TYR:CE2 | 1:A:277:ASP:HB3 | 2.22 | 0.74 |
| 1:A:222:ILE:CG2 | 1:A:226:ALA:HB2 | 2.17 | 0.74 |
| 1:A:92:PRO:HB2 | 1:A:97:PHE:CD2 | 2.22 | 0.74 |
| 1:A:384:MET:CE | 1:A:389:LEU:HD23 | 2.18 | 0.73 |
| 1:A:206:TYR:OH | 1:A:239:ILE:HD11 | 1.88 | 0.73 |
| 1:A:362:PRO:HD3 | 1:A:367:LEU:HD23 | 1.66 | 0.73 |
| 1:A:378:LEU:O | 1:A:380:ALA:O | 2.06 | 0.73 |
| 1:B:200:GLU:OE2 | 1:B:201:GLU:N | 2.22 | 0.73 |
| 1:A:382:ASN:HA | 1:B:385:THR:CG2 | 2.18 | 0.73 |
| 1:B:164:ILE:HG23 | 1:B:165:GLU:H | 1.50 | 0.73 |
| 1:A:385:THR:CG2 | 1:B:382:ASN:HA | 2.19 | 0.73 |
| 1:B:346:SER:C | 1:B:348:VAL:H | 1.92 | 0.73 |
| 1:A:346:SER:C | 1:A:348:VAL:H | 1.92 | 0.73 |
| 1:A:402:ARG:HB3 | 1:B:402:ARG:NH1 | 2.04 | 0.73 |
| 1:B:206:TYR:OH | 1:B:239:ILE:HD11 | 1.88 | 0.73 |
| 1:B:356:GLY:O | 1:B:357:ILE:CG1 | 2.31 | 0.73 |
| 1:A:373:LYS:HE3 | 1:A:377:TRP:CH2 | 2.24 | 0.73 |
| 1:A:385:THR:HG21 | 1:B:382:ASN:CA | 2.19 | 0.73 |
| 1:B:349:LEU:HD22 | 1:B:371:GLU:HG2 | 1.70 | 0.72 |
| 1:A:95:LEU:HD23 | 1:A:97:PHE:CD1 | 2.24 | 0.72 |
| 1:A:123:ARG:NH1 | 1:B:318:GLU:CD | 2.42 | 0.72 |
| 1:A:318:GLU:CD | 1:B:123:ARG:NH1 | 2.43 | 0.72 |
| 1:B:174:PHE:O | 1:B:179:MET:HB2 | 1.90 | 0.72 |
| 1:A:155:TYR:CD2 | 1:A:170:GLY:HA2 | 2.24 | 0.72 |
| 1:A:342:MET:O | 1:A:348:VAL:HG21 | 1.90 | 0.72 |
| 1:B:155:TYR:CD2 | 1:B:170:GLY:HA2 | 2.24 | 0.72 |
| 1:B:373:LYS:HE3 | 1:B:377:TRP:CH2 | 2.24 | 0.72 |
| 1:B:384:MET:HE2 | 1:B:389:LEU:HD23 | 1.69 | 0.72 |
| 1:B:383:SER:HB3 | 1:B:403:ILE:CG2 | 2.19 | 0.72 |
| 1:A:372:GLU:O | 1:A:374:ILE:HG22 | 1.88 | 0.72 |
| 1:B:95:LEU:HD23 | 1:B:97:PHE:CD1 | 2.24 | 0.72 |
| 1:A:281:THR:HG21 | 1:B:315:LYS:CE | 2.19 | 0.72 |
| 1:A:357:ILE:O | 1:A:358:MET:HB2 | 1.88 | 0.72 |
| 1:B:164:ILE:HG13 | 1:B:208:VAL:HG21 | 1.70 | 0.72 |
| 1:B:342:MET:O | 1:B:348:VAL:HG21 | 1.90 | 0.72 |
| 1:A:83:GLY:N | 1:A:261:VAL:HG11 | 2.05 | 0.72 |
| 1:B:234:HIS:NE2 | 1:B:265:ALA:HB2 | 2.04 | 0.72 |
| 1:B:372:GLU:O | 1:B:374:ILE:HG22 | 1.88 | 0.72 |



| | | Interatomic | Clash |
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| Atom-1 | Atom-2 | distance (Å) | overlap (Å) |
| 1:A:123:ARG:NH1 | 1:B:318:GLU:OE2 | 2.23 | 0.72 |
| 1:B:334:ALA:O | 1:B:337:ILE:HG22 | 1.90 | 0.72 |
| 1:A:200:GLU:OE2 | 1:A:201:GLU:N | 2.22 | 0.72 |
| 1:A:234:HIS:NE2 | 1:A:265:ALA:HB2 | 2.04 | 0.72 |
| 1:B:329:LEU:HD11 | 1:B:421:TYR:HB3 | 1.72 | 0.72 |
| 1:B:384:MET:CE | 1:B:389:LEU:HD23 | 2.18 | 0.72 |
| 1:B:362:PRO:HD3 | 1:B:367:LEU:HD23 | 1.66 | 0.71 |
| 1:A:329:LEU:HD11 | 1:A:421:TYR:HB3 | 1.72 | 0.71 |
| 1:A:42:LYS:O | 1:A:42:LYS:HD3 | 1.91 | 0.71 |
| 1:A:334:ALA:O | 1:A:337:ILE:HG22 | 1.90 | 0.71 |
| 1:A:164:ILE:HG13 | 1:A:208:VAL:HG21 | 1.70 | 0.71 |
| 1:B:357:ILE:O | 1:B:358:MET:HB2 | 1.88 | 0.71 |
| 1:A:301:LEU:HD21 | 1:A:305:LYS:NZ | 2.06 | 0.71 |
| 1:A:329:LEU:HD22 | 1:A:392:PRO:CB | 2.17 | 0.71 |
| 1:A:359:LEU:CD1 | 1:B:122:LYS:O | 2.35 | 0.71 |
| 1:A:169:LYS:O | 1:A:173:ILE:HG13 | 1.91 | 0.71 |
| 1:A:174:PHE:O | 1:A:179:MET:HB2 | 1.90 | 0.71 |
| 1:B:385:THR:HG22 | 1:B:386:TYR:N | 2.05 | 0.71 |
| 1:B:403:ILE:HG22 | 1:B:414:VAL:HG21 | 1.73 | 0.71 |
| 1:A:134:VAL:HA | 1:A:140:TYR:HE1 | 1.55 | 0.71 |
| 1:A:432:LYS:HE2 | 1:B:277:ASP:HB2 | 1.72 | 0.71 |
| 1:B:83:GLY:N | 1:B:261:VAL:HG11 | 2.05 | 0.71 |
| 1:B:134:VAL:HA | 1:B:140:TYR:HE1 | 1.55 | 0.71 |
| 1:A:318:GLU:OE2 | 1:B:123:ARG:NH1 | 2.24 | 0.70 |
| 1:B:355:LEU:O | 1:B:356:GLY:C | 2.29 | 0.70 |
| 1:A:403:ILE:HG22 | 1:A:414:VAL:HG21 | 1.73 | 0.70 |
| 1:A:355:LEU:O | 1:A:356:GLY:C | 2.30 | 0.70 |
| 1:A:402:ARG:NH1 | 1:B:402:ARG:HB3 | 2.05 | 0.70 |
| 1:A:402:ARG:CG | 1:B:402:ARG:CZ | 2.70 | 0.70 |
| 1:A:402:ARG:CZ | 1:B:402:ARG:CG | 2.70 | 0.70 |
| 1:A:63:VAL:O | 1:A:63:VAL:HG12 | 1.92 | 0.70 |
| 1:A:179:MET:CE | 1:A:179:MET:HA | 2.21 | 0.70 |
| 1:B:169:LYS:O | 1:B:173:ILE:HG13 | 1.91 | 0.70 |
| 1:B:301:LEU:O | 1:B:305:LYS:HD2 | 1.92 | 0.70 |
| 1:A:176:LYS:C | 1:A:178:LYS:H | 1.96 | 0.70 |
| 1:B:42:LYS:HD3 | 1:B:42:LYS:O | 1.91 | 0.70 |
| 1:A:200:GLU:CD | 1:A:200:GLU:C | 2.51 | 0.69 |
| 1:A:277:ASP:HB2 | 1:B:432:LYS:HE2 | 1.73 | 0.69 |
| 1:A:303:LYS:HG3 | 1:A:304:VAL:H | 1.57 | 0.69 |
| 1:A:315:LYS:HZ3 | 1:B:281:THR:HG21 | 1.55 | 0.69 |
| 1:B:303:LYS:HG3 | 1:B:304:VAL:H | 1.58 | 0.69 |



| | , and pagein | Interatomic | Clash |
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| Atom-1 | Atom-2 | distance (Å) | overlap (Å) |
| 1:A:385:THR:HG22 | 1:A:386:TYR:N | 2.05 | 0.69 |
| 1:B:136:ARG:HD3 | 1:B:139:ALA:HB2 | 1.74 | 0.69 |
| 1:B:200:GLU:CD | 1:B:200:GLU:C | 2.51 | 0.69 |
| 1:A:247:MET:CE | 1:A:270:ILE:HD11 | 2.23 | 0.69 |
| 1:A:301:LEU:O | 1:A:305:LYS:HD2 | 1.92 | 0.69 |
| 1:B:301:LEU:HD21 | 1:B:305:LYS:NZ | 2.06 | 0.69 |
| 1:B:397:LYS:CA | 1:B:400:MET:HE3 | 2.23 | 0.69 |
| 1:B:176:LYS:C | 1:B:178:LYS:H | 1.96 | 0.69 |
| 1:B:401:ARG:O | 1:B:405:GLU:HG2 | 1.92 | 0.69 |
| 1:A:315:LYS:CE | 1:B:281:THR:HG21 | 2.21 | 0.69 |
| 1:B:78:LEU:O | 1:B:81:LEU:HB3 | 1.93 | 0.69 |
| 1:B:179:MET:HA | 1:B:179:MET:CE | 2.21 | 0.69 |
| 1:B:310:TYR:HA | 1:B:335:GLN:HE22 | 1.57 | 0.69 |
| 1:B:384:MET:HA | 1:B:388:GLU:OE1 | 1.92 | 0.69 |
| 1:A:401:ARG:O | 1:A:405:GLU:HG2 | 1.92 | 0.69 |
| 1:B:361:THR:HG23 | 1:B:362:PRO:CD | 2.20 | 0.69 |
| 1:B:369:ILE:HG22 | 1:B:370:GLY:H | 1.58 | 0.69 |
| 1:A:78:LEU:O | 1:A:81:LEU:HB3 | 1.93 | 0.68 |
| 1:A:369:ILE:HG22 | 1:A:370:GLY:H | 1.58 | 0.68 |
| 1:A:300:ILE:O | 1:A:303:LYS:HG2 | 1.93 | 0.68 |
| 1:A:315:LYS:HZ1 | 1:B:87:GLU:HG3 | 1.57 | 0.68 |
| 1:A:384:MET:HA | 1:A:388:GLU:OE1 | 1.92 | 0.68 |
| 1:A:310:TYR:HA | 1:A:335:GLN:HE22 | 1.58 | 0.68 |
| 1:B:100:MET:CE | 1:B:205:MET:O | 2.42 | 0.68 |
| 1:B:235:GLN:O | 1:B:237:SER:N | 2.27 | 0.68 |
| 1:B:300:ILE:O | 1:B:303:LYS:HG2 | 1.93 | 0.68 |
| 1:B:247:MET:CE | 1:B:270:ILE:HD11 | 2.23 | 0.68 |
| 1:A:412:GLU:OE1 | 1:A:415:ARG:HD2 | 1.93 | 0.68 |
| 1:B:302:GLU:OE1 | 1:B:341:LYS:HE3 | 1.94 | 0.68 |
| 1:A:136:ARG:HD3 | 1:A:139:ALA:HB2 | 1.74 | 0.68 |
| 1:A:190:HIS:CD2 | 1:A:194:GLU:OE1 | 2.47 | 0.68 |
| 1:A:383:SER:HB3 | 1:A:403:ILE:CG2 | 2.19 | 0.68 |
| 1:A:394:ILE:O | 1:A:399:ARG:NH1 | 2.27 | 0.68 |
| 1:B:63:VAL:HG12 | 1:B:63:VAL:O | 1.92 | 0.68 |
| 1:A:234:HIS:CE1 | 1:A:265:ALA:HB2 | 2.30 | 0.67 |
| 1:A:409:LEU:HB3 | 1:A:413:GLU:CD | 2.14 | 0.67 |
| 1:A:378:LEU:HA | 1:A:381:LEU:HD11 | 1.76 | 0.67 |
| 1:A:397:LYS:HA | 1:A:400:MET:CE | 2.24 | 0.67 |
| 1:B:361:THR:OG1 | 1:B:367:LEU:CD1 | 2.42 | 0.67 |
| 1:B:394:ILE:O | 1:B:399:ARG:NH1 | 2.27 | 0.67 |
| 1:B:412:GLU:OE1 | 1:B:415:ARG:HD2 | 1.92 | 0.67 |



| | A L O | Interatomic | Clash |
|------------------|------------------|-------------------------|-------------|
| Atom-1 | Atom-2 | distance (\AA) | overlap (Å) |
| 1:A:100:MET:CE | 1:A:205:MET:O | 2.42 | 0.67 |
| 1:B:378:LEU:HA | 1:B:381:LEU:HD11 | 1.76 | 0.67 |
| 1:B:397:LYS:HA | 1:B:400:MET:CE | 2.24 | 0.67 |
| 1:A:235:GLN:O | 1:A:237:SER:N | 2.27 | 0.67 |
| 1:A:302:GLU:OE1 | 1:A:341:LYS:HE3 | 1.94 | 0.67 |
| 1:B:374:ILE:C | 1:B:376:ARG:H | 1.96 | 0.67 |
| 1:B:190:HIS:CD2 | 1:B:194:GLU:OE1 | 2.47 | 0.67 |
| 1:B:373:LYS:HE3 | 1:B:377:TRP:CZ3 | 2.30 | 0.67 |
| 1:B:374:ILE:HG23 | 1:B:375:ARG:H | 1.60 | 0.67 |
| 1:A:373:LYS:HE3 | 1:A:377:TRP:CZ3 | 2.30 | 0.67 |
| 1:B:369:ILE:HG22 | 1:B:370:GLY:N | 2.10 | 0.67 |
| 1:B:409:LEU:HB3 | 1:B:413:GLU:CD | 2.14 | 0.67 |
| 1:A:397:LYS:CA | 1:A:400:MET:HE3 | 2.23 | 0.67 |
| 1:A:361:THR:OG1 | 1:A:367:LEU:CD1 | 2.42 | 0.67 |
| 1:B:234:HIS:CE1 | 1:B:265:ALA:HB2 | 2.30 | 0.67 |
| 1:B:247:MET:HE2 | 1:B:257:LEU:HD21 | 1.77 | 0.67 |
| 1:A:95:LEU:CD2 | 1:A:97:PHE:HE1 | 2.08 | 0.66 |
| 1:B:75:TYR:OH | 1:B:292:LEU:HD12 | 1.95 | 0.66 |
| 1:B:301:LEU:HG | 1:B:305:LYS:CD | 2.24 | 0.66 |
| 1:A:94:LYS:C | 1:A:97:PHE:CZ | 2.69 | 0.66 |
| 1:A:369:ILE:HG22 | 1:A:370:GLY:N | 2.10 | 0.66 |
| 1:A:374:ILE:C | 1:A:376:ARG:H | 1.96 | 0.66 |
| 1:A:374:ILE:HG23 | 1:A:375:ARG:H | 1.60 | 0.66 |
| 1:B:378:LEU:O | 1:B:379:ALA:C | 2.34 | 0.66 |
| 1:A:1:MET:O | 1:A:4:ASN:N | 2.28 | 0.66 |
| 1:A:280:GLU:OE1 | 1:A:290:ARG:NH2 | 2.28 | 0.66 |
| 1:B:190:HIS:HD2 | 1:B:194:GLU:OE1 | 1.79 | 0.66 |
| 1:A:31:GLN:HG3 | 1:A:48:THR:HG21 | 1.78 | 0.66 |
| 1:A:348:VAL:HG12 | 1:A:352:ILE:HD11 | 1.77 | 0.66 |
| 1:B:95:LEU:CD2 | 1:B:97:PHE:HE1 | 2.08 | 0.66 |
| 1:B:118:TYR:HE2 | 1:B:277:ASP:CB | 2.09 | 0.66 |
| 1:B:119:PHE:CZ | 1:B:123:ARG:NH2 | 2.64 | 0.66 |
| 1:B:276:ILE:HG23 | 1:B:277:ASP:N | 2.10 | 0.66 |
| 1:A:348:VAL:O | 1:A:352:ILE:CG1 | 2.39 | 0.66 |
| 1:B:1:MET:O | 1:B:4:ASN:N | 2.28 | 0.66 |
| 1:B:31:GLN:HG3 | 1:B:48:THR:HG21 | 1.78 | 0.66 |
| 1:B:361:THR:CA | 1:B:367:LEU:CD1 | 2.44 | 0.66 |
| 1:B:379:ALA:O | 1:B:380:ALA:O | 2.14 | 0.66 |
| 1:A:164:ILE:CG2 | 1:A:165:GLU:H | 2.09 | 0.65 |
| 1:B:280:GLU:OE1 | 1:B:290:ARG:NH2 | 2.28 | 0.65 |
| 1:A:119:PHE:CZ | 1:A:123:ARG:NH2 | 2.64 | 0.65 |



| | A L O | Interatomic | Clash |
|------------------|------------------|--------------|-------------|
| Atom-1 | Atom-2 | distance (Å) | overlap (Å) |
| 1:A:276:ILE:HG23 | 1:A:277:ASP:N | 2.10 | 0.65 |
| 1:A:361:THR:HG23 | 1:A:362:PRO:CD | 2.20 | 0.65 |
| 1:A:373:LYS:HA | 1:A:376:ARG:HG3 | 1.78 | 0.65 |
| 1:B:373:LYS:HA | 1:B:376:ARG:HG3 | 1.78 | 0.65 |
| 1:B:409:LEU:CD1 | 1:B:413:GLU:OE1 | 2.41 | 0.65 |
| 1:A:301:LEU:HG | 1:A:305:LYS:CD | 2.24 | 0.65 |
| 1:B:301:LEU:HD21 | 1:B:305:LYS:HZ1 | 1.62 | 0.65 |
| 1:B:94:LYS:C | 1:B:97:PHE:CZ | 2.69 | 0.65 |
| 1:B:348:VAL:HG12 | 1:B:352:ILE:HD11 | 1.77 | 0.65 |
| 1:A:190:HIS:HD2 | 1:A:194:GLU:OE1 | 1.79 | 0.65 |
| 1:A:339:LEU:HD22 | 1:A:339:LEU:H | 1.62 | 0.65 |
| 1:B:423:ASN:O | 1:B:427:LEU:HG | 1.97 | 0.65 |
| 1:A:53:GLU:HG3 | 1:A:57:LYS:HE3 | 1.79 | 0.64 |
| 1:A:75:TYR:OH | 1:A:292:LEU:HD12 | 1.95 | 0.64 |
| 1:A:310:TYR:O | 1:A:313:ILE:HG22 | 1.97 | 0.64 |
| 1:B:53:GLU:HG3 | 1:B:57:LYS:HE3 | 1.79 | 0.64 |
| 1:A:297:ILE:O | 1:A:300:ILE:CB | 2.45 | 0.64 |
| 1:A:423:ASN:O | 1:A:427:LEU:HG | 1.97 | 0.64 |
| 1:B:164:ILE:CG2 | 1:B:165:GLU:N | 2.59 | 0.64 |
| 1:A:378:LEU:O | 1:A:379:ALA:C | 2.34 | 0.64 |
| 1:A:379:ALA:O | 1:A:380:ALA:O | 2.15 | 0.64 |
| 1:A:2:LEU:HD13 | 1:A:291:ILE:HG23 | 1.79 | 0.64 |
| 1:A:21:LYS:HD3 | 1:A:25:GLU:OE2 | 1.97 | 0.64 |
| 1:A:359:LEU:HA | 1:B:124:GLY:CA | 2.28 | 0.64 |
| 1:B:167:ALA:HB1 | 1:B:209:LEU:HD21 | 1.79 | 0.64 |
| 1:A:86:LYS:CE | 1:A:266:THR:HG23 | 2.28 | 0.64 |
| 1:A:124:GLY:CA | 1:B:359:LEU:HA | 2.27 | 0.64 |
| 1:A:361:THR:CA | 1:A:367:LEU:CD1 | 2.44 | 0.64 |
| 1:B:21:LYS:HD3 | 1:B:25:GLU:OE2 | 1.97 | 0.64 |
| 1:A:87:GLU:OE2 | 1:B:315:LYS:HD2 | 1.98 | 0.64 |
| 1:A:385:THR:CA | 1:B:384:MET:O | 2.44 | 0.64 |
| 1:B:288:VAL:O | 1:B:291:ILE:HG12 | 1.97 | 0.64 |
| 1:B:310:TYR:O | 1:B:313:ILE:HG22 | 1.98 | 0.64 |
| 1:B:335:GLN:O | 1:B:339:LEU:CD2 | 2.45 | 0.64 |
| 1:B:164:ILE:CG2 | 1:B:165:GLU:H | 2.09 | 0.64 |
| 1:A:167:ALA:HB1 | 1:A:209:LEU:HD21 | 1.79 | 0.64 |
| 1:B:176:LYS:C | 1:B:178:LYS:N | 2.51 | 0.64 |
| 1:A:119:PHE:CZ | 1:A:123:ARG:NE | 2.66 | 0.63 |
| 1:A:95:LEU:CD2 | 1:A:97:PHE:CE1 | 2.82 | 0.63 |
| 1:A:129:LEU:HD13 | 1:A:143:LEU:CD2 | 2.18 | 0.63 |
| 1:A:281:THR:HG21 | 1:B:315:LYS:HZ3 | 1.63 | 0.63 |



| | A the C | Interatomic | Clash |
|------------------|------------------|--------------|-------------|
| Atom-1 | Atom-2 | distance (Å) | overlap (Å) |
| 1:A:288:VAL:O | 1:A:291:ILE:HG12 | 1.97 | 0.63 |
| 1:A:384:MET:O | 1:B:385:THR:CA | 2.44 | 0.63 |
| 1:A:385:THR:CG2 | 1:B:382:ASN:C | 2.63 | 0.63 |
| 1:A:87:GLU:HG3 | 1:B:315:LYS:NZ | 2.14 | 0.63 |
| 1:A:335:GLN:O | 1:A:339:LEU:CD2 | 2.45 | 0.63 |
| 1:B:196:THR:OG1 | 1:B:232:ARG:NH1 | 2.32 | 0.63 |
| 1:B:244:ILE:O | 1:B:271:GLY:N | 2.24 | 0.63 |
| 1:B:339:LEU:HD22 | 1:B:339:LEU:H | 1.62 | 0.63 |
| 1:A:247:MET:HE1 | 1:A:257:LEU:HD21 | 1.81 | 0.63 |
| 1:B:372:GLU:C | 1:B:374:ILE:N | 2.52 | 0.63 |
| 1:A:118:TYR:HE2 | 1:A:277:ASP:CB | 2.09 | 0.63 |
| 1:B:362:PRO:HD3 | 1:B:367:LEU:HD21 | 0.68 | 0.63 |
| 1:A:69:TRP:NE1 | 1:A:73:ILE:HD11 | 2.14 | 0.63 |
| 1:B:2:LEU:HD13 | 1:B:291:ILE:HG23 | 1.79 | 0.63 |
| 1:B:119:PHE:HZ | 1:B:123:ARG:NH2 | 1.95 | 0.63 |
| 1:B:362:PRO:O | 1:B:363:SER:C | 2.36 | 0.63 |
| 1:A:33:SER:O | 1:A:36:SER:HB2 | 1.99 | 0.63 |
| 1:B:9:VAL:HG13 | 1:B:71:ILE:CD1 | 2.28 | 0.63 |
| 1:B:85:ASP:OD1 | 1:B:285:LYS:HD3 | 1.99 | 0.63 |
| 1:B:348:VAL:O | 1:B:352:ILE:CG1 | 2.39 | 0.63 |
| 1:A:9:VAL:HG13 | 1:A:71:ILE:CD1 | 2.28 | 0.62 |
| 1:A:167:ALA:CB | 1:A:209:LEU:HD21 | 2.29 | 0.62 |
| 1:B:357:ILE:HD12 | 1:B:358:MET:H | 1.64 | 0.62 |
| 1:A:379:ALA:HB2 | 1:A:409:LEU:HD11 | 1.80 | 0.62 |
| 1:B:379:ALA:HB2 | 1:B:409:LEU:HD11 | 1.80 | 0.62 |
| 1:A:164:ILE:CD1 | 1:A:208:VAL:CG2 | 2.51 | 0.62 |
| 1:B:33:SER:O | 1:B:36:SER:HB2 | 1.99 | 0.62 |
| 1:B:69:TRP:NE1 | 1:B:73:ILE:HD11 | 2.14 | 0.62 |
| 1:B:359:LEU:HB3 | 1:B:360:PRO:HD2 | 1.81 | 0.62 |
| 1:A:196:THR:OG1 | 1:A:232:ARG:NH1 | 2.32 | 0.62 |
| 1:A:119:PHE:HZ | 1:A:123:ARG:NH2 | 1.95 | 0.62 |
| 1:A:376:ARG:O | 1:A:377:TRP:C | 2.38 | 0.62 |
| 1:B:283:ASN:C | 1:B:283:ASN:HD22 | 2.03 | 0.62 |
| 1:B:379:ALA:CB | 1:B:409:LEU:HD11 | 2.30 | 0.62 |
| 1:A:362:PRO:HD3 | 1:A:367:LEU:HD21 | 0.68 | 0.62 |
| 1:A:283:ASN:C | 1:A:283:ASN:HD22 | 2.03 | 0.62 |
| 1:A:357:ILE:HD12 | 1:A:358:MET:H | 1.64 | 0.62 |
| 1:B:1:MET:SD | 1:B:37:SER:HB2 | 2.40 | 0.62 |
| 1:A:75:TYR:O | 1:A:76:ASP:C | 2.38 | 0.62 |
| 1:A:291:ILE:O | 1:A:292:LEU:HB2 | 2.00 | 0.62 |
| 1:A:315:LYS:NZ | 1:B:87:GLU:HG3 | 2.14 | 0.62 |



| | lo uo pugo | Interatomic | Clash |
|------------------|------------------|--------------|-------------|
| Atom-1 | Atom-2 | distance (Å) | overlap (Å) |
| 1:B:351:HIS:O | 1:B:353:PRO:HD3 | 2.00 | 0.62 |
| 1:A:82:PHE:O | 1:A:261:VAL:HG21 | 1.99 | 0.62 |
| 1:A:244:ILE:O | 1:A:271:GLY:N | 2.24 | 0.62 |
| 1:A:315:LYS:HD2 | 1:B:87:GLU:OE2 | 2.00 | 0.62 |
| 1:A:379:ALA:CB | 1:A:409:LEU:HD11 | 2.30 | 0.61 |
| 1:B:167:ALA:CB | 1:B:209:LEU:HD21 | 2.29 | 0.61 |
| 1:A:359:LEU:HB3 | 1:A:360:PRO:HD2 | 1.81 | 0.61 |
| 1:B:75:TYR:O | 1:B:76:ASP:C | 2.38 | 0.61 |
| 1:B:119:PHE:CZ | 1:B:123:ARG:NE | 2.66 | 0.61 |
| 1:A:351:HIS:O | 1:A:353:PRO:HD3 | 2.00 | 0.61 |
| 1:B:129:LEU:HD13 | 1:B:143:LEU:CD2 | 2.18 | 0.61 |
| 1:A:85:ASP:OD1 | 1:A:285:LYS:HD3 | 1.99 | 0.61 |
| 1:A:382:ASN:C | 1:B:385:THR:CG2 | 2.64 | 0.61 |
| 1:B:297:ILE:O | 1:B:300:ILE:CB | 2.45 | 0.61 |
| 1:B:394:ILE:CG2 | 1:B:399:ARG:NH1 | 2.63 | 0.61 |
| 1:A:194:GLU:CA | 1:A:197:LYS:HE3 | 2.30 | 0.61 |
| 1:A:329:LEU:HD11 | 1:A:421:TYR:CB | 2.31 | 0.61 |
| 1:A:394:ILE:CG2 | 1:A:399:ARG:HH12 | 2.14 | 0.61 |
| 1:A:394:ILE:CG2 | 1:A:399:ARG:NH1 | 2.64 | 0.61 |
| 1:B:242:VAL:CG1 | 1:B:243:ILE:N | 2.64 | 0.61 |
| 1:A:394:ILE:HG22 | 1:A:394:ILE:O | 2.00 | 0.61 |
| 1:B:116:LEU:HD11 | 1:B:120:TYR:CE2 | 2.36 | 0.61 |
| 1:B:380:ALA:C | 1:B:381:LEU:HG | 2.21 | 0.61 |
| 1:A:380:ALA:C | 1:A:381:LEU:HG | 2.21 | 0.61 |
| 1:B:82:PHE:O | 1:B:261:VAL:HG21 | 2.00 | 0.61 |
| 1:B:273:GLY:HA3 | 1:B:278:GLU:OE1 | 2.00 | 0.61 |
| 1:B:291:ILE:O | 1:B:292:LEU:HB2 | 2.00 | 0.61 |
| 1:A:87:GLU:HB3 | 1:B:312:LYS:HE2 | 1.82 | 0.61 |
| 1:B:300:ILE:HD13 | 1:B:303:LYS:CE | 2.31 | 0.61 |
| 1:B:394:ILE:HG22 | 1:B:394:ILE:O | 2.00 | 0.61 |
| 1:A:247:MET:HE1 | 1:A:270:ILE:HD11 | 1.82 | 0.60 |
| 1:A:273:GLY:HA3 | 1:A:278:GLU:OE1 | 2.00 | 0.60 |
| 1:B:6:ARG:HA | 1:B:292:LEU:HD21 | 1.83 | 0.60 |
| 1:B:377:TRP:CE3 | 1:B:377:TRP:HA | 2.35 | 0.60 |
| 1:A:6:ARG:HA | 1:A:292:LEU:HD21 | 1.83 | 0.60 |
| 1:A:91:ASN:ND2 | 1:B:357:ILE:HG21 | 2.16 | 0.60 |
| 1:A:176:LYS:C | 1:A:178:LYS:N | 2.51 | 0.60 |
| 1:A:328:THR:HG23 | 1:A:331:ASP:OD2 | 2.01 | 0.60 |
| 1:A:377:TRP:HA | 1:A:377:TRP:CE3 | 2.35 | 0.60 |
| 1:A:234:HIS:CD2 | 1:A:265:ALA:HB2 | 2.36 | 0.60 |
| 1:A:402:ARG:CD | 1:B:402:ARG:CD | 2.78 | 0.60 |



| | | Interatomic | Clash |
|------------------|------------------|--------------|-------------|
| Atom-1 | Atom-2 | distance (Å) | overlap (Å) |
| 1:B:247:MET:HE2 | 1:B:257:LEU:CD2 | 2.31 | 0.60 |
| 1:B:378:LEU:HD23 | 1:B:378:LEU:C | 2.22 | 0.60 |
| 1:B:378:LEU:CA | 1:B:381:LEU:CD1 | 2.76 | 0.60 |
| 1:B:376:ARG:O | 1:B:377:TRP:C | 2.38 | 0.60 |
| 1:B:301:LEU:CD1 | 1:B:305:LYS:HE3 | 2.28 | 0.60 |
| 1:A:30:LEU:HD23 | 1:A:48:THR:HG22 | 1.84 | 0.60 |
| 1:A:116:LEU:HD11 | 1:A:120:TYR:CE2 | 2.36 | 0.60 |
| 1:A:300:ILE:HD13 | 1:A:303:LYS:CE | 2.31 | 0.60 |
| 1:A:327:LEU:HB2 | 1:A:390:GLU:O | 2.01 | 0.60 |
| 1:A:378:LEU:C | 1:A:378:LEU:HD23 | 2.22 | 0.60 |
| 1:B:122:LYS:C | 1:B:124:GLY:H | 2.05 | 0.60 |
| 1:B:234:HIS:CD2 | 1:B:265:ALA:HB2 | 2.36 | 0.60 |
| 1:B:329:LEU:HD11 | 1:B:421:TYR:CB | 2.31 | 0.60 |
| 1:A:119:PHE:HZ | 1:A:123:ARG:HH21 | 1.48 | 0.60 |
| 1:B:327:LEU:HB2 | 1:B:390:GLU:O | 2.01 | 0.60 |
| 1:A:378:LEU:CA | 1:A:381:LEU:CD1 | 2.76 | 0.60 |
| 1:B:328:THR:HG23 | 1:B:331:ASP:OD2 | 2.01 | 0.60 |
| 1:B:394:ILE:CG2 | 1:B:399:ARG:HH12 | 2.14 | 0.60 |
| 1:B:194:GLU:CA | 1:B:197:LYS:HE3 | 2.30 | 0.60 |
| 1:A:123:ARG:NH2 | 1:B:318:GLU:OE1 | 2.35 | 0.59 |
| 1:A:276:ILE:CG2 | 1:A:277:ASP:N | 2.65 | 0.59 |
| 1:B:85:ASP:OD1 | 1:B:285:LYS:CD | 2.50 | 0.59 |
| 1:A:302:GLU:OE1 | 1:A:341:LYS:HG3 | 2.02 | 0.59 |
| 1:A:382:ASN:CA | 1:B:385:THR:CG2 | 2.79 | 0.59 |
| 1:A:41:VAL:HG12 | 1:A:41:VAL:O | 2.02 | 0.59 |
| 1:A:85:ASP:OD1 | 1:A:285:LYS:CD | 2.50 | 0.59 |
| 1:A:122:LYS:C | 1:A:124:GLY:H | 2.05 | 0.59 |
| 1:A:312:LYS:HE2 | 1:B:87:GLU:HB3 | 1.83 | 0.59 |
| 1:A:242:VAL:CG1 | 1:A:243:ILE:N | 2.64 | 0.59 |
| 1:A:372:GLU:C | 1:A:374:ILE:N | 2.52 | 0.59 |
| 1:A:385:THR:CG2 | 1:B:382:ASN:CA | 2.79 | 0.59 |
| 1:B:276:ILE:CG2 | 1:B:277:ASP:N | 2.65 | 0.59 |
| 1:A:377:TRP:CE3 | 1:A:377:TRP:CA | 2.85 | 0.59 |
| 1:B:30:LEU:HD23 | 1:B:48:THR:HG22 | 1.84 | 0.59 |
| 1:B:302:GLU:OE1 | 1:B:341:LYS:HG3 | 2.02 | 0.59 |
| 1:A:331:ASP:O | 1:A:332:VAL:CG2 | 2.49 | 0.59 |
| 1:A:357:ILE:HG21 | 1:B:91:ASN:ND2 | 2.18 | 0.59 |
| 1:B:86:LYS:CE | 1:B:266:THR:HG23 | 2.28 | 0.59 |
| 1:B:346:SER:C | 1:B:348:VAL:N | 2.55 | 0.59 |
| 1:B:348:VAL:CG1 | 1:B:352:ILE:HD11 | 2.33 | 0.59 |
| 1:A:362:PRO:O | 1:A:363:SER:C | 2.36 | 0.59 |



| | | Interatomic | Clash |
|------------------|------------------|-------------------------|-------------|
| Atom-1 | Atom-2 | distance (\AA) | overlap (Å) |
| 1:B:331:ASP:O | 1:B:332:VAL:CG2 | 2.49 | 0.59 |
| 1:A:318:GLU:OE1 | 1:B:123:ARG:NH2 | 2.36 | 0.58 |
| 1:B:109:LYS:O | 1:B:110:THR:CB | 2.51 | 0.58 |
| 1:B:377:TRP:CE3 | 1:B:377:TRP:CA | 2.85 | 0.58 |
| 1:B:318:GLU:O | 1:B:319:ASP:OD1 | 2.22 | 0.58 |
| 1:B:418:LEU:HA | 1:B:421:TYR:CD1 | 2.34 | 0.58 |
| 1:B:41:VAL:HG12 | 1:B:41:VAL:O | 2.02 | 0.58 |
| 1:A:109:LYS:O | 1:A:110:THR:CB | 2.51 | 0.58 |
| 1:B:377:TRP:N | 1:B:377:TRP:HE3 | 2.02 | 0.58 |
| 1:B:100:MET:CE | 1:B:209:LEU:HD12 | 2.34 | 0.58 |
| 1:A:2:LEU:HB3 | 1:A:291:ILE:CG2 | 2.34 | 0.58 |
| 1:A:335:GLN:HB3 | 1:A:355:LEU:CD2 | 2.33 | 0.58 |
| 1:A:409:LEU:CD1 | 1:A:413:GLU:OE1 | 2.41 | 0.58 |
| 1:A:346:SER:C | 1:A:348:VAL:N | 2.55 | 0.57 |
| 1:B:335:GLN:HB3 | 1:B:355:LEU:CD2 | 2.33 | 0.57 |
| 1:A:123:ARG:O | 1:B:358:MET:O | 2.22 | 0.57 |
| 1:A:301:LEU:O | 1:A:305:LYS:HB2 | 2.04 | 0.57 |
| 1:B:131:ALA:O | 1:B:140:TYR:HE2 | 1.87 | 0.57 |
| 1:B:359:LEU:HB3 | 1:B:360:PRO:CD | 2.33 | 0.57 |
| 1:A:1:MET:SD | 1:A:37:SER:HB2 | 2.40 | 0.57 |
| 1:B:199:LEU:CD2 | 1:B:202:MET:SD | 2.92 | 0.57 |
| 1:A:402:ARG:CD | 1:B:402:ARG:NE | 2.68 | 0.57 |
| 1:A:402:ARG:NE | 1:B:402:ARG:NE | 2.51 | 0.57 |
| 1:A:359:LEU:HB3 | 1:A:360:PRO:CD | 2.33 | 0.57 |
| 1:A:367:LEU:O | 1:A:368:LYS:HB2 | 2.04 | 0.57 |
| 1:B:359:LEU:CD1 | 1:B:360:PRO:CD | 2.60 | 0.57 |
| 1:A:87:GLU:HG2 | 1:B:312:LYS:HG2 | 1.86 | 0.57 |
| 1:B:2:LEU:HB3 | 1:B:291:ILE:CG2 | 2.34 | 0.57 |
| 1:B:118:TYR:OH | 1:B:122:LYS:HE3 | 2.04 | 0.57 |
| 1:A:299:SER:O | 1:A:303:LYS:N | 2.37 | 0.57 |
| 1:A:300:ILE:HG22 | 1:A:301:LEU:N | 2.20 | 0.57 |
| 1:A:348:VAL:CG1 | 1:A:352:ILE:HD11 | 2.33 | 0.57 |
| 1:B:367:LEU:O | 1:B:368:LYS:HB2 | 2.04 | 0.57 |
| 1:A:199:LEU:CD2 | 1:A:202:MET:SD | 2.92 | 0.57 |
| 1:A:377:TRP:HE3 | 1:A:377:TRP:N | 2.02 | 0.57 |
| 1:B:301:LEU:O | 1:B:305:LYS:HB2 | 2.04 | 0.57 |
| 1:B:283:ASN:O | 1:B:284:ALA:C | 2.42 | 0.57 |
| 1:A:361:THR:OG1 | 1:A:367:LEU:HD12 | 2.04 | 0.56 |
| 1:B:369:ILE:CG2 | 1:B:370:GLY:H | 2.18 | 0.56 |
| 1:A:100:MET:CE | 1:A:209:LEU:HD12 | 2.34 | 0.56 |
| 1:A:402:ARG:NE | 1:B:402:ARG:CD | 2.69 | 0.56 |



| | | Interatomic | Clash |
|------------------|------------------|-------------------------|-------------|
| Atom-1 | Atom-2 | distance (\AA) | overlap (Å) |
| 1:A:283:ASN:O | 1:A:284:ALA:C | 2.42 | 0.56 |
| 1:A:318:GLU:OE1 | 1:B:123:ARG:NH1 | 2.39 | 0.56 |
| 1:A:318:GLU:O | 1:A:319:ASP:OD1 | 2.21 | 0.56 |
| 1:B:77:GLU:O | 1:B:78:LEU:C | 2.41 | 0.56 |
| 1:B:299:SER:O | 1:B:303:LYS:N | 2.37 | 0.56 |
| 1:B:300:ILE:HG22 | 1:B:301:LEU:N | 2.20 | 0.56 |
| 1:B:361:THR:OG1 | 1:B:367:LEU:HD12 | 2.04 | 0.56 |
| 1:A:116:LEU:HD11 | 1:A:120:TYR:HE2 | 1.69 | 0.56 |
| 1:A:118:TYR:OH | 1:A:122:LYS:HE3 | 2.04 | 0.56 |
| 1:A:300:ILE:HD13 | 1:A:303:LYS:HE3 | 1.88 | 0.56 |
| 1:A:342:MET:O | 1:A:343:GLY:O | 2.23 | 0.56 |
| 1:A:131:ALA:O | 1:A:140:TYR:HE2 | 1.87 | 0.56 |
| 1:A:358:MET:O | 1:B:123:ARG:O | 2.23 | 0.56 |
| 1:B:116:LEU:HD11 | 1:B:120:TYR:HE2 | 1.69 | 0.56 |
| 1:A:143:LEU:HD13 | 1:A:154:VAL:HG13 | 1.88 | 0.56 |
| 1:A:301:LEU:CD1 | 1:A:305:LYS:HE3 | 2.28 | 0.56 |
| 1:B:95:LEU:CD2 | 1:B:97:PHE:CE1 | 2.82 | 0.56 |
| 1:B:427:LEU:O | 1:B:431:VAL:HG23 | 2.06 | 0.56 |
| 1:A:135:TYR:CD1 | 1:A:189:ARG:CZ | 2.88 | 0.56 |
| 1:A:293:GLY:HA3 | 1:A:296:ASP:OD2 | 2.06 | 0.56 |
| 1:B:293:GLY:HA3 | 1:B:296:ASP:OD2 | 2.06 | 0.56 |
| 1:B:347:LYS:O | 1:B:347:LYS:HG3 | 2.06 | 0.56 |
| 1:A:312:LYS:HG2 | 1:B:87:GLU:HG2 | 1.87 | 0.56 |
| 1:A:427:LEU:O | 1:A:431:VAL:HG23 | 2.05 | 0.56 |
| 1:B:1:MET:CG | 1:B:37:SER:HB3 | 2.36 | 0.56 |
| 1:B:135:TYR:CD1 | 1:B:189:ARG:CZ | 2.88 | 0.56 |
| 1:B:300:ILE:HD13 | 1:B:303:LYS:HE3 | 1.88 | 0.56 |
| 1:B:380:ALA:C | 1:B:381:LEU:CG | 2.74 | 0.56 |
| 1:A:347:LYS:HG3 | 1:A:347:LYS:O | 2.06 | 0.56 |
| 1:A:385:THR:CG2 | 1:A:386:TYR:N | 2.69 | 0.56 |
| 1:A:293:GLY:O | 1:A:296:ASP:N | 2.32 | 0.55 |
| 1:A:369:ILE:CG2 | 1:A:370:GLY:H | 2.18 | 0.55 |
| 1:B:95:LEU:HD23 | 1:B:97:PHE:HE1 | 1.63 | 0.55 |
| 1:B:219:ASP:OD1 | 1:B:221:SER:OG | 2.23 | 0.55 |
| 1:B:247:MET:HE2 | 1:B:270:ILE:HD11 | 1.89 | 0.55 |
| 1:A:123:ARG:NH1 | 1:B:318:GLU:OE1 | 2.39 | 0.55 |
| 1:A:219:ASP:OD1 | 1:A:221:SER:OG | 2.23 | 0.55 |
| 1:B:342:MET:O | 1:B:343:GLY:O | 2.24 | 0.55 |
| 1:B:376:ARG:O | 1:B:379:ALA:N | 2.40 | 0.55 |
| 1:B:425:ASN:O | 1:B:429:LYS:HG3 | 2.06 | 0.55 |
| 1:B:75:TYR:CD2 | 1:B:297:ILE:CG2 | 2.85 | 0.55 |



| | A h C | Interatomic | Clash |
|------------------|------------------|-------------------------|-------------|
| Atom-1 | Atom-2 | distance (\AA) | overlap (Å) |
| 1:B:427:LEU:O | 1:B:428:LEU:C | 2.45 | 0.55 |
| 1:A:376:ARG:O | 1:A:379:ALA:N | 2.40 | 0.55 |
| 1:A:379:ALA:HB3 | 1:A:417:LEU:HD11 | 1.88 | 0.55 |
| 1:B:293:GLY:O | 1:B:296:ASP:N | 2.32 | 0.55 |
| 1:A:51:ILE:HD13 | 1:A:74:VAL:HG22 | 1.88 | 0.55 |
| 1:B:85:ASP:OD1 | 1:B:285:LYS:CE | 2.54 | 0.55 |
| 1:A:416:GLU:O | 1:A:417:LEU:C | 2.45 | 0.55 |
| 1:B:267:ILE:O | 1:B:267:ILE:HG22 | 2.07 | 0.55 |
| 1:A:85:ASP:OD1 | 1:A:285:LYS:CE | 2.54 | 0.55 |
| 1:A:409:LEU:HB3 | 1:A:413:GLU:OE1 | 2.07 | 0.55 |
| 1:B:379:ALA:HB3 | 1:B:417:LEU:HD11 | 1.88 | 0.54 |
| 1:B:143:LEU:HD13 | 1:B:154:VAL:HG13 | 1.88 | 0.54 |
| 1:B:329:LEU:HG | 1:B:329:LEU:O | 2.07 | 0.54 |
| 1:B:385:THR:CG2 | 1:B:386:TYR:N | 2.69 | 0.54 |
| 1:A:40:ASN:HD22 | 1:A:42:LYS:CB | 2.20 | 0.54 |
| 1:A:300:ILE:HD13 | 1:A:303:LYS:HZ2 | 1.72 | 0.54 |
| 1:B:129:LEU:HD23 | 1:B:183:ILE:HB | 1.89 | 0.54 |
| 1:B:416:GLU:O | 1:B:417:LEU:C | 2.45 | 0.54 |
| 1:A:1:MET:CG | 1:A:37:SER:HB3 | 2.36 | 0.54 |
| 1:A:77:GLU:O | 1:A:78:LEU:C | 2.41 | 0.54 |
| 1:A:247:MET:HE1 | 1:A:257:LEU:CD2 | 2.37 | 0.54 |
| 1:A:270:ILE:HG23 | 1:A:270:ILE:O | 2.08 | 0.54 |
| 1:B:75:TYR:CE2 | 1:B:297:ILE:HG23 | 2.42 | 0.54 |
| 1:A:129:LEU:HD23 | 1:A:183:ILE:HB | 1.89 | 0.54 |
| 1:A:163:PRO:O | 1:A:164:ILE:C | 2.46 | 0.54 |
| 1:A:221:SER:CA | 1:A:250:THR:HG21 | 2.33 | 0.54 |
| 1:B:361:THR:CB | 1:B:367:LEU:HG | 2.38 | 0.54 |
| 1:A:329:LEU:O | 1:A:329:LEU:HG | 2.07 | 0.54 |
| 1:B:28:LYS:O | 1:B:32:LYS:HD3 | 2.07 | 0.54 |
| 1:B:361:THR:HA | 1:B:367:LEU:HD11 | 0.66 | 0.54 |
| 1:B:369:ILE:HA | 1:B:373:LYS:HG2 | 1.89 | 0.54 |
| 1:A:101:LEU:HD12 | 1:A:113:ALA:HB2 | 1.90 | 0.54 |
| 1:A:267:ILE:HG22 | 1:A:267:ILE:O | 2.07 | 0.54 |
| 1:A:336:ILE:HD11 | 1:A:377:TRP:HD1 | 1.73 | 0.54 |
| 1:A:425:ASN:O | 1:A:429:LYS:HG3 | 2.06 | 0.54 |
| 1:B:409:LEU:HB3 | 1:B:413:GLU:OE1 | 2.07 | 0.54 |
| 1:A:369:ILE:HA | 1:A:373:LYS:HG2 | 1.89 | 0.54 |
| 1:B:190:HIS:HB3 | 1:B:194:GLU:HB2 | 1.89 | 0.54 |
| 1:B:101:LEU:HD12 | 1:B:113:ALA:HB2 | 1.90 | 0.54 |
| 1:A:28:LYS:O | 1:A:32:LYS:HD3 | 2.07 | 0.54 |
| 1:A:75:TYR:CE2 | 1:A:297:ILE:HG23 | 2.42 | 0.54 |



| | A h C | Interatomic | Clash |
|------------------|------------------|--------------|-------------|
| Atom-1 | Atom-2 | distance (Å) | overlap (Å) |
| 1:A:247:MET:HG3 | 1:A:270:ILE:HD11 | 1.90 | 0.54 |
| 1:A:293:GLY:CA | 1:A:296:ASP:OD2 | 2.56 | 0.54 |
| 1:A:385:THR:HG23 | 1:B:384:MET:O | 2.08 | 0.54 |
| 1:B:94:LYS:N | 1:B:97:PHE:CE2 | 2.68 | 0.54 |
| 1:B:155:TYR:CE1 | 1:B:173:ILE:HD12 | 2.43 | 0.54 |
| 1:A:359:LEU:CD1 | 1:A:360:PRO:CD | 2.60 | 0.53 |
| 1:A:403:ILE:CG2 | 1:A:414:VAL:HG21 | 2.38 | 0.53 |
| 1:B:51:ILE:HD13 | 1:B:74:VAL:HG22 | 1.88 | 0.53 |
| 1:B:105:GLN:O | 1:B:106:GLY:O | 2.26 | 0.53 |
| 1:B:162:ASN:O | 1:B:166:ILE:HG13 | 2.08 | 0.53 |
| 1:B:209:LEU:O | 1:B:210:LYS:C | 2.46 | 0.53 |
| 1:B:381:LEU:N | 1:B:381:LEU:CD2 | 2.62 | 0.53 |
| 1:B:403:ILE:CG2 | 1:B:414:VAL:HG21 | 2.37 | 0.53 |
| 1:A:19:TYR:CD2 | 1:A:66:ARG:NH2 | 2.76 | 0.53 |
| 1:A:105:GLN:O | 1:A:106:GLY:O | 2.26 | 0.53 |
| 1:A:361:THR:CB | 1:A:367:LEU:HG | 2.38 | 0.53 |
| 1:B:40:ASN:HD22 | 1:B:42:LYS:CB | 2.20 | 0.53 |
| 1:B:380:ALA:O | 1:B:381:LEU:CB | 2.56 | 0.53 |
| 1:B:380:ALA:O | 1:B:381:LEU:HG | 2.08 | 0.53 |
| 1:A:380:ALA:O | 1:A:382:ASN:OD1 | 2.26 | 0.53 |
| 1:A:380:ALA:C | 1:A:381:LEU:CG | 2.74 | 0.53 |
| 1:A:427:LEU:O | 1:A:428:LEU:C | 2.45 | 0.53 |
| 1:B:270:ILE:O | 1:B:270:ILE:HG23 | 2.08 | 0.53 |
| 1:B:336:ILE:HD11 | 1:B:377:TRP:HD1 | 1.73 | 0.53 |
| 1:A:162:ASN:O | 1:A:166:ILE:HG13 | 2.08 | 0.53 |
| 1:B:19:TYR:CD2 | 1:B:66:ARG:NH2 | 2.76 | 0.53 |
| 1:B:118:TYR:CZ | 1:B:122:LYS:HE3 | 2.44 | 0.53 |
| 1:B:247:MET:HG3 | 1:B:270:ILE:HD11 | 1.91 | 0.53 |
| 1:B:343:GLY:O | 1:B:348:VAL:HG21 | 2.09 | 0.53 |
| 1:A:9:VAL:HG13 | 1:A:71:ILE:HD12 | 1.90 | 0.53 |
| 1:B:1:MET:HG2 | 1:B:37:SER:HB3 | 1.91 | 0.53 |
| 1:B:75:TYR:OH | 1:B:292:LEU:CD1 | 2.55 | 0.53 |
| 1:B:310:TYR:CZ | 1:B:355:LEU:HD23 | 2.44 | 0.53 |
| 1:A:380:ALA:O | 1:A:381:LEU:HG | 2.08 | 0.53 |
| 1:B:9:VAL:HG13 | 1:B:71:ILE:HD12 | 1.90 | 0.53 |
| 1:B:380:ALA:O | 1:B:382:ASN:OD1 | 2.26 | 0.53 |
| 1:A:23:VAL:O | 1:A:24:ASP:C | 2.46 | 0.53 |
| 1:B:155:TYR:CD2 | 1:B:170:GLY:CA | 2.91 | 0.53 |
| 1:A:190:HIS:HB3 | 1:A:194:GLU:HB2 | 1.89 | 0.53 |
| 1:A:394:ILE:HG22 | 1:A:399:ARG:CZ | 2.39 | 0.53 |
| 1:A:75:TYR:OH | 1:A:292:LEU:CD1 | 2.55 | 0.53 |



| | A i a | Interatomic | Clash |
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| Atom-1 | Atom-2 | distance (Å) | overlap (Å) |
| 1:A:155:TYR:CE1 | 1:A:173:ILE:HD12 | 2.43 | 0.53 |
| 1:A:167:ALA:HB1 | 1:A:209:LEU:CD1 | 2.36 | 0.53 |
| 1:A:300:ILE:O | 1:A:303:LYS:CG | 2.57 | 0.53 |
| 1:B:163:PRO:O | 1:B:164:ILE:C | 2.46 | 0.53 |
| 1:B:167:ALA:HB1 | 1:B:209:LEU:CD1 | 2.36 | 0.53 |
| 1:B:293:GLY:CA | 1:B:296:ASP:OD2 | 2.56 | 0.53 |
| 1:A:70:PHE:O | 1:A:71:ILE:C | 2.46 | 0.53 |
| 1:A:380:ALA:O | 1:A:381:LEU:CB | 2.56 | 0.53 |
| 1:B:300:ILE:O | 1:B:303:LYS:CG | 2.57 | 0.53 |
| 1:A:15:GLY:HA2 | 1:A:67:LYS:HZ2 | 1.71 | 0.52 |
| 1:B:70:PHE:O | 1:B:71:ILE:C | 2.46 | 0.52 |
| 1:A:155:TYR:CD2 | 1:A:170:GLY:CA | 2.91 | 0.52 |
| 1:A:299:SER:O | 1:A:303:LYS:CG | 2.56 | 0.52 |
| 1:B:23:VAL:O | 1:B:24:ASP:C | 2.45 | 0.52 |
| 1:B:431:VAL:O | 1:B:432:LYS:HB2 | 2.09 | 0.52 |
| 1:A:313:ILE:CD1 | 1:A:331:ASP:OD1 | 2.56 | 0.52 |
| 1:B:143:LEU:O | 1:B:143:LEU:HD22 | 2.10 | 0.52 |
| 1:B:394:ILE:HG22 | 1:B:399:ARG:CZ | 2.39 | 0.52 |
| 1:A:372:GLU:C | 1:A:374:ILE:HG22 | 2.30 | 0.52 |
| 1:B:64:LEU:HD11 | 1:B:303:LYS:HZ3 | 1.73 | 0.52 |
| 1:B:345:LEU:HG | 1:B:346:SER:H | 1.74 | 0.52 |
| 1:B:362:PRO:CD | 1:B:367:LEU:HD23 | 2.33 | 0.52 |
| 1:A:1:MET:HG2 | 1:A:37:SER:HB3 | 1.91 | 0.52 |
| 1:A:75:TYR:CE1 | 1:A:292:LEU:HD12 | 2.44 | 0.52 |
| 1:A:343:GLY:O | 1:A:348:VAL:HG21 | 2.09 | 0.52 |
| 1:A:357:ILE:O | 1:A:358:MET:CB | 2.57 | 0.52 |
| 1:A:377:TRP:CZ3 | 1:A:417:LEU:CD2 | 2.93 | 0.52 |
| 1:B:428:LEU:O | 1:B:431:VAL:HG23 | 2.10 | 0.52 |
| 1:A:310:TYR:CZ | 1:A:355:LEU:HD23 | 2.44 | 0.52 |
| 1:B:75:TYR:HD2 | 1:B:297:ILE:CG2 | 2.19 | 0.52 |
| 1:B:225:LYS:C | 1:B:227:TYR:H | 2.12 | 0.52 |
| 1:A:100:MET:HE3 | 1:A:209:LEU:HD12 | 1.90 | 0.52 |
| 1:A:384:MET:O | 1:B:385:THR:HG23 | 2.09 | 0.52 |
| 1:A:428:LEU:O | 1:A:431:VAL:HG23 | 2.10 | 0.52 |
| 1:B:372:GLU:C | 1:B:374:ILE:HG22 | 2.30 | 0.52 |
| 1:A:118:TYR:CZ | 1:A:122:LYS:HE3 | 2.44 | 0.52 |
| 1:A:209:LEU:O | 1:A:210:LYS:C | 2.46 | 0.52 |
| 1:B:295:GLY:HA2 | 1:B:298:GLU:CB | 2.33 | 0.52 |
| 1:B:361:THR:CG2 | 1:B:365:ASP:O | 2.58 | 0.52 |
| 1:B:374:ILE:HG23 | 1:B:375:ARG:N | 2.24 | 0.52 |
| 1:A:58:GLU:O | 1:A:69:TRP:NE1 | 2.43 | 0.51 |



| | | Interatomic | Clash |
|------------------|------------------|-------------------------|-------------|
| Atom-1 | Atom-2 | distance (\AA) | overlap (Å) |
| 1:A:225:LYS:C | 1:A:227:TYR:H | 2.13 | 0.51 |
| 1:A:330:ARG:HB3 | 1:A:389:LEU:O | 2.10 | 0.51 |
| 1:B:377:TRP:CZ3 | 1:B:417:LEU:CD2 | 2.93 | 0.51 |
| 1:A:133:ASP:OD1 | 1:A:187:ALA:HB2 | 2.09 | 0.51 |
| 1:A:164:ILE:CG2 | 1:A:165:GLU:N | 2.59 | 0.51 |
| 1:A:190:HIS:CG | 1:A:197:LYS:CD | 2.79 | 0.51 |
| 1:A:283:ASN:C | 1:A:283:ASN:ND2 | 2.62 | 0.51 |
| 1:B:133:ASP:OD1 | 1:B:187:ALA:HB2 | 2.09 | 0.51 |
| 1:A:75:TYR:HD2 | 1:A:297:ILE:CG2 | 2.19 | 0.51 |
| 1:A:329:LEU:HD11 | 1:A:421:TYR:CG | 2.45 | 0.51 |
| 1:B:83:GLY:HA2 | 1:B:261:VAL:HG13 | 1.92 | 0.51 |
| 1:B:329:LEU:HD11 | 1:B:421:TYR:CG | 2.45 | 0.51 |
| 1:A:361:THR:CG2 | 1:A:365:ASP:O | 2.58 | 0.51 |
| 1:A:417:LEU:O | 1:A:421:TYR:CD1 | 2.64 | 0.51 |
| 1:A:431:VAL:O | 1:A:432:LYS:HB2 | 2.09 | 0.51 |
| 1:B:75:TYR:CE1 | 1:B:292:LEU:HD12 | 2.44 | 0.51 |
| 1:A:40:ASN:ND2 | 1:A:42:LYS:CB | 2.73 | 0.51 |
| 1:A:225:LYS:C | 1:A:227:TYR:N | 2.64 | 0.51 |
| 1:A:380:ALA:HB1 | 1:A:384:MET:SD | 2.51 | 0.51 |
| 1:B:417:LEU:O | 1:B:421:TYR:CD1 | 2.64 | 0.51 |
| 1:A:143:LEU:HD22 | 1:A:143:LEU:O | 2.10 | 0.51 |
| 1:B:144:LEU:HD23 | 1:B:154:VAL:HB | 1.91 | 0.51 |
| 1:B:168:LYS:HE3 | 1:B:208:VAL:HG13 | 1.93 | 0.51 |
| 1:A:40:ASN:HB3 | 1:A:43:LEU:HG | 1.92 | 0.51 |
| 1:A:53:GLU:CG | 1:A:57:LYS:HE3 | 2.40 | 0.51 |
| 1:A:259:ALA:O | 1:A:262:ALA:HB3 | 2.11 | 0.51 |
| 1:A:310:TYR:OH | 1:A:355:LEU:HA | 2.11 | 0.51 |
| 1:A:346:SER:O | 1:A:349:LEU:N | 2.43 | 0.51 |
| 1:A:361:THR:HA | 1:A:367:LEU:HD11 | 0.66 | 0.51 |
| 1:A:374:ILE:HG23 | 1:A:375:ARG:N | 2.24 | 0.51 |
| 1:B:53:GLU:CG | 1:B:57:LYS:HE3 | 2.40 | 0.51 |
| 1:B:225:LYS:C | 1:B:227:TYR:N | 2.64 | 0.51 |
| 1:B:283:ASN:C | 1:B:283:ASN:ND2 | 2.62 | 0.51 |
| 1:B:310:TYR:OH | 1:B:355:LEU:HA | 2.11 | 0.51 |
| 1:B:374:ILE:C | 1:B:376:ARG:N | 2.64 | 0.51 |
| 1:A:163:PRO:HG2 | 1:A:164:ILE:N | 2.22 | 0.51 |
| 1:A:295:GLY:HA2 | 1:A:298:GLU:CB | 2.33 | 0.51 |
| 1:B:40:ASN:HB3 | 1:B:43:LEU:HG | 1.92 | 0.51 |
| 1:B:330:ARG:HB3 | 1:B:389:LEU:O | 2.10 | 0.51 |
| 1:B:380:ALA:HB1 | 1:B:384:MET:SD | 2.51 | 0.51 |
| 1:A:168:LYS:HE3 | 1:A:208:VAL:HG13 | 1.93 | 0.51 |



| | A L C | Interatomic | Clash |
|------------------|------------------|--------------|-------------|
| Atom-1 | Atom-2 | distance (Å) | overlap (Å) |
| 1:B:299:SER:O | 1:B:303:LYS:CG | 2.56 | 0.51 |
| 1:A:63:VAL:O | 1:A:63:VAL:CG1 | 2.59 | 0.50 |
| 1:A:75:TYR:CD2 | 1:A:297:ILE:CG2 | 2.85 | 0.50 |
| 1:A:384:MET:O | 1:B:385:THR:CB | 2.59 | 0.50 |
| 1:B:40:ASN:ND2 | 1:B:42:LYS:CB | 2.73 | 0.50 |
| 1:B:61:PRO:O | 1:B:62:SER:C | 2.48 | 0.50 |
| 1:B:301:LEU:HG | 1:B:301:LEU:O | 2.11 | 0.50 |
| 1:A:61:PRO:O | 1:A:62:SER:C | 2.48 | 0.50 |
| 1:A:114:GLY:O | 1:A:115:LYS:C | 2.49 | 0.50 |
| 1:A:301:LEU:HG | 1:A:301:LEU:O | 2.11 | 0.50 |
| 1:B:131:ALA:HB2 | 1:B:143:LEU:HD12 | 1.92 | 0.50 |
| 1:A:6:ARG:HG3 | 1:A:292:LEU:CD2 | 2.37 | 0.50 |
| 1:A:83:GLY:HA2 | 1:A:261:VAL:HG13 | 1.92 | 0.50 |
| 1:A:195:GLU:O | 1:A:196:THR:C | 2.49 | 0.50 |
| 1:A:345:LEU:HG | 1:A:346:SER:H | 1.74 | 0.50 |
| 1:B:369:ILE:CG2 | 1:B:370:GLY:N | 2.75 | 0.50 |
| 1:A:420:TRP:O | 1:A:423:ASN:N | 2.45 | 0.50 |
| 1:B:6:ARG:HG3 | 1:B:292:LEU:CD2 | 2.37 | 0.50 |
| 1:A:119:PHE:CE1 | 1:A:123:ARG:NE | 2.73 | 0.50 |
| 1:B:101:LEU:HD23 | 1:B:215:ILE:HB | 1.94 | 0.50 |
| 1:B:374:ILE:C | 1:B:374:ILE:HD13 | 2.31 | 0.50 |
| 1:A:101:LEU:HD23 | 1:A:215:ILE:HB | 1.94 | 0.50 |
| 1:A:144:LEU:HD23 | 1:A:154:VAL:HB | 1.91 | 0.50 |
| 1:A:359:LEU:CB | 1:A:360:PRO:HD2 | 2.36 | 0.50 |
| 1:A:369:ILE:CG2 | 1:A:370:GLY:N | 2.75 | 0.50 |
| 1:B:346:SER:O | 1:B:349:LEU:N | 2.43 | 0.50 |
| 1:B:420:TRP:O | 1:B:423:ASN:N | 2.45 | 0.50 |
| 1:A:243:ILE:HG12 | 1:A:269:PHE:HB2 | 1.94 | 0.50 |
| 1:A:374:ILE:C | 1:A:374:ILE:HD13 | 2.31 | 0.50 |
| 1:B:374:ILE:HD13 | 1:B:375:ARG:N | 2.27 | 0.50 |
| 1:A:123:ARG:C | 1:B:358:MET:O | 2.50 | 0.50 |
| 1:B:115:LYS:O | 1:B:118:TYR:HB3 | 2.12 | 0.50 |
| 1:B:349:LEU:HA | 1:B:352:ILE:CB | 2.36 | 0.50 |
| 1:A:374:ILE:HD13 | 1:A:375:ARG:N | 2.27 | 0.50 |
| 1:B:87:GLU:OE1 | 1:B:283:ASN:OD1 | 2.30 | 0.49 |
| 1:B:259:ALA:O | 1:B:262:ALA:HB3 | 2.11 | 0.49 |
| 1:A:244:ILE:HB | 1:A:270:ILE:HG13 | 1.94 | 0.49 |
| 1:A:385:THR:CB | 1:B:384:MET:O | 2.60 | 0.49 |
| 1:A:418:LEU:HA | 1:A:421:TYR:CD1 | 2.34 | 0.49 |
| 1:A:131:ALA:HB2 | 1:A:143:LEU:HD12 | 1.92 | 0.49 |
| 1:A:374:ILE:C | 1:A:376:ARG:N | 2.64 | 0.49 |



| | loue page | Interatomic | Clash |
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| Atom-1 | Atom-2 | distance (Å) | overlap (Å) |
| 1:B:58:GLU:O | 1:B:69:TRP:NE1 | 2.44 | 0.49 |
| 1:B:114:GLY:O | 1:B:115:LYS:C | 2.49 | 0.49 |
| 1:B:195:GLU:O | 1:B:196:THR:C | 2.49 | 0.49 |
| 1:B:243:ILE:HG12 | 1:B:269:PHE:HB2 | 1.94 | 0.49 |
| 1:A:300:ILE:HA | 1:A:303:LYS:HE3 | 1.94 | 0.49 |
| 1:B:200:GLU:OE2 | 1:B:200:GLU:C | 2.49 | 0.49 |
| 1:B:300:ILE:HD13 | 1:B:303:LYS:HZ2 | 1.77 | 0.49 |
| 1:A:281:THR:CB | 1:B:315:LYS:HD3 | 2.42 | 0.49 |
| 1:A:115:LYS:O | 1:A:118:TYR:HB3 | 2.12 | 0.49 |
| 1:A:40:ASN:HD22 | 1:A:42:LYS:H | 1.61 | 0.49 |
| 1:A:200:GLU:OE1 | 1:A:201:GLU:N | 2.46 | 0.49 |
| 1:B:63:VAL:O | 1:B:63:VAL:CG1 | 2.59 | 0.49 |
| 1:A:242:VAL:HG12 | 1:A:243:ILE:N | 2.27 | 0.49 |
| 1:B:357:ILE:O | 1:B:358:MET:CB | 2.57 | 0.49 |
| 1:B:377:TRP:CE3 | 1:B:377:TRP:N | 2.81 | 0.49 |
| 1:A:349:LEU:O | 1:A:352:ILE:N | 2.43 | 0.48 |
| 1:B:163:PRO:CG | 1:B:164:ILE:H | 2.23 | 0.48 |
| 1:A:127:VAL:HA | 1:A:181:ILE:O | 2.14 | 0.48 |
| 1:B:100:MET:HE2 | 1:B:209:LEU:HD12 | 1.95 | 0.48 |
| 1:B:244:ILE:HB | 1:B:270:ILE:HG13 | 1.94 | 0.48 |
| 1:A:207:ASP:C | 1:A:207:ASP:OD1 | 2.52 | 0.48 |
| 1:B:100:MET:HE3 | 1:B:209:LEU:HD12 | 1.95 | 0.48 |
| 1:B:207:ASP:OD1 | 1:B:207:ASP:C | 2.52 | 0.48 |
| 1:B:242:VAL:HG12 | 1:B:243:ILE:N | 2.27 | 0.48 |
| 1:A:215:ILE:HG21 | 1:A:243:ILE:CD1 | 2.43 | 0.48 |
| 1:A:358:MET:O | 1:B:123:ARG:C | 2.52 | 0.48 |
| 1:B:300:ILE:HA | 1:B:303:LYS:HE3 | 1.94 | 0.48 |
| 1:B:330:ARG:HB3 | 1:B:389:LEU:HB3 | 1.95 | 0.48 |
| 1:A:87:GLU:OE1 | 1:A:283:ASN:OD1 | 2.30 | 0.48 |
| 1:A:200:GLU:OE2 | 1:A:200:GLU:C | 2.49 | 0.48 |
| 1:A:432:LYS:HE2 | 1:B:277:ASP:CB | 2.40 | 0.48 |
| 1:B:107:SER:OG | 1:B:109:LYS:HB2 | 2.13 | 0.48 |
| 1:B:168:LYS:CE | 1:B:208:VAL:HG13 | 2.44 | 0.48 |
| 1:A:108:GLY:O | 1:A:112:THR:OG1 | 2.25 | 0.48 |
| 1:A:234:HIS:NE2 | 1:A:265:ALA:CB | 2.75 | 0.48 |
| 1:A:362:PRO:HD2 | 1:A:367:LEU:CD2 | 2.38 | 0.48 |
| 1:A:432:LYS:HE2 | 1:B:277:ASP:OD2 | 2.14 | 0.48 |
| 1:B:396:ASP:OD1 | 1:B:396:ASP:C | 2.52 | 0.48 |
| 1:A:20:GLU:O | 1:A:24:ASP:OD2 | 2.32 | 0.48 |
| 1:B:164:ILE:HD11 | 1:B:208:VAL:HG22 | 1.88 | 0.48 |
| 1:A:107:SER:OG | 1:A:109:LYS:HB2 | 2.13 | 0.48 |



| | | Interatomic | Clash |
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| Atom-1 | Atom-2 | distance (Å) | overlap (Å) |
| 1:A:277:ASP:OD2 | 1:B:432:LYS:HE2 | 2.14 | 0.48 |
| 1:B:40:ASN:HD22 | 1:B:42:LYS:H | 1.61 | 0.48 |
| 1:B:430:MET:HE3 | 1:B:430:MET:HA | 1.95 | 0.48 |
| 1:A:168:LYS:CE | 1:A:208:VAL:HG13 | 2.44 | 0.48 |
| 1:A:373:LYS:HE3 | 1:A:377:TRP:HH2 | 1.78 | 0.48 |
| 1:B:194:GLU:O | 1:B:197:LYS:HG2 | 2.14 | 0.48 |
| 1:B:215:ILE:HG21 | 1:B:243:ILE:CD1 | 2.43 | 0.48 |
| 1:B:303:LYS:C | 1:B:307:LEU:HG | 2.31 | 0.48 |
| 1:B:370:GLY:O | 1:B:373:LYS:HB3 | 2.14 | 0.48 |
| 1:A:315:LYS:HD3 | 1:B:281:THR:CB | 2.44 | 0.47 |
| 1:A:377:TRP:CE3 | 1:A:377:TRP:N | 2.81 | 0.47 |
| 1:B:127:VAL:HA | 1:B:181:ILE:O | 2.14 | 0.47 |
| 1:A:194:GLU:HA | 1:A:197:LYS:HE3 | 1.96 | 0.47 |
| 1:A:194:GLU:O | 1:A:197:LYS:HG2 | 2.14 | 0.47 |
| 1:A:376:ARG:O | 1:A:379:ALA:CB | 2.62 | 0.47 |
| 1:A:417:LEU:C | 1:A:421:TYR:CD1 | 2.88 | 0.47 |
| 1:A:430:MET:HE3 | 1:A:430:MET:HA | 1.96 | 0.47 |
| 1:A:74:VAL:O | 1:A:75:TYR:C | 2.53 | 0.47 |
| 1:A:291:ILE:O | 1:A:292:LEU:CB | 2.62 | 0.47 |
| 1:B:177:ASN:O | 1:B:178:LYS:HB2 | 2.14 | 0.47 |
| 1:A:70:PHE:O | 1:A:73:ILE:N | 2.47 | 0.47 |
| 1:A:277:ASP:CB | 1:B:432:LYS:HE2 | 2.41 | 0.47 |
| 1:A:383:SER:HB3 | 1:A:403:ILE:CA | 2.44 | 0.47 |
| 1:B:163:PRO:HG2 | 1:B:164:ILE:N | 2.22 | 0.47 |
| 1:B:247:MET:SD | 1:B:270:ILE:HD11 | 2.55 | 0.47 |
| 1:B:221:SER:CA | 1:B:250:THR:HG21 | 2.33 | 0.47 |
| 1:B:300:ILE:HD13 | 1:B:303:LYS:NZ | 2.29 | 0.47 |
| 1:B:302:GLU:CD | 1:B:341:LYS:HE3 | 2.35 | 0.47 |
| 1:B:417:LEU:C | 1:B:421:TYR:CD1 | 2.88 | 0.47 |
| 1:A:141:ASP:O | 1:A:145:GLN:HG3 | 2.15 | 0.47 |
| 1:B:376:ARG:O | 1:B:379:ALA:CB | 2.62 | 0.47 |
| 1:B:383:SER:HB3 | 1:B:403:ILE:CA | 2.44 | 0.47 |
| 1:A:98:ILE:HD13 | 1:A:171:VAL:HG11 | 1.97 | 0.47 |
| 1:A:177:ASN:O | 1:A:178:LYS:HB2 | 2.14 | 0.47 |
| 1:A:247:MET:SD | 1:A:270:ILE:HD11 | 2.55 | 0.47 |
| 1:A:302:GLU:HB3 | 1:A:341:LYS:HB3 | 1.97 | 0.47 |
| 1:A:334:ALA:HA | 1:A:337:ILE:HG22 | 1.97 | 0.47 |
| 1:A:370:GLY:O | 1:A:373:LYS:HB3 | 2.14 | 0.47 |
| 1:A:418:LEU:CA | 1:A:421:TYR:HD1 | 2.21 | 0.47 |
| 1:B:20:GLU:O | 1:B:24:ASP:OD2 | 2.32 | 0.47 |
| 1:B:61:PRO:O | 1:B:62:SER:O | 2.33 | 0.47 |



| | • • • • • • | Interatomic | Clash |
|------------------|------------------|-------------------------|-------------|
| Atom-1 | Atom-2 | distance (\AA) | overlap (Å) |
| 1:B:194:GLU:HA | 1:B:197:LYS:HE3 | 1.96 | 0.47 |
| 1:B:200:GLU:OE1 | 1:B:201:GLU:N | 2.46 | 0.47 |
| 1:A:61:PRO:O | 1:A:62:SER:O | 2.33 | 0.47 |
| 1:A:317:MET:CE | 1:A:328:THR:HB | 2.45 | 0.47 |
| 1:B:98:ILE:HD13 | 1:B:171:VAL:HG11 | 1.97 | 0.47 |
| 1:A:362:PRO:CD | 1:A:367:LEU:HD23 | 2.33 | 0.47 |
| 1:B:302:GLU:HB3 | 1:B:341:LYS:HB3 | 1.97 | 0.47 |
| 1:A:85:ASP:OD1 | 1:A:285:LYS:HE2 | 2.15 | 0.47 |
| 1:A:300:ILE:HD13 | 1:A:303:LYS:NZ | 2.29 | 0.47 |
| 1:A:302:GLU:CD | 1:A:341:LYS:HE3 | 2.34 | 0.47 |
| 1:B:235:GLN:C | 1:B:237:SER:H | 2.18 | 0.47 |
| 1:B:367:LEU:O | 1:B:368:LYS:CB | 2.63 | 0.47 |
| 1:A:115:LYS:HG2 | 1:A:276:ILE:O | 2.14 | 0.46 |
| 1:A:235:GLN:C | 1:A:237:SER:H | 2.18 | 0.46 |
| 1:A:330:ARG:HB3 | 1:A:389:LEU:HB3 | 1.95 | 0.46 |
| 1:B:40:ASN:ND2 | 1:B:42:LYS:H | 2.13 | 0.46 |
| 1:B:115:LYS:HG2 | 1:B:276:ILE:O | 2.14 | 0.46 |
| 1:B:190:HIS:CG | 1:B:197:LYS:CD | 2.79 | 0.46 |
| 1:B:378:LEU:O | 1:B:381:LEU:CG | 2.60 | 0.46 |
| 1:A:40:ASN:ND2 | 1:A:42:LYS:HB2 | 2.31 | 0.46 |
| 1:A:119:PHE:CZ | 1:A:123:ARG:CZ | 2.98 | 0.46 |
| 1:A:135:TYR:CE1 | 1:A:189:ARG:NE | 2.83 | 0.46 |
| 1:A:301:LEU:HD21 | 1:A:305:LYS:HZ1 | 1.77 | 0.46 |
| 1:A:367:LEU:O | 1:A:368:LYS:CB | 2.63 | 0.46 |
| 1:A:417:LEU:C | 1:A:421:TYR:CE1 | 2.89 | 0.46 |
| 1:B:300:ILE:HA | 1:B:303:LYS:HG2 | 1.97 | 0.46 |
| 1:B:317:MET:CE | 1:B:328:THR:HB | 2.45 | 0.46 |
| 1:B:334:ALA:CA | 1:B:337:ILE:HG22 | 2.46 | 0.46 |
| 1:A:94:LYS:N | 1:A:97:PHE:CE2 | 2.68 | 0.46 |
| 1:B:74:VAL:O | 1:B:75:TYR:C | 2.53 | 0.46 |
| 1:B:85:ASP:OD1 | 1:B:285:LYS:HE2 | 2.15 | 0.46 |
| 1:B:119:PHE:CE1 | 1:B:123:ARG:NE | 2.74 | 0.46 |
| 1:B:230:ALA:O | 1:B:231:SER:C | 2.54 | 0.46 |
| 1:A:40:ASN:ND2 | 1:A:42:LYS:H | 2.13 | 0.46 |
| 1:A:317:MET:SD | 1:A:328:THR:CB | 3.04 | 0.46 |
| 1:B:207:ASP:O | 1:B:210:LYS:HG3 | 2.16 | 0.46 |
| 1:B:313:ILE:CD1 | 1:B:331:ASP:OD1 | 2.56 | 0.46 |
| 1:B:336:ILE:HG13 | 1:B:377:TRP:HB3 | 1.98 | 0.46 |
| 1:B:379:ALA:C | 1:B:380:ALA:O | 2.52 | 0.46 |
| 1:A:109:LYS:O | 1:A:110:THR:HB | 2.16 | 0.46 |
| 1:A:163:PRO:CG | 1:A:164:ILE:H | 2.23 | 0.46 |



| | A L O | Interatomic | Clash | |
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| Atom-1 | Atom-2 | distance (Å) | overlap (Å) | |
| 1:A:215:ILE:CG2 | 1:A:243:ILE:HG13 | 2.46 | 0.46 | |
| 1:A:230:ALA:O | 1:A:231:SER:C | 2.54 | 0.46 | |
| 1:A:300:ILE:HA | 1:A:303:LYS:HG2 | 1.97 | 0.46 | |
| 1:B:270:ILE:O | 1:B:270:ILE:CG2 | 2.64 | 0.46 | |
| 1:B:298:GLU:O | 1:B:302:GLU:HG2 | 2.16 | 0.46 | |
| 1:A:193:GLY:N | 1:A:195:GLU:OE2 | 2.42 | 0.46 | |
| 1:A:334:ALA:CA | 1:A:337:ILE:HG22 | 2.46 | 0.46 | |
| 1:A:361:THR:HG23 | 1:A:367:LEU:HG | 1.98 | 0.46 | |
| 1:A:361:THR:CB | 1:A:367:LEU:CD1 | 2.93 | 0.46 | |
| 1:B:141:ASP:O | 1:B:145:GLN:HG3 | 2.15 | 0.46 | |
| 1:B:362:PRO:HD2 | 1:B:367:LEU:CD2 | 2.38 | 0.46 | |
| 1:B:417:LEU:C | 1:B:421:TYR:CE1 | 2.89 | 0.46 | |
| 1:A:270:ILE:O | 1:A:270:ILE:CG2 | 2.63 | 0.46 | |
| 1:A:300:ILE:C | 1:A:302:GLU:N | 2.69 | 0.46 | |
| 1:A:301:LEU:O | 1:A:305:LYS:CD | 2.61 | 0.46 | |
| 1:A:303:LYS:C | 1:A:307:LEU:HG | 2.31 | 0.46 | |
| 1:B:9:VAL:HG11 | 1:B:292:LEU:HD13 | 1.98 | 0.46 | |
| 1:B:135:TYR:CE1 | 1:B:189:ARG:NE | 2.83 | 0.46 | |
| 1:B:397:LYS:O | 1:B:398:SER:C | 2.53 | 0.46 | |
| 1:A:125:TYR:CD2 | 1:B:358:MET:SD | 3.09 | 0.46 | |
| 1:A:336:ILE:HG13 | 1:A:377:TRP:HB3 | 1.98 | 0.46 | |
| 1:B:303:LYS:O | 1:B:307:LEU:CG | 2.49 | 0.46 | |
| 1:A:330:ARG:CB | 1:A:389:LEU:HB3 | 2.46 | 0.46 | |
| 1:A:300:ILE:CD1 | 1:A:303:LYS:HZ2 | 2.28 | 0.46 | |
| 1:B:298:GLU:C | 1:B:300:ILE:N | 2.67 | 0.46 | |
| 1:B:310:TYR:HA | 1:B:335:GLN:NE2 | 2.29 | 0.46 | |
| 1:B:334:ALA:HA | 1:B:337:ILE:HG22 | 1.97 | 0.46 | |
| 1:B:361:THR:CB | 1:B:367:LEU:CD1 | 2.93 | 0.46 | |
| 1:B:378:LEU:CA | 1:B:381:LEU:HD11 | 2.45 | 0.46 | |
| 1:A:75:TYR:CZ | 1:A:292:LEU:HD12 | 2.50 | 0.45 | |
| 1:A:122:LYS:C | 1:A:124:GLY:N | 2.70 | 0.45 | |
| 1:B:307:LEU:HD23 | 1:B:307:LEU:N | 2.31 | 0.45 | |
| 1:A:292:LEU:HD23 | 1:A:292:LEU:HA | 1.61 | 0.45 | |
| 1:A:396:ASP:OD1 | 1:A:396:ASP:C | 2.52 | 0.45 | |
| 1:B:392:PRO:O | 1:B:395:ILE:HG13 | 2.16 | 0.45 | |
| 1:A:378:LEU:O | 1:A:381:LEU:CG | 2.60 | 0.45 | |
| 1:B:2:LEU:HD13 | 1:B:291:ILE:CG2 | 2.46 | 0.45 | |
| 1:B:94:LYS:O | 1:B:96:PRO:O | 2.34 | 0.45 | |
| 1:B:40:ASN:ND2 | 1:B:42:LYS:HB2 | 2.31 | 0.45 | |
| 1:B:70:PHE:O | 1:B:73:ILE:N | 2.47 | 0.45 | |
| 1:B:119:PHE:CZ | 1:B:123:ARG:CZ | 2.98 | 0.45 | |



| | lo uo pugom | Interatomic | Clash | |
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| Atom-1 | Atom-2 | distance (Å) | overlap (Å) | |
| 1:B:215:ILE:CG2 | 1:B:243:ILE:HG13 | 2.46 | 0.45 | |
| 1:B:301:LEU:O | 1:B:305:LYS:CD | 2.61 | 0.45 | |
| 1:A:235:GLN:C | 1:A:237:SER:N | 2.70 | 0.45 | |
| 1:A:307:LEU:N | 1:A:307:LEU:HD23 | 2.31 | 0.45 | |
| 1:A:335:GLN:O | 1:A:338:ALA:HB3 | 2.17 | 0.45 | |
| 1:B:2:LEU:HD11 | 1:B:288:VAL:HA | 1.98 | 0.45 | |
| 1:B:75:TYR:CZ | 1:B:292:LEU:HD12 | 2.50 | 0.45 | |
| 1:A:9:VAL:HG11 | 1:A:292:LEU:HD13 | 1.98 | 0.45 | |
| 1:A:93:THR:HG22 | 1:A:93:THR:O | 2.16 | 0.45 | |
| 1:A:207:ASP:O | 1:A:210:LYS:HG3 | 2.16 | 0.45 | |
| 1:A:298:GLU:O | 1:A:302:GLU:HG2 | 2.16 | 0.45 | |
| 1:A:349:LEU:HA | 1:A:352:ILE:CB | 2.36 | 0.45 | |
| 1:A:392:PRO:O | 1:A:395:ILE:HG13 | 2.17 | 0.45 | |
| 1:B:93:THR:O | 1:B:93:THR:HG22 | 2.16 | 0.45 | |
| 1:B:109:LYS:O | 1:B:110:THR:HB | 2.16 | 0.45 | |
| 1:B:111:THR:HG22 | 1:B:115:LYS:HE3 | 1.98 | 0.45 | |
| 1:B:116:LEU:HD12 | 1:B:116:LEU:HA | 1.70 | 0.45 | |
| 1:B:212:ASP:O | 1:B:213:ASP:OD1 | 2.35 | 0.45 | |
| 1:B:335:GLN:O | 1:B:338:ALA:HB3 | 2.17 | 0.45 | |
| 1:A:2:LEU:HD11 | 1:A:288:VAL:HA | 1.98 | 0.45 | |
| 1:A:125:TYR:CG | 1:B:358:MET:SD | 3.10 | 0.45 | |
| 1:A:417:LEU:CB | 1:A:421:TYR:HE1 | 2.21 | 0.45 | |
| 1:B:300:ILE:CA | 1:B:303:LYS:HG2 | 2.47 | 0.45 | |
| 1:B:317:MET:SD | 1:B:328:THR:CB | 3.04 | 0.45 | |
| 1:B:391:ASN:O | 1:B:392:PRO:C | 2.55 | 0.45 | |
| 1:A:94:LYS:O | 1:A:96:PRO:O | 2.34 | 0.45 | |
| 1:A:164:ILE:HD11 | 1:A:208:VAL:HG22 | 1.88 | 0.45 | |
| 1:A:168:LYS:HG3 | 1:A:172:ASP:OD2 | 2.17 | 0.45 | |
| 1:B:300:ILE:C | 1:B:302:GLU:H | 2.19 | 0.45 | |
| 1:B:40:ASN:HD22 | 1:B:42:LYS:HB3 | 1.82 | 0.45 | |
| 1:B:300:ILE:HA | 1:B:303:LYS:CD | 2.47 | 0.45 | |
| 1:A:50:LYS:HD3 | 1:A:77:GLU:OE1 | 2.17 | 0.45 | |
| 1:A:94:LYS:CA | 1:A:97:PHE:CZ | 3.00 | 0.45 | |
| 1:A:336:ILE:HD11 | 1:A:377:TRP:CD1 | 2.52 | 0.45 | |
| 1:A:397:LYS:O | 1:A:398:SER:C | 2.53 | 0.45 | |
| 1:B:301:LEU:O | 1:B:305:LYS:CG | 2.65 | 0.45 | |
| 1:B:330:ARG:CB | 1:B:389:LEU:HB3 | 2.46 | 0.45 | |
| 1:B:372:GLU:O | 1:B:374:ILE:CG2 | 2.62 | 0.45 | |
| 1:A:100:MET:HE2 | 1:A:209:LEU:HD12 | 2.00 | 0.44 | |
| 1:A:300:ILE:C | 1:A:302:GLU:H | 2.19 | 0.44 | |
| 1:A:300:ILE:CA | 1:A:303:LYS:HG2 | 2.47 | 0.44 | |



| | lo ao pagom | Interatomic | Clash | |
|------------------|------------------|--------------|-------------|--|
| Atom-1 | Atom-2 | distance (Å) | overlap (Å) | |
| 1:A:373:LYS:O | 1:A:373:LYS:HG3 | 2.17 | 0.44 | |
| 1:B:373:LYS:HG3 | 1:B:373:LYS:O | 2.17 | 0.44 | |
| 1:A:212:ASP:O | 1:A:213:ASP:OD1 | 2.35 | 0.44 | |
| 1:A:300:ILE:HA | 1:A:303:LYS:CD | 2.47 | 0.44 | |
| 1:A:301:LEU:O | 1:A:305:LYS:CG | 2.65 | 0.44 | |
| 1:A:335:GLN:HA | 1:A:335:GLN:OE1 | 2.17 | 0.44 | |
| 1:B:207:ASP:OD1 | 1:B:210:LYS:NZ | 2.50 | 0.44 | |
| 1:B:234:HIS:NE2 | 1:B:265:ALA:CB | 2.75 | 0.44 | |
| 1:B:418:LEU:CA | 1:B:421:TYR:HD1 | 2.22 | 0.44 | |
| 1:A:157:GLU:OE2 | 1:A:169:LYS:HD2 | 2.17 | 0.44 | |
| 1:A:336:ILE:HA | 1:A:339:LEU:HD23 | 1.99 | 0.44 | |
| 1:B:30:LEU:HD23 | 1:B:48:THR:CG2 | 2.47 | 0.44 | |
| 1:B:47:LEU:CD1 | 1:B:77:GLU:HB3 | 2.48 | 0.44 | |
| 1:B:150:ILE:HG13 | 1:B:152:VAL:CG2 | 2.39 | 0.44 | |
| 1:B:168:LYS:HG3 | 1:B:172:ASP:OD2 | 2.17 | 0.44 | |
| 1:B:349:LEU:O | 1:B:352:ILE:N | 2.43 | 0.44 | |
| 1:B:361:THR:HG23 | 1:B:367:LEU:HG | 1.98 | 0.44 | |
| 1:A:298:GLU:C | 1:A:300:ILE:N | 2.67 | 0.44 | |
| 1:B:23:VAL:HG13 | 1:B:70:PHE:CZ | 2.53 | 0.44 | |
| 1:B:192:TYR:HE1 | 1:B:229:LEU:HD23 | 1.83 | 0.44 | |
| 1:B:336:ILE:HA | 1:B:339:LEU:HD23 | 1.99 | 0.44 | |
| 1:A:47:LEU:CD1 | 1:A:77:GLU:HB3 | 2.48 | 0.44 | |
| 1:A:53:GLU:O | 1:A:57:LYS:HG3 | 2.18 | 0.44 | |
| 1:A:111:THR:HG22 | 1:A:115:LYS:HE3 | 1.98 | 0.44 | |
| 1:A:198:LEU:O | 1:A:201:GLU:HB3 | 2.18 | 0.44 | |
| 1:B:53:GLU:O | 1:B:57:LYS:HG3 | 2.18 | 0.44 | |
| 1:B:157:GLU:OE2 | 1:B:169:LYS:HD2 | 2.17 | 0.44 | |
| 1:B:333:TYR:O | 1:B:334:ALA:C | 2.55 | 0.44 | |
| 1:A:71:ILE:O | 1:A:74:VAL:HB | 2.18 | 0.44 | |
| 1:A:378:LEU:CA | 1:A:381:LEU:HD11 | 2.45 | 0.44 | |
| 1:B:94:LYS:CA | 1:B:97:PHE:CZ | 3.00 | 0.44 | |
| 1:A:40:ASN:HD22 | 1:A:42:LYS:HB3 | 1.82 | 0.44 | |
| 1:A:302:GLU:CD | 1:A:341:LYS:CD | 2.86 | 0.44 | |
| 1:A:402:ARG:CB | 1:B:402:ARG:NH1 | 2.79 | 0.44 | |
| 1:B:410:GLU:HG2 | 1:B:411:VAL:N | 2.33 | 0.44 | |
| 1:A:23:VAL:HG13 | 1:A:70:PHE:CZ | 2.53 | 0.44 | |
| 1:B:50:LYS:HD3 | 1:B:77:GLU:OE1 | 2.17 | 0.44 | |
| 1:B:164:ILE:O | 1:B:165:GLU:C | 2.56 | 0.44 | |
| 1:B:291:ILE:O | 1:B:292:LEU:CB | 2.62 | 0.44 | |
| 1:B:300:ILE:C | 1:B:302:GLU:N | 2.69 | 0.44 | |
| 1:B:335:GLN:HA | 1:B:335:GLN:OE1 | 2.17 | 0.44 | |



| | | Interatomic | Clash | |
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| Atom-1 | Atom-2 | distance (Å) | overlap (Å) | |
| 1:B:361:THR:HA | 1:B:367:LEU:CG | 2.40 | 0.44 | |
| 1:A:164:ILE:O | 1:A:165:GLU:C | 2.56 | 0.44 | |
| 1:A:303:LYS:HG3 | 1:A:304:VAL:N | 2.30 | 0.44 | |
| 1:A:348:VAL:HG12 | 1:A:352:ILE:CD1 | 2.45 | 0.44 | |
| 1:B:69:TRP:CD1 | 1:B:73:ILE:HD11 | 2.53 | 0.44 | |
| 1:B:298:GLU:O | 1:B:299:SER:C | 2.56 | 0.44 | |
| 1:A:207:ASP:OD1 | 1:A:210:LYS:NZ | 2.50 | 0.43 | |
| 1:A:244:ILE:HG13 | 1:A:267:ILE:HD13 | 1.99 | 0.43 | |
| 1:B:122:LYS:C | 1:B:124:GLY:N | 2.70 | 0.43 | |
| 1:B:198:LEU:O | 1:B:201:GLU:HB3 | 2.18 | 0.43 | |
| 1:A:41:VAL:O | 1:A:41:VAL:CG1 | 2.65 | 0.43 | |
| 1:A:64:LEU:HD11 | 1:A:303:LYS:HZ3 | 1.83 | 0.43 | |
| 1:A:69:TRP:CD1 | 1:A:73:ILE:HD11 | 2.53 | 0.43 | |
| 1:B:71:ILE:O | 1:B:74:VAL:HB | 2.18 | 0.43 | |
| 1:B:78:LEU:O | 1:B:79:SER:C | 2.56 | 0.43 | |
| 1:B:302:GLU:CD | 1:B:341:LYS:CD | 2.86 | 0.43 | |
| 1:A:2:LEU:HD23 | 1:A:2:LEU:HA | 1.79 | 0.43 | |
| 1:A:104:VAL:HG21 | 1:A:192:TYR:CE2 | 2.53 | 0.43 | |
| 1:A:109:LYS:HE2 | 1:A:186:THR:O | 2.18 | 0.43 | |
| 1:A:176:LYS:O | 1:A:177:ASN:C | 2.56 | 0.43 | |
| 1:A:176:LYS:O | 1:A:178:LYS:HG2 | 2.18 | 0.43 | |
| 1:A:298:GLU:O | 1:A:299:SER:C | 2.56 | 0.43 | |
| 1:A:349:LEU:HA | 1:A:352:ILE:HD12 | 2.00 | 0.43 | |
| 1:A:372:GLU:O | 1:A:374:ILE:CG2 | 2.62 | 0.43 | |
| 1:B:41:VAL:O | 1:B:41:VAL:CG1 | 2.65 | 0.43 | |
| 1:A:2:LEU:HD13 | 1:A:291:ILE:CG2 | 2.46 | 0.43 | |
| 1:B:235:GLN:C | 1:B:237:SER:N | 2.70 | 0.43 | |
| 1:B:349:LEU:HA | 1:B:352:ILE:HD12 | 2.00 | 0.43 | |
| 1:A:83:GLY:HA2 | 1:A:261:VAL:CG1 | 2.48 | 0.43 | |
| 1:A:163:PRO:O | 1:A:166:ILE:N | 2.52 | 0.43 | |
| 1:A:199:LEU:HA | 1:A:202:MET:SD | 2.59 | 0.43 | |
| 1:A:410:GLU:HG2 | 1:A:411:VAL:N | 2.33 | 0.43 | |
| 1:B:131:ALA:O | 1:B:140:TYR:CE2 | 2.69 | 0.43 | |
| 1:A:192:TYR:HE1 | 1:A:229:LEU:HD23 | 1.83 | 0.43 | |
| 1:B:2:LEU:HD23 | 1:B:2:LEU:HA | 1.79 | 0.43 | |
| 1:B:119:PHE:HZ | 1:B:123:ARG:HH21 | 1.48 | 0.43 | |
| 1:B:244:ILE:HG13 | 1:B:267:ILE:HD13 | 1.99 | 0.43 | |
| 1:B:293:GLY:O | 1:B:296:ASP:HB2 | 2.18 | 0.43 | |
| 1:B:403:ILE:HG22 | 1:B:414:VAL:CG2 | 2.45 | 0.43 | |
| 1:B:417:LEU:CB | 1:B:421:TYR:HE1 | 2.21 | 0.43 | |
| 1:A:293:GLY:O | 1:A:296:ASP:HB2 | 2.18 | 0.43 | |



| | A L O | Interatomic | Clash | |
|------------------|--------------------------|-------------------------|-------------|--|
| Atom-1 | Atom-2 | distance (\AA) | overlap (Å) | |
| 1:B:105:GLN:O | 1:B:106:GLY:C | 2.56 | 0.43 | |
| 1:B:163:PRO:O | 1:B:166:ILE:N | 2.52 | 0.43 | |
| 1:B:302:GLU:CD | 1:B:341:LYS:HD2 | 2.39 | 0.43 | |
| 1:A:247:MET:HG3 | 1:A:270:ILE:CD1 | 2.48 | 0.43 | |
| 1:A:291:ILE:O | 1:A:291:ILE:HG13 | 2.19 | 0.43 | |
| 1:A:301:LEU:HD21 | 1:A:305:LYS:HZ2 | 1.83 | 0.43 | |
| 1:A:358:MET:SD | 1:B:125:TYR:CD2 | 3.12 | 0.43 | |
| 1:B:2:LEU:HB3 | 1:B:291:ILE:HG22 | 2.01 | 0.43 | |
| 1:B:199:LEU:HA | 1:B:202:MET:SD | 2.59 | 0.43 | |
| 1:B:336:ILE:HD11 | 1:B:377:TRP:CD1 | 2.52 | 0.43 | |
| 1:B:348:VAL:HG12 | 1:B:352:ILE:CD1 | 2.45 | 0.43 | |
| 1:B:109:LYS:HE2 | 1:B:186:THR:O | 2.18 | 0.43 | |
| 1:B:247:MET:HG3 | 1:B:270:ILE:CD1 | 2.48 | 0.43 | |
| 1:B:291:ILE:O | 1:B:291:ILE:HG13 | 2.19 | 0.43 | |
| 1:B:303:LYS:HG3 | 1:B:304:VAL:N | 2.30 | 0.43 | |
| 1:A:131:ALA:O | 1:A:140:TYR:CE2 | 2.69 | 0.43 | |
| 1:A:175:VAL:HG12 | 1:A:175:VAL:O | 2.19 | 0.43 | |
| 1:B:127:VAL:HG12 | 1:B:128:GLY:N | 2.34 | 0.43 | |
| 1:B:146:LEU:HD22 | 1:B:276:ILE:HD13 | 2.00 | 0.43 | |
| 1:B:210:LYS:N | 1:B:211:PRO:CD | 2.82 | 0.43 | |
| 1:A:124:GLY:HA3 | 24:GLY:HA3 1:B:359:LEU:N | | 0.42 | |
| 1:A:219:ASP:CG | 1:A:221:SER:HG | 2.19 | 0.42 | |
| 1:A:333:TYR:O | 1:A:334:ALA:C | 2.55 | 0.42 | |
| 1:A:391:ASN:O | 1:A:392:PRO:C | 2.55 | 0.42 | |
| 1:B:104:VAL:HG21 | 1:B:192:TYR:CE2 | 2.53 | 0.42 | |
| 1:B:163:PRO:CG | 1:B:164:ILE:N | 2.82 | 0.42 | |
| 1:A:403:ILE:HG22 | 1:A:414:VAL:CG2 | 2.45 | 0.42 | |
| 1:B:40:ASN:O | 1:B:44:VAL:HG23 | 2.19 | 0.42 | |
| 1:B:176:LYS:O | 1:B:178:LYS:HG2 | 2.18 | 0.42 | |
| 1:A:302:GLU:CD | 1:A:341:LYS:HD2 | 2.39 | 0.42 | |
| 1:B:107:SER:C | 1:B:109:LYS:N | 2.71 | 0.42 | |
| 1:B:335:GLN:CB | 1:B:355:LEU:HD22 | 2.46 | 0.42 | |
| 1:A:37:SER:O | 1:A:38:ASP:HB3 | 2.19 | 0.42 | |
| 1:B:83:GLY:HA2 | 1:B:261:VAL:CG1 | 2.48 | 0.42 | |
| 1:B:157:GLU:HB2 | 1:B:160:ASN:HD22 | 1.77 | 0.42 | |
| 1:A:210:LYS:N | 1:A:211:PRO:CD | 2.82 | 0.42 | |
| 1:B:383:SER:O | 1:B:384:MET:HG3 | 2.20 | 0.42 | |
| 1:A:2:LEU:HB3 | 1:A:291:ILE:HG22 | 2.01 | 0.42 | |
| 1:A:30:LEU:HD23 | 1:A:48:THR:CG2 | 2.47 | 0.42 | |
| 1:A:72:SER:OG | 1:A:73:ILE:N | 2.53 | 0.42 | |
| 1:A:76:ASP:O | 1:A:79:SER:HB3 | 2.19 | 0.42 | |



| | | Interatomic | Clash | |
|------------------|------------------|-------------------------|-------------|--|
| Atom-1 | Atom-2 | distance (\AA) | overlap (Å) | |
| 1:A:222:ILE:HD12 | 1:A:222:ILE:HA | 1.93 | 0.42 | |
| 1:A:299:SER:C | 1:A:303:LYS:HE3 | 2.40 | 0.42 | |
| 1:A:383:SER:O | 1:A:384:MET:HG3 | 2.20 | 0.42 | |
| 1:B:302:GLU:CD | 1:B:341:LYS:CE | 2.88 | 0.42 | |
| 1:B:368:LYS:O | 1:B:369:ILE:HB | 2.20 | 0.42 | |
| 1:A:310:TYR:OH | 1:A:354:GLY:O | 2.37 | 0.42 | |
| 1:A:358:MET:SD | 1:B:125:TYR:CG | 3.13 | 0.42 | |
| 1:A:376:ARG:O | 1:A:379:ALA:HB3 | 2.19 | 0.42 | |
| 1:B:283:ASN:HD21 | 1:B:285:LYS:HG2 | 1.85 | 0.42 | |
| 1:A:40:ASN:O | 1:A:44:VAL:HG23 | 2.19 | 0.42 | |
| 1:A:146:LEU:HD22 | 1:A:276:ILE:HD13 | 2.00 | 0.42 | |
| 1:A:334:ALA:C | 1:A:337:ILE:HG22 | 2.40 | 0.42 | |
| 1:A:383:SER:HB2 | 1:A:403:ILE:HG23 | 1.97 | 0.42 | |
| 1:B:35:ILE:O | 1:B:36:SER:C | 2.57 | 0.42 | |
| 1:B:37:SER:O | 1:B:38:ASP:HB3 | 2.20 | 0.42 | |
| 1:A:167:ALA:C | 1:A:209:LEU:HD21 | 2.40 | 0.42 | |
| 1:A:227:TYR:O | 1:A:228:ASP:C | 2.57 | 0.42 | |
| 1:A:303:LYS:O | 1:A:307:LEU:CG | 2.49 | 0.42 | |
| 1:B:13:LEU:HA | 1:B:13:LEU:HD23 | 1.84 | 0.42 | |
| 1:A:283:ASN:HD21 | 1:A:285:LYS:HG2 | 1.85 | 0.42 | |
| 1:B:76:ASP:O | 1:B:79:SER:HB3 | 2.19 | 0.42 | |
| 1:B:227:TYR:O | 1:B:228:ASP:C | 2.57 | 0.42 | |
| 1:A:105:GLN:O | 1:A:106:GLY:C | 2.56 | 0.41 | |
| 1:A:302:GLU:CD | 1:A:341:LYS:CE | 2.88 | 0.41 | |
| 1:B:121:LYS:O | 1:B:124:GLY:N | 2.52 | 0.41 | |
| 1:B:202:MET:O | 1:B:203:LYS:C | 2.59 | 0.41 | |
| 1:B:347:LYS:HD2 | 1:B:350:GLN:HE21 | 1.84 | 0.41 | |
| 1:A:127:VAL:HG12 | 1:A:128:GLY:N | 2.34 | 0.41 | |
| 1:B:20:GLU:HA | 1:B:20:GLU:OE1 | 2.20 | 0.41 | |
| 1:B:298:GLU:O | 1:B:300:ILE:N | 2.54 | 0.41 | |
| 1:B:377:TRP:CA | 1:B:377:TRP:HE3 | 2.33 | 0.41 | |
| 1:A:284:ALA:O | 1:A:286:ARG:N | 2.52 | 0.41 | |
| 1:B:64:LEU:CD1 | 1:B:303:LYS:HZ3 | 2.33 | 0.41 | |
| 1:B:113:ALA:O | 1:B:129:LEU:HD21 | 2.21 | 0.41 | |
| 1:B:116:LEU:HD23 | 1:B:183:ILE:HD13 | 2.03 | 0.41 | |
| 1:A:1:MET:SD | 1:A:37:SER:OG | 2.79 | 0.41 | |
| 1:A:116:LEU:HD23 | 1:A:183:ILE:HD13 | 2.03 | 0.41 | |
| 1:A:138:ALA:O | 1:A:142:GLN:HB2 | 2.20 | 0.41 | |
| 1:A:379:ALA:C | 1:A:380:ALA:O | 2.52 | 0.41 | |
| 1:A:381:LEU:HB2 | 1:A:382:ASN:H | 1.54 | 0.41 | |
| 1:B:299:SER:C | 1:B:303:LYS:HE3 | 2.40 | 0.41 | |



| Interatomic Clash | | | | | |
|-------------------|------------------|--------------|-------------|--|--|
| Atom-1 | Atom-2 | distance (Å) | overlap (Å) | | |
| 1:B:334:ALA:C | 1:B:337:ILE:HG22 | 2.39 | 0.41 | | |
| 1:B:373:LYS:HE3 | 1:B:377:TRP:HH2 | 1.78 | 0.41 | | |
| 1:B:383:SER:HB3 | 1:B:403:ILE:HA | 2.03 | 0.41 | | |
| 1:A:350:GLN:HG3 | 1:A:351:HIS:CD2 | 2.56 | 0.41 | | |
| 1:B:15:GLY:HA2 | 1:B:67:LYS:HZ2 | 1.78 | 0.41 | | |
| 1:B:138:ALA:O | 1:B:142:GLN:HB2 | 2.20 | 0.41 | | |
| 1:B:284:ALA:O | 1:B:286:ARG:N | 2.52 | 0.41 | | |
| 1:B:350:GLN:HG3 | 1:B:351:HIS:CD2 | 2.56 | 0.41 | | |
| 1:B:376:ARG:O | 1:B:379:ALA:HB3 | 2.19 | 0.41 | | |
| 1:A:368:LYS:O | 1:A:369:ILE:HB | 2.20 | 0.41 | | |
| 1:A:381:LEU:N | 1:A:381:LEU:CD2 | 2.62 | 0.41 | | |
| 1:B:219:ASP:CG | 1:B:221:SER:HG | 2.21 | 0.41 | | |
| 1:B:244:ILE:HG21 | 1:B:257:LEU:CD1 | 2.51 | 0.41 | | |
| 1:A:107:SER:C | 1:A:109:LYS:N | 2.71 | 0.41 | | |
| 1:A:202:MET:O | 1:A:203:LYS:C | 2.58 | 0.41 | | |
| 1:A:333:TYR:O | 1:A:337:ILE:HG22 | 2.21 | 0.41 | | |
| 1:A:402:ARG:NH1 | 1:B:402:ARG:CB | 2.79 | 0.41 | | |
| 1:B:383:SER:HB2 | 1:B:403:ILE:HG23 | 1.97 | 0.41 | | |
| 1:A:143:LEU:HA | 1:A:143:LEU:HD23 | 1.81 | 0.41 | | |
| 1:A:335:GLN:CB | 1:A:355:LEU:HD22 | 2.46 | 0.41 | | |
| 1:A:379:ALA:HB1 | 1:A:409:LEU:HD11 | 2.03 | 0.41 | | |
| 1:A:430:MET:HA | 1:A:430:MET:CE | 2.50 | 0.41 | | |
| 1:B:168:LYS:HE3 | 1:B:208:VAL:CG1 | 2.51 | 0.41 | | |
| 1:A:20:GLU:HA | 1:A:20:GLU:OE1 | 2.20 | 0.41 | | |
| 1:A:78:LEU:O | 1:A:79:SER:C | 2.56 | 0.41 | | |
| 1:A:113:ALA:O | 1:A:129:LEU:HD21 | 2.20 | 0.41 | | |
| 1:A:116:LEU:HA | 1:A:116:LEU:HD12 | 1.70 | 0.41 | | |
| 1:A:131:ALA:HB1 | 1:A:140:TYR:CD2 | 2.56 | 0.41 | | |
| 1:A:157:GLU:HB2 | 1:A:160:ASN:HD22 | 1.77 | 0.41 | | |
| 1:A:284:ALA:O | 1:A:287:PHE:N | 2.54 | 0.41 | | |
| 1:A:347:LYS:HD2 | 1:A:350:GLN:HE21 | 1.84 | 0.41 | | |
| 1:B:167:ALA:C | 1:B:209:LEU:HD21 | 2.40 | 0.41 | | |
| 1:B:175:VAL:O | 1:B:175:VAL:HG12 | 2.19 | 0.41 | | |
| 1:B:300:ILE:CD1 | 1:B:303:LYS:HZ2 | 2.33 | 0.41 | | |
| 1:A:47:LEU:C | 1:A:49:ALA:H | 2.24 | 0.41 | | |
| 1:A:168:LYS:HE3 | 1:A:208:VAL:CG1 | 2.51 | 0.41 | | |
| 1:A:179:MET:HA | 1:A:179:MET:HE1 | 1.99 | 0.41 | | |
| 1:A:310:TYR:HA | 1:A:335:GLN:NE2 | 2.29 | 0.41 | | |
| 1:B:264:GLY:O | 1:B:265:ALA:O | 2.39 | 0.41 | | |
| 1:B:381:LEU:HB2 | 1:B:382:ASN:H | 1.53 | 0.41 | | |
| 1:A:347:LYS:O | 1:A:347:LYS:CG | 2.69 | 0.40 | | |



| Atom 1 | A + a | Interatomic | Clash |
|------------------|------------------|-------------------------|-------------|
| Atom-1 | Atom-2 | distance (\AA) | overlap (Å) |
| 1:A:430:MET:O | 1:A:432:LYS:N | 2.55 | 0.40 |
| 1:B:6:ARG:CA | 1:B:292:LEU:HD21 | 2.51 | 0.40 |
| 1:B:131:ALA:HB1 | 1:B:140:TYR:CD2 | 2.56 | 0.40 |
| 1:B:377:TRP:O | 1:B:381:LEU:HD11 | 2.22 | 0.40 |
| 1:B:423:ASN:O | 1:B:423:ASN:ND2 | 2.55 | 0.40 |
| 1:A:35:ILE:O | 1:A:36:SER:C | 2.57 | 0.40 |
| 1:A:119:PHE:CE1 | 1:A:123:ARG:NH2 | 2.88 | 0.40 |
| 1:A:121:LYS:O | 1:A:124:GLY:N | 2.52 | 0.40 |
| 1:A:264:GLY:O | 1:A:265:ALA:O | 2.39 | 0.40 |
| 1:A:281:THR:HG21 | 1:B:315:LYS:HZ2 | 1.77 | 0.40 |
| 1:A:383:SER:HB3 | 1:A:403:ILE:HA | 2.03 | 0.40 |
| 1:A:420:TRP:O | 1:A:421:TYR:C | 2.60 | 0.40 |
| 1:B:127:VAL:HG13 | 1:B:181:ILE:O | 2.22 | 0.40 |
| 1:B:312:LYS:O | 1:B:315:LYS:N | 2.54 | 0.40 |
| 1:B:331:ASP:O | 1:B:332:VAL:CB | 2.70 | 0.40 |
| 1:A:298:GLU:O | 1:A:300:ILE:N | 2.54 | 0.40 |
| 1:A:377:TRP:O | 1:A:381:LEU:HD11 | 2.21 | 0.40 |
| 1:A:397:LYS:N | 1:A:400:MET:CE | 2.85 | 0.40 |
| 1:A:419:GLU:O | 1:A:419:GLU:HG3 | 2.21 | 0.40 |
| 1:B:47:LEU:C | 1:B:49:ALA:H | 2.24 | 0.40 |
| 1:B:329:LEU:HD22 | 1:B:392:PRO:CG | 2.51 | 0.40 |
| 1:B:349:LEU:N | 1:B:352:ILE:HD12 | 2.37 | 0.40 |
| 1:B:380:ALA:O | 1:B:381:LEU:CG | 2.70 | 0.40 |
| 1:A:127:VAL:HG13 | 1:A:181:ILE:O | 2.22 | 0.40 |
| 1:A:313:ILE:HG21 | 1:A:335:GLN:NE2 | 2.37 | 0.40 |
| 1:B:333:TYR:O | 1:B:337:ILE:HG22 | 2.21 | 0.40 |
| 1:B:83:GLY:CA | 1:B:261:VAL:CG1 | 3.00 | 0.40 |
| 1:B:430:MET:HA | 1:B:430:MET:CE | 2.51 | 0.40 |

All (43) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic | Clash |
|----------------|-------------------------|--------------|-------------|
| Atom-1 | At0111-2 | distance (Å) | overlap (Å) |
| 1:A:360:PRO:CB | 1:B:362:PRO:CA[8_454] | 1.18 | 1.02 |
| 1:A:362:PRO:CA | 1:B:360:PRO:CB[8_454] | 1.24 | 0.96 |
| 1:A:200:GLU:CB | 1:B:203:LYS:CB[6_555] | 1.41 | 0.79 |
| 1:A:203:LYS:CB | $1:B:200:GLU:CB[6_555]$ | 1.45 | 0.75 |
| 1:A:360:PRO:CB | 1:B:362:PRO:CB[8_454] | 1.57 | 0.63 |
| 1:A:362:PRO:CB | 1:B:360:PRO:CB[8_454] | 1.69 | 0.51 |
| 1:A:362:PRO:C | 1:B:360:PRO:CB[8_454] | 1.78 | 0.42 |



| 1 | O7V | |
|---|--------------------|--|
| Т | $Q \Delta \Lambda$ | |

| A 4 amo 1 | | Interatomic | Clash | |
|-----------------|-------------------------|-------------------------|-------------|--|
| Atom-1 | Atom-2 | distance (\AA) | overlap (Å) | |
| 1:A:360:PRO:CB | 1:B:362:PRO:C[8_454] | 1.79 | 0.41 | |
| 1:A:367:LEU:CD1 | 1:B:367:LEU:CD2[8_454] | 1.83 | 0.37 | |
| 1:A:196:THR:CB | 1:B:207:ASP:CB[6_555] | 1.85 | 0.35 | |
| 1:A:207:ASP:CB | 1:B:196:THR:CB[6_555] | 1.85 | 0.35 | |
| 1:A:200:GLU:O | $1:B:200:GLU:O[6_555]$ | 1.89 | 0.31 | |
| 1:A:204:GLU:CB | 1:B:197:LYS:CA[6_555] | 1.90 | 0.30 | |
| 1:A:367:LEU:CD2 | 1:B:367:LEU:CD1[8_454] | 1.90 | 0.30 | |
| 1:A:197:LYS:CA | 1:B:204:GLU:CB[6_555] | 1.92 | 0.28 | |
| 1:A:207:ASP:CB | 1:B:196:THR:CG2[6_555] | 1.92 | 0.28 | |
| 1:A:196:THR:CG2 | 1:B:207:ASP:CB[6_555] | 1.93 | 0.27 | |
| 1:A:200:GLU:CG | $1:B:204:GLU:N[6_555]$ | 2.03 | 0.17 | |
| 1:A:204:GLU:N | $1:B:200:GLU:CG[6_555]$ | 2.03 | 0.17 | |
| 1:A:41:VAL:CG1 | 1:B:41:VAL:CG1[6_554] | 2.04 | 0.16 | |
| 1:A:207:ASP:OD2 | 1:B:196:THR:OG1[6_555] | 2.04 | 0.16 | |
| 1:A:360:PRO:CA | 1:B:362:PRO:CA[8_454] | 2.04 | 0.16 | |
| 1:A:196:THR:OG1 | 1:B:207:ASP:OD2[6_555] | 2.07 | 0.13 | |
| 1:A:207:ASP:CG | 1:B:196:THR:OG1[6_555] | 2.10 | 0.10 | |
| 1:A:362:PRO:CA | 1:B:360:PRO:CA[8_454] | 2.10 | 0.10 | |
| 1:A:207:ASP:OD2 | 1:B:196:THR:CB[6_555] | 2.12 | 0.08 | |
| 1:A:363:SER:N | 1:B:360:PRO:CB[8_454] | 2.12 | 0.08 | |
| 1:A:196:THR:OG1 | $1:B:207:ASP:CG[6_555]$ | 2.13 | 0.07 | |
| 1:A:196:THR:CB | 1:B:207:ASP:OD2[6_555] | 2.13 | 0.07 | |
| 1:A:197:LYS:CA | $1:B:204:GLU:CA[6_555]$ | 2.14 | 0.06 | |
| 1:A:204:GLU:CA | 1:B:197:LYS:CA[6_555] | 2.14 | 0.06 | |
| 1:A:200:GLU:C | $1:B:200:GLU:O[6_555]$ | 2.15 | 0.05 | |
| 1:A:200:GLU:O | $1:B:200:GLU:C[6_555]$ | 2.15 | 0.05 | |
| 1:A:197:LYS:CB | $1:B:204:GLU:CB[6_555]$ | 2.16 | 0.04 | |
| 1:A:200:GLU:CG | 1:B:200:GLU:O[6_555] | 2.16 | 0.04 | |
| 1:A:204:GLU:CB | 1:B:197:LYS:CB[6_555] | 2.16 | 0.04 | |
| 1:A:200:GLU:O | 1:B:200:GLU:CG[6_555] | 2.17 | 0.03 | |
| 1:A:200:GLU:CA | 1:B:203:LYS:CB[6_555] | 2.17 | 0.03 | |
| 1:A:200:GLU:OE2 | 1:B:200:GLU:OE2[6_555] | 2.19 | 0.01 | |
| 1:A:200:GLU:OE1 | $1:B:204:GLU:CB[6_555]$ | 2.19 | 0.01 | |
| 1:A:200:GLU:CB | 1:B:203:LYS:CA[6_555] | 2.19 | 0.01 | |
| 1:A:203:LYS:CB | $1:B:200:GLU:CA[6_555]$ | 2.19 | 0.01 | |
| 1:A:204:GLU:CB | 1:B:200:GLU:OE1[6_555] | 2.19 | 0.01 | |



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 | Perce | entiles |
|-----|-------|---------------|-----------|-----------|----------|-------|---------|
| 1 | А | 421/440 (96%) | 294 (70%) | 87 (21%) | 40 (10%) | 0 | 10 |
| 1 | В | 421/440 (96%) | 293 (70%) | 88 (21%) | 40 (10%) | 0 | 10 |
| All | All | 842/880 (96%) | 587 (70%) | 175 (21%) | 80 (10%) | 0 | 10 |

All (80) Ramachandran outliers are listed below:

| Mol | Chain | \mathbf{Res} | Type |
|-----|-------|----------------|------|
| 1 | А | 63 | VAL |
| 1 | А | 236 | ALA |
| 1 | А | 265 | ALA |
| 1 | А | 332 | VAL |
| 1 | А | 343 | GLY |
| 1 | А | 347 | LYS |
| 1 | А | 357 | ILE |
| 1 | А | 358 | MET |
| 1 | А | 359 | LEU |
| 1 | А | 369 | ILE |
| 1 | А | 373 | LYS |
| 1 | А | 379 | ALA |
| 1 | А | 380 | ALA |
| 1 | В | 63 | VAL |
| 1 | В | 236 | ALA |
| 1 | В | 265 | ALA |
| 1 | В | 332 | VAL |
| 1 | В | 343 | GLY |
| 1 | В | 347 | LYS |
| 1 | В | 357 | ILE |
| 1 | В | 358 | MET |
| 1 | В | 359 | LEU |
| 1 | В | 369 | ILE |
| 1 | В | 373 | LYS |
| 1 | В | 379 | ALA |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | В | 380 | ALA |
| 1 | А | 15 | GLY |
| 1 | А | 16 | SER |
| 1 | А | 62 | SER |
| 1 | А | 106 | GLY |
| 1 | А | 110 | THR |
| 1 | А | 177 | ASN |
| 1 | А | 179 | MET |
| 1 | А | 284 | ALA |
| 1 | А | 292 | LEU |
| 1 | А | 300 | ILE |
| 1 | А | 329 | LEU |
| 1 | А | 356 | GLY |
| 1 | А | 368 | LYS |
| 1 | А | 404 | ALA |
| 1 | В | 15 | GLY |
| 1 | В | 16 | SER |
| 1 | В | 62 | SER |
| 1 | В | 106 | GLY |
| 1 | В | 110 | THR |
| 1 | В | 177 | ASN |
| 1 | В | 179 | MET |
| 1 | В | 284 | ALA |
| 1 | В | 292 | LEU |
| 1 | В | 300 | ILE |
| 1 | В | 329 | LEU |
| 1 | В | 356 | GLY |
| 1 | В | 368 | LYS |
| 1 | В | 404 | ALA |
| 1 | А | 195 | GLU |
| 1 | А | 316 | LYS |
| 1 | В | 195 | GLU |
| 1 | В | 316 | LYS |
| 1 | A | 84 | GLY |
| 1 | А | 285 | LYS |
| 1 | A | 315 | LYS |
| 1 | А | 397 | LYS |
| 1 | В | 84 | GLY |
| 1 | В | 285 | LYS |
| 1 | В | 315 | LYS |
| 1 | В | 397 | LYS |
| 1 | А | 18 | PRO |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | А | 361 | THR |
| 1 | А | 381 | LEU |
| 1 | А | 431 | VAL |
| 1 | В | 18 | PRO |
| 1 | В | 361 | THR |
| 1 | В | 381 | LEU |
| 1 | В | 431 | VAL |
| 1 | А | 158 | PRO |
| 1 | А | 164 | ILE |
| 1 | В | 158 | PRO |
| 1 | В | 164 | ILE |
| 1 | А | 163 | PRO |
| 1 | В | 163 | PRO |

5.3.2 Protein sidechains (i)

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 | А | 365/377~(97%) | 340~(93%) | 25~(7%) | 16 44 |
| 1 | В | 365/377~(97%) | 340~(93%) | 25~(7%) | 16 44 |
| All | All | 730/754~(97%) | 680 (93%) | 50 (7%) | 16 44 |

All (50) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | А | 1 | MET |
| 1 | А | 16 | SER |
| 1 | А | 17 | THR |
| 1 | А | 59 | LYS |
| 1 | А | 72 | SER |
| 1 | А | 136 | ARG |
| 1 | А | 143 | LEU |
| 1 | А | 200 | GLU |
| 1 | А | 250 | THR |
| 1 | А | 283 | ASN |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | А | 297 | ILE |
| 1 | А | 310 | TYR |
| 1 | А | 311 | ASP |
| 1 | А | 328 | THR |
| 1 | А | 331 | ASP |
| 1 | А | 349 | LEU |
| 1 | А | 357 | ILE |
| 1 | А | 359 | LEU |
| 1 | А | 361 | THR |
| 1 | А | 374 | ILE |
| 1 | А | 377 | TRP |
| 1 | А | 381 | LEU |
| 1 | А | 384 | MET |
| 1 | А | 386 | TYR |
| 1 | А | 423 | ASN |
| 1 | В | 1 | MET |
| 1 | В | 16 | SER |
| 1 | В | 17 | THR |
| 1 | В | 59 | LYS |
| 1 | В | 72 | SER |
| 1 | В | 136 | ARG |
| 1 | В | 143 | LEU |
| 1 | В | 200 | GLU |
| 1 | В | 250 | THR |
| 1 | В | 283 | ASN |
| 1 | В | 297 | ILE |
| 1 | В | 310 | TYR |
| 1 | В | 311 | ASP |
| 1 | В | 328 | THR |
| 1 | В | 331 | ASP |
| 1 | В | 349 | LEU |
| 1 | В | 357 | ILE |
| 1 | В | 359 | LEU |
| 1 | В | 361 | THR |
| 1 | В | 374 | ILE |
| 1 | В | 377 | TRP |
| 1 | В | 381 | LEU |
| 1 | В | 384 | MET |
| 1 | В | 386 | TYR |
| 1 | В | 423 | ASN |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | А | 4 | ASN |
| 1 | А | 31 | GLN |
| 1 | А | 40 | ASN |
| 1 | А | 91 | ASN |
| 1 | А | 148 | ASN |
| 1 | А | 160 | ASN |
| 1 | А | 190 | HIS |
| 1 | А | 224 | GLN |
| 1 | А | 234 | HIS |
| 1 | А | 235 | GLN |
| 1 | А | 283 | ASN |
| 1 | А | 350 | GLN |
| 1 | А | 351 | HIS |
| 1 | В | 4 | ASN |
| 1 | В | 31 | GLN |
| 1 | В | 40 | ASN |
| 1 | В | 91 | ASN |
| 1 | В | 148 | ASN |
| 1 | В | 160 | ASN |
| 1 | В | 190 | HIS |
| 1 | В | 224 | GLN |
| 1 | В | 234 | HIS |
| 1 | В | 235 | GLN |
| 1 | В | 283 | ASN |
| 1 | В | 350 | GLN |
| 1 | В | 351 | HIS |

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.



5.6 Ligand geometry (i)

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 (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

