



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 04:35 am BST

PDB ID : 6SB4  
Title : Crystal structure of murine perforin-2 P2 domain crystal form 2  
Authors : Ni, T.; Yu, X.; Ginger, L.; Gilbert, R.J.C.  
Deposited on : 2019-07-18  
Resolution : 3.17 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.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

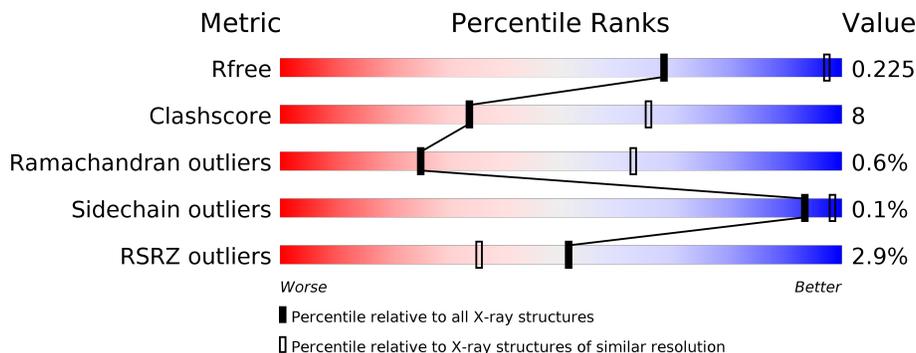
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.17 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 1467 (3.20-3.16)                                      |
| Clashscore            | 141614                      | 1599 (3.20-3.16)                                      |
| Ramachandran outliers | 138981                      | 1574 (3.20-3.16)                                      |
| Sidechain outliers    | 138945                      | 1573 (3.20-3.16)                                      |
| RSRZ outliers         | 127900                      | 1423 (3.20-3.16)                                      |

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  $\geq 3$ , 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     | 295    | <br>2% 53% 14% 34% |
| 1   | B     | 295    | <br>5% 55% 12% 33% |
| 1   | C     | 295    | <br>% 56% 11% 33%  |
| 1   | D     | 295    | <br>4% 50% 16% 34% |
| 1   | E     | 295    | <br>% 57% 10% 33%  |
| 1   | F     | 295    | <br>% 51% 15% 34%  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | G     | 295    | <br>51% 16% 34%      |
| 1   | H     | 295    | <br>%<br>53% 14% 34% |

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 11992 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 Macrophage-expressed gene 1 protein.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
|     |       |          | Total | C   | N   | O   | S  |         |         |       |
| 1   | A     | 196      | 1493  | 958 | 241 | 278 | 16 | 0       | 0       | 0     |
| 1   | B     | 198      | 1511  | 972 | 243 | 280 | 16 | 0       | 0       | 0     |
| 1   | C     | 197      | 1504  | 968 | 242 | 278 | 16 | 0       | 0       | 0     |
| 1   | D     | 195      | 1492  | 960 | 240 | 276 | 16 | 0       | 0       | 0     |
| 1   | E     | 197      | 1504  | 968 | 242 | 278 | 16 | 0       | 0       | 0     |
| 1   | F     | 196      | 1497  | 965 | 240 | 276 | 16 | 0       | 0       | 0     |
| 1   | G     | 196      | 1495  | 960 | 241 | 278 | 16 | 0       | 0       | 0     |
| 1   | H     | 196      | 1496  | 961 | 241 | 278 | 16 | 0       | 0       | 0     |

There are 96 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 346     | GLU      | -      | expression tag | UNP A1L314 |
| A     | 347     | THR      | -      | expression tag | UNP A1L314 |
| A     | 348     | GLY      | -      | expression tag | UNP A1L314 |
| A     | 632     | GLY      | -      | expression tag | UNP A1L314 |
| A     | 633     | THR      | -      | expression tag | UNP A1L314 |
| A     | 634     | LYS      | -      | expression tag | UNP A1L314 |
| A     | 635     | HIS      | -      | expression tag | UNP A1L314 |
| A     | 636     | HIS      | -      | expression tag | UNP A1L314 |
| A     | 637     | HIS      | -      | expression tag | UNP A1L314 |
| A     | 638     | HIS      | -      | expression tag | UNP A1L314 |
| A     | 639     | HIS      | -      | expression tag | UNP A1L314 |
| A     | 640     | HIS      | -      | expression tag | UNP A1L314 |
| B     | 346     | GLU      | -      | expression tag | UNP A1L314 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | 347     | THR      | -      | expression tag | UNP A1L314 |
| B     | 348     | GLY      | -      | expression tag | UNP A1L314 |
| B     | 632     | GLY      | -      | expression tag | UNP A1L314 |
| B     | 633     | THR      | -      | expression tag | UNP A1L314 |
| B     | 634     | LYS      | -      | expression tag | UNP A1L314 |
| B     | 635     | HIS      | -      | expression tag | UNP A1L314 |
| B     | 636     | HIS      | -      | expression tag | UNP A1L314 |
| B     | 637     | HIS      | -      | expression tag | UNP A1L314 |
| B     | 638     | HIS      | -      | expression tag | UNP A1L314 |
| B     | 639     | HIS      | -      | expression tag | UNP A1L314 |
| B     | 640     | HIS      | -      | expression tag | UNP A1L314 |
| C     | 346     | GLU      | -      | expression tag | UNP A1L314 |
| C     | 347     | THR      | -      | expression tag | UNP A1L314 |
| C     | 348     | GLY      | -      | expression tag | UNP A1L314 |
| C     | 632     | GLY      | -      | expression tag | UNP A1L314 |
| C     | 633     | THR      | -      | expression tag | UNP A1L314 |
| C     | 634     | LYS      | -      | expression tag | UNP A1L314 |
| C     | 635     | HIS      | -      | expression tag | UNP A1L314 |
| C     | 636     | HIS      | -      | expression tag | UNP A1L314 |
| C     | 637     | HIS      | -      | expression tag | UNP A1L314 |
| C     | 638     | HIS      | -      | expression tag | UNP A1L314 |
| C     | 639     | HIS      | -      | expression tag | UNP A1L314 |
| C     | 640     | HIS      | -      | expression tag | UNP A1L314 |
| D     | 346     | GLU      | -      | expression tag | UNP A1L314 |
| D     | 347     | THR      | -      | expression tag | UNP A1L314 |
| D     | 348     | GLY      | -      | expression tag | UNP A1L314 |
| D     | 632     | GLY      | -      | expression tag | UNP A1L314 |
| D     | 633     | THR      | -      | expression tag | UNP A1L314 |
| D     | 634     | LYS      | -      | expression tag | UNP A1L314 |
| D     | 635     | HIS      | -      | expression tag | UNP A1L314 |
| D     | 636     | HIS      | -      | expression tag | UNP A1L314 |
| D     | 637     | HIS      | -      | expression tag | UNP A1L314 |
| D     | 638     | HIS      | -      | expression tag | UNP A1L314 |
| D     | 639     | HIS      | -      | expression tag | UNP A1L314 |
| D     | 640     | HIS      | -      | expression tag | UNP A1L314 |
| E     | 346     | GLU      | -      | expression tag | UNP A1L314 |
| E     | 347     | THR      | -      | expression tag | UNP A1L314 |
| E     | 348     | GLY      | -      | expression tag | UNP A1L314 |
| E     | 632     | GLY      | -      | expression tag | UNP A1L314 |
| E     | 633     | THR      | -      | expression tag | UNP A1L314 |
| E     | 634     | LYS      | -      | expression tag | UNP A1L314 |
| E     | 635     | HIS      | -      | expression tag | UNP A1L314 |

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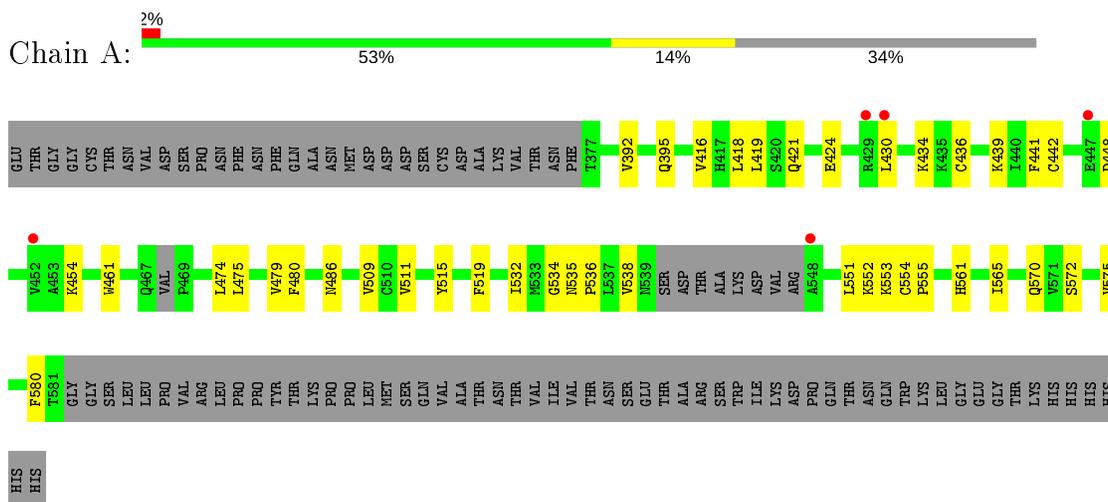
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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| E     | 636     | HIS      | -      | expression tag | UNP A1L314 |
| E     | 637     | HIS      | -      | expression tag | UNP A1L314 |
| E     | 638     | HIS      | -      | expression tag | UNP A1L314 |
| E     | 639     | HIS      | -      | expression tag | UNP A1L314 |
| E     | 640     | HIS      | -      | expression tag | UNP A1L314 |
| F     | 346     | GLU      | -      | expression tag | UNP A1L314 |
| F     | 347     | THR      | -      | expression tag | UNP A1L314 |
| F     | 348     | GLY      | -      | expression tag | UNP A1L314 |
| F     | 632     | GLY      | -      | expression tag | UNP A1L314 |
| F     | 633     | THR      | -      | expression tag | UNP A1L314 |
| F     | 634     | LYS      | -      | expression tag | UNP A1L314 |
| F     | 635     | HIS      | -      | expression tag | UNP A1L314 |
| F     | 636     | HIS      | -      | expression tag | UNP A1L314 |
| F     | 637     | HIS      | -      | expression tag | UNP A1L314 |
| F     | 638     | HIS      | -      | expression tag | UNP A1L314 |
| F     | 639     | HIS      | -      | expression tag | UNP A1L314 |
| F     | 640     | HIS      | -      | expression tag | UNP A1L314 |
| G     | 346     | GLU      | -      | expression tag | UNP A1L314 |
| G     | 347     | THR      | -      | expression tag | UNP A1L314 |
| G     | 348     | GLY      | -      | expression tag | UNP A1L314 |
| G     | 632     | GLY      | -      | expression tag | UNP A1L314 |
| G     | 633     | THR      | -      | expression tag | UNP A1L314 |
| G     | 634     | LYS      | -      | expression tag | UNP A1L314 |
| G     | 635     | HIS      | -      | expression tag | UNP A1L314 |
| G     | 636     | HIS      | -      | expression tag | UNP A1L314 |
| G     | 637     | HIS      | -      | expression tag | UNP A1L314 |
| G     | 638     | HIS      | -      | expression tag | UNP A1L314 |
| G     | 639     | HIS      | -      | expression tag | UNP A1L314 |
| G     | 640     | HIS      | -      | expression tag | UNP A1L314 |
| H     | 346     | GLU      | -      | expression tag | UNP A1L314 |
| H     | 347     | THR      | -      | expression tag | UNP A1L314 |
| H     | 348     | GLY      | -      | expression tag | UNP A1L314 |
| H     | 632     | GLY      | -      | expression tag | UNP A1L314 |
| H     | 633     | THR      | -      | expression tag | UNP A1L314 |
| H     | 634     | LYS      | -      | expression tag | UNP A1L314 |
| H     | 635     | HIS      | -      | expression tag | UNP A1L314 |
| H     | 636     | HIS      | -      | expression tag | UNP A1L314 |
| H     | 637     | HIS      | -      | expression tag | UNP A1L314 |
| H     | 638     | HIS      | -      | expression tag | UNP A1L314 |
| H     | 639     | HIS      | -      | expression tag | UNP A1L314 |
| H     | 640     | HIS      | -      | expression tag | UNP A1L314 |

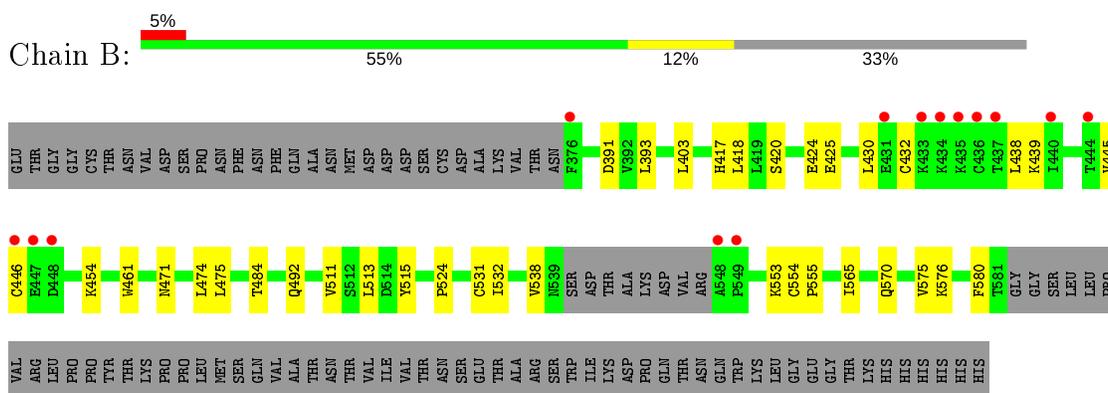
### 3 Residue-property plots [i](#)

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.

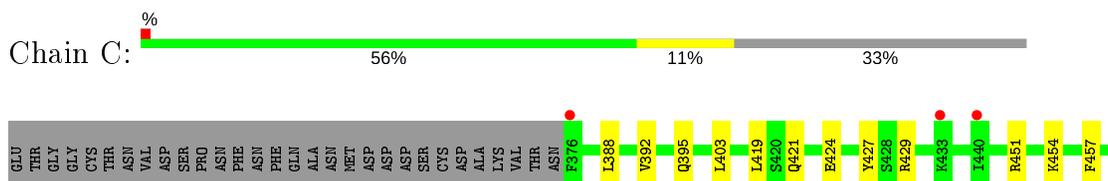
- Molecule 1: Macrophage-expressed gene 1 protein

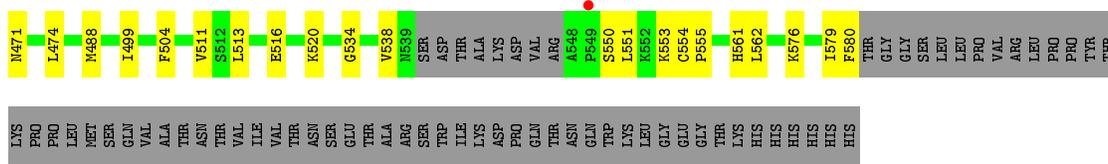


- Molecule 1: Macrophage-expressed gene 1 protein

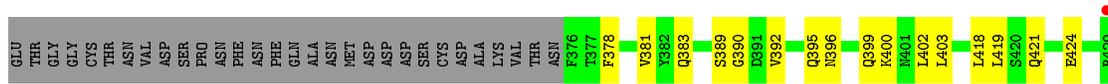


- Molecule 1: Macrophage-expressed gene 1 protein

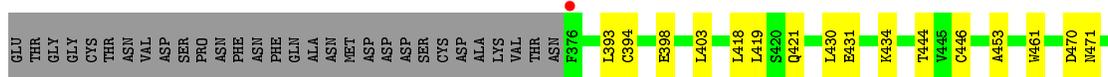




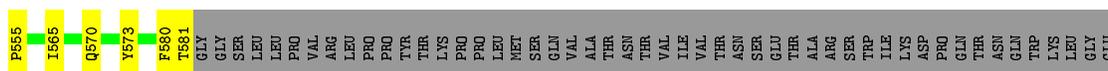
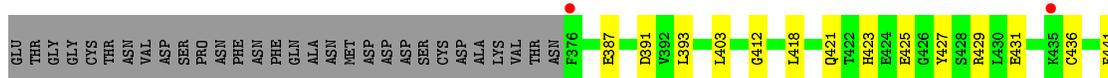
● Molecule 1: Macrophage-expressed gene 1 protein



● Molecule 1: Macrophage-expressed gene 1 protein



● Molecule 1: Macrophage-expressed gene 1 protein



GLY  
THR  
LYS  
GLY  
HIS  
HIS  
HIS  
HIS  
HIS

● Molecule 1: Macrophage-expressed gene 1 protein

Chain G: 51% 16% 34%

GLU  
THR  
GLY  
GLY  
CYS  
THR  
ASN  
VAL  
ASP  
SER  
PRO  
ASN  
PHE  
ASN  
GLN  
ALA  
ASN  
MET  
ASP  
ASP  
SER  
SER  
CYS  
ASP  
ALA  
VAL  
THR  
ASN  
PHE  
T377  
V392  
Q395  
L402  
L403  
P410  
L418  
L419  
S420  
Q421  
E424  
R429  
L430  
E431  
K434  
T437  
L438  
K439  
I440

T444  
V445  
C446  
R451  
K454  
W461  
N471  
L474  
G477  
T481  
T484  
I485  
M488  
A491  
I499  
L503  
V511  
L513  
D514  
Y515  
E516  
L517  
F529  
M535  
V538  
M539  
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K553  
C554  
S559

I565  
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A577  
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● Molecule 1: Macrophage-expressed gene 1 protein

Chain H: % 53% 14% 34%

GLU  
THR  
GLY  
CYS  
THR  
ASN  
VAL  
ASP  
SER  
PRO  
ASN  
PHE  
ASN  
GLN  
ALA  
ASN  
MET  
ASP  
ASP  
SER  
SER  
CYS  
ASP  
ALA  
VAL  
THR  
ASN  
PHE  
T377  
C385  
G390  
D391  
V392  
L393  
C394  
Q395  
L402  
L403  
L418  
Q421  
E424  
Y427  
L430  
K434  
T437  
L438  
K439

T444  
V445  
C446  
F450  
R451  
V452  
K454  
F457  
W461  
A465  
GLY  
Q467  
N471  
L474  
L475  
F476  
V479  
I499  
V509  
G510  
V511  
S512  
Y515  
E516  
V523  
C531  
I532  
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K553  
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## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 70.23Å 70.05Å 128.14Å<br>78.50° 79.05° 85.01°               | Depositor        |
| Resolution (Å)  | 56.09 – 3.17<br>65.36 – 3.17                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 95.3 (56.09-3.17)<br>95.4 (65.36-3.17)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.50 (at 3.19Å)   | Xtriage          |
| Refinement program  | PHENIX dev_3488, PHENIX dev_3488                            | Depositor        |
| R, $R_{free}$   | 0.189 , 0.225<br>0.188 , 0.225                              | Depositor<br>DCC |
| $R_{free}$ test set   | 1976 reflections (5.20%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 72.0  | Xtriage          |
| Anisotropy  | 0.664   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 57.5   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction   | 0.016 for -k,-h,-l  | Xtriage          |
| $F_o, F_c$ correlation  | 0.94  | EDS              |
| Total number of atoms   | 11992   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 90.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.01% 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 [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     | 0.28         | 0/1528  | 0.54        | 0/2064  |
| 1   | B     | 0.27         | 0/1548  | 0.52        | 0/2094  |
| 1   | C     | 0.28         | 0/1541  | 0.52        | 0/2084  |
| 1   | D     | 0.27         | 0/1528  | 0.53        | 0/2065  |
| 1   | E     | 0.28         | 0/1541  | 0.54        | 0/2084  |
| 1   | F     | 0.28         | 0/1534  | 0.52        | 0/2075  |
| 1   | G     | 0.28         | 0/1531  | 0.53        | 0/2070  |
| 1   | H     | 0.27         | 0/1531  | 0.52        | 0/2070  |
| All | All   | 0.28         | 0/12282 | 0.53        | 0/16606 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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     | 1493  | 0        | 1450     | 27      | 0            |
| 1   | B     | 1511  | 0        | 1468     | 28      | 0            |
| 1   | C     | 1504  | 0        | 1461     | 24      | 0            |
| 1   | D     | 1492  | 0        | 1449     | 31      | 0            |
| 1   | E     | 1504  | 0        | 1465     | 20      | 0            |
| 1   | F     | 1497  | 0        | 1455     | 29      | 0            |
| 1   | G     | 1495  | 0        | 1453     | 30      | 0            |
| 1   | H     | 1496  | 0        | 1453     | 28      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| All | All   | 11992 | 0        | 11654    | 201     | 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 8.

The worst 5 of 201 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:B:430:LEU:HD21 | 1:B:446:CYS:HB3 | 1.52                     | 0.91              |
| 1:G:485:ILE:HD11 | 1:G:491:ALA:HA  | 1.54                     | 0.88              |
| 1:C:516:GLU:O    | 1:C:520:LYS:NZ  | 2.15                     | 0.80              |
| 1:H:427:TYR:OH   | 1:H:451:ARG:NH1 | 2.16                     | 0.79              |
| 1:B:524:PRO:HG2  | 1:B:576:LYS:HD2 | 1.64                     | 0.78              |

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     | 190/295 (64%)   | 182 (96%)  | 7 (4%)  | 1 (0%)   | 29          | 66  |
| 1   | B     | 194/295 (66%)   | 189 (97%)  | 4 (2%)  | 1 (0%)   | 29          | 66  |
| 1   | C     | 193/295 (65%)   | 186 (96%)  | 7 (4%)  | 0        | 100         | 100 |
| 1   | D     | 191/295 (65%)   | 181 (95%)  | 7 (4%)  | 3 (2%)   | 9           | 41  |
| 1   | E     | 193/295 (65%)   | 185 (96%)  | 8 (4%)  | 0        | 100         | 100 |
| 1   | F     | 192/295 (65%)   | 184 (96%)  | 7 (4%)  | 1 (0%)   | 29          | 66  |
| 1   | G     | 192/295 (65%)   | 182 (95%)  | 9 (5%)  | 1 (0%)   | 29          | 66  |
| 1   | H     | 190/295 (64%)   | 182 (96%)  | 6 (3%)  | 2 (1%)   | 14          | 50  |
| All | All   | 1535/2360 (65%) | 1471 (96%) | 55 (4%) | 9 (1%)   | 25          | 63  |

5 of 9 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 579 | ILE  |
| 1   | H     | 390 | GLY  |
| 1   | G     | 439 | LYS  |
| 1   | H     | 577 | ALA  |
| 1   | A     | 439 | 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     | 167/255 (66%)   | 167 (100%)  | 0        | 100         | 100 |
| 1   | B     | 169/255 (66%)   | 169 (100%)  | 0        | 100         | 100 |
| 1   | C     | 168/255 (66%)   | 168 (100%)  | 0        | 100         | 100 |
| 1   | D     | 167/255 (66%)   | 167 (100%)  | 0        | 100         | 100 |
| 1   | E     | 168/255 (66%)   | 168 (100%)  | 0        | 100         | 100 |
| 1   | F     | 167/255 (66%)   | 167 (100%)  | 0        | 100         | 100 |
| 1   | G     | 168/255 (66%)   | 168 (100%)  | 0        | 100         | 100 |
| 1   | H     | 168/255 (66%)   | 166 (99%)   | 2 (1%)   | 71          | 87  |
| All | All   | 1342/2040 (66%) | 1340 (100%) | 2 (0%)   | 93          | 98  |

All (2) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 385 | CYS  |
| 1   | H     | 394 | CYS  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 423 | HIS  |
| 1   | H     | 395 | 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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     | 196/295 (66%)   | -0.09  | 5 (2%) 56 40  | 41, 72, 144, 178      | 0       |
| 1   | B     | 198/295 (67%)   | 0.08   | 14 (7%) 16 9  | 38, 73, 167, 205      | 0       |
| 1   | C     | 197/295 (66%)   | -0.06  | 4 (2%) 65 50  | 44, 74, 133, 196      | 0       |
| 1   | D     | 195/295 (66%)   | 0.11   | 13 (6%) 17 10 | 46, 88, 183, 214      | 0       |
| 1   | E     | 197/295 (66%)   | -0.12  | 1 (0%) 91 86  | 43, 75, 145, 192      | 0       |
| 1   | F     | 196/295 (66%)   | 0.00   | 4 (2%) 65 50  | 48, 90, 138, 166      | 0       |
| 1   | G     | 196/295 (66%)   | -0.16  | 1 (0%) 91 86  | 47, 85, 141, 152      | 0       |
| 1   | H     | 196/295 (66%)   | 0.00   | 4 (2%) 65 50  | 53, 100, 149, 180     | 0       |
| All | All   | 1571/2360 (66%) | -0.03  | 46 (2%) 51 35 | 38, 83, 150, 214      | 0       |

The worst 5 of 46 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 549 | PRO  | 5.5  |
| 1   | E     | 376 | PHE  | 4.2  |
| 1   | D     | 438 | LEU  | 4.1  |
| 1   | D     | 445 | VAL  | 4.1  |
| 1   | D     | 446 | CYS  | 3.9  |

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.