# Full wwPDB X-ray Structure Validation Report (i)

Nov 20, 2023 – 01:09 PM EST

| | | |
|---|---|---|
| PDB ID | : | 3VD2 |
| Title | : | structure of p73 DNA binding domain tetramer modulates p73 transactivation |
| Authors | : | Ethayathulla, A.S.; Tse, P.W.; Nguyen, S.; Viadiu, H. |
| Deposited on | : | 2012-01-04 |
| Resolution | : | 4.00 Å(reported) |

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

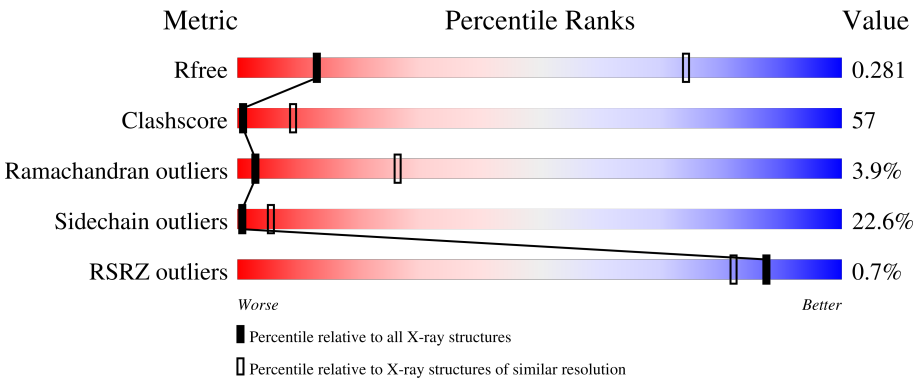
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.36 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36 |

# 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 4.00 Å.

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




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 130704 | 1087 (4.30-3.70) |
| Clashscore | 141614 | 1148 (4.30-3.70) |
| Ramachandran outliers | 138981 | 1108 (4.30-3.70) |
| Sidechain outliers | 138945 | 1099 (4.30-3.70) |
| RSRZ outliers | 127900 | 1028 (4.34-3.66) |

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 | 210 | 29% 51% 15% • • |
| 1 | B | 210 | 21% 56% 18% • 5% |
| 1 | C | 210 | 32% 50% 13% • |
| 1 | D | 210 | % 31% 50% 14% 5% |
| 1 | I | 210 | % 20% 56% 19% • • |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | J | 210 | 29% 47% 20% |
| 2 | E | 14 | 14% 29% 71% |
| 2 | F | 14 | 14% 79% 7% |
| 2 | G | 14 | 7% 86% 7% |
| 2 | H | 14 | 21% 79% |
| 2 | K | 14 | 7% 64% 21% 7% |
| 2 | L | 14 | 7% 21% 50% 21% 7% |

# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11152 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 Tumor protein p73.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 1 | A | 203 | 1590 | 994 | 289 | 296 | 11 | 0 | 0 | 0 |
| 1 | B | 200 | 1569 | 981 | 283 | 294 | 11 | 0 | 0 | 0 |
| 1 | C | 203 | 1596 | 997 | 291 | 297 | 11 | 0 | 0 | 0 |
| 1 | D | 199 | 1563 | 981 | 282 | 289 | 11 | 0 | 0 | 0 |
| 1 | I | 202 | 1576 | 985 | 284 | 296 | 11 | 0 | 0 | 0 |
| 1 | J | 202 | 1586 | 993 | 284 | 298 | 11 | 0 | 0 | 0 |

There are 72 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 103 | MET | - | initiating methionine | UNP O15350 |
| A | 104 | GLY | - | expression tag | UNP O15350 |
| A | 105 | HIS | - | expression tag | UNP O15350 |
| A | 106 | HIS | - | expression tag | UNP O15350 |
| A | 107 | HIS | - | expression tag | UNP O15350 |
| A | 108 | HIS | - | expression tag | UNP O15350 |
| A | 109 | HIS | - | expression tag | UNP O15350 |
| A | 110 | HIS | - | expression tag | UNP O15350 |
| A | 111 | HIS | - | expression tag | UNP O15350 |
| A | 112 | HIS | - | expression tag | UNP O15350 |
| A | 113 | GLU | - | expression tag | UNP O15350 |
| A | 114 | PHE | - | expression tag | UNP O15350 |
| B | 103 | MET | - | initiating methionine | UNP O15350 |
| B | 104 | GLY | - | expression tag | UNP O15350 |
| B | 105 | HIS | - | expression tag | UNP O15350 |
| B | 106 | HIS | - | expression tag | UNP O15350 |
| B | 107 | HIS | - | expression tag | UNP O15350 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | 108 | HIS | - | expression tag | UNP O15350 |
| B | 109 | HIS | - | expression tag | UNP O15350 |
| B | 110 | HIS | - | expression tag | UNP O15350 |
| B | 111 | HIS | - | expression tag | UNP O15350 |
| B | 112 | HIS | - | expression tag | UNP O15350 |
| B | 113 | GLU | - | expression tag | UNP O15350 |
| B | 114 | PHE | - | expression tag | UNP O15350 |
| C | 103 | MET | - | initiating methionine | UNP O15350 |
| C | 104 | GLY | - | expression tag | UNP O15350 |
| C | 105 | HIS | - | expression tag | UNP O15350 |
| C | 106 | HIS | - | expression tag | UNP O15350 |
| C | 107 | HIS | - | expression tag | UNP O15350 |
| C | 108 | HIS | - | expression tag | UNP O15350 |
| C | 109 | HIS | - | expression tag | UNP O15350 |
| C | 110 | HIS | - | expression tag | UNP O15350 |
| C | 111 | HIS | - | expression tag | UNP O15350 |
| C | 112 | HIS | - | expression tag | UNP O15350 |
| C | 113 | GLU | - | expression tag | UNP O15350 |
| C | 114 | PHE | - | expression tag | UNP O15350 |
| D | 103 | MET | - | initiating methionine | UNP O15350 |
| D | 104 | GLY | - | expression tag | UNP O15350 |
| D | 105 | HIS | - | expression tag | UNP O15350 |
| D | 106 | HIS | - | expression tag | UNP O15350 |
| D | 107 | HIS | - | expression tag | UNP O15350 |
| D | 108 | HIS | - | expression tag | UNP O15350 |
| D | 109 | HIS | - | expression tag | UNP O15350 |
| D | 110 | HIS | - | expression tag | UNP O15350 |
| D | 111 | HIS | - | expression tag | UNP O15350 |
| D | 112 | HIS | - | expression tag | UNP O15350 |
| D | 113 | GLU | - | expression tag | UNP O15350 |
| D | 114 | PHE | - | expression tag | UNP O15350 |
| I | 103 | MET | - | initiating methionine | UNP O15350 |
| I | 104 | GLY | - | expression tag | UNP O15350 |
| I | 105 | HIS | - | expression tag | UNP O15350 |
| I | 106 | HIS | - | expression tag | UNP O15350 |
| I | 107 | HIS | - | expression tag | UNP O15350 |
| I | 108 | HIS | - | expression tag | UNP O15350 |
| I | 109 | HIS | - | expression tag | UNP O15350 |
| I | 110 | HIS | - | expression tag | UNP O15350 |
| I | 111 | HIS | - | expression tag | UNP O15350 |
| I | 112 | HIS | - | expression tag | UNP O15350 |
| I | 113 | GLU | - | expression tag | UNP O15350 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| I | 114 | PHE | - | expression tag | UNP O15350 |
| J | 103 | MET | - | initiating methionine | UNP O15350 |
| J | 104 | GLY | - | expression tag | UNP O15350 |
| J | 105 | HIS | - | expression tag | UNP O15350 |
| J | 106 | HIS | - | expression tag | UNP O15350 |
| J | 107 | HIS | - | expression tag | UNP O15350 |
| J | 108 | HIS | - | expression tag | UNP O15350 |
| J | 109 | HIS | - | expression tag | UNP O15350 |
| J | 110 | HIS | - | expression tag | UNP O15350 |
| J | 111 | HIS | - | expression tag | UNP O15350 |
| J | 112 | HIS | - | expression tag | UNP O15350 |
| J | 113 | GLU | - | expression tag | UNP O15350 |
| J | 114 | PHE | - | expression tag | UNP O15350 |

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*TP*GP*GP*AP*CP*AP*TP*GP*TP*CP*CP*AP*T)-3').

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | | |
| 2 | E | 14 | 284 | 137 | 52 | 82 | 13 | 0 | 0 | 0 |
| 2 | F | 14 | 284 | 137 | 52 | 82 | 13 | 0 | 0 | 0 |
| 2 | G | 14 | 284 | 137 | 52 | 82 | 13 | 0 | 0 | 0 |
| 2 | H | 14 | 284 | 137 | 52 | 82 | 13 | 0 | 0 | 0 |
| 2 | L | 13 | 266 | 127 | 47 | 79 | 13 | 0 | 0 | 0 |
| 2 | K | 13 | 264 | 127 | 50 | 75 | 12 | 0 | 0 | 0 |

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Zn | | |
| 3 | A | 1 | 1 | 1 | 0 | 0 |
| 3 | B | 1 | 1 | 1 | 0 | 0 |
| 3 | C | 1 | 1 | 1 | 0 | 0 |
| 3 | D | 1 | 1 | 1 | 0 | 0 |

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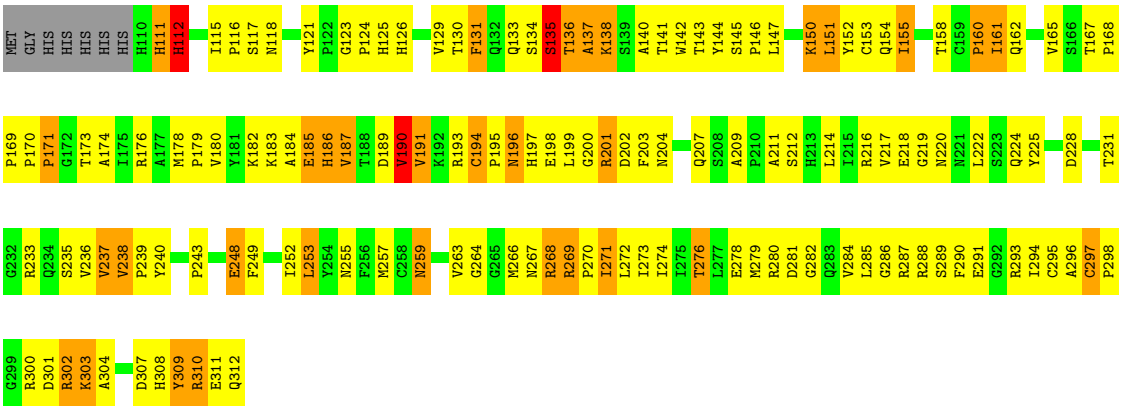
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Zn | | |
| 3 | I | 1 | 1 | 1 | 0 | 0 |
| | | | Total | Zn | | |
| 3 | J | 1 | 1 | 1 | 0 | 0 |

# 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.

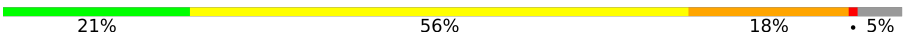
- Molecule 1: Tumor protein p73

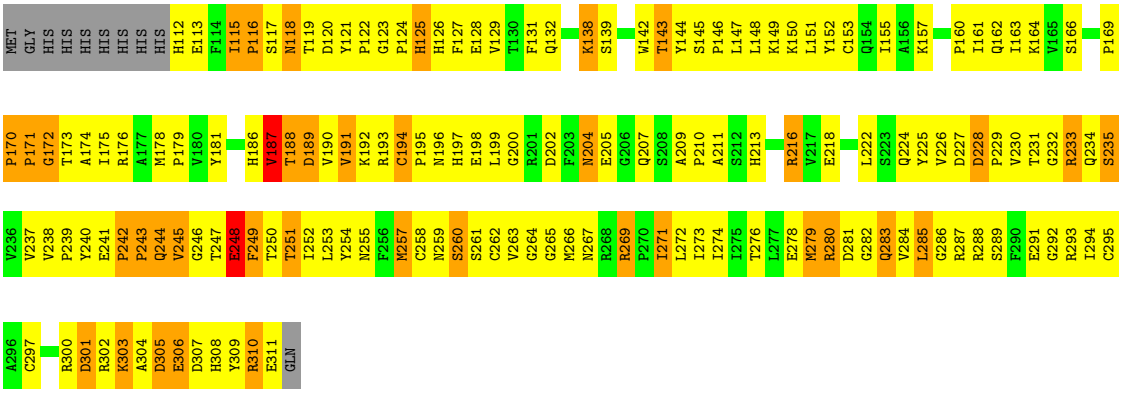
Chain A:




- Molecule 1: Tumor protein p73

Chain B:




- Molecule 1: Tumor protein p73

Chain C:

P168 P169 P170 P171 G172 T173 R176 A177 M178 P179 A184 V187 T188 D189 V190 V191 K192 R193 N196 H197 E198 L199 G200 R201 D202 F203 N204 Q207 P210 A211 S212 H213 L214 I215 R216 V217 E218 Y225 V226 D227 D228 P229 V230 R233 Q234 V237 V238 P239 Y240 E241 P242

P243 Q244 V245 G246 T247 E248 F249 T250 L253 Y254 N255 F256 M257 C258 N259 S260 S261 C262 V263 M266 N267 R268 R269 P270 I271 L272 I275 T276 L277 E278 M279 R280 D281 G282 Q283 V284 L285 G286 R287 R288 S289 F290 E291 I294 C295 A296 C297 P298 G299 R300 D301 R302 K303 A304 D305 E306

D307 R310 E311 Q312

- Molecule 1: Tumor protein p73

Chain D:

MET GLY HIS HIS HIS HIS HIS HIS H112 E113 F114 S117 N118 T119 D120 Y121 P122 G123 P124 H125 H126 F127 F131 A137 K138 S139 A140 T141 W142 T143 Y144 S145 P146 L147 L148 K149 K150 L151 Y152 C153 Q154 I155 A156 K157 T158 C159 P160 I161 Q162 I163 K164 V165 S166 G172 T173

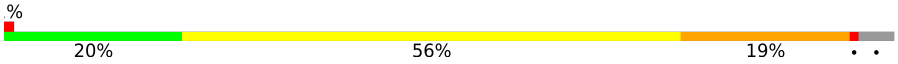
A174 I175 R176 P179 V180 Y181 K182 K183 A184 E185 H186 V187 T188 D189 V190 V191 K192 R193 C194 P195 N196 H197 E198 L199 G200 R201 D202 F203 N204 Q207 S208 A209 S212 H213 L214 I215 R216 V217 E218 G219 N220 N221 L222 S223 Q224 Y225 V226 D227 D228 P229 V230 T231 G232 R233 Q234 S235 V236

V237 V238 P239 Y240 E241 P242 P243 Q244 V245 E248 F249 T250 T251 I252 L253 Y254 N255 F256 M257 C258 N259 S260 S261 C262 V263 G264 G265 M266 N267 R268 R269 P270 I271 L272 T276 L277 E278 M279 R280 D281 G282 Q283 V284 L285 G286 R287 R288 S289 F290 E291 G292 R293 I294 C295 P298 G299 R300

D301 R302 K303 A304 D305 H308 Y309 R310 GLU GLN

- Molecule 1: Tumor protein p73

Chain I:




MET GLY HIS HIS HIS HIS HIS HIS H111 I115 P116 S117 N118 T119 D120 Y121 P122 G123 P124 H125 E128 V129 T130 F131 S134 S135 T136 A137 K138 S139 A140 T141 W142 T143 Y144 S145 P146 L147 L148 K149 K150 L151 Y152 C153 Q154 I155 A156 K157 T158 C159 P160 I161 Q162 I163 K164 V165 S166

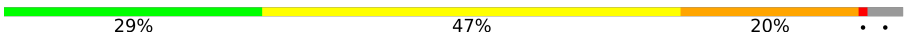
T167 P168 P169 G172 T173 A174 I175 R176 A177 M178 P179 V180 Y181 K182 K183 A184 E185 H186 V187 T188 D189 V190 V191 K192 R193 C194 P195 N196 H197 E198 L199 G200 R201 D202 F203 N204 E205 G206 Q207 S208 A209 P210 A211 S212 H213 L214 I215 R216 V217 E218 G219 N220 N221 L222 S223 Q224 Y225 V226 D227

D228 P229 V230 T231 Q234 S235 V236 P239 Y240 E241 P242 P243 Q244 V245 G246 T247 E248 F249 T250 T251 I252 L253 Y254 N255 F256 M257 C258 N259 S260 S261 C262 V263 G264 G265 M266 N267 R268 R269 P270 I271 I274 I275 T276 L277 E278 M279 R280 D281 G282 Q283 V284 L285 G286 R287 R288 S289 F290

E291 G292 R293 I294 C295 A296 C297 P298 G299 R300 A304 D305 E306 D307 H308 Y309 R310 E311 Q312

- Molecule 1: Tumor protein p73

Chain J:




MET GLY HIS HIS HIS HIS HIS HIS H111 H112 E113 F114 I115 P116 S117 Y121 P122 G123 P124 H125 H126 F127 E128 V129 T130 F131 Q132 Q133 S134 S135 T136 A137 K138 S139 A140 T141 W142 T143 Y144 S145 P146 L147 L148 K149 K150 L151 Y152 C153 Q154 I155 A156 K157 T158 C159 P160 I161 Q162 I163 K164

V165 S166 T167 P168 P169 P170 T173 A174 I175 M178 P179 V180 Y181 K182 K183 A184 E185 H186 V187 T188 D189 V190 V191 K192 R193 C194 P195 N196 H197 E198 L199 G200 R201 D202 F203 N204 E205 G206 P210 A211 S212 H213 L214 I215 R216 V217 N220 N221 L222 Y225 V226 D227 T231 G232

R233 Q234 S235 V236 V237 V238 P239 Y240 E241 P242 P243 Q244 V245 T250 L253 Y254 N255 F256 M257 C258 N259 S260 S261 C262 V263 G264 G265 M266 N267 R268 R269 P270 I271 L272 I273 I274 I275 T276 L277 E278 M279 R280 D281 G282 L285 G286 R287 R288 E291 G292 R293 I294 C295 A296 C297 P298

G299 R300 D301 R302 K303 E311 Q312

• Molecule 2: DNA (5'-D(*AP*TP*GP*GP*AP*CP*AP*TP*GP*TP*CP*CP*AP*T)-3')

Chain E: 14% 29% 71%

A402 T403 G404 G405 A406 C407 A408 T409 G410 T411 T415

• Molecule 2: DNA (5'-D(*AP*TP*GP*GP*AP*CP*AP*TP*GP*TP*CP*CP*AP*T)-3')

Chain F: 14% 79% 7%

A500 T501 G502 G503 A504 C505 A506 T507 G508 C511 A512 T513

• Molecule 2: DNA (5'-D(*AP*TP*GP*GP*AP*CP*AP*TP*GP*TP*CP*CP*AP*T)-3')

Chain G: 7% 86% 7%

A602 T603 G604 G605 A606 C607 A608 T609 G610 T611 C612 C613 A614 T615

• Molecule 2: DNA (5'-D(*AP*TP*GP*GP*AP*CP*AP*TP*GP*TP*CP*CP*AP*T)-3')

Chain H: 21% 79%

A700 T701 G702 G703 A704 C705 A706 T707 G708 C711 A712 T713

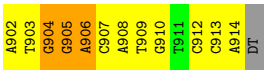
• Molecule 2: DNA (5'-D(*AP*TP*GP*GP*AP*CP*AP*TP*GP*TP*CP*CP*AP*T)-3')

Chain L: 7% 21% 50% 21% 7%

DA T801 G802 G803 A806 T807 G808 T809 C810 C811 A812 T813

• Molecule 2: DNA (5'-D(*AP*TP*GP*GP*AP*CP*AP*TP*GP*TP*CP*CP*AP*T)-3')

Chain K: 7% 64% 21% 7%


A902
T903
G904
G905
A906
C907
A908
T909
G910
T911
C912
C913
A914
DT

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | C 1 2 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 158.40Å 91.13Å 137.47Å<br>90.00° 90.20° 90.00° | Depositor |
| Resolution (Å) | 45.69 – 4.00<br>45.69 – 4.00 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 99.1 (45.69-4.00)<br>98.1 (45.69-4.00) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | 0.12 | Depositor |
| $< I/\sigma(I) >$ [1] | 3.59 (at 4.00Å) | Xtriage |
| Refinement program | CNS 1.3 | Depositor |
| R, $R_{free}$ | 0.248 , 0.284<br>0.246 , 0.281 | Depositor<br>DCC |
| $R_{free}$ test set | 350 reflections (2.10%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 91.2 | Xtriage |
| Anisotropy | 0.255 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.21 , -0.1 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.50$, $< L^2 > = 0.33$ | Xtriage |
| Estimated twinning fraction | 0.019 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l<br>0.018 for -1/2*h+3/2*k,1/2*h+1/2*k,-l<br>0.429 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l<br>0.429 for 1/2*h+3/2*k,1/2*h-1/2*k,-l<br>0.020 for -h,-k,l | Xtriage |
| $F_o$,$F_c$ correlation | 0.88 | EDS |
| Total number of atoms | 11152 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 86.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% 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 (i)

## 5.1 Standard geometry (i)

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|$ >5 | RMSZ | #$\|Z\|$ >5 |
| 1 | A | 0.53 | 0/1631 | 0.87 | 3/2218 (0.1%) |
| 1 | B | 0.46 | 0/1609 | 0.93 | 2/2187 (0.1%) |
| 1 | C | 0.49 | 0/1638 | 0.83 | 2/2226 (0.1%) |
| 1 | D | 0.49 | 0/1604 | 0.81 | 0/2181 |
| 1 | I | 0.51 | 0/1615 | 0.86 | 5/2195 (0.2%) |
| 1 | J | 0.49 | 0/1626 | 0.83 | 2/2209 (0.1%) |
| 2 | E | 0.59 | 0/318 | 0.92 | 0/489 |
| 2 | F | 0.71 | 0/318 | 0.98 | 1/489 (0.2%) |
| 2 | G | 0.71 | 0/318 | 1.01 | 2/489 (0.4%) |
| 2 | H | 0.63 | 0/318 | 0.96 | 0/489 |
| 2 | K | 1.03 | 1/296 (0.3%) | 1.29 | 2/455 (0.4%) |
| 2 | L | 1.10 | 0/297 | 1.40 | 7/456 (1.5%) |
| All | All | 0.56 | 1/11588 (0.0%) | 0.91 | 26/16083 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 2 | F | 0 | 1 |
| 2 | K | 0 | 1 |
| 2 | L | 0 | 1 |
| All | All | 0 | 3 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | K | 905 | DG | C2'-C1' | -5.78 | 1.46 | 1.52 |

All (26) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 242 | PRO | C-N-CD | -12.21 | 93.73 | 120.60 |
| 1 | J | 115 | ILE | C-N-CD | -10.49 | 97.52 | 120.60 |
| 2 | L | 810 | DC | O5'-P-OP2 | 8.05 | 120.36 | 110.70 |
| 2 | L | 810 | DC | OP2-P-O3' | 7.14 | 120.90 | 105.20 |
| 2 | G | 602 | DA | O3'-P-O5' | -6.97 | 90.77 | 104.00 |
| 2 | L | 806 | DA | O5'-P-OP1 | -6.97 | 99.43 | 105.70 |
| 2 | L | 810 | DC | OP1-P-O3' | -5.99 | 92.02 | 105.20 |
| 1 | A | 112 | HIS | N-CA-C | 5.78 | 126.60 | 111.00 |
| 2 | L | 806 | DA | C5'-C4'-O4' | 5.68 | 120.09 | 109.30 |
| 1 | I | 245 | VAL | N-CA-C | -5.62 | 95.83 | 111.00 |
| 1 | A | 219 | GLY | N-CA-C | 5.47 | 126.77 | 113.10 |
| 1 | I | 139 | SER | N-CA-C | 5.43 | 125.67 | 111.00 |
| 2 | L | 806 | DA | C3'-C2'-C1' | -5.41 | 96.01 | 102.50 |
| 1 | J | 250 | THR | N-CA-C | -5.41 | 96.41 | 111.00 |
| 2 | K | 906 | DA | C3'-C2'-C1' | -5.35 | 96.08 | 102.50 |
| 1 | I | 219 | GLY | N-CA-C | 5.32 | 126.40 | 113.10 |
| 2 | L | 801 | DT | OP1-P-OP2 | -5.30 | 111.65 | 119.60 |
| 2 | K | 905 | DG | O4'-C4'-C3' | -5.29 | 102.39 | 104.50 |
| 2 | G | 602 | DA | O4'-C1'-N9 | -5.19 | 104.37 | 108.00 |
| 1 | I | 202 | ASP | N-CA-C | 5.18 | 124.99 | 111.00 |
| 1 | A | 190 | VAL | N-CA-C | 5.17 | 124.96 | 111.00 |
| 2 | F | 503 | DG | OP1-P-O3' | 5.12 | 116.47 | 105.20 |
| 1 | B | 244 | GLN | N-CA-C | -5.09 | 97.25 | 111.00 |
| 1 | C | 115 | ILE | N-CA-C | -5.08 | 97.29 | 111.00 |
| 1 | C | 132 | GLN | N-CA-C | -5.06 | 97.33 | 111.00 |
| 1 | I | 140 | ALA | N-CA-C | -5.00 | 97.50 | 111.00 |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | F | 506 | DA | Sidechain |
| 2 | K | 904 | DG | Sidechain |
| 2 | L | 809 | DT | Sidechain |

## 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 | 1590 | 0 | 1549 | 192 | 0 |
| 1 | B | 1569 | 0 | 1535 | 233 | 0 |
| 1 | C | 1596 | 0 | 1554 | 152 | 0 |
| 1 | D | 1563 | 0 | 1533 | 194 | 0 |
| 1 | I | 1576 | 0 | 1537 | 202 | 0 |
| 1 | J | 1586 | 0 | 1548 | 175 | 0 |
| 2 | E | 284 | 0 | 160 | 12 | 0 |
| 2 | F | 284 | 0 | 160 | 18 | 0 |
| 2 | G | 284 | 0 | 160 | 19 | 0 |
| 2 | H | 284 | 0 | 160 | 16 | 0 |
| 2 | K | 264 | 0 | 148 | 14 | 0 |
| 2 | L | 266 | 0 | 148 | 16 | 0 |
| 3 | A | 1 | 0 | 0 | 0 | 0 |
| 3 | B | 1 | 0 | 0 | 0 | 0 |
| 3 | C | 1 | 0 | 0 | 0 | 0 |
| 3 | D | 1 | 0 | 0 | 0 | 0 |
| 3 | I | 1 | 0 | 0 | 0 | 0 |
| 3 | J | 1 | 0 | 0 | 0 | 0 |
| All | All | 11152 | 0 | 10192 | 1211 | 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 57.

All (1211) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:176:ARG:HG3 | 1:B:237:VAL:HG22 | 1.32 | 1.10 |
| 1:B:163:ILE:O | 1:B:249:PHE:HB2 | 1.56 | 1.06 |
| 1:I:243:PRO:HB2 | 1:I:246:GLY:HA2 | 1.36 | 1.04 |
| 1:I:215:ILE:HD13 | 1:I:215:ILE:H | 1.17 | 1.03 |
| 1:J:214:LEU:HD23 | 1:J:215:ILE:HG13 | 1.39 | 1.03 |
| 1:B:310:ARG:HD3 | 1:B:311:GLU:H | 1.21 | 1.02 |
| 1:J:145:SER:OG | 1:J:302:ARG:HD3 | 1.59 | 1.02 |
| 1:A:193:ARG:HE | 1:A:257:MET:CB | 1.74 | 1.00 |
| 1:A:193:ARG:HE | 1:A:257:MET:HB3 | 1.27 | 0.99 |
| 1:C:145:SER:HA | 1:C:302:ARG:NH1 | 1.77 | 0.98 |
| 1:A:169:PRO:HB2 | 1:A:173:THR:HG21 | 1.44 | 0.98 |
| 1:I:220:ASN:ND2 | 1:I:222:LEU:H | 1.60 | 0.98 |
| 1:J:141:THR:HA | 1:J:154:GLN:HE21 | 1.26 | 0.98 |
| 1:A:279:MET:HG2 | 1:A:285:LEU:HD21 | 1.41 | 0.97 |
| 1:D:175:ILE:HG22 | 1:D:277:LEU:HA | 1.46 | 0.96 |
| 1:A:259:ASN:HA | 1:A:294:ILE:HB | 1.45 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:248:GLU:H | 1:C:248:GLU:CD | 1.67 | 0.95 |
| 1:J:181:TYR:HA | 1:J:271:ILE:HG22 | 1.48 | 0.94 |
| 1:C:306:GLU:O | 1:C:310:ARG:HB2 | 1.68 | 0.93 |
| 1:I:152:TYR:HB3 | 1:I:298:PRO:HB3 | 1.47 | 0.93 |
| 1:B:179:PRO:O | 1:B:191:VAL:HG21 | 1.69 | 0.92 |
| 1:I:201:ARG:H | 1:I:201:ARG:HD3 | 1.35 | 0.92 |
| 1:I:218:GLU:HB2 | 1:I:255:ASN:ND2 | 1.84 | 0.92 |
| 1:I:243:PRO:HB2 | 1:I:246:GLY:CA | 1.98 | 0.92 |
| 2:L:807:DT:H2" | 2:L:808:DG:H5' | 1.52 | 0.92 |
| 1:J:138:LYS:HA | 1:J:299:GLY:HA3 | 1.50 | 0.91 |
| 1:I:220:ASN:HD22 | 1:I:222:LEU:H | 1.10 | 0.91 |
| 1:A:307:ASP:HA | 1:A:310:ARG:HG3 | 1.52 | 0.91 |
| 1:J:194:CYS:SG | 1:J:262:CYS:HB3 | 2.11 | 0.91 |
| 1:I:278:GLU:HG2 | 1:I:284:VAL:HG22 | 1.52 | 0.90 |
| 1:A:196:ASN:HB2 | 1:B:196:ASN:HD21 | 1.35 | 0.89 |
| 2:H:706:DA:H2" | 2:H:707:DT:H5' | 1.52 | 0.88 |
| 1:B:179:PRO:HA | 1:B:273:ILE:HG22 | 1.55 | 0.88 |
| 1:D:243:PRO:HB2 | 1:D:248:GLU:HB3 | 1.55 | 0.87 |
| 1:C:131:PHE:HE2 | 1:C:151:LEU:HD13 | 1.38 | 0.87 |
| 1:I:201:ARG:HG2 | 1:I:202:ASP:H | 1.38 | 0.86 |
| 1:I:119:THR:O | 1:I:287:ARG:HD2 | 1.76 | 0.86 |
| 1:I:226:VAL:O | 1:I:234:GLN:HA | 1.76 | 0.86 |
| 1:J:134:SER:HB2 | 1:J:143:THR:HA | 1.58 | 0.85 |
| 1:I:224:GLN:O | 1:I:226:VAL:HG23 | 1.76 | 0.84 |
| 1:B:310:ARG:HD3 | 1:B:311:GLU:N | 1.91 | 0.84 |
| 1:I:215:ILE:H | 1:I:215:ILE:CD1 | 1.89 | 0.84 |
| 1:B:121:TYR:HD1 | 1:B:122:PRO:HD2 | 1.43 | 0.84 |
| 1:I:161:ILE:HD11 | 1:I:254:TYR:CD1 | 2.13 | 0.83 |
| 1:C:145:SER:HA | 1:C:302:ARG:HH11 | 1.43 | 0.83 |
| 1:I:143:THR:CG2 | 1:I:298:PRO:HB2 | 2.09 | 0.82 |
| 2:F:506:DA:H2" | 2:F:507:DT:H5' | 1.61 | 0.82 |
| 1:A:263:VAL:HG13 | 1:A:264:GLY:H | 1.44 | 0.82 |
| 1:B:244:GLN:C | 1:B:246:GLY:H | 1.82 | 0.81 |
| 1:I:194:CYS:HB2 | 1:I:263:VAL:O | 1.79 | 0.81 |
| 1:A:303:LYS:HG3 | 1:A:304:ALA:N | 1.93 | 0.81 |
| 1:B:293:ARG:HG2 | 1:B:295:CYS:SG | 2.19 | 0.81 |
| 1:J:279:MET:HG2 | 1:J:285:LEU:HD21 | 1.62 | 0.81 |
| 1:B:279:MET:HG3 | 1:B:283:GLN:HB3 | 1.61 | 0.81 |
| 2:L:812:DA:H2" | 2:L:813:DT:OP2 | 1.79 | 0.81 |
| 1:A:179:PRO:O | 1:A:191:VAL:HG21 | 1.81 | 0.81 |
| 1:C:259:ASN:HA | 1:C:294:ILE:HG22 | 1.63 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:220:ASN:HD22 | 1:I:221:ASN:N | 1.78 | 0.80 |
| 2:K:904:DG:H2" | 2:K:905:DG:C8 | 2.16 | 0.80 |
| 1:B:129:VAL:HG21 | 1:B:288:ARG:HB3 | 1.64 | 0.80 |
| 1:B:272:LEU:HA | 1:B:291:GLU:HA | 1.63 | 0.80 |
| 1:D:283:GLN:NE2 | 1:J:245:VAL:HG11 | 1.96 | 0.80 |
| 1:J:193:ARG:HH21 | 1:J:257:MET:HB3 | 1.46 | 0.79 |
| 1:D:218:GLU:HG2 | 1:D:255:ASN:OD1 | 1.82 | 0.79 |
| 1:B:193:ARG:HD2 | 1:B:198:GLU:HA | 1.64 | 0.79 |
| 1:J:186:HIS:CE1 | 1:J:269:ARG:HD3 | 2.18 | 0.79 |
| 1:D:126:HIS:HB3 | 1:D:166:SER:HB2 | 1.63 | 0.79 |
| 1:J:143:THR:HG22 | 1:J:298:PRO:HB3 | 1.63 | 0.79 |
| 1:B:179:PRO:HB2 | 1:B:191:VAL:HG11 | 1.65 | 0.79 |
| 1:B:303:LYS:HA | 1:B:306:GLU:HB2 | 1.64 | 0.79 |
| 1:A:310:ARG:HD3 | 1:A:311:GLU:N | 1.98 | 0.78 |
| 1:B:148:LEU:HD11 | 1:B:305:ASP:HB2 | 1.65 | 0.78 |
| 1:C:176:ARG:HB2 | 1:C:237:VAL:HG23 | 1.65 | 0.78 |
| 1:B:120:ASP:OD1 | 1:B:288:ARG:HD3 | 1.82 | 0.78 |
| 1:A:193:ARG:HD3 | 1:A:211:ALA:O | 1.84 | 0.78 |
| 1:D:165:VAL:HG12 | 1:D:166:SER:H | 1.47 | 0.78 |
| 1:C:201:ARG:HH21 | 1:C:202:ASP:HB2 | 1.49 | 0.77 |
| 1:B:258:CYS:HB3 | 1:B:262:CYS:SG | 2.24 | 0.77 |
| 1:B:274:ILE:HG22 | 1:B:289:SER:HB3 | 1.66 | 0.77 |
| 1:C:193:ARG:NE | 1:C:197:HIS:HB3 | 1.99 | 0.77 |
| 1:D:201:ARG:HD2 | 1:D:202:ASP:H | 1.49 | 0.77 |
| 1:A:182:LYS:HG3 | 1:A:272:LEU:HD11 | 1.65 | 0.77 |
| 1:I:150:LYS:HD2 | 1:I:291:GLU:OE2 | 1.85 | 0.77 |
| 1:B:174:ALA:HA | 1:B:239:PRO:HA | 1.66 | 0.77 |
| 1:B:247:THR:O | 1:B:249:PHE:HD2 | 1.68 | 0.77 |
| 1:D:117:SER:HB3 | 1:D:287:ARG:HH12 | 1.47 | 0.77 |
| 1:D:259:ASN:HA | 1:D:294:ILE:HB | 1.67 | 0.77 |
| 1:J:131:PHE:HD1 | 1:J:131:PHE:H | 1.32 | 0.77 |
| 1:C:131:PHE:CE2 | 1:C:151:LEU:HD13 | 2.20 | 0.76 |
| 1:J:296:ALA:HB3 | 2:L:809:DT:H72 | 1.67 | 0.76 |
| 1:B:147:LEU:HB3 | 1:B:148:LEU:HD12 | 1.67 | 0.76 |
| 1:D:279:MET:HB2 | 1:D:283:GLN:HB3 | 1.67 | 0.76 |
| 1:B:119:THR:HG22 | 1:B:287:ARG:NH1 | 1.99 | 0.76 |
| 1:B:197:HIS:HB3 | 1:B:257:MET:SD | 2.25 | 0.76 |
| 1:D:279:MET:HG3 | 1:D:280:ARG:H | 1.50 | 0.76 |
| 1:B:285:LEU:HD12 | 1:B:285:LEU:N | 2.00 | 0.76 |
| 1:D:225:TYR:CD2 | 1:D:236:VAL:HG12 | 2.20 | 0.76 |
| 1:J:193:ARG:HE | 1:J:257:MET:HB3 | 1.49 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:259:ASN:O | 1:J:262:CYS:HB2 | 1.86 | 0.76 |
| 2:F:511:DC:H2" | 2:F:512:DA:OP2 | 1.86 | 0.76 |
| 1:I:293:ARG:HG2 | 1:I:295:CYS:SG | 2.26 | 0.76 |
| 1:J:185:GLU:H | 1:J:185:GLU:CD | 1.89 | 0.76 |
| 1:D:174:ALA:HA | 1:D:239:PRO:HA | 1.68 | 0.75 |
| 1:A:201:ARG:NH1 | 1:A:202:ASP:HB2 | 2.01 | 0.75 |
| 1:C:120:ASP:HB2 | 1:C:287:ARG:O | 1.87 | 0.75 |
| 2:F:512:DA:OP2 | 2:F:512:DA:H8 | 1.69 | 0.75 |
| 1:I:193:ARG:HD3 | 1:I:211:ALA:O | 1.87 | 0.75 |
| 2:G:602:DA:H2" | 2:G:603:DT:H5' | 1.68 | 0.75 |
| 1:J:141:THR:HA | 1:J:154:GLN:NE2 | 2.01 | 0.75 |
| 1:J:231:THR:OG1 | 1:J:233:ARG:HG2 | 1.86 | 0.74 |
| 1:D:193:ARG:HG3 | 1:D:213:HIS:O | 1.88 | 0.74 |
| 1:J:150:LYS:HB2 | 1:J:291:GLU:HB3 | 1.68 | 0.74 |
| 1:A:196:ASN:HB2 | 1:B:196:ASN:ND2 | 2.03 | 0.74 |
| 1:A:303:LYS:HG3 | 1:A:304:ALA:H | 1.52 | 0.74 |
| 1:I:218:GLU:HB2 | 1:I:255:ASN:HD22 | 1.52 | 0.74 |
| 1:A:218:GLU:HB2 | 1:A:255:ASN:ND2 | 2.03 | 0.74 |
| 1:B:266:MET:O | 1:B:269:ARG:HG2 | 1.88 | 0.74 |
| 1:I:225:TYR:CD1 | 1:I:236:VAL:HG12 | 2.23 | 0.74 |
| 1:D:278:GLU:HG2 | 1:D:284:VAL:HG22 | 1.69 | 0.74 |
| 1:J:126:HIS:HB2 | 1:J:166:SER:HB2 | 1.70 | 0.74 |
| 1:J:193:ARG:NH2 | 1:J:257:MET:HB3 | 2.02 | 0.74 |
| 1:B:151:LEU:HD12 | 1:B:152:TYR:H | 1.53 | 0.73 |
| 1:D:243:PRO:HB2 | 1:D:248:GLU:CB | 2.17 | 0.73 |
| 1:D:256:PHE:N | 1:D:256:PHE:HD1 | 1.85 | 0.73 |
| 1:A:263:VAL:HG13 | 1:A:264:GLY:N | 2.02 | 0.73 |
| 1:B:301:ASP:OD1 | 1:B:304:ALA:HB2 | 1.88 | 0.73 |
| 1:A:263:VAL:O | 1:A:267:ASN:ND2 | 2.20 | 0.73 |
| 1:B:176:ARG:HD2 | 1:B:278:GLU:OE1 | 1.87 | 0.73 |
| 1:D:121:TYR:HB3 | 1:D:286:GLY:HA2 | 1.70 | 0.73 |
| 1:B:186:HIS:CD2 | 1:B:269:ARG:HD2 | 2.23 | 0.73 |
| 2:L:806:DA:H2" | 2:L:807:DT:H72 | 1.71 | 0.73 |
| 1:B:129:VAL:HG22 | 1:B:288:ARG:HD2 | 1.71 | 0.73 |
| 1:A:193:ARG:HE | 1:A:257:MET:HB2 | 1.53 | 0.73 |
| 1:D:179:PRO:HG2 | 1:D:191:VAL:HG11 | 1.68 | 0.73 |
| 1:J:302:ARG:HH22 | 1:J:303:LYS:HE3 | 1.53 | 0.73 |
| 1:A:274:ILE:HG22 | 1:A:276:THR:HG22 | 1.70 | 0.73 |
| 1:A:280:ARG:HG3 | 1:A:280:ARG:HH11 | 1.54 | 0.73 |
| 1:C:184:ALA:O | 1:C:187:VAL:HG12 | 1.89 | 0.72 |
| 1:J:155:ILE:HG23 | 1:J:156:ALA:N | 2.03 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:207:GLN:HE21 | 1:D:209:ALA:H | 1.37 | 0.72 |
| 1:D:186:HIS:ND1 | 1:D:269:ARG:HD3 | 2.04 | 0.72 |
| 2:H:707:DT:H2" | 2:H:708:DG:OP2 | 1.88 | 0.72 |
| 1:B:131:PHE:HE2 | 1:B:151:LEU:HD22 | 1.54 | 0.72 |
| 1:B:148:LEU:HD12 | 1:B:148:LEU:N | 2.05 | 0.72 |
| 1:D:186:HIS:CE1 | 1:D:269:ARG:HD3 | 2.24 | 0.72 |
| 1:J:190:VAL:HG12 | 1:J:233:ARG:HD2 | 1.72 | 0.72 |
| 1:B:252:ILE:HG22 | 1:B:253:LEU:N | 2.04 | 0.72 |
| 1:B:150:LYS:HB3 | 1:B:291:GLU:HB3 | 1.71 | 0.72 |
| 1:B:243:PRO:HA | 1:B:250:THR:H | 1.54 | 0.72 |
| 1:I:163:ILE:O | 1:I:249:PHE:HB3 | 1.89 | 0.72 |
| 1:I:196:ASN:OD1 | 1:J:196:ASN:HB2 | 1.90 | 0.72 |
| 1:A:231:THR:OG1 | 1:A:233:ARG:HG2 | 1.90 | 0.71 |
| 1:D:172:GLY:O | 1:D:280:ARG:HA | 1.90 | 0.71 |
| 1:C:201:ARG:NH2 | 1:C:202:ASP:HB2 | 2.05 | 0.71 |
| 1:I:129:VAL:HG23 | 1:I:288:ARG:HG3 | 1.72 | 0.71 |
| 1:A:117:SER:HB2 | 1:A:287:ARG:NH1 | 2.06 | 0.71 |
| 1:B:263:VAL:CG1 | 1:B:264:GLY:N | 2.54 | 0.71 |
| 1:J:155:ILE:HD11 | 1:J:258:CYS:HA | 1.71 | 0.71 |
| 1:A:130:THR:HB | 1:A:162:GLN:HB2 | 1.73 | 0.71 |
| 1:D:193:ARG:HB2 | 1:D:212:SER:O | 1.90 | 0.71 |
| 1:A:126:HIS:O | 1:A:165:VAL:HA | 1.91 | 0.70 |
| 1:A:193:ARG:NE | 1:A:257:MET:HB3 | 2.03 | 0.70 |
| 1:A:178:MET:HB2 | 1:A:235:SER:HB3 | 1.72 | 0.70 |
| 1:B:307:ASP:O | 1:B:310:ARG:HD2 | 1.90 | 0.70 |
| 1:D:121:TYR:HD1 | 1:D:122:PRO:HD2 | 1.55 | 0.70 |
| 1:B:125:HIS:HA | 1:B:166:SER:OG | 1.92 | 0.70 |
| 1:J:193:ARG:NE | 1:J:257:MET:HB3 | 2.06 | 0.70 |
| 1:I:167:THR:HG22 | 1:I:168:PRO:HD2 | 1.71 | 0.70 |
| 1:J:143:THR:HG22 | 1:J:298:PRO:CB | 2.21 | 0.70 |
| 1:J:186:HIS:ND1 | 1:J:269:ARG:HD3 | 2.06 | 0.70 |
| 1:B:119:THR:HG22 | 1:B:287:ARG:HH12 | 1.56 | 0.70 |
| 1:J:193:ARG:HG2 | 1:J:258:CYS:SG | 2.31 | 0.70 |
| 1:A:142:TRP:HA | 1:A:152:TYR:O | 1.91 | 0.70 |
| 1:A:115:ILE:HD12 | 1:A:116:PRO:O | 1.92 | 0.70 |
| 1:C:135:SER:O | 1:C:140:ALA:HB2 | 1.91 | 0.70 |
| 1:B:131:PHE:CE2 | 1:B:151:LEU:HD22 | 2.27 | 0.69 |
| 1:C:200:GLY:O | 1:C:204:ASN:ND2 | 2.24 | 0.69 |
| 1:C:307:ASP:O | 1:C:311:GLU:HB2 | 1.91 | 0.69 |
| 2:H:700:DA:H2" | 2:H:701:DT:H72 | 1.71 | 0.69 |
| 1:A:193:ARG:NH1 | 1:A:197:HIS:HB3 | 2.08 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:150:LYS:HG3 | 1:C:291:GLU:HB3 | 1.75 | 0.69 |
| 1:I:138:LYS:HA | 1:I:138:LYS:HE2 | 1.73 | 0.69 |
| 1:I:150:LYS:HA | 1:I:291:GLU:O | 1.93 | 0.69 |
| 1:I:152:TYR:CB | 1:I:298:PRO:HB3 | 2.21 | 0.69 |
| 1:B:259:ASN:HA | 1:B:294:ILE:CG2 | 2.22 | 0.69 |
| 1:A:201:ARG:HH12 | 1:A:202:ASP:HB2 | 1.57 | 0.69 |
| 1:D:255:ASN:C | 1:D:256:PHE:HD1 | 1.96 | 0.69 |
| 1:I:249:PHE:N | 1:I:249:PHE:CD1 | 2.60 | 0.69 |
| 1:B:287:ARG:O | 1:B:288:ARG:HG2 | 1.93 | 0.69 |
| 1:J:163:ILE:CG2 | 1:J:250:THR:HB | 2.23 | 0.69 |
| 1:C:145:SER:HB2 | 1:C:302:ARG:CD | 2.21 | 0.69 |
| 1:D:175:ILE:HD11 | 1:D:252:ILE:HD11 | 1.75 | 0.69 |
| 1:D:256:PHE:N | 1:D:256:PHE:CD1 | 2.57 | 0.69 |
| 1:I:115:ILE:HD11 | 1:I:231:THR:HG21 | 1.75 | 0.69 |
| 1:A:182:LYS:HA | 1:A:272:LEU:HD13 | 1.75 | 0.68 |
| 1:C:303:LYS:HE3 | 1:C:307:ASP:OD2 | 1.93 | 0.68 |
| 1:I:309:TYR:CD1 | 1:I:309:TYR:C | 2.66 | 0.68 |
| 1:I:143:THR:HG22 | 1:I:298:PRO:HB2 | 1.74 | 0.68 |
| 1:I:243:PRO:HG2 | 1:I:246:GLY:HA3 | 1.75 | 0.68 |
| 1:D:138:LYS:HG3 | 1:D:139:SER:N | 2.07 | 0.68 |
| 1:J:181:TYR:CE1 | 1:J:269:ARG:HD2 | 2.28 | 0.68 |
| 1:J:297:CYS:HB2 | 1:J:300:ARG:HB2 | 1.75 | 0.68 |
| 1:C:193:ARG:NH1 | 1:C:204:ASN:OD1 | 2.27 | 0.68 |
| 1:D:279:MET:CE | 1:D:279:MET:HA | 2.23 | 0.68 |
| 1:D:125:HIS:N | 1:D:125:HIS:CD2 | 2.61 | 0.68 |
| 1:D:228:ASP:OD1 | 1:D:230:VAL:HB | 1.94 | 0.68 |
| 1:J:256:PHE:HD1 | 1:J:256:PHE:N | 1.91 | 0.68 |
| 1:D:179:PRO:HG2 | 1:D:191:VAL:CG1 | 2.23 | 0.68 |
| 1:I:118:ASN:HA | 1:I:274:ILE:HD11 | 1.74 | 0.68 |
| 2:G:614:DA:OP2 | 2:G:614:DA:H2' | 1.94 | 0.68 |
| 1:B:216:ARG:HA | 1:B:225:TYR:HE2 | 1.58 | 0.67 |
| 1:B:178:MET:HE3 | 1:B:274:ILE:HD11 | 1.77 | 0.67 |
| 1:C:153:CYS:SG | 1:C:159:CYS:HB2 | 2.34 | 0.67 |
| 1:I:215:ILE:HG12 | 1:I:236:VAL:HG13 | 1.75 | 0.67 |
| 2:L:808:DG:H2" | 2:L:809:DT:H71 | 1.74 | 0.67 |
| 2:F:512:DA:C8 | 2:F:513:DT:H72 | 2.29 | 0.67 |
| 1:A:259:ASN:HB2 | 1:A:294:ILE:O | 1.93 | 0.67 |
| 1:A:278:GLU:HB2 | 1:A:282:GLY:O | 1.94 | 0.67 |
| 1:C:272:LEU:HD21 | 1:C:289:SER:HB2 | 1.77 | 0.67 |
| 1:J:302:ARG:NH2 | 1:J:303:LYS:HE3 | 2.10 | 0.67 |
| 1:A:167:THR:HB | 1:A:168:PRO:HD2 | 1.76 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:260:SER:HA | 1:C:266:MET:SD | 2.35 | 0.67 |
| 1:B:247:THR:O | 1:B:249:PHE:CD2 | 2.48 | 0.67 |
| 1:J:256:PHE:N | 1:J:256:PHE:CD1 | 2.58 | 0.67 |
| 1:D:114:PHE:CD2 | 1:D:231:THR:HG21 | 2.30 | 0.66 |
| 1:A:152:TYR:CB | 1:A:298:PRO:HB3 | 2.25 | 0.66 |
| 1:I:280:ARG:HG3 | 1:I:281:ASP:H | 1.59 | 0.66 |
| 1:J:131:PHE:N | 1:J:131:PHE:CD1 | 2.59 | 0.66 |
| 1:J:214:LEU:CD2 | 1:J:215:ILE:HG13 | 2.21 | 0.66 |
| 1:D:218:GLU:HG3 | 1:D:218:GLU:O | 1.94 | 0.66 |
| 1:D:123:GLY:HA2 | 1:D:285:LEU:O | 1.95 | 0.66 |
| 2:E:403:DT:H2" | 2:E:404:DG:C8 | 2.30 | 0.66 |
| 1:A:184:ALA:HA | 1:A:187:VAL:HB | 1.77 | 0.66 |
| 1:B:305:ASP:O | 1:B:308:HIS:HB3 | 1.95 | 0.66 |
| 1:I:147:LEU:HG | 1:I:148:LEU:CD2 | 2.26 | 0.66 |
| 2:K:902:DA:H1' | 2:K:903:DT:H5' | 1.77 | 0.66 |
| 1:I:193:ARG:HG2 | 1:I:258:CYS:SG | 2.36 | 0.66 |
| 1:I:140:ALA:O | 1:I:141:THR:C | 2.34 | 0.66 |
| 1:J:151:LEU:HG | 1:J:152:TYR:N | 2.10 | 0.66 |
| 1:B:179:PRO:CA | 1:B:273:ILE:HG22 | 2.25 | 0.66 |
| 1:I:201:ARG:HG2 | 1:I:202:ASP:N | 2.11 | 0.66 |
| 1:A:140:ALA:O | 1:A:298:PRO:HG2 | 1.95 | 0.66 |
| 1:I:169:PRO:HG3 | 1:I:240:TYR:CD2 | 2.31 | 0.66 |
| 1:A:216:ARG:HD2 | 1:A:257:MET:HE2 | 1.78 | 0.65 |
| 1:B:244:GLN:C | 1:B:246:GLY:N | 2.49 | 0.65 |
| 1:D:127:PHE:HE1 | 1:D:163:ILE:HG23 | 1.61 | 0.65 |
| 1:J:155:ILE:CG2 | 1:J:156:ALA:N | 2.59 | 0.65 |
| 1:D:143:THR:HG23 | 1:D:152:TYR:HB2 | 1.77 | 0.65 |
| 1:C:193:ARG:HB2 | 1:C:213:HIS:O | 1.95 | 0.65 |
| 1:A:121:TYR:CD2 | 1:A:286:GLY:HA2 | 2.31 | 0.65 |
| 1:I:177:ALA:HB3 | 1:I:254:TYR:HE2 | 1.61 | 0.65 |
| 1:I:215:ILE:HD13 | 1:I:215:ILE:N | 2.00 | 0.65 |
| 1:A:150:LYS:HB2 | 1:A:291:GLU:O | 1.97 | 0.65 |
| 1:A:259:ASN:HA | 1:A:294:ILE:CB | 2.22 | 0.65 |
| 1:C:247:THR:HG22 | 1:C:248:GLU:OE2 | 1.96 | 0.65 |
| 1:I:124:PRO:HG2 | 1:I:125:HIS:ND1 | 2.12 | 0.65 |
| 1:I:147:LEU:HG | 1:I:148:LEU:HD21 | 1.79 | 0.65 |
| 1:B:122:PRO:HG2 | 1:B:123:GLY:H | 1.62 | 0.65 |
| 1:B:186:HIS:NE2 | 1:B:269:ARG:HD2 | 2.11 | 0.65 |
| 1:I:123:GLY:HA3 | 1:I:285:LEU:O | 1.97 | 0.65 |
| 2:H:713:DT:OP2 | 2:H:713:DT:H2' | 1.96 | 0.65 |
| 1:A:152:TYR:HB3 | 1:A:298:PRO:HB3 | 1.79 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:220:ASN:HD22 | 1:I:222:LEU:N | 1.91 | 0.65 |
| 1:J:257:MET:SD | 1:J:257:MET:N | 2.69 | 0.65 |
| 2:F:507:DT:H1' | 2:F:508:DG:C8 | 2.32 | 0.65 |
| 1:B:193:ARG:HD3 | 1:B:257:MET:SD | 2.36 | 0.65 |
| 1:C:187:VAL:HG13 | 1:C:188:THR:N | 2.12 | 0.65 |
| 1:A:271:ILE:HG12 | 1:A:272:LEU:N | 2.12 | 0.65 |
| 1:B:161:ILE:HG12 | 1:B:254:TYR:HD2 | 1.62 | 0.65 |
| 1:C:145:SER:HB2 | 1:C:302:ARG:HD3 | 1.79 | 0.65 |
| 1:C:218:GLU:O | 1:C:253:LEU:HB2 | 1.97 | 0.64 |
| 1:B:131:PHE:HD2 | 1:B:142:TRP:HZ3 | 1.43 | 0.64 |
| 1:D:122:PRO:O | 1:D:127:PHE:N | 2.31 | 0.64 |
| 1:I:147:LEU:C | 1:I:148:LEU:HD23 | 2.18 | 0.64 |
| 1:I:167:THR:CG2 | 1:I:168:PRO:HD2 | 2.27 | 0.64 |
| 1:C:279:MET:HB2 | 1:C:281:ASP:HB2 | 1.78 | 0.64 |
| 1:I:146:PRO:CD | 1:I:147:LEU:H | 2.10 | 0.64 |
| 1:C:163:ILE:O | 1:C:250:THR:CG2 | 2.45 | 0.64 |
| 1:D:279:MET:HA | 1:D:279:MET:HE3 | 1.80 | 0.64 |
| 1:A:216:ARG:HB3 | 1:A:225:TYR:OH | 1.98 | 0.64 |
| 1:B:195:PRO:HG2 | 1:B:196:ASN:H | 1.63 | 0.64 |
| 1:B:218:GLU:HB2 | 1:B:255:ASN:ND2 | 2.13 | 0.64 |
| 1:B:222:LEU:O | 1:B:222:LEU:HD23 | 1.97 | 0.64 |
| 1:B:193:ARG:CZ | 1:B:257:MET:HG3 | 2.28 | 0.64 |
| 1:C:161:ILE:HG13 | 1:C:161:ILE:O | 1.97 | 0.64 |
| 1:D:121:TYR:CD1 | 1:D:122:PRO:HD2 | 2.33 | 0.63 |
| 1:D:119:THR:O | 1:D:287:ARG:NE | 2.31 | 0.63 |
| 1:D:198:GLU:O | 1:D:204:ASN:ND2 | 2.30 | 0.63 |
| 1:A:271:ILE:HD11 | 1:A:273:ILE:CD1 | 2.28 | 0.63 |
| 1:C:148:LEU:O | 1:C:149:LYS:HG2 | 1.98 | 0.63 |
| 2:K:902:DA:H2" | 2:K:903:DT:OP2 | 1.98 | 0.63 |
| 1:A:125:HIS:CD2 | 1:A:169:PRO:HA | 2.33 | 0.63 |
| 1:A:138:LYS:HB3 | 2:E:404:DG:OP2 | 1.98 | 0.63 |
| 1:A:196:ASN:CB | 1:B:196:ASN:HD21 | 2.10 | 0.63 |
| 1:B:117:SER:HB3 | 1:B:287:ARG:CZ | 2.28 | 0.63 |
| 1:D:300:ARG:HD2 | 1:D:300:ARG:O | 1.98 | 0.63 |
| 1:A:117:SER:HB2 | 1:A:287:ARG:CZ | 2.28 | 0.63 |
| 1:B:152:TYR:CZ | 1:B:301:ASP:HB3 | 2.34 | 0.63 |
| 1:J:145:SER:HG | 1:J:302:ARG:HD3 | 1.61 | 0.63 |
| 1:B:263:VAL:C | 1:B:265:GLY:H | 2.00 | 0.63 |
| 1:J:163:ILE:HG22 | 1:J:250:THR:HB | 1.81 | 0.63 |
| 1:J:127:PHE:HD2 | 1:J:286:GLY:HA3 | 1.62 | 0.63 |
| 1:J:202:ASP:O | 1:J:203:PHE:HB2 | 1.99 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:L:807:DT:C2' | 2:L:808:DG:H5' | 2.28 | 0.63 |
| 1:A:198:GLU:HG3 | 1:A:212:SER:HA | 1.81 | 0.62 |
| 1:A:280:ARG:HG3 | 1:A:280:ARG:NH1 | 2.13 | 0.62 |
| 1:D:240:TYR:HE2 | 1:D:242:PRO:HG3 | 1.63 | 0.62 |
| 1:I:188:THR:HG23 | 1:I:189:ASP:N | 2.13 | 0.62 |
| 1:A:182:LYS:HA | 1:A:272:LEU:CD1 | 2.28 | 0.62 |
| 1:A:307:ASP:C | 1:A:309:TYR:H | 2.02 | 0.62 |
| 1:I:263:VAL:HG12 | 1:I:264:GLY:N | 2.14 | 0.62 |
| 1:I:125:HIS:CD2 | 1:I:167:THR:HB | 2.34 | 0.62 |
| 1:C:138:LYS:HA | 1:C:299:GLY:HA3 | 1.81 | 0.62 |
| 1:A:278:GLU:OE1 | 1:A:282:GLY:HA2 | 2.00 | 0.62 |
| 1:D:188:THR:O | 1:D:189:ASP:C | 2.38 | 0.62 |
| 1:I:196:ASN:O | 1:I:200:GLY:N | 2.29 | 0.62 |
| 1:A:307:ASP:HA | 1:A:310:ARG:CG | 2.28 | 0.62 |
| 1:I:249:PHE:HD1 | 1:I:249:PHE:H | 1.46 | 0.62 |
| 1:J:255:ASN:C | 1:J:256:PHE:CD1 | 2.73 | 0.62 |
| 1:A:143:THR:HG22 | 1:A:298:PRO:HB2 | 1.82 | 0.62 |
| 2:H:700:DA:H2" | 2:H:701:DT:C7 | 2.28 | 0.62 |
| 1:C:116:PRO:HB3 | 1:C:178:MET:CE | 2.30 | 0.62 |
| 1:A:296:ALA:O | 1:A:297:CYS:CB | 2.45 | 0.61 |
| 1:A:271:ILE:HD11 | 1:A:273:ILE:HD11 | 1.82 | 0.61 |
| 1:D:193:ARG:HH21 | 1:D:197:HIS:HB3 | 1.64 | 0.61 |
| 1:I:204:ASN:HD22 | 1:I:211:ALA:HB2 | 1.65 | 0.61 |
| 1:B:263:VAL:HG13 | 1:B:264:GLY:H | 1.65 | 0.61 |
| 1:D:277:LEU:HB3 | 1:D:286:GLY:O | 1.99 | 0.61 |
| 1:B:138:LYS:HZ3 | 2:F:502:DG:H2' | 1.64 | 0.61 |
| 1:C:259:ASN:N | 1:C:262:CYS:SG | 2.73 | 0.61 |
| 1:A:145:SER:HA | 1:A:302:ARG:NH1 | 2.16 | 0.61 |
| 1:I:274:ILE:HG22 | 1:I:274:ILE:O | 2.00 | 0.61 |
| 1:C:163:ILE:O | 1:C:250:THR:HG22 | 2.00 | 0.61 |
| 1:I:193:ARG:HB2 | 1:I:212:SER:O | 2.01 | 0.61 |
| 1:D:131:PHE:HE2 | 1:D:151:LEU:HD13 | 1.66 | 0.61 |
| 1:J:125:HIS:ND1 | 1:J:167:THR:HG23 | 2.16 | 0.61 |
| 2:H:711:DC:OP2 | 2:H:711:DC:H2' | 2.00 | 0.61 |
| 1:D:240:TYR:CE2 | 1:D:242:PRO:HG3 | 2.36 | 0.60 |
| 1:A:135:SER:O | 1:A:137:ALA:N | 2.34 | 0.60 |
| 1:B:252:ILE:CG2 | 1:B:253:LEU:N | 2.63 | 0.60 |
| 1:C:198:GLU:HG3 | 1:C:212:SER:HA | 1.83 | 0.60 |
| 1:D:158:THR:HG22 | 1:D:218:GLU:OE1 | 2.01 | 0.60 |
| 1:I:214:LEU:HD23 | 1:I:215:ILE:HG23 | 1.81 | 0.60 |
| 1:D:155:ILE:HG21 | 1:D:259:ASN:OD1 | 2.02 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:225:TYR:CE2 | 1:D:236:VAL:HG12 | 2.37 | 0.60 |
| 2:H:700:DA:C2' | 2:H:701:DT:H72 | 2.31 | 0.60 |
| 1:B:118:ASN:ND2 | 1:B:118:ASN:H | 1.98 | 0.60 |
| 1:D:121:TYR:HB3 | 1:D:287:ARG:H | 1.66 | 0.60 |
| 1:I:122:PRO:HD2 | 1:I:123:GLY:H | 1.67 | 0.60 |
| 1:B:279:MET:HE2 | 1:B:280:ARG:H | 1.66 | 0.60 |
| 1:C:193:ARG:CZ | 1:C:197:HIS:HB3 | 2.32 | 0.60 |
| 1:I:222:LEU:O | 1:I:222:LEU:HG | 2.01 | 0.60 |
| 1:J:193:ARG:CZ | 1:J:257:MET:HB3 | 2.32 | 0.60 |
| 1:A:197:HIS:O | 1:A:200:GLY:N | 2.31 | 0.60 |
| 1:B:147:LEU:O | 1:B:147:LEU:HD23 | 2.01 | 0.60 |
| 1:J:134:SER:CB | 1:J:143:THR:HA | 2.30 | 0.60 |
| 1:J:255:ASN:C | 1:J:256:PHE:HD1 | 2.04 | 0.60 |
| 1:D:175:ILE:CD1 | 1:D:252:ILE:HD11 | 2.31 | 0.60 |
| 2:K:913:DC:H2" | 2:K:914:DA:C8 | 2.37 | 0.60 |
| 1:I:243:PRO:CG | 1:I:246:GLY:HA3 | 2.31 | 0.60 |
| 1:I:280:ARG:HG3 | 1:I:281:ASP:N | 2.16 | 0.60 |
| 1:J:170:PRO:HD2 | 1:J:173:THR:OG1 | 2.02 | 0.60 |
| 1:D:117:SER:CB | 1:D:287:ARG:HH12 | 2.15 | 0.60 |
| 1:A:259:ASN:HB3 | 1:A:294:ILE:HG22 | 1.84 | 0.59 |
| 1:B:162:GLN:HE21 | 1:B:251:THR:HG21 | 1.66 | 0.59 |
| 1:B:213:HIS:CE1 | 1:B:235:SER:C | 2.76 | 0.59 |
| 1:I:201:ARG:H | 1:I:201:ARG:CD | 2.11 | 0.59 |
| 1:A:216:ARG:HD2 | 1:A:257:MET:CE | 2.32 | 0.59 |
| 1:C:173:THR:HG22 | 1:C:240:TYR:HB2 | 1.84 | 0.59 |
| 1:D:216:ARG:HD2 | 1:D:257:MET:CE | 2.31 | 0.59 |
| 1:D:279:MET:HG2 | 1:D:281:ASP:OD2 | 2.03 | 0.59 |
| 1:J:164:LYS:HG2 | 1:J:165:VAL:O | 2.03 | 0.59 |
| 1:A:121:TYR:CE1 | 1:A:123:GLY:HA2 | 2.37 | 0.59 |
| 1:I:215:ILE:CD1 | 1:I:215:ILE:N | 2.63 | 0.59 |
| 1:B:213:HIS:HB2 | 1:B:234:GLN:OE1 | 2.03 | 0.59 |
| 1:A:124:PRO:HG2 | 1:A:125:HIS:H | 1.67 | 0.59 |
| 1:A:218:GLU:HB2 | 1:A:255:ASN:HD21 | 1.68 | 0.59 |
| 1:D:259:ASN:HA | 1:D:294:ILE:CB | 2.32 | 0.59 |
| 1:I:293:ARG:NH2 | 2:K:909:DT:OP2 | 2.28 | 0.59 |
| 1:D:263:VAL:HG23 | 1:D:267:ASN:ND2 | 2.18 | 0.59 |
| 1:J:260:SER:O | 1:J:268:ARG:N | 2.27 | 0.59 |
| 1:B:266:MET:CE | 1:B:271:ILE:HG21 | 2.32 | 0.59 |
| 2:L:808:DG:H2" | 2:L:809:DT:OP2 | 2.02 | 0.59 |
| 1:D:185:GLU:HB2 | 1:D:186:HIS:ND1 | 2.18 | 0.59 |
| 1:I:174:ALA:HA | 1:I:239:PRO:HA | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:138:LYS:HD3 | 1:B:138:LYS:C | 2.23 | 0.59 |
| 1:I:147:LEU:O | 1:I:147:LEU:HD12 | 2.03 | 0.58 |
| 1:I:188:THR:HG23 | 1:I:189:ASP:H | 1.68 | 0.58 |
| 2:L:806:DA:H2" | 2:L:807:DT:C7 | 2.33 | 0.58 |
| 1:B:132:GLN:HB2 | 1:B:142:TRP:CH2 | 2.38 | 0.58 |
| 1:D:175:ILE:HA | 1:D:276:THR:O | 2.03 | 0.58 |
| 1:I:159:CYS:HB3 | 1:I:254:TYR:O | 2.03 | 0.58 |
| 1:J:194:CYS:C | 1:J:196:ASN:N | 2.55 | 0.58 |
| 1:J:160:PRO:O | 1:J:161:ILE:HG23 | 2.02 | 0.58 |
| 2:G:614:DA:H1' | 2:G:615:DT:H5' | 1.85 | 0.58 |
| 1:A:193:ARG:HB2 | 1:A:212:SER:O | 2.03 | 0.58 |
| 1:D:126:HIS:O | 1:D:126:HIS:CD2 | 2.57 | 0.58 |
| 1:I:119:THR:HG22 | 1:I:287:ARG:NH2 | 2.18 | 0.58 |
| 1:B:279:MET:HG2 | 1:B:285:LEU:HD11 | 1.86 | 0.58 |
| 1:D:201:ARG:HD2 | 1:D:202:ASP:N | 2.19 | 0.58 |
| 1:A:303:LYS:CG | 1:A:304:ALA:N | 2.66 | 0.58 |
| 1:C:145:SER:HB2 | 1:C:302:ARG:HD2 | 1.84 | 0.58 |
| 1:D:155:ILE:HG12 | 1:D:256:PHE:O | 2.04 | 0.58 |
| 1:I:216:ARG:HA | 1:I:225:TYR:HE1 | 1.68 | 0.58 |
| 2:K:903:DT:H2" | 2:K:904:DG:C8 | 2.39 | 0.58 |
| 1:D:215:ILE:O | 1:D:236:VAL:CG1 | 2.52 | 0.58 |
| 1:I:220:ASN:ND2 | 1:I:222:LEU:N | 2.43 | 0.58 |
| 1:J:121:TYR:O | 1:J:286:GLY:HA2 | 2.04 | 0.58 |
| 1:A:220:ASN:ND2 | 1:A:238:VAL:HG23 | 2.19 | 0.58 |
| 1:C:259:ASN:HA | 1:C:294:ILE:CG2 | 2.32 | 0.58 |
| 1:C:266:MET:O | 1:C:269:ARG:HB2 | 2.04 | 0.58 |
| 1:J:188:THR:HG23 | 1:J:189:ASP:OD1 | 2.04 | 0.58 |
| 1:J:194:CYS:O | 1:J:196:ASN:N | 2.36 | 0.58 |
| 2:G:602:DA:C2' | 2:G:603:DT:H5' | 2.34 | 0.58 |
| 1:A:152:TYR:CZ | 1:A:302:ARG:HA | 2.39 | 0.58 |
| 1:I:259:ASN:N | 1:I:262:CYS:SG | 2.72 | 0.58 |
| 1:B:300:ARG:HG3 | 1:B:300:ARG:HH11 | 1.69 | 0.58 |
| 1:D:181:TYR:CE2 | 1:D:269:ARG:NH1 | 2.72 | 0.58 |
| 2:K:913:DC:H2" | 2:K:914:DA:H8 | 1.69 | 0.58 |
| 1:D:279:MET:HG2 | 1:D:281:ASP:CG | 2.23 | 0.57 |
| 1:D:293:ARG:HG2 | 1:D:295:CYS:SG | 2.44 | 0.57 |
| 1:A:150:LYS:HE2 | 1:A:152:TYR:OH | 2.04 | 0.57 |
| 1:C:248:GLU:CD | 1:C:248:GLU:N | 2.46 | 0.57 |
| 1:B:247:THR:O | 1:B:249:PHE:N | 2.37 | 0.57 |
| 1:C:154:GLN:HG2 | 1:C:295:CYS:O | 2.03 | 0.57 |
| 1:I:186:HIS:CD2 | 1:I:269:ARG:HE | 2.23 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:135:SER:HB2 | 1:J:140:ALA:CB | 2.34 | 0.57 |
| 1:J:183:LYS:HB2 | 1:J:186:HIS:HD2 | 1.69 | 0.57 |
| 1:C:257:MET:SD | 1:C:257:MET:N | 2.77 | 0.57 |
| 1:C:307:ASP:HA | 1:C:310:ARG:HB3 | 1.86 | 0.57 |
| 1:I:240:TYR:CE1 | 1:I:250:THR:HG21 | 2.40 | 0.57 |
| 1:J:175:ILE:HD11 | 1:J:240:TYR:HA | 1.86 | 0.57 |
| 1:A:111:HIS:N | 1:A:111:HIS:CD2 | 2.72 | 0.57 |
| 1:A:176:ARG:HB2 | 1:A:237:VAL:HG23 | 1.85 | 0.57 |
| 1:B:197:HIS:HB3 | 1:B:257:MET:CE | 2.35 | 0.57 |
| 1:B:243:PRO:HA | 1:B:250:THR:N | 2.20 | 0.56 |
| 1:B:307:ASP:HA | 1:B:310:ARG:HB3 | 1.86 | 0.56 |
| 1:D:155:ILE:HB | 1:D:294:ILE:HG21 | 1.85 | 0.56 |
| 1:D:164:LYS:HG2 | 1:D:165:VAL:H | 1.68 | 0.56 |
| 1:D:213:HIS:HA | 1:D:234:GLN:NE2 | 2.21 | 0.56 |
| 1:C:277:LEU:HB3 | 1:C:286:GLY:H | 1.70 | 0.56 |
| 1:J:193:ARG:HE | 1:J:257:MET:CB | 2.17 | 0.56 |
| 1:A:217:VAL:HG23 | 1:A:236:VAL:HG21 | 1.88 | 0.56 |
| 1:D:243:PRO:CB | 1:D:248:GLU:HB3 | 2.33 | 0.56 |
| 1:I:138:LYS:NZ | 1:I:139:SER:H | 2.04 | 0.56 |
| 1:A:160:PRO:C | 1:A:161:ILE:HD13 | 2.26 | 0.56 |
| 1:A:201:ARG:H | 1:A:201:ARG:HD3 | 1.70 | 0.56 |
| 1:B:310:ARG:CD | 1:B:311:GLU:N | 2.67 | 0.56 |
| 1:D:276:THR:HG22 | 1:D:287:ARG:HB3 | 1.86 | 0.56 |
| 1:I:121:TYR:HB3 | 1:I:287:ARG:HB3 | 1.88 | 0.56 |
| 1:J:195:PRO:O | 1:J:199:LEU:HB2 | 2.05 | 0.56 |
| 1:A:295:CYS:SG | 1:A:298:PRO:HD3 | 2.46 | 0.56 |
| 1:B:125:HIS:N | 1:B:125:HIS:ND1 | 2.54 | 0.56 |
| 1:D:216:ARG:HD2 | 1:D:257:MET:SD | 2.46 | 0.56 |
| 1:I:164:LYS:C | 1:I:165:VAL:HG22 | 2.25 | 0.56 |
| 1:A:248:GLU:N | 1:A:248:GLU:OE1 | 2.39 | 0.56 |
| 1:B:193:ARG:CD | 1:B:198:GLU:HA | 2.35 | 0.56 |
| 1:B:252:ILE:CG2 | 1:B:253:LEU:H | 2.19 | 0.56 |
| 1:I:218:GLU:HB2 | 1:I:255:ASN:HD21 | 1.69 | 0.56 |
| 1:I:274:ILE:HD13 | 1:I:289:SER:HB3 | 1.88 | 0.56 |
| 2:F:506:DA:C2' | 2:F:507:DT:H5' | 2.34 | 0.56 |
| 2:G:613:DC:H2" | 2:G:614:DA:C8 | 2.40 | 0.56 |
| 1:A:209:ALA:HB2 | 1:A:225:TYR:CZ | 2.41 | 0.55 |
| 1:B:163:ILE:HG22 | 1:B:164:LYS:N | 2.21 | 0.55 |
| 1:B:263:VAL:HG13 | 1:B:267:ASN:ND2 | 2.20 | 0.55 |
| 1:D:198:GLU:HG3 | 1:D:212:SER:HA | 1.87 | 0.55 |
| 1:C:263:VAL:HB | 1:D:196:ASN:ND2 | 2.21 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:152:TYR:HB3 | 1:I:298:PRO:CB | 2.31 | 0.55 |
| 1:I:228:ASP:OD1 | 1:I:229:PRO:HD2 | 2.05 | 0.55 |
| 1:I:309:TYR:O | 1:I:312:GLN:HG3 | 2.06 | 0.55 |
| 1:A:155:ILE:HG23 | 1:A:155:ILE:O | 2.05 | 0.55 |
| 1:I:136:THR:HG22 | 1:I:137:ALA:N | 2.21 | 0.55 |
| 1:A:160:PRO:O | 1:A:161:ILE:HD13 | 2.06 | 0.55 |
| 1:C:279:MET:CB | 1:C:281:ASP:HB2 | 2.36 | 0.55 |
| 1:I:186:HIS:CD2 | 1:I:269:ARG:HH11 | 2.24 | 0.55 |
| 1:J:217:VAL:HG22 | 1:J:254:TYR:CE1 | 2.42 | 0.55 |
| 1:A:296:ALA:O | 1:A:297:CYS:SG | 2.65 | 0.55 |
| 1:C:130:THR:OG1 | 1:C:162:GLN:HB2 | 2.07 | 0.55 |
| 1:C:146:PRO:HD2 | 1:C:302:ARG:HH12 | 1.71 | 0.55 |
| 1:C:179:PRO:HG2 | 1:C:191:VAL:CG2 | 2.37 | 0.55 |
| 1:J:236:VAL:HG13 | 1:J:236:VAL:O | 2.07 | 0.55 |
| 1:C:145:SER:OG | 1:C:306:GLU:OE2 | 2.24 | 0.55 |
| 1:C:179:PRO:O | 1:C:191:VAL:HG21 | 2.07 | 0.55 |
| 1:J:155:ILE:HD11 | 1:J:258:CYS:CA | 2.37 | 0.55 |
| 2:H:711:DC:H2" | 2:H:712:DA:C8 | 2.42 | 0.55 |
| 1:B:199:LEU:O | 1:B:199:LEU:HD12 | 2.06 | 0.55 |
| 1:C:127:PHE:HD2 | 1:C:286:GLY:HA3 | 1.71 | 0.55 |
| 1:A:236:VAL:HG13 | 1:A:236:VAL:O | 2.06 | 0.55 |
| 1:B:132:GLN:HB2 | 1:B:142:TRP:HH2 | 1.72 | 0.55 |
| 1:B:271:ILE:HG12 | 1:B:272:LEU:N | 2.19 | 0.55 |
| 1:C:138:LYS:CG | 1:C:139:SER:N | 2.70 | 0.55 |
| 1:D:155:ILE:HB | 1:D:294:ILE:CG2 | 2.37 | 0.55 |
| 1:D:245:VAL:O | 1:D:245:VAL:HG23 | 2.06 | 0.55 |
| 1:A:158:THR:HB | 1:A:218:GLU:OE2 | 2.06 | 0.55 |
| 1:B:123:GLY:HA3 | 1:B:285:LEU:O | 2.06 | 0.55 |
| 1:C:201:ARG:HE | 1:C:202:ASP:N | 2.05 | 0.55 |
| 1:D:152:TYR:HB3 | 1:D:298:PRO:HB2 | 1.89 | 0.55 |
| 2:K:906:DA:C2 | 2:K:907:DC:C2 | 2.94 | 0.55 |
| 1:D:179:PRO:CG | 1:D:191:VAL:HG11 | 2.37 | 0.54 |
| 1:I:213:HIS:CD2 | 1:I:234:GLN:HB3 | 2.43 | 0.54 |
| 1:C:116:PRO:HB3 | 1:C:178:MET:HE1 | 1.89 | 0.54 |
| 1:D:112:HIS:C | 1:D:114:PHE:H | 2.11 | 0.54 |
| 1:D:155:ILE:HG12 | 1:D:156:ALA:N | 2.23 | 0.54 |
| 1:D:237:VAL:HG12 | 1:D:238:VAL:N | 2.21 | 0.54 |
| 1:I:212:SER:CB | 1:I:234:GLN:HE22 | 2.20 | 0.54 |
| 1:B:241:GLU:O | 1:B:250:THR:HB | 2.07 | 0.54 |
| 1:I:145:SER:O | 1:I:148:LEU:O | 2.25 | 0.54 |
| 1:D:215:ILE:O | 1:D:236:VAL:HG11 | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:179:PRO:HG2 | 1:C:191:VAL:HG21 | 1.90 | 0.54 |
| 1:J:279:MET:O | 1:J:282:GLY:N | 2.34 | 0.54 |
| 1:B:147:LEU:HB3 | 1:B:148:LEU:CD1 | 2.37 | 0.54 |
| 1:C:152:TYR:HB3 | 1:C:298:PRO:HB3 | 1.89 | 0.54 |
| 1:D:279:MET:HG2 | 1:D:281:ASP:OD1 | 2.07 | 0.54 |
| 1:I:248:GLU:HB3 | 1:I:249:PHE:CD1 | 2.43 | 0.54 |
| 2:L:807:DT:H2" | 2:L:808:DG:C5' | 2.33 | 0.54 |
| 1:C:277:LEU:HB3 | 1:C:286:GLY:N | 2.22 | 0.54 |
| 1:D:121:TYR:CE2 | 1:J:244:GLN:HB2 | 2.43 | 0.54 |
| 1:J:113:GLU:HA | 1:J:113:GLU:OE2 | 2.07 | 0.54 |
| 1:B:115:ILE:HB | 1:B:116:PRO:CD | 2.37 | 0.54 |
| 1:B:263:VAL:HG13 | 1:B:264:GLY:N | 2.22 | 0.54 |
| 1:C:144:TYR:CE2 | 1:C:146:PRO:HA | 2.43 | 0.54 |
| 1:A:141:THR:OG1 | 1:A:142:TRP:N | 2.38 | 0.53 |
| 1:B:188:THR:OG1 | 1:B:189:ASP:N | 2.40 | 0.53 |
| 1:B:294:ILE:HD12 | 1:B:294:ILE:N | 2.23 | 0.53 |
| 1:C:178:MET:HG3 | 1:C:179:PRO:HD2 | 1.91 | 0.53 |
| 1:D:156:ALA:HB1 | 1:D:203:PHE:CE2 | 2.43 | 0.53 |
| 1:D:276:THR:HG22 | 1:D:287:ARG:HG2 | 1.90 | 0.53 |
| 1:I:178:MET:HB2 | 1:I:235:SER:HB3 | 1.90 | 0.53 |
| 1:I:256:PHE:N | 1:I:256:PHE:CD2 | 2.74 | 0.53 |
| 1:J:256:PHE:CD2 | 1:J:294:ILE:HD11 | 2.42 | 0.53 |
| 1:A:125:HIS:HB3 | 1:A:165:VAL:HG23 | 1.90 | 0.53 |
| 1:B:213:HIS:HE1 | 1:B:235:SER:C | 2.12 | 0.53 |
| 1:B:274:ILE:HG13 | 1:B:274:ILE:O | 2.08 | 0.53 |
| 1:B:285:LEU:N | 1:B:285:LEU:CD1 | 2.69 | 0.53 |
| 1:D:263:VAL:C | 1:D:265:GLY:H | 2.10 | 0.53 |
| 1:J:198:GLU:C | 1:J:200:GLY:H | 2.10 | 0.53 |
| 1:B:300:ARG:C | 1:B:302:ARG:H | 2.11 | 0.53 |
| 1:B:301:ASP:OD1 | 1:B:304:ALA:CB | 2.57 | 0.53 |
| 1:C:143:THR:HG22 | 1:C:298:PRO:HB2 | 1.91 | 0.53 |
| 1:A:152:TYR:HB2 | 1:A:298:PRO:HB3 | 1.90 | 0.53 |
| 1:A:266:MET:O | 1:A:269:ARG:CD | 2.57 | 0.53 |
| 1:B:272:LEU:O | 1:B:272:LEU:HD23 | 2.08 | 0.53 |
| 1:C:263:VAL:HB | 1:D:196:ASN:HD22 | 1.73 | 0.53 |
| 1:I:147:LEU:O | 1:I:148:LEU:HD23 | 2.09 | 0.53 |
| 1:J:202:ASP:OD1 | 1:J:203:PHE:N | 2.41 | 0.53 |
| 1:A:125:HIS:HB3 | 1:A:165:VAL:CG2 | 2.38 | 0.53 |
| 1:C:202:ASP:C | 1:C:204:ASN:H | 2.12 | 0.53 |
| 1:C:301:ASP:O | 1:C:304:ALA:HB3 | 2.09 | 0.53 |
| 1:D:127:PHE:CE1 | 1:D:163:ILE:HG23 | 2.41 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:261:SER:HA | 1:I:268:ARG:H | 1.73 | 0.53 |
| 1:I:138:LYS:HG2 | 2:L:802:DG:C2' | 2.39 | 0.53 |
| 1:A:266:MET:HA | 1:A:269:ARG:HD3 | 1.90 | 0.53 |
| 1:B:122:PRO:HG2 | 1:B:123:GLY:N | 2.24 | 0.53 |
| 1:I:146:PRO:HD2 | 1:I:147:LEU:H | 1.73 | 0.53 |
| 2:G:612:DC:H2" | 2:G:613:DC:OP2 | 2.09 | 0.53 |
| 1:D:127:PHE:CD2 | 1:D:277:LEU:HB2 | 2.44 | 0.53 |
| 2:E:410:DG:C8 | 2:E:411:DT:H72 | 2.43 | 0.53 |
| 1:B:142:TRP:C | 1:B:143:THR:HG22 | 2.29 | 0.53 |
| 1:C:213:HIS:HA | 1:C:234:GLN:OE1 | 2.09 | 0.53 |
| 1:I:128:GLU:HB2 | 1:I:164:LYS:HB2 | 1.91 | 0.53 |
| 1:I:210:PRO:HD2 | 1:I:225:TYR:CD2 | 2.43 | 0.53 |
| 1:J:201:ARG:HG2 | 1:J:202:ASP:N | 2.23 | 0.53 |
| 1:J:279:MET:CG | 1:J:285:LEU:HD21 | 2.38 | 0.53 |
| 1:A:279:MET:CG | 1:A:285:LEU:HD21 | 2.29 | 0.52 |
| 1:B:310:ARG:HG2 | 1:B:311:GLU:O | 2.09 | 0.52 |
| 1:D:121:TYR:HD1 | 1:D:122:PRO:CD | 2.22 | 0.52 |
| 1:I:136:THR:HG22 | 1:I:137:ALA:H | 1.74 | 0.52 |
| 1:I:141:THR:O | 1:I:154:GLN:HB2 | 2.08 | 0.52 |
| 1:A:135:SER:HB2 | 1:A:140:ALA:HB1 | 1.91 | 0.52 |
| 1:B:240:TYR:HE1 | 1:B:250:THR:HG21 | 1.75 | 0.52 |
| 1:C:135:SER:C | 1:C:137:ALA:H | 2.12 | 0.52 |
| 1:C:190:VAL:HA | 1:C:233:ARG:NH1 | 2.24 | 0.52 |
| 1:D:287:ARG:HD2 | 1:D:287:ARG:O | 2.09 | 0.52 |
| 2:G:602:DA:H2' | 2:G:603:DT:H71 | 1.90 | 0.52 |
| 1:B:244:GLN:HB2 | 1:B:248:GLU:HG2 | 1.92 | 0.52 |
| 1:C:144:TYR:CZ | 1:C:146:PRO:HA | 2.44 | 0.52 |
| 1:C:163:ILE:O | 1:C:250:THR:HG23 | 2.10 | 0.52 |
| 1:D:193:ARG:HD3 | 1:D:257:MET:O | 2.10 | 0.52 |
| 1:J:144:TYR:CG | 1:J:145:SER:N | 2.78 | 0.52 |
| 1:J:254:TYR:C | 1:J:255:ASN:HD22 | 2.12 | 0.52 |
| 1:J:261:SER:O | 1:J:262:CYS:C | 2.47 | 0.52 |
| 1:B:179:PRO:C | 1:B:191:VAL:HG21 | 2.30 | 0.52 |
| 1:C:306:GLU:O | 1:C:310:ARG:CB | 2.50 | 0.52 |
| 1:I:177:ALA:CB | 1:I:254:TYR:HE2 | 2.23 | 0.52 |
| 1:J:158:THR:CG2 | 1:J:253:LEU:HB3 | 2.40 | 0.52 |
| 1:J:238:VAL:HG23 | 1:J:239:PRO:HD2 | 1.91 | 0.52 |
| 1:C:152:TYR:HB3 | 1:C:298:PRO:CB | 2.39 | 0.52 |
| 1:C:164:LYS:HD3 | 1:C:248:GLU:HB2 | 1.91 | 0.52 |
| 1:D:172:GLY:HA3 | 1:D:280:ARG:CB | 2.40 | 0.52 |
| 1:A:207:GLN:NE2 | 1:A:216:ARG:HH11 | 2.08 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:126:HIS:O | 1:D:126:HIS:CG | 2.62 | 0.52 |
| 1:J:193:ARG:NE | 1:J:257:MET:O | 2.42 | 0.52 |
| 1:A:186:HIS:ND1 | 1:A:269:ARG:NE | 2.57 | 0.52 |
| 2:L:802:DG:H2" | 2:L:803:DG:C8 | 2.45 | 0.52 |
| 1:C:210:PRO:HB2 | 1:C:213:HIS:HD2 | 1.75 | 0.51 |
| 1:D:125:HIS:C | 1:D:166:SER:HB3 | 2.30 | 0.51 |
| 1:I:175:ILE:HD13 | 1:I:277:LEU:HA | 1.91 | 0.51 |
| 1:A:155:ILE:O | 1:A:155:ILE:CG2 | 2.58 | 0.51 |
| 1:B:198:GLU:HG3 | 1:B:211:ALA:O | 2.10 | 0.51 |
| 1:B:207:GLN:C | 1:B:209:ALA:N | 2.64 | 0.51 |
| 1:C:210:PRO:HB2 | 1:C:213:HIS:CD2 | 2.44 | 0.51 |
| 1:D:145:SER:HB2 | 1:D:302:ARG:HD2 | 1.92 | 0.51 |
| 1:I:158:THR:HG23 | 1:I:218:GLU:OE1 | 2.10 | 0.51 |
| 1:I:309:TYR:C | 1:I:309:TYR:HD1 | 2.14 | 0.51 |
| 1:J:150:LYS:HD3 | 1:J:291:GLU:CD | 2.31 | 0.51 |
| 1:B:152:TYR:CE2 | 1:B:301:ASP:HB3 | 2.46 | 0.51 |
| 1:B:169:PRO:O | 1:B:170:PRO:O | 2.28 | 0.51 |
| 1:B:249:PHE:CD2 | 1:B:249:PHE:N | 2.77 | 0.51 |
| 1:C:126:HIS:HD2 | 1:C:128:GLU:HG2 | 1.76 | 0.51 |
| 1:I:140:ALA:O | 1:I:142:TRP:N | 2.43 | 0.51 |
| 1:I:243:PRO:CB | 1:I:246:GLY:HA3 | 2.40 | 0.51 |
| 1:J:266:MET:O | 1:J:269:ARG:HG3 | 2.10 | 0.51 |
| 1:A:189:ASP:OD2 | 1:A:269:ARG:NH2 | 2.44 | 0.51 |
| 1:B:125:HIS:O | 1:B:127:PHE:N | 2.44 | 0.51 |
| 1:B:231:THR:OG1 | 1:B:233:ARG:HG2 | 2.10 | 0.51 |
| 2:G:603:DT:H2" | 2:G:604:DG:C8 | 2.45 | 0.51 |
| 1:B:210:PRO:HD2 | 1:B:225:TYR:CD1 | 2.46 | 0.51 |
| 1:D:127:PHE:HB2 | 1:D:277:LEU:HD22 | 1.92 | 0.51 |
| 1:D:237:VAL:CG1 | 1:D:238:VAL:N | 2.73 | 0.51 |
| 1:I:179:PRO:O | 1:I:191:VAL:HG11 | 2.10 | 0.51 |
| 1:I:244:GLN:HG2 | 1:I:245:VAL:N | 2.25 | 0.51 |
| 1:J:117:SER:O | 1:J:287:ARG:HD2 | 2.11 | 0.51 |
| 1:A:217:VAL:HG23 | 1:A:236:VAL:CG2 | 2.39 | 0.51 |
| 1:A:310:ARG:HD3 | 1:A:310:ARG:C | 2.31 | 0.51 |
| 1:C:117:SER:HB2 | 1:C:287:ARG:CZ | 2.39 | 0.51 |
| 1:J:263:VAL:HG22 | 1:J:264:GLY:N | 2.25 | 0.51 |
| 1:C:187:VAL:CG1 | 1:C:188:THR:N | 2.74 | 0.51 |
| 1:C:238:VAL:HB | 1:C:239:PRO:HD2 | 1.93 | 0.51 |
| 1:I:198:GLU:O | 1:I:211:ALA:HB1 | 2.10 | 0.51 |
| 1:I:209:ALA:HB2 | 1:I:216:ARG:HE | 1.75 | 0.51 |
| 1:I:243:PRO:CB | 1:I:246:GLY:CA | 2.79 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:278:GLU:OE1 | 1:J:282:GLY:HA2 | 2.11 | 0.51 |
| 1:B:240:TYR:CE2 | 1:B:242:PRO:HG3 | 2.46 | 0.51 |
| 1:C:259:ASN:ND2 | 1:C:295:CYS:HA | 2.25 | 0.51 |
| 1:A:207:GLN:OE1 | 1:A:209:ALA:HB3 | 2.11 | 0.51 |
| 1:B:151:LEU:HD12 | 1:B:152:TYR:N | 2.24 | 0.51 |
| 1:B:240:TYR:CE1 | 1:B:250:THR:HG21 | 2.46 | 0.51 |
| 1:J:127:PHE:CD2 | 1:J:286:GLY:HA3 | 2.43 | 0.51 |
| 1:A:118:ASN:HD21 | 1:A:272:LEU:HD22 | 1.74 | 0.50 |
| 1:A:220:ASN:HD22 | 1:A:238:VAL:CG2 | 2.23 | 0.50 |
| 1:J:274:ILE:HD12 | 1:J:274:ILE:N | 2.26 | 0.50 |
| 1:B:163:ILE:O | 1:B:249:PHE:O | 2.30 | 0.50 |
| 1:D:241:GLU:O | 1:D:250:THR:CG2 | 2.59 | 0.50 |
| 1:I:157:LYS:HE3 | 1:I:157:LYS:HA | 1.93 | 0.50 |
| 1:I:177:ALA:CB | 1:I:254:TYR:CE2 | 2.94 | 0.50 |
| 1:I:213:HIS:HA | 1:I:234:GLN:OE1 | 2.12 | 0.50 |
| 1:J:179:PRO:O | 1:J:191:VAL:HG21 | 2.12 | 0.50 |
| 1:C:121:TYR:CE1 | 1:C:123:GLY:HA2 | 2.47 | 0.50 |
| 1:C:167:THR:HB | 1:C:168:PRO:HD2 | 1.93 | 0.50 |
| 1:D:222:LEU:O | 1:D:224:GLN:HG3 | 2.12 | 0.50 |
| 1:I:142:TRP:HB3 | 1:I:153:CYS:HA | 1.93 | 0.50 |
| 1:B:144:TYR:HE1 | 1:B:146:PRO:HA | 1.76 | 0.50 |
| 1:D:214:LEU:HD22 | 1:D:214:LEU:O | 2.10 | 0.50 |
| 2:F:512:DA:OP2 | 2:F:512:DA:C8 | 2.58 | 0.50 |
| 1:B:127:PHE:HE1 | 1:B:163:ILE:HG23 | 1.77 | 0.50 |
| 1:C:279:MET:O | 1:C:282:GLY:N | 2.43 | 0.50 |
| 1:C:216:ARG:NE | 1:C:257:MET:HG2 | 2.26 | 0.50 |
| 1:I:214:LEU:HG | 1:I:214:LEU:O | 2.12 | 0.50 |
| 2:K:906:DA:H2" | 2:K:907:DC:C6 | 2.47 | 0.50 |
| 1:A:135:SER:HB2 | 1:A:140:ALA:CB | 2.41 | 0.50 |
| 1:A:263:VAL:CG1 | 1:A:264:GLY:H | 2.21 | 0.50 |
| 1:D:138:LYS:HG2 | 2:H:702:DG:OP2 | 2.11 | 0.50 |
| 1:I:161:ILE:HD11 | 1:I:254:TYR:CG | 2.46 | 0.50 |
| 1:A:253:LEU:HD23 | 1:A:253:LEU:N | 2.26 | 0.50 |
| 1:B:129:VAL:CG2 | 1:B:288:ARG:HD2 | 2.42 | 0.50 |
| 1:B:216:ARG:HG3 | 1:B:225:TYR:CE2 | 2.46 | 0.50 |
| 1:D:173:THR:HG22 | 1:D:240:TYR:HB2 | 1.94 | 0.50 |
| 1:A:174:ALA:HB1 | 1:A:238:VAL:O | 2.11 | 0.50 |
| 1:A:165:VAL:HG22 | 1:A:167:THR:O | 2.12 | 0.49 |
| 1:A:195:PRO:HD2 | 1:A:264:GLY:HA3 | 1.94 | 0.49 |
| 1:B:148:LEU:N | 1:B:148:LEU:CD1 | 2.74 | 0.49 |
| 1:B:173:THR:HG22 | 1:B:240:TYR:HB2 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:204:ASN:C | 1:B:204:ASN:HD22 | 2.14 | 0.49 |
| 1:C:135:SER:O | 1:C:137:ALA:N | 2.45 | 0.49 |
| 1:D:201:ARG:N | 1:D:201:ARG:CD | 2.74 | 0.49 |
| 1:I:122:PRO:HA | 1:I:288:ARG:HH21 | 1.76 | 0.49 |
| 1:B:163:ILE:HD13 | 1:B:175:ILE:HD13 | 1.93 | 0.49 |
| 1:B:280:ARG:HG3 | 1:B:281:ASP:H | 1.77 | 0.49 |
| 1:D:121:TYR:HB3 | 1:D:287:ARG:N | 2.27 | 0.49 |
| 1:D:276:THR:HA | 1:D:287:ARG:HB3 | 1.92 | 0.49 |
| 1:D:293:ARG:NE | 1:D:295:CYS:SG | 2.86 | 0.49 |
| 1:I:306:GLU:O | 1:I:310:ARG:HB2 | 2.12 | 0.49 |
| 1:C:150:LYS:HE2 | 1:C:152:TYR:CZ | 2.48 | 0.49 |
| 1:D:123:GLY:O | 1:D:126:HIS:N | 2.42 | 0.49 |
| 1:I:118:ASN:HA | 1:I:274:ILE:CD1 | 2.42 | 0.49 |
| 1:I:279:MET:N | 1:I:283:GLN:O | 2.35 | 0.49 |
| 1:B:192:LYS:HG2 | 1:B:234:GLN:HE21 | 1.77 | 0.49 |
| 1:C:116:PRO:HB3 | 1:C:178:MET:HE3 | 1.94 | 0.49 |
| 1:I:146:PRO:CD | 1:I:147:LEU:N | 2.75 | 0.49 |
| 1:J:121:TYR:CE1 | 1:J:123:GLY:HA2 | 2.47 | 0.49 |
| 1:J:213:HIS:HA | 1:J:234:GLN:OE1 | 2.13 | 0.49 |
| 1:D:259:ASN:CA | 1:D:294:ILE:HB | 2.40 | 0.49 |
| 1:J:194:CYS:O | 1:J:195:PRO:C | 2.49 | 0.49 |
| 1:J:240:TYR:OH | 1:J:243:PRO:HD3 | 2.12 | 0.49 |
| 1:A:194:CYS:SG | 1:A:196:ASN:HB3 | 2.52 | 0.49 |
| 1:B:266:MET:HE1 | 1:B:271:ILE:HG21 | 1.94 | 0.49 |
| 1:D:117:SER:HA | 1:J:241:GLU:OE2 | 2.12 | 0.49 |
| 1:D:164:LYS:HG2 | 1:D:165:VAL:N | 2.28 | 0.49 |
| 1:D:276:THR:HG22 | 1:D:287:ARG:CB | 2.43 | 0.49 |
| 1:J:277:LEU:HD12 | 1:J:285:LEU:HD12 | 1.95 | 0.49 |
| 1:A:312:GLN:HA | 1:A:312:GLN:OE1 | 2.13 | 0.49 |
| 1:D:259:ASN:HA | 1:D:294:ILE:CG2 | 2.43 | 0.49 |
| 1:I:244:GLN:CD | 1:I:245:VAL:HG23 | 2.33 | 0.49 |
| 1:A:263:VAL:CG1 | 1:A:264:GLY:N | 2.74 | 0.49 |
| 1:B:204:ASN:C | 1:B:204:ASN:ND2 | 2.66 | 0.49 |
| 1:B:266:MET:HE3 | 1:B:271:ILE:HG21 | 1.93 | 0.49 |
| 1:B:279:MET:CG | 1:B:283:GLN:HB3 | 2.39 | 0.49 |
| 1:C:121:TYR:CE2 | 1:C:285:LEU:O | 2.65 | 0.49 |
| 1:C:135:SER:C | 1:C:137:ALA:N | 2.66 | 0.49 |
| 1:C:277:LEU:HD12 | 1:C:285:LEU:HD12 | 1.95 | 0.49 |
| 1:D:279:MET:HG3 | 1:D:280:ARG:N | 2.24 | 0.49 |
| 1:J:237:VAL:HG13 | 1:J:238:VAL:N | 2.27 | 0.49 |
| 2:H:712:DA:OP2 | 2:H:712:DA:H8 | 1.96 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:K:902:DA:C2 | 2:K:903:DT:C2 | 3.01 | 0.49 |
| 1:A:134:SER:O | 1:A:136:THR:N | 2.44 | 0.48 |
| 1:A:160:PRO:HA | 1:A:253:LEU:HA | 1.94 | 0.48 |
| 1:B:280:ARG:HG3 | 1:B:281:ASP:N | 2.27 | 0.48 |
| 1:D:154:GLN:HA | 1:D:295:CYS:O | 2.13 | 0.48 |
| 1:J:194:CYS:C | 1:J:196:ASN:H | 2.14 | 0.48 |
| 2:G:614:DA:H1' | 2:G:615:DT:C5' | 2.42 | 0.48 |
| 1:A:150:LYS:HB2 | 1:A:291:GLU:HB3 | 1.94 | 0.48 |
| 1:B:293:ARG:NH2 | 2:E:409:DT:P | 2.86 | 0.48 |
| 1:I:164:LYS:O | 1:I:165:VAL:HG22 | 2.13 | 0.48 |
| 1:A:112:HIS:C | 1:A:112:HIS:CD2 | 2.85 | 0.48 |
| 1:A:121:TYR:O | 1:A:286:GLY:HA2 | 2.13 | 0.48 |
| 1:D:299:GLY:O | 1:D:303:LYS:HB2 | 2.14 | 0.48 |
| 1:I:203:PHE:O | 1:I:207:GLN:HB2 | 2.13 | 0.48 |
| 1:B:209:ALA:HB3 | 1:B:216:ARG:HD2 | 1.96 | 0.48 |
| 1:D:256:PHE:HD2 | 1:D:294:ILE:HD11 | 1.79 | 0.48 |
| 1:A:142:TRP:HB3 | 1:A:153:CYS:HA | 1.94 | 0.48 |
| 1:A:296:ALA:O | 1:A:297:CYS:HB2 | 2.13 | 0.48 |
| 1:I:193:ARG:NE | 1:I:197:HIS:HB3 | 2.28 | 0.48 |
| 2:K:904:DG:H2" | 2:K:905:DG:H8 | 1.75 | 0.48 |
| 1:A:179:PRO:O | 1:A:191:VAL:CG2 | 2.58 | 0.48 |
| 1:A:190:VAL:O | 1:A:191:VAL:C | 2.51 | 0.48 |
| 1:A:220:ASN:ND2 | 1:A:238:VAL:CG2 | 2.77 | 0.48 |
| 1:A:233:ARG:HD3 | 1:A:233:ARG:HA | 1.60 | 0.48 |
| 1:C:146:PRO:HD2 | 1:C:302:ARG:NH1 | 2.28 | 0.48 |
| 1:C:197:HIS:O | 1:C:198:GLU:C | 2.52 | 0.48 |
| 1:J:226:VAL:HG12 | 1:J:227:ASP:N | 2.29 | 0.48 |
| 1:A:216:ARG:HA | 1:A:225:TYR:HE2 | 1.79 | 0.48 |
| 1:A:238:VAL:HG23 | 1:A:239:PRO:HD2 | 1.95 | 0.48 |
| 1:C:111:HIS:HB2 | 1:C:112:HIS:HD2 | 1.77 | 0.48 |
| 1:I:138:LYS:CE | 1:I:299:GLY:HA3 | 2.43 | 0.48 |
| 1:J:210:PRO:HB2 | 1:J:213:HIS:HD2 | 1.78 | 0.48 |
| 1:A:167:THR:HB | 1:A:168:PRO:CD | 2.43 | 0.48 |
| 1:B:291:GLU:HG2 | 1:B:292:GLY:N | 2.29 | 0.48 |
| 1:C:218:GLU:HB2 | 1:C:255:ASN:OD1 | 2.13 | 0.48 |
| 1:D:145:SER:O | 1:D:149:LYS:N | 2.46 | 0.48 |
| 1:D:272:LEU:HA | 1:D:291:GLU:HA | 1.96 | 0.48 |
| 1:I:115:ILE:N | 1:I:116:PRO:HD3 | 2.28 | 0.48 |
| 1:I:125:HIS:ND1 | 1:I:125:HIS:N | 2.61 | 0.48 |
| 1:I:195:PRO:HG2 | 1:I:196:ASN:H | 1.79 | 0.48 |
| 1:J:225:TYR:O | 1:J:226:VAL:HG23 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:277:LEU:HB3 | 1:J:286:GLY:H | 1.79 | 0.48 |
| 2:G:602:DA:C2 | 2:H:713:DT:O2 | 2.67 | 0.48 |
| 1:A:214:LEU:O | 1:A:257:MET:HG2 | 2.13 | 0.48 |
| 1:C:140:ALA:O | 1:C:141:THR:C | 2.52 | 0.48 |
| 1:D:123:GLY:C | 1:D:125:HIS:N | 2.66 | 0.48 |
| 1:D:125:HIS:N | 1:D:125:HIS:HD2 | 2.09 | 0.48 |
| 1:D:220:ASN:OD1 | 1:D:222:LEU:HB3 | 2.14 | 0.48 |
| 1:B:244:GLN:HB2 | 1:B:248:GLU:CG | 2.43 | 0.48 |
| 1:C:127:PHE:CD2 | 1:C:277:LEU:HD23 | 2.49 | 0.48 |
| 1:C:145:SER:CA | 1:C:302:ARG:HH11 | 2.20 | 0.48 |
| 1:I:163:ILE:O | 1:I:249:PHE:CB | 2.61 | 0.48 |
| 1:J:142:TRP:HA | 1:J:152:TYR:O | 2.14 | 0.48 |
| 1:D:117:SER:HB3 | 1:J:241:GLU:HG3 | 1.96 | 0.47 |
| 1:D:259:ASN:N | 1:D:262:CYS:SG | 2.87 | 0.47 |
| 1:I:263:VAL:HG13 | 1:I:267:ASN:HD21 | 1.79 | 0.47 |
| 1:I:263:VAL:CG1 | 1:I:264:GLY:N | 2.77 | 0.47 |
| 1:J:201:ARG:HE | 1:J:202:ASP:H | 1.62 | 0.47 |
| 1:B:115:ILE:HD13 | 1:B:115:ILE:N | 2.29 | 0.47 |
| 1:B:172:GLY:HA3 | 1:B:280:ARG:HB3 | 1.95 | 0.47 |
| 1:B:179:PRO:HG2 | 1:B:191:VAL:HB | 1.96 | 0.47 |
| 1:C:134:SER:O | 1:C:136:THR:N | 2.47 | 0.47 |
| 1:D:249:PHE:CD1 | 1:D:249:PHE:N | 2.79 | 0.47 |
| 1:I:210:PRO:HD2 | 1:I:225:TYR:CG | 2.49 | 0.47 |
| 1:A:151:LEU:HD12 | 1:A:290:PHE:CD2 | 2.49 | 0.47 |
| 1:A:220:ASN:C | 1:A:222:LEU:H | 2.16 | 0.47 |
| 1:C:193:ARG:NE | 1:C:257:MET:HB3 | 2.29 | 0.47 |
| 1:J:298:PRO:O | 1:J:300:ARG:N | 2.48 | 0.47 |
| 1:D:160:PRO:HA | 1:D:252:ILE:O | 2.14 | 0.47 |
| 1:D:284:VAL:O | 1:J:245:VAL:HG23 | 2.14 | 0.47 |
| 1:I:151:LEU:HG | 1:I:152:TYR:N | 2.29 | 0.47 |
| 1:I:209:ALA:CB | 1:I:216:ARG:HE | 2.27 | 0.47 |
| 1:C:228:ASP:HB3 | 1:C:233:ARG:H | 1.80 | 0.47 |
| 1:D:227:ASP:O | 1:D:228:ASP:C | 2.52 | 0.47 |
| 1:I:195:PRO:O | 1:I:198:GLU:HB3 | 2.15 | 0.47 |
| 1:I:311:GLU:O | 1:I:312:GLN:OXT | 2.32 | 0.47 |
| 1:J:280:ARG:C | 1:J:282:GLY:H | 2.18 | 0.47 |
| 1:A:131:PHE:CZ | 1:A:151:LEU:HG | 2.49 | 0.47 |
| 1:B:163:ILE:CG2 | 1:B:164:LYS:N | 2.77 | 0.47 |
| 1:B:187:VAL:HG12 | 1:B:188:THR:N | 2.29 | 0.47 |
| 1:B:252:ILE:HG22 | 1:B:253:LEU:H | 1.76 | 0.47 |
| 1:B:263:VAL:HG12 | 1:B:264:GLY:N | 2.27 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:272:LEU:HD23 | 1:B:272:LEU:H | 1.80 | 0.47 |
| 1:B:305:ASP:C | 1:B:305:ASP:OD1 | 2.53 | 0.47 |
| 1:D:190:VAL:CG2 | 1:D:191:VAL:N | 2.77 | 0.47 |
| 1:J:127:PHE:CD1 | 1:J:128:GLU:N | 2.83 | 0.47 |
| 2:G:602:DA:C2 | 2:G:603:DT:C2 | 3.03 | 0.47 |
| 1:B:272:LEU:CA | 1:B:291:GLU:HA | 2.40 | 0.47 |
| 1:C:138:LYS:HG2 | 1:C:139:SER:N | 2.30 | 0.47 |
| 1:C:156:ALA:O | 1:C:255:ASN:ND2 | 2.48 | 0.47 |
| 1:D:248:GLU:C | 1:D:249:PHE:HD1 | 2.18 | 0.47 |
| 1:J:259:ASN:HA | 1:J:294:ILE:CG2 | 2.44 | 0.47 |
| 2:E:405:DG:H2" | 2:E:406:DA:C8 | 2.50 | 0.47 |
| 1:D:152:TYR:CD1 | 1:D:152:TYR:N | 2.82 | 0.47 |
| 1:D:218:GLU:O | 1:D:253:LEU:HB2 | 2.14 | 0.47 |
| 1:I:252:ILE:HG22 | 1:I:253:LEU:N | 2.30 | 0.47 |
| 1:J:170:PRO:HG3 | 1:J:279:MET:SD | 2.54 | 0.47 |
| 1:B:131:PHE:HD2 | 1:B:142:TRP:CZ3 | 2.27 | 0.47 |
| 1:B:259:ASN:HA | 1:B:294:ILE:HB | 1.97 | 0.47 |
| 1:C:214:LEU:CD1 | 1:C:258:CYS:HB2 | 2.45 | 0.47 |
| 1:D:151:LEU:HD22 | 1:D:290:PHE:CE1 | 2.50 | 0.47 |
| 1:D:191:VAL:O | 1:D:191:VAL:HG13 | 2.13 | 0.47 |
| 1:D:248:GLU:C | 1:D:249:PHE:CD1 | 2.89 | 0.47 |
| 1:J:181:TYR:CD1 | 1:J:269:ARG:HD2 | 2.50 | 0.46 |
| 1:A:118:ASN:ND2 | 1:A:272:LEU:HD22 | 2.31 | 0.46 |
| 1:B:226:VAL:HG12 | 1:B:227:ASP:N | 2.30 | 0.46 |
| 1:B:263:VAL:C | 1:B:265:GLY:N | 2.63 | 0.46 |
| 1:D:179:PRO:O | 1:D:191:VAL:HG11 | 2.15 | 0.46 |
| 1:D:291:GLU:HG2 | 1:D:292:GLY:H | 1.79 | 0.46 |
| 1:D:310:ARG:HH21 | 1:J:206:GLY:H | 1.62 | 0.46 |
| 1:I:125:HIS:CG | 1:I:167:THR:HB | 2.50 | 0.46 |
| 1:I:246:GLY:O | 1:I:247:THR:C | 2.54 | 0.46 |
| 1:J:184:ALA:HA | 1:J:187:VAL:HG23 | 1.97 | 0.46 |
| 1:J:225:TYR:O | 1:J:226:VAL:CG2 | 2.63 | 0.46 |
| 1:A:129:VAL:HG12 | 1:A:129:VAL:O | 2.15 | 0.46 |
| 1:B:121:TYR:CD1 | 1:B:122:PRO:HD2 | 2.35 | 0.46 |
| 1:B:243:PRO:HB2 | 1:B:245:VAL:H | 1.80 | 0.46 |
| 1:I:212:SER:OG | 1:I:234:GLN:NE2 | 2.47 | 0.46 |
| 1:I:224:GLN:O | 1:I:225:TYR:C | 2.53 | 0.46 |
| 1:J:199:LEU:HA | 1:J:199:LEU:HD23 | 1.52 | 0.46 |
| 1:A:130:THR:HG21 | 1:A:249:PHE:CZ | 2.50 | 0.46 |
| 1:A:178:MET:HB2 | 1:A:235:SER:CB | 2.45 | 0.46 |
| 1:C:196:ASN:OD1 | 1:D:195:PRO:HG2 | 2.14 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:125:HIS:CD2 | 1:D:125:HIS:H | 2.32 | 0.46 |
| 2:F:507:DT:H2" | 2:F:508:DG:OP2 | 2.15 | 0.46 |
| 1:A:240:TYR:OH | 1:A:243:PRO:HD3 | 2.14 | 0.46 |
| 1:B:113:GLU:HG3 | 1:B:231:THR:HA | 1.98 | 0.46 |
| 1:B:118:ASN:ND2 | 1:B:118:ASN:N | 2.61 | 0.46 |
| 1:C:127:PHE:CE2 | 1:C:277:LEU:HB2 | 2.51 | 0.46 |
| 1:J:300:ARG:HE | 1:J:300:ARG:HB3 | 1.32 | 0.46 |
| 1:I:122:PRO:CD | 1:I:123:GLY:H | 2.28 | 0.46 |
| 1:I:193:ARG:HE | 1:I:197:HIS:HB3 | 1.80 | 0.46 |
| 1:J:217:VAL:HG22 | 1:J:254:TYR:HE1 | 1.80 | 0.46 |
| 1:J:259:ASN:ND2 | 1:J:294:ILE:HG22 | 2.30 | 0.46 |
| 1:A:266:MET:O | 1:A:267:ASN:C | 2.54 | 0.46 |
| 1:B:115:ILE:CD1 | 1:B:115:ILE:H | 2.29 | 0.46 |
| 1:B:144:TYR:CE1 | 1:B:146:PRO:HA | 2.50 | 0.46 |
| 1:C:228:ASP:OD1 | 1:C:230:VAL:HG23 | 2.15 | 0.46 |
| 1:J:169:PRO:HB2 | 1:J:170:PRO:HD2 | 1.98 | 0.46 |
| 2:H:706:DA:H2" | 2:H:707:DT:C5' | 2.35 | 0.46 |
| 1:A:170:PRO:HA | 1:A:171:PRO:HD2 | 1.79 | 0.46 |
| 1:I:246:GLY:C | 1:I:248:GLU:N | 2.64 | 0.46 |
| 1:J:237:VAL:CG1 | 1:J:238:VAL:N | 2.79 | 0.46 |
| 2:G:614:DA:H2" | 2:G:615:DT:OP2 | 2.14 | 0.46 |
| 1:A:151:LEU:HD12 | 1:A:290:PHE:HD2 | 1.81 | 0.46 |
| 1:A:152:TYR:OH | 1:A:302:ARG:HA | 2.16 | 0.46 |
| 1:A:193:ARG:NE | 1:A:257:MET:CB | 2.59 | 0.46 |
| 1:B:284:VAL:C | 1:B:285:LEU:HD12 | 2.36 | 0.46 |
| 1:B:294:ILE:HD12 | 1:B:294:ILE:H | 1.81 | 0.46 |
| 1:D:127:PHE:CE2 | 1:D:277:LEU:HB2 | 2.51 | 0.46 |
| 1:J:131:PHE:CE1 | 1:J:144:TYR:CE2 | 3.03 | 0.46 |
| 1:B:127:PHE:HD2 | 1:B:286:GLY:HA3 | 1.81 | 0.46 |
| 1:D:122:PRO:HA | 1:D:288:ARG:HH21 | 1.79 | 0.46 |
| 1:I:138:LYS:HZ3 | 1:I:139:SER:H | 1.64 | 0.46 |
| 1:I:143:THR:HG22 | 1:I:298:PRO:CB | 2.42 | 0.46 |
| 1:I:184:ALA:O | 1:I:185:GLU:C | 2.54 | 0.46 |
| 1:J:175:ILE:CD1 | 1:J:240:TYR:HA | 2.46 | 0.46 |
| 2:K:907:DC:H1' | 2:K:908:DA:C8 | 2.51 | 0.46 |
| 1:B:129:VAL:CG2 | 1:B:288:ARG:HB3 | 2.42 | 0.45 |
| 1:D:256:PHE:CD2 | 1:D:294:ILE:HD11 | 2.51 | 0.45 |
| 2:E:402:DA:N9 | 2:E:403:DT:H72 | 2.32 | 0.45 |
| 1:B:260:SER:HA | 1:B:266:MET:HE2 | 1.97 | 0.45 |
| 1:C:202:ASP:OD1 | 1:C:203:PHE:N | 2.49 | 0.45 |
| 1:C:279:MET:SD | 1:C:285:LEU:HD21 | 2.56 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:283:GLN:HE21 | 1:J:245:VAL:HG21 | 1.79 | 0.45 |
| 1:I:172:GLY:HA3 | 1:I:280:ARG:HB3 | 1.98 | 0.45 |
| 1:J:193:ARG:HD2 | 1:J:211:ALA:O | 2.16 | 0.45 |
| 1:B:115:ILE:HB | 1:B:116:PRO:HD3 | 1.98 | 0.45 |
| 1:B:197:HIS:O | 1:B:198:GLU:C | 2.53 | 0.45 |
| 1:D:150:LYS:HA | 1:D:291:GLU:O | 2.15 | 0.45 |
| 1:J:170:PRO:CG | 1:J:279:MET:SD | 3.03 | 0.45 |
| 1:J:198:GLU:C | 1:J:200:GLY:N | 2.70 | 0.45 |
| 1:A:118:ASN:C | 1:A:118:ASN:OD1 | 2.54 | 0.45 |
| 1:A:125:HIS:NE2 | 1:A:170:PRO:HD3 | 2.31 | 0.45 |
| 1:A:150:LYS:CB | 1:A:291:GLU:HB3 | 2.46 | 0.45 |
| 1:B:176:ARG:HG3 | 1:B:237:VAL:CG2 | 2.23 | 0.45 |
| 1:B:228:ASP:HB3 | 1:B:231:THR:H | 1.82 | 0.45 |
| 1:C:201:ARG:HH21 | 1:C:202:ASP:CB | 2.24 | 0.45 |
| 1:D:121:TYR:CB | 1:D:286:GLY:HA2 | 2.42 | 0.45 |
| 1:J:148:LEU:C | 1:J:149:LYS:HG3 | 2.36 | 0.45 |
| 1:J:198:GLU:O | 1:J:200:GLY:N | 2.50 | 0.45 |
| 2:E:409:DT:H2" | 2:E:410:DG:OP2 | 2.17 | 0.45 |
| 2:G:606:DA:H2" | 2:G:607:DC:H6 | 1.82 | 0.45 |
| 1:A:273:ILE:O | 1:A:289:SER:HA | 2.16 | 0.45 |
| 1:B:258:CYS:CB | 1:B:262:CYS:SG | 2.95 | 0.45 |
| 1:C:179:PRO:HD3 | 1:C:215:ILE:HD12 | 1.99 | 0.45 |
| 1:C:259:ASN:HD22 | 1:C:295:CYS:HA | 1.81 | 0.45 |
| 1:D:255:ASN:C | 1:D:256:PHE:CD1 | 2.83 | 0.45 |
| 1:D:283:GLN:HG2 | 1:J:245:VAL:HG21 | 1.98 | 0.45 |
| 1:B:150:LYS:HD2 | 1:B:291:GLU:CD | 2.37 | 0.45 |
| 1:B:200:GLY:C | 1:B:202:ASP:N | 2.66 | 0.45 |
| 1:C:152:TYR:OH | 1:C:305:ASP:OD2 | 2.25 | 0.45 |
| 1:C:154:GLN:HE21 | 1:C:296:ALA:HA | 1.82 | 0.45 |
| 1:I:236:VAL:HG23 | 1:I:236:VAL:O | 2.16 | 0.45 |
| 1:J:150:LYS:HG2 | 1:J:152:TYR:CE1 | 2.52 | 0.45 |
| 1:A:140:ALA:O | 1:A:141:THR:C | 2.55 | 0.45 |
| 1:A:144:TYR:CZ | 1:A:146:PRO:HA | 2.51 | 0.45 |
| 1:B:197:HIS:HB3 | 1:B:257:MET:HE1 | 1.99 | 0.45 |
| 1:C:271:ILE:HD13 | 1:C:271:ILE:C | 2.37 | 0.45 |
| 1:J:125:HIS:NE2 | 1:J:169:PRO:HA | 2.32 | 0.45 |
| 1:J:296:ALA:HB3 | 2:L:809:DT:C7 | 2.43 | 0.45 |
| 1:B:193:ARG:HD3 | 1:B:257:MET:HE3 | 1.99 | 0.45 |
| 1:C:145:SER:CB | 1:C:302:ARG:HD2 | 2.46 | 0.45 |
| 1:D:187:VAL:HG13 | 1:D:188:THR:N | 2.32 | 0.45 |
| 1:D:207:GLN:HG2 | 1:D:216:ARG:NH2 | 2.31 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:156:ALA:N | 1:I:256:PHE:O | 2.43 | 0.45 |
| 1:I:252:ILE:CG2 | 1:I:253:LEU:N | 2.80 | 0.45 |
| 1:I:289:SER:O | 1:I:290:PHE:HB3 | 2.16 | 0.45 |
| 1:J:194:CYS:N | 1:J:258:CYS:SG | 2.88 | 0.45 |
| 1:C:112:HIS:N | 1:C:112:HIS:CD2 | 2.85 | 0.45 |
| 1:C:120:ASP:CB | 1:C:288:ARG:HA | 2.47 | 0.45 |
| 1:D:161:ILE:O | 1:D:161:ILE:HG13 | 2.16 | 0.45 |
| 1:I:122:PRO:HB3 | 1:I:288:ARG:NH2 | 2.32 | 0.45 |
| 1:I:188:THR:CG2 | 1:I:189:ASP:H | 2.29 | 0.45 |
| 1:A:135:SER:O | 1:A:140:ALA:HB2 | 2.17 | 0.44 |
| 1:C:184:ALA:HA | 1:C:187:VAL:HB | 1.99 | 0.44 |
| 1:D:244:GLN:OE1 | 1:D:244:GLN:HA | 2.17 | 0.44 |
| 2:G:605:DG:C6 | 2:G:606:DA:N6 | 2.85 | 0.44 |
| 1:A:307:ASP:C | 1:A:309:TYR:N | 2.69 | 0.44 |
| 1:B:122:PRO:HA | 1:B:288:ARG:HH21 | 1.82 | 0.44 |
| 1:B:194:CYS:HB2 | 1:B:263:VAL:O | 2.17 | 0.44 |
| 1:D:174:ALA:CA | 1:D:239:PRO:HA | 2.44 | 0.44 |
| 1:I:153:CYS:HB2 | 1:I:159:CYS:SG | 2.58 | 0.44 |
| 1:A:202:ASP:O | 1:A:204:ASN:N | 2.51 | 0.44 |
| 1:B:228:ASP:HB3 | 1:B:232:GLY:H | 1.83 | 0.44 |
| 1:B:244:GLN:O | 1:B:244:GLN:HG3 | 2.17 | 0.44 |
| 1:C:150:LYS:HB3 | 1:C:152:TYR:CE1 | 2.51 | 0.44 |
| 1:D:131:PHE:CE2 | 1:D:151:LEU:HD13 | 2.51 | 0.44 |
| 2:L:801:DT:C2 | 2:L:802:DG:N7 | 2.85 | 0.44 |
| 1:B:195:PRO:HG2 | 1:B:196:ASN:ND2 | 2.32 | 0.44 |
| 1:D:161:ILE:C | 1:D:161:ILE:HD12 | 2.38 | 0.44 |
| 1:J:197:HIS:O | 1:J:200:GLY:N | 2.42 | 0.44 |
| 1:B:300:ARG:HG3 | 1:B:300:ARG:NH1 | 2.32 | 0.44 |
| 1:C:259:ASN:C | 1:C:261:SER:N | 2.71 | 0.44 |
| 1:J:297:CYS:O | 1:J:298:PRO:C | 2.55 | 0.44 |
| 1:A:125:HIS:O | 1:A:126:HIS:C | 2.54 | 0.44 |
| 1:J:194:CYS:SG | 1:J:262:CYS:CB | 2.88 | 0.44 |
| 1:I:139:SER:HB2 | 1:I:298:PRO:HG2 | 1.99 | 0.44 |
| 1:I:155:ILE:CG1 | 1:I:156:ALA:N | 2.81 | 0.44 |
| 1:I:195:PRO:HG2 | 1:I:196:ASN:N | 2.32 | 0.44 |
| 1:I:240:TYR:CE2 | 1:I:242:PRO:HA | 2.53 | 0.44 |
| 1:A:150:LYS:CE | 1:A:152:TYR:CZ | 3.01 | 0.44 |
| 1:A:220:ASN:HD22 | 1:A:238:VAL:HG21 | 1.82 | 0.44 |
| 1:B:192:LYS:HG2 | 1:B:234:GLN:NE2 | 2.32 | 0.44 |
| 1:J:178:MET:HB2 | 1:J:235:SER:HB3 | 1.99 | 0.44 |
| 1:B:207:GLN:C | 1:B:209:ALA:H | 2.21 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:259:ASN:O | 1:B:262:CYS:SG | 2.76 | 0.44 |
| 1:D:310:ARG:HH21 | 1:J:205:GLU:HA | 1.82 | 0.44 |
| 1:I:261:SER:O | 1:I:262:CYS:C | 2.56 | 0.44 |
| 1:I:298:PRO:O | 1:I:299:GLY:C | 2.56 | 0.44 |
| 1:J:210:PRO:O | 1:J:213:HIS:HB2 | 2.18 | 0.44 |
| 2:F:500:DA:H2" | 2:F:501:DT:H71 | 2.00 | 0.43 |
| 2:G:602:DA:H1' | 2:G:603:DT:C5' | 2.48 | 0.43 |
| 1:A:268:ARG:HE | 1:A:268:ARG:HB2 | 1.46 | 0.43 |
| 1:B:138:LYS:HD3 | 1:B:139:SER:OG | 2.18 | 0.43 |
| 1:I:154:GLN:HA | 1:I:295:CYS:O | 2.18 | 0.43 |
| 1:I:162:GLN:OE1 | 1:I:251:THR:HB | 2.18 | 0.43 |
| 2:F:507:DT:C1' | 2:F:508:DG:C8 | 3.00 | 0.43 |
| 1:D:165:VAL:HG12 | 1:D:166:SER:N | 2.25 | 0.43 |
| 1:D:181:TYR:CZ | 1:D:269:ARG:NH1 | 2.86 | 0.43 |
| 1:D:197:HIS:O | 1:D:198:GLU:C | 2.56 | 0.43 |
| 1:D:263:VAL:C | 1:D:265:GLY:N | 2.72 | 0.43 |
| 1:I:246:GLY:O | 1:I:248:GLU:N | 2.51 | 0.43 |
| 1:I:256:PHE:CD1 | 1:I:294:ILE:HD11 | 2.54 | 0.43 |
| 1:J:190:VAL:HG12 | 1:J:233:ARG:CD | 2.46 | 0.43 |
| 1:A:289:SER:C | 1:A:290:PHE:HD1 | 2.21 | 0.43 |
| 1:B:147:LEU:C | 1:B:148:LEU:HD12 | 2.38 | 0.43 |
| 1:B:161:ILE:CG1 | 1:B:254:TYR:HD2 | 2.30 | 0.43 |
| 1:C:120:ASP:HB2 | 1:C:288:ARG:HA | 2.00 | 0.43 |
| 1:C:121:TYR:CZ | 1:C:123:GLY:HA2 | 2.53 | 0.43 |
| 1:I:138:LYS:HE2 | 1:I:299:GLY:HA3 | 1.99 | 0.43 |
| 1:A:183:LYS:HB3 | 1:A:185:GLU:HG3 | 2.00 | 0.43 |
| 1:A:271:ILE:HD11 | 1:A:273:ILE:HD12 | 2.00 | 0.43 |
| 1:B:120:ASP:OD1 | 1:B:288:ARG:CD | 2.60 | 0.43 |
| 1:C:145:SER:O | 1:C:149:LYS:N | 2.50 | 0.43 |
| 1:D:277:LEU:O | 1:D:284:VAL:HG13 | 2.19 | 0.43 |
| 1:I:131:PHE:CE1 | 1:I:144:TYR:CE1 | 3.07 | 0.43 |
| 1:I:259:ASN:HB2 | 1:I:262:CYS:SG | 2.59 | 0.43 |
| 1:J:173:THR:HG22 | 1:J:240:TYR:HB2 | 1.99 | 0.43 |
| 1:J:296:ALA:CB | 2:L:809:DT:H72 | 2.44 | 0.43 |
| 1:A:173:THR:HG23 | 1:A:240:TYR:HB3 | 1.99 | 0.43 |
| 1:A:220:ASN:C | 1:A:222:LEU:N | 2.72 | 0.43 |
| 1:A:281:ASP:OD1 | 1:A:281:ASP:C | 2.57 | 0.43 |
| 1:A:297:CYS:N | 1:A:298:PRO:CD | 2.81 | 0.43 |
| 1:A:308:HIS:CD2 | 1:A:308:HIS:O | 2.72 | 0.43 |
| 1:B:124:PRO:HG2 | 1:B:125:HIS:ND1 | 2.34 | 0.43 |
| 1:B:193:ARG:CD | 1:B:257:MET:SD | 3.05 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:193:ARG:NH1 | 1:B:211:ALA:HA | 2.33 | 0.43 |
| 1:B:259:ASN:HA | 1:B:294:ILE:CB | 2.48 | 0.43 |
| 1:B:300:ARG:C | 1:B:302:ARG:N | 2.72 | 0.43 |
| 1:C:302:ARG:O | 1:C:306:GLU:HG3 | 2.19 | 0.43 |
| 1:D:119:THR:OG1 | 1:J:241:GLU:OE1 | 2.31 | 0.43 |
| 1:D:237:VAL:O | 1:D:238:VAL:HG12 | 2.18 | 0.43 |
| 1:I:130:THR:OG1 | 1:I:131:PHE:N | 2.51 | 0.43 |
| 1:I:201:ARG:O | 1:I:203:PHE:N | 2.52 | 0.43 |
| 1:J:117:SER:HB2 | 1:J:287:ARG:CZ | 2.49 | 0.43 |
| 1:J:260:SER:HA | 1:J:266:MET:HE2 | 2.01 | 0.43 |
| 1:B:162:GLN:HG3 | 1:B:251:THR:HG22 | 1.99 | 0.43 |
| 1:B:199:LEU:O | 1:B:199:LEU:CD1 | 2.67 | 0.43 |
| 1:B:283:GLN:HE21 | 1:B:283:GLN:HB2 | 1.59 | 0.43 |
| 1:D:190:VAL:HG22 | 1:D:191:VAL:N | 2.31 | 0.43 |
| 1:D:276:THR:HG22 | 1:D:287:ARG:CG | 2.48 | 0.43 |
| 1:I:120:ASP:OD1 | 1:I:288:ARG:HA | 2.18 | 0.43 |
| 1:J:128:GLU:HG3 | 1:J:288:ARG:CZ | 2.48 | 0.43 |
| 1:J:150:LYS:HD3 | 1:J:291:GLU:HG2 | 2.01 | 0.43 |
| 1:A:228:ASP:HB3 | 1:A:233:ARG:H | 1.84 | 0.43 |
| 1:B:178:MET:CE | 1:B:274:ILE:HD11 | 2.44 | 0.43 |
| 1:C:216:ARG:HA | 1:C:225:TYR:HE1 | 1.83 | 0.43 |
| 1:D:263:VAL:HG23 | 1:D:267:ASN:HD21 | 1.83 | 0.43 |
| 1:J:163:ILE:HG22 | 1:J:250:THR:O | 2.19 | 0.43 |
| 1:J:193:ARG:HB2 | 1:J:213:HIS:O | 2.18 | 0.43 |
| 2:E:402:DA:C8 | 2:E:403:DT:H72 | 2.54 | 0.43 |
| 1:B:240:TYR:OH | 1:B:243:PRO:HD3 | 2.19 | 0.43 |
| 1:D:172:GLY:HA3 | 1:D:280:ARG:HB3 | 2.00 | 0.43 |
| 1:D:271:ILE:O | 1:D:291:GLU:HG3 | 2.19 | 0.43 |
| 2:E:402:DA:H2" | 2:E:403:DT:C7 | 2.49 | 0.43 |
| 1:A:116:PRO:HB2 | 1:A:180:VAL:HG21 | 2.00 | 0.43 |
| 1:C:170:PRO:O | 1:C:171:PRO:C | 2.56 | 0.43 |
| 1:D:186:HIS:CG | 1:D:269:ARG:CD | 3.02 | 0.43 |
| 1:I:280:ARG:C | 1:I:282:GLY:H | 2.22 | 0.43 |
| 1:J:135:SER:HB2 | 1:J:140:ALA:HB2 | 2.01 | 0.43 |
| 1:J:275:ILE:N | 1:J:275:ILE:HD12 | 2.34 | 0.43 |
| 1:A:150:LYS:HE2 | 1:A:152:TYR:CZ | 2.54 | 0.42 |
| 1:D:152:TYR:HB3 | 1:D:298:PRO:CB | 2.49 | 0.42 |
| 1:D:202:ASP:C | 1:D:204:ASN:N | 2.70 | 0.42 |
| 1:D:279:MET:CG | 1:D:281:ASP:OD1 | 2.67 | 0.42 |
| 1:I:242:PRO:O | 1:I:243:PRO:C | 2.57 | 0.42 |
| 1:J:127:PHE:CE1 | 1:J:163:ILE:HD11 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:157:LYS:HA | 1:B:157:LYS:HD3 | 1.62 | 0.42 |
| 1:B:263:VAL:HG13 | 1:B:267:ASN:HD21 | 1.83 | 0.42 |
| 1:D:291:GLU:HG2 | 1:D:292:GLY:N | 2.34 | 0.42 |
| 1:J:302:ARG:HH22 | 1:J:303:LYS:CE | 2.27 | 0.42 |
| 2:K:909:DT:H2" | 2:K:910:DG:OP2 | 2.19 | 0.42 |
| 1:B:138:LYS:HG3 | 2:F:502:DG:C5' | 2.49 | 0.42 |
| 1:C:170:PRO:HA | 1:C:171:PRO:HD3 | 1.94 | 0.42 |
| 1:D:121:TYR:CG | 1:D:286:GLY:HA2 | 2.54 | 0.42 |
| 1:D:237:VAL:C | 1:D:238:VAL:HG12 | 2.39 | 0.42 |
| 1:I:122:PRO:HB3 | 1:I:288:ARG:HH21 | 1.84 | 0.42 |
| 1:I:220:ASN:HD22 | 1:I:220:ASN:C | 2.21 | 0.42 |
| 1:J:154:GLN:HA | 1:J:295:CYS:O | 2.19 | 0.42 |
| 1:J:259:ASN:HA | 1:J:294:ILE:HG22 | 2.01 | 0.42 |
| 1:J:273:ILE:HG22 | 1:J:275:ILE:HD12 | 1.99 | 0.42 |
| 2:F:504:DA:C2 | 2:F:505:DC:C2 | 3.08 | 0.42 |
| 2:G:605:DG:C6 | 2:G:606:DA:C6 | 3.06 | 0.42 |
| 1:B:240:TYR:CZ | 1:B:242:PRO:HA | 2.55 | 0.42 |
| 1:B:244:GLN:C | 1:B:245:VAL:HG23 | 2.40 | 0.42 |
| 1:C:126:HIS:CD2 | 1:C:128:GLU:HG2 | 2.54 | 0.42 |
| 1:C:216:ARG:HD2 | 1:C:257:MET:CE | 2.50 | 0.42 |
| 1:D:126:HIS:O | 1:D:127:PHE:C | 2.57 | 0.42 |
| 1:D:157:LYS:N | 1:D:157:LYS:HD2 | 2.33 | 0.42 |
| 1:I:150:LYS:HE2 | 1:I:152:TYR:CZ | 2.55 | 0.42 |
| 2:H:704:DA:C5 | 2:H:705:DC:C4 | 3.06 | 0.42 |
| 1:A:151:LEU:HD12 | 1:A:151:LEU:H | 1.84 | 0.42 |
| 1:A:158:THR:HB | 1:A:218:GLU:CD | 2.40 | 0.42 |
| 1:B:138:LYS:NZ | 2:F:502:DG:H2' | 2.33 | 0.42 |
| 1:B:149:LYS:HB3 | 1:B:149:LYS:HE3 | 1.84 | 0.42 |
| 1:C:145:SER:HA | 1:C:146:PRO:HD2 | 1.75 | 0.42 |
| 1:D:241:GLU:O | 1:D:250:THR:HG21 | 2.19 | 0.42 |
| 1:I:150:LYS:CG | 1:I:291:GLU:HB3 | 2.49 | 0.42 |
| 1:J:150:LYS:HB3 | 1:J:150:LYS:HE2 | 1.80 | 0.42 |
| 2:E:407:DC:H2" | 2:E:408:DA:OP2 | 2.20 | 0.42 |
| 1:A:289:SER:C | 1:A:290:PHE:CD1 | 2.92 | 0.42 |
| 1:B:115:ILE:HD13 | 1:B:115:ILE:H | 1.84 | 0.42 |
| 1:B:171:PRO:O | 1:B:173:THR:N | 2.52 | 0.42 |
| 1:B:171:PRO:C | 1:B:173:THR:H | 2.22 | 0.42 |
| 1:I:129:VAL:HG21 | 1:I:288:ARG:HB2 | 2.02 | 0.42 |
| 1:J:128:GLU:HG3 | 1:J:288:ARG:HD2 | 2.01 | 0.42 |
| 1:A:140:ALA:O | 1:A:298:PRO:CG | 2.67 | 0.42 |
| 1:B:240:TYR:CE2 | 1:B:242:PRO:HA | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:134:SER:OG | 1:C:143:THR:HA | 2.19 | 0.42 |
| 1:C:197:HIS:O | 1:C:200:GLY:N | 2.50 | 0.42 |
| 1:D:176:ARG:HB2 | 1:D:237:VAL:HG22 | 2.01 | 0.42 |
| 1:I:138:LYS:CE | 1:I:139:SER:H | 2.32 | 0.42 |
| 1:A:266:MET:O | 1:A:269:ARG:HD2 | 2.20 | 0.42 |
| 1:A:296:ALA:C | 1:A:297:CYS:SG | 2.98 | 0.42 |
| 1:B:303:LYS:HE3 | 1:B:306:GLU:HG2 | 2.01 | 0.42 |
| 1:B:310:ARG:O | 1:B:311:GLU:HB2 | 2.20 | 0.42 |
| 1:C:176:ARG:HB2 | 1:C:237:VAL:CG2 | 2.44 | 0.42 |
| 1:C:240:TYR:OH | 1:C:242:PRO:HA | 2.20 | 0.42 |
| 1:C:256:PHE:CB | 1:C:294:ILE:HG12 | 2.50 | 0.42 |
| 1:D:151:LEU:HD23 | 1:D:151:LEU:H | 1.85 | 0.42 |
| 1:J:121:TYR:CE2 | 1:J:285:LEU:O | 2.72 | 0.42 |
| 1:J:239:PRO:O | 1:J:240:TYR:C | 2.57 | 0.42 |
| 1:J:273:ILE:HG22 | 1:J:275:ILE:CD1 | 2.50 | 0.42 |
| 1:A:154:GLN:HA | 1:A:295:CYS:O | 2.19 | 0.42 |
| 1:B:163:ILE:HB | 1:B:250:THR:HG23 | 2.00 | 0.42 |
| 1:B:259:ASN:HA | 1:B:294:ILE:HG21 | 2.00 | 0.42 |
| 1:C:144:TYR:O | 1:C:302:ARG:CZ | 2.68 | 0.42 |
| 1:D:127:PHE:CD2 | 1:D:277:LEU:CB | 3.03 | 0.42 |
| 1:I:214:LEU:HD12 | 1:I:258:CYS:HB2 | 2.02 | 0.42 |
| 2:L:801:DT:H2" | 2:L:802:DG:H8 | 1.84 | 0.42 |
| 1:A:216:ARG:HA | 1:A:225:TYR:CE2 | 2.55 | 0.42 |
| 1:A:280:ARG:C | 1:A:282:GLY:N | 2.73 | 0.42 |
| 1:B:162:GLN:HG3 | 1:B:251:THR:CG2 | 2.50 | 0.42 |
| 1:I:220:ASN:ND2 | 1:I:221:ASN:N | 2.58 | 0.42 |
| 1:A:111:HIS:N | 1:A:111:HIS:HD2 | 2.17 | 0.41 |
| 1:I:257:MET:N | 1:I:257:MET:SD | 2.92 | 0.41 |
| 1:I:279:MET:SD | 1:I:281:ASP:OD1 | 2.78 | 0.41 |
| 1:J:268:ARG:O | 1:J:268:ARG:HG3 | 2.20 | 0.41 |
| 1:A:170:PRO:O | 1:A:171:PRO:C | 2.58 | 0.41 |
| 1:B:121:TYR:HD1 | 1:B:122:PRO:CD | 2.23 | 0.41 |
| 1:B:150:LYS:HA | 1:B:291:GLU:O | 2.20 | 0.41 |
| 1:B:252:ILE:O | 1:B:253:LEU:HD23 | 2.20 | 0.41 |
| 1:C:272:LEU:CD2 | 1:C:289:SER:HB2 | 2.49 | 0.41 |
| 1:I:195:PRO:HD3 | 1:I:264:GLY:HA3 | 2.02 | 0.41 |
| 2:H:712:DA:H2" | 2:H:713:DT:OP2 | 2.20 | 0.41 |
| 1:A:272:LEU:HA | 1:A:290:PHE:O | 2.19 | 0.41 |
| 1:A:293:ARG:NE | 1:A:301:ASP:OD2 | 2.52 | 0.41 |
| 1:B:181:TYR:CE2 | 1:B:269:ARG:NH1 | 2.88 | 0.41 |
| 1:C:207:GLN:HG3 | 1:C:216:ARG:HH12 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:180:VAL:O | 1:I:271:ILE:HB | 2.19 | 0.41 |
| 1:J:150:LYS:HD3 | 1:J:291:GLU:CG | 2.49 | 0.41 |
| 1:J:178:MET:HG3 | 1:J:179:PRO:HD2 | 2.03 | 0.41 |
| 2:E:406:DA:H2" | 2:E:407:DC:H6 | 1.85 | 0.41 |
| 1:D:222:LEU:O | 1:D:223:SER:C | 2.58 | 0.41 |
| 1:J:131:PHE:CZ | 1:J:144:TYR:CE1 | 3.08 | 0.41 |
| 2:F:500:DA:H1' | 2:F:501:DT:C6 | 2.55 | 0.41 |
| 2:G:602:DA:H1' | 2:G:603:DT:H5" | 2.02 | 0.41 |
| 2:G:609:DT:H2" | 2:G:610:DG:H8 | 1.86 | 0.41 |
| 2:K:912:DC:H2" | 2:K:913:DC:C6 | 2.56 | 0.41 |
| 1:A:142:TRP:NE1 | 1:A:160:PRO:HD2 | 2.35 | 0.41 |
| 1:B:131:PHE:CD2 | 1:B:144:TYR:HB2 | 2.55 | 0.41 |
| 1:C:176:ARG:O | 1:C:275:ILE:HA | 2.19 | 0.41 |
| 1:C:179:PRO:C | 1:C:191:VAL:HG21 | 2.41 | 0.41 |
| 1:D:261:SER:O | 1:D:262:CYS:C | 2.59 | 0.41 |
| 1:I:164:LYS:C | 1:I:165:VAL:CG2 | 2.89 | 0.41 |
| 1:I:307:ASP:O | 1:I:311:GLU:N | 2.25 | 0.41 |
| 2:E:408:DA:H61 | 2:F:507:DT:H3 | 1.68 | 0.41 |
| 2:F:507:DT:C2 | 2:F:508:DG:N7 | 2.88 | 0.41 |
| 1:A:259:ASN:CB | 1:A:294:ILE:O | 2.64 | 0.41 |
| 1:B:122:PRO:CG | 1:B:123:GLY:H | 2.31 | 0.41 |
| 1:D:300:ARG:HD2 | 1:D:300:ARG:C | 2.40 | 0.41 |
| 1:C:245:VAL:O | 1:C:245:VAL:CG2 | 2.69 | 0.41 |
| 1:C:267:ASN:O | 1:C:268:ARG:HB2 | 2.20 | 0.41 |
| 1:I:129:VAL:CG2 | 1:I:288:ARG:HB2 | 2.50 | 0.41 |
| 1:I:150:LYS:HG2 | 1:I:291:GLU:HB3 | 2.02 | 0.41 |
| 1:I:212:SER:HB2 | 1:I:234:GLN:HE22 | 1.84 | 0.41 |
| 1:J:300:ARG:O | 1:J:301:ASP:C | 2.59 | 0.41 |
| 1:A:202:ASP:C | 1:A:204:ASN:N | 2.74 | 0.41 |
| 1:A:257:MET:N | 1:A:257:MET:SD | 2.90 | 0.41 |
| 1:B:228:ASP:HA | 1:B:229:PRO:HD3 | 1.87 | 0.41 |
| 1:B:261:SER:O | 1:B:262:CYS:C | 2.59 | 0.41 |
| 1:C:132:GLN:OE1 | 1:C:160:PRO:HG3 | 2.21 | 0.41 |
| 1:C:169:PRO:HB2 | 1:C:173:THR:OG1 | 2.21 | 0.41 |
| 1:I:119:THR:CG2 | 1:I:287:ARG:NH2 | 2.83 | 0.41 |
| 1:I:214:LEU:HD13 | 1:I:266:MET:CE | 2.51 | 0.41 |
| 1:A:193:ARG:NE | 1:A:257:MET:HB2 | 2.29 | 0.41 |
| 1:A:228:ASP:HB3 | 1:A:231:THR:OG1 | 2.21 | 0.41 |
| 1:A:252:ILE:C | 1:A:253:LEU:HD23 | 2.41 | 0.41 |
| 1:A:311:GLU:CG | 1:A:312:GLN:H | 2.34 | 0.41 |
| 1:B:171:PRO:HG2 | 1:B:172:GLY:H | 1.86 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:276:THR:CG2 | 1:B:287:ARG:HG3 | 2.51 | 0.41 |
| 1:B:300:ARG:O | 1:B:302:ARG:N | 2.54 | 0.41 |
| 1:C:202:ASP:C | 1:C:204:ASN:N | 2.74 | 0.41 |
| 1:C:216:ARG:HB2 | 1:C:255:ASN:HB2 | 2.03 | 0.41 |
| 1:C:240:TYR:CG | 1:C:241:GLU:N | 2.89 | 0.41 |
| 1:D:122:PRO:HG2 | 1:D:123:GLY:H | 1.86 | 0.41 |
| 1:D:125:HIS:O | 1:D:126:HIS:C | 2.57 | 0.41 |
| 1:D:125:HIS:O | 1:D:166:SER:N | 2.53 | 0.41 |
| 1:I:193:ARG:CG | 1:I:258:CYS:SG | 3.08 | 0.41 |
| 1:J:214:LEU:O | 1:J:256:PHE:HA | 2.21 | 0.41 |
| 1:A:176:ARG:HB3 | 1:A:276:THR:OG1 | 2.21 | 0.41 |
| 1:A:197:HIS:O | 1:A:198:GLU:C | 2.59 | 0.41 |
| 1:B:121:TYR:HB3 | 1:B:287:ARG:H | 1.86 | 0.41 |
| 1:C:245:VAL:O | 1:C:245:VAL:HG23 | 2.21 | 0.41 |
| 1:C:297:CYS:O | 1:C:298:PRO:C | 2.56 | 0.41 |
| 1:D:186:HIS:ND1 | 1:D:269:ARG:CD | 2.81 | 0.41 |
| 1:D:288:ARG:HA | 1:D:288:ARG:HD3 | 1.70 | 0.41 |
| 1:I:178:MET:HA | 1:I:179:PRO:HD3 | 1.90 | 0.41 |
| 1:I:225:TYR:HD1 | 1:I:236:VAL:HG12 | 1.77 | 0.41 |
| 1:J:255:ASN:HD22 | 1:J:255:ASN:N | 2.19 | 0.41 |
| 1:A:134:SER:CB | 1:A:144:TYR:H | 2.34 | 0.40 |
| 1:A:269:ARG:HA | 1:A:270:PRO:HD3 | 1.94 | 0.40 |
| 1:J:167:THR:OG1 | 1:J:168:PRO:HD2 | 2.22 | 0.40 |
| 1:J:226:VAL:CG1 | 1:J:227:ASP:N | 2.83 | 0.40 |
| 2:L:801:DT:C2 | 2:L:802:DG:C5 | 3.09 | 0.40 |
| 1:J:216:ARG:HG3 | 1:J:217:VAL:N | 2.36 | 0.40 |
| 2:H:712:DA:C5 | 2:H:713:DT:C4 | 3.10 | 0.40 |
| 1:B:138:LYS:HG3 | 2:F:502:DG:H5” | 2.03 | 0.40 |
| 1:B:224:GLN:HG2 | 1:I:229:PRO:HB3 | 2.02 | 0.40 |
| 1:C:126:HIS:HD2 | 1:C:128:GLU:CG | 2.34 | 0.40 |
| 1:D:222:LEU:C | 1:D:222:LEU:HD23 | 2.41 | 0.40 |
| 1:I:136:THR:HG22 | 1:I:138:LYS:H | 1.87 | 0.40 |
| 1:J:220:ASN:C | 1:J:222:LEU:H | 2.24 | 0.40 |
| 2:G:608:DA:C8 | 2:G:609:DT:C7 | 3.05 | 0.40 |
| 1:A:297:CYS:N | 1:A:298:PRO:HD2 | 2.36 | 0.40 |
| 1:B:119:THR:OG1 | 1:B:120:ASP:N | 2.55 | 0.40 |
| 1:B:138:LYS:HD3 | 1:B:138:LYS:O | 2.21 | 0.40 |
| 1:J:161:ILE:HD11 | 1:J:254:TYR:CE2 | 2.56 | 0.40 |
| 2:H:707:DT:C2’ | 2:H:708:DG:OP2 | 2.62 | 0.40 |
| 1:A:197:HIS:C | 1:A:200:GLY:H | 2.22 | 0.40 |
| 1:A:279:MET:O | 1:A:282:GLY:N | 2.54 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:160:PRO:HA | 1:B:252:ILE:O | 2.22 | 0.40 |
| 1:B:169:PRO:HA | 1:B:170:PRO:HD2 | 1.82 | 0.40 |
| 1:B:204:ASN:O | 1:B:207:GLN:N | 2.45 | 0.40 |
| 1:I:244:GLN:CG | 1:I:245:VAL:N | 2.84 | 0.40 |
| 1:J:116:PRO:HG3 | 1:J:233:ARG:NH2 | 2.37 | 0.40 |
| 1:J:163:ILE:HG23 | 1:J:250:THR:HB | 2.01 | 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 | 201/210 (96%) | 162 (81%) | 31 (15%) | 8 (4%) | 3 26 |
| 1 | B | 198/210 (94%) | 150 (76%) | 35 (18%) | 13 (7%) | 1 17 |
| 1 | C | 201/210 (96%) | 158 (79%) | 40 (20%) | 3 (2%) | 10 45 |
| 1 | D | 197/210 (94%) | 152 (77%) | 38 (19%) | 7 (4%) | 3 28 |
| 1 | I | 200/210 (95%) | 159 (80%) | 33 (16%) | 8 (4%) | 3 26 |
| 1 | J | 200/210 (95%) | 161 (80%) | 31 (16%) | 8 (4%) | 3 26 |
| All | All | 1197/1260 (95%) | 942 (79%) | 208 (17%) | 47 (4%) | 3 26 |

All (47) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 136 | THR |
| 1 | B | 170 | PRO |
| 1 | B | 243 | PRO |
| 1 | B | 245 | VAL |
| 1 | B | 248 | GLU |
| 1 | I | 202 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 135 | SER |
| 1 | A | 137 | ALA |
| 1 | B | 172 | GLY |
| 1 | B | 189 | ASP |
| 1 | C | 135 | SER |
| 1 | D | 200 | GLY |
| 1 | D | 233 | ARG |
| 1 | D | 279 | MET |
| 1 | I | 165 | VAL |
| 1 | J | 116 | PRO |
| 1 | A | 171 | PRO |
| 1 | A | 203 | PHE |
| 1 | A | 297 | CYS |
| 1 | B | 126 | HIS |
| 1 | B | 233 | ARG |
| 1 | B | 282 | GLY |
| 1 | B | 301 | ASP |
| 1 | C | 136 | THR |
| 1 | D | 184 | ALA |
| 1 | D | 282 | GLY |
| 1 | J | 157 | LYS |
| 1 | J | 199 | LEU |
| 1 | J | 262 | CYS |
| 1 | B | 187 | VAL |
| 1 | I | 156 | ALA |
| 1 | I | 218 | GLU |
| 1 | I | 281 | ASP |
| 1 | J | 221 | ASN |
| 1 | B | 171 | PRO |
| 1 | I | 304 | ALA |
| 1 | B | 116 | PRO |
| 1 | C | 203 | PHE |
| 1 | D | 188 | THR |
| 1 | J | 301 | ASP |
| 1 | I | 230 | VAL |
| 1 | I | 155 | ILE |
| 1 | A | 191 | VAL |
| 1 | A | 190 | VAL |
| 1 | D | 160 | PRO |
| 1 | J | 187 | VAL |
| 1 | J | 299 | 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 | 177/186 (95%) | 140 (79%) | 37 (21%) | 1 6 |
| 1 | B | 176/186 (95%) | 137 (78%) | 39 (22%) | 1 6 |
| 1 | C | 178/186 (96%) | 145 (82%) | 33 (18%) | 1 10 |
| 1 | D | 175/186 (94%) | 139 (79%) | 36 (21%) | 1 7 |
| 1 | I | 175/186 (94%) | 128 (73%) | 47 (27%) | 0 3 |
| 1 | J | 177/186 (95%) | 130 (73%) | 47 (27%) | 0 3 |
| All | All | 1058/1116 (95%) | 819 (77%) | 239 (23%) | 1 5 |

All (239) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 111 | HIS |
| 1 | A | 112 | HIS |
| 1 | A | 131 | PHE |
| 1 | A | 133 | GLN |
| 1 | A | 135 | SER |
| 1 | A | 138 | LYS |
| 1 | A | 147 | LEU |
| 1 | A | 150 | LYS |
| 1 | A | 151 | LEU |
| 1 | A | 155 | ILE |
| 1 | A | 160 | PRO |
| 1 | A | 161 | ILE |
| 1 | A | 185 | GLU |
| 1 | A | 186 | HIS |
| 1 | A | 187 | VAL |
| 1 | A | 190 | VAL |
| 1 | A | 194 | CYS |
| 1 | A | 196 | ASN |
| 1 | A | 199 | LEU |
| 1 | A | 201 | ARG |
| 1 | A | 224 | GLN |
| 1 | A | 237 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 238 | VAL |
| 1 | A | 248 | GLU |
| 1 | A | 253 | LEU |
| 1 | A | 259 | ASN |
| 1 | A | 268 | ARG |
| 1 | A | 269 | ARG |
| 1 | A | 271 | ILE |
| 1 | A | 276 | THR |
| 1 | A | 284 | VAL |
| 1 | A | 288 | ARG |
| 1 | A | 300 | ARG |
| 1 | A | 302 | ARG |
| 1 | A | 303 | LYS |
| 1 | A | 309 | TYR |
| 1 | A | 310 | ARG |
| 1 | B | 112 | HIS |
| 1 | B | 115 | ILE |
| 1 | B | 118 | ASN |
| 1 | B | 125 | HIS |
| 1 | B | 128 | GLU |
| 1 | B | 138 | LYS |
| 1 | B | 143 | THR |
| 1 | B | 145 | SER |
| 1 | B | 153 | CYS |
| 1 | B | 155 | ILE |
| 1 | B | 187 | VAL |
| 1 | B | 188 | THR |
| 1 | B | 190 | VAL |
| 1 | B | 191 | VAL |
| 1 | B | 194 | CYS |
| 1 | B | 204 | ASN |
| 1 | B | 205 | GLU |
| 1 | B | 216 | ARG |
| 1 | B | 228 | ASP |
| 1 | B | 230 | VAL |
| 1 | B | 235 | SER |
| 1 | B | 238 | VAL |
| 1 | B | 248 | GLU |
| 1 | B | 249 | PHE |
| 1 | B | 251 | THR |
| 1 | B | 257 | MET |
| 1 | B | 260 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 269 | ARG |
| 1 | B | 271 | ILE |
| 1 | B | 279 | MET |
| 1 | B | 280 | ARG |
| 1 | B | 283 | GLN |
| 1 | B | 285 | LEU |
| 1 | B | 297 | CYS |
| 1 | B | 303 | LYS |
| 1 | B | 305 | ASP |
| 1 | B | 306 | GLU |
| 1 | B | 309 | TYR |
| 1 | B | 310 | ARG |
| 1 | C | 111 | HIS |
| 1 | C | 115 | ILE |
| 1 | C | 117 | SER |
| 1 | C | 122 | PRO |
| 1 | C | 135 | SER |
| 1 | C | 139 | SER |
| 1 | C | 147 | LEU |
| 1 | C | 148 | LEU |
| 1 | C | 150 | LYS |
| 1 | C | 160 | PRO |
| 1 | C | 164 | LYS |
| 1 | C | 188 | THR |
| 1 | C | 191 | VAL |
| 1 | C | 201 | ARG |
| 1 | C | 227 | ASP |
| 1 | C | 230 | VAL |
| 1 | C | 237 | VAL |
| 1 | C | 244 | GLN |
| 1 | C | 245 | VAL |
| 1 | C | 247 | THR |
| 1 | C | 248 | GLU |
| 1 | C | 250 | THR |
| 1 | C | 257 | MET |
| 1 | C | 258 | CYS |
| 1 | C | 260 | SER |
| 1 | C | 271 | ILE |
| 1 | C | 276 | THR |
| 1 | C | 277 | LEU |
| 1 | C | 283 | GLN |
| 1 | C | 285 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 301 | ASP |
| 1 | C | 302 | ARG |
| 1 | C | 312 | GLN |
| 1 | D | 121 | TYR |
| 1 | D | 125 | HIS |
| 1 | D | 127 | PHE |
| 1 | D | 141 | THR |
| 1 | D | 143 | THR |
| 1 | D | 147 | LEU |
| 1 | D | 152 | TYR |
| 1 | D | 154 | GLN |
| 1 | D | 155 | ILE |
| 1 | D | 157 | LYS |
| 1 | D | 160 | PRO |
| 1 | D | 161 | ILE |
| 1 | D | 183 | LYS |
| 1 | D | 192 | LYS |
| 1 | D | 193 | ARG |
| 1 | D | 194 | CYS |
| 1 | D | 198 | GLU |
| 1 | D | 201 | ARG |
| 1 | D | 212 | SER |
| 1 | D | 214 | LEU |
| 1 | D | 224 | GLN |
| 1 | D | 238 | VAL |
| 1 | D | 244 | GLN |
| 1 | D | 249 | PHE |
| 1 | D | 255 | ASN |
| 1 | D | 256 | PHE |
| 1 | D | 271 | ILE |
| 1 | D | 272 | LEU |
| 1 | D | 276 | THR |
| 1 | D | 281 | ASP |
| 1 | D | 285 | LEU |
| 1 | D | 287 | ARG |
| 1 | D | 301 | ASP |
| 1 | D | 303 | LYS |
| 1 | D | 305 | ASP |
| 1 | D | 308 | HIS |
| 1 | I | 115 | ILE |
| 1 | I | 125 | HIS |
| 1 | I | 134 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | I | 135 | SER |
| 1 | I | 138 | LYS |
| 1 | I | 148 | LEU |
| 1 | I | 151 | LEU |
| 1 | I | 153 | CYS |
| 1 | I | 157 | LYS |
| 1 | I | 158 | THR |
| 1 | I | 161 | ILE |
| 1 | I | 165 | VAL |
| 1 | I | 173 | THR |
| 1 | I | 180 | VAL |
| 1 | I | 182 | LYS |
| 1 | I | 190 | VAL |
| 1 | I | 194 | CYS |
| 1 | I | 199 | LEU |
| 1 | I | 201 | ARG |
| 1 | I | 202 | ASP |
| 1 | I | 205 | GLU |
| 1 | I | 207 | GLN |
| 1 | I | 214 | LEU |
| 1 | I | 215 | ILE |
| 1 | I | 220 | ASN |
| 1 | I | 221 | ASN |
| 1 | I | 222 | LEU |
| 1 | I | 227 | ASP |
| 1 | I | 235 | SER |
| 1 | I | 245 | VAL |
| 1 | I | 249 | PHE |
| 1 | I | 250 | THR |
| 1 | I | 251 | THR |
| 1 | I | 256 | PHE |
| 1 | I | 258 | CYS |
| 1 | I | 266 | MET |
| 1 | I | 268 | ARG |
| 1 | I | 269 | ARG |
| 1 | I | 271 | ILE |
| 1 | I | 276 | THR |
| 1 | I | 277 | LEU |
| 1 | I | 283 | GLN |
| 1 | I | 285 | LEU |
| 1 | I | 297 | CYS |
| 1 | I | 300 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | I | 309 | TYR |
| 1 | I | 311 | GLU |
| 1 | J | 113 | GLU |
| 1 | J | 115 | ILE |
| 1 | J | 117 | SER |
| 1 | J | 127 | PHE |
| 1 | J | 130 | THR |
| 1 | J | 131 | PHE |
| 1 | J | 133 | GLN |
| 1 | J | 134 | SER |
| 1 | J | 135 | SER |
| 1 | J | 136 | THR |
| 1 | J | 138 | LYS |
| 1 | J | 141 | THR |
| 1 | J | 147 | LEU |
| 1 | J | 148 | LEU |
| 1 | J | 155 | ILE |
| 1 | J | 162 | GLN |
| 1 | J | 166 | SER |
| 1 | J | 167 | THR |
| 1 | J | 179 | PRO |
| 1 | J | 190 | VAL |
| 1 | J | 191 | VAL |
| 1 | J | 195 | PRO |
| 1 | J | 201 | ARG |
| 1 | J | 214 | LEU |
| 1 | J | 216 | ARG |
| 1 | J | 227 | ASP |
| 1 | J | 233 | ARG |
| 1 | J | 237 | VAL |
| 1 | J | 238 | VAL |
| 1 | J | 241 | GLU |
| 1 | J | 244 | GLN |
| 1 | J | 253 | LEU |
| 1 | J | 256 | PHE |
| 1 | J | 257 | MET |
| 1 | J | 258 | CYS |
| 1 | J | 259 | ASN |
| 1 | J | 261 | SER |
| 1 | J | 262 | CYS |
| 1 | J | 267 | ASN |
| 1 | J | 268 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | J | 276 | THR |
| 1 | J | 277 | LEU |
| 1 | J | 293 | ARG |
| 1 | J | 297 | CYS |
| 1 | J | 300 | ARG |
| 1 | J | 301 | ASP |
| 1 | J | 311 | GLU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 112 | HIS |
| 1 | A | 196 | ASN |
| 1 | A | 255 | ASN |
| 1 | A | 259 | ASN |
| 1 | A | 308 | HIS |
| 1 | B | 118 | ASN |
| 1 | B | 162 | GLN |
| 1 | B | 196 | ASN |
| 1 | B | 204 | ASN |
| 1 | B | 244 | GLN |
| 1 | B | 267 | ASN |
| 1 | B | 283 | GLN |
| 1 | C | 111 | HIS |
| 1 | C | 112 | HIS |
| 1 | C | 126 | HIS |
| 1 | C | 154 | GLN |
| 1 | C | 186 | HIS |
| 1 | C | 213 | HIS |
| 1 | C | 259 | ASN |
| 1 | C | 308 | HIS |
| 1 | D | 125 | HIS |
| 1 | D | 207 | GLN |
| 1 | D | 224 | GLN |
| 1 | D | 267 | ASN |
| 1 | D | 283 | GLN |
| 1 | I | 204 | ASN |
| 1 | I | 220 | ASN |
| 1 | I | 255 | ASN |
| 1 | J | 154 | GLN |
| 1 | J | 186 | HIS |
| 1 | J | 213 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | J | 255 | ASN |
| 1 | J | 259 | ASN |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 6 Fit of model and data (i)

## 6.1 Protein, DNA and RNA chains (i)

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 | 203/210 (96%) | -0.38 | 0 | 100 | 100 | 45, 74, 104, 125 | 3 (1%) |
| 1 | B | 200/210 (95%) | -0.33 | 0 | 100 | 100 | 67, 88, 112, 123 | 1 (0%) |
| 1 | C | 203/210 (96%) | -0.33 | 1 (0%) | 91 | 85 | 50, 77, 103, 123 | 2 (0%) |
| 1 | D | 199/210 (94%) | -0.20 | 3 (1%) | 73 | 64 | 60, 87, 118, 127 | 2 (1%) |
| 1 | I | 202/210 (96%) | -0.33 | 2 (0%) | 82 | 74 | 57, 84, 111, 125 | 2 (0%) |
| 1 | J | 202/210 (96%) | -0.35 | 0 | 100 | 100 | 54, 78, 108, 132 | 2 (0%) |
| 2 | E | 14/14 (100%) | 0.41 | 2 (14%) | 2 | 3 | 76, 98, 132, 142 | 0 |
| 2 | F | 14/14 (100%) | -0.25 | 0 | 100 | 100 | 76, 104, 126, 137 | 0 |
| 2 | G | 14/14 (100%) | -0.31 | 0 | 100 | 100 | 74, 102, 142, 159 | 0 |
| 2 | H | 14/14 (100%) | -0.15 | 0 | 100 | 100 | 76, 100, 140, 151 | 0 |
| 2 | K | 13/14 (92%) | 0.20 | 0 | 100 | 100 | 81, 103, 122, 137 | 0 |
| 2 | L | 13/14 (92%) | 0.20 | 1 (7%) | 13 | 11 | 90, 109, 135, 148 | 0 |
| All | All | 1291/1344 (96%) | -0.30 | 9 (0%) | 87 | 82 | 45, 83, 117, 159 | 12 (0%) |

All (9) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | I | 136 | THR | 4.6 |
| 1 | C | 281 | ASP | 3.2 |
| 1 | I | 137 | ALA | 2.9 |
| 1 | D | 283 | GLN | 2.9 |
| 2 | E | 410 | DG | 2.6 |
| 1 | D | 137 | ALA | 2.5 |
| 1 | D | 282 | GLY | 2.4 |
| 2 | L | 813 | DT | 2.1 |
| 2 | E | 415 | DT | 2.1 |

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

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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 3 | ZN | D | 401 | 1/1 | 0.97 | 0.05 | 84,84,84,84 | 0 |
| 3 | ZN | B | 401 | 1/1 | 0.98 | 0.14 | 89,89,89,89 | 0 |
| 3 | ZN | C | 401 | 1/1 | 0.98 | 0.09 | 58,58,58,58 | 0 |
| 3 | ZN | A | 401 | 1/1 | 0.98 | 0.08 | 73,73,73,73 | 0 |
| 3 | ZN | I | 401 | 1/1 | 0.98 | 0.07 | 76,76,76,76 | 0 |
| 3 | ZN | J | 401 | 1/1 | 1.00 | 0.15 | 56,56,56,56 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.