



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 04:11 PM UTC

PDB ID : 1N0F / pdb\_00001n0f  
Title : CRYSTAL STRUCTURE OF A CELL DIVISION AND CELL WALL BIOSYNTHESIS PROTEIN UPF0040 FROM MYCOPLASMA PNEUMONIAE: INDICATION OF A NOVEL FOLD WITH A POSSIBLE NEW CONSERVED SEQUENCE MOTIF  
Authors : Chen, S.; Jancrick, J.; Yokota, H.; Kim, R.; Kim, S.-H.; Berkeley Structural Genomics Center (BSGC)  
Deposited on : 2002-10-13  
Resolution : 2.80 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

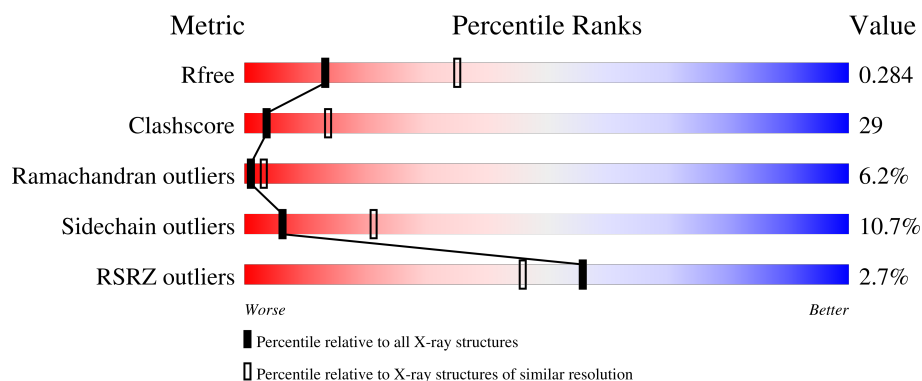
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 3866 (2.80-2.80)                                      |
| Clashscore            | 190562                      | 4276 (2.80-2.80)                                      |
| Ramachandran outliers | 187476                      | 4196 (2.80-2.80)                                      |
| Sidechain outliers    | 187428                      | 4198 (2.80-2.80)                                      |
| RSRZ outliers         | 180081                      | 3869 (2.80-2.80)                                      |

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  $\geq 3$ , 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  $\leq 5\%$ . 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     | 166    | <div> <div>2%</div> <div> <div>34%</div> <div>37%</div> <div>13%</div> <div>•</div> <div>15%</div> </div> </div> |
| 1   | B     | 166    | <div> <div>0%</div> <div> <div>42%</div> <div>26%</div> <div>14%</div> <div>•</div> <div>16%</div> </div> </div> |
| 1   | C     | 166    | <div> <div>2%</div> <div> <div>43%</div> <div>27%</div> <div>11%</div> <div>•</div> <div>17%</div> </div> </div> |
| 1   | D     | 166    | <div> <div>0%</div> <div> <div>40%</div> <div>27%</div> <div>13%</div> <div>•</div> <div>17%</div> </div> </div> |

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| Mol | Chain | Length | Quality of chain                                                                                        |
|-----|-------|--------|---------------------------------------------------------------------------------------------------------|
| 1   | E     | 166    | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>5%37%31%13%•17%</div></div> |
| 1   | F     | 166    | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>%42%28%11%•17%</div></div>  |
| 1   | G     | 166    | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>%36%32%13%•17%</div></div>  |
| 1   | H     | 166    | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>5%36%31%13%•17%</div></div> |

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 9184 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 Protein mraZ.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | A     | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1153  | 739 | 197 | 214 | 3 |         |         |       |
| 1   | B     | 139      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1133  | 725 | 194 | 211 | 3 |         |         |       |
| 1   | C     | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1119  | 717 | 190 | 209 | 3 |         |         |       |
| 1   | D     | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1119  | 717 | 190 | 209 | 3 |         |         |       |
| 1   | E     | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1119  | 717 | 190 | 209 | 3 |         |         |       |
| 1   | F     | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1119  | 717 | 190 | 209 | 3 |         |         |       |
| 1   | G     | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1119  | 717 | 190 | 209 | 3 |         |         |       |
| 1   | H     | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1119  | 717 | 190 | 209 | 3 |         |         |       |

There are 200 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 1       | MET      | -      | expression tag | UNP P75467 |
| A     | 2       | GLY      | -      | expression tag | UNP P75467 |
| A     | 3       | SER      | -      | expression tag | UNP P75467 |
| A     | 4       | SER      | -      | expression tag | UNP P75467 |
| A     | 5       | HIS      | -      | expression tag | UNP P75467 |
| A     | 6       | HIS      | -      | expression tag | UNP P75467 |
| A     | 7       | HIS      | -      | expression tag | UNP P75467 |
| A     | 8       | HIS      | -      | expression tag | UNP P75467 |
| A     | 9       | HIS      | -      | expression tag | UNP P75467 |
| A     | 10      | HIS      | -      | expression tag | UNP P75467 |
| A     | 11      | ASP      | -      | expression tag | UNP P75467 |
| A     | 12      | TYR      | -      | expression tag | UNP P75467 |
| A     | 13      | ASP      | -      | expression tag | UNP P75467 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 14      | ILE      | -      | expression tag | UNP P75467 |
| A     | 15      | PRO      | -      | expression tag | UNP P75467 |
| A     | 16      | THR      | -      | expression tag | UNP P75467 |
| A     | 17      | THR      | -      | expression tag | UNP P75467 |
| A     | 18      | GLU      | -      | expression tag | UNP P75467 |
| A     | 19      | ASN      | -      | expression tag | UNP P75467 |
| A     | 20      | LEU      | -      | expression tag | UNP P75467 |
| A     | 21      | TYR      | -      | expression tag | UNP P75467 |
| A     | 22      | PHE      | -      | expression tag | UNP P75467 |
| A     | 23      | GLN      | -      | expression tag | UNP P75467 |
| A     | 24      | GLY      | -      | expression tag | UNP P75467 |
| A     | 25      | HIS      | -      | expression tag | UNP P75467 |
| B     | 1       | MET      | -      | expression tag | UNP P75467 |
| B     | 2       | GLY      | -      | expression tag | UNP P75467 |
| B     | 3       | SER      | -      | expression tag | UNP P75467 |
| B     | 4       | SER      | -      | expression tag | UNP P75467 |
| B     | 5       | HIS      | -      | expression tag | UNP P75467 |
| B     | 6       | HIS      | -      | expression tag | UNP P75467 |
| B     | 7       | HIS      | -      | expression tag | UNP P75467 |
| B     | 8       | HIS      | -      | expression tag | UNP P75467 |
| B     | 9       | HIS      | -      | expression tag | UNP P75467 |
| B     | 10      | HIS      | -      | expression tag | UNP P75467 |
| B     | 11      | ASP      | -      | expression tag | UNP P75467 |
| B     | 12      | TYR      | -      | expression tag | UNP P75467 |
| B     | 13      | ASP      | -      | expression tag | UNP P75467 |
| B     | 14      | ILE      | -      | expression tag | UNP P75467 |
| B     | 15      | PRO      | -      | expression tag | UNP P75467 |
| B     | 16      | THR      | -      | expression tag | UNP P75467 |
| B     | 17      | THR      | -      | expression tag | UNP P75467 |
| B     | 18      | GLU      | -      | expression tag | UNP P75467 |
| B     | 19      | ASN      | -      | expression tag | UNP P75467 |
| B     | 20      | LEU      | -      | expression tag | UNP P75467 |
| B     | 21      | TYR      | -      | expression tag | UNP P75467 |
| B     | 22      | PHE      | -      | expression tag | UNP P75467 |
| B     | 23      | GLN      | -      | expression tag | UNP P75467 |
| B     | 24      | GLY      | -      | expression tag | UNP P75467 |
| B     | 25      | HIS      | -      | expression tag | UNP P75467 |
| C     | 1       | MET      | -      | expression tag | UNP P75467 |
| C     | 2       | GLY      | -      | expression tag | UNP P75467 |
| C     | 3       | SER      | -      | expression tag | UNP P75467 |
| C     | 4       | SER      | -      | expression tag | UNP P75467 |
| C     | 5       | HIS      | -      | expression tag | UNP P75467 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | 6       | HIS      | -      | expression tag | UNP P75467 |
| C     | 7       | HIS      | -      | expression tag | UNP P75467 |
| C     | 8       | HIS      | -      | expression tag | UNP P75467 |
| C     | 9       | HIS      | -      | expression tag | UNP P75467 |
| C     | 10      | HIS      | -      | expression tag | UNP P75467 |
| C     | 11      | ASP      | -      | expression tag | UNP P75467 |
| C     | 12      | TYR      | -      | expression tag | UNP P75467 |
| C     | 13      | ASP      | -      | expression tag | UNP P75467 |
| C     | 14      | ILE      | -      | expression tag | UNP P75467 |
| C     | 15      | PRO      | -      | expression tag | UNP P75467 |
| C     | 16      | THR      | -      | expression tag | UNP P75467 |
| C     | 17      | THR      | -      | expression tag | UNP P75467 |
| C     | 18      | GLU      | -      | expression tag | UNP P75467 |
| C     | 19      | ASN      | -      | expression tag | UNP P75467 |
| C     | 20      | LEU      | -      | expression tag | UNP P75467 |
| C     | 21      | TYR      | -      | expression tag | UNP P75467 |
| C     | 22      | PHE      | -      | expression tag | UNP P75467 |
| C     | 23      | GLN      | -      | expression tag | UNP P75467 |
| C     | 24      | GLY      | -      | expression tag | UNP P75467 |
| C     | 25      | HIS      | -      | expression tag | UNP P75467 |
| D     | 1       | MET      | -      | expression tag | UNP P75467 |
| D     | 2       | GLY      | -      | expression tag | UNP P75467 |
| D     | 3       | SER      | -      | expression tag | UNP P75467 |
| D     | 4       | SER      | -      | expression tag | UNP P75467 |
| D     | 5       | HIS      | -      | expression tag | UNP P75467 |
| D     | 6       | HIS      | -      | expression tag | UNP P75467 |
| D     | 7       | HIS      | -      | expression tag | UNP P75467 |
| D     | 8       | HIS      | -      | expression tag | UNP P75467 |
| D     | 9       | HIS      | -      | expression tag | UNP P75467 |
| D     | 10      | HIS      | -      | expression tag | UNP P75467 |
| D     | 11      | ASP      | -      | expression tag | UNP P75467 |
| D     | 12      | TYR      | -      | expression tag | UNP P75467 |
| D     | 13      | ASP      | -      | expression tag | UNP P75467 |
| D     | 14      | ILE      | -      | expression tag | UNP P75467 |
| D     | 15      | PRO      | -      | expression tag | UNP P75467 |
| D     | 16      | THR      | -      | expression tag | UNP P75467 |
| D     | 17      | THR      | -      | expression tag | UNP P75467 |
| D     | 18      | GLU      | -      | expression tag | UNP P75467 |
| D     | 19      | ASN      | -      | expression tag | UNP P75467 |
| D     | 20      | LEU      | -      | expression tag | UNP P75467 |
| D     | 21      | TYR      | -      | expression tag | UNP P75467 |
| D     | 22      | PHE      | -      | expression tag | UNP P75467 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| D     | 23      | GLN      | -      | expression tag | UNP P75467 |
| D     | 24      | GLY      | -      | expression tag | UNP P75467 |
| D     | 25      | HIS      | -      | expression tag | UNP P75467 |
| E     | 1       | MET      | -      | expression tag | UNP P75467 |
| E     | 2       | GLY      | -      | expression tag | UNP P75467 |
| E     | 3       | SER      | -      | expression tag | UNP P75467 |
| E     | 4       | SER      | -      | expression tag | UNP P75467 |
| E     | 5       | HIS      | -      | expression tag | UNP P75467 |
| E     | 6       | HIS      | -      | expression tag | UNP P75467 |
| E     | 7       | HIS      | -      | expression tag | UNP P75467 |
| E     | 8       | HIS      | -      | expression tag | UNP P75467 |
| E     | 9       | HIS      | -      | expression tag | UNP P75467 |
| E     | 10      | HIS      | -      | expression tag | UNP P75467 |
| E     | 11      | ASP      | -      | expression tag | UNP P75467 |
| E     | 12      | TYR      | -      | expression tag | UNP P75467 |
| E     | 13      | ASP      | -      | expression tag | UNP P75467 |
| E     | 14      | ILE      | -      | expression tag | UNP P75467 |
| E     | 15      | PRO      | -      | expression tag | UNP P75467 |
| E     | 16      | THR      | -      | expression tag | UNP P75467 |
| E     | 17      | THR      | -      | expression tag | UNP P75467 |
| E     | 18      | GLU      | -      | expression tag | UNP P75467 |
| E     | 19      | ASN      | -      | expression tag | UNP P75467 |
| E     | 20      | LEU      | -      | expression tag | UNP P75467 |
| E     | 21      | TYR      | -      | expression tag | UNP P75467 |
| E     | 22      | PHE      | -      | expression tag | UNP P75467 |
| E     | 23      | GLN      | -      | expression tag | UNP P75467 |
| E     | 24      | GLY      | -      | expression tag | UNP P75467 |
| E     | 25      | HIS      | -      | expression tag | UNP P75467 |
| F     | 1       | MET      | -      | expression tag | UNP P75467 |
| F     | 2       | GLY      | -      | expression tag | UNP P75467 |
| F     | 3       | SER      | -      | expression tag | UNP P75467 |
| F     | 4       | SER      | -      | expression tag | UNP P75467 |
| F     | 5       | HIS      | -      | expression tag | UNP P75467 |
| F     | 6       | HIS      | -      | expression tag | UNP P75467 |
| F     | 7       | HIS      | -      | expression tag | UNP P75467 |
| F     | 8       | HIS      | -      | expression tag | UNP P75467 |
| F     | 9       | HIS      | -      | expression tag | UNP P75467 |
| F     | 10      | HIS      | -      | expression tag | UNP P75467 |
| F     | 11      | ASP      | -      | expression tag | UNP P75467 |
| F     | 12      | TYR      | -      | expression tag | UNP P75467 |
| F     | 13      | ASP      | -      | expression tag | UNP P75467 |
| F     | 14      | ILE      | -      | expression tag | UNP P75467 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| F     | 15      | PRO      | -      | expression tag | UNP P75467 |
| F     | 16      | THR      | -      | expression tag | UNP P75467 |
| F     | 17      | THR      | -      | expression tag | UNP P75467 |
| F     | 18      | GLU      | -      | expression tag | UNP P75467 |
| F     | 19      | ASN      | -      | expression tag | UNP P75467 |
| F     | 20      | LEU      | -      | expression tag | UNP P75467 |
| F     | 21      | TYR      | -      | expression tag | UNP P75467 |
| F     | 22      | PHE      | -      | expression tag | UNP P75467 |
| F     | 23      | GLN      | -      | expression tag | UNP P75467 |
| F     | 24      | GLY      | -      | expression tag | UNP P75467 |
| F     | 25      | HIS      | -      | expression tag | UNP P75467 |
| G     | 1       | MET      | -      | expression tag | UNP P75467 |
| G     | 2       | GLY      | -      | expression tag | UNP P75467 |
| G     | 3       | SER      | -      | expression tag | UNP P75467 |
| G     | 4       | SER      | -      | expression tag | UNP P75467 |
| G     | 5       | HIS      | -      | expression tag | UNP P75467 |
| G     | 6       | HIS      | -      | expression tag | UNP P75467 |
| G     | 7       | HIS      | -      | expression tag | UNP P75467 |
| G     | 8       | HIS      | -      | expression tag | UNP P75467 |
| G     | 9       | HIS      | -      | expression tag | UNP P75467 |
| G     | 10      | HIS      | -      | expression tag | UNP P75467 |
| G     | 11      | ASP      | -      | expression tag | UNP P75467 |
| G     | 12      | TYR      | -      | expression tag | UNP P75467 |
| G     | 13      | ASP      | -      | expression tag | UNP P75467 |
| G     | 14      | ILE      | -      | expression tag | UNP P75467 |
| G     | 15      | PRO      | -      | expression tag | UNP P75467 |
| G     | 16      | THR      | -      | expression tag | UNP P75467 |
| G     | 17      | THR      | -      | expression tag | UNP P75467 |
| G     | 18      | GLU      | -      | expression tag | UNP P75467 |
| G     | 19      | ASN      | -      | expression tag | UNP P75467 |
| G     | 20      | LEU      | -      | expression tag | UNP P75467 |
| G     | 21      | TYR      | -      | expression tag | UNP P75467 |
| G     | 22      | PHE      | -      | expression tag | UNP P75467 |
| G     | 23      | GLN      | -      | expression tag | UNP P75467 |
| G     | 24      | GLY      | -      | expression tag | UNP P75467 |
| G     | 25      | HIS      | -      | expression tag | UNP P75467 |
| H     | 1       | MET      | -      | expression tag | UNP P75467 |
| H     | 2       | GLY      | -      | expression tag | UNP P75467 |
| H     | 3       | SER      | -      | expression tag | UNP P75467 |
| H     | 4       | SER      | -      | expression tag | UNP P75467 |
| H     | 5       | HIS      | -      | expression tag | UNP P75467 |
| H     | 6       | HIS      | -      | expression tag | UNP P75467 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| H     | 7       | HIS      | -      | expression tag | UNP P75467 |
| H     | 8       | HIS      | -      | expression tag | UNP P75467 |
| H     | 9       | HIS      | -      | expression tag | UNP P75467 |
| H     | 10      | HIS      | -      | expression tag | UNP P75467 |
| H     | 11      | ASP      | -      | expression tag | UNP P75467 |
| H     | 12      | TYR      | -      | expression tag | UNP P75467 |
| H     | 13      | ASP      | -      | expression tag | UNP P75467 |
| H     | 14      | ILE      | -      | expression tag | UNP P75467 |
| H     | 15      | PRO      | -      | expression tag | UNP P75467 |
| H     | 16      | THR      | -      | expression tag | UNP P75467 |
| H     | 17      | THR      | -      | expression tag | UNP P75467 |
| H     | 18      | GLU      | -      | expression tag | UNP P75467 |
| H     | 19      | ASN      | -      | expression tag | UNP P75467 |
| H     | 20      | LEU      | -      | expression tag | UNP P75467 |
| H     | 21      | TYR      | -      | expression tag | UNP P75467 |
| H     | 22      | PHE      | -      | expression tag | UNP P75467 |
| H     | 23      | GLN      | -      | expression tag | UNP P75467 |
| H     | 24      | GLY      | -      | expression tag | UNP P75467 |
| H     | 25      | HIS      | -      | expression tag | UNP P75467 |

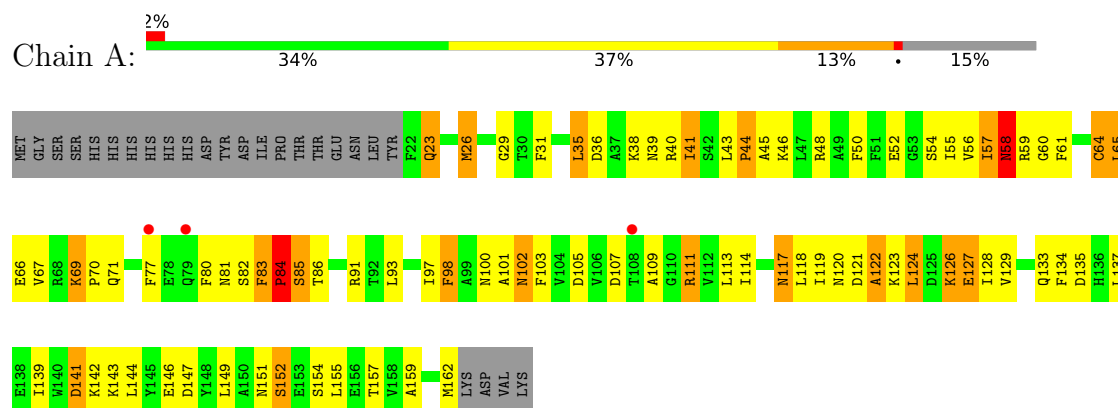
- Molecule 2 is water.

| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 2   | A     | 21       | Total O<br>21 21 | 0       | 0       |
| 2   | B     | 31       | Total O<br>31 31 | 0       | 0       |
| 2   | C     | 23       | Total O<br>23 23 | 0       | 0       |
| 2   | D     | 30       | Total O<br>30 30 | 0       | 0       |
| 2   | E     | 15       | Total O<br>15 15 | 0       | 0       |
| 2   | F     | 10       | Total O<br>10 10 | 0       | 0       |
| 2   | G     | 14       | Total O<br>14 14 | 0       | 0       |
| 2   | H     | 40       | Total O<br>40 40 | 0       | 0       |

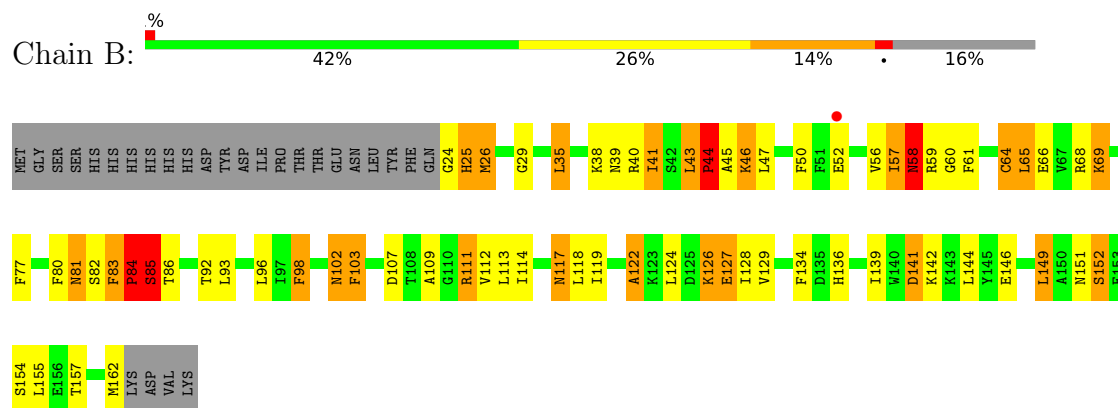
### 3 Residue-property plots [i](#)

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.

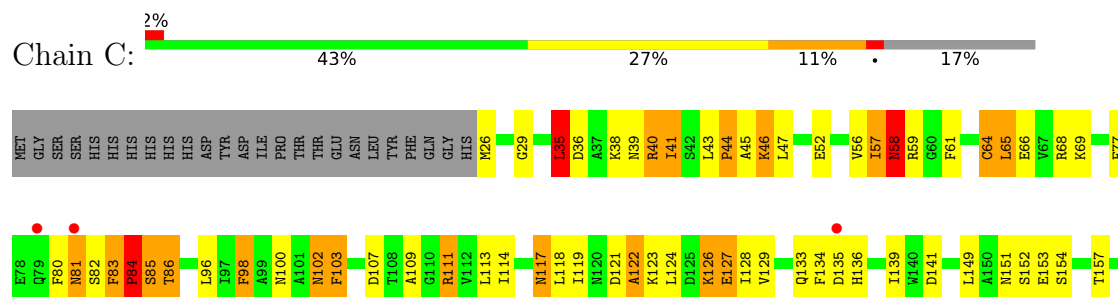
#### • Molecule 1: Protein mraZ



#### • Molecule 1: Protein mraZ

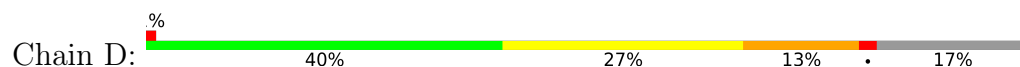


#### • Molecule 1: Protein mraZ



M162  
LYS  
ASP  
VAL  
LYS

• Molecule 1: Protein mraZ



MET GLY SER SER HIS HIS HIS HIS HIS ASP TYR ASP ILE PRO THR THR GLU ASN LEU TYR PHE GLN GLY HIS M26 G29 I33 T34 L35 D36 A37 K38 N39 R40 I41 S42 L43 P44 A45 K46 L47 R48 A49 F50 E51 E52 I55 V56 I57 N58 R59 G60 F61 E62 C64

L65 E66 V67 R68 K69 F77 E76 E79 F80 N81 ASP S82 ASP F83 ILE S85 T86 L93 L96 I97 F98 A99 N100 GLY A101 N102 F103 D107 T108 A109 G110 R111 V112 L113 N114 N117 L118 I119 A122 K123 L124 D125 K126 E127 F51 I128 F134 D135 H136 I139 W140 D141 L144 Y148

L149 A150 M151 S152 E153 S154 L155 E156 T157 M162 LYS ASP VAL LYS

• Molecule 1: Protein mraZ

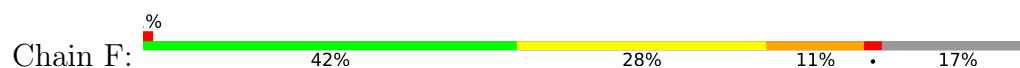


MET GLY SER SER HIS HIS HIS HIS HIS ASP TYR ASP ILE PRO THR THR GLU ASN LEU TYR PHE GLN GLY HIS M26 L27 L28 I33 T34 L35 D36 A37 K38 N39 R40 I41 S42 L43 P44 A45 K46 L47 R48 A49 F50 E51 E52 V56 I57 N58 R59 G60 F61 C64 L65 E66

V67 R68 K69 F70 Q71 F77 F80 N81 ASP S82 ASP F83 ILE S85 T86 L93 L94 K95 F98 A99 N100 GLY A101 N102 F103 D107 T108 A109 G110 R111 V112 L113 N114 P115 M116 N117 L118 I119 A120 D121 A122 K123 L124 D125 K126 E127 F51 I128 W129 L130 F134 D135 H136 L137 E138 I139 W140 D141

K142 K143 D147 Y148 L149 A150 M151 S152 E153 S154 T157 M162 LYS ASP VAL LYS

• Molecule 1: Protein mraZ



MET GLY SER SER HIS HIS HIS HIS HIS ASP TYR ASP ILE PRO THR THR GLU ASN LEU TYR PHE GLN GLY HIS M26 G29 I33 T34 L35 D36 A37 K38 N39 R40 I41 S42 L43 P44 A45 K46 F51 E52 I55 V56 I57 N58 R59 G60 C64 E66 V67 R68 K69

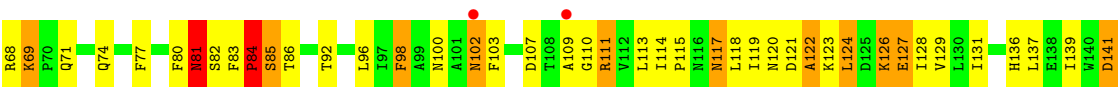
P70 Q71 Q74 F77 E78 Q79 F80 N81 ASP S82 ASP F83 ILE S85 T86 F98 A99 N100 GLY A101 N102 F103 D107 T108 A109 G110 R111 V112 L113 N114 M117 L118 I119 N120 D121 A122 K123 L124 D125 K126 E127 V128 H136 L137 E138 I139 W140 D141 K143 D147 Y148 L149 S152

E153 S154 T157 V158 E162 LYS ASP VAL LYS

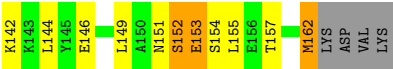
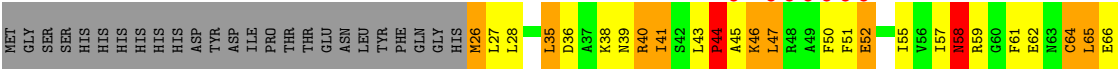
• Molecule 1: Protein mraZ



MET GLY SER SER HIS HIS HIS HIS HIS ASP TYR ASP ILE PRO THR THR GLU ASN LEU TYR PHE GLN GLY HIS M26 G29 I33 T34 L35 D36 A37 K38 N39 R40 I41 S42 L43 P44 A45 K46 L47 R48 A49 F50 F51 E52 V56 I57 N58 R59 G60 C64 L65 E66 V67



● Molecule 1: Protein mraZ



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 84.89Å 101.18Å 169.05Å<br>90.00° 90.00° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 13.01 – 2.80<br>13.01 – 2.80                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 97.5 (13.01-2.80)<br>98.2 (13.01-2.80)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.10                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.64 (at 2.60Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.0                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.240 , 0.284<br>0.240 , 0.284                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1786 reflections (4.00%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 48.2                                                        | Xtriage          |
| Anisotropy                                                              | 0.039                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 54.2                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.91                                                        | EDS              |
| Total number of atoms                                                   | 9184                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 48.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |               | Bond angles |                  |
|-----|-------|--------------|---------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$   | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 0.81         | 1/1175 (0.1%) | 1.37        | 20/1584 (1.3%)   |
| 1   | B     | 0.92         | 1/1154 (0.1%) | 1.33        | 22/1556 (1.4%)   |
| 1   | C     | 0.82         | 1/1139 (0.1%) | 1.34        | 21/1536 (1.4%)   |
| 1   | D     | 0.82         | 0/1139        | 1.35        | 19/1536 (1.2%)   |
| 1   | E     | 0.78         | 1/1139 (0.1%) | 1.32        | 18/1536 (1.2%)   |
| 1   | F     | 0.70         | 0/1139        | 1.32        | 19/1536 (1.2%)   |
| 1   | G     | 0.75         | 1/1139 (0.1%) | 1.31        | 17/1536 (1.1%)   |
| 1   | H     | 0.91         | 2/1139 (0.2%) | 1.34        | 16/1536 (1.0%)   |
| All | All   | 0.82         | 7/9163 (0.1%) | 1.34        | 152/12356 (1.2%) |

The worst 5 of 7 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1   | G     | 162 | MET  | SD-CE | -11.23 | 1.51        | 1.79     |
| 1   | H     | 26  | MET  | SD-CE | 8.87   | 2.01        | 1.79     |
| 1   | H     | 162 | MET  | SD-CE | -8.11  | 1.59        | 1.79     |
| 1   | E     | 162 | MET  | SD-CE | -6.82  | 1.62        | 1.79     |
| 1   | A     | 26  | MET  | SD-CE | -6.51  | 1.63        | 1.79     |

The worst 5 of 152 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | F     | 57  | ILE  | N-CA-C | 13.08 | 122.81      | 111.56   |
| 1   | G     | 57  | ILE  | N-CA-C | 12.76 | 122.53      | 111.56   |
| 1   | A     | 57  | ILE  | N-CA-C | 11.44 | 121.40      | 111.56   |
| 1   | D     | 102 | ASN  | N-CA-C | 11.43 | 129.15      | 114.75   |
| 1   | G     | 102 | ASN  | N-CA-C | 11.08 | 127.25      | 114.62   |

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     | 1153  | 0        | 1148     | 71      | 1            |
| 1   | B     | 1133  | 0        | 1131     | 68      | 0            |
| 1   | C     | 1119  | 0        | 1121     | 66      | 0            |
| 1   | D     | 1119  | 0        | 1121     | 67      | 0            |
| 1   | E     | 1119  | 0        | 1121     | 82      | 0            |
| 1   | F     | 1119  | 0        | 1121     | 63      | 0            |
| 1   | G     | 1119  | 0        | 1121     | 71      | 0            |
| 1   | H     | 1119  | 0        | 1121     | 82      | 1            |
| 2   | A     | 21    | 0        | 0        | 1       | 0            |
| 2   | B     | 31    | 0        | 0        | 3       | 0            |
| 2   | C     | 23    | 0        | 0        | 0       | 0            |
| 2   | D     | 30    | 0        | 0        | 3       | 0            |
| 2   | E     | 15    | 0        | 0        | 2       | 0            |
| 2   | F     | 10    | 0        | 0        | 0       | 0            |
| 2   | G     | 14    | 0        | 0        | 2       | 0            |
| 2   | H     | 40    | 0        | 0        | 2       | 0            |
| All | All   | 9184  | 0        | 9005     | 524     | 1            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

The worst 5 of 524 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:H:26:MET:SD   | 1:H:26:MET:CE    | 2.01                     | 1.48              |
| 1:F:41:ILE:HD12 | 1:F:114:ILE:HD11 | 1.57                     | 0.87              |
| 1:H:126:LYS:O   | 1:H:127:GLU:HB2  | 1.76                     | 0.86              |
| 1:H:27:LEU:HA   | 2:H:169:HOH:O    | 1.75                     | 0.85              |
| 1:H:109:ALA:HB3 | 1:H:111:ARG:HD2  | 1.58                     | 0.83              |

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

| Atom-1         | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------------|--------------------------|-------------------|
| 1:A:48:ARG:NH2 | 1:H:153:GLU:OE2[4_456] | 2.19                     | 0.01              |

## 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     | 139/166 (84%)   | 118 (85%) | 13 (9%)   | 8 (6%)   | 1           | 4 |
| 1   | B     | 137/166 (82%)   | 116 (85%) | 12 (9%)   | 9 (7%)   | 1           | 3 |
| 1   | C     | 135/166 (81%)   | 112 (83%) | 14 (10%)  | 9 (7%)   | 1           | 3 |
| 1   | D     | 135/166 (81%)   | 115 (85%) | 12 (9%)   | 8 (6%)   | 1           | 3 |
| 1   | E     | 135/166 (81%)   | 114 (84%) | 13 (10%)  | 8 (6%)   | 1           | 3 |
| 1   | F     | 135/166 (81%)   | 111 (82%) | 16 (12%)  | 8 (6%)   | 1           | 3 |
| 1   | G     | 135/166 (81%)   | 110 (82%) | 17 (13%)  | 8 (6%)   | 1           | 3 |
| 1   | H     | 135/166 (81%)   | 111 (82%) | 15 (11%)  | 9 (7%)   | 1           | 3 |
| All | All   | 1086/1328 (82%) | 907 (84%) | 112 (10%) | 67 (6%)  | 1           | 3 |

5 of 67 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 44  | PRO  |
| 1   | A     | 58  | ASN  |
| 1   | A     | 127 | GLU  |
| 1   | B     | 58  | ASN  |
| 1   | B     | 152 | SER  |

### 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     | 126/150 (84%)  | 114 (90%) | 12 (10%)  | 8           | 26 |
| 1   | B     | 124/150 (83%)  | 111 (90%) | 13 (10%)  | 6           | 22 |
| 1   | C     | 123/150 (82%)  | 110 (89%) | 13 (11%)  | 6           | 22 |
| 1   | D     | 123/150 (82%)  | 110 (89%) | 13 (11%)  | 6           | 22 |
| 1   | E     | 123/150 (82%)  | 107 (87%) | 16 (13%)  | 4           | 14 |
| 1   | F     | 123/150 (82%)  | 111 (90%) | 12 (10%)  | 7           | 25 |
| 1   | G     | 123/150 (82%)  | 109 (89%) | 14 (11%)  | 5           | 19 |
| 1   | H     | 123/150 (82%)  | 110 (89%) | 13 (11%)  | 6           | 22 |
| All | All   | 988/1200 (82%) | 882 (89%) | 106 (11%) | 6           | 21 |

5 of 106 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 81  | ASN  |
| 1   | F     | 81  | ASN  |
| 1   | H     | 84  | PRO  |
| 1   | E     | 113 | LEU  |
| 1   | E     | 137 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 133 | GLN  |
| 1   | G     | 79  | GLN  |
| 1   | F     | 39  | ASN  |
| 1   | F     | 117 | ASN  |
| 1   | G     | 117 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides 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<sup>th</sup> 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 <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 141/166 (84%)   | 0.02   | 3 (2%) 63 54  | 26, 46, 71, 95        | 0     |
| 1   | B     | 139/166 (83%)   | -0.18  | 1 (0%) 84 77  | 19, 36, 59, 80        | 0     |
| 1   | C     | 137/166 (82%)   | -0.13  | 3 (2%) 62 52  | 23, 42, 70, 80        | 0     |
| 1   | D     | 137/166 (82%)   | -0.16  | 2 (1%) 72 63  | 24, 39, 66, 83        | 0     |
| 1   | E     | 137/166 (82%)   | 0.43   | 8 (5%) 29 22  | 26, 53, 84, 102       | 0     |
| 1   | F     | 137/166 (82%)   | 0.18   | 2 (1%) 72 63  | 31, 57, 76, 85        | 0     |
| 1   | G     | 137/166 (82%)   | 0.26   | 2 (1%) 72 63  | 31, 58, 80, 91        | 0     |
| 1   | H     | 137/166 (82%)   | -0.01  | 9 (6%) 24 18  | 20, 38, 74, 91        | 0     |
| All | All   | 1102/1328 (82%) | 0.05   | 30 (2%) 56 46 | 19, 46, 77, 102       | 0     |

The worst 5 of 30 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 50  | PHE  | 5.8  |
| 1   | H     | 50  | PHE  | 5.7  |
| 1   | E     | 48  | ARG  | 4.2  |
| 1   | H     | 47  | LEU  | 3.9  |
| 1   | E     | 49  | ALA  | 3.6  |

### 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 oligosaccharides 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.