



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 03:49 PM GMT

PDB ID : 4DEJ
Title : Crystal structure of glutathione transferase-like protein IL0419 (Target EFI-501089) from Idiomarina loihiensis L2TR
Authors : Patskovsky, Y.; Toro, R.; Bhosle, R.; Zencheck, W.D.; Hillerich, B.; Seidel, R.D.; Washington, E.; Scott Glenn, A.; Chowdhury, S.; Evans, B.; Hammonds, J.; Imker, H.J.; Armstrong, R.N.; Gerlt, J.A.; Almo, S.C.; Enzyme Function Initiative (EFI)
Deposited on : 2012-01-20
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

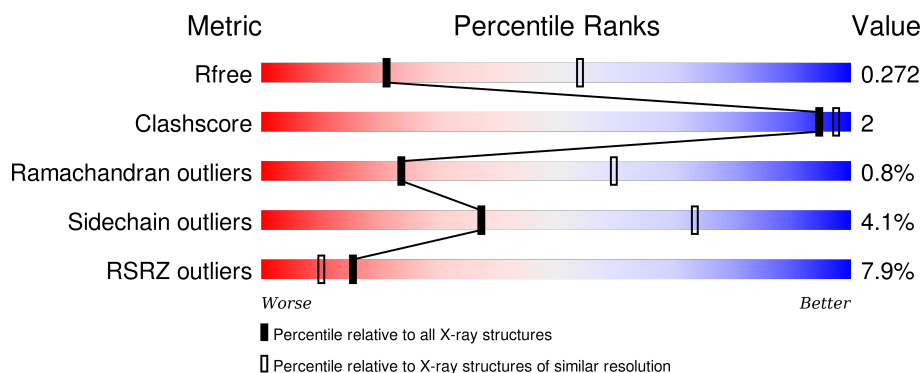
1 Overall quality at a glance

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 $\leq 5\%$. 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 | 231 | <div> <div>7%</div> <div>78% 8% • 13%</div> </div> |
| 1 | B | 231 | <div> <div>81% 5% • 13%</div> </div> |
| 1 | C | 231 | <div> <div>3%</div> <div>79% 8% 13%</div> </div> |
| 1 | D | 231 | <div> <div>6%</div> <div>83% • • 12%</div> </div> |
| 1 | E | 231 | <div> <div>4%</div> <div>79% 6% • 13%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | F | 231 | |
| 1 | G | 231 | |
| 1 | H | 231 | |
| 1 | I | 231 | |
| 1 | J | 231 | |
| 1 | K | 231 | |
| 1 | L | 231 | |

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19591 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 Glutathione S-transferase related protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1 | A | 202 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1639 | 1051 | 268 | 312 | 8 | | | |
| 1 | B | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1634 | 1048 | 267 | 311 | 8 | | | |
| 1 | C | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1634 | 1048 | 267 | 311 | 8 | | | |
| 1 | D | 203 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1653 | 1058 | 273 | 314 | 8 | | | |
| 1 | E | 200 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1625 | 1042 | 265 | 310 | 8 | | | |
| 1 | F | 197 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1601 | 1030 | 258 | 305 | 8 | | | |
| 1 | G | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1625 | 1044 | 263 | 310 | 8 | | | |
| 1 | H | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1636 | 1048 | 269 | 311 | 8 | | | |
| 1 | I | 200 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1629 | 1045 | 266 | 310 | 8 | | | |
| 1 | J | 202 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1643 | 1053 | 268 | 314 | 8 | | | |
| 1 | K | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1640 | 1051 | 270 | 311 | 8 | | | |
| 1 | L | 200 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1618 | 1038 | 263 | 309 | 8 | | | |

There are 288 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | -1 | MET | - | EXPRESSION TAG | UNP Q5R0K1 |
| A | 0 | VAL | - | EXPRESSION TAG | UNP Q5R0K1 |
| A | 208 | ALA | - | EXPRESSION TAG | UNP Q5R0K1 |
| A | 209 | GLU | - | EXPRESSION TAG | UNP Q5R0K1 |
| A | 210 | ASN | - | EXPRESSION TAG | UNP Q5R0K1 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | 211 | LEU | - | EXPRESSION TAG | UNP Q5R0K1 |
| A | 212 | TYR | - | EXPRESSION TAG | UNP Q5R0K1 |
| A | 213 | PHE | - | EXPRESSION TAG | UNP Q5R0K1 |
| A | 214 | GLN | - | EXPRESSION TAG | UNP Q5R0K1 |
| A | 215 | SER | - | EXPRESSION TAG | UNP Q5R0K1 |
| A | 216 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| A | 217 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| A | 218 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| A | 219 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| A | 220 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| A | 221 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| A | 222 | TRP | - | EXPRESSION TAG | UNP Q5R0K1 |
| A | 223 | SER | - | EXPRESSION TAG | UNP Q5R0K1 |
| A | 224 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| A | 225 | PRO | - | EXPRESSION TAG | UNP Q5R0K1 |
| A | 226 | GLN | - | EXPRESSION TAG | UNP Q5R0K1 |
| A | 227 | PHE | - | EXPRESSION TAG | UNP Q5R0K1 |
| A | 228 | GLU | - | EXPRESSION TAG | UNP Q5R0K1 |
| A | 229 | LYS | - | EXPRESSION TAG | UNP Q5R0K1 |
| B | -1 | MET | - | EXPRESSION TAG | UNP Q5R0K1 |
| B | 0 | VAL | - | EXPRESSION TAG | UNP Q5R0K1 |
| B | 208 | ALA | - | EXPRESSION TAG | UNP Q5R0K1 |
| B | 209 | GLU | - | EXPRESSION TAG | UNP Q5R0K1 |
| B | 210 | ASN | - | EXPRESSION TAG | UNP Q5R0K1 |
| B | 211 | LEU | - | EXPRESSION TAG | UNP Q5R0K1 |
| B | 212 | TYR | - | EXPRESSION TAG | UNP Q5R0K1 |
| B | 213 | PHE | - | EXPRESSION TAG | UNP Q5R0K1 |
| B | 214 | GLN | - | EXPRESSION TAG | UNP Q5R0K1 |
| B | 215 | SER | - | EXPRESSION TAG | UNP Q5R0K1 |
| B | 216 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| B | 217 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| B | 218 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| B | 219 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| B | 220 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| B | 221 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| B | 222 | TRP | - | EXPRESSION TAG | UNP Q5R0K1 |
| B | 223 | SER | - | EXPRESSION TAG | UNP Q5R0K1 |
| B | 224 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| B | 225 | PRO | - | EXPRESSION TAG | UNP Q5R0K1 |
| B | 226 | GLN | - | EXPRESSION TAG | UNP Q5R0K1 |
| B | 227 | PHE | - | EXPRESSION TAG | UNP Q5R0K1 |
| B | 228 | GLU | - | EXPRESSION TAG | UNP Q5R0K1 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| B | 229 | LYS | - | EXPRESSION TAG | UNP Q5R0K1 |
| C | -1 | MET | - | EXPRESSION TAG | UNP Q5R0K1 |
| C | 0 | VAL | - | EXPRESSION TAG | UNP Q5R0K1 |
| C | 208 | ALA | - | EXPRESSION TAG | UNP Q5R0K1 |
| C | 209 | GLU | - | EXPRESSION TAG | UNP Q5R0K1 |
| C | 210 | ASN | - | EXPRESSION TAG | UNP Q5R0K1 |
| C | 211 | LEU | - | EXPRESSION TAG | UNP Q5R0K1 |
| C | 212 | TYR | - | EXPRESSION TAG | UNP Q5R0K1 |
| C | 213 | PHE | - | EXPRESSION TAG | UNP Q5R0K1 |
| C | 214 | GLN | - | EXPRESSION TAG | UNP Q5R0K1 |
| C | 215 | SER | - | EXPRESSION TAG | UNP Q5R0K1 |
| C | 216 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| C | 217 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| C | 218 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| C | 219 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| C | 220 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| C | 221 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| C | 222 | TRP | - | EXPRESSION TAG | UNP Q5R0K1 |
| C | 223 | SER | - | EXPRESSION TAG | UNP Q5R0K1 |
| C | 224 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| C | 225 | PRO | - | EXPRESSION TAG | UNP Q5R0K1 |
| C | 226 | GLN | - | EXPRESSION TAG | UNP Q5R0K1 |
| C | 227 | PHE | - | EXPRESSION TAG | UNP Q5R0K1 |
| C | 228 | GLU | - | EXPRESSION TAG | UNP Q5R0K1 |
| C | 229 | LYS | - | EXPRESSION TAG | UNP Q5R0K1 |
| D | -1 | MET | - | EXPRESSION TAG | UNP Q5R0K1 |
| D | 0 | VAL | - | EXPRESSION TAG | UNP Q5R0K1 |
| D | 208 | ALA | - | EXPRESSION TAG | UNP Q5R0K1 |
| D | 209 | GLU | - | EXPRESSION TAG | UNP Q5R0K1 |
| D | 210 | ASN | - | EXPRESSION TAG | UNP Q5R0K1 |
| D | 211 | LEU | - | EXPRESSION TAG | UNP Q5R0K1 |
| D | 212 | TYR | - | EXPRESSION TAG | UNP Q5R0K1 |
| D | 213 | PHE | - | EXPRESSION TAG | UNP Q5R0K1 |
| D | 214 | GLN | - | EXPRESSION TAG | UNP Q5R0K1 |
| D | 215 | SER | - | EXPRESSION TAG | UNP Q5R0K1 |
| D | 216 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| D | 217 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| D | 218 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| D | 219 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| D | 220 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| D | 221 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| D | 222 | TRP | - | EXPRESSION TAG | UNP Q5R0K1 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| D | 223 | SER | - | EXPRESSION TAG | UNP Q5R0K1 |
| D | 224 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| D | 225 | PRO | - | EXPRESSION TAG | UNP Q5R0K1 |
| D | 226 | GLN | - | EXPRESSION TAG | UNP Q5R0K1 |
| D | 227 | PHE | - | EXPRESSION TAG | UNP Q5R0K1 |
| D | 228 | GLU | - | EXPRESSION TAG | UNP Q5R0K1 |
| D | 229 | LYS | - | EXPRESSION TAG | UNP Q5R0K1 |
| E | -1 | MET | - | EXPRESSION TAG | UNP Q5R0K1 |
| E | 0 | VAL | - | EXPRESSION TAG | UNP Q5R0K1 |
| E | 208 | ALA | - | EXPRESSION TAG | UNP Q5R0K1 |
| E | 209 | GLU | - | EXPRESSION TAG | UNP Q5R0K1 |
| E | 210 | ASN | - | EXPRESSION TAG | UNP Q5R0K1 |
| E | 211 | LEU | - | EXPRESSION TAG | UNP Q5R0K1 |
| E | 212 | TYR | - | EXPRESSION TAG | UNP Q5R0K1 |
| E | 213 | PHE | - | EXPRESSION TAG | UNP Q5R0K1 |
| E | 214 | GLN | - | EXPRESSION TAG | UNP Q5R0K1 |
| E | 215 | SER | - | EXPRESSION TAG | UNP Q5R0K1 |
| E | 216 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| E | 217 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| E | 218 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| E | 219 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| E | 220 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| E | 221 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| E | 222 | TRP | - | EXPRESSION TAG | UNP Q5R0K1 |
| E | 223 | SER | - | EXPRESSION TAG | UNP Q5R0K1 |
| E | 224 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| E | 225 | PRO | - | EXPRESSION TAG | UNP Q5R0K1 |
| E | 226 | GLN | - | EXPRESSION TAG | UNP Q5R0K1 |
| E | 227 | PHE | - | EXPRESSION TAG | UNP Q5R0K1 |
| E | 228 | GLU | - | EXPRESSION TAG | UNP Q5R0K1 |
| E | 229 | LYS | - | EXPRESSION TAG | UNP Q5R0K1 |
| F | -1 | MET | - | EXPRESSION TAG | UNP Q5R0K1 |
| F | 0 | VAL | - | EXPRESSION TAG | UNP Q5R0K1 |
| F | 208 | ALA | - | EXPRESSION TAG | UNP Q5R0K1 |
| F | 209 | GLU | - | EXPRESSION TAG | UNP Q5R0K1 |
| F | 210 | ASN | - | EXPRESSION TAG | UNP Q5R0K1 |
| F | 211 | LEU | - | EXPRESSION TAG | UNP Q5R0K1 |
| F | 212 | TYR | - | EXPRESSION TAG | UNP Q5R0K1 |
| F | 213 | PHE | - | EXPRESSION TAG | UNP Q5R0K1 |
| F | 214 | GLN | - | EXPRESSION TAG | UNP Q5R0K1 |
| F | 215 | SER | - | EXPRESSION TAG | UNP Q5R0K1 |
| F | 216 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| F | 217 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| F | 218 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| F | 219 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| F | 220 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| F | 221 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| F | 222 | TRP | - | EXPRESSION TAG | UNP Q5R0K1 |
| F | 223 | SER | - | EXPRESSION TAG | UNP Q5R0K1 |
| F | 224 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| F | 225 | PRO | - | EXPRESSION TAG | UNP Q5R0K1 |
| F | 226 | GLN | - | EXPRESSION TAG | UNP Q5R0K1 |
| F | 227 | PHE | - | EXPRESSION TAG | UNP Q5R0K1 |
| F | 228 | GLU | - | EXPRESSION TAG | UNP Q5R0K1 |
| F | 229 | LYS | - | EXPRESSION TAG | UNP Q5R0K1 |
| G | -1 | MET | - | EXPRESSION TAG | UNP Q5R0K1 |
| G | 0 | VAL | - | EXPRESSION TAG | UNP Q5R0K1 |
| G | 208 | ALA | - | EXPRESSION TAG | UNP Q5R0K1 |
| G | 209 | GLU | - | EXPRESSION TAG | UNP Q5R0K1 |
| G | 210 | ASN | - | EXPRESSION TAG | UNP Q5R0K1 |
| G | 211 | LEU | - | EXPRESSION TAG | UNP Q5R0K1 |
| G | 212 | TYR | - | EXPRESSION TAG | UNP Q5R0K1 |
| G | 213 | PHE | - | EXPRESSION TAG | UNP Q5R0K1 |
| G | 214 | GLN | - | EXPRESSION TAG | UNP Q5R0K1 |
| G | 215 | SER | - | EXPRESSION TAG | UNP Q5R0K1 |
| G | 216 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| G | 217 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| G | 218 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| G | 219 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| G | 220 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| G | 221 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| G | 222 | TRP | - | EXPRESSION TAG | UNP Q5R0K1 |
| G | 223 | SER | - | EXPRESSION TAG | UNP Q5R0K1 |
| G | 224 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| G | 225 | PRO | - | EXPRESSION TAG | UNP Q5R0K1 |
| G | 226 | GLN | - | EXPRESSION TAG | UNP Q5R0K1 |
| G | 227 | PHE | - | EXPRESSION TAG | UNP Q5R0K1 |
| G | 228 | GLU | - | EXPRESSION TAG | UNP Q5R0K1 |
| G | 229 | LYS | - | EXPRESSION TAG | UNP Q5R0K1 |
| H | -1 | MET | - | EXPRESSION TAG | UNP Q5R0K1 |
| H | 0 | VAL | - | EXPRESSION TAG | UNP Q5R0K1 |
| H | 208 | ALA | - | EXPRESSION TAG | UNP Q5R0K1 |
| H | 209 | GLU | - | EXPRESSION TAG | UNP Q5R0K1 |
| H | 210 | ASN | - | EXPRESSION TAG | UNP Q5R0K1 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| H | 211 | LEU | - | EXPRESSION TAG | UNP Q5R0K1 |
| H | 212 | TYR | - | EXPRESSION TAG | UNP Q5R0K1 |
| H | 213 | PHE | - | EXPRESSION TAG | UNP Q5R0K1 |
| H | 214 | GLN | - | EXPRESSION TAG | UNP Q5R0K1 |
| H | 215 | SER | - | EXPRESSION TAG | UNP Q5R0K1 |
| H | 216 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| H | 217 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| H | 218 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| H | 219 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| H | 220 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| H | 221 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| H | 222 | TRP | - | EXPRESSION TAG | UNP Q5R0K1 |
| H | 223 | SER | - | EXPRESSION TAG | UNP Q5R0K1 |
| H | 224 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| H | 225 | PRO | - | EXPRESSION TAG | UNP Q5R0K1 |
| H | 226 | GLN | - | EXPRESSION TAG | UNP Q5R0K1 |
| H | 227 | PHE | - | EXPRESSION TAG | UNP Q5R0K1 |
| H | 228 | GLU | - | EXPRESSION TAG | UNP Q5R0K1 |
| H | 229 | LYS | - | EXPRESSION TAG | UNP Q5R0K1 |
| I | -1 | MET | - | EXPRESSION TAG | UNP Q5R0K1 |
| I | 0 | VAL | - | EXPRESSION TAG | UNP Q5R0K1 |
| I | 208 | ALA | - | EXPRESSION TAG | UNP Q5R0K1 |
| I | 209 | GLU | - | EXPRESSION TAG | UNP Q5R0K1 |
| I | 210 | ASN | - | EXPRESSION TAG | UNP Q5R0K1 |
| I | 211 | LEU | - | EXPRESSION TAG | UNP Q5R0K1 |
| I | 212 | TYR | - | EXPRESSION TAG | UNP Q5R0K1 |
| I | 213 | PHE | - | EXPRESSION TAG | UNP Q5R0K1 |
| I | 214 | GLN | - | EXPRESSION TAG | UNP Q5R0K1 |
| I | 215 | SER | - | EXPRESSION TAG | UNP Q5R0K1 |
| I | 216 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| I | 217 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| I | 218 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| I | 219 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| I | 220 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| I | 221 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| I | 222 | TRP | - | EXPRESSION TAG | UNP Q5R0K1 |
| I | 223 | SER | - | EXPRESSION TAG | UNP Q5R0K1 |
| I | 224 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| I | 225 | PRO | - | EXPRESSION TAG | UNP Q5R0K1 |
| I | 226 | GLN | - | EXPRESSION TAG | UNP Q5R0K1 |
| I | 227 | PHE | - | EXPRESSION TAG | UNP Q5R0K1 |
| I | 228 | GLU | - | EXPRESSION TAG | UNP Q5R0K1 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| I | 229 | LYS | - | EXPRESSION TAG | UNP Q5R0K1 |
| J | -1 | MET | - | EXPRESSION TAG | UNP Q5R0K1 |
| J | 0 | VAL | - | EXPRESSION TAG | UNP Q5R0K1 |
| J | 208 | ALA | - | EXPRESSION TAG | UNP Q5R0K1 |
| J | 209 | GLU | - | EXPRESSION TAG | UNP Q5R0K1 |
| J | 210 | ASN | - | EXPRESSION TAG | UNP Q5R0K1 |
| J | 211 | LEU | - | EXPRESSION TAG | UNP Q5R0K1 |
| J | 212 | TYR | - | EXPRESSION TAG | UNP Q5R0K1 |
| J | 213 | PHE | - | EXPRESSION TAG | UNP Q5R0K1 |
| J | 214 | GLN | - | EXPRESSION TAG | UNP Q5R0K1 |
| J | 215 | SER | - | EXPRESSION TAG | UNP Q5R0K1 |
| J | 216 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| J | 217 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| J | 218 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| J | 219 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| J | 220 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| J | 221 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| J | 222 | TRP | - | EXPRESSION TAG | UNP Q5R0K1 |
| J | 223 | SER | - | EXPRESSION TAG | UNP Q5R0K1 |
| J | 224 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| J | 225 | PRO | - | EXPRESSION TAG | UNP Q5R0K1 |
| J | 226 | GLN | - | EXPRESSION TAG | UNP Q5R0K1 |
| J | 227 | PHE | - | EXPRESSION TAG | UNP Q5R0K1 |
| J | 228 | GLU | - | EXPRESSION TAG | UNP Q5R0K1 |
| J | 229 | LYS | - | EXPRESSION TAG | UNP Q5R0K1 |
| K | -1 | MET | - | EXPRESSION TAG | UNP Q5R0K1 |
| K | 0 | VAL | - | EXPRESSION TAG | UNP Q5R0K1 |
| K | 208 | ALA | - | EXPRESSION TAG | UNP Q5R0K1 |
| K | 209 | GLU | - | EXPRESSION TAG | UNP Q5R0K1 |
| K | 210 | ASN | - | EXPRESSION TAG | UNP Q5R0K1 |
| K | 211 | LEU | - | EXPRESSION TAG | UNP Q5R0K1 |
| K | 212 | TYR | - | EXPRESSION TAG | UNP Q5R0K1 |
| K | 213 | PHE | - | EXPRESSION TAG | UNP Q5R0K1 |
| K | 214 | GLN | - | EXPRESSION TAG | UNP Q5R0K1 |
| K | 215 | SER | - | EXPRESSION TAG | UNP Q5R0K1 |
| K | 216 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| K | 217 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| K | 218 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| K | 219 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| K | 220 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| K | 221 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| K | 222 | TRP | - | EXPRESSION TAG | UNP Q5R0K1 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| K | 223 | SER | - | EXPRESSION TAG | UNP Q5R0K1 |
| K | 224 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| K | 225 | PRO | - | EXPRESSION TAG | UNP Q5R0K1 |
| K | 226 | GLN | - | EXPRESSION TAG | UNP Q5R0K1 |
| K | 227 | PHE | - | EXPRESSION TAG | UNP Q5R0K1 |
| K | 228 | GLU | - | EXPRESSION TAG | UNP Q5R0K1 |
| K | 229 | LYS | - | EXPRESSION TAG | UNP Q5R0K1 |
| L | -1 | MET | - | EXPRESSION TAG | UNP Q5R0K1 |
| L | 0 | VAL | - | EXPRESSION TAG | UNP Q5R0K1 |
| L | 208 | ALA | - | EXPRESSION TAG | UNP Q5R0K1 |
| L | 209 | GLU | - | EXPRESSION TAG | UNP Q5R0K1 |
| L | 210 | ASN | - | EXPRESSION TAG | UNP Q5R0K1 |
| L | 211 | LEU | - | EXPRESSION TAG | UNP Q5R0K1 |
| L | 212 | TYR | - | EXPRESSION TAG | UNP Q5R0K1 |
| L | 213 | PHE | - | EXPRESSION TAG | UNP Q5R0K1 |
| L | 214 | GLN | - | EXPRESSION TAG | UNP Q5R0K1 |
| L | 215 | SER | - | EXPRESSION TAG | UNP Q5R0K1 |
| L | 216 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| L | 217 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| L | 218 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| L | 219 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| L | 220 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| L | 221 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| L | 222 | TRP | - | EXPRESSION TAG | UNP Q5R0K1 |
| L | 223 | SER | - | EXPRESSION TAG | UNP Q5R0K1 |
| L | 224 | HIS | - | EXPRESSION TAG | UNP Q5R0K1 |
| L | 225 | PRO | - | EXPRESSION TAG | UNP Q5R0K1 |
| L | 226 | GLN | - | EXPRESSION TAG | UNP Q5R0K1 |
| L | 227 | PHE | - | EXPRESSION TAG | UNP Q5R0K1 |
| L | 228 | GLU | - | EXPRESSION TAG | UNP Q5R0K1 |
| L | 229 | LYS | - | EXPRESSION TAG | UNP Q5R0K1 |

- Molecule 2 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 2 | A | 4 | Total O 4 4 | 0 | 0 |
| 2 | B | 3 | Total O 3 3 | 0 | 0 |
| 2 | C | 1 | Total O 1 1 | 0 | 0 |
| 2 | E | 1 | Total O 1 1 | 0 | 0 |

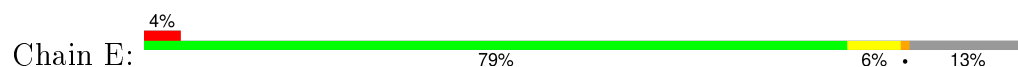
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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 2 | F | 1 | Total 1 | O 1 | 0 | 0 |
| 2 | I | 2 | Total 2 | O 2 | 0 | 0 |
| 2 | J | 1 | Total 1 | O 1 | 0 | 0 |
| 2 | L | 1 | Total 1 | O 1 | 0 | 0 |

HIS
HIS
HIS
HIS
HIS
TRP
SER
HIS
PRO
GLN
PHE
GLU
LYS

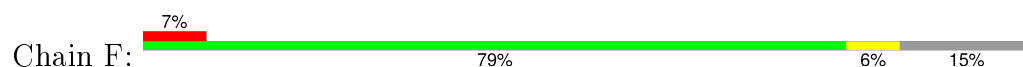
- Molecule 1: Glutathione S-transferase related protein



MET VAL MET MET VAL ALA VAL ALA ALA ASN ASN LYS S9 L20 Q24 L27 V28 L29 V34 G35 V36 V41 T42 D43 E44 S45 E48 D49 L50 L51 Q52 L53 K60 R66 E67 L68 V69 N72 I75 R83 I118 A123 Y157 I170 A208 GLU

ASN LEU TYR PHE GLN SER HIS HIS HIS HIS HIS TRP SER HIS PRO GLN PHE GLU LYS

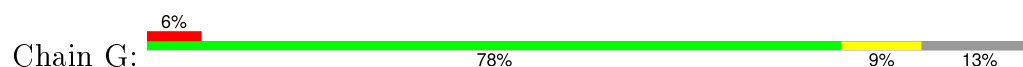
- Molecule 1: Glutathione S-transferase related protein



MET VAL MET MET VAL ALA VAL ALA ALA ASN ASN LYS S9 Q24 L27 V28 L29 V36 V41 E44 S45 L53 K60 V69 N72 W111 N121 I134 S135 L136 I139 V154 Y157 L158 L161 L172 E173 G174 Q175 G176 A177 K178 E179 I180

V185 E199 A205 ARG ASN ALA ALA ASN ASN LEU TYR PHE GLN SER HIS HIS HIS HIS HIS TRP SER PRO GLN PHE GLU LYS

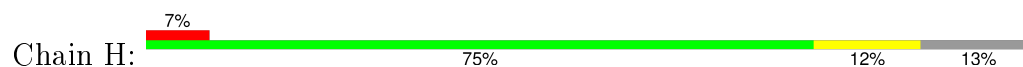
- Molecule 1: Glutathione S-transferase related protein



MET VAL MET MET VAL ALA VAL ALA ALA ASN LYS R8 V36 E44 L53 K60 R66 E67 L68 V69 L70 Y71 N72 A73 Q74 E78 R83 E108 Y112 A137 P138 I139 F140 A141 A159 L162 L165 L172 E173 G174 Q175 G176 A177 K178 E179 I180 D195

L204 A205 R206 L207 A208 GLU ASN LEU TYR PHE GLN SER HIS HIS HIS HIS HIS TRP SER HIS PRO GLN PHE GLU LYS

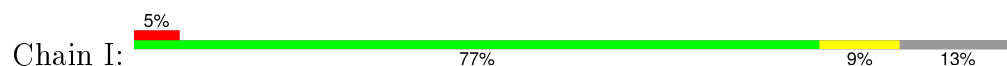
- Molecule 1: Glutathione S-transferase related protein

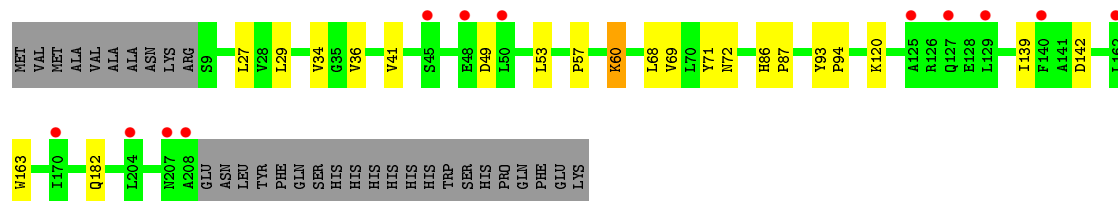


MET VAL MET MET VAL ALA VAL ALA ALA ASN LYS R8 D18 Q24 L27 V28 L29 V36 E44 D49 L53 K60 V64 D65 R66 Y71 N72 R83 Y92 Y93 P94 E108 W111 Y112 K120 N121 D122 A123 Q124 K130 I133 I134 I139

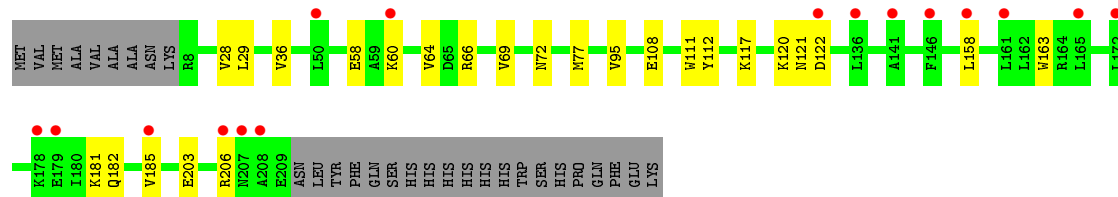
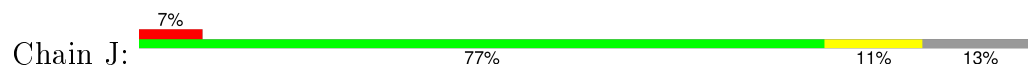
Y157 L158 A159 L162 W163 W164 L165 L172 A177 K181 V185 K191 L207 A208 GLU ASN TYR PHE GLN SER HIS HIS HIS HIS HIS TRP SER PRO GLN PHE GLU LYS

- Molecule 1: Glutathione S-transferase related protein

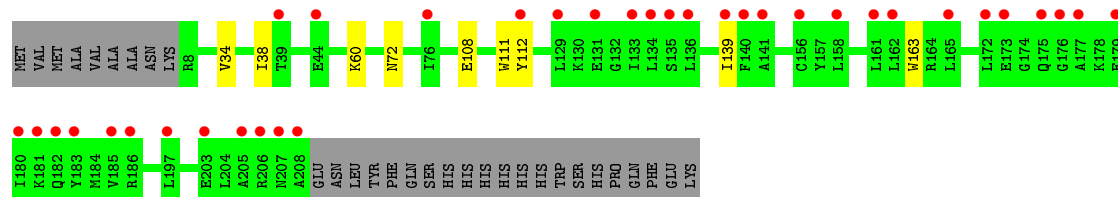
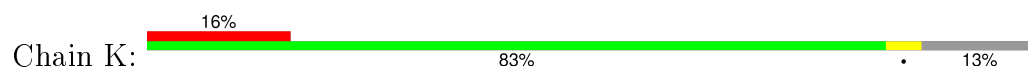




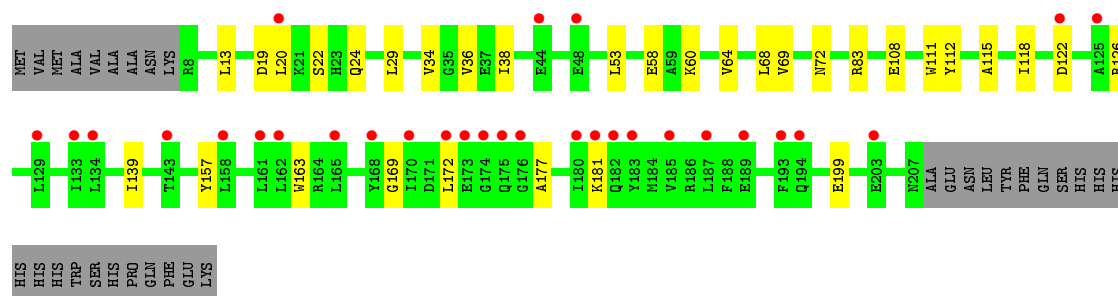
- Molecule 1: Glutathione S-transferase related protein



- Molecule 1: Glutathione S-transferase related protein



- Molecule 1: Glutathione S-transferase related protein



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 91.36Å 156.99Å 244.12Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 40.00 – 2.90 48.10 – 2.80 | Depositor EDS |
| % Data completeness (in resolution range) | 99.7 (40.00-2.90) 99.1 (48.10-2.80) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | 0.08 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.13 (at 2.81Å) | Xtriage |
| Refinement program | REFMAC 5.6.0117 | Depositor |
| R, R_{free} | 0.207 , 0.275 0.210 , 0.272 | Depositor DCC |
| R_{free} test set | 2357 reflections (3.10%) | DCC |
| Wilson B-factor (Å ²) | 87.9 | Xtriage |
| Anisotropy | 0.166 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.32 , 75.9 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$ | Xtriage |
| Outliers | 0 of 86599 reflections | Xtriage |
| F_o, F_c correlation | 0.95 | EDS |
| Total number of atoms | 19591 | wwPDB-VP |
| Average B, all atoms (Å ²) | 104.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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 | 0.43 | 1/1675 (0.1%) | 0.62 | 0/2271 |
| 1 | B | 0.43 | 1/1670 (0.1%) | 0.64 | 0/2264 |
| 1 | C | 0.42 | 1/1670 (0.1%) | 0.62 | 0/2264 |
| 1 | D | 0.43 | 1/1689 (0.1%) | 0.61 | 0/2289 |
| 1 | E | 0.43 | 0/1661 | 0.63 | 0/2253 |
| 1 | F | 0.43 | 1/1637 (0.1%) | 0.60 | 0/2220 |
| 1 | G | 0.43 | 0/1661 | 0.62 | 0/2253 |
| 1 | H | 0.44 | 2/1672 (0.1%) | 0.61 | 0/2267 |
| 1 | I | 0.42 | 1/1665 (0.1%) | 0.61 | 0/2257 |
| 1 | J | 0.43 | 2/1679 (0.1%) | 0.59 | 0/2276 |
| 1 | K | 0.43 | 2/1676 (0.1%) | 0.60 | 0/2271 |
| 1 | L | 0.43 | 2/1654 (0.1%) | 0.59 | 0/2245 |
| All | All | 0.43 | 14/20009 (0.1%) | 0.61 | 0/27130 |

The worst 5 of 14 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 1 | J | 111 | TRP | CD2-CE2 | 5.29 | 1.47 | 1.41 |
| 1 | A | 111 | TRP | CD2-CE2 | 5.27 | 1.47 | 1.41 |
| 1 | F | 111 | TRP | CD2-CE2 | 5.26 | 1.47 | 1.41 |
| 1 | D | 111 | TRP | CD2-CE2 | 5.19 | 1.47 | 1.41 |
| 1 | H | 163 | TRP | CD2-CE2 | 5.18 | 1.47 | 1.41 |

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 | 1639 | 0 | 1627 | 6 | 0 |
| 1 | B | 1634 | 0 | 1625 | 5 | 0 |
| 1 | C | 1634 | 0 | 1625 | 3 | 0 |
| 1 | D | 1653 | 0 | 1644 | 4 | 0 |
| 1 | E | 1625 | 0 | 1612 | 7 | 0 |
| 1 | F | 1601 | 0 | 1593 | 4 | 0 |
| 1 | G | 1625 | 0 | 1610 | 5 | 0 |
| 1 | H | 1636 | 0 | 1625 | 6 | 0 |
| 1 | I | 1629 | 0 | 1623 | 7 | 0 |
| 1 | J | 1643 | 0 | 1631 | 10 | 0 |
| 1 | K | 1640 | 0 | 1636 | 2 | 0 |
| 1 | L | 1618 | 0 | 1594 | 11 | 0 |
| 2 | A | 4 | 0 | 0 | 0 | 0 |
| 2 | B | 3 | 0 | 0 | 0 | 0 |
| 2 | C | 1 | 0 | 0 | 0 | 0 |
| 2 | E | 1 | 0 | 0 | 0 | 0 |
| 2 | F | 1 | 0 | 0 | 0 | 0 |
| 2 | I | 2 | 0 | 0 | 0 | 0 |
| 2 | J | 1 | 0 | 0 | 0 | 0 |
| 2 | L | 1 | 0 | 0 | 0 | 0 |
| All | All | 19591 | 0 | 19445 | 67 | 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 2.

The worst 5 of 67 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:J:121:ASN:O | 1:J:121:ASN:ND2 | 2.30 | 0.64 |
| 1:I:29:LEU:HD13 | 1:I:36:VAL:HG11 | 1.85 | 0.57 |
| 1:E:29:LEU:HD13 | 1:E:36:VAL:HG11 | 1.87 | 0.56 |
| 1:J:120:LYS:O | 1:J:121:ASN:HB3 | 2.06 | 0.56 |
| 1:L:29:LEU:HD13 | 1:L:36:VAL:HG11 | 1.88 | 0.56 |

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 | 200/231 (87%) | 191 (96%) | 8 (4%) | 1 (0%) | 34 | 71 |
| 1 | B | 199/231 (86%) | 195 (98%) | 2 (1%) | 2 (1%) | 19 | 54 |
| 1 | C | 199/231 (86%) | 189 (95%) | 8 (4%) | 2 (1%) | 19 | 54 |
| 1 | D | 201/231 (87%) | 195 (97%) | 5 (2%) | 1 (0%) | 34 | 71 |
| 1 | E | 198/231 (86%) | 194 (98%) | 2 (1%) | 2 (1%) | 19 | 54 |
| 1 | F | 195/231 (84%) | 189 (97%) | 5 (3%) | 1 (0%) | 34 | 71 |
| 1 | G | 199/231 (86%) | 192 (96%) | 5 (2%) | 2 (1%) | 19 | 54 |
| 1 | H | 199/231 (86%) | 193 (97%) | 3 (2%) | 3 (2%) | 13 | 42 |
| 1 | I | 198/231 (86%) | 191 (96%) | 5 (2%) | 2 (1%) | 19 | 54 |
| 1 | J | 200/231 (87%) | 194 (97%) | 4 (2%) | 2 (1%) | 19 | 54 |
| 1 | K | 199/231 (86%) | 188 (94%) | 10 (5%) | 1 (0%) | 34 | 71 |
| 1 | L | 198/231 (86%) | 190 (96%) | 7 (4%) | 1 (0%) | 34 | 71 |
| All | All | 2385/2772 (86%) | 2301 (96%) | 64 (3%) | 20 (1%) | 24 | 60 |

5 of 20 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 72 | ASN |
| 1 | B | 72 | ASN |
| 1 | E | 66 | ARG |
| 1 | F | 72 | ASN |
| 1 | G | 66 | ARG |

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 | 178/206 (86%) | 167 (94%) | 11 (6%) | 23 | 55 |
| 1 | B | 178/206 (86%) | 173 (97%) | 5 (3%) | 51 | 84 |
| 1 | C | 178/206 (86%) | 167 (94%) | 11 (6%) | 23 | 55 |
| 1 | D | 180/206 (87%) | 175 (97%) | 5 (3%) | 51 | 84 |
| 1 | E | 177/206 (86%) | 172 (97%) | 5 (3%) | 51 | 84 |
| 1 | F | 175/206 (85%) | 170 (97%) | 5 (3%) | 50 | 83 |
| 1 | G | 176/206 (85%) | 166 (94%) | 10 (6%) | 25 | 59 |
| 1 | H | 178/206 (86%) | 168 (94%) | 10 (6%) | 26 | 60 |
| 1 | I | 178/206 (86%) | 170 (96%) | 8 (4%) | 34 | 70 |
| 1 | J | 179/206 (87%) | 173 (97%) | 6 (3%) | 44 | 79 |
| 1 | K | 179/206 (87%) | 176 (98%) | 3 (2%) | 68 | 91 |
| 1 | L | 175/206 (85%) | 166 (95%) | 9 (5%) | 29 | 65 |
| All | All | 2131/2472 (86%) | 2043 (96%) | 88 (4%) | 37 | 73 |

5 of 88 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 121 | ASN |
| 1 | G | 172 | LEU |
| 1 | L | 60 | LYS |
| 1 | F | 139 | ILE |
| 1 | G | 68 | LEU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | H | 24 | GLN |
| 1 | H | 119 | GLN |
| 1 | J | 121 | ASN |
| 1 | G | 182 | GLN |
| 1 | J | 182 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 | 202/231 (87%) | 0.63 | 16 (7%) 15 10 | 57, 94, 148, 176 | 0 |
| 1 | B | 201/231 (87%) | 0.33 | 1 (0%) 91 90 | 47, 77, 123, 184 | 0 |
| 1 | C | 201/231 (87%) | 0.41 | 8 (3%) 42 35 | 56, 93, 142, 173 | 0 |
| 1 | D | 203/231 (87%) | 0.58 | 15 (7%) 17 11 | 63, 95, 144, 173 | 0 |
| 1 | E | 200/231 (86%) | 0.52 | 10 (5%) 32 26 | 56, 84, 140, 184 | 0 |
| 1 | F | 197/231 (85%) | 0.65 | 16 (8%) 15 9 | 59, 103, 151, 169 | 0 |
| 1 | G | 201/231 (87%) | 0.71 | 14 (6%) 19 13 | 55, 100, 149, 180 | 0 |
| 1 | H | 201/231 (87%) | 0.54 | 17 (8%) 13 8 | 69, 105, 150, 169 | 0 |
| 1 | I | 200/231 (86%) | 0.49 | 12 (6%) 25 18 | 67, 101, 147, 188 | 0 |
| 1 | J | 202/231 (87%) | 0.56 | 16 (7%) 15 10 | 68, 104, 149, 187 | 0 |
| 1 | K | 201/231 (87%) | 0.99 | 36 (17%) 2 1 | 76, 124, 163, 180 | 0 |
| 1 | L | 200/231 (86%) | 0.88 | 30 (15%) 3 2 | 76, 126, 165, 182 | 0 |
| All | All | 2409/2772 (86%) | 0.61 | 191 (7%) 15 10 | 47, 100, 155, 188 | 0 |

The worst 5 of 191 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | K | 208 | ALA | 7.6 |
| 1 | G | 207 | ASN | 7.1 |
| 1 | D | 6 | ASN | 6.4 |
| 1 | L | 183 | TYR | 6.4 |
| 1 | K | 185 | VAL | 6.1 |

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 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.