# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 09:16 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 2EXW |
| Title | : | Crystal structure of a EcClC-Fab complex in the absence of bound ions |
| Authors | : | Lobet, S.; Dutzler, R. |
| Deposited on | : | 2005-11-09 |
| Resolution | : | 3.20 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 ⓘ symbol.

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

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

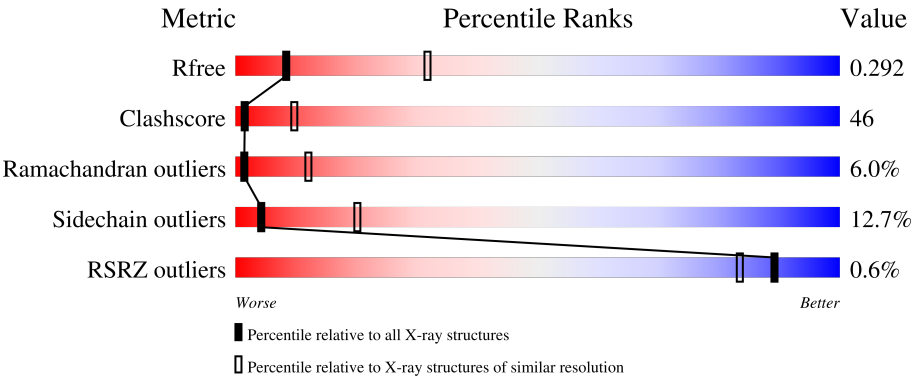
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.35 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & 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-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 130704 | 1133 (3.20-3.20) |
| Clashscore | 141614 | 1253 (3.20-3.20) |
| Ramachandran outliers | 138981 | 1234 (3.20-3.20) |
| Sidechain outliers | 138945 | 1233 (3.20-3.20) |
| RSRZ outliers | 127900 | 1095 (3.20-3.20) |

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 473 | 42% 46% 5% 6% |
| 1 | B | 473 | 42% 45% 6% 7% |
| 2 | C | 222 | % 36% 47% 14% . |
| 2 | E | 222 | % 31% 50% 17% . |
| 3 | D | 211 | 29% 54% 16% . |

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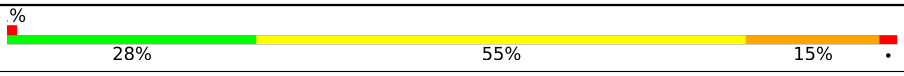
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 3 | F | 211 |   |

# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13223 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called H(+)/Cl(-) exchange transporter clcA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 444 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3333 | 2190 | 560 | 563 | 20 | | | |
| 1 | B | 441 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3304 | 2174 | 553 | 557 | 20 | | | |

- Molecule 2 is a protein called Fab Fragment (Heavy Chain).

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | C | 221 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1672 | 1077 | 274 | 315 | 6 | | | |
| 2 | E | 221 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1672 | 1077 | 274 | 315 | 6 | | | |

- Molecule 3 is a protein called Fab Fragment (Light Chain).

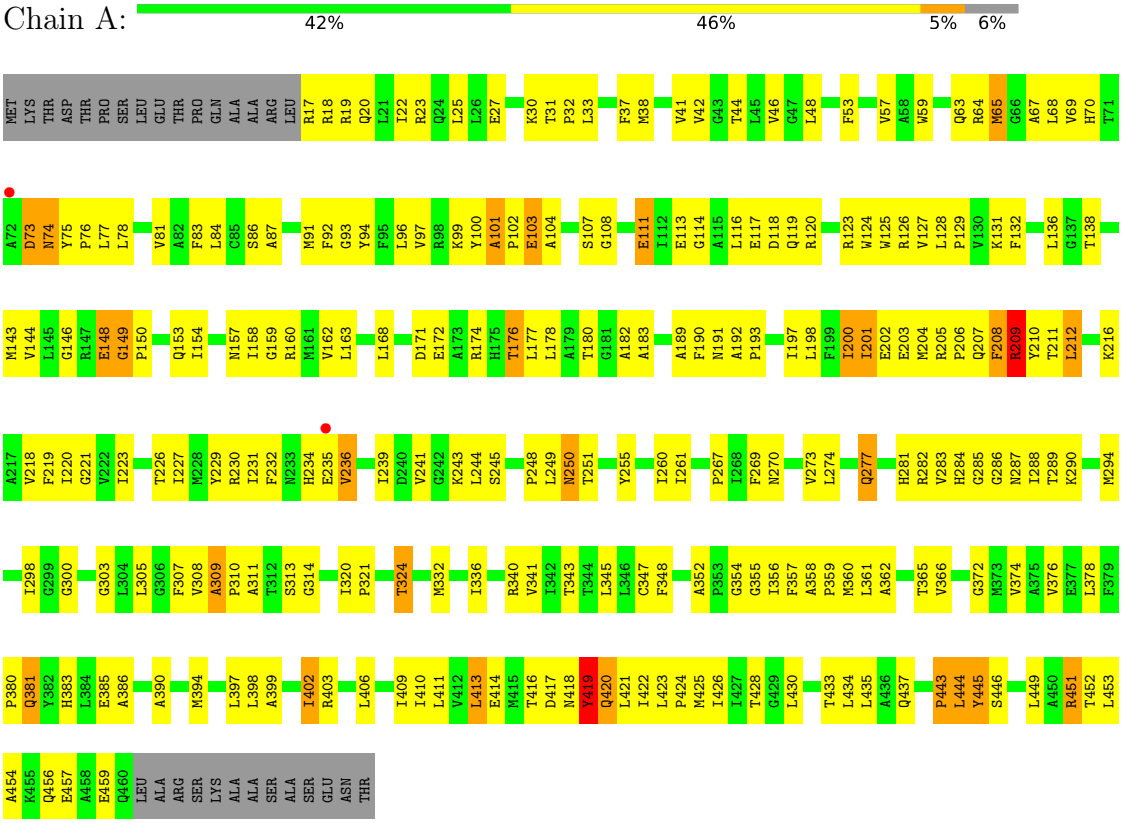
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | D | 211 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1621 | 1008 | 271 | 334 | 8 | | | |
| 3 | F | 211 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1621 | 1008 | 271 | 334 | 8 | | | |

# 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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

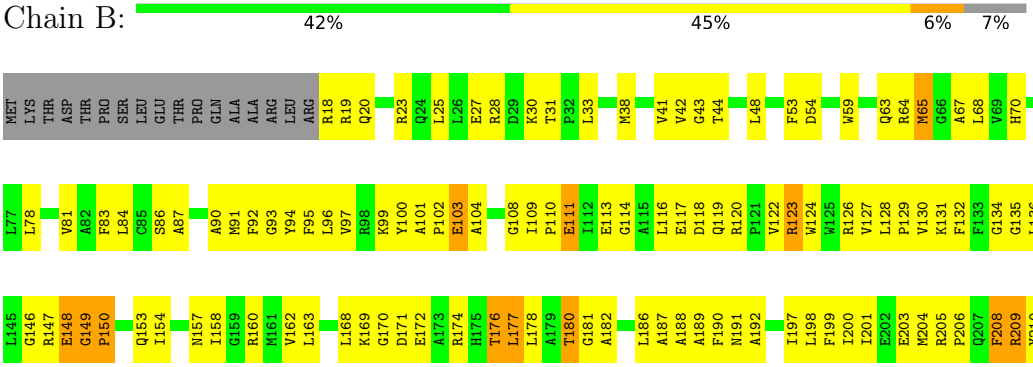
• Molecule 1: H(+)/Cl(-) exchange transporter clcA

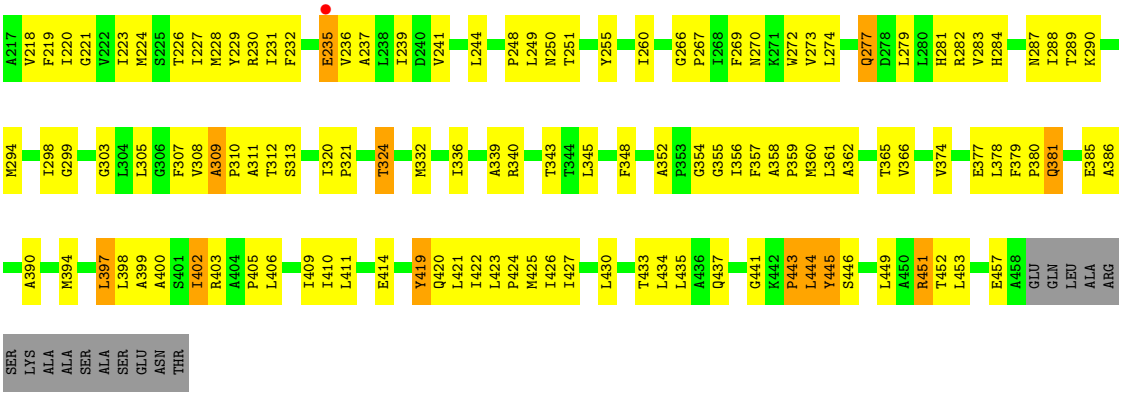
Chain A:



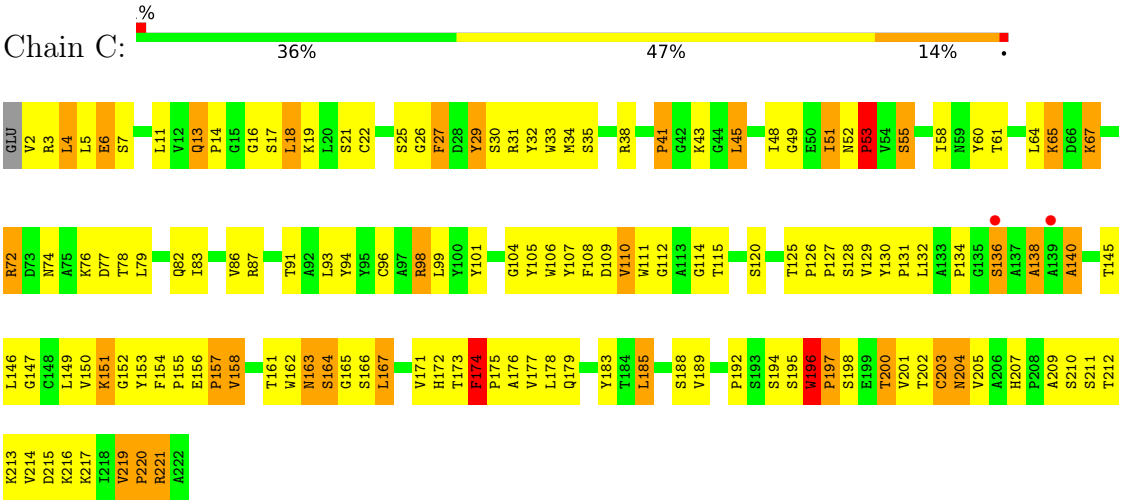

• Molecule 1: H(+)/Cl(-) exchange transporter clcA

Chain B:

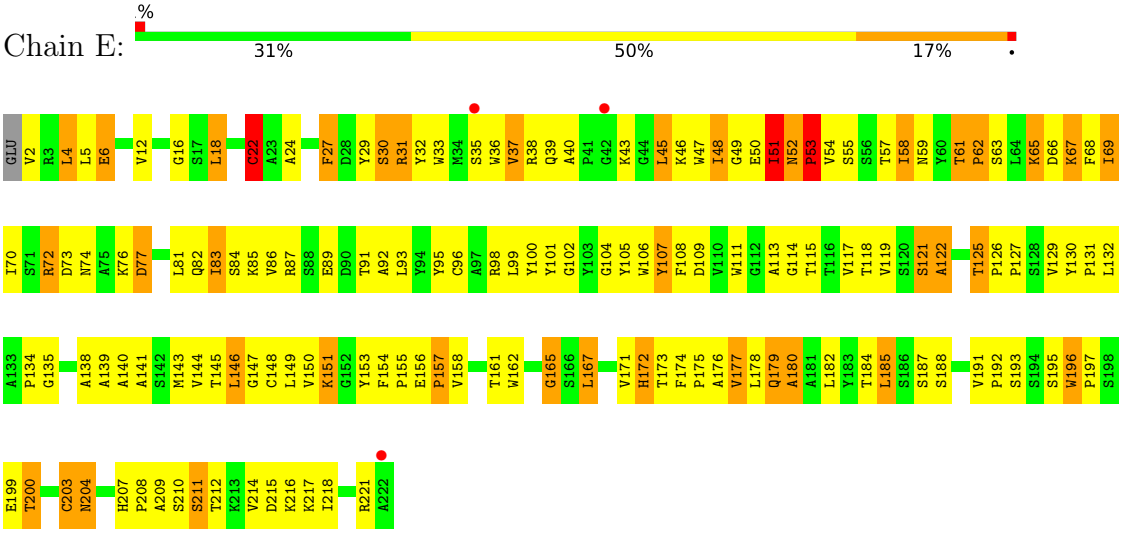




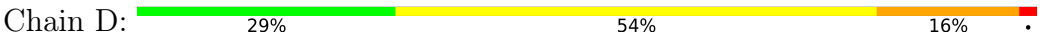
• Molecule 2: Fab Fragment (Heavy Chain)

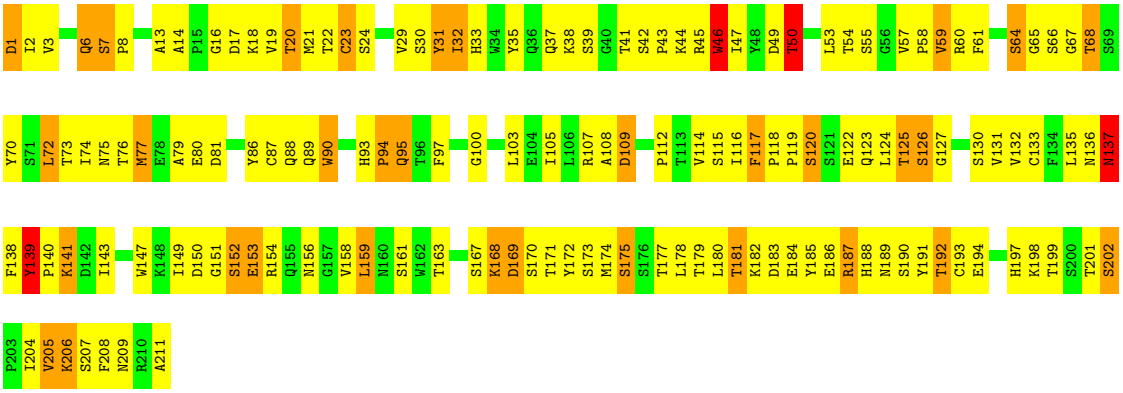



• Molecule 2: Fab Fragment (Heavy Chain)



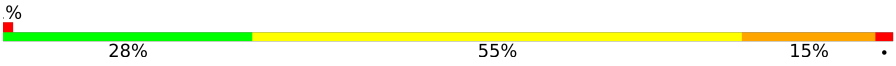

• Molecule 3: Fab Fragment (Light Chain)

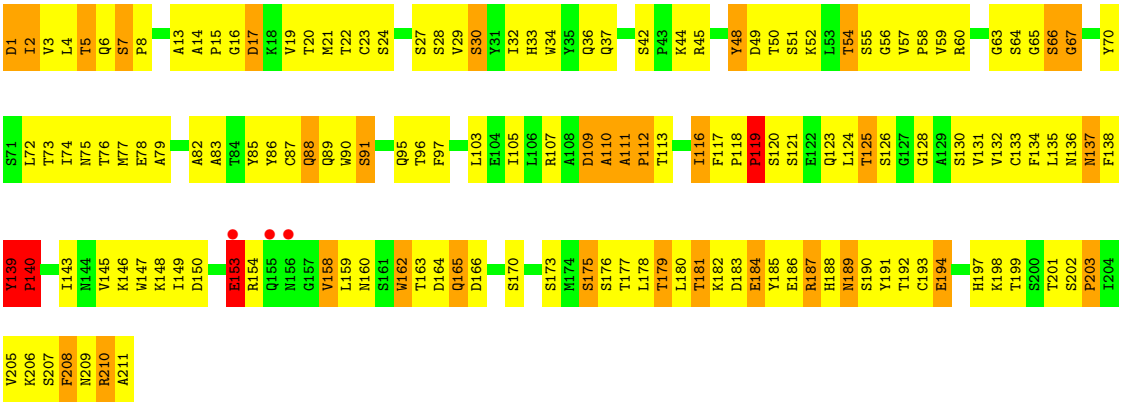





• Molecule 3: Fab Fragment (Light Chain)

Chain F:



# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | C 1 2 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 219.83Å 122.44Å 151.34Å<br>90.00° 128.16° 90.00° | Depositor |
| Resolution (Å) | 19.98 – 3.20<br>19.98 – 3.20 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 98.0 (19.98-3.20)<br>98.1 (19.98-3.20) | Depositor<br>EDS |
| $R_{merge}$ | 0.10 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 3.93 (at 3.22Å) | Xtriage |
| Refinement program | CNS 1.1 | Depositor |
| R, $R_{free}$ | 0.268 , 0.314<br>0.261 , 0.292 | Depositor<br>DCC |
| $R_{free}$ test set | 2524 reflections (4.86%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 86.6 | Xtriage |
| Anisotropy | 0.519 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.28 , 61.7 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.51$, $< L^2 > = 0.35$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.91 | EDS |
| Total number of atoms | 13223 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 79.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

# 5 Model quality

## 5.1 Standard geometry

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|$ >5 | RMSZ | #$\|Z\|$ >5 |
| 1 | A | 0.43 | 0/3405 | 0.65 | 0/4621 |
| 1 | B | 0.48 | 0/3376 | 0.68 | 0/4583 |
| 2 | C | 0.56 | 0/1721 | 0.94 | 4/2355 (0.2%) |
| 2 | E | 0.56 | 0/1721 | 0.94 | 4/2355 (0.2%) |
| 3 | D | 0.44 | 0/1660 | 0.85 | 1/2257 (0.0%) |
| 3 | F | 0.72 | 6/1660 (0.4%) | 1.04 | 8/2257 (0.4%) |
| All | All | 0.52 | 6/13543 (0.0%) | 0.82 | 17/18428 (0.1%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | A | 0 | 1 |
| 1 | B | 0 | 1 |
| 2 | C | 0 | 1 |
| 2 | E | 0 | 1 |
| 3 | D | 0 | 1 |
| 3 | F | 0 | 1 |
| All | All | 0 | 6 |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | F | 139 | TYR | C-O | -8.93 | 1.06 | 1.23 |
| 3 | F | 140 | PRO | CA-C | 7.08 | 1.67 | 1.52 |
| 3 | F | 140 | PRO | C-O | 5.35 | 1.33 | 1.23 |
| 3 | F | 139 | TYR | CD2-CE2 | 5.27 | 1.47 | 1.39 |
| 3 | F | 140 | PRO | N-CA | 5.16 | 1.56 | 1.47 |
| 3 | F | 139 | TYR | CG-CD2 | 5.00 | 1.45 | 1.39 |

All (17) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | F | 139 | TYR | C-N-CA | -8.08 | 88.07 | 122.00 |
| 3 | F | 110 | ALA | N-CA-C | 7.11 | 130.20 | 111.00 |
| 3 | F | 140 | PRO | CA-N-CD | -6.57 | 102.30 | 111.50 |
| 3 | F | 140 | PRO | CA-C-O | 6.33 | 135.38 | 120.20 |
| 2 | E | 22 | CYS | CA-CB-SG | 6.07 | 124.92 | 114.00 |
| 2 | C | 158 | VAL | N-CA-C | -6.03 | 94.73 | 111.00 |
| 2 | C | 93 | LEU | CA-CB-CG | 5.52 | 127.99 | 115.30 |
| 2 | C | 196 | TRP | N-CA-C | 5.43 | 125.66 | 111.00 |
| 3 | F | 140 | PRO | N-CA-C | 5.42 | 126.19 | 112.10 |
| 2 | C | 61 | THR | N-CA-C | -5.40 | 96.41 | 111.00 |
| 3 | F | 139 | TYR | C-N-CD | 5.28 | 139.48 | 128.40 |
| 3 | D | 139 | TYR | C-N-CD | 5.20 | 139.32 | 128.40 |
| 2 | E | 148 | CYS | CA-CB-SG | 5.18 | 123.33 | 114.00 |
| 3 | F | 140 | PRO | CA-C-N | -5.17 | 105.82 | 117.20 |
| 2 | E | 31 | ARG | CG-CD-NE | -5.17 | 100.95 | 111.80 |
| 2 | E | 102 | GLY | N-CA-C | -5.11 | 100.32 | 113.10 |
| 3 | F | 139 | TYR | N-CA-CB | 5.10 | 119.77 | 110.60 |

There are no chirality outliers.

All (6) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 419 | TYR | Sidechain |
| 1 | B | 419 | TYR | Sidechain |
| 2 | C | 29 | TYR | Sidechain |
| 3 | D | 139 | TYR | Sidechain |
| 2 | E | 101 | TYR | Sidechain |
| 3 | F | 139 | TYR | Mainchain |

## 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 | A | 3333 | 0 | 3484 | 289 | 0 |
| 1 | B | 3304 | 0 | 3457 | 269 | 0 |
| 2 | C | 1672 | 0 | 1654 | 183 | 0 |
| 2 | E | 1672 | 0 | 1654 | 165 | 0 |
| 3 | D | 1621 | 0 | 1546 | 194 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 3 | F | 1621 | 0 | 1546 | 234 | 0 |
| All | All | 13223 | 0 | 13341 | 1220 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 46.

All (1220) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:E:207:HIS:ND1 | 2:E:210:SER:HB2 | 1.52 | 1.23 |
| 1:A:235:GLU:O | 1:A:236:VAL:HG23 | 1.47 | 1.12 |
| 1:A:223:ILE:HD11 | 1:B:426:ILE:HG22 | 1.33 | 1.10 |
| 3:F:7:SER:HB2 | 3:F:22:THR:HB | 1.34 | 1.08 |
| 3:D:16:GLY:HA2 | 3:D:76:THR:HG23 | 1.35 | 1.07 |
| 3:F:192:THR:HA | 3:F:207:SER:HB3 | 1.38 | 1.06 |
| 1:A:381:GLN:HE21 | 1:A:381:GLN:N | 1.54 | 1.05 |
| 3:F:13:ALA:HB3 | 3:F:77:MET:HE1 | 1.39 | 1.03 |
| 2:C:51:ILE:HD11 | 2:C:55:SER:HB3 | 1.41 | 1.02 |
| 3:F:36:GLN:HG3 | 3:F:85:TYR:HE2 | 1.17 | 1.02 |
| 3:F:194:GLU:HG2 | 3:F:205:VAL:HG12 | 1.42 | 1.02 |
| 2:C:51:ILE:HD13 | 2:C:72:ARG:HD2 | 1.41 | 1.02 |
| 3:F:111:ALA:H | 3:F:199:THR:HG21 | 1.25 | 1.01 |
| 1:B:381:GLN:HE21 | 1:B:381:GLN:N | 1.57 | 1.01 |
| 3:F:139:TYR:O | 3:F:140:PRO:C | 1.86 | 1.01 |
| 1:B:287:ASN:ND2 | 1:B:290:LYS:H | 1.58 | 1.00 |
| 3:D:31:TYR:HA | 3:D:50:THR:OG1 | 1.61 | 1.00 |
| 1:A:381:GLN:H | 1:A:381:GLN:NE2 | 1.59 | 0.99 |
| 1:B:381:GLN:H | 1:B:381:GLN:NE2 | 1.61 | 0.99 |
| 1:A:426:ILE:HG22 | 1:B:223:ILE:HD11 | 1.44 | 0.99 |
| 2:C:177:VAL:HG21 | 3:D:159:LEU:HD13 | 1.43 | 0.97 |
| 1:A:287:ASN:ND2 | 1:A:290:LYS:H | 1.60 | 0.97 |
| 1:A:423:LEU:HB3 | 1:A:424:PRO:HD3 | 1.44 | 0.96 |
| 1:A:216:LYS:HE2 | 1:B:433:THR:HG22 | 1.48 | 0.95 |
| 2:E:45:LEU:HD11 | 3:F:86:TYR:CD1 | 2.01 | 0.95 |
| 2:E:107:TYR:HB3 | 3:F:33:HIS:CD2 | 2.01 | 0.94 |
| 3:D:22:THR:HG22 | 3:D:23:CYS:H | 1.30 | 0.94 |
| 1:A:18:ARG:HH11 | 1:B:457:GLU:HB3 | 1.31 | 0.94 |
| 1:A:457:GLU:HG3 | 1:B:18:ARG:HH11 | 1.32 | 0.94 |
| 3:F:190:SER:HA | 3:F:209:ASN:OD1 | 1.69 | 0.93 |
| 3:F:65:GLY:HA3 | 3:F:70:TYR:CD2 | 2.04 | 0.92 |
| 2:C:2:VAL:HG23 | 2:C:27:PHE:CD1 | 2.05 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:223:ILE:HD11 | 1:B:426:ILE:CG2 | 2.01 | 0.91 |
| 1:A:38:MET:HG3 | 1:A:168:LEU:HD11 | 1.53 | 0.91 |
| 1:B:176:THR:O | 1:B:180:THR:HG23 | 1.71 | 0.91 |
| 3:F:139:TYR:O | 3:F:140:PRO:O | 1.88 | 0.91 |
| 1:A:241:VAL:HG12 | 1:A:244:LEU:HD21 | 1.53 | 0.90 |
| 1:B:38:MET:HG3 | 1:B:168:LEU:HD11 | 1.50 | 0.90 |
| 3:F:36:GLN:HG3 | 3:F:85:TYR:CE2 | 2.06 | 0.90 |
| 1:A:116:LEU:HD23 | 1:A:178:LEU:HD23 | 1.54 | 0.90 |
| 3:F:14:ALA:O | 3:F:17:ASP:HB2 | 1.70 | 0.89 |
| 1:A:443:PRO:HB2 | 1:A:446:SER:HB2 | 1.51 | 0.89 |
| 1:A:212:LEU:HD12 | 1:A:212:LEU:H | 1.38 | 0.89 |
| 1:B:320:ILE:HG21 | 1:B:394:MET:HE1 | 1.54 | 0.89 |
| 2:E:162:TRP:CZ3 | 2:E:203:CYS:HB3 | 2.09 | 0.88 |
| 3:F:20:THR:HG23 | 3:F:73:THR:OG1 | 1.74 | 0.88 |
| 2:C:127:PRO:HB3 | 2:C:153:TYR:HB3 | 1.55 | 0.87 |
| 2:E:207:HIS:ND1 | 2:E:210:SER:CB | 2.38 | 0.87 |
| 1:B:212:LEU:HD12 | 1:B:212:LEU:H | 1.40 | 0.86 |
| 3:D:95:GLN:CD | 3:D:95:GLN:H | 1.72 | 0.86 |
| 2:C:35:SER:HB2 | 2:C:49:GLY:O | 1.76 | 0.86 |
| 1:B:443:PRO:HB2 | 1:B:446:SER:HB2 | 1.58 | 0.86 |
| 2:C:178:LEU:HD12 | 2:C:179:GLN:H | 1.41 | 0.85 |
| 3:F:111:ALA:N | 3:F:199:THR:HG21 | 1.90 | 0.85 |
| 1:A:433:THR:HG22 | 1:B:216:LYS:HE2 | 1.60 | 0.84 |
| 1:A:250:ASN:HD22 | 2:C:105:TYR:HE1 | 1.23 | 0.83 |
| 3:D:150:ASP:HA | 3:D:190:SER:HB3 | 1.59 | 0.83 |
| 3:F:88:GLN:HB2 | 3:F:97:PHE:CD1 | 2.14 | 0.83 |
| 2:C:132:LEU:HB2 | 2:C:147:GLY:O | 1.79 | 0.83 |
| 1:A:75:TYR:HB3 | 1:A:76:PRO:HD3 | 1.59 | 0.83 |
| 1:B:75:TYR:HB3 | 1:B:76:PRO:HD3 | 1.60 | 0.83 |
| 3:F:153:GLU:HG3 | 3:F:154:ARG:N | 1.92 | 0.82 |
| 2:C:129:VAL:HG21 | 2:C:214:VAL:HG21 | 1.59 | 0.82 |
| 3:D:95:GLN:OE1 | 3:D:95:GLN:N | 2.12 | 0.82 |
| 3:D:112:PRO:HG2 | 3:D:204:ILE:HD12 | 1.61 | 0.81 |
| 2:C:147:GLY:HA2 | 2:C:162:TRP:HH2 | 1.44 | 0.81 |
| 1:B:116:LEU:HD23 | 1:B:178:LEU:HD23 | 1.61 | 0.81 |
| 3:F:7:SER:HB3 | 3:F:8:PRO:HD3 | 1.62 | 0.81 |
| 3:F:192:THR:CA | 3:F:207:SER:HB3 | 2.10 | 0.81 |
| 2:C:147:GLY:HA2 | 2:C:162:TRP:CH2 | 2.15 | 0.80 |
| 1:A:216:LYS:HE2 | 1:B:433:THR:CG2 | 2.10 | 0.80 |
| 2:C:98:ARG:HD2 | 2:C:110:VAL:HG23 | 1.61 | 0.80 |
| 2:E:91:THR:OG1 | 2:E:119:VAL:HG23 | 1.80 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:192:ALA:HB1 | 1:A:414:GLU:OE2 | 1.80 | 0.80 |
| 2:E:16:GLY:H | 2:E:86:VAL:HG22 | 1.46 | 0.79 |
| 3:F:7:SER:HB3 | 3:F:8:PRO:CD | 2.12 | 0.79 |
| 1:A:200:ILE:HA | 1:A:204:MET:HB2 | 1.64 | 0.79 |
| 3:D:13:ALA:HB3 | 3:D:77:MET:HE3 | 1.62 | 0.79 |
| 2:E:125:THR:HG22 | 2:E:153:TYR:HA | 1.64 | 0.79 |
| 2:E:18:LEU:HD23 | 2:E:18:LEU:H | 1.48 | 0.79 |
| 1:B:227:ILE:O | 1:B:231:ILE:HG12 | 1.84 | 0.78 |
| 3:D:14:ALA:O | 3:D:17:ASP:HB2 | 1.82 | 0.78 |
| 1:A:171:ASP:HB2 | 1:A:212:LEU:HD22 | 1.65 | 0.78 |
| 1:A:457:GLU:HG3 | 1:B:18:ARG:NH1 | 1.98 | 0.78 |
| 1:A:426:ILE:CG2 | 1:B:223:ILE:HD11 | 2.14 | 0.78 |
| 3:D:54:THR:O | 3:D:57:VAL:HG23 | 1.84 | 0.78 |
| 3:D:13:ALA:HB3 | 3:D:77:MET:CE | 2.13 | 0.77 |
| 3:F:210:ARG:HB3 | 3:F:210:ARG:NH1 | 1.98 | 0.77 |
| 1:B:200:ILE:HA | 1:B:204:MET:HB2 | 1.66 | 0.77 |
| 1:B:409:ILE:HD13 | 1:B:426:ILE:HG12 | 1.66 | 0.77 |
| 3:D:7:SER:HB3 | 3:D:8:PRO:HD3 | 1.66 | 0.77 |
| 1:A:320:ILE:HD13 | 1:A:394:MET:CE | 2.15 | 0.77 |
| 3:F:7:SER:CB | 3:F:8:PRO:HD3 | 2.14 | 0.77 |
| 1:B:127:VAL:HB | 1:B:157:ASN:ND2 | 1.99 | 0.77 |
| 1:B:171:ASP:HB2 | 1:B:212:LEU:HD22 | 1.67 | 0.77 |
| 1:B:200:ILE:HG22 | 1:B:201:ILE:N | 2.00 | 0.77 |
| 1:A:208:PHE:O | 1:A:209:ARG:HB3 | 1.85 | 0.76 |
| 2:C:107:TYR:HB3 | 3:D:33:HIS:CD2 | 2.20 | 0.76 |
| 3:D:158:VAL:O | 3:D:159:LEU:HD23 | 1.85 | 0.76 |
| 2:C:196:TRP:O | 2:C:197:PRO:C | 2.20 | 0.76 |
| 1:A:398:LEU:O | 1:A:402:ILE:HG23 | 1.85 | 0.76 |
| 1:A:18:ARG:NH1 | 1:B:457:GLU:HB3 | 2.00 | 0.76 |
| 1:B:208:PHE:O | 1:B:209:ARG:HB3 | 1.85 | 0.76 |
| 2:C:174:PHE:H | 2:C:174:PHE:HD2 | 1.30 | 0.76 |
| 2:E:73:ASP:OD2 | 2:E:76:LYS:HD2 | 1.86 | 0.76 |
| 1:B:59:TRP:O | 1:B:63:GLN:HG2 | 1.86 | 0.76 |
| 2:C:30:SER:C | 2:C:32:TYR:H | 1.85 | 0.76 |
| 3:D:7:SER:HB2 | 3:D:22:THR:HB | 1.67 | 0.76 |
| 1:A:86:SER:OG | 1:A:303:GLY:HA3 | 1.85 | 0.76 |
| 3:F:124:LEU:HD23 | 3:F:128:GLY:O | 1.87 | 0.75 |
| 3:F:22:THR:HG22 | 3:F:23:CYS:N | 1.99 | 0.75 |
| 1:B:131:LYS:HE3 | 1:B:150:PRO:HA | 1.68 | 0.75 |
| 3:D:125:THR:HG22 | 3:D:125:THR:O | 1.85 | 0.75 |
| 2:E:204:ASN:HB3 | 2:E:215:ASP:OD1 | 1.85 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:2:ILE:HD11 | 3:F:27:SER:HB2 | 1.68 | 0.74 |
| 2:C:2:VAL:HG23 | 2:C:27:PHE:HD1 | 1.48 | 0.74 |
| 3:F:48:TYR:CE2 | 3:F:52:LYS:HB2 | 2.23 | 0.74 |
| 1:B:423:LEU:HB3 | 1:B:424:PRO:HD3 | 1.70 | 0.74 |
| 3:F:188:HIS:O | 3:F:210:ARG:HD3 | 1.87 | 0.74 |
| 3:D:6:GLN:HG3 | 3:D:100:GLY:H | 1.52 | 0.74 |
| 3:D:90:TRP:CE2 | 3:D:95:GLN:NE2 | 2.56 | 0.74 |
| 2:E:107:TYR:HE2 | 3:F:48:TYR:CD1 | 2.06 | 0.74 |
| 3:F:19:VAL:HG12 | 3:F:74:ILE:HB | 1.68 | 0.74 |
| 2:C:172:HIS:HB2 | 2:C:188:SER:HB3 | 1.70 | 0.74 |
| 2:E:61:THR:O | 2:E:63:SER:N | 2.21 | 0.74 |
| 2:C:51:ILE:HD11 | 2:C:55:SER:CB | 2.18 | 0.73 |
| 3:F:16:GLY:HA2 | 3:F:76:THR:HG23 | 1.68 | 0.73 |
| 1:A:38:MET:HA | 1:A:41:VAL:HG12 | 1.70 | 0.73 |
| 2:C:129:VAL:HG21 | 2:C:214:VAL:CG2 | 2.18 | 0.73 |
| 2:E:100:TYR:HB3 | 2:E:107:TYR:HE1 | 1.54 | 0.73 |
| 1:A:234:HIS:CE1 | 3:F:52:LYS:NZ | 2.57 | 0.73 |
| 1:A:124:TRP:HA | 1:A:157:ASN:HD22 | 1.52 | 0.73 |
| 1:A:248:PRO:O | 1:A:251:THR:HB | 1.89 | 0.73 |
| 1:B:123:ARG:HE | 1:B:126:ARG:HD2 | 1.51 | 0.73 |
| 3:F:187:ARG:HG2 | 3:F:188:HIS:CD2 | 2.24 | 0.72 |
| 1:B:320:ILE:HD13 | 1:B:394:MET:CE | 2.20 | 0.72 |
| 3:D:60:ARG:HG2 | 3:D:74:ILE:HG22 | 1.71 | 0.72 |
| 2:C:72:ARG:NH1 | 2:C:74:ASN:OD1 | 2.22 | 0.72 |
| 1:A:433:THR:CG2 | 1:B:216:LYS:HE2 | 2.18 | 0.72 |
| 3:D:136:ASN:HB3 | 3:D:137:ASN:ND2 | 2.05 | 0.72 |
| 3:F:95:GLN:N | 3:F:95:GLN:OE1 | 2.23 | 0.72 |
| 1:A:419:TYR:CZ | 1:B:414:GLU:HG2 | 2.24 | 0.72 |
| 3:F:116:ILE:HD12 | 3:F:193:CYS:HB2 | 1.70 | 0.72 |
| 1:B:154:ILE:O | 1:B:158:ILE:HG12 | 1.89 | 0.71 |
| 3:F:210:ARG:HH11 | 3:F:210:ARG:CG | 2.02 | 0.71 |
| 3:F:7:SER:CB | 3:F:22:THR:HB | 2.16 | 0.71 |
| 3:F:149:ILE:HD12 | 3:F:154:ARG:HH11 | 1.55 | 0.71 |
| 2:C:52:ASN:HB2 | 2:C:53:PRO:HD2 | 1.72 | 0.71 |
| 1:A:294:MET:O | 1:A:298:ILE:HG13 | 1.90 | 0.71 |
| 1:A:287:ASN:HD22 | 1:A:290:LYS:HG3 | 1.56 | 0.70 |
| 3:D:90:TRP:CZ2 | 3:D:95:GLN:NE2 | 2.59 | 0.70 |
| 1:A:17:ARG:HG3 | 1:A:18:ARG:N | 2.05 | 0.70 |
| 2:E:36:TRP:O | 2:E:37:VAL:HG23 | 1.91 | 0.70 |
| 1:A:241:VAL:HG11 | 1:A:324:THR:HG21 | 1.72 | 0.70 |
| 2:C:109:ASP:HA | 3:D:45:ARG:HE | 1.56 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:177:VAL:HG21 | 3:D:159:LEU:CD1 | 2.21 | 0.70 |
| 1:A:123:ARG:HE | 1:A:126:ARG:HD2 | 1.56 | 0.70 |
| 1:B:212:LEU:HD12 | 1:B:212:LEU:N | 2.06 | 0.70 |
| 2:E:30:SER:O | 2:E:31:ARG:HB2 | 1.91 | 0.70 |
| 1:B:260:ILE:HG23 | 1:B:435:LEU:HG | 1.73 | 0.70 |
| 3:D:65:GLY:HA3 | 3:D:70:TYR:HA | 1.74 | 0.70 |
| 1:A:332:MET:O | 1:A:336:ILE:HG13 | 1.91 | 0.70 |
| 2:C:52:ASN:HB2 | 2:C:53:PRO:CD | 2.22 | 0.69 |
| 3:F:22:THR:CG2 | 3:F:23:CYS:N | 2.55 | 0.69 |
| 1:A:451:ARG:HH11 | 1:A:451:ARG:HB3 | 1.56 | 0.69 |
| 3:D:201:THR:HG23 | 3:D:202:SER:H | 1.58 | 0.69 |
| 3:F:82:ALA:HB2 | 3:F:105:ILE:CD1 | 2.22 | 0.69 |
| 1:A:20:GLN:O | 1:A:23:ARG:HB3 | 1.93 | 0.69 |
| 1:B:287:ASN:HD22 | 1:B:290:LYS:HG3 | 1.58 | 0.69 |
| 2:C:196:TRP:O | 2:C:198:SER:N | 2.26 | 0.69 |
| 3:F:72:LEU:C | 3:F:72:LEU:HD23 | 2.13 | 0.69 |
| 2:C:6:GLU:O | 2:C:115:THR:HG23 | 1.93 | 0.69 |
| 1:A:409:ILE:HD13 | 1:A:426:ILE:HG12 | 1.75 | 0.69 |
| 3:F:134:PHE:O | 3:F:135:LEU:HD23 | 1.93 | 0.68 |
| 3:F:150:ASP:HA | 3:F:190:SER:HB3 | 1.75 | 0.68 |
| 1:A:200:ILE:HG22 | 1:A:201:ILE:N | 2.07 | 0.68 |
| 1:A:414:GLU:HG2 | 1:B:419:TYR:CZ | 2.28 | 0.68 |
| 2:E:39:GLN:O | 2:E:92:ALA:HB1 | 1.93 | 0.68 |
| 1:B:380:PRO:HD2 | 1:B:381:GLN:HE22 | 1.58 | 0.68 |
| 3:D:123:GLN:HE22 | 3:D:130:SER:HB2 | 1.57 | 0.68 |
| 1:B:108:GLY:HA3 | 1:B:153:GLN:NE2 | 2.08 | 0.68 |
| 1:B:374:VAL:O | 1:B:378:LEU:HG | 1.94 | 0.68 |
| 3:D:125:THR:O | 3:D:125:THR:CG2 | 2.42 | 0.68 |
| 1:A:287:ASN:HD22 | 1:A:290:LYS:H | 1.41 | 0.68 |
| 2:E:146:LEU:N | 2:E:146:LEU:HD23 | 2.08 | 0.68 |
| 3:F:197:HIS:CE1 | 3:F:199:THR:HG23 | 2.29 | 0.68 |
| 2:C:51:ILE:CD1 | 2:C:55:SER:HB3 | 2.21 | 0.68 |
| 2:C:130:TYR:CE2 | 3:D:123:GLN:HG3 | 2.28 | 0.68 |
| 3:D:6:GLN:OE1 | 3:D:87:CYS:N | 2.23 | 0.68 |
| 3:D:94:PRO:HA | 3:D:95:GLN:OE1 | 1.92 | 0.68 |
| 1:B:443:PRO:O | 1:B:446:SER:N | 2.28 | 0.67 |
| 3:F:72:LEU:HD23 | 3:F:73:THR:N | 2.08 | 0.67 |
| 3:F:88:GLN:HB2 | 3:F:97:PHE:HD1 | 1.59 | 0.67 |
| 2:C:29:TYR:OH | 2:C:34:MET:HG3 | 1.93 | 0.67 |
| 3:F:7:SER:CB | 3:F:8:PRO:CD | 2.70 | 0.67 |
| 3:F:32:ILE:CD1 | 3:F:89:GLN:HB3 | 2.24 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:241:VAL:HG12 | 1:B:244:LEU:HD21 | 1.77 | 0.67 |
| 1:B:287:ASN:HD22 | 1:B:290:LYS:H | 1.38 | 0.67 |
| 3:F:34:TRP:CZ3 | 3:F:87:CYS:HB3 | 2.28 | 0.67 |
| 1:B:74:ASN:HD22 | 1:B:75:TYR:N | 1.93 | 0.67 |
| 1:B:127:VAL:HB | 1:B:157:ASN:HD21 | 1.58 | 0.67 |
| 2:E:100:TYR:HB3 | 2:E:107:TYR:CE1 | 2.29 | 0.67 |
| 3:F:2:ILE:CD1 | 3:F:27:SER:HB2 | 2.24 | 0.67 |
| 1:A:320:ILE:HG23 | 1:A:365:THR:HG21 | 1.77 | 0.67 |
| 3:F:37:GLN:O | 3:F:83:ALA:HB1 | 1.94 | 0.67 |
| 2:E:196:TRP:HB3 | 2:E:197:PRO:HD3 | 1.77 | 0.67 |
| 2:C:51:ILE:CD1 | 2:C:72:ARG:HD2 | 2.24 | 0.67 |
| 3:D:31:TYR:HB3 | 3:D:49:ASP:HA | 1.76 | 0.66 |
| 1:B:38:MET:HA | 1:B:41:VAL:HG12 | 1.78 | 0.66 |
| 1:A:176:THR:HG22 | 1:A:177:LEU:HD23 | 1.77 | 0.66 |
| 1:A:235:GLU:O | 1:A:236:VAL:CG2 | 2.34 | 0.66 |
| 2:C:45:LEU:HD12 | 2:C:45:LEU:H | 1.61 | 0.66 |
| 3:F:7:SER:O | 3:F:8:PRO:C | 2.32 | 0.66 |
| 2:C:30:SER:O | 2:C:32:TYR:N | 2.25 | 0.66 |
| 1:A:92:PHE:O | 1:A:96:LEU:HD23 | 1.96 | 0.66 |
| 1:A:255:TYR:HB3 | 1:A:428:THR:OG1 | 1.95 | 0.66 |
| 3:F:13:ALA:HB3 | 3:F:77:MET:CE | 2.22 | 0.66 |
| 2:C:204:ASN:HB3 | 2:C:215:ASP:OD1 | 1.96 | 0.66 |
| 3:F:210:ARG:HH11 | 3:F:210:ARG:HG2 | 1.59 | 0.66 |
| 1:B:294:MET:O | 1:B:298:ILE:HG13 | 1.96 | 0.66 |
| 1:A:150:PRO:O | 1:A:154:ILE:HG13 | 1.96 | 0.66 |
| 3:D:22:THR:HG22 | 3:D:23:CYS:N | 2.06 | 0.66 |
| 2:C:105:TYR:CD2 | 3:D:31:TYR:HD1 | 2.14 | 0.65 |
| 3:F:148:LYS:HB2 | 3:F:192:THR:OG1 | 1.95 | 0.65 |
| 3:D:50:THR:HG23 | 3:D:70:TYR:CD2 | 2.31 | 0.65 |
| 3:F:192:THR:HA | 3:F:207:SER:CB | 2.23 | 0.65 |
| 2:E:108:PHE:CE1 | 3:F:88:GLN:NE2 | 2.64 | 0.65 |
| 2:C:26:GLY:O | 2:C:27:PHE:HB3 | 1.96 | 0.65 |
| 2:C:192:PRO:O | 2:C:195:SER:HB3 | 1.95 | 0.65 |
| 2:E:145:THR:C | 2:E:146:LEU:HD23 | 2.17 | 0.65 |
| 1:A:87:ALA:O | 1:A:91:MET:HG3 | 1.97 | 0.65 |
| 3:F:187:ARG:HG3 | 3:F:187:ARG:O | 1.97 | 0.65 |
| 1:A:234:HIS:CE1 | 3:F:52:LYS:HZ1 | 2.14 | 0.65 |
| 2:E:108:PHE:CD1 | 3:F:88:GLN:NE2 | 2.64 | 0.65 |
| 1:A:131:LYS:HE3 | 1:A:150:PRO:HA | 1.79 | 0.65 |
| 1:B:287:ASN:ND2 | 1:B:290:LYS:N | 2.39 | 0.65 |
| 2:E:45:LEU:HD11 | 3:F:86:TYR:CE1 | 2.32 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:E:132:LEU:HD13 | 3:F:132:VAL:HG21 | 1.79 | 0.65 |
| 3:F:194:GLU:CG | 3:F:205:VAL:HG12 | 2.25 | 0.65 |
| 1:A:154:ILE:O | 1:A:158:ILE:HG12 | 1.97 | 0.64 |
| 1:B:421:LEU:O | 1:B:424:PRO:HD2 | 1.97 | 0.64 |
| 1:A:449:LEU:O | 1:A:453:LEU:HB2 | 1.98 | 0.64 |
| 1:B:332:MET:O | 1:B:336:ILE:HG13 | 1.97 | 0.64 |
| 2:C:178:LEU:HB2 | 2:C:183:TYR:CE2 | 2.32 | 0.64 |
| 3:F:158:VAL:HG23 | 3:F:178:LEU:HD13 | 1.79 | 0.64 |
| 1:A:176:THR:O | 1:A:180:THR:HG23 | 1.98 | 0.64 |
| 1:A:320:ILE:HD13 | 1:A:394:MET:HE1 | 1.80 | 0.64 |
| 3:D:117:PHE:CD1 | 3:D:117:PHE:N | 2.64 | 0.64 |
| 3:D:180:LEU:HD12 | 3:D:185:TYR:HB2 | 1.78 | 0.64 |
| 1:B:281:HIS:HA | 1:B:284:HIS:CE1 | 2.33 | 0.64 |
| 3:D:31:TYR:HA | 3:D:50:THR:HG1 | 1.60 | 0.64 |
| 2:C:32:TYR:CE2 | 2:C:98:ARG:NE | 2.66 | 0.64 |
| 2:E:6:GLU:HA | 2:E:22:CYS:HA | 1.80 | 0.64 |
| 3:F:82:ALA:HB2 | 3:F:105:ILE:HD11 | 1.80 | 0.64 |
| 1:A:443:PRO:O | 1:A:446:SER:N | 2.30 | 0.63 |
| 1:B:92:PHE:O | 1:B:96:LEU:HD23 | 1.98 | 0.63 |
| 3:D:47:ILE:HG13 | 3:D:53:LEU:HD23 | 1.80 | 0.63 |
| 1:A:127:VAL:HB | 1:A:157:ASN:ND2 | 2.12 | 0.63 |
| 3:D:95:GLN:CD | 3:D:95:GLN:N | 2.48 | 0.63 |
| 3:D:182:LYS:HG2 | 3:D:186:GLU:OE1 | 1.98 | 0.63 |
| 1:B:20:GLN:O | 1:B:23:ARG:HB3 | 1.98 | 0.63 |
| 1:A:399:ALA:O | 1:A:403:ARG:HA | 1.99 | 0.63 |
| 3:D:50:THR:HG23 | 3:D:70:TYR:HD2 | 1.64 | 0.63 |
| 3:F:45:ARG:HH12 | 3:F:54:THR:HG23 | 1.63 | 0.63 |
| 1:A:38:MET:HG3 | 1:A:168:LEU:CD1 | 2.28 | 0.63 |
| 1:B:451:ARG:HB3 | 1:B:451:ARG:HH11 | 1.64 | 0.63 |
| 2:E:130:TYR:HB3 | 3:F:120:SER:OG | 1.98 | 0.63 |
| 3:F:77:MET:SD | 3:F:103:LEU:HD21 | 2.38 | 0.63 |
| 1:A:423:LEU:HB3 | 1:A:424:PRO:CD | 2.21 | 0.63 |
| 1:B:74:ASN:O | 1:B:78:LEU:HB2 | 1.99 | 0.63 |
| 1:B:86:SER:OG | 1:B:303:GLY:HA3 | 1.99 | 0.63 |
| 3:F:178:LEU:HD12 | 3:F:179:THR:N | 2.14 | 0.63 |
| 3:F:182:LYS:O | 3:F:186:GLU:HG3 | 1.99 | 0.63 |
| 1:A:226:THR:O | 1:A:230:ARG:HG2 | 1.99 | 0.63 |
| 2:C:2:VAL:O | 2:C:2:VAL:HG13 | 1.99 | 0.63 |
| 2:E:196:TRP:O | 2:E:197:PRO:C | 2.36 | 0.63 |
| 1:A:172:GLU:O | 1:A:176:THR:HB | 1.99 | 0.62 |
| 2:C:32:TYR:HD2 | 2:C:98:ARG:HG2 | 1.64 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:146:LYS:HD3 | 3:F:148:LYS:HE3 | 1.80 | 0.62 |
| 1:A:212:LEU:HD12 | 1:A:212:LEU:N | 2.10 | 0.62 |
| 1:B:320:ILE:HG23 | 1:B:365:THR:HG21 | 1.81 | 0.62 |
| 3:D:117:PHE:N | 3:D:117:PHE:HD1 | 1.97 | 0.62 |
| 3:F:210:ARG:HB3 | 3:F:210:ARG:HH11 | 1.63 | 0.62 |
| 1:A:59:TRP:O | 1:A:63:GLN:HG2 | 1.98 | 0.62 |
| 2:C:192:PRO:HB2 | 2:C:195:SER:HB2 | 1.80 | 0.62 |
| 2:C:22:CYS:O | 2:C:78:THR:HG23 | 2.00 | 0.62 |
| 2:C:174:PHE:CD2 | 2:C:174:PHE:N | 2.60 | 0.62 |
| 2:E:108:PHE:HE1 | 3:F:88:GLN:HE21 | 1.44 | 0.62 |
| 1:B:176:THR:HG22 | 1:B:177:LEU:HD23 | 1.81 | 0.62 |
| 3:F:133:CYS:HB2 | 3:F:147:TRP:CH2 | 2.34 | 0.62 |
| 3:F:153:GLU:HG3 | 3:F:154:ARG:H | 1.64 | 0.62 |
| 2:C:32:TYR:CD2 | 2:C:98:ARG:HG2 | 2.35 | 0.62 |
| 2:E:33:TRP:CH2 | 2:E:52:ASN:HB3 | 2.35 | 0.62 |
| 3:F:210:ARG:HH11 | 3:F:210:ARG:CB | 2.12 | 0.62 |
| 1:A:374:VAL:O | 1:A:378:LEU:HG | 2.00 | 0.61 |
| 2:C:178:LEU:HD12 | 2:C:179:GLN:N | 2.12 | 0.61 |
| 3:D:201:THR:HG23 | 3:D:202:SER:N | 2.14 | 0.61 |
| 2:E:33:TRP:O | 2:E:99:LEU:HB2 | 2.01 | 0.61 |
| 3:F:187:ARG:O | 3:F:187:ARG:CG | 2.47 | 0.61 |
| 1:A:148:GLU:OE1 | 1:A:355:GLY:HA3 | 2.00 | 0.61 |
| 2:E:162:TRP:CZ3 | 2:E:203:CYS:CB | 2.81 | 0.61 |
| 3:F:125:THR:O | 3:F:125:THR:HG22 | 1.99 | 0.61 |
| 2:C:172:HIS:HD2 | 3:D:136:ASN:ND2 | 1.97 | 0.61 |
| 1:B:94:TYR:CZ | 1:B:352:ALA:HB2 | 2.35 | 0.61 |
| 3:F:107:ARG:HD3 | 3:F:170:SER:O | 2.00 | 0.61 |
| 3:D:30:SER:HA | 3:D:70:TYR:OH | 2.01 | 0.61 |
| 3:D:168:LYS:O | 3:D:170:SER:N | 2.33 | 0.61 |
| 2:E:18:LEU:HD23 | 2:E:18:LEU:N | 2.13 | 0.61 |
| 1:A:281:HIS:HA | 1:A:284:HIS:CE1 | 2.35 | 0.61 |
| 3:F:34:TRP:CZ2 | 3:F:72:LEU:HB2 | 2.36 | 0.61 |
| 1:A:94:TYR:CZ | 1:A:352:ALA:HB2 | 2.36 | 0.61 |
| 1:A:239:ILE:HD13 | 1:A:394:MET:HE1 | 1.83 | 0.61 |
| 1:A:274:LEU:HD23 | 1:A:277:GLN:HE22 | 1.65 | 0.61 |
| 1:B:87:ALA:O | 1:B:91:MET:HG3 | 2.01 | 0.61 |
| 2:C:7:SER:HA | 2:C:115:THR:HG21 | 1.82 | 0.61 |
| 3:D:7:SER:CB | 3:D:8:PRO:HD3 | 2.31 | 0.61 |
| 3:D:136:ASN:HB3 | 3:D:137:ASN:HD22 | 1.66 | 0.61 |
| 1:A:108:GLY:HA3 | 1:A:153:GLN:NE2 | 2.15 | 0.61 |
| 3:F:191:TYR:HB2 | 3:F:208:PHE:CE2 | 2.34 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:E:36:TRP:HE3 | 2:E:95:TYR:O | 1.82 | 0.61 |
| 1:A:113:GLU:OE2 | 1:A:203:GLU:HG3 | 2.00 | 0.60 |
| 2:C:105:TYR:CE2 | 3:D:31:TYR:HD1 | 2.19 | 0.60 |
| 3:D:143:ILE:HG23 | 3:D:174:MET:CE | 2.30 | 0.60 |
| 2:E:200:THR:OG1 | 2:E:217:LYS:HE3 | 2.01 | 0.60 |
| 1:A:31:THR:H | 1:B:437:GLN:HE22 | 1.47 | 0.60 |
| 1:A:269:PHE:O | 1:A:273:VAL:HG12 | 2.00 | 0.60 |
| 1:B:163:LEU:CD2 | 1:B:174:ARG:HA | 2.31 | 0.60 |
| 3:F:139:TYR:CG | 3:F:140:PRO:N | 2.70 | 0.60 |
| 1:A:74:ASN:O | 1:A:78:LEU:HB2 | 2.00 | 0.60 |
| 3:D:17:ASP:O | 3:D:76:THR:HA | 2.01 | 0.60 |
| 3:D:139:TYR:CD1 | 3:D:140:PRO:HD3 | 2.37 | 0.60 |
| 1:A:409:ILE:HD11 | 1:A:426:ILE:HA | 1.84 | 0.60 |
| 2:C:30:SER:C | 2:C:32:TYR:N | 2.55 | 0.60 |
| 1:A:171:ASP:CB | 1:A:212:LEU:HD22 | 2.31 | 0.60 |
| 3:D:192:THR:HA | 3:D:207:SER:HB3 | 1.84 | 0.60 |
| 2:C:200:THR:HG22 | 2:C:200:THR:O | 2.00 | 0.60 |
| 3:D:137:ASN:HA | 3:D:172:TYR:O | 2.02 | 0.60 |
| 1:B:138:THR:HG21 | 1:B:352:ALA:HB1 | 1.84 | 0.60 |
| 1:B:273:VAL:HA | 1:B:345:LEU:HD22 | 1.83 | 0.60 |
| 2:E:107:TYR:HE2 | 3:F:48:TYR:HD1 | 1.47 | 0.60 |
| 2:E:179:GLN:O | 2:E:180:ALA:HB3 | 2.02 | 0.60 |
| 2:C:156:GLU:OE2 | 2:C:176:ALA:HB3 | 2.02 | 0.60 |
| 1:A:220:ILE:HG13 | 1:B:430:LEU:HD21 | 1.84 | 0.59 |
| 1:B:131:LYS:HE2 | 1:B:153:GLN:NE2 | 2.15 | 0.59 |
| 1:A:99:LYS:HG2 | 1:A:100:TYR:CE1 | 2.37 | 0.59 |
| 2:E:69:ILE:HB | 2:E:82:GLN:HB2 | 1.85 | 0.59 |
| 2:E:69:ILE:HG22 | 2:E:69:ILE:O | 2.02 | 0.59 |
| 2:E:132:LEU:CD1 | 3:F:132:VAL:HG21 | 2.32 | 0.59 |
| 1:B:248:PRO:O | 1:B:251:THR:HB | 2.03 | 0.59 |
| 1:A:250:ASN:ND2 | 2:C:105:TYR:CE1 | 2.62 | 0.59 |
| 1:B:117:GLU:OE1 | 1:B:209:ARG:NH1 | 2.34 | 0.59 |
| 3:F:178:LEU:HD12 | 3:F:179:THR:H | 1.67 | 0.59 |
| 1:A:108:GLY:HA3 | 1:A:153:GLN:HE21 | 1.68 | 0.59 |
| 1:A:249:LEU:C | 1:A:251:THR:H | 2.04 | 0.59 |
| 2:E:144:VAL:O | 2:E:144:VAL:HG13 | 2.01 | 0.59 |
| 3:F:197:HIS:ND1 | 3:F:198:LYS:N | 2.49 | 0.59 |
| 1:A:357:PHE:CE1 | 1:A:398:LEU:HD22 | 2.37 | 0.59 |
| 1:A:383:HIS:CE1 | 3:D:90:TRP:CZ2 | 2.91 | 0.59 |
| 3:D:46:TRP:HA | 3:D:46:TRP:CE3 | 2.37 | 0.59 |
| 2:E:192:PRO:HB2 | 2:E:195:SER:HB2 | 1.82 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:116:ILE:CD1 | 3:F:193:CYS:HB2 | 2.33 | 0.59 |
| 1:A:223:ILE:CD1 | 1:B:426:ILE:HG22 | 2.22 | 0.59 |
| 3:D:114:VAL:O | 3:D:206:LYS:HD2 | 2.03 | 0.59 |
| 1:A:220:ILE:CG1 | 1:B:430:LEU:HD21 | 2.32 | 0.59 |
| 2:C:38:ARG:HD3 | 2:C:48:ILE:HD11 | 1.84 | 0.59 |
| 2:C:45:LEU:HD11 | 3:D:86:TYR:CD1 | 2.37 | 0.59 |
| 3:D:21:MET:SD | 3:D:72:LEU:HD22 | 2.43 | 0.59 |
| 3:D:89:GLN:OE1 | 3:D:90:TRP:N | 2.36 | 0.59 |
| 3:D:190:SER:HA | 3:D:209:ASN:OD1 | 2.03 | 0.59 |
| 2:E:98:ARG:NH1 | 2:E:109:ASP:OD2 | 2.35 | 0.59 |
| 3:F:65:GLY:HA3 | 3:F:70:TYR:HD2 | 1.66 | 0.59 |
| 1:A:212:LEU:H | 1:A:212:LEU:CD1 | 2.14 | 0.58 |
| 3:D:79:ALA:HB1 | 3:D:105:ILE:CD1 | 2.33 | 0.58 |
| 3:D:141:LYS:HB3 | 3:D:172:TYR:CD1 | 2.38 | 0.58 |
| 1:A:33:LEU:O | 1:A:33:LEU:HD23 | 2.02 | 0.58 |
| 3:F:45:ARG:NH1 | 3:F:54:THR:HG23 | 2.18 | 0.58 |
| 1:B:241:VAL:HG11 | 1:B:324:THR:HG21 | 1.85 | 0.58 |
| 3:F:188:HIS:O | 3:F:210:ARG:CD | 2.50 | 0.58 |
| 1:A:287:ASN:ND2 | 1:A:290:LYS:HG3 | 2.18 | 0.58 |
| 1:A:414:GLU:HG2 | 1:B:419:TYR:OH | 2.02 | 0.58 |
| 2:E:131:PRO:HD3 | 2:E:216:LYS:HG2 | 1.83 | 0.58 |
| 2:C:146:LEU:HB2 | 2:C:189:VAL:CG1 | 2.33 | 0.58 |
| 3:F:205:VAL:O | 3:F:206:LYS:HG2 | 2.03 | 0.58 |
| 1:A:160:ARG:O | 1:A:163:LEU:HB3 | 2.04 | 0.58 |
| 1:B:27:GLU:O | 1:B:30:LYS:HG3 | 2.02 | 0.58 |
| 3:F:64:SER:OG | 3:F:65:GLY:N | 2.37 | 0.58 |
| 1:A:202:GLU:HG2 | 1:A:202:GLU:O | 2.02 | 0.58 |
| 2:C:150:VAL:CG2 | 2:C:205:VAL:HG21 | 2.33 | 0.58 |
| 3:F:89:GLN:HE21 | 3:F:96:THR:H | 1.50 | 0.58 |
| 3:D:94:PRO:CA | 3:D:95:GLN:OE1 | 2.51 | 0.58 |
| 3:F:21:MET:SD | 3:F:85:TYR:HD1 | 2.26 | 0.58 |
| 3:D:141:LYS:HB3 | 3:D:172:TYR:CE1 | 2.39 | 0.57 |
| 2:E:40:ALA:HA | 2:E:92:ALA:HB2 | 1.86 | 0.57 |
| 3:F:89:GLN:NE2 | 3:F:95:GLN:HA | 2.19 | 0.57 |
| 1:A:372:GLY:O | 1:A:376:VAL:HG23 | 2.04 | 0.57 |
| 1:B:449:LEU:O | 1:B:453:LEU:HB2 | 2.03 | 0.57 |
| 2:C:177:VAL:CG2 | 3:D:159:LEU:HD13 | 2.26 | 0.57 |
| 3:F:189:ASN:ND2 | 3:F:210:ARG:HB2 | 2.18 | 0.57 |
| 1:A:287:ASN:ND2 | 1:A:290:LYS:N | 2.42 | 0.57 |
| 1:B:172:GLU:O | 1:B:176:THR:HB | 2.05 | 0.57 |
| 1:B:273:VAL:HG11 | 1:B:444:LEU:HD21 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:17:SER:O | 2:C:18:LEU:HB3 | 2.04 | 0.57 |
| 2:C:173:THR:HG22 | 2:C:173:THR:O | 2.03 | 0.57 |
| 2:C:185:LEU:O | 2:C:185:LEU:HD12 | 2.03 | 0.57 |
| 1:A:74:ASN:HD22 | 1:A:75:TYR:N | 2.02 | 0.57 |
| 1:A:198:LEU:HD11 | 1:B:198:LEU:HD21 | 1.85 | 0.57 |
| 1:B:208:PHE:CD1 | 1:B:208:PHE:N | 2.70 | 0.57 |
| 3:F:73:THR:HG22 | 3:F:74:ILE:N | 2.17 | 0.57 |
| 1:A:53:PHE:O | 1:A:57:VAL:HG23 | 2.04 | 0.57 |
| 1:A:200:ILE:HD12 | 1:A:204:MET:HG3 | 1.86 | 0.57 |
| 1:B:160:ARG:O | 1:B:163:LEU:N | 2.35 | 0.57 |
| 2:E:158:VAL:HG21 | 2:E:185:LEU:HD11 | 1.86 | 0.57 |
| 3:F:73:THR:CG2 | 3:F:74:ILE:N | 2.66 | 0.57 |
| 1:B:380:PRO:HD2 | 1:B:381:GLN:NE2 | 2.19 | 0.57 |
| 2:C:132:LEU:HB3 | 3:D:117:PHE:CD2 | 2.38 | 0.57 |
| 1:B:38:MET:HG3 | 1:B:168:LEU:CD1 | 2.30 | 0.57 |
| 3:D:81:ASP:O | 3:D:103:LEU:HD23 | 2.05 | 0.57 |
| 3:F:32:ILE:HG22 | 3:F:33:HIS:N | 2.20 | 0.57 |
| 1:B:191:ASN:HB2 | 1:B:229:TYR:CE2 | 2.40 | 0.57 |
| 1:B:398:LEU:O | 1:B:402:ILE:HG23 | 2.04 | 0.57 |
| 2:E:171:VAL:C | 2:E:172:HIS:HD1 | 2.07 | 0.57 |
| 1:B:163:LEU:HD21 | 1:B:174:ARG:HA | 1.86 | 0.57 |
| 2:C:162:TRP:CE2 | 2:C:189:VAL:HB | 2.40 | 0.57 |
| 3:D:114:VAL:HG22 | 3:D:135:LEU:CD2 | 2.34 | 0.57 |
| 1:B:65:MET:C | 1:B:67:ALA:H | 2.08 | 0.56 |
| 2:E:107:TYR:CE2 | 3:F:48:TYR:HD1 | 2.22 | 0.56 |
| 2:E:32:TYR:O | 2:E:72:ARG:NH2 | 2.38 | 0.56 |
| 3:F:22:THR:CG2 | 3:F:23:CYS:H | 2.17 | 0.56 |
| 1:A:192:ALA:HB1 | 1:A:414:GLU:CD | 2.24 | 0.56 |
| 1:A:250:ASN:ND2 | 2:C:105:TYR:HE1 | 2.00 | 0.56 |
| 1:B:150:PRO:O | 1:B:154:ILE:HG13 | 2.05 | 0.56 |
| 2:C:16:GLY:O | 2:C:86:VAL:HG13 | 2.04 | 0.56 |
| 3:D:7:SER:CB | 3:D:22:THR:HB | 2.34 | 0.56 |
| 3:F:15:PRO:HD3 | 3:F:105:ILE:HG23 | 1.88 | 0.56 |
| 1:A:409:ILE:CD1 | 1:A:426:ILE:HA | 2.34 | 0.56 |
| 1:B:160:ARG:HH12 | 1:B:174:ARG:HD2 | 1.69 | 0.56 |
| 1:B:287:ASN:ND2 | 1:B:290:LYS:HG3 | 2.19 | 0.56 |
| 2:C:150:VAL:HB | 2:C:185:LEU:CD1 | 2.36 | 0.56 |
| 2:C:213:LYS:O | 2:C:214:VAL:HG13 | 2.04 | 0.56 |
| 2:E:68:PHE:CD2 | 2:E:83:ILE:HG23 | 2.41 | 0.56 |
| 3:F:192:THR:HG22 | 3:F:207:SER:CB | 2.35 | 0.56 |
| 1:A:410:ILE:O | 1:A:414:GLU:HB2 | 2.06 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:212:LEU:H | 1:B:212:LEU:CD1 | 2.17 | 0.56 |
| 2:C:98:ARG:HD2 | 2:C:110:VAL:CG2 | 2.33 | 0.56 |
| 3:D:138:PHE:CE1 | 3:D:172:TYR:HB2 | 2.41 | 0.56 |
| 1:A:311:ALA:HB1 | 1:A:336:ILE:HD13 | 1.88 | 0.56 |
| 1:B:358:ALA:HB3 | 1:B:359:PRO:HD3 | 1.88 | 0.56 |
| 2:E:72:ARG:HD3 | 2:E:74:ASN:OD1 | 2.04 | 0.56 |
| 3:F:159:LEU:O | 3:F:177:THR:N | 2.31 | 0.56 |
| 1:A:17:ARG:HG3 | 1:A:18:ARG:H | 1.69 | 0.56 |
| 1:A:198:LEU:HD12 | 1:A:406:LEU:HG | 1.88 | 0.56 |
| 3:D:93:HIS:CD2 | 3:D:94:PRO:HB3 | 2.40 | 0.56 |
| 3:F:110:ALA:HB3 | 3:F:139:TYR:N | 2.20 | 0.56 |
| 1:A:198:LEU:HD21 | 1:B:198:LEU:HD11 | 1.88 | 0.56 |
| 2:E:107:TYR:HB3 | 3:F:33:HIS:NE2 | 2.18 | 0.56 |
| 1:A:116:LEU:CD2 | 1:A:178:LEU:HD23 | 2.33 | 0.56 |
| 1:A:146:GLY:HA3 | 1:A:148:GLU:OE2 | 2.06 | 0.56 |
| 2:C:2:VAL:HA | 2:C:25:SER:O | 2.06 | 0.56 |
| 2:E:200:THR:HG22 | 2:E:200:THR:O | 2.05 | 0.56 |
| 1:A:119:GLN:HB3 | 1:A:453:LEU:HD11 | 1.88 | 0.55 |
| 2:E:221:ARG:HD2 | 3:F:118:PRO:HG2 | 1.87 | 0.55 |
| 3:F:149:ILE:HD12 | 3:F:154:ARG:NH1 | 2.20 | 0.55 |
| 1:A:144:VAL:HG21 | 1:A:343:THR:HB | 1.88 | 0.55 |
| 2:E:195:SER:O | 2:E:199:GLU:HG3 | 2.06 | 0.55 |
| 1:B:113:GLU:OE2 | 1:B:203:GLU:HG3 | 2.07 | 0.55 |
| 1:B:274:LEU:O | 1:B:277:GLN:HB2 | 2.06 | 0.55 |
| 1:B:356:ILE:HG23 | 1:B:360:MET:HE2 | 1.87 | 0.55 |
| 2:E:207:HIS:CE1 | 2:E:210:SER:HB2 | 2.37 | 0.55 |
| 3:F:118:PRO:O | 3:F:119:PRO:C | 2.44 | 0.55 |
| 1:B:218:VAL:O | 1:B:221:GLY:N | 2.39 | 0.55 |
| 1:B:226:THR:O | 1:B:230:ARG:HG2 | 2.07 | 0.55 |
| 1:B:284:HIS:HA | 1:B:290:LYS:HB3 | 1.89 | 0.55 |
| 2:E:32:TYR:CE2 | 2:E:98:ARG:HD3 | 2.41 | 0.55 |
| 2:E:132:LEU:HB2 | 2:E:147:GLY:O | 2.07 | 0.55 |
| 1:A:287:ASN:HD22 | 1:A:290:LYS:CG | 2.20 | 0.55 |
| 1:B:192:ALA:HB1 | 1:B:414:GLU:OE2 | 2.06 | 0.55 |
| 1:B:218:VAL:O | 1:B:219:PHE:C | 2.44 | 0.55 |
| 3:D:116:ILE:HD12 | 3:D:193:CYS:HB3 | 1.88 | 0.55 |
| 1:A:210:TYR:CE1 | 1:B:208:PHE:HA | 2.42 | 0.55 |
| 2:C:106:TRP:CD1 | 2:C:106:TRP:N | 2.74 | 0.55 |
| 2:C:178:LEU:HB2 | 2:C:183:TYR:HE2 | 1.71 | 0.55 |
| 2:E:67:LYS:NZ | 2:E:85:LYS:O | 2.36 | 0.55 |
| 3:F:132:VAL:HG12 | 3:F:133:CYS:N | 2.22 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:207:HIS:CE1 | 2:C:209:ALA:HB3 | 2.41 | 0.55 |
| 3:F:7:SER:OG | 3:F:8:PRO:HD3 | 2.07 | 0.55 |
| 3:F:30:SER:HA | 3:F:70:TYR:OH | 2.06 | 0.55 |
| 1:B:160:ARG:O | 1:B:163:LEU:HB3 | 2.07 | 0.55 |
| 2:C:105:TYR:HD2 | 3:D:30:SER:O | 1.89 | 0.55 |
| 3:D:124:LEU:C | 3:D:126:SER:H | 2.10 | 0.55 |
| 1:B:53:PHE:CE1 | 1:B:136:LEU:HD12 | 2.41 | 0.54 |
| 1:B:287:ASN:HD22 | 1:B:290:LYS:CG | 2.20 | 0.54 |
| 1:B:362:ALA:O | 1:B:366:VAL:HG23 | 2.07 | 0.54 |
| 2:C:7:SER:HA | 2:C:115:THR:CG2 | 2.38 | 0.54 |
| 2:E:49:GLY:HA3 | 2:E:70:ILE:HD11 | 1.90 | 0.54 |
| 1:B:169:LYS:HG2 | 1:B:170:GLY:N | 2.22 | 0.54 |
| 3:D:29:VAL:HG23 | 3:D:70:TYR:CE1 | 2.43 | 0.54 |
| 1:A:42:VAL:HG23 | 1:A:162:VAL:HG21 | 1.88 | 0.54 |
| 1:A:216:LYS:HD3 | 1:B:434:LEU:HD23 | 1.90 | 0.54 |
| 1:A:434:LEU:HD23 | 1:B:216:LYS:HD3 | 1.88 | 0.54 |
| 2:E:50:GLU:OE1 | 3:F:90:TRP:HH2 | 1.90 | 0.54 |
| 1:A:190:PHE:HD1 | 1:A:411:LEU:HD11 | 1.73 | 0.54 |
| 3:F:95:GLN:H | 3:F:95:GLN:CD | 2.11 | 0.54 |
| 3:F:191:TYR:O | 3:F:207:SER:HB2 | 2.07 | 0.54 |
| 1:A:150:PRO:HD3 | 1:A:354:GLY:HA2 | 1.88 | 0.54 |
| 1:B:444:LEU:HD13 | 1:B:444:LEU:O | 2.08 | 0.54 |
| 2:E:104:GLY:O | 2:E:106:TRP:CD1 | 2.61 | 0.54 |
| 2:E:150:VAL:HB | 2:E:185:LEU:HD12 | 1.90 | 0.54 |
| 3:D:178:LEU:HD12 | 3:D:179:THR:N | 2.23 | 0.54 |
| 2:E:57:THR:C | 2:E:58:ILE:HG12 | 2.28 | 0.54 |
| 3:F:4:LEU:HD22 | 3:F:23:CYS:SG | 2.48 | 0.54 |
| 1:A:381:GLN:HE21 | 1:A:381:GLN:H | 0.74 | 0.54 |
| 1:B:108:GLY:CA | 1:B:153:GLN:NE2 | 2.70 | 0.54 |
| 3:D:114:VAL:HG22 | 3:D:135:LEU:HD22 | 1.89 | 0.54 |
| 1:A:320:ILE:HG21 | 1:A:394:MET:HE1 | 1.89 | 0.54 |
| 1:B:274:LEU:HD23 | 1:B:277:GLN:HE22 | 1.73 | 0.54 |
| 2:E:107:TYR:CE2 | 3:F:48:TYR:CD1 | 2.92 | 0.54 |
| 1:A:250:ASN:ND2 | 2:C:105:TYR:CD1 | 2.74 | 0.54 |
| 1:B:33:LEU:HD23 | 1:B:33:LEU:O | 2.08 | 0.54 |
| 2:C:106:TRP:H | 2:C:106:TRP:HD1 | 1.52 | 0.54 |
| 2:E:132:LEU:HD11 | 2:E:149:LEU:HB2 | 1.90 | 0.54 |
| 1:A:108:GLY:CA | 1:A:153:GLN:NE2 | 2.71 | 0.53 |
| 1:B:128:LEU:HB2 | 1:B:129:PRO:CD | 2.38 | 0.53 |
| 3:D:139:TYR:O | 3:D:172:TYR:HD1 | 1.91 | 0.53 |
| 3:F:185:TYR:CD1 | 3:F:191:TYR:CE1 | 2.96 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:200:ILE:CG2 | 1:B:201:ILE:N | 2.71 | 0.53 |
| 1:B:267:PRO:O | 1:B:270:ASN:HB2 | 2.07 | 0.53 |
| 3:D:76:THR:HG22 | 3:D:76:THR:O | 2.08 | 0.53 |
| 3:D:90:TRP:CH2 | 3:D:95:GLN:NE2 | 2.76 | 0.53 |
| 3:D:139:TYR:HB3 | 3:D:140:PRO:CD | 2.39 | 0.53 |
| 3:D:185:TYR:HA | 3:D:191:TYR:OH | 2.07 | 0.53 |
| 3:D:90:TRP:CD2 | 3:D:95:GLN:NE2 | 2.77 | 0.53 |
| 3:F:145:VAL:HG11 | 3:F:176:SER:OG | 2.08 | 0.53 |
| 2:C:83:ILE:HD11 | 2:C:94:TYR:CE1 | 2.43 | 0.53 |
| 3:D:186:GLU:C | 3:D:188:HIS:H | 2.12 | 0.53 |
| 3:D:192:THR:HA | 3:D:207:SER:CB | 2.39 | 0.53 |
| 1:A:190:PHE:CD1 | 1:A:411:LEU:HD21 | 2.43 | 0.53 |
| 1:B:144:VAL:HG21 | 1:B:343:THR:HB | 1.90 | 0.53 |
| 1:B:288:ILE:CG2 | 1:B:289:THR:N | 2.72 | 0.53 |
| 2:C:185:LEU:CD1 | 2:C:185:LEU:C | 2.77 | 0.53 |
| 3:D:58:PRO:C | 3:D:60:ARG:H | 2.12 | 0.53 |
| 3:F:54:THR:HG22 | 3:F:55:SER:H | 1.74 | 0.53 |
| 3:F:76:THR:HG22 | 3:F:76:THR:O | 2.09 | 0.53 |
| 3:F:82:ALA:HB2 | 3:F:105:ILE:HD12 | 1.90 | 0.53 |
| 1:A:308:VAL:O | 1:A:309:ALA:HB2 | 2.08 | 0.53 |
| 1:B:282:ARG:O | 1:B:284:HIS:N | 2.41 | 0.53 |
| 2:C:41:PRO:C | 2:C:43:LYS:H | 2.12 | 0.53 |
| 3:F:181:THR:OG1 | 3:F:184:GLU:HB3 | 2.08 | 0.53 |
| 1:A:270:ASN:HA | 1:A:273:VAL:HG12 | 1.90 | 0.53 |
| 1:B:108:GLY:HA3 | 1:B:153:GLN:HE21 | 1.73 | 0.53 |
| 2:C:165:GLY:C | 2:C:167:LEU:H | 2.12 | 0.53 |
| 3:F:74:ILE:CG2 | 3:F:77:MET:HA | 2.39 | 0.53 |
| 1:B:358:ALA:O | 1:B:361:LEU:HB2 | 2.09 | 0.53 |
| 2:C:99:LEU:HD21 | 2:C:108:PHE:CD2 | 2.43 | 0.53 |
| 2:C:126:PRO:HA | 2:C:210:SER:OG | 2.09 | 0.53 |
| 1:A:171:ASP:HB3 | 1:A:212:LEU:HD13 | 1.90 | 0.53 |
| 1:A:419:TYR:OH | 1:B:414:GLU:HG2 | 2.08 | 0.53 |
| 2:C:6:GLU:OE2 | 2:C:96:CYS:N | 2.42 | 0.53 |
| 1:A:31:THR:H | 1:B:437:GLN:NE2 | 2.08 | 0.52 |
| 1:A:437:GLN:HE22 | 1:B:31:THR:H | 1.56 | 0.52 |
| 1:B:99:LYS:HG2 | 1:B:100:TYR:CE1 | 2.44 | 0.52 |
| 2:C:51:ILE:HG13 | 2:C:58:ILE:HG12 | 1.91 | 0.52 |
| 3:D:169:ASP:OD1 | 3:D:171:THR:HG23 | 2.09 | 0.52 |
| 3:F:133:CYS:HB2 | 3:F:147:TRP:HH2 | 1.74 | 0.52 |
| 1:B:422:ILE:HD12 | 1:B:425:MET:HE3 | 1.91 | 0.52 |
| 3:D:19:VAL:O | 3:D:73:THR:HG23 | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:D:37:GLN:HE21 | 3:D:43:PRO:HD3 | 1.73 | 0.52 |
| 2:E:87:ARG:HG3 | 2:E:89:GLU:OE2 | 2.08 | 0.52 |
| 2:E:196:TRP:CD1 | 2:E:196:TRP:C | 2.83 | 0.52 |
| 3:F:132:VAL:HA | 3:F:177:THR:HG23 | 1.90 | 0.52 |
| 3:F:136:ASN:HB3 | 3:F:137:ASN:HD22 | 1.75 | 0.52 |
| 1:A:419:TYR:CE1 | 1:B:414:GLU:HG2 | 2.44 | 0.52 |
| 1:B:324:THR:HG23 | 1:B:390:ALA:HB3 | 1.91 | 0.52 |
| 2:C:177:VAL:CG2 | 3:D:159:LEU:CD1 | 2.86 | 0.52 |
| 1:A:143:MET:HB3 | 1:A:347:CYS:SG | 2.49 | 0.52 |
| 1:A:274:LEU:HD23 | 1:A:277:GLN:NE2 | 2.24 | 0.52 |
| 1:A:422:ILE:HG23 | 1:A:423:LEU:N | 2.24 | 0.52 |
| 1:B:116:LEU:CD2 | 1:B:178:LEU:HD23 | 2.37 | 0.52 |
| 3:D:112:PRO:HG2 | 3:D:204:ILE:CD1 | 2.38 | 0.52 |
| 3:F:162:TRP:N | 3:F:162:TRP:HE3 | 2.08 | 0.52 |
| 2:C:7:SER:CA | 2:C:115:THR:HG21 | 2.39 | 0.52 |
| 2:C:174:PHE:CE1 | 3:D:175:SER:HB3 | 2.45 | 0.52 |
| 2:E:47:TRP:CZ2 | 2:E:49:GLY:HA2 | 2.45 | 0.52 |
| 3:F:164:ASP:O | 3:F:165:GLN:C | 2.47 | 0.52 |
| 1:A:208:PHE:HA | 1:B:210:TYR:CE1 | 2.45 | 0.52 |
| 1:A:270:ASN:HA | 1:A:273:VAL:CG1 | 2.38 | 0.52 |
| 1:A:444:LEU:O | 1:A:444:LEU:HD13 | 2.10 | 0.52 |
| 2:C:45:LEU:HD11 | 3:D:86:TYR:CE1 | 2.45 | 0.52 |
| 2:C:194:SER:O | 2:C:198:SER:OG | 2.26 | 0.52 |
| 3:F:29:VAL:HA | 3:F:91:SER:OG | 2.09 | 0.52 |
| 3:F:29:VAL:HG23 | 3:F:70:TYR:HE1 | 1.74 | 0.52 |
| 1:B:249:LEU:C | 1:B:251:THR:H | 2.12 | 0.52 |
| 2:C:111:TRP:N | 2:C:111:TRP:CD1 | 2.78 | 0.52 |
| 3:D:119:PRO:HD3 | 3:D:131:VAL:HG22 | 1.92 | 0.52 |
| 2:E:143:MET:SD | 2:E:192:PRO:HA | 2.49 | 0.52 |
| 1:B:320:ILE:HD13 | 1:B:394:MET:HE1 | 1.89 | 0.52 |
| 3:D:79:ALA:HB1 | 3:D:105:ILE:HD11 | 1.91 | 0.52 |
| 3:F:162:TRP:HE3 | 3:F:162:TRP:H | 1.58 | 0.52 |
| 2:C:6:GLU:CG | 2:C:114:GLY:HA2 | 2.40 | 0.52 |
| 3:D:107:ARG:NH2 | 3:D:108:ALA:O | 2.26 | 0.52 |
| 3:F:48:TYR:CD2 | 3:F:52:LYS:HB2 | 2.45 | 0.52 |
| 1:A:19:ARG:HB2 | 1:A:19:ARG:NH1 | 2.25 | 0.52 |
| 1:A:183:ALA:HB2 | 1:A:200:ILE:HD13 | 1.92 | 0.52 |
| 1:A:340:ARG:HA | 1:A:343:THR:OG1 | 2.10 | 0.52 |
| 3:D:22:THR:CG2 | 3:D:23:CYS:H | 2.13 | 0.52 |
| 2:E:151:LYS:HB2 | 2:E:184:THR:OG1 | 2.10 | 0.52 |
| 2:E:162:TRP:CD1 | 2:E:171:VAL:HG13 | 2.45 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:148:GLU:OE1 | 1:B:355:GLY:HA3 | 2.10 | 0.51 |
| 3:D:167:SER:OG | 3:D:168:LYS:HE3 | 2.10 | 0.51 |
| 2:E:200:THR:O | 2:E:200:THR:CG2 | 2.57 | 0.51 |
| 3:F:189:ASN:HD21 | 3:F:211:ALA:H | 1.58 | 0.51 |
| 1:A:305:LEU:HA | 1:A:308:VAL:HG22 | 1.91 | 0.51 |
| 2:C:145:THR:O | 2:C:146:LEU:HD23 | 2.10 | 0.51 |
| 2:C:163:ASN:O | 2:C:164:SER:HB2 | 2.10 | 0.51 |
| 1:A:65:MET:C | 1:A:67:ALA:H | 2.14 | 0.51 |
| 1:A:100:TYR:O | 1:A:101:ALA:HB2 | 2.10 | 0.51 |
| 1:B:74:ASN:ND2 | 1:B:76:PRO:HD2 | 2.25 | 0.51 |
| 1:A:358:ALA:HB3 | 1:A:359:PRO:HD3 | 1.91 | 0.51 |
| 2:C:161:THR:O | 2:C:204:ASN:OD1 | 2.29 | 0.51 |
| 1:A:358:ALA:O | 1:A:361:LEU:HB2 | 2.10 | 0.51 |
| 1:A:380:PRO:HD2 | 1:A:381:GLN:HE22 | 1.74 | 0.51 |
| 3:F:131:VAL:HG12 | 3:F:147:TRP:CZ3 | 2.45 | 0.51 |
| 1:A:158:ILE:O | 1:A:162:VAL:HG13 | 2.10 | 0.51 |
| 1:B:381:GLN:HE21 | 1:B:381:GLN:H | 0.75 | 0.51 |
| 3:D:73:THR:HG22 | 3:D:74:ILE:N | 2.25 | 0.51 |
| 3:D:131:VAL:HG12 | 3:D:147:TRP:CH2 | 2.45 | 0.51 |
| 2:E:36:TRP:CZ3 | 2:E:96:CYS:HB3 | 2.46 | 0.51 |
| 3:F:210:ARG:NH1 | 3:F:210:ARG:CB | 2.68 | 0.51 |
| 2:C:6:GLU:HA | 2:C:21:SER:O | 2.10 | 0.51 |
| 3:F:150:ASP:OD1 | 3:F:189:ASN:N | 2.35 | 0.51 |
| 1:A:227:ILE:O | 1:A:231:ILE:HG12 | 2.11 | 0.51 |
| 1:A:423:LEU:CB | 1:A:424:PRO:HD3 | 2.30 | 0.51 |
| 2:C:127:PRO:CB | 2:C:153:TYR:HB3 | 2.37 | 0.51 |
| 3:F:48:TYR:H | 3:F:48:TYR:HD2 | 1.57 | 0.51 |
| 1:A:356:ILE:HG23 | 1:A:356:ILE:O | 2.11 | 0.51 |
| 1:B:320:ILE:HG21 | 1:B:394:MET:CE | 2.32 | 0.51 |
| 2:C:146:LEU:HB2 | 2:C:189:VAL:HG12 | 1.93 | 0.51 |
| 3:F:48:TYR:CD2 | 3:F:52:LYS:O | 2.64 | 0.51 |
| 3:F:179:THR:O | 3:F:180:LEU:HD23 | 2.11 | 0.51 |
| 1:A:251:THR:HG22 | 1:A:255:TYR:HE1 | 1.75 | 0.50 |
| 2:E:50:GLU:OE1 | 3:F:90:TRP:CH2 | 2.64 | 0.50 |
| 1:A:208:PHE:N | 1:A:208:PHE:CD1 | 2.80 | 0.50 |
| 1:A:459:GLU:HG3 | 1:A:459:GLU:O | 2.12 | 0.50 |
| 1:B:190:PHE:HD1 | 1:B:411:LEU:HD11 | 1.76 | 0.50 |
| 2:C:45:LEU:HD12 | 2:C:45:LEU:N | 2.25 | 0.50 |
| 3:D:47:ILE:HG13 | 3:D:53:LEU:CD2 | 2.41 | 0.50 |
| 2:E:107:TYR:CB | 3:F:33:HIS:CD2 | 2.85 | 0.50 |
| 3:F:191:TYR:O | 3:F:207:SER:CB | 2.59 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:192:PRO:O | 2:C:195:SER:CB | 2.59 | 0.50 |
| 2:E:18:LEU:N | 2:E:18:LEU:CD2 | 2.75 | 0.50 |
| 2:E:91:THR:O | 2:E:92:ALA:HB2 | 2.11 | 0.50 |
| 2:E:125:THR:O | 2:E:153:TYR:HA | 2.11 | 0.50 |
| 3:F:148:LYS:HB2 | 3:F:192:THR:HG1 | 1.75 | 0.50 |
| 1:A:27:GLU:OE1 | 1:A:27:GLU:HA | 2.11 | 0.50 |
| 1:A:75:TYR:HB3 | 1:A:76:PRO:CD | 2.36 | 0.50 |
| 1:A:117:GLU:O | 1:A:118:ASP:HB2 | 2.11 | 0.50 |
| 3:D:3:VAL:HG12 | 3:D:3:VAL:O | 2.11 | 0.50 |
| 3:F:162:TRP:N | 3:F:162:TRP:CE3 | 2.79 | 0.50 |
| 1:A:116:LEU:HD12 | 1:A:204:MET:O | 2.12 | 0.50 |
| 1:A:148:GLU:O | 1:A:149:GLY:C | 2.50 | 0.50 |
| 3:D:123:GLN:HE22 | 3:D:130:SER:CB | 2.25 | 0.50 |
| 3:D:132:VAL:HG22 | 3:D:177:THR:HG23 | 1.92 | 0.50 |
| 2:E:29:TYR:CD2 | 2:E:77:ASP:HA | 2.46 | 0.50 |
| 2:E:129:VAL:HG21 | 2:E:214:VAL:HG23 | 1.94 | 0.50 |
| 1:A:17:ARG:O | 1:A:20:GLN:HB3 | 2.12 | 0.50 |
| 1:A:234:HIS:HE1 | 3:F:52:LYS:HZ3 | 1.59 | 0.50 |
| 1:A:273:VAL:HG11 | 1:A:444:LEU:HD21 | 1.93 | 0.50 |
| 1:B:163:LEU:HD12 | 1:B:168:LEU:HB2 | 1.93 | 0.50 |
| 2:C:19:LYS:HG3 | 2:C:82:GLN:HG2 | 1.93 | 0.50 |
| 3:F:159:LEU:O | 3:F:176:SER:HA | 2.12 | 0.50 |
| 3:F:164:ASP:OD2 | 3:F:165:GLN:N | 2.44 | 0.50 |
| 1:A:120:ARG:NH1 | 1:A:452:THR:CG2 | 2.75 | 0.50 |
| 1:B:74:ASN:HD21 | 1:B:76:PRO:HD2 | 1.77 | 0.50 |
| 1:B:270:ASN:HA | 1:B:273:VAL:HG12 | 1.94 | 0.50 |
| 3:F:124:LEU:C | 3:F:126:SER:H | 2.15 | 0.50 |
| 1:A:131:LYS:CE | 1:A:150:PRO:HA | 2.40 | 0.50 |
| 1:A:191:ASN:HB2 | 1:A:229:TYR:CE2 | 2.47 | 0.50 |
| 1:A:218:VAL:O | 1:A:219:PHE:C | 2.49 | 0.50 |
| 1:A:241:VAL:HG12 | 1:A:241:VAL:O | 2.11 | 0.50 |
| 1:A:383:HIS:HD2 | 2:C:33:TRP:CZ3 | 2.30 | 0.50 |
| 1:B:117:GLU:O | 1:B:118:ASP:HB2 | 2.11 | 0.50 |
| 1:B:148:GLU:O | 1:B:149:GLY:C | 2.47 | 0.50 |
| 2:E:93:LEU:HD12 | 2:E:115:THR:O | 2.12 | 0.50 |
| 3:F:56:GLY:O | 3:F:57:VAL:C | 2.49 | 0.50 |
| 1:A:284:HIS:HA | 1:A:290:LYS:HB3 | 1.94 | 0.50 |
| 1:A:288:ILE:CG2 | 1:A:289:THR:N | 2.74 | 0.50 |
| 1:A:383:HIS:HD2 | 2:C:33:TRP:CE3 | 2.30 | 0.50 |
| 1:B:356:ILE:HG23 | 1:B:356:ILE:O | 2.11 | 0.50 |
| 2:C:163:ASN:O | 2:C:164:SER:CB | 2.60 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:D:46:TRP:HA | 3:D:46:TRP:HE3 | 1.76 | 0.50 |
| 3:D:79:ALA:C | 3:D:81:ASP:H | 2.14 | 0.50 |
| 3:F:48:TYR:HD2 | 3:F:48:TYR:N | 2.10 | 0.50 |
| 1:B:279:LEU:O | 1:B:279:LEU:HD23 | 2.12 | 0.49 |
| 2:C:175:PRO:HD2 | 3:D:161:SER:OG | 2.12 | 0.49 |
| 2:E:150:VAL:HB | 2:E:185:LEU:CD1 | 2.41 | 0.49 |
| 1:A:97:VAL:HG22 | 1:A:104:ALA:HB3 | 1.94 | 0.49 |
| 1:A:241:VAL:CG1 | 1:A:244:LEU:HD21 | 2.34 | 0.49 |
| 2:C:162:TRP:C | 2:C:164:SER:H | 2.15 | 0.49 |
| 2:E:68:PHE:HD2 | 2:E:83:ILE:HG23 | 1.76 | 0.49 |
| 2:E:40:ALA:HA | 2:E:92:ALA:CB | 2.42 | 0.49 |
| 2:C:108:PHE:CD1 | 3:D:97:PHE:HZ | 2.30 | 0.49 |
| 2:C:129:VAL:CG2 | 2:C:214:VAL:HG21 | 2.39 | 0.49 |
| 2:C:200:THR:O | 2:C:200:THR:CG2 | 2.60 | 0.49 |
| 3:D:107:ARG:HG3 | 3:D:139:TYR:CD2 | 2.47 | 0.49 |
| 2:E:93:LEU:HD11 | 2:E:114:GLY:HA3 | 1.94 | 0.49 |
| 2:E:131:PRO:CB | 2:E:218:ILE:HD13 | 2.43 | 0.49 |
| 3:F:150:ASP:OD2 | 3:F:188:HIS:CB | 2.61 | 0.49 |
| 3:D:205:VAL:O | 3:D:206:LYS:HG2 | 2.12 | 0.49 |
| 2:E:52:ASN:OD1 | 2:E:52:ASN:O | 2.30 | 0.49 |
| 2:E:106:TRP:CD1 | 2:E:106:TRP:N | 2.80 | 0.49 |
| 1:A:348:PHE:CD1 | 1:A:356:ILE:HB | 2.48 | 0.49 |
| 1:B:44:THR:O | 1:B:48:LEU:HG | 2.12 | 0.49 |
| 1:B:74:ASN:HD22 | 1:B:74:ASN:C | 2.15 | 0.49 |
| 1:B:198:LEU:HD12 | 1:B:406:LEU:HG | 1.94 | 0.49 |
| 1:B:200:ILE:HD12 | 1:B:204:MET:HG3 | 1.94 | 0.49 |
| 3:D:66:SER:O | 3:D:68:THR:N | 2.45 | 0.49 |
| 1:A:208:PHE:O | 1:A:209:ARG:CB | 2.59 | 0.49 |
| 3:F:48:TYR:CD2 | 3:F:48:TYR:N | 2.80 | 0.49 |
| 3:F:88:GLN:CB | 3:F:97:PHE:CD1 | 2.91 | 0.49 |
| 3:F:150:ASP:OD2 | 3:F:188:HIS:ND1 | 2.46 | 0.49 |
| 1:A:274:LEU:O | 1:A:277:GLN:HB2 | 2.13 | 0.49 |
| 1:B:235:GLU:O | 1:B:236:VAL:CG2 | 2.61 | 0.49 |
| 1:B:305:LEU:HA | 1:B:308:VAL:HG22 | 1.94 | 0.49 |
| 1:B:308:VAL:O | 1:B:309:ALA:HB2 | 2.13 | 0.49 |
| 2:E:93:LEU:CD1 | 2:E:115:THR:H | 2.25 | 0.49 |
| 1:A:18:ARG:HB2 | 1:B:119:GLN:OE1 | 2.13 | 0.49 |
| 1:B:75:TYR:HB3 | 1:B:76:PRO:CD | 2.38 | 0.49 |
| 3:D:151:GLY:O | 3:D:152:SER:HB2 | 2.13 | 0.49 |
| 1:B:313:SER:O | 1:B:340:ARG:NH2 | 2.46 | 0.48 |
| 2:C:196:TRP:HD1 | 2:C:201:VAL:HG23 | 1.77 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:D:184:GLU:HA | 3:D:187:ARG:NH1 | 2.28 | 0.48 |
| 3:D:185:TYR:HD1 | 3:D:191:TYR:CZ | 2.31 | 0.48 |
| 1:B:148:GLU:HG2 | 1:B:357:PHE:CD2 | 2.48 | 0.48 |
| 1:B:309:ALA:O | 1:B:311:ALA:N | 2.45 | 0.48 |
| 2:C:196:TRP:HB3 | 2:C:197:PRO:HD3 | 1.95 | 0.48 |
| 3:D:172:TYR:O | 3:D:173:SER:OG | 2.31 | 0.48 |
| 3:F:191:TYR:CB | 3:F:208:PHE:CE2 | 2.96 | 0.48 |
| 1:A:320:ILE:HG21 | 1:A:394:MET:CE | 2.43 | 0.48 |
| 3:D:1:ASP:OD1 | 3:D:1:ASP:O | 2.30 | 0.48 |
| 3:D:139:TYR:O | 3:D:172:TYR:CD1 | 2.66 | 0.48 |
| 3:D:153:GLU:HG3 | 3:D:154:ARG:N | 2.27 | 0.48 |
| 2:E:131:PRO:HD3 | 2:E:216:LYS:CG | 2.42 | 0.48 |
| 2:E:191:VAL:HB | 2:E:192:PRO:CD | 2.43 | 0.48 |
| 1:A:127:VAL:HB | 1:A:157:ASN:HD21 | 1.77 | 0.48 |
| 1:A:380:PRO:HG2 | 3:D:93:HIS:HB2 | 1.96 | 0.48 |
| 1:B:294:MET:O | 1:B:294:MET:HG2 | 2.14 | 0.48 |
| 2:C:11:LEU:CD1 | 2:C:154:PHE:HE2 | 2.26 | 0.48 |
| 2:E:51:ILE:HG23 | 2:E:51:ILE:O | 2.13 | 0.48 |
| 1:A:356:ILE:HG23 | 1:A:360:MET:HE2 | 1.96 | 0.48 |
| 1:A:416:THR:O | 1:A:418:ASN:ND2 | 2.42 | 0.48 |
| 2:E:125:THR:HG22 | 2:E:125:THR:O | 2.13 | 0.48 |
| 3:F:194:GLU:OE1 | 3:F:203:PRO:HB2 | 2.12 | 0.48 |
| 1:A:83:PHE:CD1 | 1:A:83:PHE:C | 2.86 | 0.48 |
| 1:A:282:ARG:O | 1:A:284:HIS:N | 2.47 | 0.48 |
| 1:A:362:ALA:O | 1:A:366:VAL:HG23 | 2.14 | 0.48 |
| 1:A:383:HIS:NE2 | 3:D:90:TRP:CZ2 | 2.81 | 0.48 |
| 1:B:100:TYR:O | 1:B:101:ALA:HB2 | 2.13 | 0.48 |
| 1:B:190:PHE:CD1 | 1:B:411:LEU:HD11 | 2.49 | 0.48 |
| 1:B:235:GLU:O | 1:B:236:VAL:HG23 | 2.13 | 0.48 |
| 3:D:38:LYS:O | 3:D:39:SER:C | 2.51 | 0.48 |
| 3:D:90:TRP:O | 3:D:90:TRP:CD1 | 2.66 | 0.48 |
| 2:E:49:GLY:HA3 | 2:E:70:ILE:CD1 | 2.43 | 0.48 |
| 3:F:29:VAL:HG23 | 3:F:70:TYR:CE1 | 2.48 | 0.48 |
| 1:A:273:VAL:HA | 1:A:345:LEU:HD22 | 1.94 | 0.48 |
| 1:A:313:SER:OG | 1:A:314:GLY:N | 2.47 | 0.48 |
| 1:B:443:PRO:O | 1:B:445:TYR:N | 2.46 | 0.48 |
| 2:C:32:TYR:HE2 | 2:C:98:ARG:CD | 2.26 | 0.48 |
| 3:D:181:THR:O | 3:D:182:LYS:C | 2.52 | 0.48 |
| 1:A:148:GLU:HG2 | 1:A:357:PHE:HD2 | 1.79 | 0.48 |
| 1:B:64:ARG:O | 1:B:67:ALA:HB3 | 2.14 | 0.48 |
| 1:B:86:SER:HB3 | 1:B:299:GLY:O | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:174:PHE:CD1 | 3:D:175:SER:HB3 | 2.48 | 0.48 |
| 3:F:123:GLN:HE22 | 3:F:130:SER:CB | 2.26 | 0.48 |
| 3:D:33:HIS:HB2 | 3:D:88:GLN:OE1 | 2.13 | 0.48 |
| 3:D:137:ASN:ND2 | 3:D:137:ASN:N | 2.62 | 0.48 |
| 3:F:17:ASP:O | 3:F:76:THR:HA | 2.13 | 0.48 |
| 3:F:189:ASN:HA | 3:F:210:ARG:HD3 | 1.94 | 0.48 |
| 1:A:18:ARG:O | 1:A:22:ILE:HG13 | 2.14 | 0.48 |
| 1:A:75:TYR:O | 1:A:78:LEU:HB3 | 2.14 | 0.48 |
| 1:B:83:PHE:CD1 | 1:B:84:LEU:HD23 | 2.49 | 0.48 |
| 1:B:128:LEU:HD21 | 1:B:157:ASN:HB2 | 1.94 | 0.48 |
| 1:B:224:MET:O | 1:B:228:MET:HG2 | 2.14 | 0.48 |
| 2:E:87:ARG:HG3 | 2:E:89:GLU:H | 1.79 | 0.48 |
| 1:A:189:ALA:O | 1:A:190:PHE:HD2 | 1.98 | 0.47 |
| 1:B:305:LEU:C | 1:B:307:PHE:H | 2.17 | 0.47 |
| 1:B:422:ILE:HG23 | 1:B:423:LEU:N | 2.29 | 0.47 |
| 2:C:53:PRO:O | 2:C:74:ASN:ND2 | 2.43 | 0.47 |
| 2:E:127:PRO:HB2 | 2:E:150:VAL:HG12 | 1.95 | 0.47 |
| 2:E:179:GLN:O | 2:E:180:ALA:CB | 2.62 | 0.47 |
| 1:B:410:ILE:O | 1:B:414:GLU:HB2 | 2.13 | 0.47 |
| 2:C:177:VAL:O | 2:C:177:VAL:HG23 | 2.14 | 0.47 |
| 2:C:189:VAL:HG13 | 2:C:189:VAL:O | 2.13 | 0.47 |
| 1:A:454:ALA:C | 1:A:456:GLN:H | 2.17 | 0.47 |
| 2:C:131:PRO:HD3 | 2:C:216:LYS:HD2 | 1.96 | 0.47 |
| 2:C:185:LEU:HD12 | 2:C:185:LEU:C | 2.35 | 0.47 |
| 3:D:116:ILE:HG21 | 3:D:206:LYS:O | 2.15 | 0.47 |
| 3:D:149:ILE:HD11 | 3:D:178:LEU:HD21 | 1.96 | 0.47 |
| 3:F:34:TRP:CE2 | 3:F:72:LEU:HB2 | 2.49 | 0.47 |
| 3:F:192:THR:CB | 3:F:207:SER:HB3 | 2.43 | 0.47 |
| 1:A:320:ILE:N | 1:A:321:PRO:CD | 2.78 | 0.47 |
| 1:B:274:LEU:HD23 | 1:B:277:GLN:NE2 | 2.30 | 0.47 |
| 2:C:147:GLY:CA | 2:C:162:TRP:HH2 | 2.22 | 0.47 |
| 3:D:13:ALA:CB | 3:D:77:MET:HE3 | 2.38 | 0.47 |
| 2:E:132:LEU:HB3 | 3:F:117:PHE:CD2 | 2.49 | 0.47 |
| 3:F:72:LEU:C | 3:F:72:LEU:CD2 | 2.83 | 0.47 |
| 3:F:150:ASP:OD2 | 3:F:188:HIS:HA | 2.14 | 0.47 |
| 1:A:437:GLN:NE2 | 1:B:30:LYS:HA | 2.29 | 0.47 |
| 2:C:178:LEU:HD22 | 2:C:183:TYR:CZ | 2.49 | 0.47 |
| 3:D:7:SER:CB | 3:D:8:PRO:CD | 2.91 | 0.47 |
| 3:D:150:ASP:OD2 | 3:D:188:HIS:HB3 | 2.13 | 0.47 |
| 2:E:127:PRO:HB3 | 2:E:153:TYR:HB3 | 1.95 | 0.47 |
| 3:D:139:TYR:HD1 | 3:D:140:PRO:HD3 | 1.77 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:18:ARG:O | 1:A:18:ARG:HG2 | 2.12 | 0.47 |
| 1:A:182:ALA:HB1 | 1:A:204:MET:HE2 | 1.96 | 0.47 |
| 1:A:270:ASN:ND2 | 1:A:444:LEU:HD23 | 2.29 | 0.47 |
| 1:A:409:ILE:CD1 | 1:A:426:ILE:HG12 | 2.44 | 0.47 |
| 2:C:98:ARG:NH1 | 2:C:109:ASP:OD2 | 2.48 | 0.47 |
| 3:D:143:ILE:HG23 | 3:D:174:MET:HE1 | 1.96 | 0.47 |
| 2:E:24:ALA:HB1 | 2:E:27:PHE:HE1 | 1.80 | 0.47 |
| 2:E:27:PHE:HE2 | 2:E:98:ARG:HG3 | 1.79 | 0.47 |
| 3:F:20:THR:HG23 | 3:F:73:THR:HG1 | 1.77 | 0.47 |
| 3:F:59:VAL:HG12 | 3:F:59:VAL:O | 2.14 | 0.47 |
| 1:A:457:GLU:OE2 | 1:B:19:ARG:HD3 | 2.14 | 0.47 |
| 1:B:150:PRO:HD3 | 1:B:354:GLY:HA2 | 1.97 | 0.47 |
| 3:F:1:ASP:OD1 | 3:F:1:ASP:N | 2.42 | 0.47 |
| 3:F:75:ASN:O | 3:F:76:THR:HB | 2.14 | 0.47 |
| 3:D:136:ASN:C | 3:D:137:ASN:HD22 | 2.17 | 0.47 |
| 3:F:48:TYR:CE2 | 3:F:52:LYS:CB | 2.96 | 0.47 |
| 1:A:260:ILE:HG23 | 1:A:435:LEU:HG | 1.96 | 0.47 |
| 1:B:220:ILE:O | 1:B:224:MET:HG2 | 2.15 | 0.47 |
| 2:C:125:THR:HA | 2:C:126:PRO:HD2 | 1.56 | 0.47 |
| 2:E:176:ALA:HA | 2:E:185:LEU:HB3 | 1.95 | 0.47 |
| 1:A:53:PHE:CE1 | 1:A:136:LEU:HD12 | 2.50 | 0.46 |
| 2:C:167:LEU:C | 2:C:167:LEU:HD12 | 2.35 | 0.46 |
| 2:C:203:CYS:SG | 2:C:203:CYS:O | 2.72 | 0.46 |
| 3:F:60:ARG:HD3 | 3:F:78:GLU:HG2 | 1.97 | 0.46 |
| 2:C:126:PRO:CA | 2:C:210:SER:OG | 2.62 | 0.46 |
| 2:E:36:TRP:CE3 | 2:E:96:CYS:HB3 | 2.50 | 0.46 |
| 2:E:87:ARG:O | 2:E:119:VAL:HG21 | 2.15 | 0.46 |
| 3:F:110:ALA:HB3 | 3:F:139:TYR:CB | 2.45 | 0.46 |
| 1:B:148:GLU:HG2 | 1:B:357:PHE:HD2 | 1.79 | 0.46 |
| 3:D:179:THR:O | 3:D:180:LEU:HD23 | 2.16 | 0.46 |
| 3:F:183:ASP:O | 3:F:185:TYR:N | 2.48 | 0.46 |
| 1:A:176:THR:HG22 | 1:A:177:LEU:N | 2.30 | 0.46 |
| 1:A:182:ALA:HB1 | 1:A:204:MET:CE | 2.46 | 0.46 |
| 1:B:114:GLY:O | 1:B:117:GLU:N | 2.44 | 0.46 |
| 2:C:174:PHE:CE1 | 3:D:175:SER:N | 2.82 | 0.46 |
| 3:D:60:ARG:HH11 | 3:D:81:ASP:CG | 2.18 | 0.46 |
| 2:E:30:SER:C | 2:E:32:TYR:H | 2.18 | 0.46 |
| 2:C:134:PRO:O | 2:C:221:ARG:HG3 | 2.16 | 0.46 |
| 3:D:143:ILE:HG23 | 3:D:174:MET:HE3 | 1.96 | 0.46 |
| 1:B:250:ASN:HB2 | 2:E:105:TYR:HE1 | 1.80 | 0.46 |
| 2:C:136:SER:C | 2:C:138:ALA:H | 2.19 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:150:VAL:HB | 2:C:185:LEU:HD11 | 1.97 | 0.46 |
| 3:D:7:SER:O | 3:D:8:PRO:C | 2.53 | 0.46 |
| 1:A:248:PRO:HG3 | 2:C:101:TYR:CZ | 2.50 | 0.46 |
| 1:B:269:PHE:O | 1:B:273:VAL:HG12 | 2.15 | 0.46 |
| 2:C:126:PRO:HB3 | 2:C:210:SER:OG | 2.15 | 0.46 |
| 2:E:6:GLU:H | 2:E:6:GLU:CD | 2.18 | 0.46 |
| 1:A:148:GLU:HG2 | 1:A:357:PHE:CD2 | 2.51 | 0.46 |
| 1:A:437:GLN:NE2 | 1:B:31:THR:H | 2.14 | 0.46 |
| 2:C:6:GLU:CD | 2:C:114:GLY:HA2 | 2.36 | 0.46 |
| 2:C:67:LYS:HA | 2:C:67:LYS:HD3 | 1.69 | 0.46 |
| 3:D:109:ASP:HA | 3:D:139:TYR:HB3 | 1.98 | 0.46 |
| 2:E:67:LYS:HE2 | 2:E:84:SER:O | 2.16 | 0.46 |
| 1:A:83:PHE:CD1 | 1:A:84:LEU:HD23 | 2.50 | 0.46 |
| 1:B:423:LEU:HB3 | 1:B:424:PRO:CD | 2.44 | 0.46 |
| 2:C:32:TYR:CE2 | 2:C:98:ARG:CD | 2.99 | 0.46 |
| 1:A:232:PHE:CD1 | 1:A:232:PHE:N | 2.84 | 0.45 |
| 1:A:422:ILE:CG2 | 1:A:423:LEU:N | 2.78 | 0.45 |
| 3:D:190:SER:O | 3:D:191:TYR:CD1 | 2.69 | 0.45 |
| 3:F:89:GLN:HE21 | 3:F:96:THR:N | 2.13 | 0.45 |
| 3:F:120:SER:OG | 3:F:123:GLN:HB2 | 2.15 | 0.45 |
| 1:A:25:LEU:HD23 | 1:B:208:PHE:CZ | 2.51 | 0.45 |
| 1:A:74:ASN:HD22 | 1:A:74:ASN:C | 2.18 | 0.45 |
| 1:A:138:THR:HG21 | 1:A:352:ALA:HB1 | 1.97 | 0.45 |
| 1:B:83:PHE:CD1 | 1:B:83:PHE:C | 2.89 | 0.45 |
| 1:B:116:LEU:HD12 | 1:B:204:MET:O | 2.16 | 0.45 |
| 1:B:312:THR:HG22 | 1:B:339:ALA:CB | 2.46 | 0.45 |
| 3:D:47:ILE:HD11 | 3:D:61:PHE:HB3 | 1.97 | 0.45 |
| 3:D:116:ILE:O | 3:D:116:ILE:HG23 | 2.16 | 0.45 |
| 3:F:32:ILE:HD13 | 3:F:89:GLN:HB3 | 1.94 | 0.45 |
| 1:A:361:LEU:HD23 | 1:A:394:MET:O | 2.15 | 0.45 |
| 1:B:163:LEU:HD22 | 1:B:174:ARG:HA | 1.98 | 0.45 |
| 1:B:357:PHE:CE1 | 1:B:398:LEU:HD22 | 2.51 | 0.45 |
| 1:B:422:ILE:CG2 | 1:B:423:LEU:N | 2.79 | 0.45 |
| 2:C:32:TYR:CD2 | 2:C:98:ARG:CG | 2.99 | 0.45 |
| 3:D:47:ILE:HD13 | 3:D:72:LEU:HD12 | 1.98 | 0.45 |
| 3:D:139:TYR:O | 3:D:140:PRO:C | 2.53 | 0.45 |
| 2:E:178:LEU:HD12 | 2:E:182:LEU:O | 2.16 | 0.45 |
| 1:A:30:LYS:HA | 1:B:437:GLN:NE2 | 2.31 | 0.45 |
| 2:C:130:TYR:HB3 | 3:D:120:SER:HG | 1.81 | 0.45 |
| 2:E:174:PHE:CG | 3:F:175:SER:HB3 | 2.51 | 0.45 |
| 2:E:210:SER:O | 2:E:211:SER:HB3 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:183:ASP:O | 3:F:186:GLU:N | 2.50 | 0.45 |
| 1:A:68:LEU:CD2 | 1:A:81:VAL:HG23 | 2.47 | 0.45 |
| 1:B:385:GLU:O | 1:B:386:ALA:C | 2.55 | 0.45 |
| 1:B:402:ILE:O | 1:B:402:ILE:CG1 | 2.64 | 0.45 |
| 2:E:35:SER:HB2 | 2:E:49:GLY:O | 2.16 | 0.45 |
| 3:F:48:TYR:HD2 | 3:F:52:LYS:O | 1.99 | 0.45 |
| 1:A:37:PHE:HD2 | 1:A:38:MET:HE2 | 1.81 | 0.45 |
| 1:A:207:GLN:HG2 | 1:B:28:ARG:HD2 | 1.99 | 0.45 |
| 1:B:284:HIS:HB3 | 1:B:290:LYS:O | 2.17 | 0.45 |
| 2:E:16:GLY:N | 2:E:86:VAL:HG22 | 2.25 | 0.45 |
| 3:F:138:PHE:CD1 | 3:F:140:PRO:O | 2.69 | 0.45 |
| 1:B:171:ASP:CB | 1:B:212:LEU:HD22 | 2.39 | 0.45 |
| 1:B:312:THR:HG22 | 1:B:339:ALA:HB3 | 1.98 | 0.45 |
| 1:B:399:ALA:O | 1:B:403:ARG:HA | 2.16 | 0.45 |
| 2:C:105:TYR:CE2 | 3:D:31:TYR:CD1 | 3.01 | 0.45 |
| 2:E:38:ARG:HE | 2:E:46:LYS:HE3 | 1.81 | 0.45 |
| 3:F:185:TYR:CE1 | 3:F:191:TYR:HE1 | 2.34 | 0.45 |
| 1:A:42:VAL:CG2 | 1:A:162:VAL:HG21 | 2.46 | 0.45 |
| 1:B:127:VAL:CB | 1:B:157:ASN:HD21 | 2.27 | 0.45 |
| 2:E:36:TRP:CE2 | 2:E:81:LEU:HB2 | 2.52 | 0.45 |
| 1:A:74:ASN:ND2 | 1:A:76:PRO:HD2 | 2.32 | 0.45 |
| 1:B:131:LYS:HE2 | 1:B:153:GLN:HE21 | 1.80 | 0.45 |
| 2:C:104:GLY:C | 2:C:105:TYR:HD1 | 2.19 | 0.45 |
| 3:D:1:ASP:O | 3:D:1:ASP:CG | 2.55 | 0.45 |
| 2:E:18:LEU:HD11 | 2:E:117:VAL:HG11 | 1.99 | 0.45 |
| 2:E:108:PHE:HD1 | 3:F:88:GLN:NE2 | 2.11 | 0.45 |
| 3:F:5:THR:O | 3:F:5:THR:HG22 | 2.16 | 0.45 |
| 1:B:68:LEU:CD2 | 1:B:81:VAL:HG23 | 2.47 | 0.45 |
| 1:B:228:MET:O | 1:B:232:PHE:HD1 | 2.00 | 0.45 |
| 1:B:270:ASN:O | 1:B:273:VAL:CG1 | 2.65 | 0.45 |
| 3:D:197:HIS:CE1 | 3:D:199:THR:HG23 | 2.52 | 0.45 |
| 1:B:42:VAL:HG23 | 1:B:162:VAL:HG21 | 1.97 | 0.44 |
| 1:B:54:ASP:OD1 | 1:B:147:ARG:NE | 2.45 | 0.44 |
| 2:C:150:VAL:HB | 2:C:185:LEU:HD12 | 1.99 | 0.44 |
| 2:E:95:TYR:OH | 3:F:37:GLN:NE2 | 2.50 | 0.44 |
| 3:F:131:VAL:HG12 | 3:F:147:TRP:CH2 | 2.52 | 0.44 |
| 3:F:210:ARG:NH1 | 3:F:210:ARG:CG | 2.70 | 0.44 |
| 1:A:124:TRP:HB3 | 1:A:157:ASN:HB3 | 1.99 | 0.44 |
| 1:A:416:THR:O | 1:A:417:ASP:C | 2.56 | 0.44 |
| 2:C:33:TRP:CE2 | 2:C:52:ASN:HB3 | 2.52 | 0.44 |
| 3:D:114:VAL:HG11 | 3:D:206:LYS:HB2 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:E:18:LEU:HD11 | 2:E:117:VAL:CG1 | 2.47 | 0.44 |
| 1:A:413:LEU:HD22 | 1:A:422:ILE:HD13 | 1.98 | 0.44 |
| 1:B:236:VAL:HG12 | 1:B:237:ALA:N | 2.33 | 0.44 |
| 2:C:13:GLN:HA | 2:C:120:SER:O | 2.18 | 0.44 |
| 3:D:19:VAL:O | 3:D:73:THR:HA | 2.18 | 0.44 |
| 3:D:58:PRO:CB | 3:D:60:ARG:NH2 | 2.81 | 0.44 |
| 2:E:98:ARG:O | 2:E:109:ASP:HB3 | 2.18 | 0.44 |
| 3:F:34:TRP:CE3 | 3:F:87:CYS:HB3 | 2.53 | 0.44 |
| 3:F:111:ALA:CA | 3:F:199:THR:HG21 | 2.46 | 0.44 |
| 3:F:191:TYR:CB | 3:F:208:PHE:HE2 | 2.30 | 0.44 |
| 1:A:190:PHE:CE1 | 1:A:411:LEU:HD21 | 2.52 | 0.44 |
| 1:A:231:ILE:HB | 1:A:232:PHE:CD1 | 2.53 | 0.44 |
| 1:A:234:HIS:HE1 | 3:F:52:LYS:NZ | 2.09 | 0.44 |
| 1:A:380:PRO:HG2 | 3:D:93:HIS:CB | 2.47 | 0.44 |
| 1:B:190:PHE:HD1 | 1:B:411:LEU:CD1 | 2.31 | 0.44 |
| 3:F:88:GLN:HG3 | 3:F:97:PHE:CD1 | 2.52 | 0.44 |
| 1:A:267:PRO:O | 1:A:270:ASN:HB2 | 2.17 | 0.44 |
| 2:E:29:TYR:HB2 | 2:E:77:ASP:OD2 | 2.17 | 0.44 |
| 2:E:122:ALA:HB3 | 2:E:154:PHE:CE2 | 2.52 | 0.44 |
| 1:B:287:ASN:HD22 | 1:B:290:LYS:N | 2.11 | 0.44 |
| 1:B:340:ARG:HA | 1:B:343:THR:OG1 | 2.17 | 0.44 |
| 1:B:422:ILE:HA | 1:B:425:MET:HE2 | 2.00 | 0.44 |
| 2:C:11:LEU:HD11 | 2:C:154:PHE:HE2 | 1.82 | 0.44 |
| 2:C:105:TYR:CD1 | 2:C:105:TYR:N | 2.86 | 0.44 |
| 3:D:124:LEU:HD22 | 3:D:182:LYS:HG3 | 2.00 | 0.44 |
| 2:E:175:PRO:HG2 | 3:F:162:TRP:O | 2.18 | 0.44 |
| 3:F:185:TYR:CE1 | 3:F:191:TYR:CE1 | 3.06 | 0.44 |
| 1:A:270:ASN:CG | 1:A:444:LEU:HD23 | 2.38 | 0.44 |
| 2:C:162:TRP:C | 2:C:164:SER:N | 2.69 | 0.44 |
| 2:E:52:ASN:OD1 | 2:E:52:ASN:C | 2.56 | 0.44 |
| 3:F:66:SER:N | 3:F:70:TYR:CE2 | 2.85 | 0.44 |
| 3:F:119:PRO:HD3 | 3:F:131:VAL:HG22 | 1.99 | 0.44 |
| 1:A:249:LEU:C | 1:A:251:THR:N | 2.69 | 0.44 |
| 1:B:209:ARG:HG3 | 1:B:210:TYR:O | 2.17 | 0.44 |
| 1:B:287:ASN:HD22 | 1:B:290:LYS:CB | 2.30 | 0.44 |
| 2:C:151:LYS:HG3 | 2:C:152:GLY:N | 2.33 | 0.44 |
| 3:D:50:THR:CG2 | 3:D:70:TYR:CD2 | 3.00 | 0.44 |
| 3:F:109:ASP:OD1 | 3:F:198:LYS:HE2 | 2.18 | 0.44 |
| 1:B:187:ALA:O | 1:B:189:ALA:N | 2.51 | 0.44 |
| 1:B:405:PRO:HG2 | 1:B:406:LEU:H | 1.82 | 0.44 |
| 2:C:64:LEU:O | 2:C:65:LYS:C | 2.55 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:176:ALA:HA | 2:C:185:LEU:HB3 | 2.00 | 0.44 |
| 3:D:73:THR:CG2 | 3:D:74:ILE:N | 2.80 | 0.44 |
| 1:A:44:THR:O | 1:A:48:LEU:HG | 2.18 | 0.43 |
| 1:B:90:ALA:CB | 1:B:299:GLY:HA3 | 2.48 | 0.43 |
| 1:B:239:ILE:HD13 | 1:B:394:MET:HE1 | 2.00 | 0.43 |
| 2:C:138:ALA:O | 2:C:140:ALA:N | 2.49 | 0.43 |
| 2:E:134:PRO:O | 2:E:221:ARG:HG3 | 2.17 | 0.43 |
| 3:F:4:LEU:HA | 3:F:24:SER:O | 2.18 | 0.43 |
| 1:B:27:GLU:HA | 1:B:27:GLU:OE1 | 2.18 | 0.43 |
| 2:C:108:PHE:CE1 | 3:D:97:PHE:CZ | 3.06 | 0.43 |
| 2:E:48:ILE:HD13 | 2:E:48:ILE:N | 2.34 | 0.43 |
| 3:F:185:TYR:HD1 | 3:F:191:TYR:CE1 | 2.36 | 0.43 |
| 1:A:128:LEU:HD21 | 1:A:157:ASN:HB2 | 1.98 | 0.43 |
| 1:B:378:LEU:HB2 | 1:B:379:PHE:CE1 | 2.54 | 0.43 |
| 2:C:7:SER:C | 2:C:115:THR:HG21 | 2.38 | 0.43 |
| 2:C:78:THR:HG22 | 2:C:79:LEU:N | 2.32 | 0.43 |
| 2:C:132:LEU:HD11 | 2:C:149:LEU:HB2 | 1.99 | 0.43 |
| 3:D:61:PHE:HA | 3:D:73:THR:O | 2.17 | 0.43 |
| 2:E:172:HIS:CD2 | 3:F:173:SER:OG | 2.71 | 0.43 |
| 2:E:210:SER:OG | 2:E:212:THR:HG23 | 2.18 | 0.43 |
| 1:B:279:LEU:HD23 | 1:B:279:LEU:C | 2.39 | 0.43 |
| 3:D:189:ASN:HD21 | 3:D:209:ASN:HB3 | 1.83 | 0.43 |
| 3:F:88:GLN:HG2 | 3:F:89:GLN:N | 2.33 | 0.43 |
| 3:F:119:PRO:HG3 | 3:F:130:SER:C | 2.39 | 0.43 |
| 3:F:185:TYR:CD1 | 3:F:191:TYR:HE1 | 2.35 | 0.43 |
| 1:B:171:ASP:HB3 | 1:B:212:LEU:HD13 | 1.99 | 0.43 |
| 1:B:320:ILE:N | 1:B:321:PRO:CD | 2.81 | 0.43 |
| 2:C:156:GLU:HG2 | 2:C:183:TYR:CE1 | 2.52 | 0.43 |
| 3:D:30:SER:O | 3:D:31:TYR:HB2 | 2.18 | 0.43 |
| 3:D:117:PHE:HA | 3:D:118:PRO:HD3 | 1.92 | 0.43 |
| 3:D:133:CYS:HB2 | 3:D:147:TRP:CH2 | 2.54 | 0.43 |
| 3:D:192:THR:HB | 3:D:207:SER:HB3 | 2.00 | 0.43 |
| 1:A:255:TYR:O | 1:A:428:THR:HA | 2.18 | 0.43 |
| 1:A:422:ILE:HD12 | 1:A:425:MET:HE3 | 2.00 | 0.43 |
| 1:B:320:ILE:O | 1:B:324:THR:OG1 | 2.34 | 0.43 |
| 1:B:423:LEU:O | 1:B:427:ILE:HG13 | 2.18 | 0.43 |
| 2:C:196:TRP:C | 2:C:198:SER:N | 2.71 | 0.43 |
| 3:D:138:PHE:HE1 | 3:D:141:LYS:HA | 1.84 | 0.43 |
| 2:E:177:VAL:HG21 | 3:F:159:LEU:HD13 | 2.00 | 0.43 |
| 1:A:124:TRP:CB | 1:A:157:ASN:HB3 | 2.49 | 0.43 |
| 1:A:430:LEU:HD21 | 1:B:220:ILE:CG1 | 2.48 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:180:THR:O | 1:B:181:GLY:C | 2.56 | 0.43 |
| 1:B:445:TYR:HD2 | 1:B:445:TYR:HA | 1.72 | 0.43 |
| 2:C:112:GLY:O | 3:D:42:SER:CB | 2.66 | 0.43 |
| 3:F:194:GLU:OE1 | 3:F:203:PRO:CB | 2.67 | 0.43 |
| 3:D:18:LYS:HG3 | 3:D:75:ASN:HA | 2.00 | 0.43 |
| 3:D:58:PRO:O | 3:D:60:ARG:N | 2.51 | 0.43 |
| 2:E:52:ASN:HB2 | 2:E:53:PRO:HD2 | 2.00 | 0.43 |
| 2:E:111:TRP:N | 2:E:111:TRP:CD1 | 2.87 | 0.43 |
| 2:E:139:ALA:O | 2:E:141:ALA:N | 2.52 | 0.43 |
| 2:E:144:VAL:HG22 | 2:E:146:LEU:CD2 | 2.48 | 0.43 |
| 3:F:32:ILE:HG23 | 3:F:88:GLN:O | 2.18 | 0.43 |
| 3:F:113:THR:HG22 | 3:F:113:THR:O | 2.19 | 0.43 |
| 3:F:124:LEU:O | 3:F:126:SER:N | 2.49 | 0.43 |
| 1:A:288:ILE:HG23 | 1:A:289:THR:N | 2.33 | 0.43 |
| 2:E:156:GLU:HA | 2:E:157:PRO:HA | 1.80 | 0.43 |
| 3:F:187:ARG:HG2 | 3:F:188:HIS:HD2 | 1.78 | 0.43 |
| 1:A:30:LYS:HE2 | 1:A:30:LYS:HB3 | 1.87 | 0.43 |
| 1:A:42:VAL:O | 1:A:46:VAL:HG23 | 2.19 | 0.43 |
| 1:A:208:PHE:CZ | 1:B:25:LEU:HD23 | 2.54 | 0.43 |
| 1:A:324:THR:HG23 | 1:A:390:ALA:HB3 | 2.01 | 0.43 |
| 1:B:251:THR:HG22 | 1:B:255:TYR:HE1 | 1.84 | 0.43 |
| 1:B:348:PHE:CD1 | 1:B:356:ILE:HB | 2.54 | 0.43 |
| 2:C:162:TRP:CZ2 | 2:C:189:VAL:HB | 2.53 | 0.43 |
| 3:D:46:TRP:O | 3:D:54:THR:OG1 | 2.27 | 0.43 |
| 1:A:220:ILE:HG12 | 1:B:430:LEU:HD21 | 2.00 | 0.42 |
| 1:A:245:SER:O | 1:A:420:GLN:NE2 | 2.50 | 0.42 |
| 1:A:250:ASN:ND2 | 2:C:104:GLY:O | 2.50 | 0.42 |
| 1:A:421:LEU:O | 1:A:424:PRO:HD2 | 2.19 | 0.42 |
| 1:B:38:MET:O | 1:B:41:VAL:HG12 | 2.18 | 0.42 |
| 1:B:130:VAL:O | 1:B:134:GLY:N | 2.52 | 0.42 |
| 1:B:250:ASN:CB | 2:E:105:TYR:HE1 | 2.32 | 0.42 |
| 2:C:149:LEU:HD22 | 3:D:132:VAL:CG2 | 2.49 | 0.42 |
| 2:E:107:TYR:HD1 | 2:E:107:TYR:C | 2.23 | 0.42 |
| 1:A:83:PHE:HD1 | 1:A:84:LEU:N | 2.18 | 0.42 |
| 1:A:409:ILE:HD13 | 1:A:426:ILE:CG1 | 2.47 | 0.42 |
| 1:B:117:GLU:HA | 1:B:209:ARG:HH12 | 1.84 | 0.42 |
| 2:C:171:VAL:O | 2:C:171:VAL:HG12 | 2.18 | 0.42 |
| 3:D:60:ARG:NH1 | 3:D:81:ASP:OD1 | 2.52 | 0.42 |
| 3:D:75:ASN:O | 3:D:76:THR:HB | 2.19 | 0.42 |
| 3:D:194:GLU:HG2 | 3:D:205:VAL:HG12 | 2.00 | 0.42 |
| 3:F:58:PRO:C | 3:F:60:ARG:H | 2.22 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:91:MET:C | 1:A:93:GLY:N | 2.72 | 0.42 |
| 1:A:99:LYS:O | 1:A:99:LYS:HG3 | 2.20 | 0.42 |
| 1:A:101:ALA:O | 1:A:103:GLU:N | 2.52 | 0.42 |
| 1:A:197:ILE:HD13 | 1:A:219:PHE:CE1 | 2.54 | 0.42 |
| 1:B:97:VAL:HG22 | 1:B:104:ALA:HB3 | 2.01 | 0.42 |
| 1:B:146:GLY:HA3 | 1:B:148:GLU:OE2 | 2.19 | 0.42 |
| 2:C:32:TYR:HE2 | 2:C:98:ARG:NE | 2.17 | 0.42 |
| 3:D:47:ILE:CG1 | 3:D:53:LEU:HD23 | 2.48 | 0.42 |
| 3:F:124:LEU:HA | 3:F:128:GLY:O | 2.19 | 0.42 |
| 1:A:86:SER:HB2 | 1:A:300:GLY:HA2 | 2.02 | 0.42 |
| 1:A:103:GLU:HB3 | 1:A:111:GLU:HG2 | 2.01 | 0.42 |
| 1:A:385:GLU:O | 1:A:386:ALA:C | 2.58 | 0.42 |
| 1:B:120:ARG:NH1 | 1:B:452:THR:CG2 | 2.82 | 0.42 |
| 3:D:60:ARG:HD3 | 3:D:76:THR:O | 2.19 | 0.42 |
| 3:D:189:ASN:ND2 | 3:D:211:ALA:H | 2.17 | 0.42 |
| 1:A:443:PRO:O | 1:A:445:TYR:N | 2.53 | 0.42 |
| 1:B:128:LEU:HD21 | 1:B:157:ASN:CB | 2.49 | 0.42 |
| 1:B:270:ASN:HA | 1:B:273:VAL:CG1 | 2.48 | 0.42 |
| 2:E:4:LEU:HD12 | 2:E:4:LEU:HA | 1.94 | 0.42 |
| 2:E:57:THR:O | 2:E:58:ILE:HG12 | 2.18 | 0.42 |
| 2:E:66:ASP:O | 2:E:67:LYS:C | 2.55 | 0.42 |
| 2:E:208:PRO:O | 2:E:209:ALA:C | 2.58 | 0.42 |
| 3:F:77:MET:CG | 3:F:78:GLU:N | 2.80 | 0.42 |
| 1:A:38:MET:CA | 1:A:41:VAL:HG12 | 2.44 | 0.42 |
| 1:A:172:GLU:HA | 1:A:212:LEU:O | 2.19 | 0.42 |
| 1:A:216:LYS:HD3 | 1:B:434:LEU:CD2 | 2.49 | 0.42 |
| 2:C:99:LEU:HD21 | 2:C:108:PHE:CE2 | 2.55 | 0.42 |
| 3:D:2:ILE:HG21 | 3:D:29:VAL:CG1 | 2.50 | 0.42 |
| 3:D:118:PRO:HB3 | 3:D:208:PHE:CZ | 2.55 | 0.42 |
| 3:D:178:LEU:HD12 | 3:D:179:THR:H | 1.83 | 0.42 |
| 1:A:19:ARG:HB2 | 1:A:19:ARG:HH11 | 1.84 | 0.42 |
| 1:A:31:THR:HA | 1:A:32:PRO:HD3 | 1.95 | 0.42 |
| 1:B:266:GLY:HA3 | 1:B:400:ALA:HB1 | 2.02 | 0.42 |
| 2:E:104:GLY:O | 2:E:106:TRP:HD1 | 2.02 | 0.42 |
| 3:F:4:LEU:HD12 | 3:F:96:THR:O | 2.20 | 0.42 |
| 3:F:111:ALA:HA | 3:F:112:PRO:HD2 | 1.91 | 0.42 |
| 3:F:119:PRO:HG3 | 3:F:130:SER:O | 2.20 | 0.42 |
| 1:B:135:GLY:O | 1:B:136:LEU:C | 2.58 | 0.42 |
| 3:D:79:ALA:HB1 | 3:D:105:ILE:HD13 | 2.02 | 0.42 |
| 1:A:234:HIS:CE1 | 3:F:52:LYS:HZ3 | 2.32 | 0.42 |
| 1:A:249:LEU:O | 1:A:251:THR:N | 2.53 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:43:GLY:O | 1:B:44:THR:C | 2.57 | 0.42 |
| 1:B:83:PHE:HD1 | 1:B:84:LEU:HD23 | 1.85 | 0.42 |
| 1:B:311:ALA:HB1 | 1:B:336:ILE:HD13 | 2.01 | 0.42 |
| 1:B:397:LEU:C | 1:B:399:ALA:N | 2.71 | 0.42 |
| 3:D:20:THR:HG23 | 3:D:73:THR:OG1 | 2.20 | 0.42 |
| 3:D:79:ALA:CA | 3:D:105:ILE:HD11 | 2.49 | 0.42 |
| 2:E:173:THR:O | 3:F:163:THR:HG22 | 2.19 | 0.42 |
| 2:E:174:PHE:HA | 2:E:175:PRO:HD3 | 1.96 | 0.42 |
| 3:F:150:ASP:OD2 | 3:F:188:HIS:HB3 | 2.20 | 0.42 |
| 1:A:210:TYR:HE1 | 1:B:208:PHE:HA | 1.84 | 0.42 |
| 1:A:305:LEU:C | 1:A:307:PHE:H | 2.22 | 0.42 |
| 2:C:108:PHE:N | 3:D:35:TYR:OH | 2.43 | 0.42 |
| 3:F:3:VAL:HG12 | 3:F:3:VAL:O | 2.19 | 0.42 |
| 3:F:48:TYR:O | 3:F:49:ASP:C | 2.58 | 0.42 |
| 1:A:107:SER:HB2 | 1:A:348:PHE:CZ | 2.55 | 0.41 |
| 1:B:272:TRP:HB3 | 1:B:345:LEU:CD1 | 2.49 | 0.41 |
| 2:C:60:TYR:CD1 | 2:C:60:TYR:N | 2.88 | 0.41 |
| 2:C:165:GLY:C | 2:C:167:LEU:N | 2.73 | 0.41 |
| 2:E:29:TYR:O | 2:E:32:TYR:HB2 | 2.19 | 0.41 |
| 3:F:77:MET:HG3 | 3:F:78:GLU:N | 2.35 | 0.41 |
| 3:D:168:LYS:C | 3:D:170:SER:H | 2.23 | 0.41 |
| 2:E:146:LEU:N | 2:E:146:LEU:CD2 | 2.80 | 0.41 |
| 3:F:49:ASP:O | 3:F:51:SER:N | 2.51 | 0.41 |
| 1:B:182:ALA:HB3 | 1:B:200:ILE:HD11 | 2.03 | 0.41 |
| 1:B:186:LEU:HD22 | 1:B:199:PHE:CD2 | 2.55 | 0.41 |
| 1:B:435:LEU:HA | 1:B:435:LEU:HD13 | 1.87 | 0.41 |
| 3:D:205:VAL:O | 3:D:206:LYS:CG | 2.68 | 0.41 |
| 3:F:160:ASN:HB3 | 3:F:162:TRP:CZ3 | 2.55 | 0.41 |
| 3:F:192:THR:HG22 | 3:F:207:SER:HB3 | 2.00 | 0.41 |
| 1:B:169:LYS:HG2 | 1:B:170:GLY:H | 1.85 | 0.41 |
| 1:B:241:VAL:HG12 | 1:B:241:VAL:O | 2.20 | 0.41 |
| 2:C:2:VAL:HG23 | 2:C:27:PHE:CE1 | 2.53 | 0.41 |
| 2:C:4:LEU:HD12 | 2:C:4:LEU:HA | 1.82 | 0.41 |
| 2:C:13:GLN:O | 2:C:14:PRO:C | 2.58 | 0.41 |
| 2:C:91:THR:O | 2:C:91:THR:HG22 | 2.19 | 0.41 |
| 2:C:163:ASN:HD21 | 2:C:201:VAL:HA | 1.84 | 0.41 |
| 3:D:136:ASN:HD22 | 3:D:173:SER:HB3 | 1.85 | 0.41 |
| 2:E:36:TRP:HA | 2:E:96:CYS:HA | 2.03 | 0.41 |
| 2:E:99:LEU:HD21 | 2:E:108:PHE:CD2 | 2.55 | 0.41 |
| 2:E:107:TYR:C | 2:E:107:TYR:CD1 | 2.93 | 0.41 |
| 2:E:144:VAL:O | 2:E:144:VAL:CG1 | 2.68 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:74:ILE:HG21 | 3:F:77:MET:HA | 2.01 | 0.41 |
| 1:B:212:LEU:N | 1:B:212:LEU:CD1 | 2.76 | 0.41 |
| 1:B:270:ASN:O | 1:B:273:VAL:HG12 | 2.21 | 0.41 |
| 2:C:127:PRO:HB3 | 2:C:153:TYR:CB | 2.39 | 0.41 |
| 1:A:309:ALA:O | 1:A:311:ALA:N | 2.53 | 0.41 |
| 1:B:103:GLU:HB3 | 1:B:111:GLU:HG2 | 2.02 | 0.41 |
| 1:B:423:LEU:CB | 1:B:424:PRO:HD3 | 2.47 | 0.41 |
| 2:E:161:THR:HB | 2:E:165:GLY:H | 1.85 | 0.41 |
| 2:E:162:TRP:NE1 | 2:E:171:VAL:HG13 | 2.34 | 0.41 |
| 3:F:32:ILE:CG2 | 3:F:33:HIS:N | 2.83 | 0.41 |
| 3:F:51:SER:HB3 | 3:F:63:GLY:O | 2.20 | 0.41 |
| 3:F:202:SER:HA | 3:F:203:PRO:HD2 | 1.84 | 0.41 |
| 1:A:219:PHE:O | 1:A:220:ILE:C | 2.57 | 0.41 |
| 1:A:287:ASN:HD22 | 1:A:290:LYS:CB | 2.34 | 0.41 |
| 1:B:75:TYR:O | 1:B:78:LEU:HB3 | 2.19 | 0.41 |
| 1:B:250:ASN:ND2 | 2:E:105:TYR:CD1 | 2.88 | 0.41 |
| 2:C:109:ASP:C | 2:C:109:ASP:OD1 | 2.58 | 0.41 |
| 2:C:219:VAL:CB | 2:C:220:PRO:HD2 | 2.51 | 0.41 |
| 3:D:64:SER:OG | 3:D:65:GLY:N | 2.53 | 0.41 |
| 2:E:33:TRP:CZ3 | 2:E:52:ASN:HB3 | 2.55 | 0.41 |
| 2:E:43:LYS:HB3 | 2:E:43:LYS:HE3 | 1.86 | 0.41 |
| 3:F:29:VAL:O | 3:F:67:GLY:HA2 | 2.21 | 0.41 |
| 1:B:287:ASN:HD21 | 1:B:289:THR:HB | 1.84 | 0.41 |
| 1:B:377:GLU:HG3 | 1:B:378:LEU:N | 2.36 | 0.41 |
| 1:A:128:LEU:HB2 | 1:A:129:PRO:CD | 2.51 | 0.41 |
| 1:A:192:ALA:HA | 1:A:193:PRO:HD2 | 1.90 | 0.41 |
| 1:A:218:VAL:O | 1:A:221:GLY:N | 2.54 | 0.41 |
| 1:A:305:LEU:HA | 1:A:308:VAL:CG2 | 2.51 | 0.41 |
| 1:A:341:VAL:O | 1:A:345:LEU:HG | 2.21 | 0.41 |
| 2:C:165:GLY:O | 2:C:167:LEU:N | 2.53 | 0.41 |
| 3:D:168:LYS:H | 3:D:168:LYS:HG2 | 1.72 | 0.41 |
| 2:E:65:LYS:HB2 | 2:E:66:ASP:H | 1.31 | 0.41 |
| 2:E:125:THR:HA | 2:E:126:PRO:HD2 | 1.83 | 0.41 |
| 2:E:127:PRO:HB2 | 2:E:150:VAL:CG1 | 2.50 | 0.41 |
| 3:F:197:HIS:ND1 | 3:F:197:HIS:C | 2.74 | 0.41 |
| 1:A:125:TRP:CD1 | 1:A:126:ARG:HG3 | 2.55 | 0.41 |
| 1:B:109:ILE:N | 1:B:110:PRO:CD | 2.84 | 0.41 |
| 1:B:197:ILE:HD13 | 1:B:219:PHE:CE1 | 2.55 | 0.41 |
| 1:B:409:ILE:HD11 | 1:B:426:ILE:HA | 2.03 | 0.41 |
| 2:C:150:VAL:CG2 | 2:C:205:VAL:CG2 | 2.99 | 0.41 |
| 2:C:156:GLU:OE1 | 2:C:157:PRO:HA | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:D:58:PRO:HB3 | 3:D:60:ARG:NH2 | 2.36 | 0.41 |
| 2:E:18:LEU:CD1 | 2:E:117:VAL:HG13 | 2.50 | 0.41 |
| 2:E:87:ARG:CZ | 2:E:89:GLU:HB2 | 2.51 | 0.41 |
| 2:E:121:SER:O | 2:E:122:ALA:O | 2.38 | 0.41 |
| 1:B:91:MET:C | 1:B:93:GLY:N | 2.72 | 0.40 |
| 2:C:196:TRP:CD1 | 2:C:201:VAL:HG23 | 2.56 | 0.40 |
| 2:E:167:LEU:HD13 | 2:E:167:LEU:HA | 1.79 | 0.40 |
| 3:F:138:PHE:HD1 | 3:F:140:PRO:O | 2.05 | 0.40 |
| 3:F:187:ARG:O | 3:F:188:HIS:CD2 | 2.74 | 0.40 |
| 1:A:243:LYS:O | 1:A:243:LYS:HG3 | 2.19 | 0.40 |
| 1:B:65:MET:C | 1:B:67:ALA:N | 2.75 | 0.40 |
| 1:B:101:ALA:HB3 | 1:B:130:VAL:HG11 | 2.02 | 0.40 |
| 2:C:27:PHE:CD2 | 2:C:27:PHE:C | 2.95 | 0.40 |
| 3:D:32:ILE:HD12 | 3:D:32:ILE:HA | 1.81 | 0.40 |
| 3:D:168:LYS:HB2 | 3:D:169:ASP:H | 1.67 | 0.40 |
| 2:E:154:PHE:HA | 2:E:155:PRO:HA | 1.79 | 0.40 |
| 3:F:117:PHE:HA | 3:F:118:PRO:HD3 | 1.74 | 0.40 |
| 1:A:163:LEU:HD21 | 1:A:174:ARG:HG3 | 2.02 | 0.40 |
| 1:B:122:VAL:O | 1:B:124:TRP:N | 2.52 | 0.40 |
| 1:B:274:LEU:O | 1:B:277:GLN:N | 2.50 | 0.40 |
| 2:C:76:LYS:O | 2:C:77:ASP:C | 2.60 | 0.40 |
| 3:D:201:THR:CG2 | 3:D:202:SER:H | 2.30 | 0.40 |
| 2:E:99:LEU:HD23 | 2:E:107:TYR:O | 2.21 | 0.40 |
| 1:A:64:ARG:O | 1:A:68:LEU:HG | 2.20 | 0.40 |
| 1:A:74:ASN:HB3 | 1:A:77:LEU:HB3 | 2.04 | 0.40 |
| 1:A:120:ARG:NH1 | 1:A:452:THR:HG22 | 2.37 | 0.40 |
| 1:A:284:HIS:C | 1:A:286:GLY:H | 2.25 | 0.40 |
| 1:A:348:PHE:CG | 1:A:356:ILE:HB | 2.56 | 0.40 |
| 1:B:176:THR:HG22 | 1:B:177:LEU:N | 2.36 | 0.40 |
| 2:C:6:GLU:HA | 2:C:22:CYS:HA | 2.03 | 0.40 |
| 2:E:135:GLY:HA2 | 3:F:118:PRO:CG | 2.51 | 0.40 |
| 1:A:42:VAL:CG2 | 1:A:159:GLY:HA2 | 2.52 | 0.40 |
| 1:A:114:GLY:HA2 | 1:A:449:LEU:HD21 | 2.02 | 0.40 |
| 1:A:270:ASN:CA | 1:A:273:VAL:HG12 | 2.52 | 0.40 |
| 1:A:356:ILE:O | 1:A:360:MET:HE3 | 2.21 | 0.40 |
| 1:A:358:ALA:N | 1:A:359:PRO:CD | 2.84 | 0.40 |
| 1:B:135:GLY:HA2 | 1:B:138:THR:OG1 | 2.22 | 0.40 |
| 2:C:105:TYR:CD2 | 3:D:30:SER:O | 2.73 | 0.40 |
| 2:C:162:TRP:O | 2:C:164:SER:N | 2.55 | 0.40 |
| 2:C:217:LYS:O | 2:C:219:VAL:HG13 | 2.22 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 1 | A | 442/473 (93%) | 361 (82%) | 62 (14%) | 19 (4%) | 2 20 |
| 1 | B | 439/473 (93%) | 342 (78%) | 81 (18%) | 16 (4%) | 3 23 |
| 2 | C | 219/222 (99%) | 166 (76%) | 39 (18%) | 14 (6%) | 1 10 |
| 2 | E | 219/222 (99%) | 173 (79%) | 30 (14%) | 16 (7%) | 1 7 |
| 3 | D | 209/211 (99%) | 159 (76%) | 28 (13%) | 22 (10%) | 0 3 |
| 3 | F | 209/211 (99%) | 158 (76%) | 33 (16%) | 18 (9%) | 1 4 |
| All | All | 1737/1812 (96%) | 1359 (78%) | 273 (16%) | 105 (6%) | 1 12 |

All (105) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 73 | ASP |
| 1 | A | 209 | ARG |
| 1 | A | 236 | VAL |
| 1 | A | 309 | ALA |
| 1 | B | 73 | ASP |
| 1 | B | 132 | PHE |
| 2 | C | 27 | PHE |
| 2 | C | 65 | LYS |
| 2 | C | 140 | ALA |
| 3 | D | 7 | SER |
| 3 | D | 67 | GLY |
| 3 | D | 126 | SER |
| 3 | D | 137 | ASN |
| 3 | D | 168 | LYS |
| 3 | D | 169 | ASP |
| 2 | E | 51 | ILE |
| 2 | E | 65 | LYS |
| 2 | E | 113 | ALA |
| 2 | E | 122 | ALA |
| 2 | E | 140 | ALA |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | F | 2 | ILE |
| 3 | F | 7 | SER |
| 3 | F | 109 | ASP |
| 3 | F | 111 | ALA |
| 3 | F | 139 | TYR |
| 3 | F | 140 | PRO |
| 3 | F | 153 | GLU |
| 1 | A | 283 | VAL |
| 1 | A | 419 | TYR |
| 1 | B | 209 | ARG |
| 1 | B | 283 | VAL |
| 1 | B | 309 | ALA |
| 1 | B | 441 | GLY |
| 1 | B | 444 | LEU |
| 2 | C | 164 | SER |
| 2 | C | 166 | SER |
| 2 | C | 196 | TRP |
| 3 | D | 31 | TYR |
| 3 | D | 55 | SER |
| 3 | D | 109 | ASP |
| 3 | D | 127 | GLY |
| 3 | D | 139 | TYR |
| 3 | D | 153 | GLU |
| 3 | D | 198 | LYS |
| 2 | E | 138 | ALA |
| 2 | E | 180 | ALA |
| 3 | F | 66 | SER |
| 3 | F | 67 | GLY |
| 3 | F | 119 | PRO |
| 3 | F | 125 | THR |
| 3 | F | 184 | GLU |
| 1 | A | 102 | PRO |
| 1 | A | 132 | PHE |
| 1 | A | 149 | GLY |
| 1 | A | 413 | LEU |
| 1 | A | 444 | LEU |
| 1 | B | 102 | PRO |
| 1 | B | 310 | PRO |
| 2 | C | 18 | LEU |
| 2 | C | 138 | ALA |
| 2 | C | 220 | PRO |
| 3 | D | 46 | TRP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | D | 50 | THR |
| 3 | D | 90 | TRP |
| 2 | E | 62 | PRO |
| 3 | F | 137 | ASN |
| 3 | F | 203 | PRO |
| 1 | A | 250 | ASN |
| 1 | A | 310 | PRO |
| 1 | B | 95 | PHE |
| 1 | B | 188 | ALA |
| 2 | C | 31 | ARG |
| 2 | C | 163 | ASN |
| 3 | D | 23 | CYS |
| 3 | D | 59 | VAL |
| 3 | D | 141 | LYS |
| 3 | D | 152 | SER |
| 3 | F | 50 | THR |
| 3 | F | 79 | ALA |
| 3 | F | 112 | PRO |
| 1 | A | 206 | PRO |
| 1 | B | 206 | PRO |
| 1 | B | 443 | PRO |
| 3 | D | 187 | ARG |
| 2 | E | 52 | ASN |
| 2 | E | 157 | PRO |
| 2 | E | 165 | GLY |
| 2 | E | 211 | SER |
| 3 | F | 165 | GLN |
| 1 | B | 123 | ARG |
| 1 | B | 235 | GLU |
| 2 | C | 53 | PRO |
| 2 | C | 197 | PRO |
| 3 | D | 80 | GLU |
| 2 | E | 196 | TRP |
| 1 | A | 201 | ILE |
| 2 | E | 37 | VAL |
| 2 | E | 53 | PRO |
| 2 | C | 174 | PHE |
| 2 | E | 69 | ILE |
| 1 | A | 261 | ILE |
| 1 | B | 149 | GLY |
| 1 | A | 101 | ALA |
| 1 | A | 443 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 285 | GLY |

### 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 | A | 335/358 (94%) | 312 (93%) | 23 (7%) | 15 49 |
| 1 | B | 332/358 (93%) | 310 (93%) | 22 (7%) | 16 51 |
| 2 | C | 181/182 (100%) | 149 (82%) | 32 (18%) | 2 9 |
| 2 | E | 181/182 (100%) | 141 (78%) | 40 (22%) | 1 4 |
| 3 | D | 185/185 (100%) | 153 (83%) | 32 (17%) | 2 10 |
| 3 | F | 185/185 (100%) | 156 (84%) | 29 (16%) | 2 12 |
| All | All | 1399/1450 (96%) | 1221 (87%) | 178 (13%) | 4 20 |

All (178) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 65 | MET |
| 1 | A | 69 | VAL |
| 1 | A | 70 | HIS |
| 1 | A | 73 | ASP |
| 1 | A | 74 | ASN |
| 1 | A | 103 | GLU |
| 1 | A | 111 | GLU |
| 1 | A | 148 | GLU |
| 1 | A | 176 | THR |
| 1 | A | 200 | ILE |
| 1 | A | 205 | ARG |
| 1 | A | 208 | PHE |
| 1 | A | 209 | ARG |
| 1 | A | 211 | THR |
| 1 | A | 212 | LEU |
| 1 | A | 277 | GLN |
| 1 | A | 324 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 381 | GLN |
| 1 | A | 397 | LEU |
| 1 | A | 402 | ILE |
| 1 | A | 420 | GLN |
| 1 | A | 445 | TYR |
| 1 | A | 451 | ARG |
| 1 | B | 65 | MET |
| 1 | B | 70 | HIS |
| 1 | B | 73 | ASP |
| 1 | B | 74 | ASN |
| 1 | B | 103 | GLU |
| 1 | B | 111 | GLU |
| 1 | B | 148 | GLU |
| 1 | B | 150 | PRO |
| 1 | B | 176 | THR |
| 1 | B | 177 | LEU |
| 1 | B | 180 | THR |
| 1 | B | 205 | ARG |
| 1 | B | 208 | PHE |
| 1 | B | 212 | LEU |
| 1 | B | 277 | GLN |
| 1 | B | 324 | THR |
| 1 | B | 381 | GLN |
| 1 | B | 397 | LEU |
| 1 | B | 402 | ILE |
| 1 | B | 420 | GLN |
| 1 | B | 445 | TYR |
| 1 | B | 451 | ARG |
| 2 | C | 3 | ARG |
| 2 | C | 4 | LEU |
| 2 | C | 5 | LEU |
| 2 | C | 6 | GLU |
| 2 | C | 13 | GLN |
| 2 | C | 41 | PRO |
| 2 | C | 45 | LEU |
| 2 | C | 51 | ILE |
| 2 | C | 53 | PRO |
| 2 | C | 55 | SER |
| 2 | C | 67 | LYS |
| 2 | C | 72 | ARG |
| 2 | C | 87 | ARG |
| 2 | C | 98 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | C | 110 | VAL |
| 2 | C | 128 | SER |
| 2 | C | 136 | SER |
| 2 | C | 151 | LYS |
| 2 | C | 155 | PRO |
| 2 | C | 157 | PRO |
| 2 | C | 158 | VAL |
| 2 | C | 167 | LEU |
| 2 | C | 174 | PHE |
| 2 | C | 185 | LEU |
| 2 | C | 200 | THR |
| 2 | C | 202 | THR |
| 2 | C | 203 | CYS |
| 2 | C | 204 | ASN |
| 2 | C | 211 | SER |
| 2 | C | 212 | THR |
| 2 | C | 219 | VAL |
| 2 | C | 221 | ARG |
| 3 | D | 1 | ASP |
| 3 | D | 6 | GLN |
| 3 | D | 20 | THR |
| 3 | D | 24 | SER |
| 3 | D | 32 | ILE |
| 3 | D | 41 | THR |
| 3 | D | 44 | LYS |
| 3 | D | 46 | TRP |
| 3 | D | 50 | THR |
| 3 | D | 59 | VAL |
| 3 | D | 64 | SER |
| 3 | D | 68 | THR |
| 3 | D | 72 | LEU |
| 3 | D | 77 | MET |
| 3 | D | 94 | PRO |
| 3 | D | 95 | GLN |
| 3 | D | 115 | SER |
| 3 | D | 117 | PHE |
| 3 | D | 120 | SER |
| 3 | D | 122 | GLU |
| 3 | D | 125 | THR |
| 3 | D | 137 | ASN |
| 3 | D | 156 | ASN |
| 3 | D | 159 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | D | 163 | THR |
| 3 | D | 175 | SER |
| 3 | D | 181 | THR |
| 3 | D | 183 | ASP |
| 3 | D | 192 | THR |
| 3 | D | 202 | SER |
| 3 | D | 205 | VAL |
| 3 | D | 206 | LYS |
| 2 | E | 2 | VAL |
| 2 | E | 4 | LEU |
| 2 | E | 5 | LEU |
| 2 | E | 6 | GLU |
| 2 | E | 12 | VAL |
| 2 | E | 18 | LEU |
| 2 | E | 22 | CYS |
| 2 | E | 27 | PHE |
| 2 | E | 30 | SER |
| 2 | E | 45 | LEU |
| 2 | E | 48 | ILE |
| 2 | E | 51 | ILE |
| 2 | E | 53 | PRO |
| 2 | E | 54 | VAL |
| 2 | E | 55 | SER |
| 2 | E | 58 | ILE |
| 2 | E | 59 | ASN |
| 2 | E | 61 | THR |
| 2 | E | 62 | PRO |
| 2 | E | 67 | LYS |
| 2 | E | 72 | ARG |
| 2 | E | 77 | ASP |
| 2 | E | 83 | ILE |
| 2 | E | 107 | TYR |
| 2 | E | 118 | THR |
| 2 | E | 121 | SER |
| 2 | E | 125 | THR |
| 2 | E | 146 | LEU |
| 2 | E | 151 | LYS |
| 2 | E | 167 | LEU |
| 2 | E | 172 | HIS |
| 2 | E | 177 | VAL |
| 2 | E | 179 | GLN |
| 2 | E | 185 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | E | 187 | SER |
| 2 | E | 188 | SER |
| 2 | E | 193 | SER |
| 2 | E | 200 | THR |
| 2 | E | 203 | CYS |
| 2 | E | 204 | ASN |
| 3 | F | 1 | ASP |
| 3 | F | 5 | THR |
| 3 | F | 6 | GLN |
| 3 | F | 17 | ASP |
| 3 | F | 28 | SER |
| 3 | F | 30 | SER |
| 3 | F | 42 | SER |
| 3 | F | 44 | LYS |
| 3 | F | 48 | TYR |
| 3 | F | 54 | THR |
| 3 | F | 88 | GLN |
| 3 | F | 91 | SER |
| 3 | F | 116 | ILE |
| 3 | F | 119 | PRO |
| 3 | F | 121 | SER |
| 3 | F | 143 | ILE |
| 3 | F | 153 | GLU |
| 3 | F | 158 | VAL |
| 3 | F | 162 | TRP |
| 3 | F | 166 | ASP |
| 3 | F | 175 | SER |
| 3 | F | 179 | THR |
| 3 | F | 181 | THR |
| 3 | F | 187 | ARG |
| 3 | F | 189 | ASN |
| 3 | F | 194 | GLU |
| 3 | F | 201 | THR |
| 3 | F | 208 | PHE |
| 3 | F | 210 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 74 | ASN |
| 1 | A | 153 | GLN |
| 1 | A | 157 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 207 | GLN |
| 1 | A | 270 | ASN |
| 1 | A | 277 | GLN |
| 1 | A | 284 | HIS |
| 1 | A | 287 | ASN |
| 1 | A | 327 | ASN |
| 1 | A | 381 | GLN |
| 1 | A | 420 | GLN |
| 1 | A | 437 | GLN |
| 1 | B | 74 | ASN |
| 1 | B | 153 | GLN |
| 1 | B | 157 | ASN |
| 1 | B | 207 | GLN |
| 1 | B | 270 | ASN |
| 1 | B | 277 | GLN |
| 1 | B | 284 | HIS |
| 1 | B | 287 | ASN |
| 1 | B | 327 | ASN |
| 1 | B | 381 | GLN |
| 1 | B | 437 | GLN |
| 2 | C | 39 | GLN |
| 2 | C | 172 | HIS |
| 3 | D | 37 | GLN |
| 3 | D | 93 | HIS |
| 3 | D | 136 | ASN |
| 3 | D | 137 | ASN |
| 3 | D | 155 | GLN |
| 3 | D | 189 | ASN |
| 2 | E | 39 | GLN |
| 3 | F | 37 | GLN |
| 3 | F | 89 | GLN |
| 3 | F | 137 | ASN |
| 3 | F | 189 | ASN |

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

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

## 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 1 | A | 444/473 (93%) | -0.37 | 2 (0%) 91 86 | 48, 77, 111, 138 | 0 |
| 1 | B | 441/473 (93%) | -0.44 | 1 (0%) 95 94 | 41, 71, 115, 151 | 0 |
| 2 | C | 221/222 (99%) | -0.25 | 2 (0%) 84 75 | 43, 71, 106, 160 | 0 |
| 2 | E | 221/222 (99%) | -0.07 | 3 (1%) 75 63 | 37, 78, 121, 145 | 0 |
| 3 | D | 211/211 (100%) | -0.03 | 0 100 100 | 52, 91, 118, 128 | 0 |
| 3 | F | 211/211 (100%) | -0.12 | 3 (1%) 75 63 | 26, 70, 123, 140 | 0 |
| All | All | 1749/1812 (96%) | -0.26 | 11 (0%) 89 83 | 26, 76, 117, 160 | 0 |

All (11) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 2 | E | 222 | ALA | 3.6 |
| 1 | B | 235 | GLU | 3.4 |
| 1 | A | 235 | GLU | 2.8 |
| 1 | A | 72 | ALA | 2.7 |
| 2 | C | 136 | SER | 2.3 |
| 3 | F | 156 | ASN | 2.2 |
| 2 | C | 139 | ALA | 2.1 |
| 2 | E | 35 | SER | 2.1 |
| 2 | E | 42 | GLY | 2.1 |
| 3 | F | 153 | GLU | 2.1 |
| 3 | F | 155 | GLN | 2.0 |

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

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

## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.4 Ligands (i)

There are no ligands in this entry.

## 6.5 Other polymers (i)

There are no such residues in this entry.