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

Jan 31, 2016 – 07:00 PM GMT

| | | |
|---|---|---|
| PDB ID | : | 1DN0 |
| Title | : | STRUCTURE OF THE FAB FRAGMENT FROM A HUMAN IGM COLD AGGLUTININ |
| Authors | : | Cauerhff, A.; Braden, B.; Carvalho, J.G.; Leoni, J.; Polikarpov, I.; Goldbaum, F. |
| Deposited on | : | 1999-12-15 |
| Resolution | : | 2.28 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 (i)) were used in the production of this report:

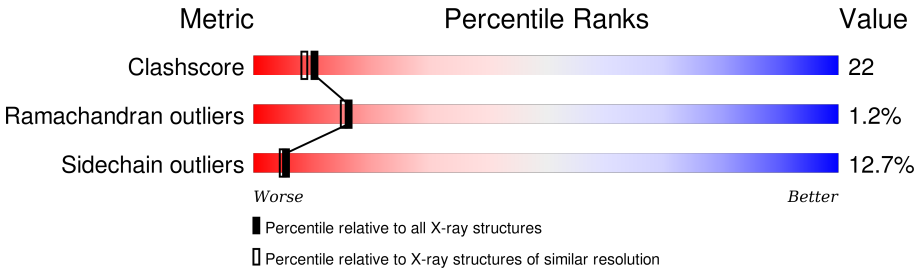
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7 (RC4), CSD as536be (2015) |
| Xtriage (Phenix) | : | NOT EXECUTED |
| EDS | : | NOT EXECUTED |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Ideal geometry (proteins) | : | Engh & 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 2.28 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)) |
|---|---|---|
| Clashscore | 102246 | 5929 (2.30-2.26) |
| Ramachandran outliers | 100387 | 5851 (2.30-2.26) |
| Sidechain outliers | 100360 | 5850 (2.30-2.26) |

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.

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 215 | 59% 32% 8% • |
| 1 | C | 215 | 65% 25% 10% |
| 2 | B | 232 | 57% 25% 9% • 7% |
| 2 | D | 232 | 62% 24% 7% 6% |

# 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7208 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 IGM-KAPPA COLD AGGLUTININ (LIGHT CHAIN).

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 215 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1638 | 1023 | 275 | 335 | 5 | | | |
| 1 | C | 215 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1638 | 1023 | 275 | 335 | 5 | | | |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 23 | CYS | GLY | CONFLICT | PIR A23746 |
| A | 89 | CYS | GLY | CONFLICT | PIR A23746 |
| A | 215 | CYS | GLY | CONFLICT | PIR A23746 |
| C | 23 | CYS | GLY | CONFLICT | PIR A23746 |
| C | 89 | CYS | GLY | CONFLICT | PIR A23746 |
| C | 215 | CYS | GLY | CONFLICT | PIR A23746 |

- Molecule 2 is a protein called IGM-KAPPA COLD AGGLUTININ (HEAVY CHAIN).

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | B | 216 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1657 | 1052 | 279 | 321 | 5 | | | |
| 2 | D | 217 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1661 | 1055 | 280 | 320 | 6 | | | |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | 1 | GLU | - | CONFLICT | PIR B23746 |
| B | 200 | ALA | GLN | CONFLICT | PIR B23746 |
| D | 1 | GLU | - | CONFLICT | PIR B23746 |
| D | 200 | ALA | GLN | CONFLICT | PIR B23746 |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 3 | A | 163 | Total O<br>163 163 | 0 | 0 |
| 3 | B | 156 | Total O<br>156 156 | 0 | 0 |
| 3 | C | 149 | Total O<br>149 149 | 0 | 0 |
| 3 | D | 146 | Total O<br>146 146 | 0 | 0 |

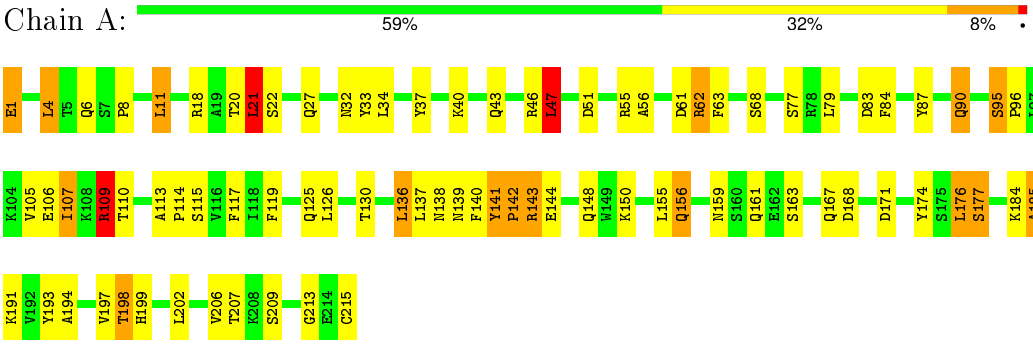
# 3 Residue-property plots (i)

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.

Note EDS was not executed.

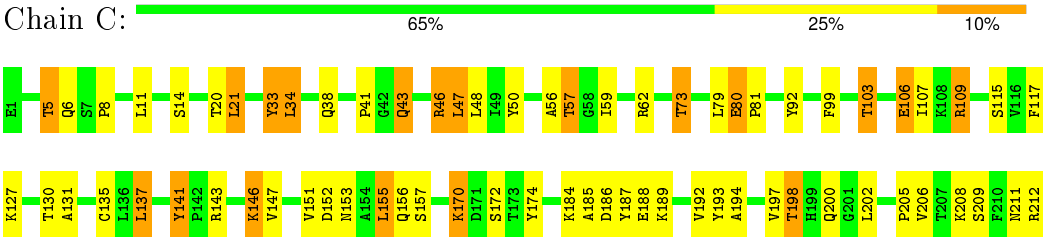
- Molecule 1: IGM-KAPPA COLD AGGLUTININ (LIGHT CHAIN)

Chain A:



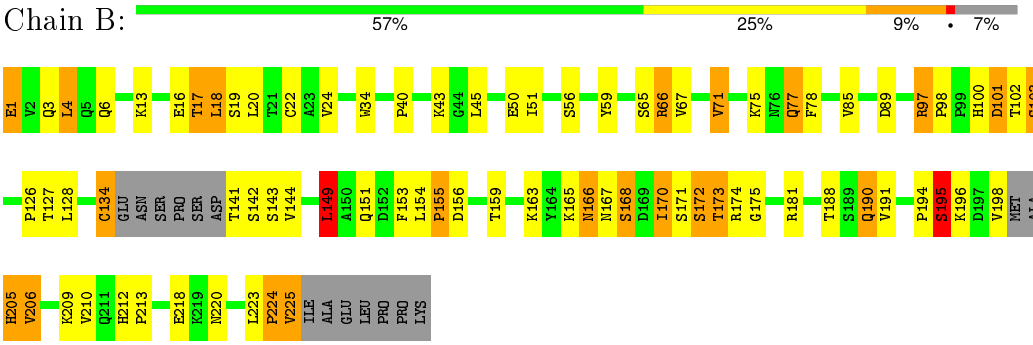

- Molecule 1: IGM-KAPPA COLD AGGLUTININ (LIGHT CHAIN)

Chain C:



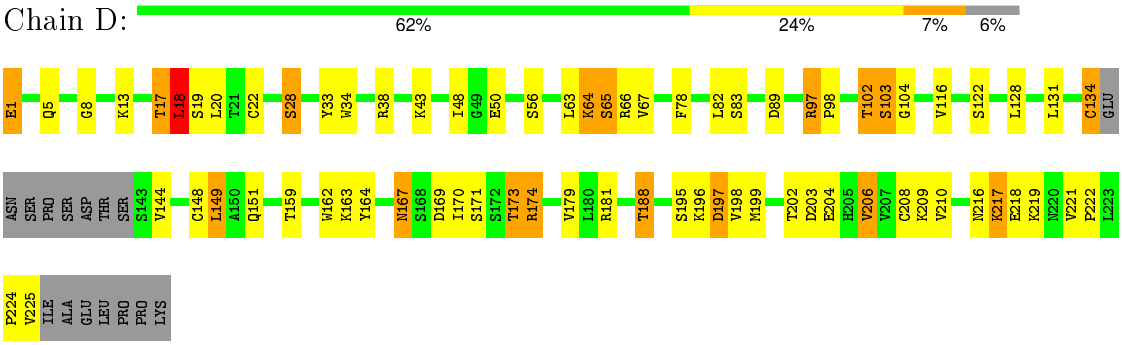

- Molecule 2: IGM-KAPPA COLD AGGLUTININ (HEAVY CHAIN)

Chain B:




- Molecule 2: IGM-KAPPA COLD AGGLUTININ (HEAVY CHAIN)

Chain D:


62%
24%
7%
6%
E1 Q5 G8 K13 T17 L18 S19 L20 T21 C22 S28 Y33 W34 R38 K43 I48 G49 E50 S56 L63 K64 S65 R66 V67 F78 L82 S83 D89 R97 P98 T102 S103 G104 V116 S122 L128 L131 C134 GLU
ASN SER PRO SER ASP THR SER S143 V144 C148 L149 A150 Q151 T159 W162 K163 Y164 N167 S168 D169 I170 S171 S172 T173 R174 V179 L180 R181 T188 S195 K196 D197 V198 M199 T202 D203 E204 H205 V206 V207 C208 K209 V210 N216 K217 E218 K219 N220 V221 P222 L223
P224 V225 ILE ALA GLU LEU PRO PRO LYS

# 4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

| Property | Value | Source |
|---|---|---|
| Space group | P 31 2 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 110.88Å 110.88Å 170.76Å<br>90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 100.00 – 2.28 | Depositor |
| % Data completeness<br>(in resolution range) | (Not available) (100.00-2.28) | Depositor |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| Refinement program | CNS | Depositor |
| R, $R_{free}$ | 0.180 , 0.240 | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 7208 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 31.0 | wwPDB-VP |

# 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 | 1.09 | 0/1673 | 1.20 | 14/2273 (0.6%) |
| 1 | C | 1.12 | 3/1673 (0.2%) | 1.27 | 11/2273 (0.5%) |
| 2 | B | 1.05 | 1/1703 (0.1%) | 1.12 | 8/2325 (0.3%) |
| 2 | D | 1.10 | 0/1708 | 1.09 | 3/2332 (0.1%) |
| All | All | 1.09 | 4/6757 (0.1%) | 1.17 | 36/9203 (0.4%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | A | 0 | 2 |
| 1 | C | 0 | 2 |
| All | All | 0 | 4 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | B | 225 | VAL | CA-CB | 5.71 | 1.66 | 1.54 |
| 1 | C | 50 | TYR | CE2-CZ | 5.63 | 1.45 | 1.38 |
| 1 | C | 99 | PHE | CE2-CZ | 5.33 | 1.47 | 1.37 |
| 1 | C | 215 | CYS | CB-SG | -5.12 | 1.73 | 1.81 |

All (36) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | C | 46 | ARG | NE-CZ-NH2 | -16.46 | 112.07 | 120.30 |
| 1 | A | 46 | ARG | NE-CZ-NH2 | -13.63 | 113.48 | 120.30 |
| 1 | C | 62 | ARG | NE-CZ-NH1 | 10.95 | 125.78 | 120.30 |
| 1 | C | 62 | ARG | NE-CZ-NH2 | -10.25 | 115.18 | 120.30 |
| 1 | C | 46 | ARG | NE-CZ-NH1 | 9.73 | 125.17 | 120.30 |
| 2 | B | 66 | ARG | NE-CZ-NH2 | -9.32 | 115.64 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 62 | ARG | NE-CZ-NH2 | -9.05 | 115.77 | 120.30 |
| 2 | B | 66 | ARG | NE-CZ-NH1 | 8.11 | 124.36 | 120.30 |
| 1 | A | 47 | LEU | CA-CB-CG | 7.14 | 131.73 | 115.30 |
| 1 | C | 46 | ARG | CG-CD-NE | -7.14 | 96.81 | 111.80 |
| 1 | A | 46 | ARG | NE-CZ-NH1 | 6.75 | 123.67 | 120.30 |
| 2 | B | 71 | VAL | CB-CA-C | -6.70 | 98.67 | 111.40 |
| 1 | A | 109 | ARG | NE-CZ-NH1 | 6.50 | 123.55 | 120.30 |
| 2 | D | 18 | LEU | CA-CB-CG | 5.93 | 128.94 | 115.30 |
| 1 | A | 46 | ARG | CG-CD-NE | -5.93 | 99.35 | 111.80 |
| 1 | C | 34 | LEU | CA-CB-CG | -5.61 | 102.39 | 115.30 |
| 1 | C | 107 | ILE | CB-CA-C | -5.59 | 100.42 | 111.60 |
| 1 | A | 109 | ARG | NE-CZ-NH2 | -5.56 | 117.52 | 120.30 |
| 1 | A | 4 | LEU | CA-CB-CG | -5.53 | 102.57 | 115.30 |
| 2 | B | 170 | ILE | N-CA-C | -5.47 | 96.23 | 111.00 |
| 1 | C | 43 | GLN | CB-CA-C | -5.44 | 99.53 | 110.40 |
| 2 | B | 149 | LEU | CA-CB-CG | 5.38 | 127.68 | 115.30 |
| 2 | D | 13 | LYS | CD-CE-NZ | -5.36 | 99.38 | 111.70 |
| 1 | C | 57 | THR | CB-CA-C | -5.34 | 97.19 | 111.60 |
| 1 | A | 62 | ARG | CG-CD-NE | -5.32 | 100.62 | 111.80 |
| 2 | D | 225 | VAL | N-CA-C | 5.25 | 125.17 | 111.00 |
| 1 | C | 57 | THR | N-CA-CB | 5.23 | 120.24 | 110.30 |
| 1 | C | 115 | SER | N-CA-C | -5.22 | 96.91 | 111.00 |
| 1 | A | 21 | LEU | CA-CB-CG | 5.17 | 127.19 | 115.30 |
| 2 | B | 101 | ASP | CB-CG-OD1 | -5.14 | 113.67 | 118.30 |
| 2 | B | 175 | GLY | N-CA-C | 5.13 | 125.92 | 113.10 |
| 2 | B | 156 | ASP | CB-CG-OD2 | 5.11 | 122.90 | 118.30 |
| 1 | A | 27 | GLN | N-CA-C | -5.08 | 97.28 | 111.00 |
| 1 | A | 115 | SER | N-CA-C | -5.07 | 97.30 | 111.00 |
| 1 | A | 51 | ASP | CB-CG-OD1 | 5.07 | 122.86 | 118.30 |
| 1 | A | 106 | GLU | N-CA-CB | -5.01 | 101.59 | 110.60 |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 141 | TYR | Sidechain |
| 1 | A | 33 | TYR | Sidechain |
| 1 | C | 141 | TYR | Sidechain |
| 1 | C | 33 | TYR | 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 | 1638 | 0 | 1587 | 78 | 0 |
| 1 | C | 1638 | 0 | 1587 | 69 | 0 |
| 2 | B | 1657 | 0 | 1601 | 72 | 0 |
| 2 | D | 1661 | 0 | 1607 | 71 | 0 |
| 3 | A | 163 | 0 | 0 | 12 | 0 |
| 3 | B | 156 | 0 | 0 | 2 | 1 |
| 3 | C | 149 | 0 | 0 | 9 | 0 |
| 3 | D | 146 | 0 | 0 | 6 | 0 |
| All | All | 7208 | 0 | 6382 | 277 | 1 |

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 22.

All (277) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:1:GLU:OE1 | 2:B:1:GLU:N | 1.75 | 1.19 |
| 1:C:198:THR:HG22 | 3:C:2200:HOH:O | 1.55 | 1.04 |
| 1:C:215:CYS:HB3 | 2:D:134:CYS:HB2 | 1.38 | 1.04 |
| 2:D:1:GLU:N | 2:D:1:GLU:OE1 | 1.91 | 1.03 |
| 2:D:181:ARG:HH11 | 2:D:181:ARG:HB3 | 1.32 | 0.94 |
| 2:B:1:GLU:CD | 2:B:1:GLU:H3 | 1.70 | 0.94 |
| 2:B:1:GLU:CD | 2:B:1:GLU:N | 2.17 | 0.94 |
| 1:A:184:LYS:O | 1:A:188:GLU:HG3 | 1.72 | 0.87 |
| 2:D:181:ARG:NH1 | 2:D:181:ARG:HB3 | 1.90 | 0.87 |
| 2:D:181:ARG:HH11 | 2:D:181:ARG:CB | 1.87 | 0.87 |
| 2:D:209:LYS:HG2 | 2:D:218:GLU:HG2 | 1.54 | 0.86 |
| 1:C:213:GLY:O | 1:C:215:CYS:N | 2.09 | 0.86 |
| 2:B:163:LYS:HD2 | 2:B:209:LYS:NZ | 1.95 | 0.81 |
| 2:D:144:VAL:HG11 | 2:D:224:PRO:HG3 | 1.63 | 0.81 |
| 1:A:176:LEU:HD23 | 1:A:176:LEU:C | 2.02 | 0.80 |
| 2:B:18:LEU:HD11 | 2:B:20:LEU:HG | 1.63 | 0.80 |
| 2:D:18:LEU:HD22 | 2:D:116:VAL:HG11 | 1.65 | 0.79 |
| 1:A:198:THR:HG23 | 3:A:2131:HOH:O | 1.83 | 0.78 |
| 2:B:97:ARG:HD3 | 2:B:98:PRO:O | 1.84 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:202:LEU:HD13 | 1:C:206:VAL:HG23 | 1.67 | 0.76 |
| 1:A:167:GLN:HG3 | 1:A:174:TYR:CZ | 2.21 | 0.75 |
| 2:B:18:LEU:HD12 | 2:B:19:SER:N | 2.01 | 0.74 |
| 2:B:181:ARG:HG2 | 3:B:2444:HOH:O | 1.87 | 0.74 |
| 1:A:198:THR:HG21 | 3:A:2507:HOH:O | 1.88 | 0.73 |
| 2:D:149:LEU:HD23 | 2:D:188:THR:HG22 | 1.69 | 0.73 |
| 2:B:17:THR:HG22 | 3:B:2138:HOH:O | 1.89 | 0.72 |
| 2:B:166:ASN:OD1 | 2:B:168:SER:HB2 | 1.90 | 0.72 |
| 1:A:8:PRO:O | 1:A:103:THR:HB | 1.90 | 0.71 |
| 2:B:143:SER:HA | 2:B:194:PRO:HA | 1.72 | 0.71 |
| 1:C:8:PRO:O | 1:C:103:THR:HB | 1.91 | 0.71 |
| 2:D:1:GLU:N | 2:D:1:GLU:CD | 2.38 | 0.70 |
| 2:B:34:TRP:CH2 | 2:B:97:ARG:HG3 | 2.26 | 0.70 |
| 1:C:215:CYS:HB3 | 2:D:134:CYS:CB | 2.20 | 0.70 |
| 2:D:103:SER:HB2 | 3:D:2351:HOH:O | 1.92 | 0.70 |
| 1:C:153:ASN:ND2 | 3:C:2599:HOH:O | 2.15 | 0.70 |
| 2:B:18:LEU:HD22 | 2:B:116:VAL:HG11 | 1.74 | 0.69 |
| 2:B:149:LEU:HD23 | 2:B:188:THR:HG22 | 1.74 | 0.69 |
| 1:C:143:ARG:HD2 | 1:C:143:ARG:O | 1.92 | 0.69 |
| 2:D:209:LYS:HG2 | 2:D:218:GLU:CG | 2.21 | 0.69 |
| 2:B:205:HIS:HD1 | 2:B:205:HIS:C | 1.95 | 0.69 |
| 2:D:63:LEU:O | 2:D:65:SER:OG | 2.10 | 0.68 |
| 1:A:20:THR:HG23 | 3:A:2491:HOH:O | 1.94 | 0.68 |
| 2:B:18:LEU:C | 2:B:18:LEU:HD12 | 2.15 | 0.68 |
| 1:C:20:THR:HG23 | 3:C:2452:HOH:O | 1.92 | 0.67 |
| 1:A:215:CYS:SG | 2:B:134:CYS:CB | 2.84 | 0.66 |
| 2:B:172:SER:O | 2:B:191:VAL:HA | 1.96 | 0.66 |
| 1:A:61:ASP:HB2 | 3:A:2460:HOH:O | 1.96 | 0.66 |
| 2:D:173:THR:HG22 | 3:D:2576:HOH:O | 1.95 | 0.66 |
| 2:B:142:SER:HA | 2:B:195:SER:HB2 | 1.78 | 0.66 |
| 2:D:34:TRP:O | 2:D:50:GLU:HA | 1.96 | 0.66 |
| 2:B:205:HIS:C | 2:B:205:HIS:ND1 | 2.48 | 0.65 |
| 2:B:40:PRO:HB2 | 2:B:43:LYS:HG3 | 1.78 | 0.65 |
| 1:A:37:TYR:OH | 1:A:90:GLN:NE2 | 2.29 | 0.65 |
| 1:A:156:GLN:HG3 | 1:A:159:ASN:HD21 | 1.61 | 0.65 |
| 1:C:146:LYS:HB3 | 1:C:198:THR:HG23 | 1.78 | 0.65 |
| 2:B:165:LYS:HG3 | 2:B:205:HIS:CE1 | 2.31 | 0.64 |
| 2:B:170:ILE:HD11 | 2:B:206:VAL:CG2 | 2.26 | 0.64 |
| 2:B:163:LYS:HD2 | 2:B:209:LYS:HZ2 | 1.62 | 0.64 |
| 1:C:143:ARG:HG2 | 1:C:143:ARG:HH11 | 1.63 | 0.64 |
| 2:B:205:HIS:CD2 | 2:B:220:ASN:HB3 | 2.33 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:16:GLU:O | 2:B:85:VAL:HG22 | 1.99 | 0.62 |
| 2:D:18:LEU:HD12 | 2:D:19:SER:N | 2.15 | 0.62 |
| 2:D:17:THR:HG22 | 3:D:2216:HOH:O | 2.01 | 0.61 |
| 3:C:2600:HOH:O | 2:D:174:ARG:HD2 | 2.00 | 0.61 |
| 1:C:192:VAL:HG22 | 1:C:211:ASN:OD1 | 2.00 | 0.61 |
| 2:D:34:TRP:CZ3 | 2:D:97:ARG:HB2 | 2.36 | 0.61 |
| 2:B:142:SER:CA | 2:B:195:SER:HB2 | 2.31 | 0.61 |
| 2:B:224:PRO:O | 2:B:225:VAL:HG12 | 2.02 | 0.60 |
| 1:C:33:TYR:HB3 | 1:C:92:TYR:CD1 | 2.37 | 0.60 |
| 1:C:188:GLU:O | 1:C:212:ARG:NH2 | 2.35 | 0.60 |
| 1:A:114:PRO:HB3 | 1:A:140:PHE:HB3 | 1.83 | 0.60 |
| 2:D:67:VAL:HG22 | 2:D:82:LEU:CD1 | 2.32 | 0.60 |
| 2:B:100:HIS:HB2 | 2:B:103:SER:HB2 | 1.83 | 0.59 |
| 1:A:103:THR:HG21 | 3:A:2086:HOH:O | 2.03 | 0.59 |
| 1:C:43:GLN:N | 1:C:43:GLN:NE2 | 2.51 | 0.59 |
| 2:D:144:VAL:HG11 | 2:D:224:PRO:CG | 2.33 | 0.58 |
| 2:B:1:GLU:CD | 2:B:1:GLU:H1 | 2.04 | 0.58 |
| 1:C:41:PRO:O | 1:C:43:GLN:NE2 | 2.37 | 0.58 |
| 1:C:170:LYS:HB3 | 1:C:170:LYS:NZ | 2.18 | 0.58 |
| 1:C:198:THR:HB | 1:C:205:PRO:HG3 | 1.84 | 0.58 |
| 2:D:97:ARG:HD3 | 2:D:98:PRO:O | 2.03 | 0.58 |
| 1:A:18:ARG:HH21 | 1:A:77:SER:HB2 | 1.69 | 0.57 |
| 2:D:1:GLU:OE1 | 2:D:1:GLU:CA | 2.53 | 0.57 |
| 2:B:174:ARG:HG3 | 2:B:190:GLN:O | 2.05 | 0.57 |
| 1:A:159:ASN:N | 1:A:159:ASN:OD1 | 2.37 | 0.56 |
| 2:D:198:VAL:HG23 | 2:D:199:MET:N | 2.20 | 0.56 |
| 1:A:109:ARG:HD3 | 1:A:110:THR:O | 2.03 | 0.56 |
| 2:B:18:LEU:CD1 | 2:B:20:LEU:HG | 2.36 | 0.56 |
| 1:A:167:GLN:HG3 | 1:A:174:TYR:OH | 2.04 | 0.56 |
| 1:A:21:LEU:HD23 | 1:A:21:LEU:N | 2.21 | 0.56 |
| 1:C:5:THR:HG23 | 3:C:2169:HOH:O | 2.06 | 0.56 |
| 2:D:144:VAL:CG1 | 2:D:224:PRO:HG3 | 2.35 | 0.55 |
| 1:C:124:GLU:OE1 | 2:D:219:LYS:NZ | 2.33 | 0.55 |
| 1:A:55:ARG:NH1 | 3:A:2402:HOH:O | 2.40 | 0.55 |
| 2:D:197:ASP:OD2 | 2:D:197:ASP:N | 2.39 | 0.55 |
| 1:C:184:LYS:O | 1:C:188:GLU:HG3 | 2.07 | 0.55 |
| 2:D:148:CYS:HB2 | 2:D:162:TRP:CH2 | 2.42 | 0.55 |
| 2:D:164:TYR:CZ | 2:D:170:ILE:HG12 | 2.42 | 0.55 |
| 1:C:143:ARG:HG2 | 1:C:143:ARG:NH1 | 2.21 | 0.55 |
| 2:B:212:HIS:CG | 2:B:213:PRO:HD2 | 2.42 | 0.55 |
| 1:C:80:GLU:HG3 | 1:C:81:PRO:CD | 2.36 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:165:LYS:HG3 | 2:B:205:HIS:HE1 | 1.72 | 0.55 |
| 2:D:128:LEU:HD21 | 2:D:210:VAL:HG11 | 1.89 | 0.55 |
| 1:A:206:VAL:CG1 | 1:A:207:THR:N | 2.70 | 0.54 |
| 1:A:113:ALA:HB1 | 1:A:202:LEU:CD2 | 2.37 | 0.54 |
| 2:B:34:TRP:HB3 | 2:B:78:PHE:CZ | 2.43 | 0.54 |
| 2:B:97:ARG:CD | 2:B:98:PRO:O | 2.54 | 0.54 |
| 1:C:126:LEU:HD21 | 1:C:131:ALA:HB2 | 1.90 | 0.53 |
| 1:A:47:LEU:HD13 | 1:A:56:ALA:HB2 | 1.89 | 0.53 |
| 1:A:103:THR:CG2 | 3:A:2086:HOH:O | 2.56 | 0.53 |
| 2:D:216:ASN:C | 2:D:217:LYS:HG2 | 2.28 | 0.53 |
| 2:D:63:LEU:HD22 | 2:D:82:LEU:HD11 | 1.91 | 0.53 |
| 1:A:148:GLN:HG2 | 1:A:155:LEU:CD2 | 2.39 | 0.53 |
| 1:A:22:SER:HB3 | 3:A:2264:HOH:O | 2.08 | 0.53 |
| 2:B:170:ILE:HD11 | 2:B:206:VAL:HG21 | 1.90 | 0.53 |
| 1:C:6:GLN:HB3 | 1:C:103:THR:HG22 | 1.90 | 0.52 |
| 1:A:215:CYS:HB2 | 3:A:2424:HOH:O | 2.08 | 0.52 |
| 1:C:38:GLN:HB2 | 1:C:48:LEU:HD11 | 1.91 | 0.52 |
| 2:D:34:TRP:HB3 | 2:D:78:PHE:CZ | 2.44 | 0.52 |
| 1:A:176:LEU:CD2 | 1:A:176:LEU:C | 2.76 | 0.52 |
| 2:D:159:THR:O | 2:D:210:VAL:HA | 2.09 | 0.52 |
| 2:D:18:LEU:HD12 | 2:D:18:LEU:C | 2.30 | 0.52 |
| 1:A:189:LYS:O | 1:A:190:HIS:CG | 2.63 | 0.52 |
| 1:A:18:ARG:HD3 | 3:A:2004:HOH:O | 2.10 | 0.52 |
| 2:D:144:VAL:HG13 | 3:D:2573:HOH:O | 2.09 | 0.52 |
| 1:A:215:CYS:SG | 2:B:134:CYS:HB3 | 2.49 | 0.52 |
| 1:C:109:ARG:HD2 | 1:C:141:TYR:CG | 2.45 | 0.52 |
| 2:B:142:SER:HA | 2:B:195:SER:CB | 2.40 | 0.51 |
| 2:D:131:LEU:HD23 | 3:D:2597:HOH:O | 2.09 | 0.51 |
| 1:A:139:ASN:HD21 | 2:B:174:ARG:NH2 | 2.09 | 0.51 |
| 1:C:106:GLU:HG3 | 1:C:174:TYR:OH | 2.10 | 0.51 |
| 1:C:11:LEU:HD12 | 1:C:21:LEU:HD22 | 1.92 | 0.51 |
| 2:B:209:LYS:HE2 | 2:B:218:GLU:OE2 | 2.11 | 0.51 |
| 1:A:119:PHE:HE2 | 1:A:136:LEU:HD22 | 1.76 | 0.51 |
| 1:A:136:LEU:HD23 | 2:B:190:GLN:NE2 | 2.26 | 0.51 |
| 1:A:148:GLN:HG2 | 1:A:155:LEU:HD23 | 1.94 | 0.50 |
| 2:D:164:TYR:CE1 | 2:D:170:ILE:HG12 | 2.47 | 0.50 |
| 2:B:209:LYS:HG2 | 2:B:218:GLU:HB3 | 1.92 | 0.50 |
| 1:A:141:TYR:CD2 | 1:A:142:PRO:HA | 2.46 | 0.50 |
| 1:A:156:GLN:CG | 1:A:159:ASN:HD21 | 2.25 | 0.50 |
| 1:A:62:ARG:HD2 | 1:A:83:ASP:OD2 | 2.12 | 0.50 |
| 1:C:186:ASP:HA | 1:C:189:LYS:HE2 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:163:LYS:HD2 | 2:B:209:LYS:HZ1 | 1.75 | 0.49 |
| 2:D:198:VAL:CG2 | 2:D:199:MET:N | 2.74 | 0.49 |
| 1:A:87:TYR:O | 1:A:102:GLY:HA2 | 2.12 | 0.49 |
| 1:A:150:LYS:HB2 | 1:A:194:ALA:HB3 | 1.93 | 0.49 |
| 2:D:34:TRP:HB3 | 2:D:78:PHE:CE1 | 2.47 | 0.49 |
| 2:B:126:PRO:HB3 | 2:B:153:PHE:HB3 | 1.94 | 0.49 |
| 2:D:63:LEU:HB3 | 2:D:67:VAL:CG2 | 2.43 | 0.49 |
| 1:A:40:LYS:HB2 | 1:A:43:GLN:HG3 | 1.94 | 0.49 |
| 2:B:34:TRP:O | 2:B:50:GLU:HA | 2.11 | 0.49 |
| 2:B:34:TRP:CZ3 | 2:B:97:ARG:HG3 | 2.48 | 0.49 |
| 2:B:143:SER:HA | 2:B:195:SER:H | 1.77 | 0.49 |
| 1:A:1:GLU:HG3 | 1:A:98:THR:HG21 | 1.93 | 0.49 |
| 1:A:161:GLN:OE1 | 2:B:181:ARG:HD3 | 2.13 | 0.48 |
| 1:A:137:LEU:HD22 | 1:A:197:VAL:HG21 | 1.95 | 0.48 |
| 2:B:154:LEU:HD12 | 2:B:155:PRO:HA | 1.96 | 0.48 |
| 1:C:146:LYS:HE2 | 1:C:198:THR:CG2 | 2.43 | 0.48 |
| 2:B:142:SER:C | 2:B:195:SER:HB2 | 2.34 | 0.48 |
| 2:D:38:ARG:HD3 | 2:D:48:ILE:HD11 | 1.94 | 0.48 |
| 2:D:163:LYS:NZ | 2:D:169:ASP:OD1 | 2.43 | 0.48 |
| 2:B:170:ILE:HD11 | 2:B:206:VAL:HG22 | 1.94 | 0.48 |
| 2:B:205:HIS:HA | 2:B:223:LEU:HG | 1.95 | 0.47 |
| 2:D:8:GLY:HA3 | 2:D:20:LEU:HD23 | 1.96 | 0.47 |
| 1:C:146:LYS:HB3 | 1:C:146:LYS:HE2 | 1.74 | 0.47 |
| 1:C:146:LYS:NZ | 1:C:198:THR:HG21 | 2.29 | 0.47 |
| 2:D:181:ARG:NH1 | 2:D:181:ARG:CB | 2.60 | 0.47 |
| 1:A:37:TYR:HE2 | 1:A:90:GLN:HE21 | 1.63 | 0.47 |
| 2:B:170:ILE:CD1 | 2:B:206:VAL:HG21 | 2.45 | 0.47 |
| 2:D:17:THR:HB | 2:D:83:SER:HA | 1.95 | 0.47 |
| 1:A:119:PHE:CE2 | 1:A:136:LEU:HD22 | 2.50 | 0.47 |
| 2:B:13:LYS:HE3 | 2:B:121:GLY:O | 2.15 | 0.47 |
| 2:B:75:LYS:HB2 | 2:B:77:GLN:HG3 | 1.97 | 0.46 |
| 2:B:1:GLU:OE1 | 2:B:1:GLU:CA | 2.57 | 0.46 |
| 1:A:4:LEU:HA | 1:A:4:LEU:HD23 | 1.52 | 0.46 |
| 2:D:34:TRP:CZ3 | 2:D:97:ARG:HG3 | 2.49 | 0.46 |
| 1:A:125:GLN:HG2 | 1:A:130:THR:O | 2.16 | 0.46 |
| 1:A:144:GLU:CD | 1:A:144:GLU:H | 2.19 | 0.46 |
| 2:B:4:LEU:HB3 | 2:B:22:CYS:SG | 2.56 | 0.46 |
| 2:D:28:SER:HB2 | 3:D:2376:HOH:O | 2.16 | 0.46 |
| 2:B:34:TRP:CZ3 | 2:B:97:ARG:HB2 | 2.50 | 0.46 |
| 1:A:18:ARG:NH2 | 1:A:77:SER:HB2 | 2.30 | 0.46 |
| 2:D:34:TRP:CH2 | 2:D:97:ARG:HG3 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:34:TRP:CE3 | 2:D:97:ARG:HB2 | 2.50 | 0.45 |
| 2:B:24:VAL:HG21 | 2:B:34:TRP:CH2 | 2.51 | 0.45 |
| 1:A:6:GLN:HB3 | 1:A:103:THR:HG22 | 1.98 | 0.45 |
| 1:C:215:CYS:CB | 2:D:134:CYS:SG | 3.04 | 0.45 |
| 2:D:33:TYR:HB3 | 2:D:50:GLU:HB2 | 1.99 | 0.45 |
| 1:A:138:ASN:HB3 | 1:A:139:ASN:ND2 | 2.32 | 0.45 |
| 1:A:32:ASN:OD1 | 1:A:68:SER:HA | 2.15 | 0.45 |
| 1:C:92:TYR:CE1 | 2:D:104:GLY:HA3 | 2.51 | 0.45 |
| 2:B:128:LEU:HD11 | 2:B:210:VAL:HG22 | 1.97 | 0.45 |
| 2:D:64:LYS:HB3 | 2:D:64:LYS:NZ | 2.31 | 0.45 |
| 1:C:193:TYR:HE1 | 1:C:212:ARG:HG3 | 1.82 | 0.45 |
| 2:D:102:THR:O | 2:D:103:SER:O | 2.34 | 0.45 |
| 1:C:5:THR:CG2 | 3:C:2169:HOH:O | 2.63 | 0.45 |
| 2:D:66:ARG:NH2 | 2:D:89:ASP:OD2 | 2.49 | 0.45 |
| 1:A:176:LEU:HD23 | 1:A:176:LEU:O | 2.17 | 0.44 |
| 1:C:146:LYS:HB3 | 1:C:198:THR:CG2 | 2.45 | 0.44 |
| 1:A:198:THR:CG2 | 3:A:2131:HOH:O | 2.52 | 0.44 |
| 2:D:216:ASN:O | 2:D:217:LYS:HG2 | 2.17 | 0.44 |
| 2:B:212:HIS:HA | 2:B:213:PRO:HD3 | 1.80 | 0.44 |
| 1:A:176:LEU:HD23 | 1:A:177:SER:N | 2.32 | 0.44 |
| 1:C:109:ARG:HD2 | 1:C:141:TYR:CB | 2.48 | 0.44 |
| 1:C:6:GLN:HB3 | 1:C:103:THR:CG2 | 2.47 | 0.44 |
| 1:C:215:CYS:CB | 2:D:134:CYS:HG | 2.27 | 0.44 |
| 1:A:107:ILE:HB | 1:A:167:GLN:HE22 | 1.82 | 0.44 |
| 1:C:185:ALA:O | 1:C:189:LYS:HG3 | 2.17 | 0.44 |
| 2:B:4:LEU:N | 2:B:4:LEU:HD23 | 2.33 | 0.44 |
| 2:D:5:GLN:O | 2:D:22:CYS:HA | 2.18 | 0.44 |
| 1:A:213:GLY:O | 1:C:127:LYS:HG2 | 2.17 | 0.44 |
| 1:A:168:ASP:HB3 | 1:A:171:ASP:OD1 | 2.18 | 0.43 |
| 1:C:146:LYS:CB | 1:C:198:THR:HG23 | 2.48 | 0.43 |
| 2:D:1:GLU:H3 | 2:D:1:GLU:CD | 1.92 | 0.43 |
| 1:C:48:LEU:CD2 | 1:C:59:ILE:HD12 | 2.48 | 0.43 |
| 2:D:66:ARG:HH22 | 2:D:89:ASP:CG | 2.22 | 0.43 |
| 2:B:171:SER:O | 2:B:173:THR:N | 2.51 | 0.43 |
| 2:D:18:LEU:HD11 | 2:D:20:LEU:HG | 2.00 | 0.43 |
| 1:A:206:VAL:HG12 | 1:A:207:THR:N | 2.32 | 0.43 |
| 1:A:194:ALA:HB2 | 1:A:209:SER:HB3 | 2.01 | 0.43 |
| 1:A:117:PHE:CD1 | 1:A:117:PHE:N | 2.87 | 0.43 |
| 1:A:84:PHE:CD2 | 1:A:105:VAL:HG12 | 2.53 | 0.43 |
| 1:C:103:THR:CG2 | 3:C:2170:HOH:O | 2.67 | 0.43 |
| 1:A:43:GLN:HB2 | 3:A:2008:HOH:O | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:102:THR:HG22 | 2:D:103:SER:H | 1.84 | 0.43 |
| 1:A:136:LEU:C | 1:A:137:LEU:HD23 | 2.38 | 0.43 |
| 2:D:128:LEU:HD21 | 2:D:210:VAL:CG1 | 2.49 | 0.43 |
| 1:C:155:LEU:HD22 | 1:C:156:GLN:O | 2.18 | 0.43 |
| 1:A:185:ALA:O | 1:A:188:GLU:HB2 | 2.19 | 0.43 |
| 1:C:143:ARG:HD2 | 1:C:143:ARG:C | 2.39 | 0.43 |
| 1:C:46:ARG:HD3 | 3:C:2049:HOH:O | 2.19 | 0.43 |
| 1:C:151:VAL:HB | 1:C:156:GLN:NE2 | 2.34 | 0.43 |
| 1:C:47:LEU:HD13 | 1:C:56:ALA:HB2 | 1.99 | 0.43 |
| 1:C:43:GLN:N | 1:C:43:GLN:CD | 2.71 | 0.42 |
| 1:A:199:HIS:O | 1:A:202:LEU:HB2 | 2.18 | 0.42 |
| 2:B:59:TYR:CE2 | 2:B:67:VAL:HG12 | 2.54 | 0.42 |
| 1:C:137:LEU:HD22 | 1:C:197:VAL:HG21 | 2.02 | 0.42 |
| 1:C:33:TYR:HB3 | 1:C:92:TYR:CE1 | 2.54 | 0.42 |
| 2:B:3:GLN:C | 2:B:4:LEU:HD23 | 2.39 | 0.42 |
| 2:D:170:ILE:HD11 | 2:D:206:VAL:HG22 | 2.01 | 0.42 |
| 1:C:125:GLN:HG2 | 1:C:130:THR:O | 2.19 | 0.42 |
| 1:C:212:ARG:O | 1:C:214:GLU:N | 2.50 | 0.42 |
| 1:C:187:TYR:CE2 | 1:C:212:ARG:HD3 | 2.54 | 0.42 |
| 1:C:126:LEU:CD2 | 1:C:131:ALA:HB2 | 2.49 | 0.42 |
| 1:C:215:CYS:CB | 2:D:134:CYS:HB2 | 2.29 | 0.42 |
| 1:C:11:LEU:CD1 | 1:C:21:LEU:HD22 | 2.49 | 0.42 |
| 1:A:141:TYR:CG | 1:A:142:PRO:HA | 2.54 | 0.42 |
| 1:A:193:TYR:O | 1:A:209:SER:HA | 2.19 | 0.42 |
| 1:C:109:ARG:HG2 | 1:C:172:SER:HB2 | 2.01 | 0.42 |
| 1:C:193:TYR:O | 1:C:209:SER:HB2 | 2.20 | 0.41 |
| 2:B:66:ARG:HH22 | 2:B:89:ASP:CG | 2.23 | 0.41 |
| 1:C:117:PHE:O | 1:C:135:CYS:HA | 2.20 | 0.41 |
| 1:C:147:VAL:HG22 | 1:C:197:VAL:HG22 | 2.02 | 0.41 |
| 2:D:102:THR:CG2 | 2:D:103:SER:N | 2.84 | 0.41 |
| 1:C:194:ALA:CB | 1:C:209:SER:HB3 | 2.51 | 0.41 |
| 2:B:143:SER:CA | 2:B:195:SER:H | 2.33 | 0.41 |
| 1:A:137:LEU:CD2 | 1:A:197:VAL:HG21 | 2.51 | 0.41 |
| 1:A:144:GLU:CD | 1:A:144:GLU:N | 2.74 | 0.41 |
| 2:B:101:ASP:OD1 | 2:B:102:THR:N | 2.54 | 0.41 |
| 1:C:152:ASP:O | 1:C:153:ASN:HB2 | 2.20 | 0.41 |
| 1:A:62:ARG:HB3 | 1:A:62:ARG:HE | 1.62 | 0.41 |
| 2:B:51:ILE:HA | 2:B:56:SER:O | 2.21 | 0.41 |
| 1:C:208:LYS:HA | 1:C:208:LYS:HD3 | 1.92 | 0.41 |
| 1:A:95:SER:HA | 1:A:96:PRO:HA | 1.78 | 0.41 |
| 2:D:221:VAL:HA | 2:D:222:PRO:HD3 | 1.82 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:209:LYS:CG | 2:D:218:GLU:HG2 | 2.36 | 0.40 |
| 1:A:143:ARG:HB2 | 1:A:174:TYR:CE1 | 2.55 | 0.40 |
| 1:C:73:THR:CG2 | 3:C:2538:HOH:O | 2.68 | 0.40 |
| 1:C:211:ASN:HB2 | 1:C:214:GLU:OE2 | 2.21 | 0.40 |
| 1:A:114:PRO:HB3 | 1:A:140:PHE:CD2 | 2.56 | 0.40 |
| 1:A:11:LEU:HD12 | 1:A:21:LEU:HD22 | 2.03 | 0.40 |
| 2:D:163:LYS:HE3 | 2:D:167:ASN:OD1 | 2.22 | 0.40 |
| 1:A:148:GLN:CG | 1:A:155:LEU:HD21 | 2.51 | 0.40 |
| 2:B:101:ASP:OD1 | 2:B:102:THR:HG23 | 2.21 | 0.40 |
| 1:A:126:LEU:HD23 | 1:A:126:LEU:HA | 1.76 | 0.40 |
| 2:B:212:HIS:CD2 | 2:B:213:PRO:HD2 | 2.56 | 0.40 |
| 1:A:62:ARG:HG2 | 1:A:63:PHE:CD1 | 2.57 | 0.40 |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:B:2132:HOH:O | 3:B:2132:HOH:O[6_555] | 2.17 | 0.03 |

## 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 | 213/215 (99%) | 203 (95%) | 9 (4%) | 1 (0%) | 34 39 |
| 1 | C | 213/215 (99%) | 199 (93%) | 13 (6%) | 1 (0%) | 34 39 |
| 2 | B | 210/232 (90%) | 194 (92%) | 12 (6%) | 4 (2%) | 10 7 |
| 2 | D | 213/232 (92%) | 198 (93%) | 11 (5%) | 4 (2%) | 10 7 |
| All | All | 849/894 (95%) | 794 (94%) | 45 (5%) | 10 (1%) | 16 15 |

All (10) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 172 | SER |
| 1 | C | 214 | GLU |
| 2 | D | 64 | LYS |
| 2 | D | 103 | SER |
| 2 | D | 167 | ASN |
| 2 | B | 195 | SER |
| 2 | D | 174 | ARG |
| 2 | B | 224 | PRO |
| 1 | A | 185 | ALA |
| 2 | B | 196 | LYS |

### 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 | 185/185 (100%) | 165 (89%) | 20 (11%) | 8 8 |
| 1 | C | 185/185 (100%) | 166 (90%) | 19 (10%) | 9 9 |
| 2 | B | 187/200 (94%) | 158 (84%) | 29 (16%) | 3 3 |
| 2 | D | 186/200 (93%) | 160 (86%) | 26 (14%) | 4 3 |
| All | All | 743/770 (96%) | 649 (87%) | 94 (13%) | 5 5 |

All (94) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1 | GLU |
| 1 | A | 11 | LEU |
| 1 | A | 21 | LEU |
| 1 | A | 34 | LEU |
| 1 | A | 47 | LEU |
| 1 | A | 79 | LEU |
| 1 | A | 90 | GLN |
| 1 | A | 95 | SER |
| 1 | A | 103 | THR |
| 1 | A | 107 | ILE |
| 1 | A | 109 | ARG |
| 1 | A | 136 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 142 | PRO |
| 1 | A | 143 | ARG |
| 1 | A | 156 | GLN |
| 1 | A | 163 | SER |
| 1 | A | 176 | LEU |
| 1 | A | 177 | SER |
| 1 | A | 191 | LYS |
| 1 | A | 198 | THR |
| 2 | B | 1 | GLU |
| 2 | B | 4 | LEU |
| 2 | B | 6 | GLN |
| 2 | B | 17 | THR |
| 2 | B | 18 | LEU |
| 2 | B | 45 | LEU |
| 2 | B | 65 | SER |
| 2 | B | 71 | VAL |
| 2 | B | 77 | GLN |
| 2 | B | 97 | ARG |
| 2 | B | 103 | SER |
| 2 | B | 127 | THR |
| 2 | B | 134 | CYS |
| 2 | B | 141 | THR |
| 2 | B | 144 | VAL |
| 2 | B | 149 | LEU |
| 2 | B | 151 | GLN |
| 2 | B | 155 | PRO |
| 2 | B | 159 | THR |
| 2 | B | 166 | ASN |
| 2 | B | 167 | ASN |
| 2 | B | 168 | SER |
| 2 | B | 173 | THR |
| 2 | B | 190 | GLN |
| 2 | B | 195 | SER |
| 2 | B | 198 | VAL |
| 2 | B | 204 | GLU |
| 2 | B | 205 | HIS |
| 2 | B | 206 | VAL |
| 1 | C | 5 | THR |
| 1 | C | 14 | SER |
| 1 | C | 21 | LEU |
| 1 | C | 34 | LEU |
| 1 | C | 47 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 57 | THR |
| 1 | C | 73 | THR |
| 1 | C | 79 | LEU |
| 1 | C | 80 | GLU |
| 1 | C | 103 | THR |
| 1 | C | 106 | GLU |
| 1 | C | 109 | ARG |
| 1 | C | 137 | LEU |
| 1 | C | 146 | LYS |
| 1 | C | 155 | LEU |
| 1 | C | 157 | SER |
| 1 | C | 170 | LYS |
| 1 | C | 198 | THR |
| 1 | C | 200 | GLN |
| 2 | D | 1 | GLU |
| 2 | D | 17 | THR |
| 2 | D | 18 | LEU |
| 2 | D | 28 | SER |
| 2 | D | 43 | LYS |
| 2 | D | 56 | SER |
| 2 | D | 65 | SER |
| 2 | D | 97 | ARG |
| 2 | D | 102 | THR |
| 2 | D | 122 | SER |
| 2 | D | 134 | CYS |
| 2 | D | 149 | LEU |
| 2 | D | 151 | GLN |
| 2 | D | 171 | SER |
| 2 | D | 173 | THR |
| 2 | D | 179 | VAL |
| 2 | D | 188 | THR |
| 2 | D | 195 | SER |
| 2 | D | 196 | LYS |
| 2 | D | 197 | ASP |
| 2 | D | 202 | THR |
| 2 | D | 203 | ASP |
| 2 | D | 204 | GLU |
| 2 | D | 206 | VAL |
| 2 | D | 208 | CYS |
| 2 | D | 217 | LYS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 90 | GLN |
| 1 | A | 138 | ASN |
| 1 | A | 156 | GLN |
| 1 | A | 200 | GLN |
| 2 | B | 190 | GLN |
| 2 | B | 214 | ASN |
| 1 | C | 43 | GLN |
| 2 | D | 76 | ASN |
| 2 | D | 151 | GLN |
| 2 | D | 205 | HIS |
| 2 | D | 214 | ASN |
| 2 | D | 220 | 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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

## 6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

## 6.4 Ligands

EDS was not executed - this section will therefore be empty.

## 6.5 Other polymers

EDS was not executed - this section will therefore be empty.