# WORLDWIDE wwPDB PROTEIN DATA BANK

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

Feb 15, 2017 – 06:05 am GMT

|  |  |  |
|---|---|---|
| PDB ID | : | 4W91 |
| Title | : | Crystal structure of a cysteine desulfurase SufS from Brucella suis bound to PLP |
| Authors | : | Seattle Structural Genomics Center for Infectious Disease |
| Deposited on | : | 2014-08-26 |
| Resolution | : | 2.45 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 (i) symbol.

# 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 2.45 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.
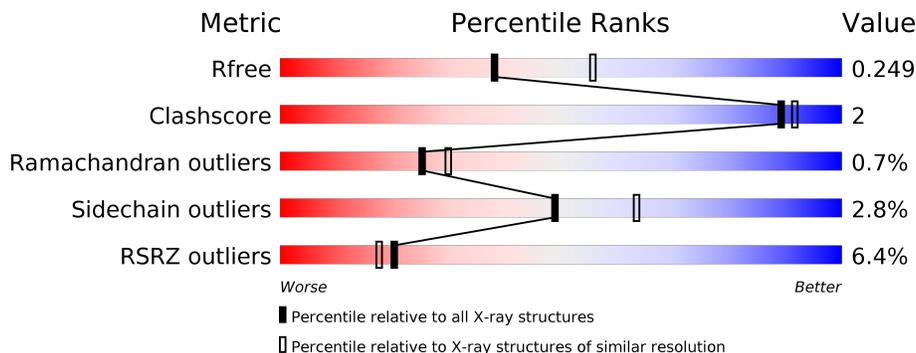


| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 100719 | 1119 (2.48-2.44) |
| Clashscore | 112137 | 1193 (2.48-2.44) |
| Ramachandran outliers | 110173 | 1185 (2.48-2.44) |
| Sidechain outliers | 110143 | 1185 (2.48-2.44) |
| RSRZ outliers | 101464 | 1126 (2.48-2.44) |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 422 |  |
| 1 | B | 422 |  |
| 1 | C | 422 |  |
| 1 | D | 422 |  |
| 1 | E | 422 |  |
| 1 | F | 422 |  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | G | 422 | 3% 87% 8% · 5% |
| 1 | H | 422 | 4% 89% 5% 5% |
| 1 | I | 422 | 28% 90% · 6% |
| 1 | J | 422 | 24% 81% · · 16% |
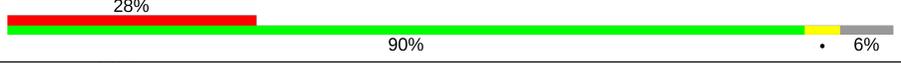
# 2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 30371 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 Aminotransferase.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 404 | Total 3117 | C 1974 | N 558 | O 573 | P 1 | S 11 | 0 | 2 | 0 |
| 1 | B | 405 | Total 3110 | C 1970 | N 555 | O 574 | P 1 | S 10 | 0 | 0 | 0 |
| 1 | C | 404 | Total 3118 | C 1973 | N 558 | O 576 | P 1 | S 10 | 0 | 0 | 0 |
| 1 | D | 404 | Total 3131 | C 1982 | N 560 | O 577 | P 1 | S 11 | 0 | 1 | 0 |
| 1 | E | 404 | Total 3083 | C 1952 | N 548 | O 572 | P 1 | S 10 | 0 | 0 | 0 |
| 1 | F | 404 | Total 3097 | C 1961 | N 552 | O 573 | P 1 | S 10 | 0 | 1 | 0 |
| 1 | G | 403 | Total 3041 | C 1931 | N 536 | O 563 | P 1 | S 10 | 0 | 0 | 0 |
| 1 | H | 400 | Total 3041 | C 1927 | N 542 | O 560 | P 1 | S 11 | 0 | 0 | 0 |
| 1 | I | 398 | Total 2764 | C 1728 | N 501 | O 525 | P 1 | S 9 | 0 | 0 | 0 |
| 1 | J | 356 | Total 2508 | C 1575 | N 449 | O 474 | P 1 | S 9 | 0 | 0 | 0 |

There are 80 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | -7 | MET | - | initiating methionine | UNP D0BBJ1 |
| A | -6 | ALA | - | expression tag | UNP D0BBJ1 |
| A | -5 | HIS | - | expression tag | UNP D0BBJ1 |
| A | -4 | HIS | - | expression tag | UNP D0BBJ1 |
| A | -3 | HIS | - | expression tag | UNP D0BBJ1 |
| A | -2 | HIS | - | expression tag | UNP D0BBJ1 |
| A | -1 | HIS | - | expression tag | UNP D0BBJ1 |
| A | 0 | HIS | - | expression tag | UNP D0BBJ1 |
| B | -7 | MET | - | initiating methionine | UNP D0BBJ1 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment | Reference |
|:-----:|:-------:|:--------:|:------:|:-------:|:---------:|
| B | -6 | ALA | - | expression tag | UNP D0BBJ1 |
| B | -5 | HIS | - | expression tag | UNP D0BBJ1 |
| B | -4 | HIS | - | expression tag | UNP D0BBJ1 |
| B | -3 | HIS | - | expression tag | UNP D0BBJ1 |
| B | -2 | HIS | - | expression tag | UNP D0BBJ1 |
| B | -1 | HIS | - | expression tag | UNP D0BBJ1 |
| B | 0 | HIS | - | expression tag | UNP D0BBJ1 |
| C | -7 | MET | - | initiating methionine | UNP D0BBJ1 |
| C | -6 | ALA | - | expression tag | UNP D0BBJ1 |
| C | -5 | HIS | - | expression tag | UNP D0BBJ1 |
| C | -4 | HIS | - | expression tag | UNP D0BBJ1 |
| C | -3 | HIS | - | expression tag | UNP D0BBJ1 |
| C | -2 | HIS | - | expression tag | UNP D0BBJ1 |
| C | -1 | HIS | - | expression tag | UNP D0BBJ1 |
| C | 0 | HIS | - | expression tag | UNP D0BBJ1 |
| D | -7 | MET | - | initiating methionine | UNP D0BBJ1 |
| D | -6 | ALA | - | expression tag | UNP D0BBJ1 |
| D | -5 | HIS | - | expression tag | UNP D0BBJ1 |
| D | -4 | HIS | - | expression tag | UNP D0BBJ1 |
| D | -3 | HIS | - | expression tag | UNP D0BBJ1 |
| D | -2 | HIS | - | expression tag | UNP D0BBJ1 |
| D | -1 | HIS | - | expression tag | UNP D0BBJ1 |
| D | 0 | HIS | - | expression tag | UNP D0BBJ1 |
| E | -7 | MET | - | initiating methionine | UNP D0BBJ1 |
| E | -6 | ALA | - | expression tag | UNP D0BBJ1 |
| E | -5 | HIS | - | expression tag | UNP D0BBJ1 |
| E | -4 | HIS | - | expression tag | UNP D0BBJ1 |
| E | -3 | HIS | - | expression tag | UNP D0BBJ1 |
| E | -2 | HIS | - | expression tag | UNP D0BBJ1 |
| E | -1 | HIS | - | expression tag | UNP D0BBJ1 |
| E | 0 | HIS | - | expression tag | UNP D0BBJ1 |
| F | -7 | MET | - | initiating methionine | UNP D0BBJ1 |
| F | -6 | ALA | - | expression tag | UNP D0BBJ1 |
| F | -5 | HIS | - | expression tag | UNP D0BBJ1 |
| F | -4 | HIS | - | expression tag | UNP D0BBJ1 |
| F | -3 | HIS | - | expression tag | UNP D0BBJ1 |
| F | -2 | HIS | - | expression tag | UNP D0BBJ1 |
| F | -1 | HIS | - | expression tag | UNP D0BBJ1 |
| F | 0 | HIS | - | expression tag | UNP D0BBJ1 |
| G | -7 | MET | - | initiating methionine | UNP D0BBJ1 |
| G | -6 | ALA | - | expression tag | UNP D0BBJ1 |
| G | -5 | HIS | - | expression tag | UNP D0BBJ1 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| G | -4 | HIS | - | expression tag | UNP D0BBJ1 |
| G | -3 | HIS | - | expression tag | UNP D0BBJ1 |
| G | -2 | HIS | - | expression tag | UNP D0BBJ1 |
| G | -1 | HIS | - | expression tag | UNP D0BBJ1 |
| G | 0 | HIS | - | expression tag | UNP D0BBJ1 |
| H | -7 | MET | - | initiating methionine | UNP D0BBJ1 |
| H | -6 | ALA | - | expression tag | UNP D0BBJ1 |
| H | -5 | HIS | - | expression tag | UNP D0BBJ1 |
| H | -4 | HIS | - | expression tag | UNP D0BBJ1 |
| H | -3 | HIS | - | expression tag | UNP D0BBJ1 |
| H | -2 | HIS | - | expression tag | UNP D0BBJ1 |
| H | -1 | HIS | - | expression tag | UNP D0BBJ1 |
| H | 0 | HIS | - | expression tag | UNP D0BBJ1 |
| I | -7 | MET | - | initiating methionine | UNP D0BBJ1 |
| I | -6 | ALA | - | expression tag | UNP D0BBJ1 |
| I | -5 | HIS | - | expression tag | UNP D0BBJ1 |
| I | -4 | HIS | - | expression tag | UNP D0BBJ1 |
| I | -3 | HIS | - | expression tag | UNP D0BBJ1 |
| I | -2 | HIS | - | expression tag | UNP D0BBJ1 |
| I | -1 | HIS | - | expression tag | UNP D0BBJ1 |
| I | 0 | HIS | - | expression tag | UNP D0BBJ1 |
| J | -7 | MET | - | initiating methionine | UNP D0BBJ1 |
| J | -6 | ALA | - | expression tag | UNP D0BBJ1 |
| J | -5 | HIS | - | expression tag | UNP D0BBJ1 |
| J | -4 | HIS | - | expression tag | UNP D0BBJ1 |
| J | -3 | HIS | - | expression tag | UNP D0BBJ1 |
| J | -2 | HIS | - | expression tag | UNP D0BBJ1 |
| J | -1 | HIS | - | expression tag | UNP D0BBJ1 |
| J | 0 | HIS | - | expression tag | UNP D0BBJ1 |

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|------|---------|---------|
| 2 | D | 1 | Total | Cl | 0 | 0 |
|   |   |   | 1 | 1 |   |   |
| 2 | E | 1 | Total | Cl | 0 | 0 |
|   |   |   | 1 | 1 |   |   |
| 2 | H | 1 | Total | Cl | 0 | 0 |
|   |   |   | 1 | 1 |   |   |
| 2 | B | 1 | Total | Cl | 0 | 0 |
|   |   |   | 1 | 1 |   |   |
| 2 | I | 1 | Total | Cl | 0 | 0 |
|   |   |   | 1 | 1 |   |   |

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 2 | C | 1 | Total 1 | Cl 1 | 0 | 0 |
| 2 | A | 1 | Total 1 | Cl 1 | 0 | 0 |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 3 | A | 46 | Total 46 | O 46 | 0 | 0 |
| 3 | B | 52 | Total 52 | O 52 | 0 | 0 |
| 3 | C | 38 | Total 38 | O 38 | 0 | 0 |
| 3 | D | 54 | Total 54 | O 54 | 0 | 0 |
| 3 | E | 41 | Total 41 | O 41 | 0 | 0 |
| 3 | F | 49 | Total 49 | O 49 | 0 | 0 |
| 3 | G | 41 | Total 41 | O 41 | 0 | 0 |
| 3 | H | 28 | Total 28 | O 28 | 0 | 0 |
| 3 | I | 2 | Total 2 | O 2 | 0 | 0 |
| 3 | J | 3 | Total 3 | O 3 | 0 | 0 |

# 3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: Aminotransferase

Chain A:

- Molecule 1: Aminotransferase

Chain B:

- Molecule 1: Aminotransferase

Chain C:

- Molecule 1: Aminotransferase

Chain D:

K339 G340 A341 I342 M357 V358 Q374 P375 R379 F380 G381 V382 T383 F412 F413 G414

• Molecule 1: Aminotransferase

Chain E:

87%    8%   • •

MET ALA HIS HIS HIS HIS MET ASP GLN LYS ASN PRO LEU THR MET ALA Y11 R18 V27 E58 V62 H63 R64 G65 L66 H67 S70 N71 S80 R85 R86 M115 P116 P153 E164 R172 R201 D208 K234 V235 R247 A248 Q249

E266 I292 E302 R317 G334 K339 V358 R367 Q374 P375 R379 T383 S384 G414

• Molecule 1: Aminotransferase

Chain F:

88%    6%   • •

MET ALA HIS HIS HIS HIS MET ASP GLN LYS ASN PRO LEU THR MET ALA Y11 V27 V62 H63 R64 H67 S70 N71 E78 K79 S80 R85 R86 N89 M115 P116 P153 E163 E164 R201 D226 V235 V243 R247 E262

E302 R317 R323 R326 S329 G334 K339 E348 M357 R361 R379 G414

• Molecule 1: Aminotransferase

Chain G:

3%

87%    8%   • 5%

MET ALA HIS HIS HIS HIS MET ASP GLN LYS ASN PRO LEU THR MET ALA Y11 V27 H28 V62 H63 R64 G65 L66 N71 E78 K79 S80 R85 R86 G91 M115 P116 P153 N157 E164 D208 G209 Y228 K234 V235 R247 E266

E269 I292 E302 R317 R323 L324 G325 R326 I327 N328 G334 K339 G349 A352 V358 V366 T370 Q374 P375 R379 R387 A409 R410 K411 F412 F413 GLY

• Molecule 1: Aminotransferase

Chain H:

4%

89%    5%   5%

MET ALA HIS HIS HIS HIS MET ASP GLN LYS ASN PRO LEU THR MET ALA Y11 D12 V13 E14 A15 I16 L23 V27 I48 N57 V62 HIS ARG GLY LEU H67 N71 S80 R85 R86 M115 P116 D122 I162 R172 D208 K234 V235

R247 M250 I292 E302 K303 I304 G305 A308 I309 V358 Q374 P375 R379 T383 S384 A391 L392 Y393 V399 F412 F413 G414

• Molecule 1: Aminotransferase

Chain I:

28%

90%    •   6%

MET ALA HIS HIS HIS HIS MET ASP GLN LYS ASN PRO LEU THR MET ALA Y11 D12 V13 E14 A15 I16 R17 R18 D19 F20 P21 V27 L32 V33 Y34 A41 Q42 K43 V51 T52 Y55 A56 N57 E58 Y59 A60 H63 ARG GLY LEU H67 F68 L69 S70 A73

• Molecule 1: Aminotransferase

# 4   Data and refinement statistics ⓘ

| Property | Value | Source |
|---|---|---|
| Space group | P 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 89.85Å    121.91Å    133.72Å<br>111.49°    106.53°      89.81° | Depositor |
| Resolution (Å) | 50.00  –  2.45<br>48.39  –  2.45 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 96.5 (50.00-2.45)<br>84.4 (48.39-2.45) | Depositor<br>EDS |
| $R_{merge}$ | 0.07 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $<I/\sigma(I)>$ [1] | 2.22 (at 2.45Å) | Xtriage |
| Refinement program | REFMAC 5.8.0073 | Depositor |
| R, $R_{free}$ | 0.237  ,  0.252<br>0.231  ,  0.249 | Depositor<br>DCC |
| $R_{free}$ test set | 8955 reflections (5.29%) | DCC |
| Wilson B-factor (Å$^2$) | 34.6 | Xtriage |
| Anisotropy | 1.233 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.32 , 38.1 | EDS |
| L-test for twinning[2] | $<\vert L \vert> = 0.49, <L^2> = 0.33$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.93 | EDS |
| Total number of atoms | 30371 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 61.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<\vert L \vert>$, $<L^2>$ 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LLP, CL

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 | 0.57 | 0/3168 | 0.77 | 7/4301 (0.2%) |
| 1 | B | 0.58 | 0/3155 | 0.70 | 3/4284 (0.1%) |
| 1 | C | 0.60 | 2/3163 (0.1%) | 0.75 | 7/4293 (0.2%) |
| 1 | D | 0.62 | 1/3179 (0.0%) | 0.73 | 4/4312 (0.1%) |
| 1 | E | 0.59 | 0/3128 | 0.76 | 11/4254 (0.3%) |
| 1 | F | 0.58 | 1/3146 (0.0%) | 0.71 | 3/4277 (0.1%) |
| 1 | G | 0.52 | 1/3084 (0.0%) | 0.70 | 3/4201 (0.1%) |
| 1 | H | 0.52 | 0/3084 | 0.73 | 5/4194 (0.1%) |
| 1 | I | 0.48 | 0/2794 | 0.66 | 2/3822 (0.1%) |
| 1 | J | 0.47 | 0/2538 | 0.64 | 3/3472 (0.1%) |
| All | All | 0.56 | 5/30439 (0.0%) | 0.72 | 48/41410 (0.1%) |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1 | D | 78 | GLU | CD-OE2 | 5.69 | 1.31 | 1.25 |
| 1 | G | 78 | GLU | CD-OE2 | 5.55 | 1.31 | 1.25 |
| 1 | F | 80 | SER | CA-CB | 5.49 | 1.61 | 1.52 |
| 1 | C | 384 | SER | CA-CB | -5.25 | 1.45 | 1.52 |
| 1 | C | 384 | SER | CB-OG | -5.04 | 1.35 | 1.42 |

The worst 5 of 48 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1 | A | 379 | ARG | NE-CZ-NH1 | 10.86 | 125.73 | 120.30 |
| 1 | C | 201 | ARG | NE-CZ-NH2 | 9.40 | 125.00 | 120.30 |
| 1 | A | 379 | ARG | NE-CZ-NH2 | -9.00 | 115.80 | 120.30 |
| 1 | D | 247 | ARG | NE-CZ-NH1 | -8.82 | 115.89 | 120.30 |
| 1 | A | 247 | ARG | NE-CZ-NH2 | -8.62 | 115.99 | 120.30 |

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 | 3117 | 0 | 3021 | 21 | 0 |
| 1 | B | 3110 | 0 | 3012 | 16 | 0 |
| 1 | C | 3118 | 0 | 3023 | 16 | 0 |
| 1 | D | 3131 | 0 | 3048 | 17 | 0 |
| 1 | E | 3083 | 0 | 2950 | 12 | 0 |
| 1 | F | 3097 | 0 | 2972 | 15 | 0 |
| 1 | G | 3041 | 0 | 2896 | 16 | 0 |
| 1 | H | 3041 | 0 | 2917 | 10 | 0 |
| 1 | I | 2764 | 0 | 2421 | 9 | 0 |
| 1 | J | 2508 | 0 | 2181 | 5 | 0 |
| 2 | A | 1 | 0 | 0 | 0 | 0 |
| 2 | B | 1 | 0 | 0 | 0 | 0 |
| 2 | C | 1 | 0 | 0 | 0 | 0 |
| 2 | D | 1 | 0 | 0 | 0 | 0 |
| 2 | E | 1 | 0 | 0 | 0 | 0 |
| 2 | H | 1 | 0 | 0 | 0 | 0 |
| 2 | I | 1 | 0 | 0 | 0 | 0 |
| 3 | A | 46 | 0 | 0 | 1 | 0 |
| 3 | B | 52 | 0 | 0 | 1 | 0 |
| 3 | C | 38 | 0 | 0 | 0 | 0 |
| 3 | D | 54 | 0 | 0 | 0 | 0 |
| 3 | E | 41 | 0 | 0 | 0 | 0 |
| 3 | F | 49 | 0 | 0 | 0 | 0 |
| 3 | G | 41 | 0 | 0 | 1 | 0 |
| 3 | H | 28 | 0 | 0 | 2 | 0 |
| 3 | I | 2 | 0 | 0 | 0 | 0 |
| 3 | J | 3 | 0 | 0 | 0 | 0 |
| All | All | 30371 | 0 | 28441 | 126 | 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 126 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:F:78:GLU:HA | 1:F:78:GLU:OE1 | 1.67 | 0.94 |
| 1:H:247:ARG:HD3 | 3:H:621:HOH:O | 1.81 | 0.79 |
| 1:C:115:MET:HB3 | 1:C:116:PRO:HD3 | 1.75 | 0.69 |
| 1:D:115:MET:HB3 | 1:D:116:PRO:HD3 | 1.76 | 0.68 |
| 1:A:115:MET:HB3 | 1:A:116:PRO:HD3 | 1.74 | 0.67 |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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 | 403/422 (96%) | 390 (97%) | 10 (2%) | 3 (1%) | 25 | 30 |
| 1 | B | 402/422 (95%) | 389 (97%) | 10 (2%) | 3 (1%) | 25 | 30 |
| 1 | C | 401/422 (95%) | 388 (97%) | 10 (2%) | 3 (1%) | 25 | 30 |
| 1 | D | 402/422 (95%) | 388 (96%) | 11 (3%) | 3 (1%) | 25 | 30 |
| 1 | E | 401/422 (95%) | 388 (97%) | 10 (2%) | 3 (1%) | 25 | 30 |
| 1 | F | 402/422 (95%) | 389 (97%) | 10 (2%) | 3 (1%) | 25 | 30 |
| 1 | G | 400/422 (95%) | 387 (97%) | 10 (2%) | 3 (1%) | 22 | 26 |
| 1 | H | 395/422 (94%) | 384 (97%) | 10 (2%) | 1 (0%) | 44 | 55 |
| 1 | I | 391/422 (93%) | 380 (97%) | 10 (3%) | 1 (0%) | 44 | 55 |
| 1 | J | 347/422 (82%) | 335 (96%) | 9 (3%) | 3 (1%) | 20 | 23 |
| All | All | 3944/4220 (94%) | 3818 (97%) | 100 (2%) | 26 (1%) | 25 | 30 |

5 of 26 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 64 | ARG |
| 1 | B | 64 | ARG |
| 1 | C | 64 | ARG |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 64  | ARG  |
| 1   | E     | 64  | ARG  |

### 5.3.2   Protein sidechains ⓘ

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     | 312/341 (92%) | 301 (96%) | 11 (4%) | 41 | 56 |
| 1   | B     | 311/341 (91%) | 303 (97%) | 8 (3%)  | 51 | 66 |
| 1   | C     | 313/341 (92%) | 303 (97%) | 10 (3%) | 44 | 58 |
| 1   | D     | 316/341 (93%) | 307 (97%) | 9 (3%)  | 49 | 63 |
| 1   | E     | 305/341 (89%) | 295 (97%) | 10 (3%) | 43 | 57 |
| 1   | F     | 308/341 (90%) | 299 (97%) | 9 (3%)  | 48 | 61 |
| 1   | G     | 297/341 (87%) | 288 (97%) | 9 (3%)  | 46 | 60 |
| 1   | H     | 300/341 (88%) | 293 (98%) | 7 (2%)  | 56 | 70 |
| 1   | I     | 233/341 (68%) | 229 (98%) | 4 (2%)  | 66 | 78 |
| 1   | J     | 215/341 (63%) | 210 (98%) | 5 (2%)  | 56 | 70 |
| All | All   | 2910/3410 (85%) | 2828 (97%) | 82 (3%) | 49 | 63 |

5 of 82 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 383 | THR  |
| 1   | E     | 379 | ARG  |
| 1   | I     | 358 | VAL  |
| 1   | E     | 27  | VAL  |
| 1   | E     | 201 | ARG  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 335 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------|------|----------|--------|------|----------|
| | | | | | Counts | RMSZ | #$|Z| > 2$ | Counts | RMSZ | #$|Z| > 2$ |
| 1 | LLP | A | 234 | 1 | 24,24,25 | 3.37 | 4 (16%) | 28,32,34 | 1.31 | 2 (7%) |
| 1 | LLP | B | 234 | 1 | 24,24,25 | 2.90 | 6 (25%) | 28,32,34 | 1.54 | 5 (17%) |
| 1 | LLP | C | 234 | 1 | 24,24,25 | 3.03 | 5 (20%) | 28,32,34 | 1.28 | 3 (10%) |
| 1 | LLP | D | 234 | 1 | 24,24,25 | 3.29 | 5 (20%) | 28,32,34 | 1.51 | 4 (14%) |
| 1 | LLP | E | 234 | 1 | 24,24,25 | 2.64 | 6 (25%) | 28,32,34 | 1.40 | 3 (10%) |
| 1 | LLP | F | 234 | 1 | 24,24,25 | 2.85 | 5 (20%) | 28,32,34 | 1.38 | 3 (10%) |
| 1 | LLP | G | 234 | 1 | 24,24,25 | 3.36 | 5 (20%) | 28,32,34 | 1.36 | 3 (10%) |
| 1 | LLP | H | 234 | 1 | 24,24,25 | 3.32 | 5 (20%) | 28,32,34 | 1.38 | 5 (17%) |
| 1 | LLP | I | 234 | 1 | 24,24,25 | 3.24 | 5 (20%) | 28,32,34 | 1.33 | 3 (10%) |
| 1 | LLP | J | 234 | 1 | 24,24,25 | 3.15 | 5 (20%) | 28,32,34 | 1.43 | 5 (17%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 1 | LLP | A | 234 | 1 | - | 0/15/17/19 | 0/1/1/1 |
| 1 | LLP | B | 234 | 1 | - | 0/15/17/19 | 0/1/1/1 |
| 1 | LLP | C | 234 | 1 | - | 0/15/17/19 | 0/1/1/1 |
| 1 | LLP | D | 234 | 1 | - | 0/15/17/19 | 0/1/1/1 |
| 1 | LLP | E | 234 | 1 | - | 0/15/17/19 | 0/1/1/1 |
| 1 | LLP | F | 234 | 1 | - | 0/15/17/19 | 0/1/1/1 |
| 1 | LLP | G | 234 | 1 | - | 0/15/17/19 | 0/1/1/1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 1 | LLP | H | 234 | 1 | - | 0/15/17/19 | 0/1/1/1 |
| 1 | LLP | I | 234 | 1 | - | 0/15/17/19 | 0/1/1/1 |
| 1 | LLP | J | 234 | 1 | - | 0/15/17/19 | 0/1/1/1 |

The worst 5 of 51 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 1 | F | 234 | LLP | C6-C5 | 2.02 | 1.41 | 1.37 |
| 1 | I | 234 | LLP | C4-C4' | 2.10 | 1.50 | 1.46 |
| 1 | D | 234 | LLP | C4-C4' | 2.11 | 1.50 | 1.46 |
| 1 | E | 234 | LLP | CA-C | 2.11 | 1.53 | 1.50 |
| 1 | C | 234 | LLP | C4-C4' | 2.43 | 1.50 | 1.46 |

The worst 5 of 36 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|-------|---|----------------|-------------|
| 1 | D | 234 | LLP | C4-C3-C2 | -4.57 | 117.34 | 120.15 |
| 1 | B | 234 | LLP | C4-C3-C2 | -4.08 | 117.64 | 120.15 |
| 1 | A | 234 | LLP | C4-C3-C2 | -4.01 | 117.69 | 120.15 |
| 1 | G | 234 | LLP | C4-C3-C2 | -3.55 | 117.97 | 120.15 |
| 1 | H | 234 | LLP | C4-C3-C2 | -3.44 | 118.04 | 120.15 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 9 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1 | A | 234 | LLP | 1 | 0 |
| 1 | B | 234 | LLP | 1 | 0 |
| 1 | C | 234 | LLP | 1 | 0 |
| 1 | D | 234 | LLP | 1 | 0 |
| 1 | E | 234 | LLP | 1 | 0 |
| 1 | G | 234 | LLP | 1 | 0 |
| 1 | H | 234 | LLP | 1 | 0 |
| 1 | I | 234 | LLP | 1 | 0 |
| 1 | J | 234 | LLP | 1 | 0 |

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

# 6   Fit of model and data ⓘ

## 6.1   Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å$^2$) | Q<0.9 |
|-----|-------|----------|--------|---------|-----|-----|-------------|-------|
| 1 | A | 403/422 (95%) | -0.06 | 3 (0%) | 87 | 89 | 39, 52, 68, 79 | 0 |
| 1 | B | 404/422 (95%) | -0.03 | 3 (0%) | 87 | 89 | 39, 50, 65, 80 | 0 |
| 1 | C | 403/422 (95%) | -0.11 | 1 (0%) | 94 | 95 | 43, 54, 65, 71 | 0 |
| 1 | D | 403/422 (95%) | -0.07 | 0 | 100 | 100 | 41, 49, 60, 67 | 0 |
| 1 | E | 403/422 (95%) | -0.10 | 2 (0%) | 90 | 92 | 40, 52, 68, 77 | 0 |
| 1 | F | 403/422 (95%) | 0.01 | 2 (0%) | 90 | 92 | 41, 55, 72, 82 | 0 |
| 1 | G | 402/422 (95%) | 0.18 | 11 (2%) | 55 | 50 | 51, 63, 87, 105 | 0 |
| 1 | H | 399/422 (94%) | 0.27 | 15 (3%) | 41 | 38 | 55, 69, 81, 89 | 0 |
| 1 | I | 397/422 (94%) | 1.57 | 118 (29%) | 1 | 0 | 66, 89, 125, 143 | 0 |
| 1 | J | 355/422 (84%) | 1.57 | 100 (28%) | 1 | 0 | 70, 85, 106, 116 | 0 |
| All | All | 3972/4220 (94%) | 0.31 | 255 (6%) | 20 | 17 | 39, 58, 98, 143 | 0 |

The worst 5 of 255 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | I | 126 | LEU | 11.6 |
| 1 | J | 203 | ILE | 7.6 |
| 1 | I | 76 | ALA | 7.2 |
| 1 | J | 373 | ALA | 7.1 |
| 1 | I | 304 | ILE | 7.0 |

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy

less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|------------------|-------|
| 1 | LLP | H | 234 | 24/25 | 0.96 | 0.16 | - | 54,56,59,61 | 0 |
| 1 | LLP | I | 234 | 24/25 | 0.89 | 0.22 | - | 72,75,80,82 | 0 |
| 1 | LLP | F | 234 | 24/25 | 0.98 | 0.17 | - | 42,44,46,47 | 0 |
| 1 | LLP | J | 234 | 24/25 | 0.90 | 0.22 | - | 75,77,79,80 | 0 |
| 1 | LLP | C | 234 | 24/25 | 0.97 | 0.15 | - | 44,46,47,47 | 0 |
| 1 | LLP | A | 234 | 24/25 | 0.97 | 0.14 | - | 40,43,44,45 | 0 |
| 1 | LLP | G | 234 | 24/25 | 0.97 | 0.15 | - | 54,57,59,59 | 0 |
| 1 | LLP | D | 234 | 24/25 | 0.97 | 0.17 | - | 41,41,42,43 | 0 |
| 1 | LLP | E | 234 | 24/25 | 0.98 | 0.15 | - | 41,42,44,45 | 0 |
| 1 | LLP | B | 234 | 24/25 | 0.98 | 0.16 | - | 38,40,41,41 | 0 |

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|------------------|-------|
| 2 | CL | I | 501 | 1/1 | 0.84 | 0.17 | - | 79,79,79,79 | 0 |
| 2 | CL | C | 501 | 1/1 | 0.85 | 0.14 | - | 86,86,86,86 | 0 |
| 2 | CL | B | 501 | 1/1 | 0.81 | 0.22 | - | 69,69,69,69 | 0 |
| 2 | CL | E | 501 | 1/1 | 0.82 | 0.20 | - | 72,72,72,72 | 0 |
| 2 | CL | D | 501 | 1/1 | 0.87 | 0.17 | - | 52,52,52,52 | 0 |
| 2 | CL | H | 501 | 1/1 | 0.70 | 0.15 | - | 71,71,71,71 | 0 |
| 2 | CL | A | 501 | 1/1 | 0.85 | 0.18 | - | 69,69,69,69 | 0 |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.