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

Jan 31, 2016 – 09:08 PM GMT

| | | |
|---|---|---|
| PDB ID | : | 1NKV |
| Title | : | X-RAY STRUCTURE OF YJHP FROM E.COLI NORTHEAST STRUCTURAL GENOMICS RESEARCH CONSORTIUM (NESG) TARGET ER13 |
| Authors | : | Kuzin, A.; Manor, P.; Benach, J.; Smith, P.; Rost, B.; Xiao, R.; Montelione, G.; Hunt, J.; Northeast Structural Genomics Consortium (NESG) |
| Deposited on | : | 2003-01-03 |
| Resolution | : | 2.90 Å(reported) |

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

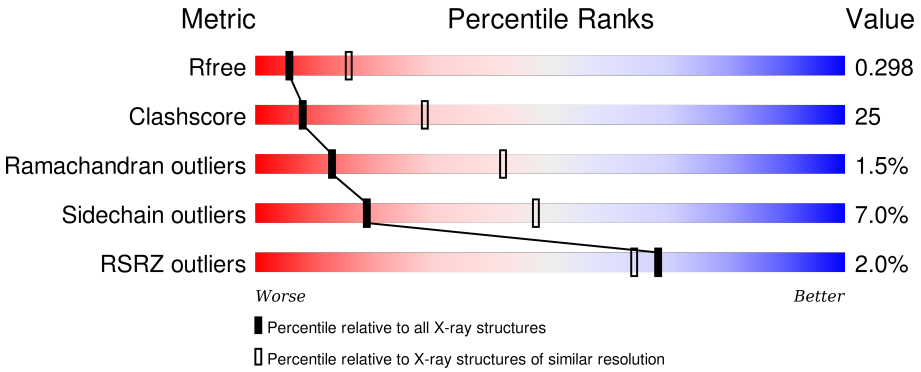
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7 (RC4), CSD as536be (2015) |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | rb-20026688 |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | trunk26865 |

# 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 2.90 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)) |
|---|---|---|
| $R_{free}$ | 91344 | 1451 (2.90-2.90) |
| Clashscore | 102246 | 1668 (2.90-2.90) |
| Ramachandran outliers | 100387 | 1630 (2.90-2.90) |
| Sidechain outliers | 100360 | 1632 (2.90-2.90) |
| RSRZ outliers | 91569 | 1456 (2.90-2.90) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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 | 256 | 55% 37% |
| 1 | B | 256 | 4% 45% 41% 5% 10% |
| 1 | C | 256 | 2% 57% 36% |

## 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5760 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 HYPOTHETICAL PROTEIN yjhP.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 245 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 1899 | 1201 | 330 | 357 | 5 | 6 | | | |
| 1 | B | 231 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 1805 | 1145 | 312 | 337 | 5 | 6 | | | |
| 1 | C | 249 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 1945 | 1228 | 340 | 365 | 5 | 7 | | | |

There are 45 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 1 | MSE | MET | MODIFIED RESIDUE | UNP P39367 |
| A | 34 | MSE | MET | MODIFIED RESIDUE | UNP P39367 |
| A | 50 | MSE | MET | MODIFIED RESIDUE | UNP P39367 |
| A | 67 | MSE | MET | MODIFIED RESIDUE | UNP P39367 |
| A | 136 | MSE | MET | MODIFIED RESIDUE | UNP P39367 |
| A | 184 | MSE | MET | MODIFIED RESIDUE | UNP P39367 |
| A | 203 | MSE | MET | MODIFIED RESIDUE | UNP P39367 |
| A | 249 | LEU | - | EXPRESSION TAG | UNP P39367 |
| A | 250 | GLU | - | EXPRESSION TAG | UNP P39367 |
| A | 251 | HIS | - | EXPRESSION TAG | UNP P39367 |
| A | 252 | HIS | - | EXPRESSION TAG | UNP P39367 |
| A | 253 | HIS | - | EXPRESSION TAG | UNP P39367 |
| A | 254 | HIS | - | EXPRESSION TAG | UNP P39367 |
| A | 255 | HIS | - | EXPRESSION TAG | UNP P39367 |
| A | 256 | HIS | - | EXPRESSION TAG | UNP P39367 |
| B | 1 | MSE | MET | MODIFIED RESIDUE | UNP P39367 |
| B | 34 | MSE | MET | MODIFIED RESIDUE | UNP P39367 |
| B | 50 | MSE | MET | MODIFIED RESIDUE | UNP P39367 |
| B | 67 | MSE | MET | MODIFIED RESIDUE | UNP P39367 |
| B | 136 | MSE | MET | MODIFIED RESIDUE | UNP P39367 |
| B | 184 | MSE | MET | MODIFIED RESIDUE | UNP P39367 |
| B | 203 | MSE | MET | MODIFIED RESIDUE | UNP P39367 |
| B | 249 | LEU | - | EXPRESSION TAG | UNP P39367 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | 250 | GLU | - | EXPRESSION TAG | UNP P39367 |
| B | 251 | HIS | - | EXPRESSION TAG | UNP P39367 |
| B | 252 | HIS | - | EXPRESSION TAG | UNP P39367 |
| B | 253 | HIS | - | EXPRESSION TAG | UNP P39367 |
| B | 254 | HIS | - | EXPRESSION TAG | UNP P39367 |
| B | 255 | HIS | - | EXPRESSION TAG | UNP P39367 |
| B | 256 | HIS | - | EXPRESSION TAG | UNP P39367 |
| C | 1 | MSE | MET | MODIFIED RESIDUE | UNP P39367 |
| C | 34 | MSE | MET | MODIFIED RESIDUE | UNP P39367 |
| C | 50 | MSE | MET | MODIFIED RESIDUE | UNP P39367 |
| C | 67 | MSE | MET | MODIFIED RESIDUE | UNP P39367 |
| C | 136 | MSE | MET | MODIFIED RESIDUE | UNP P39367 |
| C | 184 | MSE | MET | MODIFIED RESIDUE | UNP P39367 |
| C | 203 | MSE | MET | MODIFIED RESIDUE | UNP P39367 |
| C | 249 | LEU | - | EXPRESSION TAG | UNP P39367 |
| C | 250 | GLU | - | EXPRESSION TAG | UNP P39367 |
| C | 251 | HIS | - | EXPRESSION TAG | UNP P39367 |
| C | 252 | HIS | - | EXPRESSION TAG | UNP P39367 |
| C | 253 | HIS | - | EXPRESSION TAG | UNP P39367 |
| C | 254 | HIS | - | EXPRESSION TAG | UNP P39367 |
| C | 255 | HIS | - | EXPRESSION TAG | UNP P39367 |
| C | 256 | HIS | - | EXPRESSION TAG | UNP P39367 |

- Molecule 2 is water.

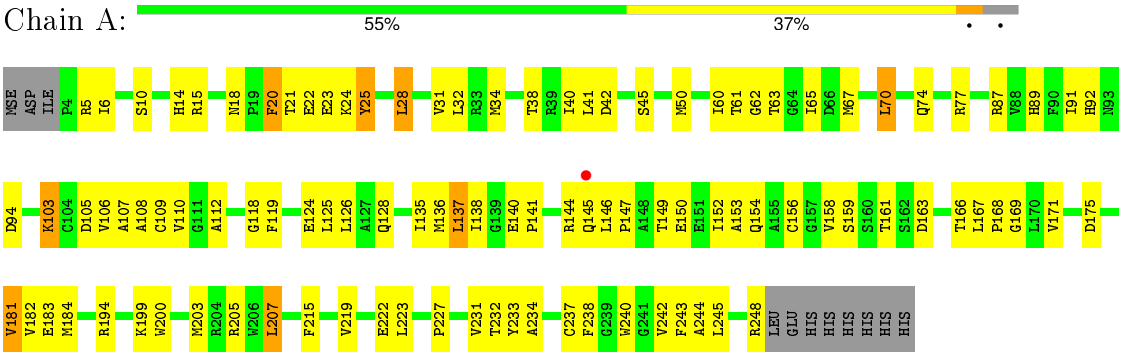
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 2 | A | 44 | Total O<br>44 44 | 0 | 0 |
| 2 | B | 26 | Total O<br>26 26 | 0 | 0 |
| 2 | C | 41 | Total O<br>41 41 | 0 | 0 |

# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

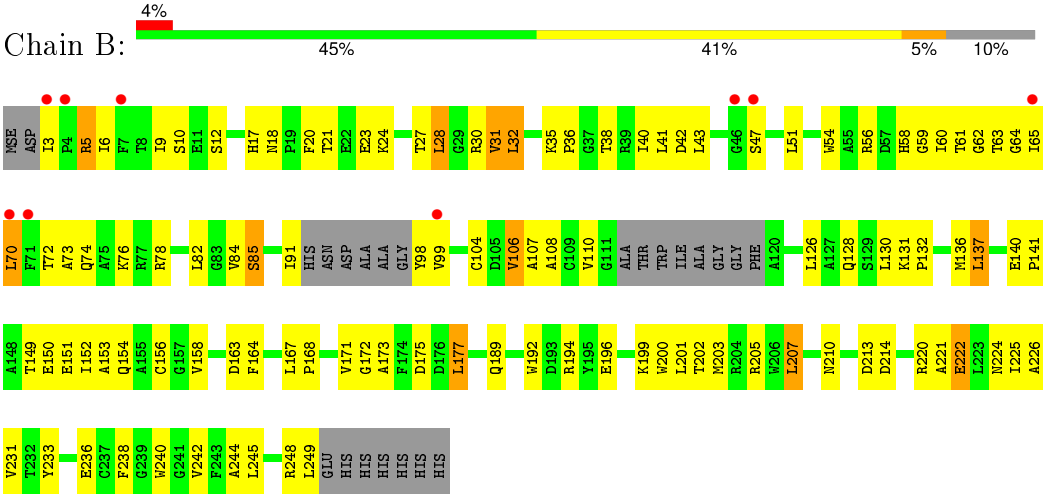
- Molecule 1: HYPOTHETICAL PROTEIN yjhP

Chain A:



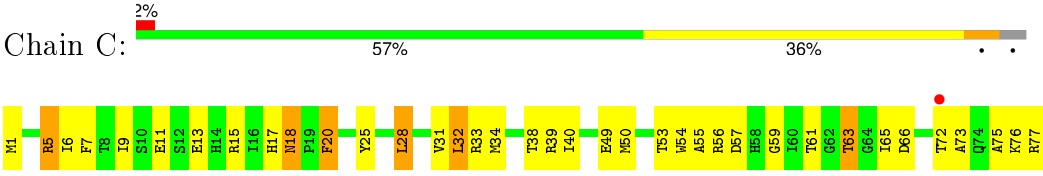

- Molecule 1: HYPOTHETICAL PROTEIN yjhP

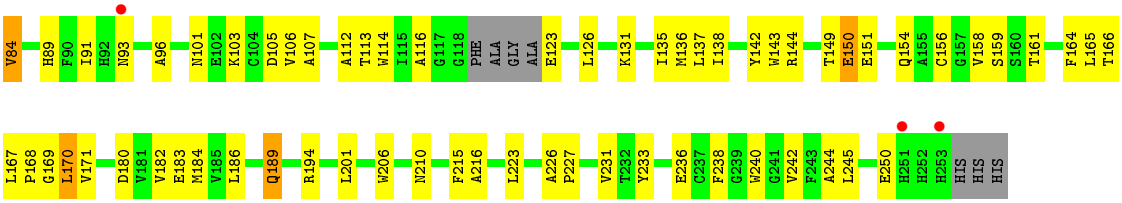
Chain B:




- Molecule 1: HYPOTHETICAL PROTEIN yjhP

Chain C:




V84 H89 F90 I91 H92 N93 A96 N101 E102 K103 C104 D105 V106 A107 A112 T113 W114 I115 A116 G117 G118 PHE ALA GLY ALA E123 L126 K131 I135 M136 L137 I138 Y142 W143 R144 T149 E150 E151 Q154 A155 C156 G157 V158 S159 S160 T161 F164 L165 T166
L167 P168 G169 L170 V171 D180 V181 V182 E183 M184 V185 L186 Q189 R194 L201 W206 N210 F215 A216 L223 A226 P227 V231 T232 Y233 E236 C237 F238 G239 W240 G241 V242 F243 A244 L245 E250 H251 H252 H253 HIS HIS HIS

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 1 21 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 59.97Å 54.42Å 118.33Å<br>90.00° 99.83° 90.00° | Depositor |
| Resolution (Å) | 19.99 – 2.90<br>20.04 – 2.80 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 93.9 (19.99-2.90)<br>97.5 (20.04-2.80) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 4.87 (at 2.79Å) | Xtriage |
| Refinement program | CNS 1.1 | Depositor |
| R, $R_{free}$ | 0.220 , 0.290<br>0.235 , 0.298 | Depositor<br>DCC |
| $R_{free}$ test set | 851 reflections (5.10%) | DCC |
| Wilson B-factor (Å$^2$) | 43.4 | Xtriage |
| Anisotropy | 0.558 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.26 , 32.1 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning[2] | $< \|L\| > = 0.49$, $< L^2 > = 0.33$ | Xtriage |
| Outliers | 1 of 35296 reflections (0.003%) | Xtriage |
| $F_o$,$F_c$ correlation | 0.90 | EDS |
| Total number of atoms | 5760 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 40.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

# 5 Model quality

## 5.1 Standard geometry

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|>5$ | RMSZ | #$\|Z\|>5$ |
| 1 | A | 0.44 | 0/1937 | 0.61 | 0/2616 |
| 1 | B | 0.42 | 0/1836 | 0.61 | 0/2474 |
| 1 | C | 0.45 | 1/1984 (0.1%) | 0.61 | 0/2679 |
| All | All | 0.44 | 1/5757 (0.0%) | 0.61 | 0/7769 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | C | 250 | GLU | C-N | 5.66 | 1.47 | 1.34 |

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 1899 | 0 | 1839 | 89 | 0 |
| 1 | B | 1805 | 0 | 1764 | 106 | 0 |
| 1 | C | 1945 | 0 | 1880 | 92 | 0 |
| 2 | A | 44 | 0 | 0 | 2 | 0 |
| 2 | B | 26 | 0 | 0 | 4 | 0 |
| 2 | C | 41 | 0 | 0 | 2 | 0 |
| All | All | 5760 | 0 | 5483 | 275 | 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 25.

All (275) 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:172:GLY:HA3 | 2:B:281:HOH:O | 1.63 | 0.97 |
| 1:A:107:ALA:HB1 | 1:A:126:LEU:HD12 | 1.47 | 0.96 |
| 1:A:103:LYS:HE3 | 1:A:103:LYS:H | 1.31 | 0.96 |
| 1:B:248:ARG:O | 1:B:249:LEU:HB2 | 1.72 | 0.90 |
| 1:B:67:MSE:HB3 | 1:B:70:LEU:HD22 | 1.56 | 0.88 |
| 1:B:17:HIS:HE1 | 1:B:74:GLN:HE22 | 1.20 | 0.87 |
| 1:A:34:MSE:HE1 | 1:A:106:VAL:HG11 | 1.60 | 0.83 |
| 1:B:84:VAL:HG23 | 1:B:85:SER:H | 1.43 | 0.83 |
| 1:C:18:ASN:ND2 | 1:C:20:PHE:HB2 | 1.94 | 0.82 |
| 1:C:166:THR:HG23 | 1:C:169:GLY:H | 1.46 | 0.79 |
| 1:B:107:ALA:HB1 | 1:B:126:LEU:HD12 | 1.64 | 0.78 |
| 1:C:156:CYS:HB3 | 1:C:238:PHE:CZ | 2.21 | 0.76 |
| 1:C:18:ASN:HD21 | 1:C:20:PHE:HB2 | 1.47 | 0.76 |
| 1:B:41:LEU:HB2 | 1:B:104:CYS:SG | 2.27 | 0.75 |
| 1:B:40:ILE:HG12 | 1:B:106:VAL:HG13 | 1.68 | 0.75 |
| 1:C:78:ARG:HE | 1:C:82:LEU:CD2 | 1.98 | 0.74 |
| 1:A:166:THR:HG23 | 1:A:169:GLY:H | 1.51 | 0.74 |
| 1:A:50:MSE:HE1 | 1:A:110:VAL:HG21 | 1.70 | 0.74 |
| 1:A:40:ILE:HG12 | 1:A:106:VAL:CG1 | 2.18 | 0.73 |
| 1:B:72:THR:O | 1:B:76:LYS:HG3 | 1.91 | 0.70 |
| 1:A:156:CYS:SG | 1:A:233:TYR:HB3 | 2.30 | 0.70 |
| 1:B:61:THR:HG22 | 1:B:62:GLY:H | 1.56 | 0.70 |
| 1:B:226:ALA:HB3 | 1:B:227:PRO:HD3 | 1.73 | 0.70 |
| 1:A:150:GLU:O | 1:A:154:GLN:HG3 | 1.92 | 0.70 |
| 1:A:146:LEU:HD12 | 1:A:147:PRO:HD2 | 1.75 | 0.69 |
| 1:C:18:ASN:HD22 | 1:C:20:PHE:H | 1.40 | 0.69 |
| 1:B:56:ARG:HD3 | 1:B:82:LEU:HD12 | 1.75 | 0.68 |
| 1:B:72:THR:HG22 | 1:B:76:LYS:HE3 | 1.74 | 0.68 |
| 1:C:183:GLU:HB3 | 1:C:244:ALA:HB3 | 1.73 | 0.68 |
| 1:B:73:ALA:HA | 1:B:76:LYS:HD2 | 1.76 | 0.68 |
| 1:B:126:LEU:H | 1:B:126:LEU:HD22 | 1.59 | 0.67 |
| 1:A:18:ASN:ND2 | 1:A:20:PHE:HB2 | 2.09 | 0.67 |
| 1:B:23:GLU:HB2 | 2:B:268:HOH:O | 1.95 | 0.66 |
| 1:C:136:MSE:HE3 | 1:C:138:ILE:HG21 | 1.76 | 0.66 |
| 1:B:136:MSE:HE2 | 1:B:245:LEU:HD12 | 1.78 | 0.66 |
| 1:C:78:ARG:HE | 1:C:82:LEU:HD21 | 1.61 | 0.65 |
| 1:C:113:THR:HG23 | 1:C:116:ALA:H | 1.61 | 0.65 |
| 1:A:136:MSE:HE3 | 1:A:138:ILE:HD11 | 1.79 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:25:TYR:HE1 | 1:A:50:MSE:HE3 | 1.60 | 0.64 |
| 1:B:35:LYS:HB2 | 1:B:36:PRO:HD2 | 1.79 | 0.64 |
| 1:B:194:ARG:NE | 1:B:194:ARG:HA | 2.13 | 0.64 |
| 1:C:5:ARG:HG3 | 1:C:9:ILE:HD13 | 1.80 | 0.64 |
| 1:A:74:GLN:HA | 1:A:77:ARG:NH2 | 2.13 | 0.63 |
| 1:B:32:LEU:HD21 | 1:B:137:LEU:HD11 | 1.80 | 0.63 |
| 1:B:196:GLU:HG3 | 1:B:230:TYR:CD1 | 2.34 | 0.62 |
| 1:C:123:GLU:HG3 | 1:C:126:LEU:HD12 | 1.80 | 0.62 |
| 1:C:11:GLU:OE2 | 1:C:17:HIS:CD2 | 2.53 | 0.61 |
| 1:B:18:ASN:ND2 | 1:B:20:PHE:HB2 | 2.16 | 0.60 |
| 1:A:89:HIS:NE2 | 1:A:91:ILE:HG22 | 2.17 | 0.59 |
| 1:B:27:THR:O | 1:B:31:VAL:HB | 2.02 | 0.59 |
| 1:C:40:ILE:HG12 | 1:C:106:VAL:HB | 1.84 | 0.59 |
| 1:B:42:ASP:HB2 | 1:B:51:LEU:HD11 | 1.82 | 0.59 |
| 1:C:5:ARG:HG2 | 1:C:215:PHE:CE2 | 2.38 | 0.59 |
| 1:A:63:THR:HA | 1:A:89:HIS:O | 2.03 | 0.59 |
| 1:A:194:ARG:HA | 1:A:194:ARG:NE | 2.18 | 0.59 |
| 1:C:6:ILE:HG13 | 1:C:7:PHE:H | 1.68 | 0.58 |
| 1:A:171:VAL:HG21 | 1:C:231:VAL:HG21 | 1.85 | 0.58 |
| 1:B:201:LEU:O | 1:B:205:ARG:HG2 | 2.04 | 0.58 |
| 1:A:34:MSE:CE | 1:A:106:VAL:HG11 | 2.33 | 0.58 |
| 1:B:248:ARG:O | 1:B:249:LEU:CB | 2.45 | 0.58 |
| 1:A:25:TYR:CE1 | 1:A:50:MSE:HE3 | 2.38 | 0.58 |
| 1:A:67:MSE:O | 1:A:92:HIS:NE2 | 2.38 | 0.57 |
| 1:B:40:ILE:HG22 | 1:B:41:LEU:N | 2.20 | 0.57 |
| 1:A:136:MSE:HE3 | 1:A:138:ILE:CD1 | 2.35 | 0.57 |
| 1:B:6:ILE:HG21 | 1:B:222:GLU:HG3 | 1.88 | 0.56 |
| 1:B:40:ILE:HG23 | 1:B:106:VAL:O | 2.05 | 0.56 |
| 1:A:28:LEU:HD11 | 1:A:242:VAL:HG11 | 1.88 | 0.56 |
| 1:A:184:MSE:HE2 | 1:A:243:PHE:CE2 | 2.41 | 0.56 |
| 1:B:40:ILE:HG12 | 1:B:106:VAL:CG1 | 2.36 | 0.55 |
| 1:B:154:GLN:HA | 1:B:158:VAL:O | 2.06 | 0.55 |
| 1:B:64:GLY:O | 1:B:65:ILE:HD13 | 2.05 | 0.55 |
| 1:C:144:ARG:HH12 | 1:C:236:GLU:HG3 | 1.71 | 0.55 |
| 1:B:84:VAL:HG23 | 1:B:85:SER:N | 2.18 | 0.55 |
| 1:A:50:MSE:CE | 1:A:110:VAL:HG21 | 2.36 | 0.55 |
| 1:C:56:ARG:HG2 | 1:C:56:ARG:HH11 | 1.72 | 0.55 |
| 1:A:40:ILE:HG12 | 1:A:106:VAL:HG13 | 1.87 | 0.54 |
| 1:C:156:CYS:HB3 | 1:C:238:PHE:CE1 | 2.42 | 0.54 |
| 1:C:31:VAL:O | 1:C:33:ARG:HD3 | 2.07 | 0.54 |
| 1:A:199:LYS:O | 1:A:203:MSE:HG3 | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:150:GLU:OE2 | 1:C:161:THR:HG22 | 2.08 | 0.54 |
| 1:B:156:CYS:HB3 | 1:B:238:PHE:CE1 | 2.43 | 0.54 |
| 1:B:78:ARG:O | 1:B:82:LEU:HD23 | 2.07 | 0.54 |
| 1:C:77:ARG:O | 1:C:77:ARG:HD3 | 2.08 | 0.54 |
| 1:B:131:LYS:HB2 | 1:B:132:PRO:HD2 | 1.89 | 0.54 |
| 1:A:231:VAL:HG21 | 1:B:171:VAL:HG21 | 1.89 | 0.53 |
| 1:B:40:ILE:HD11 | 1:B:60:ILE:CD1 | 2.39 | 0.53 |
| 1:C:206:TRP:HZ3 | 1:C:216:ALA:HA | 1.72 | 0.53 |
| 1:C:32:LEU:HB3 | 1:C:34:MSE:HG3 | 1.91 | 0.53 |
| 1:C:25:TYR:CE1 | 1:C:50:MSE:HE2 | 2.43 | 0.53 |
| 1:B:28:LEU:HD22 | 1:B:32:LEU:HD22 | 1.88 | 0.53 |
| 1:C:55:ALA:O | 1:C:59:GLY:HA2 | 2.09 | 0.53 |
| 1:A:109:CYS:HB2 | 1:A:126:LEU:HD21 | 1.90 | 0.53 |
| 1:A:40:ILE:HG22 | 1:A:41:LEU:N | 2.24 | 0.53 |
| 1:A:65:ILE:N | 1:A:65:ILE:HD12 | 2.23 | 0.53 |
| 1:C:5:ARG:HG3 | 1:C:9:ILE:CD1 | 2.39 | 0.52 |
| 1:A:21:THR:H | 1:A:24:LYS:HB2 | 1.74 | 0.52 |
| 1:B:151:GLU:HG3 | 1:B:152:ILE:N | 2.25 | 0.52 |
| 1:A:67:MSE:SE | 1:A:94:ASP:HA | 2.59 | 0.52 |
| 1:B:12:SER:HB3 | 1:B:202:THR:HG21 | 1.91 | 0.52 |
| 1:C:15:ARG:HG2 | 1:C:15:ARG:HH11 | 1.75 | 0.52 |
| 1:C:143:TRP:NE1 | 1:C:164:PHE:HB2 | 2.24 | 0.52 |
| 1:C:49:GLU:OE1 | 1:C:78:ARG:NH1 | 2.42 | 0.52 |
| 1:C:73:ALA:HA | 1:C:76:LYS:HB2 | 1.92 | 0.52 |
| 1:C:39:ARG:HH11 | 1:C:39:ARG:HG2 | 1.75 | 0.51 |
| 1:C:91:ILE:O | 1:C:91:ILE:HG13 | 2.10 | 0.51 |
| 1:C:38:THR:HG23 | 1:C:105:ASP:HB2 | 1.91 | 0.51 |
| 1:C:166:THR:HG23 | 1:C:169:GLY:N | 2.23 | 0.51 |
| 1:B:151:GLU:HG3 | 1:B:152:ILE:H | 1.76 | 0.51 |
| 1:C:63:THR:HA | 1:C:89:HIS:O | 2.10 | 0.51 |
| 1:B:244:ALA:O | 1:B:245:LEU:HD23 | 2.11 | 0.51 |
| 1:A:60:ILE:C | 1:A:60:ILE:HD12 | 2.31 | 0.51 |
| 1:C:165:LEU:HD23 | 1:C:170:LEU:HA | 1.93 | 0.51 |
| 1:C:138:ILE:HD11 | 1:C:245:LEU:HD11 | 1.93 | 0.51 |
| 1:C:78:ARG:HH21 | 1:C:82:LEU:HD21 | 1.75 | 0.51 |
| 1:C:78:ARG:HE | 1:C:82:LEU:HD23 | 1.73 | 0.51 |
| 1:B:54:TRP:O | 1:B:58:HIS:HB2 | 2.10 | 0.51 |
| 1:A:183:GLU:HB3 | 1:A:244:ALA:HB3 | 1.93 | 0.50 |
| 1:B:28:LEU:O | 1:B:31:VAL:HG12 | 2.11 | 0.50 |
| 1:C:75:ALA:O | 1:C:78:ARG:HB3 | 2.12 | 0.50 |
| 1:B:110:VAL:HG13 | 1:B:240:TRP:HH2 | 1.75 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:10:SER:O | 1:B:199:LYS:HG2 | 2.12 | 0.50 |
| 1:B:40:ILE:HG22 | 1:B:41:LEU:H | 1.75 | 0.50 |
| 1:A:183:GLU:HB3 | 1:A:244:ALA:CB | 2.42 | 0.49 |
| 1:A:14:HIS:HA | 2:A:298:HOH:O | 2.12 | 0.49 |
| 1:A:184:MSE:HE2 | 1:A:243:PHE:HE2 | 1.75 | 0.49 |
| 1:A:158:VAL:HG22 | 1:A:159:SER:H | 1.78 | 0.49 |
| 1:A:89:HIS:CE1 | 1:A:91:ILE:HG22 | 2.48 | 0.49 |
| 1:A:106:VAL:HA | 1:A:135:ILE:O | 2.13 | 0.49 |
| 1:C:18:ASN:HD22 | 1:C:20:PHE:N | 2.09 | 0.49 |
| 1:B:43:LEU:HD11 | 1:B:98:TYR:HD2 | 1.78 | 0.49 |
| 1:A:60:ILE:O | 1:A:87:ARG:HD2 | 2.13 | 0.49 |
| 1:C:184:MSE:HE3 | 1:C:186:LEU:HD11 | 1.95 | 0.49 |
| 1:B:156:CYS:SG | 1:B:233:TYR:HB3 | 2.52 | 0.49 |
| 1:A:124:GLU:O | 1:A:128:GLN:HG3 | 2.13 | 0.49 |
| 1:C:39:ARG:HH12 | 1:C:61:THR:HG21 | 1.78 | 0.49 |
| 1:A:23:GLU:H | 1:A:23:GLU:CD | 2.16 | 0.49 |
| 1:B:99:VAL:HG13 | 1:B:128:GLN:O | 2.13 | 0.48 |
| 1:B:189:GLN:HE22 | 1:B:236:GLU:HG3 | 1.78 | 0.48 |
| 1:B:201:LEU:HB2 | 1:C:182:VAL:O | 2.13 | 0.48 |
| 1:A:70:LEU:O | 1:A:74:GLN:HG3 | 2.14 | 0.48 |
| 1:B:17:HIS:CE1 | 1:B:74:GLN:HE22 | 2.13 | 0.48 |
| 1:C:6:ILE:HG13 | 1:C:7:PHE:N | 2.28 | 0.48 |
| 1:A:141:PRO:HB3 | 1:A:240:TRP:HD1 | 1.78 | 0.48 |
| 1:C:166:THR:OG1 | 1:C:168:PRO:HD2 | 2.14 | 0.48 |
| 1:C:114:TRP:HA | 2:C:258:HOH:O | 2.12 | 0.48 |
| 1:B:147:PRO:HG3 | 1:B:153:ALA:HB2 | 1.96 | 0.48 |
| 1:A:168:PRO:HA | 1:A:171:VAL:HG22 | 1.95 | 0.48 |
| 1:A:28:LEU:O | 1:A:31:VAL:HG12 | 2.14 | 0.48 |
| 1:B:173:ALA:O | 1:B:177:LEU:HD23 | 2.14 | 0.48 |
| 1:A:5:ARG:O | 1:A:5:ARG:HG2 | 2.14 | 0.47 |
| 1:C:65:ILE:HG23 | 1:C:93:ASN:HB3 | 1.96 | 0.47 |
| 1:B:203:MSE:SE | 1:B:222:GLU:HB3 | 2.65 | 0.47 |
| 1:B:221:ALA:O | 1:B:225:ILE:HG12 | 2.14 | 0.47 |
| 1:B:41:LEU:HG | 1:B:43:LEU:CD2 | 2.44 | 0.47 |
| 1:A:200:TRP:CZ2 | 1:A:227:PRO:HA | 2.50 | 0.47 |
| 1:B:167:LEU:N | 1:B:168:PRO:HD2 | 2.30 | 0.47 |
| 1:C:189:GLN:HA | 1:C:189:GLN:HE21 | 1.80 | 0.47 |
| 1:A:144:ARG:N | 1:A:237:CYS:O | 2.48 | 0.47 |
| 1:C:13:GLU:HB2 | 2:C:262:HOH:O | 2.14 | 0.46 |
| 1:B:107:ALA:H | 1:B:130:LEU:HD13 | 1.79 | 0.46 |
| 1:C:53:THR:HG23 | 1:C:54:TRP:N | 2.30 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:114:TRP:HB2 | 1:C:240:TRP:CD1 | 2.50 | 0.46 |
| 1:A:147:PRO:HG2 | 1:A:161:THR:HG22 | 1.96 | 0.46 |
| 1:B:3:ILE:HG23 | 1:B:3:ILE:O | 2.15 | 0.46 |
| 1:B:143:TRP:NE1 | 1:B:164:PHE:HB2 | 2.30 | 0.46 |
| 1:A:10:SER:HB2 | 1:A:199:LYS:HB3 | 1.98 | 0.46 |
| 1:C:180:ASP:O | 1:C:182:VAL:HG13 | 2.15 | 0.46 |
| 1:B:150:GLU:O | 1:B:154:GLN:HG3 | 2.15 | 0.46 |
| 1:A:15:ARG:HH11 | 1:A:15:ARG:HG2 | 1.81 | 0.46 |
| 1:B:58:HIS:O | 1:B:59:GLY:C | 2.54 | 0.46 |
| 1:A:215:PHE:O | 1:A:219:VAL:HG23 | 2.16 | 0.46 |
| 1:C:66:ASP:HB3 | 1:C:72:THR:HG21 | 1.97 | 0.46 |
| 1:B:40:ILE:HD11 | 1:B:60:ILE:HD13 | 1.97 | 0.46 |
| 1:A:166:THR:OG1 | 1:A:168:PRO:HD2 | 2.16 | 0.46 |
| 1:A:182:VAL:HB | 1:C:201:LEU:HA | 1.97 | 0.46 |
| 1:A:42:ASP:HB3 | 1:A:45:SER:HB3 | 1.98 | 0.46 |
| 1:B:104:CYS:O | 1:B:130:LEU:HD12 | 2.16 | 0.45 |
| 1:A:153:ALA:O | 1:A:158:VAL:HG12 | 2.16 | 0.45 |
| 1:A:175:ASP:OD1 | 1:A:248:ARG:NH2 | 2.49 | 0.45 |
| 1:C:226:ALA:HB3 | 1:C:227:PRO:HD3 | 1.96 | 0.45 |
| 1:B:126:LEU:CD2 | 1:B:126:LEU:H | 2.28 | 0.45 |
| 1:C:84:VAL:HG22 | 1:C:84:VAL:O | 2.16 | 0.45 |
| 1:A:167:LEU:N | 1:A:168:PRO:HD2 | 2.31 | 0.45 |
| 1:B:175:ASP:C | 1:B:177:LEU:H | 2.20 | 0.45 |
| 1:B:126:LEU:HD22 | 1:B:126:LEU:N | 2.30 | 0.45 |
| 1:B:38:THR:HB | 1:B:60:ILE:CD1 | 2.46 | 0.45 |
| 1:C:103:LYS:HB2 | 1:C:131:LYS:HG2 | 1.98 | 0.45 |
| 1:A:22:GLU:HB2 | 1:A:23:GLU:OE2 | 2.16 | 0.45 |
| 1:B:5:ARG:O | 1:B:9:ILE:HG12 | 2.16 | 0.45 |
| 1:A:6:ILE:HG12 | 1:A:222:GLU:HG3 | 1.98 | 0.45 |
| 1:A:140:GLU:OE1 | 1:A:141:PRO:HD2 | 2.17 | 0.45 |
| 1:B:140:GLU:CD | 1:B:141:PRO:HD2 | 2.36 | 0.45 |
| 1:B:149:THR:OG1 | 1:B:152:ILE:HG12 | 2.16 | 0.45 |
| 1:A:15:ARG:NE | 2:A:293:HOH:O | 2.50 | 0.45 |
| 1:B:43:LEU:HD23 | 1:B:126:LEU:CD1 | 2.47 | 0.45 |
| 1:B:220:ARG:O | 1:B:224:ASN:OD1 | 2.35 | 0.45 |
| 1:C:32:LEU:HD21 | 1:C:137:LEU:HD21 | 2.00 | 0.44 |
| 1:C:143:TRP:CE2 | 1:C:164:PHE:HB2 | 2.52 | 0.44 |
| 1:B:110:VAL:HG13 | 1:B:240:TRP:CH2 | 2.53 | 0.44 |
| 1:C:107:ALA:HB1 | 1:C:126:LEU:HD22 | 1.98 | 0.44 |
| 1:A:158:VAL:HG22 | 1:A:159:SER:N | 2.32 | 0.44 |
| 1:C:15:ARG:NH1 | 1:C:15:ARG:HG2 | 2.33 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:18:ASN:HD22 | 1:A:20:PHE:HB2 | 1.79 | 0.44 |
| 1:C:123:GLU:CB | 1:C:126:LEU:HD12 | 2.48 | 0.44 |
| 1:C:123:GLU:CG | 1:C:126:LEU:HD12 | 2.47 | 0.44 |
| 1:B:194:ARG:NE | 1:B:194:ARG:CA | 2.80 | 0.44 |
| 1:A:108:ALA:HB2 | 1:A:137:LEU:HB2 | 2.00 | 0.44 |
| 1:B:17:HIS:HE1 | 1:B:74:GLN:NE2 | 2.02 | 0.44 |
| 1:C:194:ARG:HA | 1:C:194:ARG:NE | 2.33 | 0.44 |
| 1:B:231:VAL:HG21 | 1:C:171:VAL:HG21 | 2.00 | 0.44 |
| 1:C:106:VAL:HG13 | 1:C:137:LEU:HD13 | 1.99 | 0.43 |
| 1:A:156:CYS:HB3 | 1:A:238:PHE:CE2 | 2.52 | 0.43 |
| 1:B:231:VAL:HG23 | 1:C:168:PRO:HA | 2.00 | 0.43 |
| 1:A:136:MSE:HE2 | 1:A:245:LEU:HD12 | 2.00 | 0.43 |
| 1:C:144:ARG:NH1 | 1:C:236:GLU:HG3 | 2.33 | 0.43 |
| 1:C:38:THR:CG2 | 1:C:105:ASP:HB2 | 2.49 | 0.43 |
| 1:B:140:GLU:OE1 | 1:B:141:PRO:HD2 | 2.18 | 0.43 |
| 1:A:181:VAL:HG22 | 1:A:181:VAL:O | 2.17 | 0.43 |
| 1:C:142:TYR:OH | 1:C:186:LEU:HD22 | 2.17 | 0.43 |
| 1:A:89:HIS:NE2 | 1:A:91:ILE:CG2 | 2.81 | 0.43 |
| 1:B:201:LEU:HA | 1:C:182:VAL:HB | 2.00 | 0.43 |
| 1:B:192:TRP:CZ2 | 1:B:238:PHE:HB3 | 2.54 | 0.43 |
| 1:A:15:ARG:NH1 | 1:A:15:ARG:HG2 | 2.34 | 0.43 |
| 1:A:38:THR:HG23 | 1:A:105:ASP:CB | 2.48 | 0.43 |
| 1:B:43:LEU:H | 1:B:43:LEU:HD22 | 1.83 | 0.43 |
| 1:A:149:THR:OG1 | 1:A:152:ILE:HG13 | 2.18 | 0.43 |
| 1:A:103:LYS:CE | 1:A:103:LYS:H | 2.16 | 0.42 |
| 1:A:40:ILE:HG23 | 1:A:106:VAL:HG13 | 2.01 | 0.42 |
| 1:C:136:MSE:HE2 | 1:C:138:ILE:HD13 | 2.00 | 0.42 |
| 1:A:231:VAL:HG21 | 1:B:171:VAL:CG2 | 2.49 | 0.42 |
| 1:A:38:THR:HG23 | 1:A:105:ASP:HB2 | 2.01 | 0.42 |
| 1:B:47:SER:HA | 1:B:74:GLN:HE21 | 1.84 | 0.42 |
| 1:A:136:MSE:CE | 1:A:245:LEU:HD12 | 2.49 | 0.42 |
| 1:A:61:THR:HG22 | 1:A:62:GLY:N | 2.33 | 0.42 |
| 1:A:32:LEU:HD23 | 1:A:34:MSE:SE | 2.69 | 0.42 |
| 1:C:5:ARG:O | 1:C:9:ILE:HD13 | 2.20 | 0.42 |
| 1:A:232:THR:HA | 1:B:168:PRO:HB3 | 2.02 | 0.42 |
| 1:A:207:LEU:HA | 1:A:207:LEU:HD12 | 1.89 | 0.42 |
| 1:B:41:LEU:HG | 1:B:43:LEU:HD22 | 2.01 | 0.42 |
| 1:B:51:LEU:HD13 | 2:B:277:HOH:O | 2.20 | 0.42 |
| 1:C:50:MSE:O | 1:C:53:THR:HG22 | 2.19 | 0.42 |
| 1:B:207:LEU:HD21 | 1:B:220:ARG:HA | 2.01 | 0.42 |
| 1:B:28:LEU:CD1 | 1:B:242:VAL:HG11 | 2.50 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:135:ILE:HG22 | 1:C:137:LEU:HD12 | 2.01 | 0.42 |
| 1:A:231:VAL:HG21 | 1:B:171:VAL:HG11 | 2.00 | 0.42 |
| 1:C:39:ARG:NH1 | 1:C:39:ARG:HG2 | 2.34 | 0.42 |
| 1:C:65:ILE:HG22 | 1:C:93:ASN:O | 2.20 | 0.42 |
| 1:B:21:THR:H | 1:B:24:LYS:HB2 | 1.85 | 0.42 |
| 1:A:31:VAL:HG22 | 1:A:183:GLU:OE2 | 2.20 | 0.42 |
| 1:C:154:GLN:HA | 1:C:158:VAL:O | 2.20 | 0.42 |
| 1:B:38:THR:HB | 1:B:60:ILE:HG13 | 2.01 | 0.41 |
| 1:B:220:ARG:NE | 1:B:224:ASN:OD1 | 2.48 | 0.41 |
| 1:A:125:LEU:O | 1:A:128:GLN:HB2 | 2.20 | 0.41 |
| 1:C:226:ALA:HB3 | 1:C:227:PRO:CD | 2.50 | 0.41 |
| 1:A:183:GLU:OE1 | 1:A:184:MSE:N | 2.43 | 0.41 |
| 1:B:229:ARG:NH1 | 2:B:280:HOH:O | 2.53 | 0.41 |
| 1:B:200:TRP:CZ2 | 1:B:227:PRO:HA | 2.56 | 0.41 |
| 1:B:28:LEU:HD13 | 1:B:54:TRP:CZ2 | 2.55 | 0.41 |
| 1:A:231:VAL:CG2 | 1:B:171:VAL:HG21 | 2.51 | 0.41 |
| 1:C:28:LEU:HD11 | 1:C:242:VAL:HG11 | 2.02 | 0.41 |
| 1:C:56:ARG:HG2 | 1:C:56:ARG:NH1 | 2.34 | 0.41 |
| 1:C:56:ARG:NH1 | 1:C:57:ASP:OD1 | 2.53 | 0.41 |
| 1:B:108:ALA:HA | 1:B:137:LEU:O | 2.20 | 0.41 |
| 1:C:39:ARG:NH1 | 1:C:61:THR:HG21 | 2.36 | 0.41 |
| 1:C:123:GLU:HB2 | 1:C:126:LEU:HB2 | 2.03 | 0.41 |
| 1:B:147:PRO:CG | 1:B:153:ALA:HB2 | 2.51 | 0.41 |
| 1:B:213:ASP:CG | 1:B:214:ASP:N | 2.74 | 0.41 |
| 1:B:30:ARG:HG3 | 1:B:31:VAL:N | 2.36 | 0.41 |
| 1:C:138:ILE:HD11 | 1:C:245:LEU:CD1 | 2.51 | 0.40 |
| 1:C:25:TYR:HE1 | 1:C:50:MSE:HE2 | 1.85 | 0.40 |
| 1:B:231:VAL:CG2 | 1:C:168:PRO:HA | 2.51 | 0.40 |
| 1:C:167:LEU:N | 1:C:168:PRO:HD2 | 2.36 | 0.40 |
| 1:B:32:LEU:HA | 1:B:32:LEU:HD12 | 1.90 | 0.40 |
| 1:A:23:GLU:N | 1:A:23:GLU:CD | 2.74 | 0.40 |
| 1:C:149:THR:HG23 | 1:C:151:GLU:HB2 | 2.03 | 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 | 243/256 (95%) | 213 (88%) | 26 (11%) | 4 (2%) | 12 | 40 |
| 1 | B | 223/256 (87%) | 187 (84%) | 33 (15%) | 3 (1%) | 15 | 46 |
| 1 | C | 245/256 (96%) | 219 (89%) | 22 (9%) | 4 (2%) | 12 | 40 |
| All | All | 711/768 (93%) | 619 (87%) | 81 (11%) | 11 (2%) | 13 | 42 |

All (11) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 234 | ALA |
| 1 | A | 118 | GLY |
| 1 | B | 66 | ASP |
| 1 | B | 85 | SER |
| 1 | C | 112 | ALA |
| 1 | A | 119 | PHE |
| 1 | B | 106 | VAL |
| 1 | C | 96 | ALA |
| 1 | C | 159 | SER |
| 1 | A | 112 | ALA |
| 1 | C | 84 | VAL |

### 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 | 191/195 (98%) | 179 (94%) | 12 (6%) | 22 | 54 |
| 1 | B | 184/195 (94%) | 170 (92%) | 14 (8%) | 16 | 43 |
| 1 | C | 198/195 (102%) | 184 (93%) | 14 (7%) | 18 | 47 |
| All | All | 573/585 (98%) | 533 (93%) | 40 (7%) | 19 | 47 |

All (40) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 20 | PHE |
| 1 | A | 25 | TYR |
| 1 | A | 28 | LEU |
| 1 | A | 70 | LEU |
| 1 | A | 103 | LYS |
| 1 | A | 137 | LEU |
| 1 | A | 145 | GLN |
| 1 | A | 163 | ASP |
| 1 | A | 181 | VAL |
| 1 | A | 205 | ARG |
| 1 | A | 207 | LEU |
| 1 | A | 223 | LEU |
| 1 | B | 5 | ARG |
| 1 | B | 28 | LEU |
| 1 | B | 31 | VAL |
| 1 | B | 32 | LEU |
| 1 | B | 63 | THR |
| 1 | B | 67 | MSE |
| 1 | B | 70 | LEU |
| 1 | B | 91 | ILE |
| 1 | B | 137 | LEU |
| 1 | B | 163 | ASP |
| 1 | B | 177 | LEU |
| 1 | B | 207 | LEU |
| 1 | B | 210 | ASN |
| 1 | B | 222 | GLU |
| 1 | C | 1 | MSE |
| 1 | C | 5 | ARG |
| 1 | C | 18 | ASN |
| 1 | C | 20 | PHE |
| 1 | C | 28 | LEU |
| 1 | C | 32 | LEU |
| 1 | C | 63 | THR |
| 1 | C | 101 | ASN |
| 1 | C | 150 | GLU |
| 1 | C | 170 | LEU |
| 1 | C | 189 | GLN |
| 1 | C | 210 | ASN |
| 1 | C | 223 | LEU |
| 1 | C | 233 | TYR |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 17 | HIS |
| 1 | A | 18 | ASN |
| 1 | A | 154 | GLN |
| 1 | A | 189 | GLN |
| 1 | A | 210 | ASN |
| 1 | A | 224 | ASN |
| 1 | B | 17 | HIS |
| 1 | B | 74 | GLN |
| 1 | B | 154 | GLN |
| 1 | C | 17 | HIS |
| 1 | C | 18 | ASN |
| 1 | C | 101 | ASN |
| 1 | C | 154 | GLN |
| 1 | C | 189 | GLN |
| 1 | C | 210 | ASN |

#### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates

There are no carbohydrates in this entry.

### 5.6 Ligand geometry

There are no ligands in this entry.

### 5.7 Other polymers

There are no such residues in this entry.

### 5.8 Polymer linkage issues

There are no chain breaks in this entry.

# 6 Fit of model and data

## 6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, $95^{th}$ 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 | 239/256 (93%) | -0.24 | 1 (0%) | 93 92 | 13, 30, 68, 72 | 0 |
| 1 | B | 225/256 (87%) | 0.11 | 9 (4%) | 42 35 | 14, 44, 89, 101 | 0 |
| 1 | C | 242/256 (94%) | -0.05 | 4 (1%) | 73 70 | 13, 37, 69, 82 | 0 |
| All | All | 706/768 (91%) | -0.06 | 14 (1%) | 68 64 | 13, 38, 79, 101 | 0 |

All (14) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | C | 72 | THR | 3.6 |
| 1 | B | 7 | PHE | 3.5 |
| 1 | C | 253 | HIS | 3.2 |
| 1 | B | 3 | ILE | 3.0 |
| 1 | B | 4 | PRO | 3.0 |
| 1 | B | 99 | VAL | 3.0 |
| 1 | B | 46 | GLY | 2.9 |
| 1 | B | 47 | SER | 2.4 |
| 1 | B | 70 | LEU | 2.4 |
| 1 | A | 145 | GLN | 2.3 |
| 1 | B | 71 | PHE | 2.3 |
| 1 | C | 93 | ASN | 2.3 |
| 1 | C | 251 | HIS | 2.1 |
| 1 | B | 65 | ILE | 2.0 |

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

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

## 6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

## 6.4 Ligands (i)

There are no ligands in this entry.

## 6.5 Other polymers (i)

There are no such residues in this entry.