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

Oct 31, 2023 – 11:04 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 3PZ6 |
| Title | : | The crystal structure of GlLeuRS-CP1 |
| Authors | : | Liu, R.J.; Du, D.H.; Wang, E.D. |
| Deposited on | : | 2010-12-14 |
| Resolution | : | 2.60 Å(reported) |

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

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

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

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

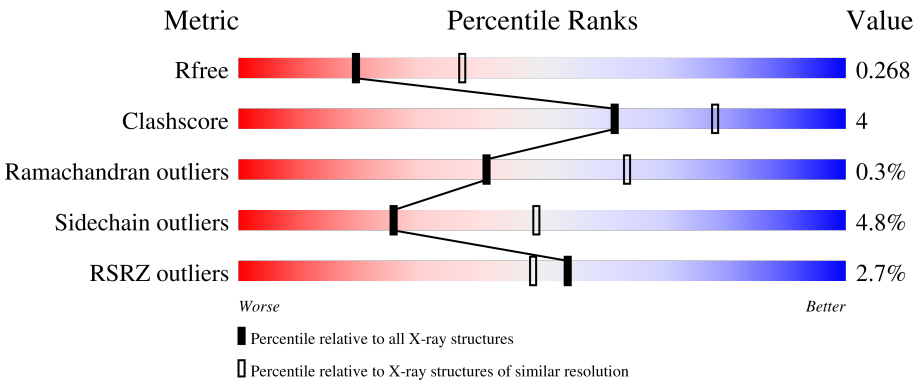
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.36 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh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

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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 | 3163 (2.60-2.60) |
| Clashscore | 141614 | 3518 (2.60-2.60) |
| Ramachandran outliers | 138981 | 3455 (2.60-2.60) |
| Sidechain outliers | 138945 | 3455 (2.60-2.60) |
| RSRZ outliers | 127900 | 3104 (2.60-2.60) |

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 | 311 | 3% 77% 13% • 10% |
| 1 | B | 311 | 5% 77% 12% • 11% |
| 1 | C | 311 | % 71% 11% 18% |
| 1 | D | 311 | % 68% 13% • 18% |
| 1 | E | 311 | % 70% 11% • 18% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | F | 311 | 3% 73% 10% • 17% |

# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12091 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 Leucyl-tRNA synthetase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 1 | A | 279 | 2084 | 1339 | 339 | 393 | 13 | 0 | 0 | 0 |
| 1 | B | 278 | 2075 | 1332 | 332 | 398 | 13 | 0 | 0 | 0 |
| 1 | C | 256 | 1934 | 1241 | 310 | 370 | 13 | 0 | 0 | 0 |
| 1 | D | 254 | 1907 | 1226 | 308 | 360 | 13 | 0 | 0 | 0 |
| 1 | E | 255 | 1913 | 1225 | 307 | 368 | 13 | 0 | 0 | 0 |
| 1 | F | 259 | 1948 | 1248 | 312 | 375 | 13 | 0 | 0 | 0 |

There are 18 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 251 | GLY | - | expression tag | UNP A8BY54 |
| A | 395 | SER | CYS | engineered mutation | UNP A8BY54 |
| A | 533 | SER | CYS | engineered mutation | UNP A8BY54 |
| B | 251 | GLY | - | expression tag | UNP A8BY54 |
| B | 395 | SER | CYS | engineered mutation | UNP A8BY54 |
| B | 533 | SER | CYS | engineered mutation | UNP A8BY54 |
| C | 251 | GLY | - | expression tag | UNP A8BY54 |
| C | 395 | SER | CYS | engineered mutation | UNP A8BY54 |
| C | 533 | SER | CYS | engineered mutation | UNP A8BY54 |
| D | 251 | GLY | - | expression tag | UNP A8BY54 |
| D | 395 | SER | CYS | engineered mutation | UNP A8BY54 |
| D | 533 | SER | CYS | engineered mutation | UNP A8BY54 |
| E | 251 | GLY | - | expression tag | UNP A8BY54 |
| E | 395 | SER | CYS | engineered mutation | UNP A8BY54 |
| E | 533 | SER | CYS | engineered mutation | UNP A8BY54 |
| F | 251 | GLY | - | expression tag | UNP A8BY54 |
| F | 395 | SER | CYS | engineered mutation | UNP A8BY54 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| F | 533 | SER | CYS | engineered mutation | UNP A8BY54 |

- Molecule 2 is water.

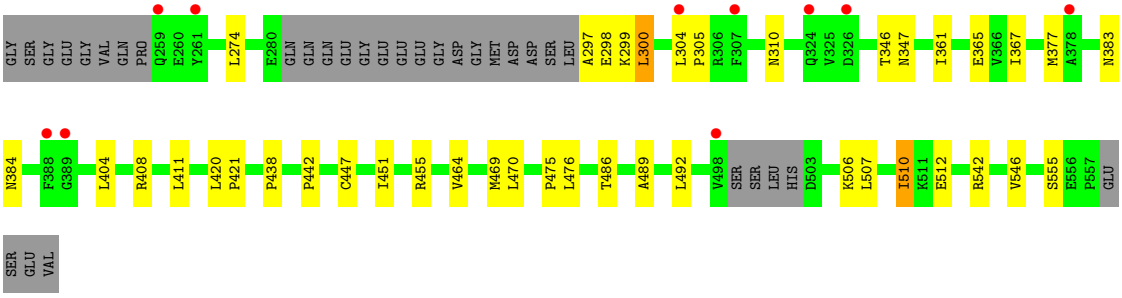
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | O | | |
| 2 | A | 42 | 42 | 42 | 0 | 0 |
| | | | Total | O | | |
| 2 | B | 37 | 37 | 37 | 0 | 0 |
| | | | Total | O | | |
| 2 | C | 26 | 26 | 26 | 0 | 0 |
| | | | Total | O | | |
| 2 | D | 30 | 30 | 30 | 0 | 0 |
| | | | Total | O | | |
| 2 | E | 50 | 50 | 50 | 0 | 0 |
| | | | Total | O | | |
| 2 | F | 45 | 45 | 45 | 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.

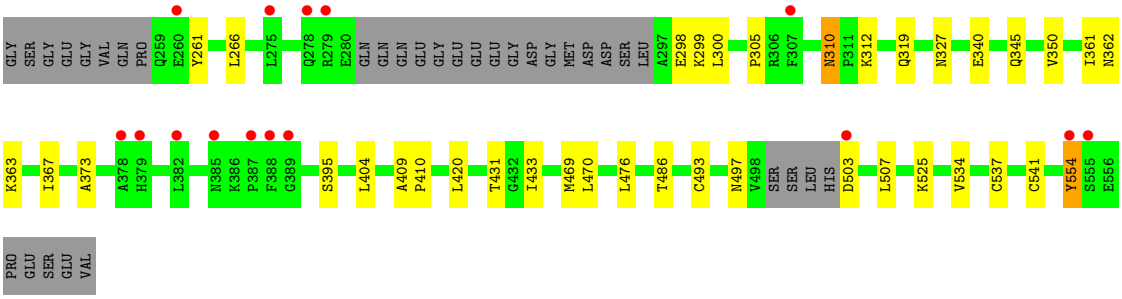
• Molecule 1: Leucyl-tRNA synthetase

Chain A:



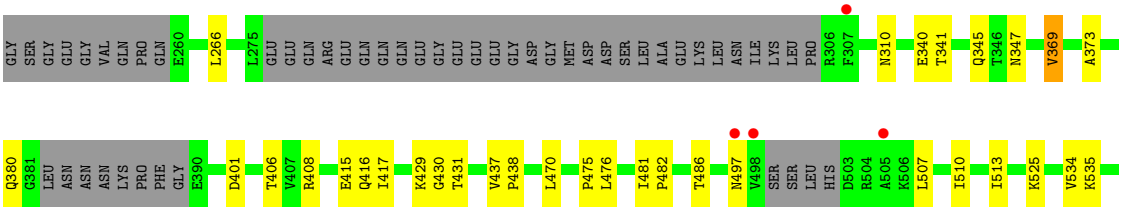

• Molecule 1: Leucyl-tRNA synthetase

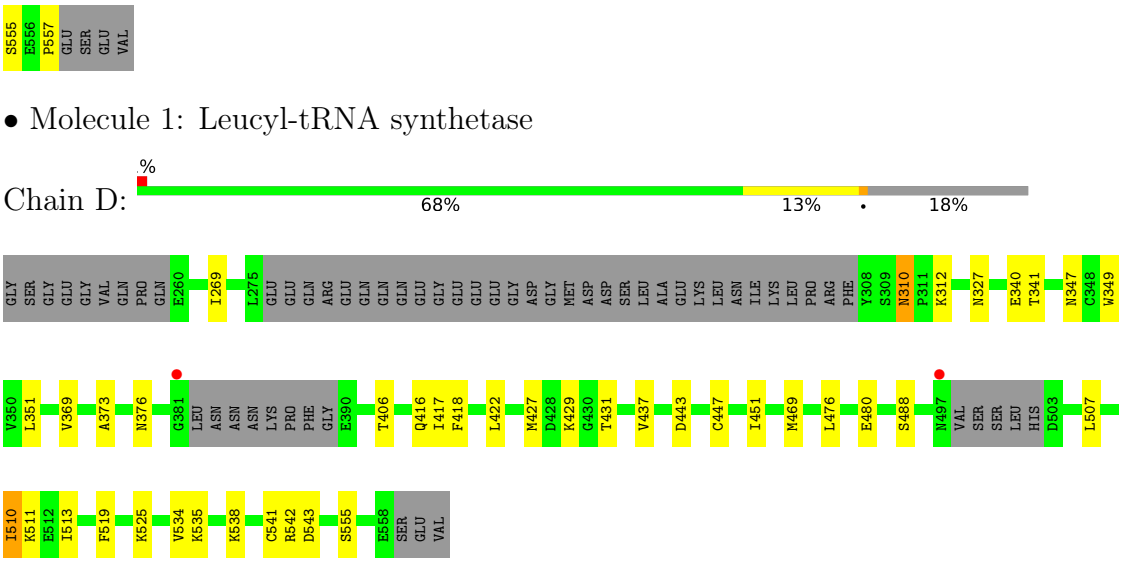
Chain B:




• Molecule 1: Leucyl-tRNA synthetase

Chain C:




S555 E556 P557 GLU SER GLU VAL
• Molecule 1: Leucyl-tRNA synthetase
Chain D:
%
68%
13%
18%
GLY SER GLY GLU GLY VAL GLN PRO GLN E260 I269 L275 GLU GLU GLN ARG GLU GLN GLN GLN GLU GLY GLU GLU GLU GLY ASP GLY MET ASP ASP SER LEU ALA GLU LYS LEU ASN ILE LYS LEU PRO ARG PHE Y308 S309 N310 P311 K312 N327 E340 T341 N347 C348 W349
V350 L351 V369 A373 N376 G381 LEU ASN ASN ASN LYS PRO PHE GLY E390 T406 Q416 I417 F418 L422 M427 D428 K429 G430 T431 V437 D443 C447 I451 M469 L476 E480 S488 N497 VAL SER SER LEU HIS D503 L507
I510 K511 E512 I513 F519 K525 V534 K535 K538 C541 R542 D543 S555 E558 SER GLU VAL
• Molecule 1: Leucyl-tRNA synthetase
Chain E:
%
70%
11%
18%
GLY SER GLY GLU GLY VAL GLN PRO Q259 E260 Y261 I264 Y271 T272 T273 L274 L275 GLU GLU GLN ARG GLU GLN GLN GLN GLU GLY GLU GLU GLU GLY ASP GLY MET ASP ASP SER LEU ALA GLU LYS LEU ASN ILE LYS LEU PRO R306 N310 E340 V343 A373 N376
M377 A378 H379 GLN GLY LEU ASN ASN ASN LYS PRO PHE GLY E390 L404 P410 L411 Y414 L420 D428 D443 C447 Y448 I451 V464 M469 L470 L476 P477 I478 L492 V498 SER SER LEU HIS D503 L507 T508 Q509 I510 Y520 V534 K535
D536 C537 K538 Q539 R542 D543 Q547 P557 GLU SER GLU VAL
• Molecule 1: Leucyl-tRNA synthetase
Chain F:
3%
73%
10%
17%
GLY SER GLY GLU GLY VAL GLN PRO GLN E260 L274 L275 GLU GLU GLN ARG GLU GLN GLN GLN GLU GLY GLU GLU GLU GLY ASP GLY MET ASP ASP SER LEU ALA GLU LYS LEU ASN ILE LYS LEU PRO ARG F307 N310 E340 V350 H372 A373 N376 H379 GLN GLY
LEU ASN ASN ASN LYS PRO PHE GLY E390 P410 L411 Y414 L420 K429 G430 T431 G432 I433 P442 C447 Y448 I451 L470 L476 E480 T486 N497 V498 S499 S500 LEU HIS D503 R504 L507 T508 Q509 I510 K511 E512 I513 K525 V534 C537
Q547 V561

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | C 1 2 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 232.28Å 72.09Å 111.25Å<br>90.00° 95.06° 90.00° | Depositor |
| Resolution (Å) | 29.85 – 2.60<br>29.85 – 2.60 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 88.7 (29.85-2.60)<br>94.2 (29.85-2.60) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 4.10 (at 2.61Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: 1.6.2_432) | Depositor |
| R, $R_{free}$ | 0.215 , 0.271<br>0.216 , 0.268 | Depositor<br>DCC |
| $R_{free}$ test set | 2693 reflections (5.03%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 39.9 | Xtriage |
| Anisotropy | 0.336 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.31 , 44.7 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.50$, $< L^2 > = 0.33$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.94 | EDS |
| Total number of atoms | 12091 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 44.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 64.89 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.7187e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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 | 0.37 | 0/2124 | 0.55 | 1/2899 (0.0%) |
| 1 | B | 0.38 | 0/2114 | 0.55 | 1/2885 (0.0%) |
| 1 | C | 0.37 | 0/1970 | 0.55 | 1/2684 (0.0%) |
| 1 | D | 0.39 | 0/1943 | 0.51 | 0/2650 |
| 1 | E | 0.38 | 0/1948 | 0.52 | 0/2657 |
| 1 | F | 0.39 | 0/1984 | 0.54 | 0/2706 |
| All | All | 0.38 | 0/12083 | 0.54 | 3/16481 (0.0%) |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | C | 557 | PRO | N-CA-CB | 5.99 | 110.49 | 103.30 |
| 1 | B | 305 | PRO | N-CA-CB | 5.68 | 110.11 | 103.30 |
| 1 | A | 305 | PRO | N-CA-CB | 5.44 | 109.83 | 103.30 |

There are no chirality outliers.

There are no planarity outliers.

## 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 | 2084 | 0 | 2008 | 18 | 0 |
| 1 | B | 2075 | 0 | 1984 | 17 | 0 |
| 1 | C | 1934 | 0 | 1875 | 14 | 0 |
| 1 | D | 1907 | 0 | 1857 | 19 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | E | 1913 | 0 | 1846 | 22 | 0 |
| 1 | F | 1948 | 0 | 1885 | 13 | 0 |
| 2 | A | 42 | 0 | 0 | 1 | 0 |
| 2 | B | 37 | 0 | 0 | 0 | 0 |
| 2 | C | 26 | 0 | 0 | 0 | 0 |
| 2 | D | 30 | 0 | 0 | 1 | 0 |
| 2 | E | 50 | 0 | 0 | 0 | 0 |
| 2 | F | 45 | 0 | 0 | 1 | 0 |
| All | All | 12091 | 0 | 11455 | 103 | 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 4.

All (103) 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:E:376:ASN:HD21 | 1:E:557:PRO:HD3 | 1.37 | 0.88 |
| 1:E:507:LEU:HA | 1:E:510:ILE:HG22 | 1.75 | 0.67 |
| 1:F:372:HIS:O | 1:F:376:ASN:HB2 | 1.95 | 0.66 |
| 1:E:414:TYR:CE2 | 1:E:476:LEU:HD21 | 2.29 | 0.66 |
| 1:E:271:TYR:O | 1:E:274:LEU:HB2 | 1.96 | 0.65 |
| 1:E:340:GLU:HG3 | 1:E:534:VAL:HG13 | 1.79 | 0.64 |
| 1:E:373:ALA:O | 1:E:377:MET:HB2 | 1.96 | 0.64 |
| 1:E:376:ASN:HD21 | 1:E:557:PRO:CD | 2.08 | 0.64 |
| 1:C:340:GLU:HG3 | 1:C:534:VAL:HG13 | 1.81 | 0.62 |
| 1:D:310:ASN:HD22 | 1:D:312:LYS:H | 1.48 | 0.62 |
| 1:F:420:LEU:HD11 | 1:F:470:LEU:HD21 | 1.82 | 0.61 |
| 1:A:420:LEU:HD11 | 1:A:470:LEU:HD21 | 1.83 | 0.61 |
| 1:F:442:PRO:HG2 | 1:F:511:LYS:HA | 1.82 | 0.61 |
| 1:E:448:TYR:CE1 | 1:E:470:LEU:HD22 | 2.35 | 0.61 |
| 1:E:414:TYR:HE2 | 1:E:476:LEU:HD21 | 1.64 | 0.60 |
| 1:F:414:TYR:CE2 | 1:F:476:LEU:HD21 | 2.37 | 0.59 |
| 1:E:447:CYS:O | 1:E:451:ILE:HG12 | 2.02 | 0.58 |
| 1:F:350:VAL:HG12 | 1:F:433:ILE:HG12 | 1.84 | 0.58 |
| 1:F:510:ILE:HA | 1:F:513:ILE:HD12 | 1.86 | 0.58 |
| 1:D:480:GLU:HB2 | 1:D:525:LYS:HD2 | 1.85 | 0.57 |
| 1:A:506:LYS:O | 1:A:510:ILE:HG22 | 2.05 | 0.56 |
| 1:D:340:GLU:HG3 | 1:D:534:VAL:HG13 | 1.87 | 0.55 |
| 1:E:404:LEU:HD21 | 1:E:464:VAL:HG22 | 1.91 | 0.53 |
| 1:D:341:THR:HB | 1:D:437:VAL:HG11 | 1.92 | 0.52 |
| 1:A:274:LEU:HD21 | 1:A:408:ARG:HH22 | 1.75 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:507:LEU:HA | 1:D:510:ILE:HG22 | 1.91 | 0.51 |
| 1:A:420:LEU:CD1 | 1:A:470:LEU:HD21 | 2.39 | 0.51 |
| 1:C:341:THR:HB | 1:C:437:VAL:HG11 | 1.93 | 0.51 |
| 1:F:447:CYS:O | 1:F:451:ILE:HG12 | 2.11 | 0.51 |
| 1:F:340:GLU:HG3 | 1:F:534:VAL:HG13 | 1.93 | 0.51 |
| 1:E:404:LEU:HD22 | 1:E:469:MET:SD | 2.51 | 0.50 |
| 1:D:510:ILE:HA | 1:D:513:ILE:HD12 | 1.93 | 0.50 |
| 1:C:380:GLN:HE22 | 1:C:555:SER:H | 1.59 | 0.50 |
| 1:B:493:CYS:O | 1:B:497:ASN:O | 2.29 | 0.49 |
| 1:E:272:THR:C | 1:E:274:LEU:H | 2.16 | 0.49 |
| 1:B:310:ASN:HD22 | 1:B:312:LYS:H | 1.60 | 0.49 |
| 1:B:525:LYS:HE2 | 1:B:525:LYS:HA | 1.95 | 0.49 |
| 1:C:266:LEU:HD21 | 1:C:345:GLN:HE22 | 1.77 | 0.49 |
| 1:D:310:ASN:ND2 | 1:D:312:LYS:H | 2.10 | 0.49 |
| 1:D:542:ARG:NH1 | 1:D:543:ASP:OD1 | 2.46 | 0.48 |
| 1:E:376:ASN:ND2 | 1:E:557:PRO:HD3 | 2.17 | 0.48 |
| 1:A:361:ILE:HG12 | 1:A:367:ILE:HG12 | 1.96 | 0.48 |
| 1:E:310:ASN:C | 1:E:310:ASN:HD22 | 2.17 | 0.48 |
| 1:E:492:LEU:HB2 | 1:E:510:ILE:HD11 | 1.95 | 0.47 |
| 1:A:346:THR:OG1 | 1:A:347:ASN:ND2 | 2.48 | 0.47 |
| 1:A:489:ALA:HA | 1:A:510:ILE:HD11 | 1.95 | 0.47 |
| 1:F:448:TYR:CE1 | 1:F:470:LEU:HD22 | 2.50 | 0.47 |
| 1:D:349:TRP:HB3 | 1:D:422:LEU:HB3 | 1.96 | 0.46 |
| 1:D:347:ASN:HA | 1:D:417:ILE:HB | 1.97 | 0.46 |
| 1:A:486:THR:O | 2:A:48:HOH:O | 2.20 | 0.46 |
| 1:D:488:SER:HB2 | 2:D:52:HOH:O | 2.15 | 0.46 |
| 1:E:340:GLU:OE1 | 1:E:538:LYS:HG2 | 2.15 | 0.46 |
| 1:B:350:VAL:HG12 | 1:B:433:ILE:HG12 | 1.98 | 0.46 |
| 1:A:298:GLU:C | 1:A:300:LEU:H | 2.19 | 0.46 |
| 1:B:362:ASN:OD1 | 1:B:363:LYS:N | 2.49 | 0.46 |
| 1:B:420:LEU:HD11 | 1:B:470:LEU:HD21 | 1.98 | 0.46 |
| 1:D:373:ALA:HB2 | 1:D:431:THR:HA | 1.97 | 0.45 |
| 1:B:373:ALA:HB1 | 1:B:554:TYR:OH | 2.17 | 0.45 |
| 1:C:415:GLU:HG2 | 1:C:416:GLN:OE1 | 2.16 | 0.45 |
| 1:B:340:GLU:HG3 | 1:B:534:VAL:HG13 | 1.98 | 0.45 |
| 1:B:409:ALA:HA | 1:B:410:PRO:HD2 | 1.85 | 0.45 |
| 1:C:438:PRO:HB2 | 1:C:475:PRO:HG3 | 1.99 | 0.45 |
| 1:F:480:GLU:HB2 | 1:F:525:LYS:HD2 | 1.99 | 0.45 |
| 1:D:519:PHE:HE1 | 1:D:538:LYS:HD2 | 1.83 | 0.44 |
| 1:F:373:ALA:HB2 | 1:F:431:THR:HA | 1.99 | 0.44 |
| 1:A:420:LEU:HB3 | 1:A:421:PRO:HD2 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:535:LYS:NZ | 1:D:535:LYS:HB3 | 2.32 | 0.44 |
| 1:C:415:GLU:HG2 | 1:C:416:GLN:CD | 2.38 | 0.44 |
| 1:B:373:ALA:HB2 | 1:B:431:THR:HA | 2.00 | 0.44 |
| 1:C:369:VAL:HG12 | 1:C:431:THR:HB | 2.00 | 0.43 |
| 1:E:543:ASP:O | 1:E:547:GLN:HB3 | 2.18 | 0.43 |
| 1:D:269:ILE:HD12 | 1:D:406:THR:HB | 2.00 | 0.43 |
| 1:A:404:LEU:HD22 | 1:A:469:MET:SD | 2.58 | 0.43 |
| 1:A:542:ARG:O | 1:A:546:VAL:HG23 | 2.19 | 0.43 |
| 1:B:361:ILE:HG12 | 1:B:367:ILE:HG12 | 2.00 | 0.43 |
| 1:D:443:ASP:OD2 | 1:D:511:LYS:HE2 | 2.19 | 0.43 |
| 1:C:373:ALA:HB2 | 1:C:430:GLY:O | 2.19 | 0.43 |
| 1:F:410:PRO:O | 1:F:411:LEU:HB2 | 2.18 | 0.43 |
| 1:B:261:TYR:HB2 | 1:B:554:TYR:HB3 | 2.01 | 0.42 |
| 1:D:418:PHE:CD1 | 1:D:469:MET:HG2 | 2.55 | 0.42 |
| 1:B:319:GLN:HE21 | 1:B:395:SER:HB3 | 1.84 | 0.42 |
| 1:F:486:THR:O | 2:F:98:HOH:O | 2.22 | 0.42 |
| 1:C:347:ASN:HA | 1:C:417:ILE:HB | 2.02 | 0.42 |
| 1:A:442:PRO:HB3 | 1:A:510:ILE:HD13 | 2.00 | 0.42 |
| 1:B:266:LEU:HD21 | 1:B:345:GLN:HE22 | 1.85 | 0.42 |
| 1:A:492:LEU:HD12 | 1:A:510:ILE:HG13 | 2.02 | 0.41 |
| 1:B:298:GLU:C | 1:B:300:LEU:H | 2.23 | 0.41 |
| 1:E:410:PRO:O | 1:E:411:LEU:HB2 | 2.20 | 0.41 |
| 1:A:447:CYS:O | 1:A:451:ILE:HG12 | 2.20 | 0.41 |
| 1:B:404:LEU:HD22 | 1:B:469:MET:SD | 2.61 | 0.41 |
| 1:B:503:ASP:O | 1:B:507:LEU:HB2 | 2.21 | 0.41 |
| 1:C:510:ILE:HA | 1:C:513:ILE:HD12 | 2.03 | 0.41 |
| 1:E:260:GLU:OE2 | 1:E:542:ARG:NE | 2.49 | 0.41 |
| 1:E:420:LEU:HD11 | 1:E:470:LEU:HD21 | 2.02 | 0.41 |
| 1:C:481:ILE:HA | 1:C:482:PRO:HD3 | 1.97 | 0.40 |
| 1:A:438:PRO:HB2 | 1:A:475:PRO:HG3 | 2.03 | 0.40 |
| 1:C:507:LEU:HA | 1:C:510:ILE:HG22 | 2.03 | 0.40 |
| 1:D:447:CYS:O | 1:D:451:ILE:HG12 | 2.21 | 0.40 |
| 1:A:297:ALA:O | 1:A:299:LYS:N | 2.44 | 0.40 |
| 1:D:351:LEU:HB3 | 1:D:427:MET:HE3 | 2.04 | 0.40 |
| 1:A:404:LEU:HD21 | 1:A:464:VAL:HG22 | 2.03 | 0.40 |
| 1:C:373:ALA:HB2 | 1:C:431:THR:HA | 2.02 | 0.40 |
| 1:E:343:VAL:HG13 | 1:E:478:ILE:HG21 | 2.02 | 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 | 273/311 (88%) | 256 (94%) | 17 (6%) | 0 | 100 | 100 |
| 1 | B | 272/311 (88%) | 250 (92%) | 20 (7%) | 2 (1%) | 22 | 43 |
| 1 | C | 248/311 (80%) | 234 (94%) | 14 (6%) | 0 | 100 | 100 |
| 1 | D | 246/311 (79%) | 228 (93%) | 17 (7%) | 1 (0%) | 34 | 57 |
| 1 | E | 247/311 (79%) | 230 (93%) | 16 (6%) | 1 (0%) | 34 | 57 |
| 1 | F | 251/311 (81%) | 240 (96%) | 10 (4%) | 1 (0%) | 34 | 57 |
| All | All | 1537/1866 (82%) | 1438 (94%) | 94 (6%) | 5 (0%) | 41 | 64 |

All (5) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 327 | ASN |
| 1 | B | 327 | ASN |
| 1 | E | 273 | THR |
| 1 | F | 504 | ARG |
| 1 | B | 299 | 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 | 215/271 (79%) | 201 (94%) | 14 (6%) | 17 | 34 |
| 1 | B | 214/271 (79%) | 208 (97%) | 6 (3%) | 43 | 69 |
| 1 | C | 205/271 (76%) | 193 (94%) | 12 (6%) | 19 | 39 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | D | 200/271 (74%) | 191 (96%) | 9 (4%) | 27 | 52 |
| 1 | E | 201/271 (74%) | 191 (95%) | 10 (5%) | 24 | 47 |
| 1 | F | 207/271 (76%) | 198 (96%) | 9 (4%) | 29 | 54 |
| All | All | 1242/1626 (76%) | 1182 (95%) | 60 (5%) | 25 | 49 |

All (60) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 300 | LEU |
| 1 | A | 304 | LEU |
| 1 | A | 310 | ASN |
| 1 | A | 365 | GLU |
| 1 | A | 377 | MET |
| 1 | A | 383 | ASN |
| 1 | A | 384 | ASN |
| 1 | A | 411 | LEU |
| 1 | A | 455 | ARG |
| 1 | A | 476 | LEU |
| 1 | A | 507 | LEU |
| 1 | A | 510 | ILE |
| 1 | A | 512 | GLU |
| 1 | A | 555 | SER |
| 1 | B | 310 | ASN |
| 1 | B | 476 | LEU |
| 1 | B | 486 | THR |
| 1 | B | 537 | CYS |
| 1 | B | 541 | CYS |
| 1 | B | 554 | TYR |
| 1 | C | 310 | ASN |
| 1 | C | 369 | VAL |
| 1 | C | 401 | ASP |
| 1 | C | 406 | THR |
| 1 | C | 408 | ARG |
| 1 | C | 429 | LYS |
| 1 | C | 470 | LEU |
| 1 | C | 476 | LEU |
| 1 | C | 486 | THR |
| 1 | C | 497 | ASN |
| 1 | C | 525 | LYS |
| 1 | C | 535 | LYS |
| 1 | D | 310 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 369 | VAL |
| 1 | D | 376 | ASN |
| 1 | D | 416 | GLN |
| 1 | D | 429 | LYS |
| 1 | D | 476 | LEU |
| 1 | D | 510 | ILE |
| 1 | D | 541 | CYS |
| 1 | D | 555 | SER |
| 1 | E | 261 | TYR |
| 1 | E | 264 | ILE |
| 1 | E | 310 | ASN |
| 1 | E | 376 | ASN |
| 1 | E | 428 | ASP |
| 1 | E | 443 | ASP |
| 1 | E | 510 | ILE |
| 1 | E | 538 | LYS |
| 1 | E | 539 | GLN |
| 1 | E | 547 | GLN |
| 1 | F | 274 | LEU |
| 1 | F | 307 | PHE |
| 1 | F | 310 | ASN |
| 1 | F | 429 | LYS |
| 1 | F | 486 | THR |
| 1 | F | 509 | GLN |
| 1 | F | 510 | ILE |
| 1 | F | 537 | CYS |
| 1 | F | 547 | GLN |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 310 | ASN |
| 1 | A | 345 | GLN |
| 1 | A | 347 | ASN |
| 1 | A | 384 | ASN |
| 1 | A | 532 | GLN |
| 1 | B | 310 | ASN |
| 1 | B | 319 | GLN |
| 1 | B | 345 | GLN |
| 1 | B | 347 | ASN |
| 1 | B | 532 | GLN |
| 1 | C | 345 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 347 | ASN |
| 1 | C | 379 | HIS |
| 1 | C | 380 | GLN |
| 1 | D | 310 | ASN |
| 1 | D | 347 | ASN |
| 1 | D | 550 | GLN |
| 1 | E | 310 | ASN |
| 1 | E | 347 | ASN |
| 1 | E | 376 | ASN |
| 1 | E | 532 | GLN |
| 1 | E | 539 | GLN |
| 1 | E | 547 | GLN |
| 1 | E | 548 | ASN |
| 1 | F | 310 | ASN |
| 1 | F | 323 | ASN |
| 1 | F | 347 | ASN |
| 1 | F | 532 | GLN |
| 1 | F | 547 | GLN |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

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, $95^{th}$ 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 | 279/311 (89%) | -0.03 | 10 (3%) | 42 | 35 | 20, 38, 78, 90 | 0 |
| 1 | B | 278/311 (89%) | 0.06 | 15 (5%) | 25 | 20 | 20, 40, 81, 93 | 0 |
| 1 | C | 256/311 (82%) | -0.07 | 4 (1%) | 72 | 68 | 24, 43, 70, 90 | 0 |
| 1 | D | 254/311 (81%) | -0.16 | 2 (0%) | 86 | 84 | 23, 44, 70, 89 | 0 |
| 1 | E | 255/311 (81%) | -0.15 | 3 (1%) | 79 | 76 | 23, 39, 66, 85 | 0 |
| 1 | F | 259/311 (83%) | -0.09 | 8 (3%) | 49 | 42 | 22, 42, 74, 83 | 0 |
| All | All | 1581/1866 (84%) | -0.07 | 42 (2%) | 54 | 48 | 20, 41, 75, 93 | 0 |

All (42) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | B | 388 | PHE | 5.1 |
| 1 | C | 307 | PHE | 4.1 |
| 1 | C | 498 | VAL | 4.1 |
| 1 | C | 497 | ASN | 3.9 |
| 1 | A | 388 | PHE | 3.8 |
| 1 | B | 378 | ALA | 3.7 |
| 1 | A | 307 | PHE | 3.7 |
| 1 | B | 260 | GLU | 3.7 |
| 1 | B | 379 | HIS | 3.7 |
| 1 | F | 497 | ASN | 3.5 |
| 1 | F | 508 | THR | 3.3 |
| 1 | A | 378 | ALA | 3.1 |
| 1 | A | 259 | GLN | 3.1 |
| 1 | A | 324 | GLN | 3.1 |
| 1 | B | 554 | TYR | 2.9 |
| 1 | D | 381 | GLY | 2.9 |
| 1 | B | 389 | GLY | 2.8 |
| 1 | B | 387 | PRO | 2.7 |
| 1 | A | 498 | VAL | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | E | 520 | TYR | 2.7 |
| 1 | B | 385 | ASN | 2.7 |
| 1 | F | 498 | VAL | 2.6 |
| 1 | B | 382 | LEU | 2.6 |
| 1 | F | 500 | SER | 2.6 |
| 1 | A | 326 | ASP | 2.6 |
| 1 | E | 508 | THR | 2.6 |
| 1 | B | 307 | PHE | 2.6 |
| 1 | F | 499 | SER | 2.5 |
| 1 | F | 561 | VAL | 2.4 |
| 1 | B | 278 | GLN | 2.3 |
| 1 | A | 304 | LEU | 2.3 |
| 1 | D | 497 | ASN | 2.3 |
| 1 | B | 503 | ASP | 2.2 |
| 1 | F | 307 | PHE | 2.2 |
| 1 | B | 275 | LEU | 2.2 |
| 1 | F | 507 | LEU | 2.2 |
| 1 | B | 555 | SER | 2.1 |
| 1 | E | 536 | ASP | 2.1 |
| 1 | A | 261 | TYR | 2.1 |
| 1 | B | 279 | ARG | 2.1 |
| 1 | C | 505 | ALA | 2.1 |
| 1 | A | 389 | GLY | 2.0 |

## 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.