



# Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 10:51 PM GMT

PDB ID : 2ABX  
Title : THE CRYSTAL STRUCTURE OF ALPHA-BUNGAROTOXIN AT 2.5  
ANGSTROMS RESOLUTION. RELATION TO SOLUTION STRUCTURE  
AND BINDING TO ACETYLCHOLINE RECEPTOR  
Authors : Love, R.; Stroud, R.  
Deposited on : 1986-02-19  
Resolution : 2.50 Å(reported)

This is a full wwPDB validation 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 <http://wwpdb.org/ValidationPDFNotes.html>

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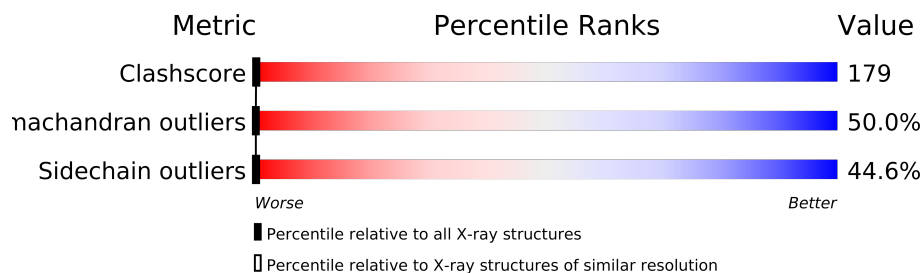
The following versions of software and data (see [references](#)) were used in the production of this report:

|                                |   |                          |
|--------------------------------|---|--------------------------|
| MolProbity                     | : | 4.02b-467                |
| Mogul                          | : | 1.15 2013                |
| Xtriage (Phenix)               | : | NOT EXECUTED             |
| EDS                            | : | NOT EXECUTED             |
| Percentile statistics          | : | 21963                    |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)      |
| Ideal geometry (DNA, RNA)      | : | Parkinson et. al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | stable22683              |

# 1 Overall quality at a glance

The reported resolution of this entry is 2.50 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 79885                       | 3562 (2.50-2.50)                                      |
| Ramachandran outliers | 78287                       | 3480 (2.50-2.50)                                      |
| Sidechain outliers    | 78261                       | 3482 (2.50-2.50)                                      |

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 74     |                  |
| 1   | B     | 74     |                  |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1118 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ALPHA-BUNGAROTOXIN.

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 1   | A     | 74       | Total | C   | N  | O   | S  | 0       | 0       | 0     |
|     |       |          | 551   | 338 | 97 | 105 | 11 |         |         |       |
| 1   | B     | 74       | Total | C   | N  | O   | S  | 0       | 0       | 0     |
|     |       |          | 551   | 338 | 97 | 105 | 11 |         |         |       |

There are 12 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 9       | ILE      | SER    | CONFLICT | UNP P60615 |
| A     | 11      | SER      | ILE    | CONFLICT | UNP P60615 |
| A     | 67      | HIS      | PRO    | CONFLICT | UNP P60615 |
| A     | 68      | PRO      | HIS    | CONFLICT | UNP P60615 |
| A     | 71      | ARG      | GLN    | CONFLICT | UNP P60615 |
| A     | 72      | GLN      | ARG    | CONFLICT | UNP P60615 |
| B     | 9       | ILE      | SER    | CONFLICT | UNP P60615 |
| B     | 11      | SER      | ILE    | CONFLICT | UNP P60615 |
| B     | 67      | HIS      | PRO    | CONFLICT | UNP P60615 |
| B     | 68      | PRO      | HIS    | CONFLICT | UNP P60615 |
| B     | 71      | ARG      | GLN    | CONFLICT | UNP P60615 |
| B     | 72      | GLN      | ARG    | CONFLICT | UNP P60615 |

- Molecule 2 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | A     | 10       | Total | O  | 0       | 0       |
|     |       |          | 10    | 10 |         |         |
| 2   | B     | 6        | Total | O  | 0       | 0       |
|     |       |          | 6     | 6  |         |         |

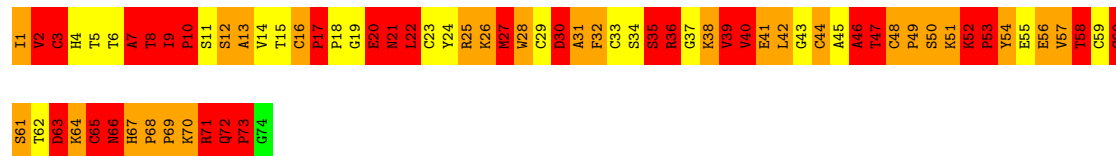
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Note EDS was not executed.

Chain A:



Chain B:



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

| Property                                                 | Value                                        | Source    |
|----------------------------------------------------------|----------------------------------------------|-----------|
| Space group                                              | P 21 21 21                                   | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 67.80Å 78.40Å 22.40Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)                                           | (Not available) – 2.50                       | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) ((Not available)-2.50)       | Depositor |
| $R_{merge}$                                              | (Not available)                              | Depositor |
| $R_{sym}$                                                | (Not available)                              | Depositor |
| Refinement program                                       | PROLSQ                                       | Depositor |
| R, $R_{free}$                                            | 0.240 , (Not available)                      | Depositor |
| Estimated twinning fraction                              | No twinning to report.                       | Xtriage   |
| Total number of atoms                                    | 1118                                         | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 15.0                                         | wwPDB-VP  |

## 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     | 1.81         | 7/565 (1.2%)   | 3.21        | 71/767 (9.3%)   |
| 1   | B     | 1.65         | 6/565 (1.1%)   | 2.92        | 64/767 (8.3%)   |
| All | All   | 1.73         | 13/1130 (1.2%) | 3.07        | 135/1534 (8.8%) |

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   | A     | 0                   | 1                   |
| 1   | B     | 0                   | 2                   |
| All | All   | 0                   | 3                   |

All (13) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | A     | 59  | CYS  | CB-SG  | -13.89 | 1.58        | 1.82     |
| 1   | A     | 56  | GLU  | CD-OE2 | 8.44   | 1.34        | 1.25     |
| 1   | A     | 48  | CYS  | CB-SG  | -7.63  | 1.69        | 1.82     |
| 1   | B     | 55  | GLU  | CD-OE2 | 7.13   | 1.33        | 1.25     |
| 1   | B     | 41  | GLU  | CD-OE2 | 6.35   | 1.32        | 1.25     |
| 1   | A     | 73  | PRO  | N-CD   | 5.94   | 1.56        | 1.47     |
| 1   | A     | 69  | PRO  | N-CD   | 5.81   | 1.55        | 1.47     |
| 1   | A     | 33  | CYS  | CB-SG  | 5.71   | 1.92        | 1.82     |
| 1   | B     | 22  | LEU  | C-O    | 5.41   | 1.33        | 1.23     |
| 1   | B     | 20  | GLU  | CD-OE2 | 5.32   | 1.31        | 1.25     |
| 1   | B     | 35  | SER  | N-CA   | 5.04   | 1.56        | 1.46     |
| 1   | B     | 55  | GLU  | CA-CB  | -5.02  | 1.43        | 1.53     |
| 1   | A     | 41  | GLU  | CD-OE2 | 5.02   | 1.31        | 1.25     |

All (135) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 59  | CYS  | CA-CB-SG   | 19.85 | 149.73      | 114.00   |
| 1   | B     | 25  | ARG  | NE-CZ-NH2  | 19.00 | 129.80      | 120.30   |
| 1   | A     | 25  | ARG  | NE-CZ-NH1  | 18.93 | 129.77      | 120.30   |
| 1   | B     | 55  | GLU  | CA-CB-CG   | 16.96 | 150.72      | 113.40   |
| 1   | A     | 36  | ARG  | NE-CZ-NH2  | 16.26 | 128.43      | 120.30   |
| 1   | A     | 54  | TYR  | CA-CB-CG   | 15.24 | 142.36      | 113.40   |
| 1   | B     | 57  | VAL  | CB-CA-C    | 15.08 | 140.04      | 111.40   |
| 1   | A     | 33  | CYS  | CB-CA-C    | 12.17 | 134.75      | 110.40   |
| 1   | A     | 54  | TYR  | CB-CG-CD1  | 12.16 | 128.29      | 121.00   |
| 1   | B     | 36  | ARG  | NE-CZ-NH1  | 11.84 | 126.22      | 120.30   |
| 1   | A     | 36  | ARG  | CD-NE-CZ   | 11.58 | 139.81      | 123.60   |
| 1   | B     | 59  | CYS  | CA-CB-SG   | 11.39 | 134.51      | 114.00   |
| 1   | A     | 30  | ASP  | CB-CG-OD1  | 10.79 | 128.01      | 118.30   |
| 1   | A     | 31  | ALA  | O-C-N      | 10.61 | 139.68      | 122.70   |
| 1   | A     | 25  | ARG  | CD-NE-CZ   | 10.36 | 138.11      | 123.60   |
| 1   | A     | 29  | CYS  | CA-CB-SG   | -9.72 | 96.50       | 114.00   |
| 1   | B     | 53  | PRO  | N-CA-C     | 9.45  | 136.66      | 112.10   |
| 1   | B     | 39  | VAL  | O-C-N      | 9.17  | 137.37      | 122.70   |
| 1   | B     | 71  | ARG  | NE-CZ-NH2  | -9.16 | 115.72      | 120.30   |
| 1   | B     | 57  | VAL  | CA-CB-CG2  | 9.07  | 124.51      | 110.90   |
| 1   | B     | 2   | VAL  | C-N-CA     | 8.90  | 143.96      | 121.70   |
| 1   | A     | 63  | ASP  | O-C-N      | 8.89  | 136.93      | 122.70   |
| 1   | A     | 21  | ASN  | O-C-N      | 8.80  | 136.78      | 122.70   |
| 1   | A     | 25  | ARG  | NE-CZ-NH2  | -8.64 | 115.98      | 120.30   |
| 1   | B     | 21  | ASN  | C-N-CA     | 8.56  | 143.09      | 121.70   |
| 1   | B     | 33  | CYS  | O-C-N      | 8.55  | 136.39      | 122.70   |
| 1   | A     | 18  | PRO  | CB-CA-C    | -8.47 | 90.83       | 112.00   |
| 1   | A     | 48  | CYS  | CA-CB-SG   | 8.39  | 129.11      | 114.00   |
| 1   | B     | 12  | SER  | C-N-CA     | 8.22  | 142.25      | 121.70   |
| 1   | B     | 17  | PRO  | CA-N-CD    | -8.19 | 100.03      | 111.50   |
| 1   | A     | 55  | GLU  | C-N-CA     | 8.17  | 142.12      | 121.70   |
| 1   | B     | 3   | CYS  | N-CA-CB    | -7.93 | 96.32       | 110.60   |
| 1   | B     | 66  | ASN  | N-CA-CB    | -7.88 | 96.41       | 110.60   |
| 1   | B     | 27  | MET  | CA-CB-CG   | 7.86  | 126.66      | 113.30   |
| 1   | A     | 66  | ASN  | N-CA-C     | 7.85  | 132.20      | 111.00   |
| 1   | A     | 11  | SER  | N-CA-CB    | -7.84 | 98.74       | 110.50   |
| 1   | B     | 63  | ASP  | CB-CG-OD2  | -7.74 | 111.34      | 118.30   |
| 1   | A     | 36  | ARG  | NH1-CZ-NH2 | -7.70 | 110.93      | 119.40   |
| 1   | A     | 29  | CYS  | N-CA-C     | 7.69  | 131.76      | 111.00   |
| 1   | A     | 24  | TYR  | CB-CG-CD1  | 7.68  | 125.61      | 121.00   |
| 1   | A     | 63  | ASP  | CB-CG-OD1  | 7.66  | 125.20      | 118.30   |
| 1   | A     | 2   | VAL  | O-C-N      | 7.54  | 134.76      | 122.70   |
| 1   | A     | 70  | LYS  | N-CA-CB    | 7.54  | 124.16      | 110.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 3   | CYS  | CA-CB-SG   | -7.42 | 100.65      | 114.00   |
| 1   | B     | 71  | ARG  | NE-CZ-NH1  | 7.38  | 123.99      | 120.30   |
| 1   | A     | 41  | GLU  | CG-CD-OE2  | -7.22 | 103.86      | 118.30   |
| 1   | B     | 33  | CYS  | CA-C-N     | -6.95 | 101.90      | 117.20   |
| 1   | B     | 10  | PRO  | CB-CA-C    | 6.83  | 129.08      | 112.00   |
| 1   | B     | 41  | GLU  | OE1-CD-OE2 | 6.82  | 131.48      | 123.30   |
| 1   | B     | 17  | PRO  | N-CA-C     | -6.81 | 94.40       | 112.10   |
| 1   | A     | 58  | THR  | N-CA-CB    | 6.80  | 123.21      | 110.30   |
| 1   | A     | 55  | GLU  | N-CA-CB    | 6.79  | 122.83      | 110.60   |
| 1   | A     | 1   | ILE  | CB-CA-C    | 6.72  | 125.03      | 111.60   |
| 1   | A     | 44  | CYS  | CA-CB-SG   | 6.71  | 126.08      | 114.00   |
| 1   | A     | 39  | VAL  | CB-CA-C    | 6.67  | 124.08      | 111.40   |
| 1   | A     | 33  | CYS  | CA-C-O     | 6.58  | 133.91      | 120.10   |
| 1   | A     | 54  | TYR  | N-CA-CB    | 6.51  | 122.31      | 110.60   |
| 1   | B     | 20  | GLU  | CA-CB-CG   | 6.50  | 127.70      | 113.40   |
| 1   | A     | 3   | CYS  | N-CA-CB    | -6.49 | 98.92       | 110.60   |
| 1   | A     | 70  | LYS  | CA-C-N     | 6.42  | 131.34      | 117.20   |
| 1   | A     | 54  | TYR  | CD1-CG-CD2 | -6.42 | 110.83      | 117.90   |
| 1   | B     | 46  | ALA  | O-C-N      | 6.41  | 132.95      | 122.70   |
| 1   | A     | 13  | ALA  | N-CA-CB    | -6.39 | 101.15      | 110.10   |
| 1   | A     | 70  | LYS  | CA-C-O     | -6.37 | 106.72      | 120.10   |
| 1   | B     | 25  | ARG  | NE-CZ-NH1  | -6.33 | 117.13      | 120.30   |
| 1   | A     | 54  | TYR  | CG-CD2-CE2 | 6.30  | 126.34      | 121.30   |
| 1   | A     | 65  | CYS  | N-CA-C     | 6.29  | 127.98      | 111.00   |
| 1   | A     | 31  | ALA  | N-CA-CB    | 6.28  | 118.90      | 110.10   |
| 1   | B     | 2   | VAL  | CA-CB-CG1  | 6.27  | 120.30      | 110.90   |
| 1   | A     | 69  | PRO  | CA-N-CD    | -6.22 | 102.79      | 111.50   |
| 1   | A     | 21  | ASN  | CA-C-N     | -6.21 | 103.55      | 117.20   |
| 1   | B     | 40  | VAL  | CA-C-O     | 6.19  | 133.11      | 120.10   |
| 1   | B     | 39  | VAL  | C-N-CA     | 6.18  | 137.16      | 121.70   |
| 1   | A     | 15  | THR  | N-CA-CB    | 6.15  | 121.98      | 110.30   |
| 1   | B     | 55  | GLU  | N-CA-CB    | 6.10  | 121.58      | 110.60   |
| 1   | B     | 41  | GLU  | CG-CD-OE2  | -6.10 | 106.11      | 118.30   |
| 1   | B     | 59  | CYS  | O-C-N      | 6.09  | 132.44      | 122.70   |
| 1   | A     | 34  | SER  | N-CA-CB    | 6.06  | 119.60      | 110.50   |
| 1   | A     | 63  | ASP  | N-CA-CB    | 6.05  | 121.50      | 110.60   |
| 1   | B     | 49  | PRO  | O-C-N      | 6.05  | 132.38      | 122.70   |
| 1   | B     | 36  | ARG  | NE-CZ-NH2  | -6.04 | 117.28      | 120.30   |
| 1   | A     | 8   | THR  | O-C-N      | 6.03  | 132.35      | 122.70   |
| 1   | B     | 8   | THR  | C-N-CA     | 6.02  | 136.74      | 121.70   |
| 1   | B     | 54  | TYR  | CG-CD1-CE1 | 6.02  | 126.11      | 121.30   |
| 1   | B     | 3   | CYS  | CB-CA-C    | -5.99 | 98.43       | 110.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 64  | LYS  | CA-C-O     | -5.96 | 107.58      | 120.10   |
| 1   | B     | 13  | ALA  | N-CA-CB    | 5.96  | 118.44      | 110.10   |
| 1   | B     | 13  | ALA  | C-N-CA     | 5.83  | 136.26      | 121.70   |
| 1   | B     | 7   | ALA  | CA-C-N     | -5.79 | 104.46      | 117.20   |
| 1   | B     | 25  | ARG  | NH1-CZ-NH2 | -5.76 | 113.06      | 119.40   |
| 1   | A     | 40  | VAL  | C-N-CA     | 5.75  | 136.06      | 121.70   |
| 1   | A     | 54  | TYR  | CG-CD1-CE1 | 5.73  | 125.89      | 121.30   |
| 1   | B     | 8   | THR  | CA-C-O     | 5.73  | 132.13      | 120.10   |
| 1   | B     | 33  | CYS  | CB-CA-C    | 5.72  | 121.84      | 110.40   |
| 1   | B     | 26  | LYS  | C-N-CA     | 5.71  | 135.96      | 121.70   |
| 1   | A     | 62  | THR  | C-N-CA     | 5.70  | 135.94      | 121.70   |
| 1   | A     | 54  | TYR  | CB-CA-C    | 5.68  | 121.76      | 110.40   |
| 1   | A     | 21  | ASN  | C-N-CA     | 5.67  | 135.88      | 121.70   |
| 1   | B     | 39  | VAL  | CA-C-N     | -5.60 | 104.89      | 117.20   |
| 1   | B     | 13  | ALA  | CA-C-O     | -5.59 | 108.37      | 120.10   |
| 1   | A     | 48  | CYS  | N-CA-CB    | -5.58 | 100.56      | 110.60   |
| 1   | A     | 25  | ARG  | NH1-CZ-NH2 | -5.58 | 113.27      | 119.40   |
| 1   | A     | 32  | PHE  | CB-CG-CD1  | -5.53 | 116.93      | 120.80   |
| 1   | A     | 58  | THR  | C-N-CA     | 5.53  | 135.52      | 121.70   |
| 1   | A     | 65  | CYS  | CA-C-N     | 5.52  | 129.35      | 117.20   |
| 1   | B     | 17  | PRO  | O-C-N      | 5.51  | 131.58      | 121.10   |
| 1   | A     | 22  | LEU  | O-C-N      | 5.51  | 131.51      | 122.70   |
| 1   | A     | 69  | PRO  | N-CD-CG    | -5.47 | 94.99       | 103.20   |
| 1   | A     | 34  | SER  | O-C-N      | 5.43  | 131.38      | 122.70   |
| 1   | B     | 10  | PRO  | CA-C-N     | -5.37 | 105.38      | 117.20   |
| 1   | B     | 59  | CYS  | N-CA-CB    | 5.37  | 120.27      | 110.60   |
| 1   | A     | 50  | SER  | CB-CA-C    | 5.35  | 120.26      | 110.10   |
| 1   | A     | 2   | VAL  | CA-C-N     | -5.31 | 105.52      | 117.20   |
| 1   | B     | 33  | CYS  | CA-CB-SG   | -5.29 | 104.47      | 114.00   |
| 1   | B     | 73  | PRO  | CA-N-CD    | -5.25 | 104.15      | 111.50   |
| 1   | A     | 56  | GLU  | CG-CD-OE2  | -5.24 | 107.81      | 118.30   |
| 1   | B     | 46  | ALA  | CA-C-N     | -5.22 | 105.72      | 117.20   |
| 1   | B     | 70  | LYS  | CB-CA-C    | -5.21 | 99.98       | 110.40   |
| 1   | A     | 41  | GLU  | OE1-CD-OE2 | 5.21  | 129.55      | 123.30   |
| 1   | A     | 67  | HIS  | O-C-N      | 5.17  | 130.93      | 121.10   |
| 1   | B     | 17  | PRO  | N-CD-CG    | -5.17 | 95.45       | 103.20   |
| 1   | B     | 7   | ALA  | N-CA-CB    | 5.12  | 117.27      | 110.10   |
| 1   | A     | 54  | TYR  | O-C-N      | -5.12 | 114.51      | 122.70   |
| 1   | B     | 26  | LYS  | CD-CE-NZ   | 5.10  | 123.44      | 111.70   |
| 1   | B     | 41  | GLU  | C-N-CA     | 5.10  | 134.45      | 121.70   |
| 1   | A     | 2   | VAL  | CA-CB-CG1  | 5.09  | 118.53      | 110.90   |
| 1   | A     | 24  | TYR  | CA-CB-CG   | 5.09  | 123.06      | 113.40   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | B     | 72  | GLN  | O-C-N    | 5.07  | 130.72      | 121.10   |
| 1   | A     | 8   | THR  | CA-C-N   | -5.06 | 106.08      | 117.20   |
| 1   | A     | 63  | ASP  | C-N-CA   | 5.05  | 134.34      | 121.70   |
| 1   | B     | 3   | CYS  | CA-C-O   | -5.05 | 109.49      | 120.10   |
| 1   | A     | 64  | LYS  | CA-CB-CG | 5.05  | 124.50      | 113.40   |
| 1   | B     | 67  | HIS  | N-CA-CB  | 5.04  | 119.68      | 110.60   |
| 1   | B     | 49  | PRO  | CA-N-CD  | 5.04  | 118.76      | 111.70   |
| 1   | B     | 66  | ASN  | N-CA-C   | 5.02  | 124.56      | 111.00   |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 71  | ARG  | Sidechain |
| 1   | B     | 36  | ARG  | Sidechain |
| 1   | B     | 71  | ARG  | Sidechain |

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 551   | 0        | 531      | 223     | 6            |
| 1   | B     | 551   | 0        | 530      | 162     | 7            |
| 2   | A     | 10    | 0        | 0        | 2       | 3            |
| 2   | B     | 6     | 0        | 0        | 0       | 0            |
| All | All   | 1118  | 0        | 1061     | 385     | 9            |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 179.

All (385) close contacts within the same asymmetric unit are listed below.

| Atom-1         | Atom-2          | Distance(Å) | Clash(Å) |
|----------------|-----------------|-------------|----------|
| 1:A:16:CYS:HB2 | 1:A:17:PRO:CD   | 1.22        | 1.52     |
| 1:B:52:LYS:HB2 | 1:B:53:PRO:CD   | 1.06        | 1.52     |
| 1:A:42:LEU:CB  | 1:A:66:ASN:HD22 | 1.25        | 1.45     |

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| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:A:17:PRO:HB2  | 1:A:18:PRO:CD   | 1.31        | 1.40     |
| 1:A:42:LEU:HB2  | 1:A:66:ASN:ND2  | 1.12        | 1.39     |
| 1:A:4:HIS:CE1   | 1:A:13:ALA:HB1  | 1.60        | 1.35     |
| 1:B:52:LYS:CB   | 1:B:53:PRO:HD3  | 1.57        | 1.35     |
| 1:A:4:HIS:CD2   | 1:A:13:ALA:HB1  | 1.61        | 1.33     |
| 1:A:9:ILE:HB    | 1:A:10:PRO:CD   | 1.58        | 1.32     |
| 1:A:50:SER:O    | 1:A:51:LYS:HG3  | 1.32        | 1.28     |
| 1:A:24:TYR:CD1  | 1:A:51:LYS:HE2  | 1.66        | 1.27     |
| 1:B:52:LYS:CB   | 1:B:53:PRO:CD   | 2.00        | 1.27     |
| 1:A:4:HIS:NE2   | 1:A:13:ALA:HB1  | 1.47        | 1.26     |
| 1:B:16:CYS:CB   | 1:B:17:PRO:HD3  | 1.60        | 1.26     |
| 1:A:26:LYS:CG   | 1:A:57:VAL:HG13 | 1.68        | 1.24     |
| 1:A:4:HIS:CE1   | 1:A:13:ALA:CB   | 2.22        | 1.23     |
| 1:A:17:PRO:CB   | 1:A:18:PRO:CD   | 2.13        | 1.22     |
| 1:B:7:ALA:O     | 1:B:14:VAL:HG21 | 1.35        | 1.21     |
| 1:A:52:LYS:HB3  | 1:A:53:PRO:CD   | 1.71        | 1.21     |
| 1:A:16:CYS:CB   | 1:A:17:PRO:CD   | 2.14        | 1.20     |
| 1:A:3:CYS:O     | 1:A:15:THR:HG22 | 1.43        | 1.17     |
| 1:A:4:HIS:CG    | 1:A:13:ALA:HB1  | 1.79        | 1.17     |
| 1:A:9:ILE:CB    | 1:A:10:PRO:HD3  | 1.74        | 1.17     |
| 1:B:38:LYS:HD3  | 1:B:71:ARG:HG3  | 1.24        | 1.17     |
| 1:A:52:LYS:HB3  | 1:A:53:PRO:HD2  | 1.21        | 1.16     |
| 1:B:60:CYS:SG   | 1:B:61:SER:N    | 2.15        | 1.15     |
| 1:A:22:LEU:HD12 | 1:A:61:SER:HB2  | 1.26        | 1.14     |
| 1:A:16:CYS:HB2  | 1:A:17:PRO:HD2  | 1.23        | 1.13     |
| 1:A:16:CYS:CB   | 1:A:17:PRO:HD3  | 1.78        | 1.13     |
| 1:A:26:LYS:HG3  | 1:A:57:VAL:CG1  | 1.79        | 1.12     |
| 1:B:38:LYS:CD   | 1:B:71:ARG:HG3  | 1.79        | 1.11     |
| 1:B:24:TYR:CZ   | 1:B:49:PRO:HG2  | 1.86        | 1.10     |
| 1:B:66:ASN:HD22 | 1:B:66:ASN:N    | 1.43        | 1.10     |
| 1:A:72:GLN:OE1  | 1:A:72:GLN:HA   | 1.42        | 1.09     |
| 1:A:22:LEU:HD12 | 1:A:61:SER:CB   | 1.81        | 1.09     |
| 1:B:66:ASN:H    | 1:B:66:ASN:ND2  | 1.33        | 1.08     |
| 1:A:2:VAL:HG11  | 1:A:22:LEU:N    | 1.68        | 1.08     |
| 1:A:6:THR:HA    | 1:A:11:SER:OG   | 1.53        | 1.08     |
| 1:B:9:ILE:HB    | 1:B:10:PRO:CD   | 1.84        | 1.08     |
| 1:B:4:HIS:HB3   | 1:B:64:LYS:HZ3  | 1.16        | 1.06     |
| 1:B:52:LYS:HB2  | 1:B:53:PRO:HD2  | 1.15        | 1.06     |
| 1:A:29:CYS:O    | 1:A:33:CYS:SG   | 2.14        | 1.06     |
| 1:A:10:PRO:O    | 1:A:11:SER:HB2  | 1.28        | 1.05     |
| 1:B:17:PRO:HB2  | 1:B:18:PRO:HD2  | 1.37        | 1.05     |
| 1:A:2:VAL:HG11  | 1:A:22:LEU:CA   | 1.85        | 1.05     |

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| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:A:22:LEU:HD11 | 1:A:60:CYS:O    | 1.57        | 1.04     |
| 1:A:22:LEU:CD1  | 1:A:61:SER:HB2  | 1.85        | 1.03     |
| 1:A:6:THR:HG22  | 1:A:7:ALA:H     | 1.21        | 1.03     |
| 1:B:9:ILE:HB    | 1:B:10:PRO:HD2  | 1.04        | 1.03     |
| 1:B:9:ILE:O     | 1:B:11:SER:N    | 1.89        | 1.03     |
| 1:A:22:LEU:CD1  | 1:A:61:SER:CB   | 2.35        | 1.03     |
| 1:A:9:ILE:HB    | 1:A:10:PRO:HD3  | 1.04        | 1.02     |
| 1:B:41:GLU:C    | 1:B:42:LEU:HD12 | 1.78        | 1.02     |
| 1:B:16:CYS:HB3  | 1:B:17:PRO:CD   | 1.90        | 1.02     |
| 1:B:17:PRO:O    | 1:B:17:PRO:HD2  | 1.59        | 1.02     |
| 1:B:7:ALA:O     | 1:B:14:VAL:CG2  | 2.08        | 1.01     |
| 1:A:17:PRO:CB   | 1:A:18:PRO:HD2  | 1.81        | 1.00     |
| 1:A:27:MET:HG3  | 1:A:28:TRP:H    | 1.25        | 1.00     |
| 1:B:23:CYS:HB2  | 1:B:60:CYS:SG   | 2.01        | 1.00     |
| 1:B:16:CYS:CB   | 1:B:17:PRO:CD   | 2.40        | 0.99     |
| 1:A:4:HIS:ND1   | 1:A:13:ALA:HB1  | 1.77        | 0.98     |
| 1:A:4:HIS:NE2   | 1:A:13:ALA:CB   | 2.22        | 0.98     |
| 1:A:10:PRO:O    | 1:A:11:SER:CB   | 2.11        | 0.98     |
| 1:B:5:THR:HG23  | 1:B:64:LYS:HG3  | 1.43        | 0.97     |
| 1:A:53:PRO:O    | 1:A:54:TYR:O    | 1.83        | 0.96     |
| 1:B:9:ILE:CB    | 1:B:10:PRO:HD2  | 1.94        | 0.96     |
| 1:A:17:PRO:HD2  | 1:A:44:CYS:SG   | 2.06        | 0.96     |
| 1:B:4:HIS:HB3   | 1:B:64:LYS:NZ   | 1.81        | 0.96     |
| 1:A:50:SER:O    | 1:A:51:LYS:CG   | 2.15        | 0.95     |
| 1:A:42:LEU:CB   | 1:A:66:ASN:ND2  | 1.96        | 0.94     |
| 1:B:16:CYS:HB3  | 1:B:17:PRO:HD3  | 0.96        | 0.94     |
| 1:A:4:HIS:CD2   | 1:A:13:ALA:CB   | 2.50        | 0.94     |
| 1:B:30:ASP:O    | 1:B:31:ALA:HB2  | 1.68        | 0.93     |
| 1:A:3:CYS:O     | 1:A:15:THR:CG2  | 2.15        | 0.93     |
| 1:B:17:PRO:HB2  | 1:B:18:PRO:CD   | 1.99        | 0.93     |
| 1:B:42:LEU:HD12 | 1:B:42:LEU:N    | 1.81        | 0.93     |
| 1:A:48:CYS:O    | 1:A:50:SER:N    | 2.02        | 0.92     |
| 1:B:56:GLU:O    | 1:B:57:VAL:HB   | 1.67        | 0.92     |
| 1:A:27:MET:O    | 1:A:28:TRP:HB2  | 1.65        | 0.91     |
| 1:A:72:GLN:OE1  | 1:A:73:PRO:HD2  | 1.70        | 0.91     |
| 1:A:5:THR:OG1   | 1:A:66:ASN:OD1  | 1.89        | 0.90     |
| 1:A:72:GLN:OE1  | 1:A:72:GLN:CA   | 2.19        | 0.90     |
| 1:B:17:PRO:CD   | 1:B:17:PRO:O    | 2.15        | 0.90     |
| 1:A:16:CYS:HB2  | 1:A:17:PRO:HD3  | 0.90        | 0.90     |
| 1:A:41:GLU:C    | 1:A:42:LEU:HD22 | 1.94        | 0.89     |
| 1:A:17:PRO:HB2  | 1:A:18:PRO:HD2  | 0.90        | 0.88     |
| 1:B:25:ARG:HD2  | 1:B:66:ASN:HB3  | 1.55        | 0.88     |

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| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:A:16:CYS:CB   | 1:A:17:PRO:HD2  | 1.94        | 0.88     |
| 1:B:45:ALA:O    | 1:B:46:ALA:HB3  | 1.73        | 0.88     |
| 1:B:30:ASP:O    | 1:B:31:ALA:CB   | 2.19        | 0.88     |
| 1:A:54:TYR:O    | 1:A:55:GLU:O    | 1.90        | 0.88     |
| 1:A:17:PRO:CB   | 1:A:18:PRO:HD3  | 2.02        | 0.88     |
| 1:B:66:ASN:N    | 1:B:66:ASN:ND2  | 2.09        | 0.88     |
| 1:A:6:THR:O     | 1:A:7:ALA:CB    | 2.22        | 0.86     |
| 1:A:41:GLU:C    | 1:A:42:LEU:CD2  | 2.44        | 0.86     |
| 1:A:22:LEU:CD1  | 1:A:61:SER:HB3  | 2.04        | 0.85     |
| 1:A:2:VAL:CG1   | 1:A:22:LEU:N    | 2.39        | 0.85     |
| 1:A:44:CYS:O    | 1:A:45:ALA:HB2  | 1.77        | 0.84     |
| 1:A:24:TYR:CD1  | 1:A:51:LYS:CE   | 2.58        | 0.84     |
| 1:A:22:LEU:HD23 | 1:A:23:CYS:O    | 1.77        | 0.84     |
| 1:A:43:GLY:O    | 1:A:44:CYS:HB2  | 1.77        | 0.84     |
| 1:A:52:LYS:CB   | 1:A:53:PRO:CD   | 2.47        | 0.84     |
| 1:B:6:THR:CG2   | 1:B:42:LEU:HB2  | 2.08        | 0.83     |
| 1:B:4:HIS:CD2   | 1:B:13:ALA:HB2  | 2.14        | 0.83     |
| 1:A:26:LYS:O    | 1:A:27:MET:CB   | 2.25        | 0.82     |
| 1:B:66:ASN:HD22 | 1:B:66:ASN:H    | 0.85        | 0.82     |
| 1:A:27:MET:SD   | 1:A:54:TYR:OH   | 2.36        | 0.82     |
| 1:B:4:HIS:CG    | 1:B:13:ALA:HB2  | 2.14        | 0.82     |
| 1:A:70:LYS:HZ2  | 1:A:70:LYS:HB3  | 1.44        | 0.82     |
| 1:A:27:MET:HG3  | 1:A:28:TRP:N    | 1.94        | 0.82     |
| 1:A:53:PRO:HB3  | 2:A:217:HOH:O   | 1.78        | 0.82     |
| 1:A:2:VAL:HG11  | 1:A:22:LEU:HA   | 1.62        | 0.81     |
| 1:A:48:CYS:C    | 1:A:50:SER:H    | 1.82        | 0.81     |
| 1:B:9:ILE:O     | 1:B:10:PRO:C    | 2.19        | 0.81     |
| 1:B:42:LEU:N    | 1:B:42:LEU:CD1  | 2.44        | 0.81     |
| 1:A:12:SER:C    | 1:A:14:VAL:H    | 1.81        | 0.81     |
| 1:B:45:ALA:O    | 1:B:46:ALA:CB   | 2.30        | 0.80     |
| 1:B:50:SER:O    | 1:B:51:LYS:HB2  | 1.80        | 0.80     |
| 1:B:28:TRP:HH2  | 1:B:69:PRO:HD2  | 1.46        | 0.80     |
| 1:B:60:CYS:O    | 1:B:61:SER:CB   | 2.28        | 0.80     |
| 1:A:70:LYS:O    | 1:A:71:ARG:HB2  | 1.81        | 0.79     |
| 1:A:14:VAL:HG12 | 1:A:16:CYS:N    | 1.98        | 0.79     |
| 1:B:52:LYS:HB2  | 1:B:53:PRO:HD3  | 0.80        | 0.79     |
| 1:A:27:MET:CG   | 1:A:28:TRP:N    | 2.46        | 0.78     |
| 1:A:42:LEU:O    | 1:A:66:ASN:ND2  | 2.14        | 0.78     |
| 1:B:66:ASN:O    | 1:B:68:PRO:HD3  | 1.83        | 0.78     |
| 1:A:26:LYS:HG3  | 1:A:57:VAL:HG13 | 0.82        | 0.78     |
| 1:B:4:HIS:CD2   | 1:B:13:ALA:CB   | 2.67        | 0.78     |
| 1:B:52:LYS:CB   | 1:B:53:PRO:HD2  | 1.93        | 0.77     |

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| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:A:41:GLU:O    | 1:A:42:LEU:HB3  | 1.81        | 0.77     |
| 1:A:6:THR:O     | 1:A:7:ALA:HB3   | 1.83        | 0.77     |
| 1:A:9:ILE:CG2   | 1:A:10:PRO:HD3  | 2.13        | 0.77     |
| 1:A:4:HIS:CG    | 1:A:13:ALA:CB   | 2.65        | 0.77     |
| 1:A:7:ALA:CB    | 1:A:43:GLY:HA2  | 2.15        | 0.76     |
| 1:A:34:SER:O    | 1:A:35:SER:HB2  | 1.83        | 0.76     |
| 1:A:50:SER:C    | 1:A:51:LYS:HG3  | 2.06        | 0.76     |
| 1:B:25:ARG:HH11 | 1:B:58:THR:HG21 | 1.51        | 0.76     |
| 1:B:5:THR:CG2   | 1:B:64:LYS:CG   | 2.64        | 0.76     |
| 1:B:5:THR:HG23  | 1:B:64:LYS:CG   | 2.14        | 0.76     |
| 1:A:64:LYS:HG3  | 1:A:65:CYS:N    | 2.01        | 0.75     |
| 1:A:6:THR:HB    | 1:A:42:LEU:HG   | 1.68        | 0.75     |
| 1:A:47:THR:O    | 1:A:49:PRO:N    | 2.18        | 0.75     |
| 1:A:4:HIS:ND1   | 1:A:13:ALA:O    | 2.18        | 0.75     |
| 1:B:2:VAL:HG12  | 1:B:3:CYS:SG    | 2.26        | 0.75     |
| 1:A:7:ALA:HA    | 1:A:43:GLY:HA2  | 1.69        | 0.75     |
| 1:A:66:ASN:O    | 1:A:67:HIS:C    | 2.25        | 0.75     |
| 1:A:22:LEU:HD11 | 1:A:61:SER:HB3  | 1.68        | 0.74     |
| 1:B:43:GLY:O    | 1:B:44:CYS:HB3  | 1.88        | 0.74     |
| 1:A:19:GLY:O    | 1:A:20:GLU:CD   | 2.25        | 0.74     |
| 1:A:22:LEU:HD23 | 1:A:23:CYS:H    | 1.53        | 0.74     |
| 1:A:42:LEU:CG   | 1:A:66:ASN:ND2  | 2.50        | 0.74     |
| 1:A:47:THR:O    | 1:A:48:CYS:C    | 2.25        | 0.74     |
| 1:B:5:THR:CG2   | 1:B:64:LYS:HG3  | 2.18        | 0.73     |
| 1:B:47:THR:O    | 1:B:48:CYS:C    | 2.26        | 0.73     |
| 1:A:19:GLY:O    | 1:A:20:GLU:CB   | 2.36        | 0.73     |
| 1:A:7:ALA:HA    | 1:A:43:GLY:CA   | 2.18        | 0.73     |
| 1:A:19:GLY:O    | 1:A:20:GLU:CG   | 2.38        | 0.72     |
| 1:A:52:LYS:HB3  | 1:A:53:PRO:HD3  | 1.71        | 0.72     |
| 1:B:72:GLN:CG   | 1:B:72:GLN:O    | 2.38        | 0.72     |
| 1:A:22:LEU:CG   | 1:A:61:SER:HB2  | 2.19        | 0.72     |
| 1:A:2:VAL:CG1   | 1:A:22:LEU:HA   | 2.20        | 0.72     |
| 1:B:28:TRP:CH2  | 1:B:69:PRO:HD2  | 2.24        | 0.71     |
| 1:A:6:THR:HG22  | 1:A:7:ALA:N     | 2.02        | 0.71     |
| 1:A:42:LEU:CG   | 1:A:66:ASN:HD22 | 2.04        | 0.71     |
| 1:B:60:CYS:O    | 1:B:61:SER:HB3  | 1.89        | 0.71     |
| 1:A:48:CYS:C    | 1:A:50:SER:N    | 2.39        | 0.70     |
| 1:B:24:TYR:CZ   | 1:B:49:PRO:CG   | 2.72        | 0.70     |
| 1:B:23:CYS:O    | 1:B:60:CYS:HB3  | 1.92        | 0.70     |
| 1:B:16:CYS:HB2  | 1:B:17:PRO:HD3  | 1.70        | 0.70     |
| 1:B:35:SER:O    | 1:B:36:ARG:HG3  | 1.92        | 0.70     |
| 1:B:43:GLY:O    | 1:B:44:CYS:CB   | 2.41        | 0.68     |

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| Atom-1         | Atom-2          | Distance(Å) | Clash(Å) |
|----------------|-----------------|-------------|----------|
| 1:A:17:PRO:CD  | 1:A:44:CYS:SG   | 2.79        | 0.68     |
| 1:B:25:ARG:HD2 | 1:B:66:ASN:CB   | 2.23        | 0.68     |
| 1:A:52:LYS:CB  | 1:A:53:PRO:HD3  | 2.22        | 0.68     |
| 1:B:25:ARG:HD3 | 1:B:58:THR:HG21 | 1.74        | 0.68     |
| 1:B:30:ASP:N   | 1:B:30:ASP:OD1  | 2.27        | 0.68     |
| 1:A:47:THR:OG1 | 1:A:47:THR:O    | 2.08        | 0.68     |
| 1:A:19:GLY:O   | 1:A:20:GLU:HB2  | 1.94        | 0.68     |
| 1:A:4:HIS:CE1  | 1:A:13:ALA:C    | 2.68        | 0.67     |
| 1:A:4:HIS:ND1  | 1:A:13:ALA:C    | 2.47        | 0.67     |
| 1:A:19:GLY:O   | 1:A:20:GLU:OE1  | 2.13        | 0.67     |
| 1:B:1:ILE:HG13 | 1:B:1:ILE:O     | 1.94        | 0.67     |
| 1:B:24:TYR:OH  | 1:B:49:PRO:HG2  | 1.95        | 0.67     |
| 1:B:67:HIS:O   | 1:B:69:PRO:HD3  | 1.94        | 0.67     |
| 1:A:12:SER:O   | 1:A:13:ALA:HB3  | 1.95        | 0.66     |
| 1:A:26:LYS:O   | 1:A:27:MET:HB2  | 1.93        | 0.66     |
| 1:B:5:THR:O    | 1:B:13:ALA:HA   | 1.93        | 0.66     |
| 1:B:6:THR:CG2  | 1:B:42:LEU:HD22 | 2.25        | 0.66     |
| 1:A:30:ASP:O   | 1:A:31:ALA:HB2  | 1.94        | 0.66     |
| 1:B:41:GLU:CA  | 1:B:42:LEU:HD12 | 2.24        | 0.66     |
| 1:A:2:VAL:CG1  | 1:A:22:LEU:H    | 2.08        | 0.65     |
| 1:A:7:ALA:CA   | 1:A:43:GLY:HA2  | 2.26        | 0.65     |
| 1:A:9:ILE:CB   | 1:A:10:PRO:CD   | 2.40        | 0.65     |
| 1:B:40:VAL:HB  | 1:B:42:LEU:HD11 | 1.77        | 0.65     |
| 1:A:13:ALA:O   | 1:A:15:THR:N    | 2.30        | 0.65     |
| 1:B:25:ARG:CD  | 1:B:66:ASN:HB3  | 2.26        | 0.65     |
| 1:A:26:LYS:O   | 1:A:41:GLU:HB3  | 1.96        | 0.65     |
| 1:A:69:PRO:O   | 1:A:71:ARG:HG3  | 1.96        | 0.65     |
| 1:A:4:HIS:ND1  | 1:A:13:ALA:CB   | 2.48        | 0.65     |
| 1:A:64:LYS:HG3 | 1:A:65:CYS:H    | 1.61        | 0.65     |
| 1:A:4:HIS:CE1  | 1:A:13:ALA:HB3  | 2.26        | 0.64     |
| 1:B:38:LYS:HD2 | 1:B:71:ARG:HG3  | 1.78        | 0.64     |
| 1:A:53:PRO:C   | 1:A:54:TYR:O    | 2.35        | 0.64     |
| 1:B:38:LYS:CD  | 1:B:71:ARG:CG   | 2.69        | 0.64     |
| 1:A:41:GLU:O   | 1:A:42:LEU:CB   | 2.45        | 0.64     |
| 1:B:6:THR:HG22 | 1:B:42:LEU:HB2  | 1.80        | 0.63     |
| 1:A:3:CYS:C    | 1:A:15:THR:HG22 | 2.17        | 0.63     |
| 1:A:58:THR:OG1 | 1:A:59:CYS:N    | 2.31        | 0.63     |
| 1:B:22:LEU:HA  | 1:B:61:SER:HB2  | 1.79        | 0.63     |
| 1:B:17:PRO:CB  | 1:B:18:PRO:CD   | 2.74        | 0.63     |
| 1:A:4:HIS:ND1  | 1:A:13:ALA:CA   | 2.62        | 0.63     |
| 1:A:68:PRO:O   | 1:A:71:ARG:HD2  | 1.98        | 0.63     |
| 1:B:48:CYS:O   | 1:B:50:SER:N    | 2.32        | 0.62     |

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| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:A:24:TYR:O    | 1:A:24:TYR:CD1  | 2.52        | 0.62     |
| 1:A:20:GLU:O    | 1:A:21:ASN:HB3  | 1.99        | 0.61     |
| 1:B:68:PRO:HD2  | 1:B:73:PRO:HD2  | 1.82        | 0.61     |
| 1:A:32:PHE:C    | 1:A:34:SER:H    | 2.04        | 0.61     |
| 1:B:64:LYS:O    | 1:B:65:CYS:CB   | 2.49        | 0.60     |
| 1:A:42:LEU:HD23 | 1:A:42:LEU:N    | 2.15        | 0.60     |
| 1:B:6:THR:HG21  | 1:B:42:LEU:HD22 | 1.82        | 0.60     |
| 1:A:17:PRO:HB3  | 1:A:18:PRO:HD3  | 1.82        | 0.60     |
| 1:A:6:THR:HG21  | 1:A:42:LEU:HD21 | 1.84        | 0.60     |
| 1:A:42:LEU:CD2  | 1:A:42:LEU:N    | 2.65        | 0.59     |
| 1:B:56:GLU:O    | 1:B:57:VAL:CB   | 2.45        | 0.59     |
| 1:A:27:MET:CG   | 1:A:28:TRP:H    | 2.00        | 0.59     |
| 1:B:8:THR:O     | 1:B:9:ILE:O     | 2.21        | 0.59     |
| 1:B:50:SER:O    | 1:B:51:LYS:CB   | 2.49        | 0.59     |
| 1:B:57:VAL:O    | 1:B:58:THR:HB   | 2.02        | 0.59     |
| 1:B:64:LYS:O    | 1:B:65:CYS:HB2  | 2.02        | 0.59     |
| 1:A:3:CYS:HA    | 1:A:64:LYS:HA   | 1.85        | 0.59     |
| 1:A:29:CYS:O    | 1:A:29:CYS:SG   | 2.61        | 0.59     |
| 1:A:5:THR:HG21  | 1:A:66:ASN:H    | 1.68        | 0.58     |
| 1:B:9:ILE:O     | 1:B:11:SER:CA   | 2.52        | 0.58     |
| 1:A:1:ILE:C     | 1:A:2:VAL:HG22  | 2.22        | 0.58     |
| 1:B:48:CYS:O    | 1:B:49:PRO:C    | 2.42        | 0.58     |
| 1:B:24:TYR:CE1  | 1:B:49:PRO:HG2  | 2.38        | 0.58     |
| 1:B:72:GLN:O    | 1:B:72:GLN:HG3  | 2.01        | 0.58     |
| 1:A:26:LYS:CG   | 1:A:57:VAL:CG1  | 2.58        | 0.58     |
| 1:A:4:HIS:CE1   | 1:A:13:ALA:CA   | 2.86        | 0.58     |
| 1:B:4:HIS:O     | 1:B:5:THR:CG2   | 2.53        | 0.57     |
| 1:A:24:TYR:HE1  | 1:A:41:GLU:CG   | 2.16        | 0.57     |
| 1:A:68:PRO:HG2  | 1:A:71:ARG:NH2  | 2.19        | 0.57     |
| 1:B:52:LYS:HB3  | 1:B:53:PRO:HD3  | 1.73        | 0.57     |
| 1:A:26:LYS:O    | 1:A:27:MET:HB3  | 2.03        | 0.57     |
| 1:B:42:LEU:HB3  | 1:B:66:ASN:OD1  | 2.04        | 0.57     |
| 1:B:2:VAL:HB    | 1:B:16:CYS:SG   | 2.45        | 0.57     |
| 1:A:52:LYS:CG   | 1:A:53:PRO:HD3  | 2.35        | 0.57     |
| 1:B:48:CYS:C    | 1:B:50:SER:N    | 2.56        | 0.57     |
| 1:A:6:THR:CG2   | 1:A:7:ALA:N     | 2.65        | 0.56     |
| 1:A:51:LYS:O    | 1:A:52:LYS:HD2  | 2.06        | 0.56     |
| 1:A:14:VAL:HG12 | 1:A:16:CYS:H    | 1.68        | 0.56     |
| 1:B:60:CYS:O    | 1:B:61:SER:HB2  | 2.04        | 0.56     |
| 1:B:25:ARG:NH2  | 1:B:28:TRP:HZ3  | 2.04        | 0.56     |
| 1:A:8:THR:O     | 1:A:9:ILE:HD12  | 2.05        | 0.56     |
| 1:A:60:CYS:O    | 1:A:61:SER:HB3  | 2.06        | 0.55     |

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| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:B:5:THR:CG2   | 1:B:64:LYS:HG2  | 2.36        | 0.55     |
| 1:A:12:SER:C    | 1:A:14:VAL:N    | 2.56        | 0.55     |
| 1:A:22:LEU:HD11 | 1:A:60:CYS:C    | 2.27        | 0.55     |
| 1:B:4:HIS:HA    | 1:B:13:ALA:HB1  | 1.88        | 0.55     |
| 1:A:30:ASP:O    | 1:A:31:ALA:CB   | 2.52        | 0.55     |
| 1:A:48:CYS:O    | 1:A:49:PRO:C    | 2.44        | 0.55     |
| 1:B:9:ILE:CB    | 1:B:10:PRO:CD   | 2.62        | 0.55     |
| 1:A:68:PRO:HG2  | 1:A:68:PRO:O    | 2.07        | 0.55     |
| 1:A:22:LEU:O    | 1:A:23:CYS:SG   | 2.65        | 0.55     |
| 1:B:6:THR:HG23  | 1:B:42:LEU:HB2  | 1.85        | 0.54     |
| 1:A:45:ALA:O    | 1:A:46:ALA:HB3  | 2.07        | 0.54     |
| 1:B:1:ILE:CG1   | 1:B:1:ILE:O     | 2.56        | 0.54     |
| 1:A:51:LYS:O    | 1:A:52:LYS:CD   | 2.56        | 0.53     |
| 1:A:41:GLU:O    | 1:A:42:LEU:HD22 | 2.07        | 0.53     |
| 1:A:6:THR:O     | 1:A:7:ALA:HB2   | 2.08        | 0.53     |
| 1:A:19:GLY:C    | 1:A:20:GLU:CD   | 2.68        | 0.53     |
| 1:B:7:ALA:HB2   | 1:B:43:GLY:HA2  | 1.91        | 0.52     |
| 1:A:9:ILE:C     | 1:A:11:SER:N    | 2.61        | 0.52     |
| 1:A:5:THR:C     | 1:A:6:THR:O     | 2.48        | 0.52     |
| 1:B:9:ILE:C     | 1:B:11:SER:N    | 2.62        | 0.52     |
| 1:A:3:CYS:SG    | 1:A:16:CYS:SG   | 3.08        | 0.51     |
| 1:A:24:TYR:CE1  | 1:A:51:LYS:HE2  | 2.34        | 0.51     |
| 1:A:64:LYS:O    | 1:A:65:CYS:HB2  | 2.11        | 0.51     |
| 1:A:9:ILE:HB    | 1:A:10:PRO:HD2  | 1.78        | 0.51     |
| 1:A:23:CYS:HB3  | 1:A:43:GLY:O    | 2.11        | 0.51     |
| 1:A:45:ALA:O    | 1:A:46:ALA:CB   | 2.59        | 0.51     |
| 1:B:22:LEU:CB   | 1:B:61:SER:HB2  | 2.41        | 0.51     |
| 1:A:33:CYS:C    | 1:A:35:SER:H    | 2.14        | 0.50     |
| 1:A:64:LYS:O    | 1:A:65:CYS:CB   | 2.59        | 0.50     |
| 1:A:41:GLU:CA   | 1:A:42:LEU:HD22 | 2.41        | 0.50     |
| 1:A:70:LYS:HZ2  | 1:A:70:LYS:CB   | 2.10        | 0.50     |
| 1:B:4:HIS:CG    | 1:B:13:ALA:CB   | 2.88        | 0.50     |
| 1:A:2:VAL:HG11  | 1:A:22:LEU:C    | 2.32        | 0.50     |
| 1:A:24:TYR:CE1  | 1:A:41:GLU:CG   | 2.94        | 0.50     |
| 1:A:24:TYR:CG   | 1:A:51:LYS:HE2  | 2.35        | 0.50     |
| 1:B:25:ARG:HB2  | 1:B:58:THR:HG22 | 1.93        | 0.50     |
| 1:B:67:HIS:O    | 1:B:69:PRO:CD   | 2.59        | 0.49     |
| 1:B:22:LEU:HA   | 1:B:61:SER:CB   | 2.42        | 0.49     |
| 1:A:22:LEU:HG   | 1:A:61:SER:HB2  | 1.92        | 0.49     |
| 1:A:7:ALA:HB2   | 1:A:43:GLY:HA2  | 1.94        | 0.49     |
| 1:B:6:THR:HG22  | 1:B:42:LEU:HD22 | 1.93        | 0.49     |
| 1:B:19:GLY:O    | 1:B:20:GLU:HB2  | 2.12        | 0.49     |

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| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:A:6:THR:CG2   | 1:A:7:ALA:H     | 1.96        | 0.48     |
| 1:B:23:CYS:CB   | 1:B:60:CYS:SG   | 2.90        | 0.48     |
| 1:B:4:HIS:O     | 1:B:5:THR:HG23  | 2.14        | 0.48     |
| 1:B:24:TYR:CE2  | 1:B:49:PRO:HD2  | 2.48        | 0.48     |
| 1:A:32:PHE:C    | 1:A:34:SER:N    | 2.66        | 0.48     |
| 1:A:7:ALA:HA    | 1:A:43:GLY:HA3  | 1.94        | 0.47     |
| 1:B:26:LYS:O    | 1:B:27:MET:HG3  | 2.14        | 0.47     |
| 1:B:21:ASN:OD1  | 1:B:22:LEU:HD13 | 2.14        | 0.47     |
| 1:A:22:LEU:CD2  | 1:A:23:CYS:H    | 2.25        | 0.47     |
| 1:B:21:ASN:OD1  | 1:B:21:ASN:C    | 2.52        | 0.47     |
| 1:A:22:LEU:CD2  | 1:A:23:CYS:O    | 2.58        | 0.47     |
| 1:B:22:LEU:HG   | 1:B:48:CYS:HB2  | 1.95        | 0.47     |
| 1:B:48:CYS:C    | 1:B:50:SER:H    | 2.18        | 0.47     |
| 1:B:25:ARG:CG   | 1:B:66:ASN:HB3  | 2.44        | 0.47     |
| 1:A:34:SER:O    | 1:A:35:SER:CB   | 2.56        | 0.47     |
| 1:A:16:CYS:SG   | 1:A:17:PRO:HD2  | 2.55        | 0.47     |
| 1:A:27:MET:HG2  | 1:A:39:VAL:O    | 2.14        | 0.47     |
| 1:A:22:LEU:C    | 1:A:23:CYS:SG   | 2.93        | 0.47     |
| 1:A:41:GLU:HG3  | 1:A:42:LEU:N    | 2.30        | 0.47     |
| 1:B:16:CYS:HB2  | 1:B:17:PRO:CD   | 2.32        | 0.47     |
| 1:B:4:HIS:CB    | 1:B:64:LYS:NZ   | 2.66        | 0.47     |
| 1:B:26:LYS:HB2  | 1:B:57:VAL:HG23 | 1.96        | 0.46     |
| 1:A:72:GLN:HA   | 1:A:73:PRO:HD2  | 1.67        | 0.46     |
| 1:A:5:THR:HG21  | 1:A:66:ASN:N    | 2.30        | 0.46     |
| 1:B:27:MET:SD   | 1:B:39:VAL:O    | 2.73        | 0.46     |
| 1:B:41:GLU:N    | 1:B:42:LEU:HD12 | 2.30        | 0.46     |
| 1:B:63:ASP:HB3  | 1:B:64:LYS:H    | 1.29        | 0.46     |
| 1:B:62:THR:O    | 1:B:63:ASP:CB   | 2.64        | 0.46     |
| 1:B:22:LEU:O    | 1:B:22:LEU:HD23 | 2.16        | 0.46     |
| 1:B:4:HIS:C     | 1:B:5:THR:HG23  | 2.36        | 0.46     |
| 1:A:4:HIS:O     | 1:A:64:LYS:HD3  | 2.16        | 0.46     |
| 1:B:42:LEU:HD23 | 1:B:66:ASN:O    | 2.16        | 0.45     |
| 1:A:22:LEU:HD12 | 1:A:61:SER:HB3  | 1.70        | 0.45     |
| 1:B:24:TYR:CD2  | 1:B:49:PRO:HD2  | 2.52        | 0.45     |
| 1:B:7:ALA:HA    | 1:B:42:LEU:O    | 2.17        | 0.45     |
| 1:A:41:GLU:N    | 1:A:42:LEU:HD22 | 2.32        | 0.45     |
| 1:A:24:TYR:CG   | 1:A:51:LYS:CE   | 2.97        | 0.45     |
| 1:B:22:LEU:CD2  | 1:B:22:LEU:O    | 2.64        | 0.45     |
| 1:B:22:LEU:CA   | 1:B:61:SER:HB2  | 2.45        | 0.45     |
| 1:A:4:HIS:HA    | 1:A:13:ALA:HA   | 1.99        | 0.45     |
| 1:A:41:GLU:C    | 1:A:42:LEU:HD23 | 2.32        | 0.45     |
| 1:A:60:CYS:HB3  | 1:A:61:SER:H    | 1.62        | 0.45     |

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| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:B:28:TRP:O    | 1:B:37:GLY:HA2  | 2.17        | 0.44     |
| 1:A:39:VAL:HA   | 2:A:200:HOH:O   | 2.17        | 0.44     |
| 1:A:26:LYS:CD   | 1:A:57:VAL:HG13 | 2.43        | 0.44     |
| 1:A:22:LEU:HD23 | 1:A:23:CYS:N    | 2.26        | 0.44     |
| 1:A:26:LYS:HE2  | 1:A:54:TYR:CE2  | 2.52        | 0.44     |
| 1:B:22:LEU:C    | 1:B:22:LEU:CD2  | 2.86        | 0.44     |
| 1:B:67:HIS:HA   | 1:B:68:PRO:HD3  | 1.82        | 0.44     |
| 1:B:48:CYS:N    | 1:B:49:PRO:CD   | 2.78        | 0.44     |
| 1:B:25:ARG:CD   | 1:B:66:ASN:CB   | 2.91        | 0.44     |
| 1:A:22:LEU:HD23 | 1:A:23:CYS:C    | 2.37        | 0.44     |
| 1:A:24:TYR:O    | 1:A:42:LEU:HA   | 2.17        | 0.43     |
| 1:A:59:CYS:O    | 1:A:60:CYS:O    | 2.36        | 0.43     |
| 1:A:42:LEU:CA   | 1:A:66:ASN:ND2  | 2.77        | 0.43     |
| 1:B:57:VAL:O    | 1:B:58:THR:CB   | 2.66        | 0.43     |
| 1:B:47:THR:O    | 1:B:49:PRO:N    | 2.50        | 0.43     |
| 1:B:25:ARG:HG2  | 1:B:66:ASN:HB3  | 2.01        | 0.43     |
| 1:B:4:HIS:HA    | 1:B:13:ALA:CB   | 2.48        | 0.43     |
| 1:B:22:LEU:C    | 1:B:22:LEU:HD23 | 2.38        | 0.43     |
| 1:A:52:LYS:HG3  | 1:A:53:PRO:HD3  | 2.00        | 0.43     |
| 1:A:68:PRO:CG   | 1:A:68:PRO:O    | 2.65        | 0.43     |
| 1:A:12:SER:O    | 1:A:14:VAL:N    | 2.50        | 0.43     |
| 1:A:24:TYR:HD1  | 1:A:51:LYS:HE2  | 1.58        | 0.43     |
| 1:B:47:THR:C    | 1:B:49:PRO:N    | 2.69        | 0.43     |
| 1:A:43:GLY:O    | 1:A:44:CYS:CB   | 2.58        | 0.43     |
| 1:A:42:LEU:HB2  | 1:A:66:ASN:HD22 | 0.38        | 0.43     |
| 1:B:4:HIS:O     | 1:B:64:LYS:HG3  | 2.19        | 0.43     |
| 1:B:29:CYS:O    | 1:B:31:ALA:N    | 2.51        | 0.43     |
| 1:A:42:LEU:HG   | 1:A:66:ASN:ND2  | 2.33        | 0.42     |
| 1:B:14:VAL:HG12 | 1:B:16:CYS:N    | 2.34        | 0.42     |
| 1:B:71:ARG:HB3  | 1:B:72:GLN:H    | 1.36        | 0.42     |
| 1:B:19:GLY:O    | 1:B:20:GLU:CB   | 2.67        | 0.42     |
| 1:B:51:LYS:C    | 1:B:52:LYS:HG2  | 2.40        | 0.42     |
| 1:A:8:THR:C     | 1:A:9:ILE:HD12  | 2.40        | 0.42     |
| 1:B:52:LYS:CG   | 1:B:53:PRO:HD2  | 2.49        | 0.42     |
| 1:B:27:MET:SD   | 1:B:40:VAL:HA   | 2.60        | 0.42     |
| 1:A:50:SER:O    | 1:A:51:LYS:CB   | 2.67        | 0.41     |
| 1:A:5:THR:CG2   | 1:A:67:HIS:H    | 2.33        | 0.41     |
| 1:B:46:ALA:HB1  | 1:B:47:THR:HG23 | 2.03        | 0.41     |
| 1:A:22:LEU:HD11 | 1:A:61:SER:CB   | 2.30        | 0.41     |
| 1:A:42:LEU:C    | 1:A:66:ASN:ND2  | 2.74        | 0.41     |
| 1:B:72:GLN:O    | 1:B:72:GLN:HG2  | 2.16        | 0.41     |
| 1:A:2:VAL:HB    | 1:A:23:CYS:SG   | 2.60        | 0.41     |

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| Atom-1         | Atom-2         | Distance(Å) | Clash(Å) |
|----------------|----------------|-------------|----------|
| 1:B:38:LYS:HD2 | 1:B:71:ARG:CG  | 2.45        | 0.41     |
| 1:B:64:LYS:HB2 | 1:B:64:LYS:HE2 | 1.38        | 0.41     |
| 1:A:55:GLU:HB3 | 1:A:56:GLU:HG2 | 2.03        | 0.40     |
| 1:B:6:THR:HG23 | 1:B:42:LEU:O   | 2.22        | 0.40     |

All (9) 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                | Distance(Å) | Clash(Å) |
|---------------|-----------------------|-------------|----------|
| 1:A:20:GLU:O  | 1:B:17:PRO:CA[4_467]  | 1.29        | 0.91     |
| 1:B:11:SER:OG | 2:A:211:HOH:O[3_655]  | 1.51        | 0.69     |
| 1:B:51:LYS:NZ | 1:B:69:PRO:O[1_556]   | 1.65        | 0.55     |
| 1:A:40:VAL:O  | 1:A:73:PRO:CG[1_556]  | 1.93        | 0.27     |
| 1:A:20:GLU:O  | 1:B:17:PRO:CB[4_467]  | 2.00        | 0.20     |
| 1:A:8:THR:O   | 1:B:9:ILE:CG2[3_646]  | 2.01        | 0.19     |
| 1:B:6:THR:OG1 | 2:A:211:HOH:O[3_655]  | 2.01        | 0.19     |
| 1:A:32:PHE:CZ | 1:B:32:PHE:CE2[3_646] | 2.11        | 0.09     |
| 1:A:73:PRO:O  | 2:A:209:HOH:O[1_554]  | 2.16        | 0.04     |

## 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     | 72/74 (97%)   | 10 (14%) | 23 (32%) | 39 (54%) | 0           | 0 |
| 1   | B     | 72/74 (97%)   | 15 (21%) | 24 (33%) | 33 (46%) | 0           | 0 |
| All | All   | 144/148 (97%) | 25 (17%) | 47 (33%) | 72 (50%) | 0           | 0 |

All (72) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 2   | VAL  |
| 1   | A     | 6   | THR  |
| 1   | A     | 7   | ALA  |
| 1   | A     | 9   | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 14  | VAL  |
| 1   | A     | 16  | CYS  |
| 1   | A     | 20  | GLU  |
| 1   | A     | 21  | ASN  |
| 1   | A     | 27  | MET  |
| 1   | A     | 28  | TRP  |
| 1   | A     | 31  | ALA  |
| 1   | A     | 35  | SER  |
| 1   | A     | 42  | LEU  |
| 1   | A     | 44  | CYS  |
| 1   | A     | 45  | ALA  |
| 1   | A     | 46  | ALA  |
| 1   | A     | 49  | PRO  |
| 1   | A     | 50  | SER  |
| 1   | A     | 51  | LYS  |
| 1   | A     | 54  | TYR  |
| 1   | A     | 55  | GLU  |
| 1   | A     | 58  | THR  |
| 1   | A     | 60  | CYS  |
| 1   | A     | 61  | SER  |
| 1   | A     | 63  | ASP  |
| 1   | A     | 65  | CYS  |
| 1   | A     | 69  | PRO  |
| 1   | A     | 73  | PRO  |
| 1   | B     | 7   | ALA  |
| 1   | B     | 9   | ILE  |
| 1   | B     | 10  | PRO  |
| 1   | B     | 17  | PRO  |
| 1   | B     | 31  | ALA  |
| 1   | B     | 39  | VAL  |
| 1   | B     | 44  | CYS  |
| 1   | B     | 46  | ALA  |
| 1   | B     | 47  | THR  |
| 1   | B     | 50  | SER  |
| 1   | B     | 51  | LYS  |
| 1   | B     | 52  | LYS  |
| 1   | B     | 53  | PRO  |
| 1   | B     | 60  | CYS  |
| 1   | B     | 61  | SER  |
| 1   | B     | 63  | ASP  |
| 1   | B     | 65  | CYS  |
| 1   | B     | 72  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 17  | PRO  |
| 1   | A     | 18  | PRO  |
| 1   | A     | 22  | LEU  |
| 1   | A     | 30  | ASP  |
| 1   | B     | 3   | CYS  |
| 1   | B     | 16  | CYS  |
| 1   | B     | 20  | GLU  |
| 1   | B     | 22  | LEU  |
| 1   | B     | 30  | ASP  |
| 1   | B     | 35  | SER  |
| 1   | B     | 36  | ARG  |
| 1   | B     | 58  | THR  |
| 1   | A     | 15  | THR  |
| 1   | A     | 36  | ARG  |
| 1   | B     | 8   | THR  |
| 1   | B     | 34  | SER  |
| 1   | B     | 56  | GLU  |
| 1   | B     | 69  | PRO  |
| 1   | A     | 52  | LYS  |
| 1   | A     | 68  | PRO  |
| 1   | B     | 68  | PRO  |
| 1   | B     | 73  | PRO  |
| 1   | A     | 37  | GLY  |
| 1   | A     | 48  | CYS  |
| 1   | A     | 67  | HIS  |
| 1   | B     | 48  | CYS  |

### 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     | 65/65 (100%)   | 34 (52%)  | 31 (48%) | 0           | 0 |
| 1   | B     | 65/65 (100%)   | 38 (58%)  | 27 (42%) | 0           | 0 |
| All | All   | 130/130 (100%) | 72 (55%)  | 58 (45%) | 0           | 0 |

All (58) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 2   | VAL  |
| 1   | A     | 4   | HIS  |
| 1   | A     | 9   | ILE  |
| 1   | A     | 12  | SER  |
| 1   | A     | 16  | CYS  |
| 1   | A     | 20  | GLU  |
| 1   | A     | 21  | ASN  |
| 1   | A     | 22  | LEU  |
| 1   | A     | 24  | TYR  |
| 1   | A     | 25  | ARG  |
| 1   | A     | 30  | ASP  |
| 1   | A     | 36  | ARG  |
| 1   | A     | 38  | LYS  |
| 1   | A     | 39  | VAL  |
| 1   | A     | 42  | LEU  |
| 1   | A     | 47  | THR  |
| 1   | A     | 48  | CYS  |
| 1   | A     | 53  | PRO  |
| 1   | A     | 54  | TYR  |
| 1   | A     | 57  | VAL  |
| 1   | A     | 59  | CYS  |
| 1   | A     | 60  | CYS  |
| 1   | A     | 61  | SER  |
| 1   | A     | 62  | THR  |
| 1   | A     | 63  | ASP  |
| 1   | A     | 64  | LYS  |
| 1   | A     | 67  | HIS  |
| 1   | A     | 68  | PRO  |
| 1   | A     | 70  | LYS  |
| 1   | A     | 72  | GLN  |
| 1   | A     | 73  | PRO  |
| 1   | B     | 1   | ILE  |
| 1   | B     | 2   | VAL  |
| 1   | B     | 9   | ILE  |
| 1   | B     | 12  | SER  |
| 1   | B     | 15  | THR  |
| 1   | B     | 20  | GLU  |
| 1   | B     | 21  | ASN  |
| 1   | B     | 22  | LEU  |
| 1   | B     | 27  | MET  |
| 1   | B     | 28  | TRP  |
| 1   | B     | 30  | ASP  |
| 1   | B     | 32  | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 38  | LYS  |
| 1   | B     | 39  | VAL  |
| 1   | B     | 40  | VAL  |
| 1   | B     | 42  | LEU  |
| 1   | B     | 47  | THR  |
| 1   | B     | 52  | LYS  |
| 1   | B     | 53  | PRO  |
| 1   | B     | 54  | TYR  |
| 1   | B     | 58  | THR  |
| 1   | B     | 60  | CYS  |
| 1   | B     | 63  | ASP  |
| 1   | B     | 65  | CYS  |
| 1   | B     | 66  | ASN  |
| 1   | B     | 70  | LYS  |
| 1   | B     | 71  | ARG  |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 66  | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.



## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.