# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 07:08 AM EST

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|---|---|---|
| PDB ID | : | 3PQE |
| Title | : | Crystal structure of L-lactate dehydrogenase from Bacillus subtilis with H171C mutation |
| Authors | : | Zhang, Y.; Garavito, R.M. |
| Deposited on | : | 2010-11-26 |
| Resolution | : | 2.20 Å(reported) |

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

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

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

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

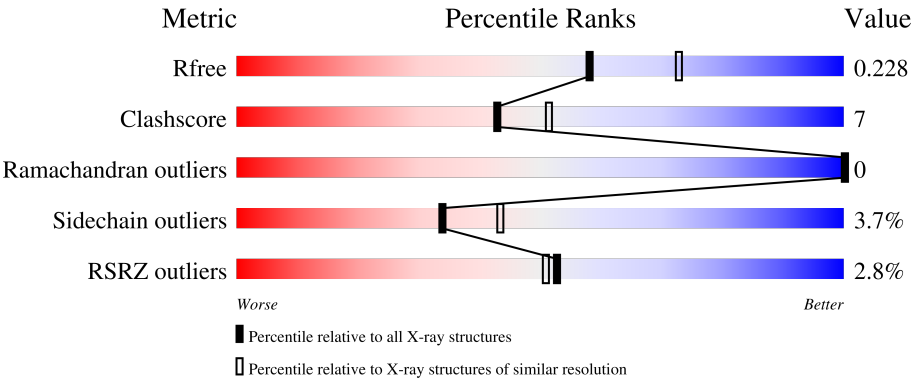
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.36 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & 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 2.20 Å.

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




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 130704 | 4898 (2.20-2.20) |
| Clashscore | 141614 | 5594 (2.20-2.20) |
| Ramachandran outliers | 138981 | 5503 (2.20-2.20) |
| Sidechain outliers | 138945 | 5504 (2.20-2.20) |
| RSRZ outliers | 127900 | 4800 (2.20-2.20) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 326 | 84% 12% |
| 1 | B | 326 | 83% 12% |
| 1 | C | 326 | 4% 76% 16% 6% |
| 1 | D | 326 | 5% 75% 18% 6% |

## 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9845 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 L-lactate dehydrogenase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 314 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2397 | 1527 | 401 | 460 | 9 | | | |
| 1 | B | 314 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2397 | 1527 | 401 | 460 | 9 | | | |
| 1 | C | 305 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2331 | 1488 | 387 | 447 | 9 | | | |
| 1 | D | 306 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2342 | 1494 | 391 | 448 | 9 | | | |

There are 28 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 171 | CYS | HIS | engineered mutation | UNP P13714 |
| A | 321 | HIS | - | expression tag | UNP P13714 |
| A | 322 | HIS | - | expression tag | UNP P13714 |
| A | 323 | HIS | - | expression tag | UNP P13714 |
| A | 324 | HIS | - | expression tag | UNP P13714 |
| A | 325 | HIS | - | expression tag | UNP P13714 |
| A | 326 | HIS | - | expression tag | UNP P13714 |
| B | 171 | CYS | HIS | engineered mutation | UNP P13714 |
| B | 321 | HIS | - | expression tag | UNP P13714 |
| B | 322 | HIS | - | expression tag | UNP P13714 |
| B | 323 | HIS | - | expression tag | UNP P13714 |
| B | 324 | HIS | - | expression tag | UNP P13714 |
| B | 325 | HIS | - | expression tag | UNP P13714 |
| B | 326 | HIS | - | expression tag | UNP P13714 |
| C | 171 | CYS | HIS | engineered mutation | UNP P13714 |
| C | 321 | HIS | - | expression tag | UNP P13714 |
| C | 322 | HIS | - | expression tag | UNP P13714 |
| C | 323 | HIS | - | expression tag | UNP P13714 |
| C | 324 | HIS | - | expression tag | UNP P13714 |
| C | 325 | HIS | - | expression tag | UNP P13714 |
| C | 326 | HIS | - | expression tag | UNP P13714 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| D | 171 | CYS | HIS | engineered mutation | UNP P13714 |
| D | 321 | HIS | - | expression tag | UNP P13714 |
| D | 322 | HIS | - | expression tag | UNP P13714 |
| D | 323 | HIS | - | expression tag | UNP P13714 |
| D | 324 | HIS | - | expression tag | UNP P13714 |
| D | 325 | HIS | - | expression tag | UNP P13714 |
| D | 326 | HIS | - | expression tag | UNP P13714 |

- Molecule 2 is water.

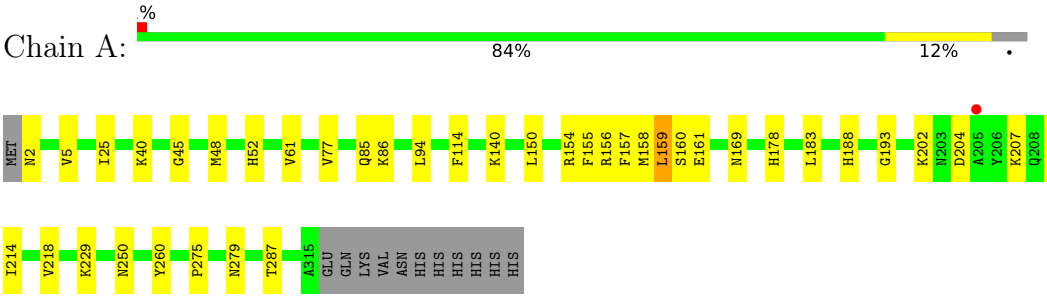
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 2 | A | 157 | Total O<br>157 157 | 0 | 0 |
| 2 | B | 154 | Total O<br>154 154 | 0 | 0 |
| 2 | C | 29 | Total O<br>29 29 | 0 | 0 |
| 2 | D | 38 | Total O<br>38 38 | 0 | 0 |

# 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.

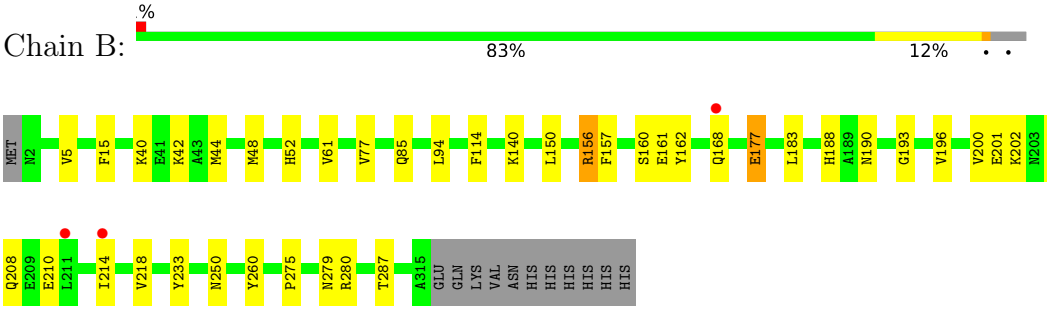
• Molecule 1: L-lactate dehydrogenase

Chain A:



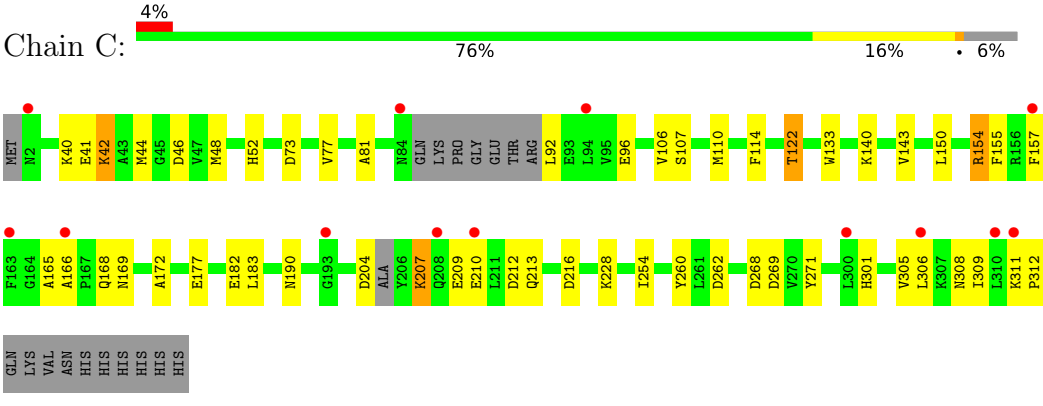

• Molecule 1: L-lactate dehydrogenase

Chain B:



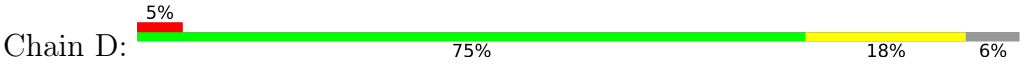

• Molecule 1: L-lactate dehydrogenase

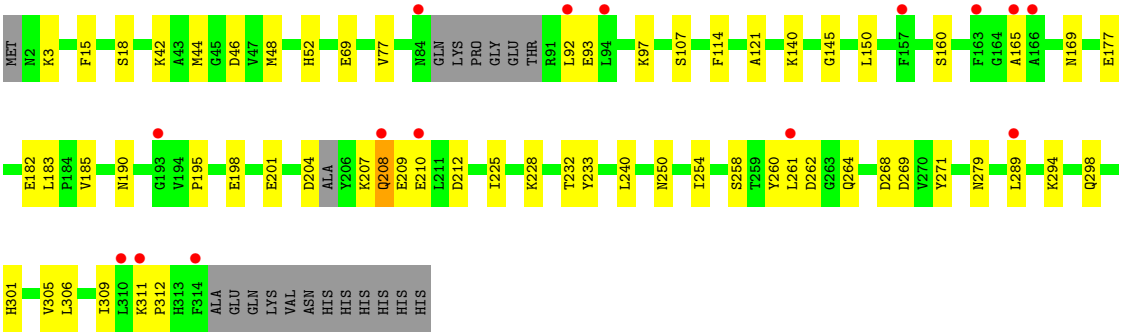
Chain C:




• Molecule 1: L-lactate dehydrogenase

Chain D:




MET N2 K3 F15 S18 K42 A43 M44 G45 D46 V47 M48 H52 E69 V77 N84 GLN LYS PRO GLY GLU THR R91 L92 E93 L94 K97 S107 F114 A121 K140 G145 L150 F157 S160 F163 G164 A165 A166 N169 E177
E182 L183 P184 V185 N190 G193 V194 P195 E198 E201 D204 ALA Y206 K207 Q208 E209 E210 L211 D212 I225 K228 T232 Y233 L240 N250 I254 S258 T259 Y260 L261 D262 G263 Q264 D268 D269 V270 Y271 N279 L289 K294 Q298
H301 V305 L306 I309 L310 K311 P312 H313 F314 ALA GLU GLN LYS VAL ASN HIS HIS HIS HIS HIS HIS

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 31 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 133.41Å 133.41Å 99.33Å<br>90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 26.93 – 2.20<br>26.93 – 2.20 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 99.5 (26.93-2.20)<br>99.5 (26.93-2.20) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 3.56 (at 2.20Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: 1.6_289) | Depositor |
| R, $R_{free}$ | 0.201 , 0.235<br>0.196 , 0.228 | Depositor<br>DCC |
| $R_{free}$ test set | 2993 reflections (3.00%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 44.3 | Xtriage |
| Anisotropy | 0.010 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.35 , 40.5 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.50$, $< L^2 > = 0.33$ | Xtriage |
| Estimated twinning fraction | 0.487 for -h,-k,l<br>0.027 for h,-h-k,-l<br>0.027 for -k,-h,-l | Xtriage |
| $F_o$,$F_c$ correlation | 0.96 | EDS |
| Total number of atoms | 9845 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 54.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

# 5 Model quality

## 5.1 Standard geometry

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\| > 5$ | RMSZ | $\#\|Z\| > 5$ |
| 1 | A | 0.49 | 0/2443 | 0.54 | 0/3311 |
| 1 | B | 0.49 | 0/2443 | 0.54 | 0/3311 |
| 1 | C | 0.34 | 0/2374 | 0.46 | 0/3215 |
| 1 | D | 0.33 | 0/2385 | 0.47 | 0/3229 |
| All | All | 0.42 | 0/9645 | 0.50 | 0/13066 |

There are no bond length outliers.

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 | 2397 | 0 | 2384 | 31 | 0 |
| 1 | B | 2397 | 0 | 2384 | 35 | 0 |
| 1 | C | 2331 | 0 | 2315 | 40 | 0 |
| 1 | D | 2342 | 0 | 2328 | 40 | 0 |
| 2 | A | 157 | 0 | 0 | 6 | 0 |
| 2 | B | 154 | 0 | 0 | 4 | 0 |
| 2 | C | 29 | 0 | 0 | 1 | 0 |
| 2 | D | 38 | 0 | 0 | 0 | 0 |
| All | All | 9845 | 0 | 9411 | 129 | 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 7.

All (129) 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:156:ARG:HH11 | 1:B:156:ARG:HG2 | 1.12 | 1.13 |
| 1:B:85:GLN:HB3 | 1:B:94:LEU:HD22 | 1.43 | 1.00 |
| 1:B:156:ARG:HG2 | 1:B:156:ARG:NH1 | 1.82 | 0.90 |
| 1:A:48:MET:CE | 1:D:228:LYS:HD2 | 2.08 | 0.84 |
| 1:A:159:LEU:N | 2:A:462:HOH:O | 2.07 | 0.81 |
| 1:C:311:LYS:HG3 | 1:C:312:PRO:HD3 | 1.63 | 0.80 |
| 1:C:209:GLU:HA | 1:C:212:ASP:HB2 | 1.67 | 0.76 |
| 1:C:254:ILE:HD12 | 1:D:169:ASN:HB3 | 1.70 | 0.74 |
| 1:C:81:ALA:O | 1:C:122:THR:HG21 | 1.89 | 0.72 |
| 1:A:156:ARG:C | 2:A:462:HOH:O | 2.28 | 0.71 |
| 1:A:48:MET:HE2 | 1:D:228:LYS:HD2 | 1.70 | 0.71 |
| 1:A:48:MET:HE1 | 1:D:228:LYS:HD2 | 1.72 | 0.70 |
| 1:A:158:MET:N | 2:A:462:HOH:O | 2.25 | 0.70 |
| 1:B:48:MET:CE | 1:C:228:LYS:HD2 | 2.23 | 0.68 |
| 1:B:156:ARG:HH11 | 1:B:156:ARG:CG | 1.97 | 0.68 |
| 1:A:52:HIS:CE1 | 1:D:150:LEU:HD21 | 2.30 | 0.66 |
| 1:A:155:PHE:O | 2:A:462:HOH:O | 2.12 | 0.66 |
| 1:B:162:TYR:HE1 | 1:B:210:GLU:HG2 | 1.62 | 0.65 |
| 1:B:48:MET:HE1 | 1:C:228:LYS:HD2 | 1.77 | 0.65 |
| 1:D:160:SER:HB2 | 1:D:165:ALA:O | 1.97 | 0.64 |
| 1:D:294:LYS:HE3 | 1:D:298:GLN:HE22 | 1.62 | 0.64 |
| 1:C:160:SER:HB2 | 1:C:165:ALA:O | 1.99 | 0.62 |
| 1:C:301:HIS:O | 1:C:305:VAL:HG23 | 2.00 | 0.61 |
| 1:B:190:ASN:C | 2:B:478:HOH:O | 2.39 | 0.61 |
| 1:C:140:LYS:HD2 | 1:C:260:TYR:CD2 | 2.36 | 0.60 |
| 1:A:188:HIS:HD2 | 1:B:193:GLY:O | 1.83 | 0.60 |
| 1:A:85:GLN:HB2 | 1:A:94:LEU:HD22 | 1.83 | 0.60 |
| 1:D:140:LYS:HD2 | 1:D:260:TYR:CD2 | 2.37 | 0.59 |
| 1:D:177:GLU:HB2 | 1:D:306:LEU:HD11 | 1.85 | 0.59 |
| 1:A:161:GLU:O | 1:A:161:GLU:HG2 | 2.04 | 0.58 |
| 1:D:301:HIS:O | 1:D:305:VAL:HG23 | 2.03 | 0.58 |
| 1:B:52:HIS:CE1 | 1:C:150:LEU:HD21 | 2.39 | 0.58 |
| 1:D:93:GLU:O | 1:D:97:LYS:HG3 | 2.03 | 0.58 |
| 1:B:44:MET:O | 1:B:48:MET:HE3 | 2.03 | 0.58 |
| 1:A:178:HIS:HD2 | 2:A:372:HOH:O | 1.87 | 0.57 |
| 1:A:193:GLY:O | 1:B:188:HIS:HD2 | 1.88 | 0.57 |
| 1:B:204:ASP:O | 1:B:207:LYS:HE2 | 2.06 | 0.55 |
| 1:D:262:ASP:HA | 1:D:268:ASP:HA | 1.89 | 0.55 |
| 1:A:214:ILE:O | 1:A:218:VAL:HG23 | 2.07 | 0.54 |
| 1:C:169:ASN:ND2 | 1:D:254:ILE:H | 2.05 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:154:ARG:O | 1:A:158:MET:HG3 | 2.08 | 0.54 |
| 1:D:305:VAL:O | 1:D:309:ILE:HG13 | 2.07 | 0.54 |
| 1:B:162:TYR:CE1 | 1:B:210:GLU:HG2 | 2.41 | 0.53 |
| 1:D:225:ILE:HG21 | 1:D:232:THR:HG22 | 1.90 | 0.52 |
| 1:D:311:LYS:HB2 | 1:D:312:PRO:HD3 | 1.90 | 0.52 |
| 1:C:177:GLU:O | 1:C:182:GLU:HB3 | 2.10 | 0.52 |
| 1:B:156:ARG:HD3 | 2:B:390:HOH:O | 2.10 | 0.52 |
| 1:D:77:VAL:HG23 | 1:D:114:PHE:CE1 | 2.45 | 0.52 |
| 1:D:225:ILE:CG2 | 1:D:232:THR:HG22 | 2.40 | 0.52 |
| 1:D:185:VAL:HG11 | 1:D:289:LEU:HD13 | 1.92 | 0.52 |
| 1:D:44:MET:O | 1:D:48:MET:HG3 | 2.11 | 0.51 |
| 1:A:2:ASN:HB3 | 1:A:5:VAL:O | 2.11 | 0.50 |
| 1:D:294:LYS:HE3 | 1:D:298:GLN:NE2 | 2.24 | 0.50 |
| 1:A:45:GLY:HA2 | 1:A:48:MET:HE3 | 1.93 | 0.50 |
| 1:A:140:LYS:HD2 | 1:A:260:TYR:CD2 | 2.46 | 0.50 |
| 1:D:260:TYR:OH | 1:D:269:ASP:HA | 2.12 | 0.50 |
| 1:A:204:ASP:O | 1:A:207:LYS:HE2 | 2.11 | 0.49 |
| 1:C:305:VAL:O | 1:C:309:ILE:HG13 | 2.12 | 0.49 |
| 1:D:260:TYR:CZ | 1:D:269:ASP:HA | 2.47 | 0.49 |
| 1:C:92:LEU:O | 1:C:96:GLU:HG3 | 2.13 | 0.49 |
| 1:C:169:ASN:HB2 | 1:D:254:ILE:HD12 | 1.95 | 0.49 |
| 1:D:250:ASN:OD1 | 1:D:279:ASN:HB2 | 2.13 | 0.49 |
| 1:B:157:PHE:CE2 | 1:B:161:GLU:OE2 | 2.66 | 0.49 |
| 1:C:157:PHE:CE2 | 1:C:161:GLU:OE1 | 2.66 | 0.49 |
| 1:B:275:PRO:HB2 | 1:B:287:THR:HB | 1.94 | 0.48 |
| 1:D:177:GLU:O | 1:D:182:GLU:HB3 | 2.13 | 0.48 |
| 1:C:155:PHE:CE2 | 1:C:172:ALA:HB1 | 2.48 | 0.48 |
| 1:C:311:LYS:CG | 1:C:312:PRO:HD3 | 2.39 | 0.48 |
| 1:B:140:LYS:HD2 | 1:B:260:TYR:CD2 | 2.48 | 0.48 |
| 1:B:214:ILE:O | 1:B:218:VAL:HG23 | 2.14 | 0.48 |
| 1:A:250:ASN:OD1 | 1:A:279:ASN:HB2 | 2.13 | 0.48 |
| 1:B:150:LEU:HD21 | 1:C:52:HIS:CE1 | 2.49 | 0.47 |
| 1:A:158:MET:SD | 2:A:457:HOH:O | 2.60 | 0.47 |
| 1:A:40:LYS:HE3 | 1:A:40:LYS:HB3 | 1.80 | 0.47 |
| 1:A:150:LEU:HD21 | 1:D:52:HIS:CE1 | 2.49 | 0.47 |
| 1:B:177:GLU:O | 1:B:177:GLU:HG2 | 2.12 | 0.47 |
| 1:C:77:VAL:HG23 | 1:C:114:PHE:CE1 | 2.50 | 0.47 |
| 1:D:195:PRO:HG2 | 1:D:198:GLU:HG3 | 1.97 | 0.47 |
| 1:A:25:ILE:HG12 | 1:A:61:VAL:HG11 | 1.95 | 0.47 |
| 1:B:202:LYS:HB2 | 1:B:202:LYS:NZ | 2.30 | 0.47 |
| 1:A:158:MET:O | 1:A:161:GLU:C | 2.53 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:280:ARG:NH2 | 1:D:3:LYS:HD3 | 2.30 | 0.46 |
| 1:A:77:VAL:HG23 | 1:A:114:PHE:CE1 | 2.51 | 0.46 |
| 1:B:196:VAL:O | 1:B:200:VAL:HG23 | 2.16 | 0.46 |
| 1:C:154:ARG:NH1 | 2:C:348:HOH:O | 2.46 | 0.46 |
| 1:D:177:GLU:HG3 | 1:D:306:LEU:HD21 | 1.96 | 0.45 |
| 1:B:77:VAL:HG23 | 1:B:114:PHE:CE1 | 2.51 | 0.45 |
| 1:D:42:LYS:HD2 | 1:D:42:LYS:HA | 1.82 | 0.45 |
| 1:D:145:GLY:HA3 | 1:D:258:SER:HB2 | 1.99 | 0.44 |
| 1:B:250:ASN:OD1 | 1:B:279:ASN:HB2 | 2.17 | 0.44 |
| 1:C:207:LYS:HD2 | 1:C:207:LYS:N | 2.32 | 0.44 |
| 1:C:40:LYS:HE3 | 1:C:41:GLU:OE1 | 2.18 | 0.44 |
| 1:C:262:ASP:HA | 1:C:268:ASP:HA | 2.00 | 0.44 |
| 1:C:177:GLU:HG3 | 1:C:306:LEU:HD21 | 1.99 | 0.44 |
| 1:C:260:TYR:OH | 1:C:269:ASP:HA | 2.18 | 0.43 |
| 1:C:157:PHE:HE2 | 1:C:161:GLU:OE1 | 2.00 | 0.43 |
| 1:D:208:GLN:HE21 | 1:D:208:GLN:HA | 1.83 | 0.43 |
| 1:B:42:LYS:NZ | 2:B:435:HOH:O | 2.51 | 0.43 |
| 1:C:133:TRP:HA | 1:C:143:VAL:HG21 | 2.00 | 0.43 |
| 1:B:48:MET:HE2 | 1:C:228:LYS:HD2 | 1.99 | 0.43 |
| 1:C:260:TYR:CZ | 1:C:269:ASP:HA | 2.53 | 0.43 |
| 1:A:209:GLU:HA | 1:A:209:GLU:OE2 | 2.18 | 0.43 |
| 1:C:106:VAL:O | 1:C:110:MET:HG2 | 2.18 | 0.43 |
| 1:A:159:LEU:HD12 | 1:A:159:LEU:HA | 1.73 | 0.42 |
| 1:B:204:ASP:HA | 2:B:342:HOH:O | 2.19 | 0.42 |
| 1:D:260:TYR:HB2 | 1:D:271:TYR:CZ | 2.54 | 0.42 |
| 1:C:213:GLN:HA | 1:C:216:ASP:OD2 | 2.20 | 0.42 |
| 1:D:15:PHE:HB3 | 1:D:233:TYR:CD2 | 2.54 | 0.42 |
| 1:C:44:MET:O | 1:C:48:MET:HG3 | 2.19 | 0.42 |
| 1:D:261:LEU:HD22 | 1:D:264:GLN:HB2 | 2.00 | 0.42 |
| 1:C:260:TYR:HB2 | 1:C:271:TYR:CZ | 2.55 | 0.42 |
| 1:D:145:GLY:CA | 1:D:258:SER:HB2 | 2.49 | 0.42 |
| 1:A:157:PHE:CD2 | 1:A:157:PHE:C | 2.93 | 0.42 |
| 1:A:275:PRO:HB2 | 1:A:287:THR:HB | 2.01 | 0.42 |
| 1:C:169:ASN:HD21 | 1:D:254:ILE:H | 1.67 | 0.41 |
| 1:B:40:LYS:HE3 | 1:B:40:LYS:HB3 | 1.90 | 0.41 |
| 1:B:61:VAL:O | 1:B:61:VAL:HG13 | 2.19 | 0.41 |
| 1:B:15:PHE:HB3 | 1:B:233:TYR:CD2 | 2.55 | 0.41 |
| 1:C:309:ILE:HG13 | 1:C:309:ILE:H | 1.65 | 0.41 |
| 1:B:207:LYS:HD3 | 1:B:207:LYS:N | 2.36 | 0.41 |
| 1:B:168:GLN:H | 1:B:168:GLN:HG2 | 1.65 | 0.41 |
| 1:B:202:LYS:NZ | 1:B:202:LYS:CB | 2.84 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:166:ALA:HB1 | 1:C:168:GLN:OE1 | 2.21 | 0.41 |
| 1:C:204:ASP:O | 1:C:207:LYS:HE3 | 2.20 | 0.41 |
| 1:C:73:ASP:OD1 | 1:C:73:ASP:N | 2.53 | 0.41 |
| 1:D:209:GLU:HA | 1:D:212:ASP:HB3 | 2.03 | 0.40 |
| 1:D:121:ALA:HB2 | 1:D:240:LEU:HD21 | 2.03 | 0.40 |
| 1:A:61:VAL:HG13 | 1:A:61:VAL:O | 2.21 | 0.40 |
| 1:C:42:LYS:HE2 | 1:C:42:LYS:HB3 | 1.90 | 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 | 312/326 (96%) | 301 (96%) | 11 (4%) | 0 | 100 | 100 |
| 1 | B | 312/326 (96%) | 301 (96%) | 11 (4%) | 0 | 100 | 100 |
| 1 | C | 299/326 (92%) | 284 (95%) | 15 (5%) | 0 | 100 | 100 |
| 1 | D | 300/326 (92%) | 291 (97%) | 9 (3%) | 0 | 100 | 100 |
| All | All | 1223/1304 (94%) | 1177 (96%) | 46 (4%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

### 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 | 255/267 (96%) | 248 (97%) | 7 (3%) | 44 | 57 |
| 1 | B | 255/267 (96%) | 247 (97%) | 8 (3%) | 40 | 51 |
| 1 | C | 249/267 (93%) | 239 (96%) | 10 (4%) | 31 | 40 |
| 1 | D | 250/267 (94%) | 238 (95%) | 12 (5%) | 25 | 32 |
| All | All | 1009/1068 (94%) | 972 (96%) | 37 (4%) | 34 | 43 |

All (37) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 86 | LYS |
| 1 | A | 159 | LEU |
| 1 | A | 160 | SER |
| 1 | A | 169 | ASN |
| 1 | A | 183 | LEU |
| 1 | A | 202 | LYS |
| 1 | A | 229 | LYS |
| 1 | B | 5 | VAL |
| 1 | B | 156 | ARG |
| 1 | B | 160 | SER |
| 1 | B | 177 | GLU |
| 1 | B | 183 | LEU |
| 1 | B | 201 | GLU |
| 1 | B | 207 | LYS |
| 1 | B | 208 | GLN |
| 1 | C | 42 | LYS |
| 1 | C | 46 | ASP |
| 1 | C | 107 | SER |
| 1 | C | 122 | THR |
| 1 | C | 154 | ARG |
| 1 | C | 183 | LEU |
| 1 | C | 190 | ASN |
| 1 | C | 207 | LYS |
| 1 | C | 210 | GLU |
| 1 | C | 308 | ASN |
| 1 | D | 18 | SER |
| 1 | D | 46 | ASP |
| 1 | D | 69 | GLU |
| 1 | D | 92 | LEU |
| 1 | D | 107 | SER |
| 1 | D | 183 | LEU |
| 1 | D | 190 | ASN |
| 1 | D | 201 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 204 | ASP |
| 1 | D | 207 | LYS |
| 1 | D | 208 | GLN |
| 1 | D | 210 | GLU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 52 | HIS |
| 1 | A | 213 | GLN |
| 1 | B | 6 | ASN |
| 1 | B | 52 | HIS |
| 1 | C | 169 | ASN |
| 1 | C | 203 | ASN |
| 1 | D | 52 | HIS |
| 1 | D | 188 | HIS |
| 1 | D | 203 | ASN |
| 1 | D | 208 | GLN |
| 1 | D | 249 | HIS |

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 6 Fit of model and data

## 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 1 | A | 314/326 (96%) | -0.03 | 2 (0%) | 89 | 88 | 27, 40, 65, 81 | 0 |
| 1 | B | 314/326 (96%) | -0.02 | 4 (1%) | 77 | 75 | 27, 40, 66, 81 | 0 |
| 1 | C | 305/326 (93%) | 0.22 | 14 (4%) | 32 | 31 | 39, 63, 92, 103 | 0 |
| 1 | D | 306/326 (93%) | 0.21 | 15 (4%) | 29 | 28 | 39, 64, 93, 110 | 0 |
| All | All | 1239/1304 (95%) | 0.09 | 35 (2%) | 53 | 51 | 27, 51, 86, 110 | 0 |

All (35) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | D | 94 | LEU | 4.3 |
| 1 | C | 193 | GLY | 4.3 |
| 1 | C | 94 | LEU | 4.2 |
| 1 | A | 205 | ALA | 4.0 |
| 1 | C | 314 | PHE | 3.8 |
| 1 | D | 193 | GLY | 3.7 |
| 1 | D | 314 | PHE | 3.6 |
| 1 | D | 163 | PHE | 3.4 |
| 1 | C | 163 | PHE | 3.3 |
| 1 | D | 210 | GLU | 3.1 |
| 1 | D | 208 | GLN | 2.9 |
| 1 | A | 211 | LEU | 2.9 |
| 1 | B | 205 | ALA | 2.9 |
| 1 | D | 157 | PHE | 2.8 |
| 1 | D | 310 | LEU | 2.8 |
| 1 | D | 311 | LYS | 2.7 |
| 1 | C | 310 | LEU | 2.7 |
| 1 | C | 208 | GLN | 2.7 |
| 1 | D | 92 | LEU | 2.7 |
| 1 | C | 157 | PHE | 2.6 |
| 1 | B | 168 | GLN | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | D | 166 | ALA | 2.6 |
| 1 | C | 306 | LEU | 2.5 |
| 1 | C | 311 | LYS | 2.4 |
| 1 | D | 261 | LEU | 2.4 |
| 1 | D | 84 | ASN | 2.4 |
| 1 | D | 289 | LEU | 2.4 |
| 1 | C | 210 | GLU | 2.3 |
| 1 | C | 166 | ALA | 2.3 |
| 1 | C | 300 | LEU | 2.3 |
| 1 | C | 2 | ASN | 2.2 |
| 1 | B | 214 | ILE | 2.2 |
| 1 | C | 84 | ASN | 2.2 |
| 1 | B | 211 | LEU | 2.2 |
| 1 | D | 165 | ALA | 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)

There are no ligands in this entry.

## 6.5 Other polymers (i)

There are no such residues in this entry.