



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 30, 2026 – 07:00 AM UTC

PDB ID : 1YDE / pdb\_00001yde  
Title : Crystal Structure of Human Retinal Short-Chain Dehydrogenase/Reductase 3  
Authors : Lukacik, P.; Bunkozci, G.; Kavanagh, K.; Sundstrom, M.; Arrowsmith, C.; Edwards, A.; von Delft, F.; Oppermann, U.; Structural Genomics Consortium (SGC)  
Deposited on : 2004-12-23  
Resolution : 2.40 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>.

---

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                                                             |

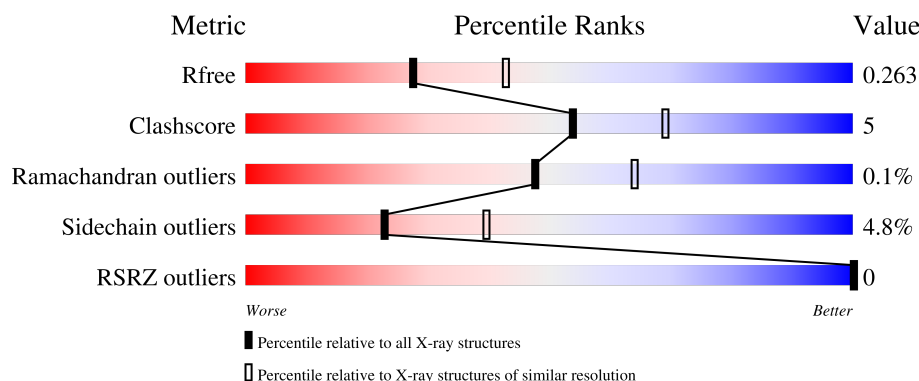
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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                      | 4912 (2.40-2.40)                                      |
| Clashscore            | 190562                      | 5391 (2.40-2.40)                                      |
| Ramachandran outliers | 187476                      | 5320 (2.40-2.40)                                      |
| Sidechain outliers    | 187428                      | 5321 (2.40-2.40)                                      |
| RSRZ outliers         | 180081                      | 4916 (2.40-2.40)                                      |

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     | 270    | <br>78% 14% • 7% |
| 1   | B     | 270    | <br>78% 14% 9%   |
| 1   | C     | 270    | <br>75% 16% • 7% |
| 1   | D     | 270    | <br>83% 11% • 6% |
| 1   | E     | 270    | <br>79% 13% • 7% |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain                                                                                |
|-----|-------|--------|-------------------------------------------------------------------------------------------------|
| 1   | F     | 270    |  81% 11% • 5% |
| 1   | G     | 270    |  77% 13% • 9% |
| 1   | H     | 270    |  82% 11% • 6% |
| 1   | I     | 270    |  83% 7% • 9%  |
| 1   | J     | 270    |  81% 13% 6%   |
| 1   | K     | 270    |  79% 12% • 7% |
| 1   | L     | 270    |  83% 10% • 6% |
| 1   | M     | 270    |  76% 13% 10%  |
| 1   | N     | 270    |  81% 7% • 11% |
| 1   | O     | 270    |  77% 11% • 9% |
| 1   | P     | 270    |  80% 11% • 6% |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 30669 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 Retinal dehydrogenase/reductase 3.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 250      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 1844  | 1162 | 324 | 349 | 9  |         |         |       |
| 1   | B     | 247      | Total | C    | N   | O   | S  | 0       | 3       | 0     |
|     |       |          | 1816  | 1140 | 324 | 342 | 10 |         |         |       |
| 1   | C     | 250      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1847  | 1162 | 327 | 349 | 9  |         |         |       |
| 1   | D     | 255      | Total | C    | N   | O   | S  | 0       | 2       | 0     |
|     |       |          | 1876  | 1179 | 330 | 356 | 11 |         |         |       |
| 1   | E     | 250      | Total | C    | N   | O   | S  | 0       | 2       | 0     |
|     |       |          | 1850  | 1165 | 325 | 350 | 10 |         |         |       |
| 1   | F     | 256      | Total | C    | N   | O   | S  | 0       | 2       | 0     |
|     |       |          | 1896  | 1191 | 337 | 358 | 10 |         |         |       |
| 1   | G     | 247      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1820  | 1144 | 323 | 344 | 9  |         |         |       |
| 1   | H     | 254      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 1861  | 1173 | 324 | 354 | 10 |         |         |       |
| 1   | I     | 247      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1825  | 1150 | 321 | 345 | 9  |         |         |       |
| 1   | J     | 255      | Total | C    | N   | O   | S  | 0       | 3       | 0     |
|     |       |          | 1881  | 1182 | 331 | 357 | 11 |         |         |       |
| 1   | K     | 250      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1843  | 1161 | 324 | 349 | 9  |         |         |       |
| 1   | L     | 255      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 1870  | 1177 | 328 | 354 | 11 |         |         |       |
| 1   | M     | 244      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1771  | 1120 | 303 | 339 | 9  |         |         |       |
| 1   | N     | 240      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1754  | 1104 | 308 | 333 | 9  |         |         |       |
| 1   | O     | 247      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1806  | 1140 | 313 | 344 | 9  |         |         |       |
| 1   | P     | 254      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1858  | 1169 | 327 | 352 | 10 |         |         |       |

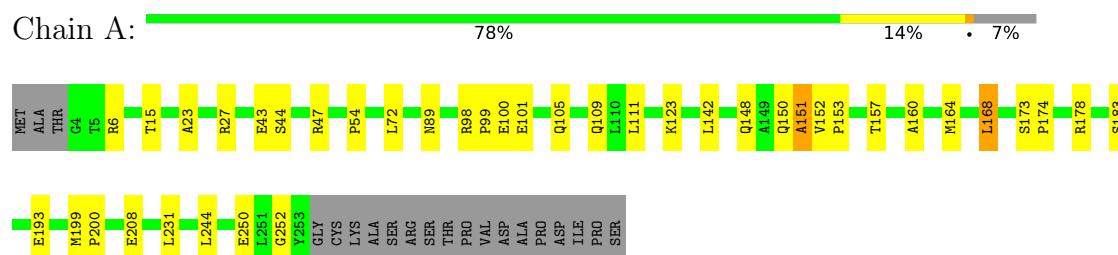
- Molecule 2 is water.

| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 2   | A     | 133      | Total<br>133 | O<br>133 | 0       | 0       |
| 2   | B     | 121      | Total<br>121 | O<br>121 | 0       | 0       |
| 2   | C     | 123      | Total<br>123 | O<br>123 | 0       | 0       |
| 2   | D     | 130      | Total<br>130 | O<br>130 | 0       | 0       |
| 2   | E     | 116      | Total<br>116 | O<br>116 | 0       | 0       |
| 2   | F     | 113      | Total<br>113 | O<br>113 | 0       | 0       |
| 2   | G     | 86       | Total<br>86  | O<br>86  | 0       | 0       |
| 2   | H     | 78       | Total<br>78  | O<br>78  | 0       | 0       |
| 2   | I     | 54       | Total<br>54  | O<br>54  | 0       | 0       |
| 2   | J     | 68       | Total<br>68  | O<br>68  | 0       | 0       |
| 2   | K     | 89       | Total<br>89  | O<br>89  | 0       | 0       |
| 2   | L     | 78       | Total<br>78  | O<br>78  | 0       | 0       |
| 2   | M     | 22       | Total<br>22  | O<br>22  | 0       | 0       |
| 2   | N     | 13       | Total<br>13  | O<br>13  | 0       | 0       |
| 2   | O     | 9        | Total<br>9   | O<br>9   | 0       | 0       |
| 2   | P     | 18       | Total<br>18  | O<br>18  | 0       | 0       |

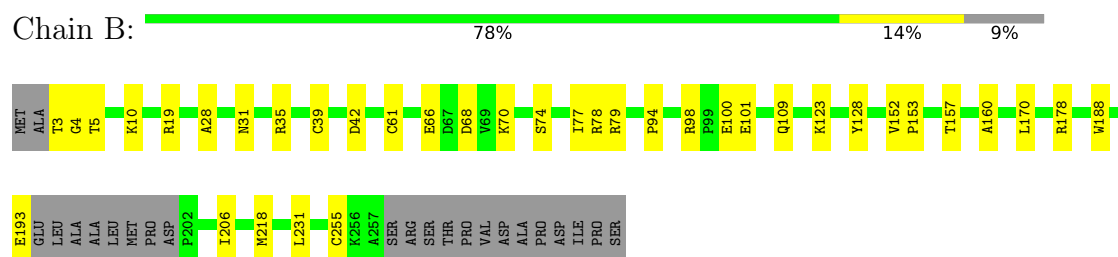
### 3 Residue-property plots

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.

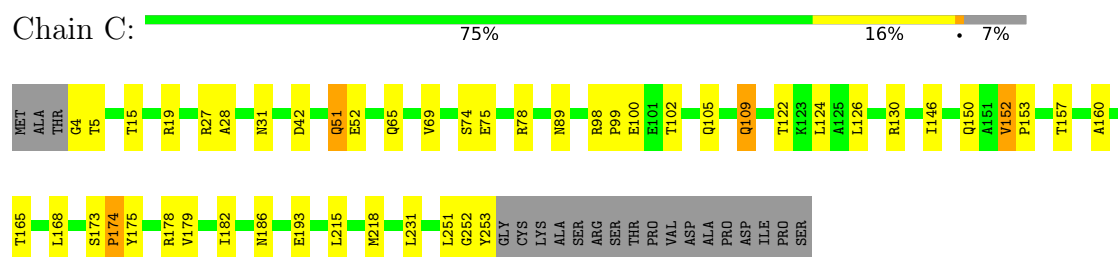
#### • Molecule 1: Retinal dehydrogenase/reductase 3



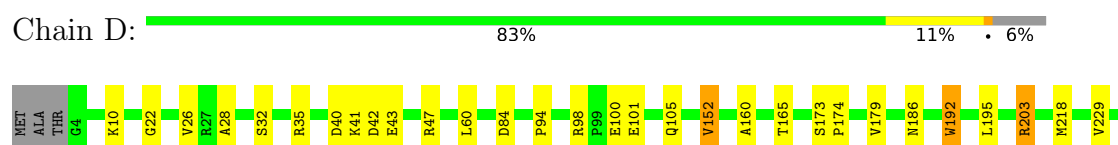
#### • Molecule 1: Retinal dehydrogenase/reductase 3

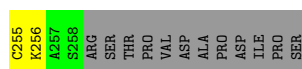


#### • Molecule 1: Retinal dehydrogenase/reductase 3



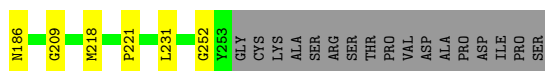
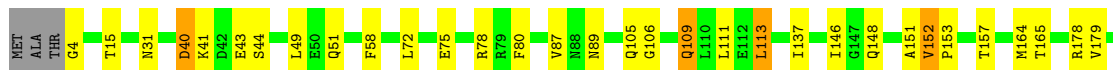
#### • Molecule 1: Retinal dehydrogenase/reductase 3





• Molecule 1: Retinal dehydrogenase/reductase 3

Chain E: 79% 13% • 7%



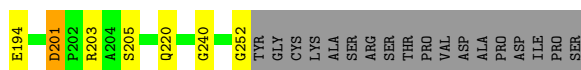
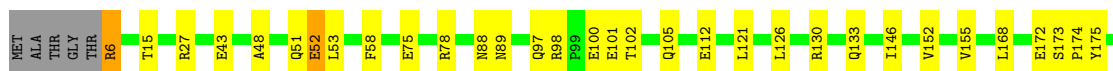
• Molecule 1: Retinal dehydrogenase/reductase 3

Chain F: 81% 11% • 5%



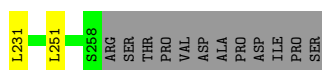
• Molecule 1: Retinal dehydrogenase/reductase 3

Chain G: 77% 13% • 9%



• Molecule 1: Retinal dehydrogenase/reductase 3

Chain H: 82% 11% • 6%



• Molecule 1: Retinal dehydrogenase/reductase 3

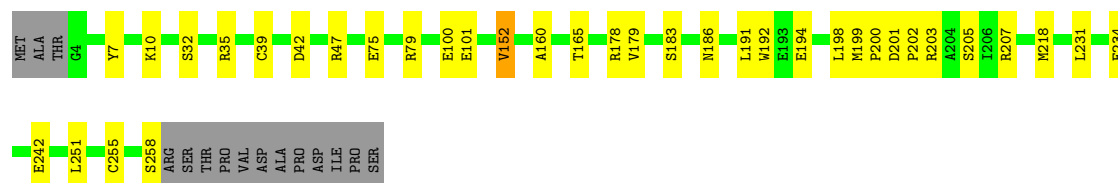
Chain I: 83% 7% • 9%



VAL  
ASP  
ALA  
PRO  
ASP  
ILE  
PRO  
SER

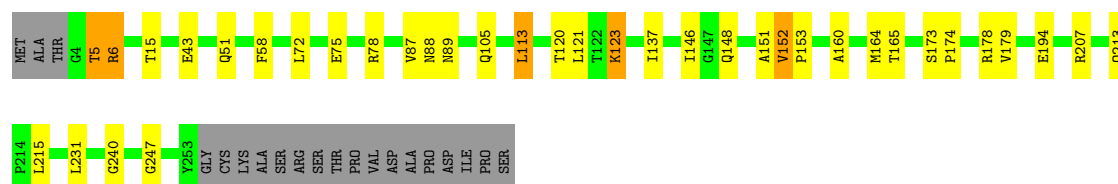
• Molecule 1: Retinal dehydrogenase/reductase 3

Chain J:  81% 13% 6%



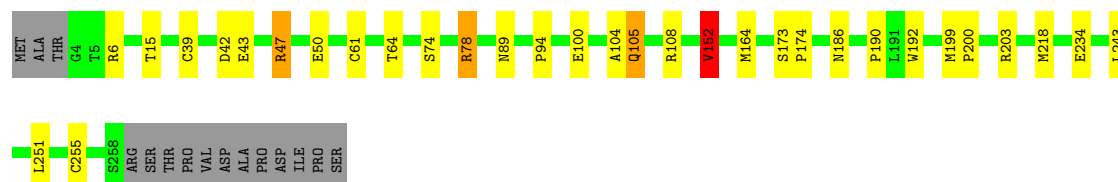
• Molecule 1: Retinal dehydrogenase/reductase 3

Chain K:  79% 12% 7%



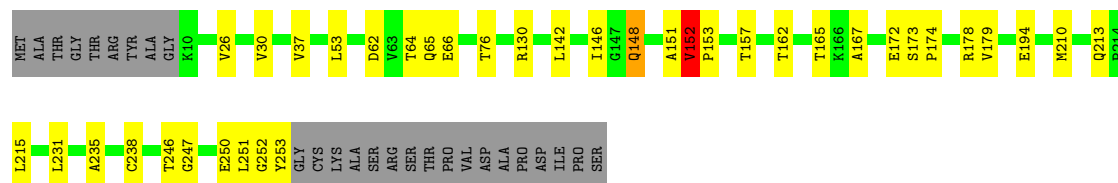
• Molecule 1: Retinal dehydrogenase/reductase 3

Chain L:  83% 10% 6%



• Molecule 1: Retinal dehydrogenase/reductase 3

Chain M:  76% 13% 10%



• Molecule 1: Retinal dehydrogenase/reductase 3

Chain N:  81% 7% 11%



ARG  
SER  
THR  
PRO  
VAL  
ASP  
ALA  
PRO  
ASP  
ILE  
PRO  
SER

● Molecule 1: Retinal dehydrogenase/reductase 3

Chain O: 

77%

11%

•

9%

MET  
ALA  
THR  
GLY  
THR  
ARG  
Y7  
T15  
V30  
N31  
S32  
V37  
E43  
Q51  
E52  
L53  
F58  
Q65  
E66  
K70  
T76  
N89  
E100  
L113  
N135  
S140  
V152  
P153  
A169  
S173  
P174  
R178  
S183  
E194  
R207  
E208  
G209  
M210

Q213  
R217  
L231  
A235  
C238  
T239  
L244  
G252  
Y253  
GLY  
CYS  
LYS  
ALA  
SER  
ARG  
SER  
THR  
PRO  
VAL  
ASP  
ALA  
PRO  
ASP  
ILE  
PRO  
SER

● Molecule 1: Retinal dehydrogenase/reductase 3

Chain P: 

80%

11%

•

6%

MET  
ALA  
THR  
GLY  
R6  
Y7  
K10  
V11  
V12  
F29  
S32  
C39  
E43  
S44  
L60  
C61  
E100  
E101  
T122  
K123  
L126  
Q133  
V152  
V155  
R178  
S183  
T189  
P190  
E193  
E194  
L195  
A196  
A197  
L198  
R199  
P200  
D201  
P202  
R203  
L231  
I241

C255  
K256  
A257  
S258  
R259  
SER  
THR  
PRO  
VAL  
ASP  
ALA  
PRO  
ASP  
ILE  
PRO  
SER

## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 167.12Å 98.82Å 167.46Å<br>90.00° 115.87° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 30.00 – 2.40<br>30.00 – 2.40                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 91.9 (30.00-2.40)<br>91.4 (30.00-2.40)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.12                                                        | Depositor        |
| $R_{sym}$                                                               | 0.12                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.45 (at 2.40Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.2.0005                                             | Depositor        |
| R, $R_{free}$                                                           | 0.181 , 0.229<br>0.247 , 0.263                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 3562 reflections (1.86%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 29.1                                                        | Xtriage          |
| Anisotropy                                                              | 0.398                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 27.7                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$ | Xtriage          |
| Estimated twinning fraction                                             | 0.368 for l,-k,h                                            | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.94                                                        | EDS              |
| Total number of atoms                                                   | 30669                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 5.0                                                         | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.97% 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     | 1.13         | 2/1879 (0.1%)   | 1.07        | 0/2555          |
| 1   | B     | 1.17         | 4/1853 (0.2%)   | 1.08        | 0/2517          |
| 1   | C     | 1.20         | 4/1878 (0.2%)   | 1.10        | 2/2553 (0.1%)   |
| 1   | D     | 1.10         | 2/1915 (0.1%)   | 1.03        | 2/2602 (0.1%)   |
| 1   | E     | 1.12         | 1/1891 (0.1%)   | 1.07        | 1/2570 (0.0%)   |
| 1   | F     | 1.00         | 3/1934 (0.2%)   | 1.03        | 5/2627 (0.2%)   |
| 1   | G     | 0.93         | 1/1850 (0.1%)   | 1.00        | 1/2516 (0.0%)   |
| 1   | H     | 0.88         | 0/1896          | 0.96        | 1/2578 (0.0%)   |
| 1   | I     | 0.87         | 1/1856 (0.1%)   | 0.98        | 0/2524          |
| 1   | J     | 0.90         | 1/1924 (0.1%)   | 0.97        | 3/2616 (0.1%)   |
| 1   | K     | 1.14         | 3/1874 (0.2%)   | 1.10        | 3/2548 (0.1%)   |
| 1   | L     | 0.95         | 1/1905 (0.1%)   | 1.03        | 3/2589 (0.1%)   |
| 1   | M     | 0.69         | 1/1801 (0.1%)   | 0.91        | 1/2455 (0.0%)   |
| 1   | N     | 0.65         | 1/1782 (0.1%)   | 0.86        | 1/2422 (0.0%)   |
| 1   | O     | 0.67         | 1/1837 (0.1%)   | 0.92        | 4/2502 (0.2%)   |
| 1   | P     | 0.65         | 0/1889          | 0.97        | 2/2569 (0.1%)   |
| All | All   | 0.96         | 26/29964 (0.1%) | 1.01        | 29/40743 (0.1%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | P     | 0                   | 2                   |

The worst 5 of 26 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | K     | 152 | VAL  | CA-CB | 16.27 | 1.63        | 1.54     |
| 1   | C     | 152 | VAL  | CA-CB | 12.62 | 1.61        | 1.54     |
| 1   | L     | 152 | VAL  | CA-CB | 11.45 | 1.60        | 1.54     |
| 1   | B     | 152 | VAL  | CA-CB | 11.26 | 1.60        | 1.54     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | M     | 152 | VAL  | CA-CB | 10.10 | 1.59        | 1.54     |

The worst 5 of 29 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | P     | 201 | ASP  | CA-C-N  | 13.80 | 137.09      | 119.84   |
| 1   | P     | 201 | ASP  | C-N-CA  | 13.80 | 137.09      | 119.84   |
| 1   | L     | 152 | VAL  | N-CA-CB | 13.13 | 120.69      | 110.45   |
| 1   | K     | 152 | VAL  | N-CA-CB | 12.64 | 120.31      | 110.45   |
| 1   | O     | 152 | VAL  | N-CA-CB | 11.04 | 117.45      | 110.50   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | P     | 198 | LEU  | Peptide |
| 1   | P     | 257 | ALA  | Peptide |

## 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     | 1844  | 0        | 1863     | 23      | 0            |
| 1   | B     | 1816  | 0        | 1828     | 22      | 0            |
| 1   | C     | 1847  | 0        | 1872     | 30      | 0            |
| 1   | D     | 1876  | 0        | 1895     | 21      | 1            |
| 1   | E     | 1850  | 0        | 1870     | 25      | 0            |
| 1   | F     | 1896  | 0        | 1922     | 18      | 0            |
| 1   | G     | 1820  | 0        | 1842     | 23      | 0            |
| 1   | H     | 1861  | 0        | 1874     | 23      | 0            |
| 1   | I     | 1825  | 0        | 1849     | 14      | 0            |
| 1   | J     | 1881  | 0        | 1892     | 13      | 0            |
| 1   | K     | 1843  | 0        | 1865     | 23      | 1            |
| 1   | L     | 1870  | 0        | 1884     | 20      | 0            |
| 1   | M     | 1771  | 0        | 1771     | 19      | 0            |
| 1   | N     | 1754  | 0        | 1766     | 10      | 0            |
| 1   | O     | 1806  | 0        | 1812     | 17      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | P     | 1858  | 0        | 1868     | 19      | 0            |
| 2   | A     | 133   | 0        | 0        | 5       | 0            |
| 2   | B     | 121   | 0        | 0        | 1       | 0            |
| 2   | C     | 123   | 0        | 0        | 4       | 0            |
| 2   | D     | 130   | 0        | 0        | 1       | 0            |
| 2   | E     | 116   | 0        | 0        | 4       | 0            |
| 2   | F     | 113   | 0        | 0        | 3       | 0            |
| 2   | G     | 86    | 0        | 0        | 0       | 0            |
| 2   | H     | 78    | 0        | 0        | 1       | 0            |
| 2   | I     | 54    | 0        | 0        | 3       | 0            |
| 2   | J     | 68    | 0        | 0        | 1       | 0            |
| 2   | K     | 89    | 0        | 0        | 3       | 0            |
| 2   | L     | 78    | 0        | 0        | 3       | 0            |
| 2   | M     | 22    | 0        | 0        | 1       | 0            |
| 2   | N     | 13    | 0        | 0        | 0       | 0            |
| 2   | O     | 9     | 0        | 0        | 0       | 0            |
| 2   | P     | 18    | 0        | 0        | 1       | 0            |
| All | All   | 30669 | 0        | 29673    | 287     | 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 5.

The worst 5 of 287 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:K:123:LYS:CE     | 1:K:123:LYS:NZ     | 1.67                     | 1.53              |
| 1:B:109:GLN:NE2    | 1:P:200:PRO:O      | 1.93                     | 1.02              |
| 1:E:186:ASN:HB3    | 1:E:218[B]:MET:HE2 | 1.41                     | 1.00              |
| 1:B:255[B]:CYS:HB3 | 1:D:255[B]:CYS:SG  | 2.06                     | 0.95              |
| 1:B:255[B]:CYS:CB  | 1:D:255[B]:CYS:SG  | 2.56                     | 0.94              |

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:D:35:ARG:NH2 | 1:K:78:ARG:O[2_444] | 2.11                     | 0.09              |

## 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     | 249/270 (92%)   | 244 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 1   | B     | 246/270 (91%)   | 241 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 1   | C     | 248/270 (92%)   | 242 (98%)  | 5 (2%)  | 1 (0%)   | 30          | 43  |
| 1   | D     | 255/270 (94%)   | 252 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 1   | E     | 250/270 (93%)   | 245 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 1   | F     | 256/270 (95%)   | 252 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 1   | G     | 245/270 (91%)   | 239 (98%)  | 6 (2%)  | 0        | 100         | 100 |
| 1   | H     | 253/270 (94%)   | 249 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 1   | I     | 245/270 (91%)   | 240 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 1   | J     | 256/270 (95%)   | 251 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 1   | K     | 248/270 (92%)   | 243 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 1   | L     | 254/270 (94%)   | 250 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 1   | M     | 242/270 (90%)   | 237 (98%)  | 4 (2%)  | 1 (0%)   | 30          | 43  |
| 1   | N     | 236/270 (87%)   | 233 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 1   | O     | 245/270 (91%)   | 240 (98%)  | 4 (2%)  | 1 (0%)   | 30          | 43  |
| 1   | P     | 252/270 (93%)   | 243 (96%)  | 8 (3%)  | 1 (0%)   | 30          | 43  |
| All | All   | 3980/4320 (92%) | 3901 (98%) | 75 (2%) | 4 (0%)   | 48          | 64  |

All (4) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 252 | GLY  |
| 1   | P     | 7   | TYR  |
| 1   | C     | 252 | GLY  |
| 1   | O     | 252 | GLY  |

### 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     | 191/208 (92%)   | 183 (96%)  | 8 (4%)   | 26          | 45 |
| 1   | B     | 188/208 (90%)   | 180 (96%)  | 8 (4%)   | 26          | 44 |
| 1   | C     | 192/208 (92%)   | 185 (96%)  | 7 (4%)   | 31          | 52 |
| 1   | D     | 196/208 (94%)   | 190 (97%)  | 6 (3%)   | 35          | 57 |
| 1   | E     | 193/208 (93%)   | 181 (94%)  | 12 (6%)  | 16          | 29 |
| 1   | F     | 197/208 (95%)   | 191 (97%)  | 6 (3%)   | 36          | 58 |
| 1   | G     | 189/208 (91%)   | 178 (94%)  | 11 (6%)  | 18          | 32 |
| 1   | H     | 192/208 (92%)   | 184 (96%)  | 8 (4%)   | 26          | 45 |
| 1   | I     | 190/208 (91%)   | 183 (96%)  | 7 (4%)   | 30          | 51 |
| 1   | J     | 196/208 (94%)   | 181 (92%)  | 15 (8%)  | 12          | 20 |
| 1   | K     | 191/208 (92%)   | 182 (95%)  | 9 (5%)   | 23          | 41 |
| 1   | L     | 193/208 (93%)   | 183 (95%)  | 10 (5%)  | 21          | 36 |
| 1   | M     | 182/208 (88%)   | 176 (97%)  | 6 (3%)   | 33          | 55 |
| 1   | N     | 182/208 (88%)   | 173 (95%)  | 9 (5%)   | 22          | 39 |
| 1   | O     | 186/208 (89%)   | 174 (94%)  | 12 (6%)  | 15          | 27 |
| 1   | P     | 191/208 (92%)   | 177 (93%)  | 14 (7%)  | 13          | 22 |
| All | All   | 3049/3328 (92%) | 2901 (95%) | 148 (5%) | 23          | 39 |

5 of 148 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | N     | 100 | GLU  |
| 1   | P     | 193 | GLU  |
| 1   | N     | 206 | ILE  |
| 1   | O     | 207 | ARG  |
| 1   | G     | 52  | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 89  | ASN  |
| 1   | O     | 51  | GLN  |
| 1   | I     | 135 | ASN  |
| 1   | N     | 236 | ASN  |
| 1   | P     | 135 | ASN  |

### 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 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     | 250/270 (92%)   | -1.46  | 0 100 100 | 2, 3, 13, 26          | 1 (0%)  |
| 1   | B     | 247/270 (91%)   | -1.39  | 0 100 100 | 2, 3, 18, 36          | 3 (1%)  |
| 1   | C     | 250/270 (92%)   | -1.44  | 0 100 100 | 2, 3, 13, 31          | 0       |
| 1   | D     | 255/270 (94%)   | -1.43  | 0 100 100 | 2, 3, 16, 36          | 2 (0%)  |
| 1   | E     | 250/270 (92%)   | -1.44  | 0 100 100 | 2, 4, 13, 29          | 2 (0%)  |
| 1   | F     | 256/270 (94%)   | -1.41  | 0 100 100 | 1, 4, 15, 25          | 2 (0%)  |
| 1   | G     | 247/270 (91%)   | -1.39  | 0 100 100 | 2, 4, 12, 22          | 0       |
| 1   | H     | 254/270 (94%)   | -1.41  | 0 100 100 | 2, 4, 13, 25          | 1 (0%)  |
| 1   | I     | 247/270 (91%)   | -1.30  | 0 100 100 | 2, 5, 13, 24          | 0       |
| 1   | J     | 255/270 (94%)   | -1.36  | 0 100 100 | 1, 4, 15, 27          | 3 (1%)  |
| 1   | K     | 250/270 (92%)   | -1.42  | 0 100 100 | 2, 4, 14, 31          | 0       |
| 1   | L     | 255/270 (94%)   | -1.34  | 0 100 100 | 2, 4, 15, 25          | 1 (0%)  |
| 1   | M     | 244/270 (90%)   | -0.98  | 0 100 100 | 2, 5, 11, 25          | 0       |
| 1   | N     | 240/270 (88%)   | -0.96  | 0 100 100 | 2, 5, 12, 18          | 0       |
| 1   | O     | 247/270 (91%)   | -0.98  | 0 100 100 | 2, 5, 11, 17          | 0       |
| 1   | P     | 254/270 (94%)   | -1.04  | 0 100 100 | 2, 5, 13, 22          | 0       |
| All | All   | 4001/4320 (92%) | -1.30  | 0 100 100 | 1, 4, 14, 36          | 15 (0%) |

There are no RSRZ outliers to report.

### 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.