



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:22 AM UTC

PDB ID : 3DP8 / pdb\_00003dp8  
Title : Structural characterization of a putative endogenous metal chelator in the periplasmic nickel transporter NikA (nickel butane-1,2,4-tricarboxylate form)  
Authors : Cherrier, M.V.; Cavazza, C.; Bochot, C.; Lemaire, D.; Fontecilla-Camps, J.C.  
Deposited on : 2008-07-07  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure 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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| 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                                                             |

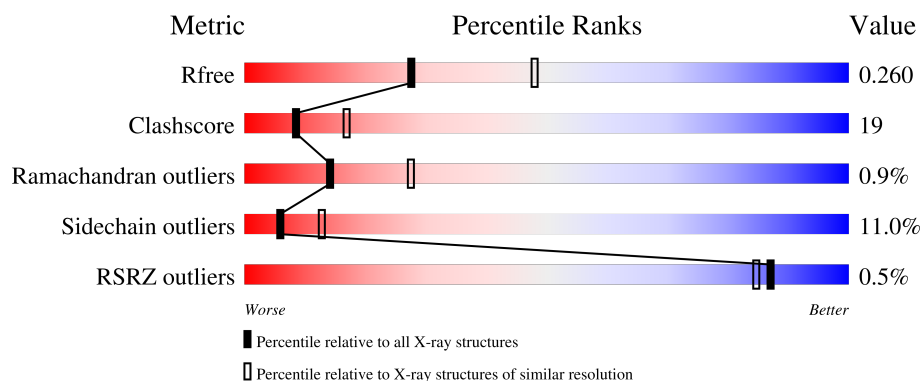
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 5829 (2.50-2.50)                                      |
| Clashscore            | 190562                      | 6492 (2.50-2.50)                                      |
| Ramachandran outliers | 187476                      | 6378 (2.50-2.50)                                      |
| Sidechain outliers    | 187428                      | 6380 (2.50-2.50)                                      |
| RSRZ outliers         | 180081                      | 5833 (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 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     | 502    | <div> <div></div> <div>64% 29% 5% ..</div> </div> |
| 1   | B     | 502    | <div> <div></div> <div>66% 27% 5% ..</div> </div> |
| 1   | C     | 502    | <div> <div></div> <div>61% 32% .. ..</div> </div> |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3   | ACT  | A     | 507 | -         | -        | X       | -                |
| 3   | ACT  | B     | 507 | -         | -        | X       | -                |
| 3   | ACT  | C     | 504 | -         | X        | X       | -                |
| 7   | GOL  | A     | 514 | -         | -        | X       | -                |
| 7   | GOL  | B     | 513 | -         | -        | X       | -                |
| 7   | GOL  | B     | 515 | -         | -        | X       | -                |

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12491 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.

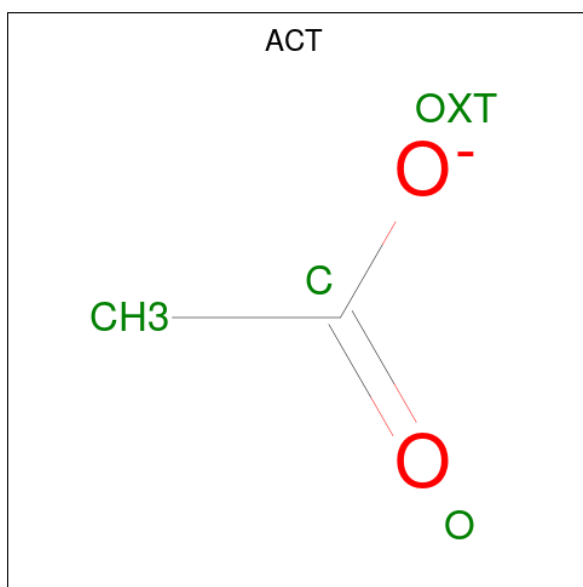
- Molecule 1 is a protein called Nickel-binding periplasmic protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 498      | Total | C    | N   | O   | S  | 0       | 15      | 0     |
|     |       |          | 4019  | 2582 | 672 | 755 | 10 |         |         |       |
| 1   | B     | 497      | Total | C    | N   | O   | S  | 6       | 18      | 0     |
|     |       |          | 4055  | 2609 | 680 | 755 | 11 |         |         |       |
| 1   | C     | 496      | Total | C    | N   | O   | S  | 0       | 11      | 0     |
|     |       |          | 4006  | 2570 | 673 | 751 | 12 |         |         |       |

- Molecule 2 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

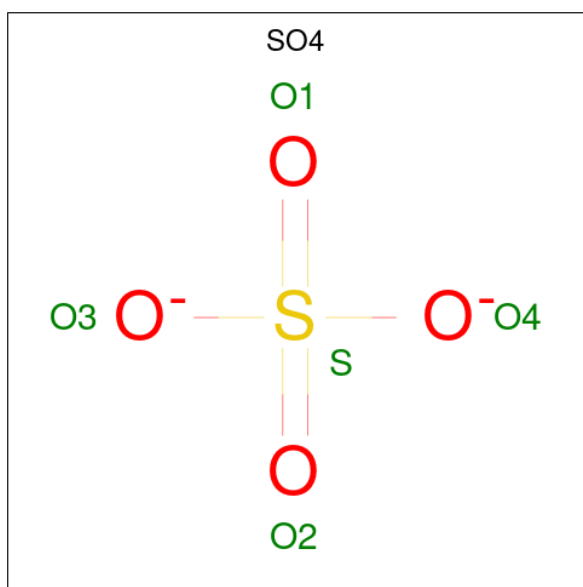
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | A     | 1        | Total | Ni | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | B     | 1        | Total | Ni | 0       | 0       |
|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

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).

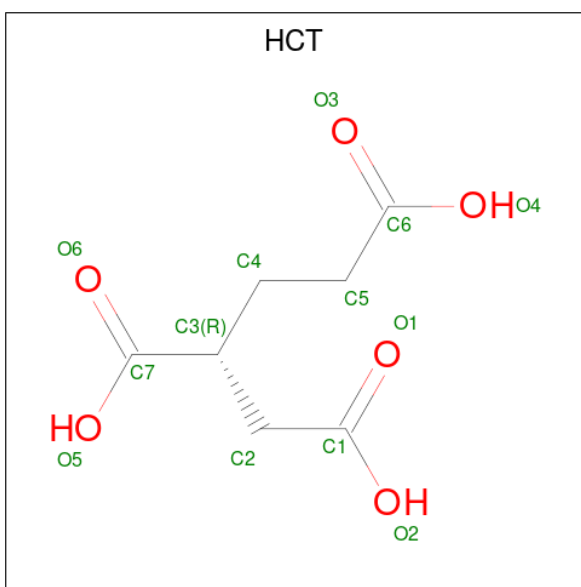


| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

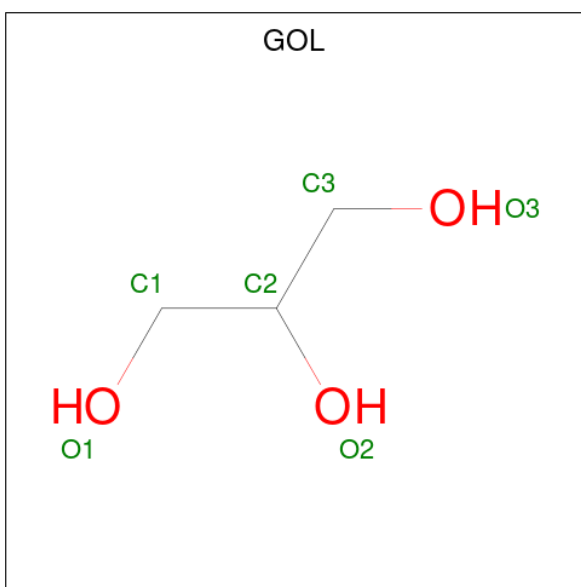
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5   | A     | 2        | Total | Cl | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 5   | B     | 3        | Total | Cl | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 5   | C     | 2        | Total | Cl | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

- Molecule 6 is (2R)-butane-1,2,4-tricarboxylic acid (CCD ID: HCT) (formula: C<sub>7</sub>H<sub>10</sub>O<sub>6</sub>).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 6   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 7 | 6 |         |         |
| 6   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 7 | 6 |         |         |
| 6   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 7 | 6 |         |         |

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 7   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |

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| Mol | Chain | Residues | Atoms      |        |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|---------|---------|
| 7   | A     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 7   | A     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 7   | A     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 7   | B     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 7   | B     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 7   | B     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 7   | B     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |

- Molecule 8 is water.

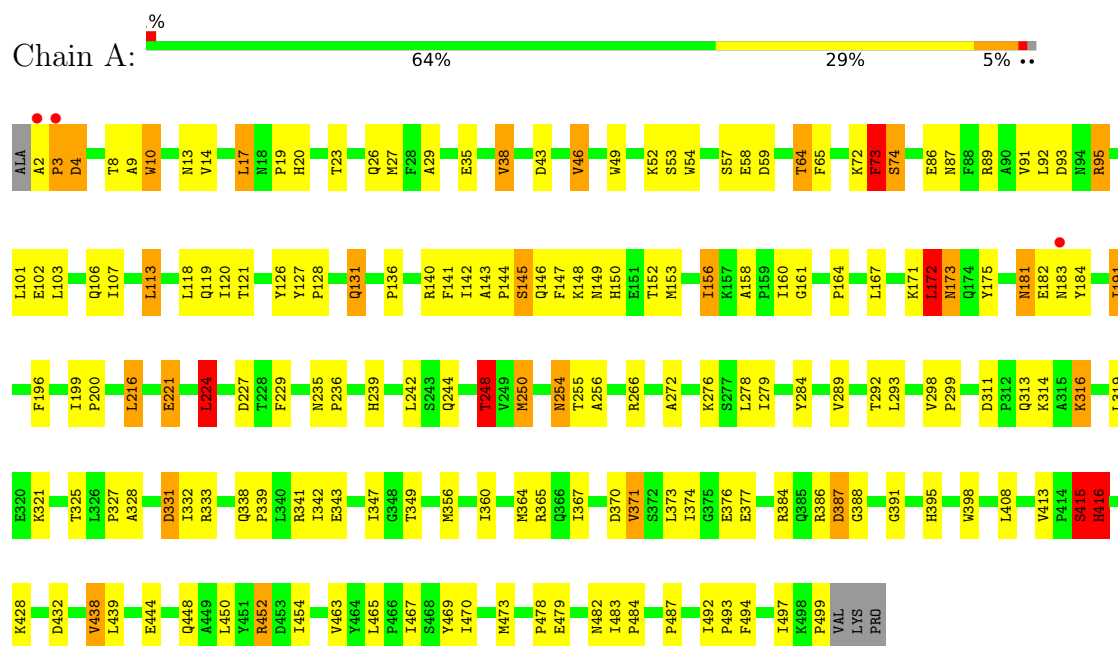
| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 8   | A     | 100      | Total<br>100 | O<br>100 | 0       | 0       |
| 8   | B     | 110      | Total<br>110 | O<br>110 | 0       | 0       |
| 8   | C     | 55       | Total<br>55  | O<br>55  | 0       | 0       |



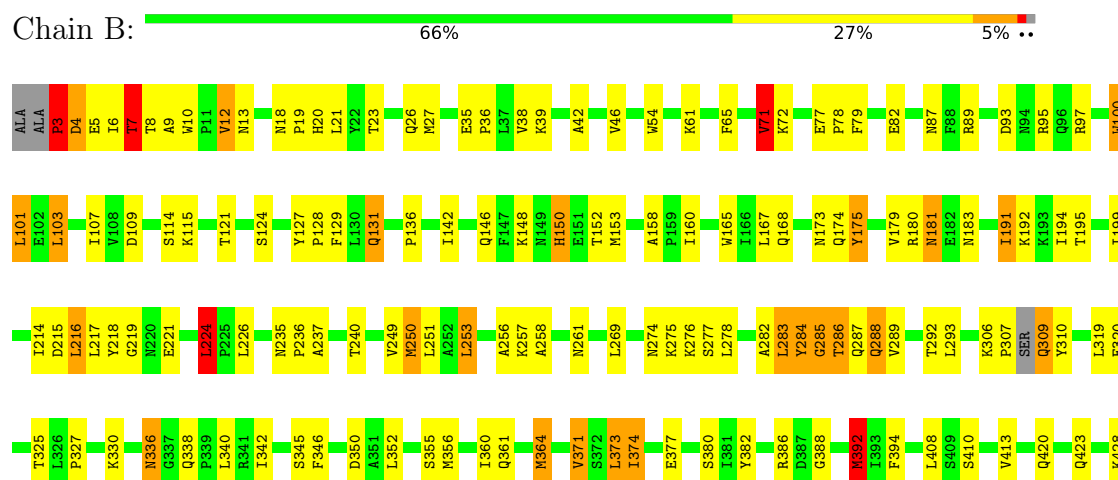
### 3 Residue-property plots

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: Nickel-binding periplasmic protein

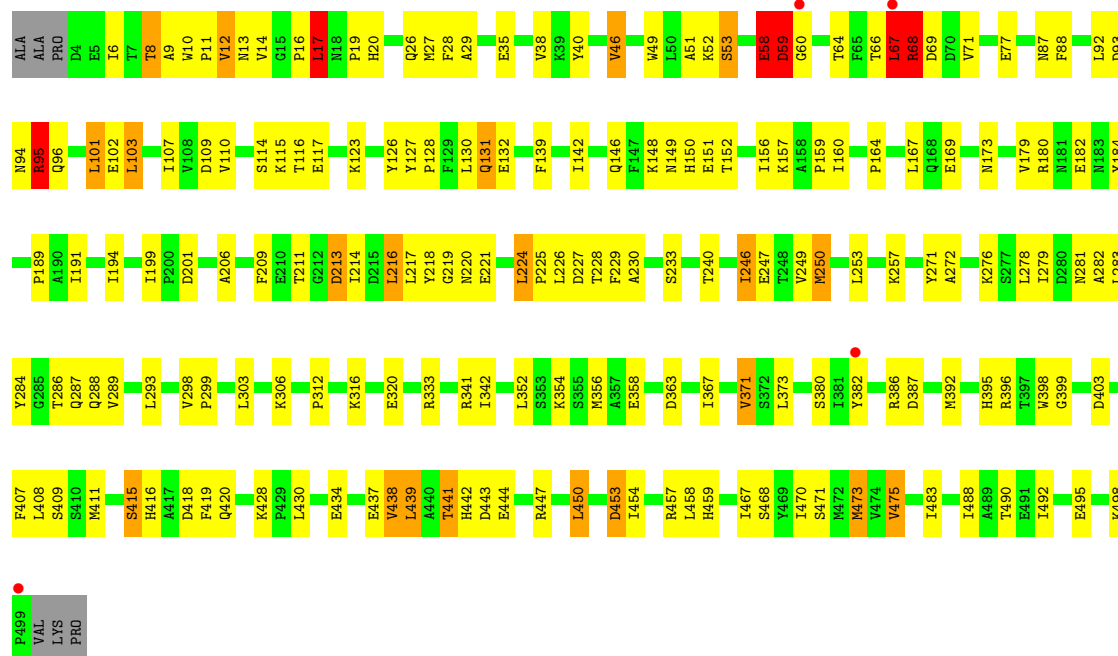


#### • Molecule 1: Nickel-binding periplasmic protein





• Molecule 1: Nickel-binding periplasmic protein



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 62                                                        | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 158.57Å 158.57Å 134.94Å<br>90.00° 90.00° 120.00°            | Depositor        |
| Resolution (Å)                                                          | 20.00 – 2.50<br>20.00 – 2.50                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.5 (20.00-2.50)<br>99.5 (20.00-2.50)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.05                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 6.20 (at 2.50Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.2.0019                                             | Depositor        |
| R, $R_{free}$                                                           | 0.199 , 0.270<br>0.194 , 0.260                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1707 reflections (2.56%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 54.2                                                        | Xtriage          |
| Anisotropy                                                              | 0.117                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 35.7                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | 0.025 for h,-h-k,-l                                         | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                        | EDS              |
| Total number of atoms                                                   | 12491                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 51.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, SO4, GOL, HCT, NI, CL

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

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5         |
| 1   | A     | 1.09         | 2/4167 (0.0%)  | 1.20        | 22/5676 (0.4%)  |
| 1   | B     | 1.09         | 3/4212 (0.1%)  | 1.21        | 20/5729 (0.3%)  |
| 1   | C     | 1.01         | 3/4139 (0.1%)  | 1.13        | 17/5634 (0.3%)  |
| All | All   | 1.07         | 8/12518 (0.1%) | 1.18        | 59/17039 (0.3%) |

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                   | 3                   |
| 1   | B     | 0                   | 3                   |
| 1   | C     | 0                   | 4                   |
| All | All   | 0                   | 10                  |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | B     | 249 | VAL  | CA-CB | 7.97  | 1.64        | 1.54     |
| 1   | B     | 257 | LYS  | C-O   | -6.09 | 1.17        | 1.24     |
| 1   | A     | 465 | LEU  | CA-C  | 5.36  | 1.58        | 1.52     |
| 1   | A     | 492 | ILE  | CA-C  | 5.16  | 1.56        | 1.52     |
| 1   | C     | 471 | SER  | CA-C  | -5.12 | 1.46        | 1.52     |
| 1   | C     | 250 | MET  | CA-C  | -5.11 | 1.46        | 1.52     |
| 1   | C     | 257 | LYS  | N-CA  | 5.06  | 1.52        | 1.46     |
| 1   | B     | 4   | ASP  | N-CA  | 5.06  | 1.52        | 1.46     |

All (59) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 1   | A     | 73  | PHE  | N-CA-C   | -13.84 | 90.73       | 110.24   |
| 1   | B     | 4   | ASP  | N-CA-C   | 9.39   | 130.80      | 110.80   |
| 1   | A     | 2   | ALA  | CA-C-N   | -9.20  | 110.06      | 119.99   |
| 1   | A     | 2   | ALA  | C-N-CA   | -9.20  | 110.06      | 119.99   |
| 1   | A     | 199 | ILE  | CA-C-N   | 7.91   | 127.98      | 119.28   |
| 1   | A     | 199 | ILE  | C-N-CA   | 7.91   | 127.98      | 119.28   |
| 1   | C     | 58  | GLU  | N-CA-C   | 7.41   | 120.29      | 111.33   |
| 1   | A     | 141 | PHE  | N-CA-C   | 7.32   | 120.72      | 108.20   |
| 1   | B     | 3   | PRO  | CA-C-N   | 7.30   | 135.49      | 121.54   |
| 1   | B     | 3   | PRO  | C-N-CA   | 7.30   | 135.49      | 121.54   |
| 1   | A     | 415 | SER  | N-CA-C   | 7.29   | 120.99      | 108.02   |
| 1   | B     | 284 | TYR  | N-CA-C   | 6.80   | 124.05      | 113.72   |
| 1   | A     | 224 | LEU  | CA-C-N   | -6.78  | 113.00      | 119.85   |
| 1   | A     | 224 | LEU  | C-N-CA   | -6.78  | 113.00      | 119.85   |
| 1   | C     | 468 | SER  | N-CA-C   | 6.77   | 118.08      | 108.74   |
| 1   | A     | 452 | ARG  | CG-CD-NE | -6.58  | 97.52       | 112.00   |
| 1   | C     | 201 | ASP  | CA-C-N   | 6.57   | 126.51      | 119.28   |
| 1   | C     | 201 | ASP  | C-N-CA   | 6.57   | 126.51      | 119.28   |
| 1   | B     | 100 | TRP  | N-CA-C   | -6.55  | 104.22      | 111.82   |
| 1   | C     | 109 | ASP  | N-CA-C   | 6.53   | 118.07      | 108.14   |
| 1   | C     | 483 | ILE  | N-CA-C   | 6.43   | 115.25      | 108.95   |
| 1   | B     | 199 | ILE  | CA-C-N   | 6.31   | 126.05      | 119.05   |
| 1   | B     | 199 | ILE  | C-N-CA   | 6.31   | 126.05      | 119.05   |
| 1   | A     | 73  | PHE  | CA-C-N   | 6.24   | 133.46      | 121.54   |
| 1   | A     | 73  | PHE  | C-N-CA   | 6.24   | 133.46      | 121.54   |
| 1   | A     | 416 | HIS  | N-CA-CB  | 6.21   | 120.99      | 110.49   |
| 1   | B     | 441 | THR  | N-CA-C   | 6.21   | 119.47      | 110.28   |
| 1   | B     | 175 | TYR  | N-CA-C   | 6.09   | 117.80      | 108.42   |
| 1   | B     | 77  | GLU  | CA-C-N   | -5.96  | 112.39      | 119.84   |
| 1   | B     | 77  | GLU  | C-N-CA   | -5.96  | 112.39      | 119.84   |
| 1   | C     | 58  | GLU  | CA-C-N   | 5.92   | 132.36      | 121.70   |
| 1   | C     | 58  | GLU  | C-N-CA   | 5.92   | 132.36      | 121.70   |
| 1   | A     | 388 | GLY  | N-CA-C   | -5.88  | 106.32      | 115.67   |
| 1   | B     | 336 | ASN  | CB-CA-C  | -5.76  | 103.71      | 111.89   |
| 1   | A     | 3   | PRO  | N-CA-C   | -5.72  | 101.53      | 111.32   |
| 1   | A     | 10  | TRP  | CA-C-N   | -5.69  | 113.89      | 120.04   |
| 1   | A     | 10  | TRP  | C-N-CA   | -5.69  | 113.89      | 120.04   |
| 1   | B     | 224 | LEU  | CA-CB-CG | 5.67   | 136.15      | 116.30   |
| 1   | C     | 67  | LEU  | CA-C-N   | 5.63   | 132.30      | 121.54   |
| 1   | C     | 67  | LEU  | C-N-CA   | 5.63   | 132.30      | 121.54   |
| 1   | C     | 53  | SER  | N-CA-C   | 5.53   | 115.68      | 107.88   |
| 1   | B     | 7   | THR  | CB-CA-C  | 5.47   | 120.10      | 109.33   |
| 1   | B     | 392 | MET  | N-CA-C   | -5.41  | 100.20      | 109.24   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | C     | 68  | ARG  | CB-CA-C | 5.39  | 121.14      | 110.42   |
| 1   | B     | 285 | GLY  | CA-C-N  | 5.37  | 131.36      | 121.70   |
| 1   | B     | 285 | GLY  | C-N-CA  | 5.37  | 131.36      | 121.70   |
| 1   | C     | 271 | TYR  | N-CA-C  | -5.34 | 106.70      | 114.12   |
| 1   | A     | 248 | THR  | CB-CA-C | 5.30  | 119.06      | 109.37   |
| 1   | A     | 106 | GLN  | N-CA-C  | 5.25  | 119.81      | 113.41   |
| 1   | B     | 71  | VAL  | N-CA-CB | 5.25  | 117.29      | 110.99   |
| 1   | A     | 413 | VAL  | CA-C-N  | 5.23  | 126.38      | 119.84   |
| 1   | A     | 413 | VAL  | C-N-CA  | 5.23  | 126.38      | 119.84   |
| 1   | C     | 407 | PHE  | N-CA-C  | -5.19 | 105.54      | 111.14   |
| 1   | B     | 191 | ILE  | CB-CA-C | -5.17 | 104.00      | 111.34   |
| 1   | C     | 35  | GLU  | CA-C-N  | 5.06  | 126.17      | 119.84   |
| 1   | C     | 35  | GLU  | C-N-CA  | 5.06  | 126.17      | 119.84   |
| 1   | C     | 453 | ASP  | N-CA-C  | 5.06  | 116.48      | 111.07   |
| 1   | A     | 463 | VAL  | CB-CA-C | -5.04 | 104.34      | 112.16   |
| 1   | B     | 423 | GLN  | N-CA-C  | 5.03  | 118.52      | 112.38   |

There are no chirality outliers.

All (10) planarity outliers are listed below:

| Mol | Chain | Res    | Type | Group     |
|-----|-------|--------|------|-----------|
| 1   | A     | 172    | LEU  | Peptide   |
| 1   | A     | 415    | SER  | Peptide   |
| 1   | A     | 73     | PHE  | Peptide   |
| 1   | B     | 215    | ASP  | Peptide   |
| 1   | B     | 3      | PRO  | Peptide   |
| 1   | B     | 309[B] | GLN  | Mainchain |
| 1   | C     | 58     | GLU  | Peptide   |
| 1   | C     | 59     | ASP  | Peptide   |
| 1   | C     | 67     | LEU  | Peptide   |
| 1   | C     | 68     | ARG  | Peptide   |

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 4019  | 0        | 4002     | 148     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | B     | 4055  | 0        | 4060     | 160     | 0            |
| 1   | C     | 4006  | 0        | 3975     | 157     | 0            |
| 2   | A     | 1     | 0        | 0        | 0       | 0            |
| 2   | B     | 1     | 0        | 0        | 0       | 0            |
| 2   | C     | 1     | 0        | 0        | 0       | 0            |
| 3   | A     | 16    | 0        | 12       | 3       | 0            |
| 3   | B     | 16    | 0        | 12       | 16      | 0            |
| 3   | C     | 12    | 0        | 9        | 3       | 0            |
| 4   | A     | 5     | 0        | 0        | 0       | 0            |
| 5   | A     | 2     | 0        | 0        | 0       | 0            |
| 5   | B     | 3     | 0        | 0        | 1       | 0            |
| 5   | C     | 2     | 0        | 0        | 0       | 0            |
| 6   | A     | 13    | 0        | 6        | 1       | 0            |
| 6   | B     | 13    | 0        | 7        | 0       | 0            |
| 6   | C     | 13    | 0        | 6        | 0       | 0            |
| 7   | A     | 24    | 0        | 32       | 12      | 0            |
| 7   | B     | 24    | 0        | 32       | 9       | 0            |
| 8   | A     | 100   | 0        | 0        | 14      | 0            |
| 8   | B     | 110   | 0        | 0        | 10      | 0            |
| 8   | C     | 55    | 0        | 0        | 5       | 0            |
| All | All   | 12491 | 0        | 12153    | 462     | 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 19.

All (462) 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:A:95:ARG:HG3   | 1:A:95:ARG:HH11    | 1.09                     | 1.11              |
| 1:C:226:LEU:CD2  | 1:C:473[B]:MET:HE1 | 1.80                     | 1.10              |
| 1:C:67:LEU:HB3   | 1:C:68:ARG:HB2     | 1.35                     | 1.08              |
| 1:A:4:ASP:HA     | 8:A:607:HOH:O      | 1.53                     | 1.07              |
| 1:A:92:LEU:HD22  | 1:A:95:ARG:HH12    | 1.23                     | 1.03              |
| 1:C:226:LEU:HD21 | 1:C:473[B]:MET:HE1 | 1.36                     | 1.02              |
| 1:A:38:VAL:HG13  | 1:A:46:VAL:HG21    | 1.40                     | 1.00              |
| 1:A:316:LYS:HE2  | 1:A:333:ARG:HH11   | 1.27                     | 0.98              |
| 1:B:9:ALA:H      | 3:B:507:ACT:H3     | 1.26                     | 0.98              |
| 1:A:95:ARG:HH11  | 1:A:95:ARG:CG      | 1.76                     | 0.97              |
| 1:A:356:MET:HE1  | 1:A:467:ILE:HG21   | 1.44                     | 0.97              |
| 1:A:13:ASN:HD21  | 1:A:173:ASN:HA     | 1.27                     | 0.95              |
| 1:B:217:LEU:HD23 | 3:B:507:ACT:H1     | 1.47                     | 0.95              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:A:35[B]:GLU:HG2   | 1:A:49:TRP:HE1     | 1.33                     | 0.91              |
| 1:C:283:LEU:HD13    | 1:C:287[B]:GLN:OE1 | 1.69                     | 0.91              |
| 1:A:95:ARG:HG3      | 1:A:95:ARG:NH1     | 1.81                     | 0.90              |
| 1:B:8:THR:OG1       | 3:B:507:ACT:CH3    | 2.20                     | 0.89              |
| 1:A:14[B]:VAL:CG2   | 1:A:29:ALA:CB      | 2.50                     | 0.88              |
| 1:C:58:GLU:OE1      | 1:C:58:GLU:HA      | 1.73                     | 0.87              |
| 1:B:388:GLY:HA3     | 7:B:513:GOL:H11    | 1.54                     | 0.87              |
| 7:A:514:GOL:H31     | 1:B:42:ALA:H       | 1.40                     | 0.86              |
| 1:B:274:ASN:OD1     | 1:B:277:SER:HB3    | 1.75                     | 0.86              |
| 1:A:239:HIS:HB2     | 1:B:448:GLN:HE22   | 1.41                     | 0.86              |
| 1:C:226:LEU:HD21    | 1:C:473[B]:MET:CE  | 2.07                     | 0.84              |
| 1:A:248:THR:HG21    | 1:A:293:LEU:O      | 1.78                     | 0.84              |
| 1:B:217:LEU:HD23    | 3:B:507:ACT:CH3    | 2.08                     | 0.83              |
| 1:B:285:GLY:HA2     | 1:B:286:THR:OG1    | 1.77                     | 0.83              |
| 1:B:224:LEU:HG      | 1:B:473[A]:MET:HE1 | 1.62                     | 0.82              |
| 1:B:364:MET:SD      | 8:B:620:HOH:O      | 2.38                     | 0.81              |
| 1:A:152[B]:THR:HG23 | 1:A:156:ILE:HG23   | 1.63                     | 0.81              |
| 1:A:313:GLN:HG2     | 8:A:604:HOH:O      | 1.81                     | 0.81              |
| 1:A:38:VAL:HG13     | 1:A:46:VAL:CG2     | 2.11                     | 0.81              |
| 1:B:269[B]:LEU:HD13 | 1:B:364:MET:SD     | 2.22                     | 0.80              |
| 1:C:13:ASN:ND2      | 1:C:173:ASN:H      | 1.79                     | 0.80              |
| 1:B:219:GLY:C       | 1:B:472:MET:HE3    | 2.06                     | 0.80              |
| 1:C:226:LEU:HD23    | 1:C:473[B]:MET:HE1 | 1.64                     | 0.80              |
| 1:B:8:THR:OG1       | 3:B:507:ACT:H2     | 1.82                     | 0.79              |
| 1:A:92:LEU:HD22     | 1:A:95:ARG:NH1     | 1.97                     | 0.79              |
| 1:C:38:VAL:HG22     | 1:C:46:VAL:HG13    | 1.65                     | 0.78              |
| 1:C:224:LEU:HD21    | 1:C:473[A]:MET:HE1 | 1.65                     | 0.78              |
| 1:B:9:ALA:H         | 3:B:507:ACT:CH3    | 1.97                     | 0.78              |
| 7:A:514:GOL:H12     | 1:B:42:ALA:HB2     | 1.66                     | 0.78              |
| 1:C:13:ASN:HD21     | 1:C:173:ASN:H      | 1.29                     | 0.78              |
| 1:C:442:HIS:HD2     | 8:C:563:HOH:O      | 1.66                     | 0.78              |
| 1:B:146:GLN:HE21    | 1:B:158:ALA:H      | 1.31                     | 0.77              |
| 1:A:360:ILE:CG2     | 1:A:364:MET:HE2    | 2.15                     | 0.77              |
| 1:B:256:ALA:HB3     | 7:B:513:GOL:H32    | 1.65                     | 0.76              |
| 1:B:269[B]:LEU:HD21 | 1:B:392:MET:SD     | 2.26                     | 0.76              |
| 1:C:438:VAL:HA      | 1:C:450:LEU:HD23   | 1.66                     | 0.76              |
| 1:A:8:THR:HG22      | 1:A:9:ALA:H        | 1.50                     | 0.75              |
| 1:B:97[B]:ARG:HH11  | 1:B:386:ARG:NH1    | 1.84                     | 0.75              |
| 1:A:14[B]:VAL:CG2   | 1:A:29:ALA:HB2     | 2.16                     | 0.75              |
| 1:B:95:ARG:NH2      | 1:B:107:ILE:O      | 2.19                     | 0.75              |
| 1:A:14[B]:VAL:HG21  | 1:A:29:ALA:CB      | 2.16                     | 0.74              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 7:A:514:GOL:C3      | 1:B:42:ALA:H        | 2.00                     | 0.74              |
| 1:C:356:MET:HE2     | 1:C:467:ILE:HG21    | 1.70                     | 0.73              |
| 1:B:221:GLU:HG2     | 1:B:473[B]:MET:HE3  | 1.71                     | 0.72              |
| 1:A:356:MET:CE      | 1:A:467:ILE:HG21    | 2.17                     | 0.72              |
| 1:A:27:MET:HG3      | 8:A:535:HOH:O       | 1.89                     | 0.72              |
| 1:B:10:TRP:HE1      | 1:B:26:GLN:HE21     | 1.36                     | 0.71              |
| 1:A:313:GLN:CG      | 8:A:604:HOH:O       | 2.37                     | 0.71              |
| 1:C:58:GLU:N        | 1:C:59:ASP:HB2      | 2.05                     | 0.71              |
| 1:B:217:LEU:CD2     | 3:B:507:ACT:H1      | 2.19                     | 0.71              |
| 1:A:152[B]:THR:HG23 | 1:A:156:ILE:CG2     | 2.21                     | 0.70              |
| 1:C:10:TRP:HE1      | 1:C:26:GLN:HE21     | 1.38                     | 0.70              |
| 1:C:286:THR:O       | 1:C:287[A]:GLN:NE2  | 2.23                     | 0.70              |
| 1:B:438:VAL:HG13    | 1:B:450:LEU:HB3     | 1.71                     | 0.70              |
| 1:C:13:ASN:HD21     | 1:C:173:ASN:N       | 1.89                     | 0.70              |
| 1:B:93:ASP:HB3      | 1:B:153:MET:HE1     | 1.74                     | 0.69              |
| 1:C:316:LYS:HG3     | 1:C:367[A]:ILE:HD13 | 1.73                     | 0.69              |
| 1:A:314[B]:LYS:HE3  | 8:A:594:HOH:O       | 1.93                     | 0.69              |
| 1:C:226:LEU:HD12    | 1:C:283:LEU:HD23    | 1.74                     | 0.69              |
| 1:B:8:THR:OG1       | 3:B:507:ACT:H3      | 1.93                     | 0.69              |
| 1:C:38:VAL:CG2      | 1:C:46:VAL:HG13     | 2.23                     | 0.68              |
| 1:C:67:LEU:HB3      | 1:C:68:ARG:CB       | 2.17                     | 0.68              |
| 1:A:360:ILE:HG23    | 1:A:364:MET:HE2     | 1.74                     | 0.68              |
| 1:B:20:HIS:HD2      | 1:B:152:THR:OG1     | 1.76                     | 0.68              |
| 1:A:272:ALA:HB2     | 1:A:367:ILE:HD13    | 1.76                     | 0.68              |
| 1:A:254:ASN:HD22    | 1:A:256:ALA:H       | 1.39                     | 0.68              |
| 1:A:316:LYS:CE      | 1:A:333:ARG:HH11    | 2.03                     | 0.68              |
| 1:A:35[B]:GLU:HG2   | 1:A:49:TRP:NE1      | 2.06                     | 0.66              |
| 1:B:216:LEU:O       | 3:B:507:ACT:H2      | 1.96                     | 0.66              |
| 1:B:253:LEU:HD12    | 1:B:392:MET:HG3     | 1.77                     | 0.66              |
| 1:A:14[A]:VAL:HG13  | 1:A:29:ALA:CB       | 2.26                     | 0.66              |
| 1:B:23:THR:HG21     | 1:B:382:TYR:CD2     | 2.31                     | 0.66              |
| 1:C:68:ARG:HB3      | 1:C:69:ASP:HA       | 1.77                     | 0.66              |
| 1:B:288[A]:GLN:H    | 1:B:288[A]:GLN:HE21 | 1.44                     | 0.65              |
| 1:B:438:VAL:CG1     | 1:B:450:LEU:HB3     | 2.26                     | 0.65              |
| 1:A:13:ASN:ND2      | 1:A:173:ASN:HA      | 2.07                     | 0.65              |
| 1:C:52:LYS:HG3      | 1:C:68:ARG:H        | 1.61                     | 0.65              |
| 1:A:64:THR:HG23     | 1:A:119:GLN:HG3     | 1.79                     | 0.65              |
| 1:B:142:ILE:HG13    | 1:B:160:ILE:O       | 1.97                     | 0.65              |
| 1:B:251:LEU:HD13    | 1:B:392:MET:HG2     | 1.78                     | 0.65              |
| 1:B:7:THR:HB        | 1:B:195:THR:HB      | 1.78                     | 0.64              |
| 1:B:278:LEU:O       | 1:B:282:ALA:HB3     | 1.98                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:C:226:LEU:CD2    | 1:C:473[B]:MET:CE  | 2.64                     | 0.64              |
| 1:B:342:ILE:O      | 1:B:371:VAL:HA     | 1.98                     | 0.64              |
| 1:B:269[B]:LEU:CD1 | 1:B:364:MET:SD     | 2.87                     | 0.63              |
| 1:B:226:LEU:CD1    | 1:B:283:LEU:HA     | 2.29                     | 0.63              |
| 1:B:250:MET:HB2    | 1:B:466:PRO:HA     | 1.80                     | 0.63              |
| 1:A:470:ILE:HD12   | 1:A:470:ILE:C      | 2.24                     | 0.63              |
| 1:A:131[A]:GLN:H   | 1:A:131[A]:GLN:NE2 | 1.97                     | 0.63              |
| 1:A:14[A]:VAL:HG12 | 1:A:17:LEU:HD13    | 1.80                     | 0.62              |
| 1:B:446[A]:GLN:HG3 | 1:B:450:LEU:HD22   | 1.80                     | 0.62              |
| 1:B:103:LEU:HD21   | 1:B:129:PHE:CD2    | 2.35                     | 0.62              |
| 1:B:217:LEU:HD13   | 1:B:224:LEU:HD22   | 1.82                     | 0.62              |
| 1:A:14[B]:VAL:HG23 | 1:A:29:ALA:HB2     | 1.81                     | 0.62              |
| 1:B:180:ARG:NH2    | 1:B:192[B]:LYS:HE2 | 2.15                     | 0.62              |
| 1:A:92:LEU:CD2     | 1:A:95:ARG:HH12    | 2.07                     | 0.62              |
| 1:B:283:LEU:HD21   | 1:B:352:LEU:HD11   | 1.81                     | 0.62              |
| 7:A:514:GOL:H12    | 1:B:42:ALA:CB      | 2.30                     | 0.62              |
| 1:C:382:TYR:HE2    | 1:C:416:HIS:CE1    | 2.16                     | 0.62              |
| 1:B:180:ARG:HH22   | 1:B:192[B]:LYS:HE2 | 1.63                     | 0.61              |
| 1:B:473[A]:MET:HE3 | 8:B:569:HOH:O      | 2.00                     | 0.61              |
| 1:C:180:ARG:HD2    | 1:C:189:PRO:HD2    | 1.82                     | 0.61              |
| 1:C:293:LEU:HB3    | 3:C:504:ACT:H3     | 1.82                     | 0.61              |
| 1:B:9:ALA:N        | 3:B:507:ACT:H3     | 2.07                     | 0.61              |
| 1:B:8:THR:HG1      | 3:B:507:ACT:H2     | 1.65                     | 0.61              |
| 1:C:103:LEU:HD13   | 1:C:139:PHE:CE1    | 2.34                     | 0.61              |
| 1:B:235:ASN:C      | 1:B:235:ASN:HD22   | 2.08                     | 0.61              |
| 1:B:127:TYR:CG     | 1:B:128:PRO:HD3    | 2.36                     | 0.61              |
| 1:C:217:LEU:HD13   | 1:C:224:LEU:HD22   | 1.82                     | 0.61              |
| 1:C:287[A]:GLN:HG3 | 1:C:470:ILE:HA     | 1.83                     | 0.61              |
| 1:C:430:LEU:C      | 1:C:430:LEU:HD23   | 2.26                     | 0.60              |
| 1:B:18:ASN:ND2     | 1:B:21:LEU:HD23    | 2.16                     | 0.60              |
| 1:C:288[B]:GLN:CD  | 1:C:289:VAL:H      | 2.09                     | 0.60              |
| 1:C:442:HIS:CD2    | 8:C:563:HOH:O      | 2.47                     | 0.60              |
| 1:C:10:TRP:HE1     | 1:C:26:GLN:NE2     | 1.99                     | 0.60              |
| 1:C:114:SER:HB3    | 1:C:117:GLU:HB2    | 1.83                     | 0.60              |
| 1:A:14[B]:VAL:HG21 | 1:A:29:ALA:HB1     | 1.82                     | 0.60              |
| 1:B:39:LYS:HE2     | 8:B:586:HOH:O      | 2.01                     | 0.60              |
| 1:B:364:MET:HG3    | 1:B:371:VAL:HG11   | 1.82                     | 0.60              |
| 1:C:283:LEU:CD2    | 1:C:352:LEU:CD1    | 2.79                     | 0.60              |
| 1:B:103:LEU:HD21   | 1:B:129:PHE:HD2    | 1.67                     | 0.60              |
| 1:A:316:LYS:HE3    | 1:A:367:ILE:HA     | 1.84                     | 0.60              |
| 1:A:4:ASP:OD2      | 1:A:4:ASP:N        | 2.35                     | 0.60              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:A:311:ASP:CG   | 1:A:314[B]:LYS:HG3 | 2.27                     | 0.60              |
| 1:A:364:MET:HG3  | 1:A:371:VAL:HG11   | 1.84                     | 0.60              |
| 1:A:20:HIS:HE1   | 1:A:140:ARG:O      | 1.85                     | 0.59              |
| 1:C:356:MET:HE2  | 1:C:467:ILE:CG2    | 2.32                     | 0.59              |
| 1:A:356:MET:HE1  | 1:A:467:ILE:CG2    | 2.28                     | 0.59              |
| 1:A:331:ASP:HB3  | 1:A:365:ARG:HH11   | 1.67                     | 0.59              |
| 1:B:278:LEU:HD21 | 1:B:356:MET:HG2    | 1.83                     | 0.59              |
| 1:A:254:ASN:ND2  | 1:A:256:ALA:H      | 2.00                     | 0.59              |
| 1:A:102:GLU:HB3  | 1:A:126:TYR:OH     | 2.03                     | 0.58              |
| 1:A:248:THR:HB   | 1:A:469:TYR:CD1    | 2.37                     | 0.58              |
| 1:A:3:PRO:HA     | 8:A:607:HOH:O      | 2.02                     | 0.58              |
| 1:C:420:GLN:HA   | 1:C:420:GLN:HE21   | 1.68                     | 0.58              |
| 1:B:146:GLN:NE2  | 1:B:158:ALA:H      | 2.00                     | 0.58              |
| 1:B:219:GLY:CA   | 1:B:472:MET:HE3    | 2.34                     | 0.58              |
| 1:B:283:LEU:HD12 | 1:B:287:GLN:HG3    | 1.84                     | 0.58              |
| 1:A:131[A]:GLN:H | 1:A:131[A]:GLN:CD  | 2.12                     | 0.58              |
| 1:B:288[A]:GLN:H | 1:B:288[A]:GLN:NE2 | 2.02                     | 0.57              |
| 1:A:13:ASN:HD21  | 1:A:172:LEU:HA     | 1.68                     | 0.57              |
| 1:B:388:GLY:HA3  | 7:B:513:GOL:C1     | 2.32                     | 0.57              |
| 1:B:278:LEU:HD23 | 1:B:278:LEU:C      | 2.29                     | 0.57              |
| 1:A:278:LEU:CD2  | 1:A:356:MET:HE3    | 2.34                     | 0.57              |
| 1:B:23:THR:HG21  | 1:B:382:TYR:HD2    | 1.67                     | 0.57              |
| 1:B:420:GLN:NE2  | 7:B:513:GOL:O3     | 2.37                     | 0.57              |
| 1:B:428:LYS:NZ   | 1:B:432:ASP:OD1    | 2.34                     | 0.57              |
| 1:C:88:PHE:HB3   | 1:C:110:VAL:HG21   | 1.86                     | 0.57              |
| 1:C:219:GLY:O    | 1:C:473[A]:MET:HG3 | 2.04                     | 0.57              |
| 1:B:61:LYS:HD3   | 1:B:124:SER:HA     | 1.86                     | 0.57              |
| 1:B:109:ASP:HB3  | 1:B:121:THR:OG1    | 2.05                     | 0.57              |
| 1:A:72:LYS:C     | 1:A:73:PHE:O       | 2.41                     | 0.57              |
| 1:B:10:TRP:HE1   | 1:B:26:GLN:NE2     | 2.02                     | 0.57              |
| 1:C:126:TYR:CZ   | 1:C:128:PRO:HG2    | 2.40                     | 0.56              |
| 1:A:248:THR:HB   | 1:A:469:TYR:HD1    | 1.70                     | 0.56              |
| 1:C:68:ARG:HB3   | 1:C:69:ASP:CA      | 2.35                     | 0.56              |
| 1:C:283:LEU:HD21 | 1:C:352:LEU:CD1    | 2.35                     | 0.56              |
| 1:A:278:LEU:HD21 | 1:A:356:MET:HG2    | 1.86                     | 0.56              |
| 1:C:438:VAL:CA   | 1:C:450:LEU:HD23   | 2.34                     | 0.56              |
| 1:A:250:MET:HE2  | 1:A:395:HIS:CD2    | 2.40                     | 0.56              |
| 1:B:373:LEU:HD22 | 7:B:515:GOL:C3     | 2.34                     | 0.56              |
| 1:A:494:PHE:HA   | 1:A:497:ILE:HD12   | 1.88                     | 0.56              |
| 1:A:43:ASP:HB3   | 7:A:514:GOL:H2     | 1.87                     | 0.56              |
| 1:B:346:PHE:HB3  | 1:B:394:PHE:CD1    | 2.41                     | 0.56              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:C:246:ILE:HD13 | 1:C:246:ILE:H      | 1.71                     | 0.56              |
| 1:C:221:GLU:OE1  | 1:C:287[A]:GLN:NE2 | 2.39                     | 0.56              |
| 1:C:443:ASP:OD1  | 1:C:443:ASP:C      | 2.49                     | 0.56              |
| 1:A:136:PRO:O    | 1:A:140:ARG:HD2    | 2.05                     | 0.56              |
| 1:B:219:GLY:CA   | 1:B:472:MET:CE     | 2.84                     | 0.56              |
| 1:C:59:ASP:HB3   | 1:C:60:GLY:HA2     | 1.88                     | 0.56              |
| 1:A:87:ASN:HD21  | 1:A:142:ILE:H      | 1.54                     | 0.55              |
| 1:A:428:LYS:HE3  | 1:A:432:ASP:OD2    | 2.06                     | 0.55              |
| 1:C:95:ARG:NH2   | 1:C:107:ILE:O      | 2.39                     | 0.55              |
| 1:B:327:PRO:HG2  | 1:B:330:LYS:HB2    | 1.87                     | 0.55              |
| 1:C:286:THR:O    | 1:C:287[A]:GLN:CD  | 2.49                     | 0.55              |
| 1:A:332:ILE:HD13 | 1:A:370:ASP:HB2    | 1.88                     | 0.55              |
| 1:B:3:PRO:N      | 1:B:5:GLU:H        | 2.04                     | 0.55              |
| 1:A:153:MET:HG2  | 8:A:578:HOH:O      | 2.07                     | 0.55              |
| 1:B:235:ASN:ND2  | 1:B:237:ALA:H      | 2.05                     | 0.55              |
| 1:C:49:TRP:C     | 1:C:51:ALA:N       | 2.64                     | 0.55              |
| 1:C:101:LEU:HD21 | 1:C:132:GLU:CD     | 2.32                     | 0.55              |
| 1:C:149:ASN:O    | 1:C:150:HIS:HB2    | 2.06                     | 0.55              |
| 1:A:10:TRP:HE1   | 1:A:26:GLN:NE2     | 2.05                     | 0.55              |
| 1:A:148:LYS:O    | 1:A:149:ASN:HB2    | 2.07                     | 0.55              |
| 1:B:219:GLY:HA2  | 1:B:472:MET:CE     | 2.37                     | 0.55              |
| 1:B:87:ASN:HD21  | 1:B:142:ILE:HG22   | 1.72                     | 0.54              |
| 1:B:274:ASN:HB2  | 1:B:310:TYR:CE1    | 2.42                     | 0.54              |
| 1:A:276:LYS:HE2  | 7:A:512:GOL:O1     | 2.07                     | 0.54              |
| 7:A:514:GOL:H31  | 1:B:42:ALA:CB      | 2.37                     | 0.54              |
| 7:A:514:GOL:H32  | 1:B:487:PRO:HG3    | 1.88                     | 0.54              |
| 1:B:13:ASN:HD21  | 1:B:173:ASN:H      | 1.56                     | 0.54              |
| 1:A:73:PHE:CE2   | 1:A:143:ALA:N      | 2.75                     | 0.54              |
| 1:C:38:VAL:CG2   | 1:C:46:VAL:CG1     | 2.86                     | 0.54              |
| 1:B:338:GLN:HE21 | 1:C:430:LEU:HB2    | 1.73                     | 0.54              |
| 1:A:87:ASN:HD21  | 1:A:142:ILE:HG22   | 1.72                     | 0.54              |
| 1:A:87:ASN:O     | 1:A:91:VAL:HG23    | 2.08                     | 0.54              |
| 1:B:373:LEU:HD22 | 7:B:515:GOL:H32    | 1.89                     | 0.54              |
| 1:C:114:SER:HB3  | 1:C:117:GLU:CB     | 2.38                     | 0.53              |
| 1:A:38:VAL:CG1   | 1:A:46:VAL:HG21    | 2.27                     | 0.53              |
| 1:A:487:PRO:HD2  | 8:A:525:HOH:O      | 2.08                     | 0.53              |
| 1:B:360:ILE:O    | 1:B:364:MET:HG2    | 2.08                     | 0.53              |
| 1:A:19:PRO:HG3   | 1:A:142:ILE:HB     | 1.89                     | 0.53              |
| 1:C:38:VAL:HG22  | 1:C:46:VAL:CG1     | 2.38                     | 0.53              |
| 1:C:437:GLU:O    | 1:C:441:THR:HG22   | 2.08                     | 0.53              |
| 1:C:382:TYR:HE2  | 1:C:416:HIS:HE1    | 1.56                     | 0.53              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:A:8:THR:HG23     | 1:A:216:LEU:O       | 2.08                     | 0.53              |
| 1:B:18:ASN:CG      | 1:B:21:LEU:HD23     | 2.33                     | 0.53              |
| 1:C:415:SER:HA     | 8:C:547:HOH:O       | 2.09                     | 0.52              |
| 1:B:71:VAL:HG22    | 1:B:79:PHE:HB3      | 1.90                     | 0.52              |
| 1:B:148:LYS:O      | 5:B:510:CL:CL       | 2.64                     | 0.52              |
| 1:B:250:MET:CB     | 1:B:466:PRO:HA      | 2.40                     | 0.52              |
| 1:B:226:LEU:HD13   | 1:B:283:LEU:HA      | 1.91                     | 0.52              |
| 1:C:19:PRO:HG3     | 1:C:142:ILE:HB      | 1.91                     | 0.52              |
| 1:A:200:PRO:HG2    | 8:A:597:HOH:O       | 2.09                     | 0.52              |
| 1:A:360:ILE:O      | 1:A:364:MET:HG2     | 2.09                     | 0.52              |
| 1:A:43:ASP:HB3     | 7:A:514:GOL:C2      | 2.39                     | 0.52              |
| 1:B:18:ASN:ND2     | 1:B:21:LEU:CD2      | 2.73                     | 0.52              |
| 1:C:92:LEU:C       | 1:C:94:ASN:H        | 2.18                     | 0.52              |
| 1:C:246:ILE:HG12   | 1:C:247:GLU:HG2     | 1.90                     | 0.52              |
| 1:A:444:GLU:O      | 1:A:448:GLN:HG3     | 2.10                     | 0.52              |
| 1:C:87:ASN:HD21    | 1:C:142:ILE:HG22    | 1.74                     | 0.51              |
| 1:A:127:TYR:CD2    | 1:A:128:PRO:HD3     | 2.45                     | 0.51              |
| 1:A:248:THR:HG22   | 8:A:521:HOH:O       | 2.10                     | 0.51              |
| 1:B:446[A]:GLN:HG2 | 8:B:623:HOH:O       | 2.10                     | 0.51              |
| 1:B:13:ASN:HD21    | 1:B:173:ASN:N       | 2.07                     | 0.51              |
| 1:C:10:TRP:CG      | 1:C:11:PRO:HD2      | 2.45                     | 0.51              |
| 1:C:246:ILE:HD13   | 1:C:470:ILE:O       | 2.09                     | 0.51              |
| 1:C:230:ALA:O      | 1:C:233:SER:HB2     | 2.11                     | 0.51              |
| 1:C:312:PRO:O      | 1:C:367[A]:ILE:HD11 | 2.11                     | 0.51              |
| 1:C:281:ASN:O      | 1:C:283:LEU:N       | 2.44                     | 0.51              |
| 1:C:316:LYS:HE2    | 8:C:511:HOH:O       | 2.10                     | 0.51              |
| 1:B:115:LYS:HA     | 8:B:580:HOH:O       | 2.09                     | 0.51              |
| 1:C:226:LEU:CD1    | 1:C:283:LEU:HD23    | 2.41                     | 0.51              |
| 1:A:364:MET:HG3    | 1:A:371:VAL:CG1     | 2.41                     | 0.50              |
| 1:A:478:PRO:HD2    | 8:A:605:HOH:O       | 2.09                     | 0.50              |
| 1:A:72:LYS:HB3     | 1:A:73:PHE:O        | 2.12                     | 0.50              |
| 1:C:102:GLU:HB3    | 1:C:126:TYR:OH      | 2.11                     | 0.50              |
| 1:A:278:LEU:HD22   | 1:A:356:MET:HE3     | 1.94                     | 0.50              |
| 1:A:13:ASN:ND2     | 1:A:172:LEU:HA      | 2.26                     | 0.50              |
| 1:B:373:LEU:C      | 1:B:374:ILE:HG12    | 2.36                     | 0.50              |
| 1:C:221:GLU:HG2    | 1:C:473[B]:MET:HG3  | 1.92                     | 0.50              |
| 1:C:226:LEU:HD12   | 1:C:283:LEU:CD2     | 2.40                     | 0.50              |
| 1:A:144:PRO:HA     | 1:A:147:PHE:CE2     | 2.47                     | 0.50              |
| 1:A:191:ILE:HG13   | 1:A:499:PRO:HG3     | 1.93                     | 0.49              |
| 1:B:235:ASN:HD22   | 1:B:237:ALA:H       | 1.58                     | 0.49              |
| 1:A:10:TRP:HE1     | 1:A:26:GLN:HE21     | 1.59                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:B:54:TRP:HB3     | 1:B:65:PHE:CD1     | 2.47                     | 0.49              |
| 1:C:14:VAL:HG12    | 1:C:17:LEU:HD23    | 1.95                     | 0.49              |
| 1:C:16:PRO:O       | 1:C:17:LEU:HB2     | 2.13                     | 0.49              |
| 1:C:66:THR:C       | 1:C:67:LEU:O       | 2.53                     | 0.49              |
| 1:A:377[A]:GLU:CD  | 1:A:377[A]:GLU:H   | 2.20                     | 0.49              |
| 1:A:181:ASN:HD22   | 1:A:184:TYR:HB2    | 1.76                     | 0.49              |
| 1:A:255:THR:HG22   | 1:A:266:ARG:CZ     | 2.43                     | 0.49              |
| 1:B:350:ASP:OD1    | 1:B:352:LEU:HB3    | 2.13                     | 0.49              |
| 1:B:20:HIS:CE1     | 1:B:87:ASN:HD22    | 2.31                     | 0.49              |
| 1:B:100:TRP:CH2    | 1:B:101:LEU:HG     | 2.47                     | 0.49              |
| 1:C:221:GLU:HG2    | 1:C:473[B]:MET:HE3 | 1.95                     | 0.49              |
| 1:A:343[B]:GLU:HG3 | 1:A:391:GLY:H      | 1.78                     | 0.49              |
| 1:C:8:THR:HG22     | 1:C:9:ALA:H        | 1.77                     | 0.49              |
| 1:A:8:THR:HG22     | 1:A:9:ALA:N        | 2.25                     | 0.48              |
| 1:C:17:LEU:HB3     | 1:C:159:PRO:HB3    | 1.95                     | 0.48              |
| 1:B:19:PRO:HG3     | 1:B:142:ILE:HB     | 1.94                     | 0.48              |
| 1:C:253:LEU:HD22   | 1:C:392:MET:HG2    | 1.95                     | 0.48              |
| 1:A:278:LEU:C      | 1:A:278:LEU:HD23   | 2.38                     | 0.48              |
| 1:A:254:ASN:HD22   | 1:A:254:ASN:C      | 2.21                     | 0.48              |
| 1:B:278:LEU:O      | 1:B:278:LEU:HD23   | 2.12                     | 0.48              |
| 1:A:164:PRO:HG3    | 1:A:184:TYR:CZ     | 2.48                     | 0.48              |
| 1:C:278:LEU:HD21   | 1:C:356:MET:HG2    | 1.94                     | 0.48              |
| 1:C:382:TYR:CE2    | 1:C:416:HIS:CE1    | 3.01                     | 0.48              |
| 1:A:74:SER:HB2     | 1:A:161:GLY:O      | 2.14                     | 0.48              |
| 1:C:164:PRO:HD3    | 1:C:184:TYR:CE1    | 2.49                     | 0.48              |
| 1:C:279:ILE:HA     | 1:C:283:LEU:HD12   | 1.96                     | 0.48              |
| 1:A:313:GLN:HG3    | 8:A:604:HOH:O      | 2.11                     | 0.48              |
| 1:C:209:PHE:HA     | 1:C:214:ILE:HG13   | 1.95                     | 0.48              |
| 1:A:311:ASP:OD2    | 1:A:314[B]:LYS:HG3 | 2.13                     | 0.47              |
| 1:B:276[A]:LYS:HD2 | 8:B:622:HOH:O      | 2.14                     | 0.47              |
| 1:C:8:THR:HG23     | 1:C:216:LEU:O      | 2.14                     | 0.47              |
| 1:C:49:TRP:C       | 1:C:51:ALA:H       | 2.20                     | 0.47              |
| 1:C:283:LEU:CD2    | 1:C:352:LEU:HD11   | 2.44                     | 0.47              |
| 1:A:14[A]:VAL:CG1  | 1:A:29:ALA:CB      | 2.91                     | 0.47              |
| 1:B:217:LEU:CD1    | 1:B:224:LEU:HD22   | 2.44                     | 0.47              |
| 1:C:428:LYS:HD2    | 1:C:428:LYS:O      | 2.14                     | 0.47              |
| 1:A:339:PRO:HB2    | 1:A:341[B]:ARG:HG3 | 1.96                     | 0.47              |
| 1:A:93:ASP:O       | 3:A:507:ACT:CH3    | 2.62                     | 0.47              |
| 1:C:226:LEU:CD1    | 1:C:283:LEU:CD2    | 2.92                     | 0.47              |
| 1:C:227:ASP:HB3    | 1:C:284:TYR:OH     | 2.14                     | 0.47              |
| 1:C:293:LEU:H      | 3:C:504:ACT:C      | 2.27                     | 0.47              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:A:349:THR:OG1     | 7:A:513:GOL:H12    | 2.15                     | 0.47              |
| 1:B:27:MET:HE2      | 1:B:136:PRO:HG2    | 1.96                     | 0.47              |
| 1:B:269[B]:LEU:HD11 | 1:B:364:MET:HE1    | 1.96                     | 0.47              |
| 1:B:364:MET:HG3     | 1:B:371:VAL:CG1    | 2.44                     | 0.47              |
| 1:C:103:LEU:HB2     | 1:C:132:GLU:OE2    | 2.15                     | 0.47              |
| 1:C:316:LYS:HG2     | 1:C:333:ARG:NH1    | 2.30                     | 0.47              |
| 1:C:354:LYS:O       | 1:C:358[A]:GLU:HG3 | 2.15                     | 0.47              |
| 1:B:258:ALA:HA      | 1:B:261:ASN:OD1    | 2.15                     | 0.46              |
| 1:A:146:GLN:HE21    | 1:A:158:ALA:H      | 1.63                     | 0.46              |
| 1:C:40:TYR:HB3      | 1:C:488:ILE:HD11   | 1.97                     | 0.46              |
| 1:C:146:GLN:OE1     | 1:C:157:LYS:HB2    | 2.14                     | 0.46              |
| 1:A:27:MET:CE       | 1:A:136:PRO:HG2    | 2.45                     | 0.46              |
| 1:B:320:GLU:OE2     | 1:B:325:THR:HG22   | 2.14                     | 0.46              |
| 7:A:514:GOL:H31     | 1:B:42:ALA:N       | 2.20                     | 0.46              |
| 1:A:316:LYS:HE2     | 1:A:333:ARG:NH1    | 2.11                     | 0.46              |
| 1:C:278:LEU:HD11    | 1:C:356:MET:HG2    | 1.98                     | 0.46              |
| 1:A:292:THR:O       | 1:A:293:LEU:C      | 2.57                     | 0.46              |
| 1:B:465:LEU:C       | 1:B:465:LEU:HD23   | 2.41                     | 0.46              |
| 1:C:93:ASP:OD2      | 1:C:151:GLU:OE1    | 2.34                     | 0.46              |
| 1:C:420:GLN:HA      | 1:C:420:GLN:NE2    | 2.30                     | 0.46              |
| 1:C:225:PRO:HB2     | 1:C:227:ASP:OD1    | 2.16                     | 0.46              |
| 1:B:226:LEU:HD12    | 1:B:283:LEU:HA     | 1.96                     | 0.46              |
| 1:B:336:ASN:HB3     | 1:C:457:ARG:HH12   | 1.80                     | 0.46              |
| 1:C:6:ILE:O         | 1:C:194:ILE:HA     | 2.15                     | 0.46              |
| 1:A:473:MET:HB2     | 1:A:473:MET:HE3    | 1.69                     | 0.45              |
| 1:B:127:TYR:CD2     | 1:B:128:PRO:HD3    | 2.51                     | 0.45              |
| 1:B:373:LEU:HD22    | 7:B:515:GOL:H31    | 1.97                     | 0.45              |
| 1:C:221:GLU:OE1     | 1:C:287[A]:GLN:CG  | 2.65                     | 0.45              |
| 1:A:331:ASP:CB      | 1:A:365:ARG:HH11   | 2.29                     | 0.45              |
| 1:B:97[B]:ARG:HH11  | 1:B:386:ARG:HH11   | 1.57                     | 0.45              |
| 1:C:253:LEU:CD2     | 1:C:392:MET:HG2    | 2.46                     | 0.45              |
| 1:A:386:ARG:CA      | 1:A:415:SER:OG     | 2.64                     | 0.45              |
| 1:A:93:ASP:O        | 3:A:507:ACT:H1     | 2.16                     | 0.45              |
| 1:A:278:LEU:HD21    | 1:A:356:MET:HE3    | 1.97                     | 0.45              |
| 1:B:218:TYR:H       | 3:B:507:ACT:C      | 2.30                     | 0.45              |
| 1:C:11:PRO:HA       | 1:C:199:ILE:O      | 2.17                     | 0.45              |
| 1:A:127:TYR:CG      | 1:A:128:PRO:HD3    | 2.51                     | 0.45              |
| 1:C:226:LEU:HD13    | 1:C:283:LEU:HA     | 1.97                     | 0.45              |
| 7:A:514:GOL:H31     | 1:B:42:ALA:HB3     | 1.99                     | 0.45              |
| 1:A:144:PRO:C       | 1:A:146:GLN:N      | 2.75                     | 0.45              |
| 1:B:191:ILE:HG21    | 1:B:194:ILE:CD1    | 2.47                     | 0.45              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:B:27:MET:CE      | 1:B:136:PRO:HG2  | 2.47                     | 0.44              |
| 1:C:283:LEU:HD22   | 1:C:352:LEU:CD1  | 2.47                     | 0.44              |
| 1:C:399:GLY:N      | 1:C:403:ASP:OD2  | 2.51                     | 0.44              |
| 1:B:364:MET:HE3    | 1:B:371:VAL:HG11 | 1.99                     | 0.44              |
| 1:C:6:ILE:HD11     | 1:C:191:ILE:HG13 | 2.00                     | 0.44              |
| 1:C:342:ILE:O      | 1:C:371:VAL:HA   | 2.17                     | 0.44              |
| 1:B:89:ARG:NH2     | 1:B:150:HIS:HB3  | 2.33                     | 0.44              |
| 1:C:14:VAL:HG13    | 1:C:29:ALA:CB    | 2.48                     | 0.44              |
| 1:C:68:ARG:HG3     | 1:C:71:VAL:HG23  | 1.99                     | 0.44              |
| 1:C:101:LEU:CD2    | 1:C:132:GLU:CD   | 2.90                     | 0.44              |
| 1:A:289:VAL:N      | 3:A:506:ACT:OXT  | 2.49                     | 0.44              |
| 1:B:373:LEU:HB2    | 7:B:515:GOL:H11  | 2.00                     | 0.44              |
| 1:B:306:LYS:HA     | 1:B:307:PRO:HD2  | 1.91                     | 0.44              |
| 1:C:68:ARG:CB      | 1:C:69:ASP:HA    | 2.46                     | 0.44              |
| 1:A:298:VAL:O      | 1:A:299:PRO:C    | 2.61                     | 0.44              |
| 1:C:298:VAL:HG13   | 1:C:299:PRO:HD2  | 2.00                     | 0.44              |
| 1:C:206:ALA:HB1    | 1:C:228:THR:HG21 | 1.99                     | 0.44              |
| 1:C:211:THR:C      | 1:C:213:ASP:H    | 2.26                     | 0.44              |
| 1:C:459:HIS:ND1    | 3:C:504:ACT:OXT  | 2.39                     | 0.44              |
| 1:A:20:HIS:CE1     | 1:A:140:ARG:O    | 2.70                     | 0.44              |
| 1:A:227:ASP:HB3    | 1:A:284:TYR:CE2  | 2.53                     | 0.44              |
| 1:A:398:TRP:CE2    | 6:A:511:HCT:H5A  | 2.53                     | 0.44              |
| 1:B:226:LEU:HD22   | 3:B:504:ACT:O    | 2.18                     | 0.44              |
| 1:A:415:SER:O      | 1:A:416:HIS:HD2  | 2.01                     | 0.43              |
| 1:B:217:LEU:HD23   | 3:B:507:ACT:H2   | 1.98                     | 0.43              |
| 1:C:131:GLN:H      | 1:C:131:GLN:HG2  | 1.16                     | 0.43              |
| 1:A:142:ILE:O      | 1:A:142:ILE:HG23 | 2.17                     | 0.43              |
| 1:B:253:LEU:HB2    | 1:B:463:VAL:O    | 2.18                     | 0.43              |
| 1:C:10:TRP:CD2     | 1:C:11:PRO:HD2   | 2.53                     | 0.43              |
| 1:C:398:TRP:HZ2    | 1:C:416:HIS:CD2  | 2.37                     | 0.43              |
| 1:A:64:THR:HA      | 1:A:118:LEU:O    | 2.18                     | 0.43              |
| 1:B:20:HIS:CD2     | 1:B:152:THR:OG1  | 2.64                     | 0.43              |
| 1:C:28:PHE:HB2     | 1:C:492:ILE:HG12 | 2.00                     | 0.43              |
| 1:C:88:PHE:CB      | 1:C:110:VAL:HG21 | 2.48                     | 0.43              |
| 1:C:458:LEU:HD23   | 1:C:458:LEU:HA   | 1.80                     | 0.43              |
| 1:A:95:ARG:HH11    | 1:A:95:ARG:CB    | 2.29                     | 0.43              |
| 1:C:444[A]:GLU:HG3 | 1:C:447:ARG:HH21 | 1.83                     | 0.43              |
| 1:B:72[B]:LYS:HD3  | 1:B:78:PRO:HA    | 2.00                     | 0.43              |
| 1:B:284:TYR:N      | 1:B:285:GLY:HA3  | 2.34                     | 0.43              |
| 1:C:218:TYR:CD2    | 1:C:492:ILE:HD12 | 2.54                     | 0.43              |
| 1:B:35:GLU:HA      | 1:B:36:PRO:HD3   | 1.89                     | 0.43              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:C:411:MET:HG2   | 1:C:418:ASP:HB3     | 2.01                     | 0.43              |
| 1:C:457:ARG:O     | 1:C:458:LEU:C       | 2.61                     | 0.43              |
| 1:B:364:MET:HE3   | 1:B:392:MET:HE1     | 2.00                     | 0.43              |
| 1:A:327:PRO:O     | 1:A:328:ALA:C       | 2.62                     | 0.43              |
| 1:B:192[B]:LYS:CE | 8:B:597:HOH:O       | 2.67                     | 0.43              |
| 1:C:272:ALA:HB2   | 1:C:367[B]:ILE:HD13 | 2.01                     | 0.43              |
| 1:C:272:ALA:O     | 1:C:363:ASP:HB3     | 2.19                     | 0.43              |
| 1:B:9:ALA:O       | 3:B:507:ACT:CH3     | 2.67                     | 0.42              |
| 1:A:158:ALA:O     | 1:A:160:ILE:N       | 2.50                     | 0.42              |
| 1:B:174:GLN:O     | 1:B:175:TYR:HB3     | 2.19                     | 0.42              |
| 1:B:361:GLN:HE22  | 7:B:515:GOL:H31     | 1.84                     | 0.42              |
| 1:C:127:TYR:CG    | 1:C:128:PRO:HD3     | 2.54                     | 0.42              |
| 1:B:235:ASN:HD22  | 1:B:236:PRO:N       | 2.17                     | 0.42              |
| 1:A:20:HIS:CE1    | 1:A:87:ASN:HD22     | 2.35                     | 0.42              |
| 1:A:144:PRO:C     | 1:A:146:GLN:H       | 2.26                     | 0.42              |
| 1:A:224:LEU:HD21  | 1:A:229:PHE:HB2     | 2.01                     | 0.42              |
| 1:B:131:GLN:H     | 1:B:131:GLN:HG2     | 1.60                     | 0.42              |
| 1:C:12:VAL:HG13   | 1:C:13:ASN:O        | 2.20                     | 0.42              |
| 1:C:408:LEU:HD13  | 1:C:454:ILE:HG21    | 2.00                     | 0.42              |
| 1:A:89:ARG:HH22   | 1:A:150:HIS:HB3     | 1.85                     | 0.42              |
| 1:B:274:ASN:OD1   | 1:B:277:SER:CB      | 2.56                     | 0.42              |
| 1:A:54:TRP:HB3    | 1:A:65:PHE:CD1      | 2.54                     | 0.42              |
| 1:A:374:ILE:HG22  | 1:A:376:GLU:HG3     | 2.00                     | 0.42              |
| 1:C:101:LEU:HD21  | 1:C:132:GLU:CG      | 2.50                     | 0.42              |
| 1:C:408:LEU:O     | 1:C:409:SER:C       | 2.62                     | 0.42              |
| 1:B:18:ASN:CG     | 1:B:21:LEU:CD2      | 2.93                     | 0.42              |
| 1:B:226:LEU:HD23  | 1:B:226:LEU:HA      | 1.93                     | 0.42              |
| 1:A:221:GLU:HG3   | 1:A:470:ILE:HB      | 2.01                     | 0.42              |
| 1:B:12:VAL:HG13   | 1:B:13:ASN:O        | 2.19                     | 0.42              |
| 1:B:219:GLY:C     | 1:B:472:MET:CE      | 2.88                     | 0.42              |
| 1:C:226:LEU:HD23  | 1:C:226:LEU:HA      | 1.83                     | 0.42              |
| 1:C:217:LEU:HD23  | 1:C:217:LEU:HA      | 1.92                     | 0.42              |
| 1:A:384:ARG:HA    | 1:A:387:ASP:HB2     | 2.02                     | 0.42              |
| 1:C:229:PHE:CD2   | 1:C:473[B]:MET:HE2  | 2.55                     | 0.42              |
| 1:A:57:SER:OG     | 1:A:59:ASP:OD1      | 2.34                     | 0.41              |
| 1:A:338:GLN:HA    | 1:A:339:PRO:HD3     | 1.95                     | 0.41              |
| 1:A:395:HIS:CE1   | 8:A:603:HOH:O       | 2.72                     | 0.41              |
| 1:B:275:LYS:HD2   | 1:B:289:VAL:HG13    | 2.02                     | 0.41              |
| 1:C:17:LEU:HD22   | 1:C:17:LEU:HA       | 1.73                     | 0.41              |
| 1:B:13:ASN:ND2    | 1:B:173:ASN:H       | 2.16                     | 0.41              |
| 1:B:181:ASN:ND2   | 1:B:183:ASN:H       | 2.19                     | 0.41              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:C:409:SER:HB2  | 1:C:439:LEU:HD21   | 2.02                     | 0.41              |
| 1:A:235:ASN:HA   | 1:A:236:PRO:HD3    | 1.94                     | 0.41              |
| 1:A:408:LEU:HD13 | 1:A:454:ILE:HG21   | 2.02                     | 0.41              |
| 1:C:419:PHE:HB3  | 8:C:535:HOH:O      | 2.20                     | 0.41              |
| 1:B:274:ASN:HB2  | 1:B:310:TYR:CD1    | 2.55                     | 0.41              |
| 1:B:153:MET:HE2  | 8:B:581:HOH:O      | 2.20                     | 0.41              |
| 1:C:20:HIS:CD2   | 1:C:152:THR:HG21   | 2.55                     | 0.41              |
| 1:C:411:MET:HG2  | 1:C:418:ASP:CB     | 2.50                     | 0.41              |
| 1:A:438:VAL:HG23 | 1:A:450:LEU:HB2    | 2.03                     | 0.41              |
| 1:B:360:ILE:HG22 | 1:B:364:MET:HE2    | 2.03                     | 0.41              |
| 1:A:181:ASN:ND2  | 1:A:184:TYR:HB2    | 2.36                     | 0.41              |
| 1:A:181:ASN:HD21 | 1:A:183:ASN:C      | 2.29                     | 0.41              |
| 1:A:483:ILE:HA   | 1:A:484:PRO:HD3    | 1.87                     | 0.41              |
| 1:B:346:PHE:HB3  | 1:B:394:PHE:HD1    | 1.86                     | 0.41              |
| 1:B:377:GLU:CD   | 8:B:621:HOH:O      | 2.64                     | 0.41              |
| 1:B:408:LEU:HD12 | 1:B:451:TYR:HE2    | 1.86                     | 0.41              |
| 1:C:6:ILE:CD1    | 1:C:191:ILE:HG13   | 2.50                     | 0.41              |
| 1:C:68:ARG:HA    | 1:C:68:ARG:HD3     | 1.45                     | 0.41              |
| 1:C:101:LEU:HD22 | 1:C:132:GLU:OE2    | 2.21                     | 0.41              |
| 1:C:180:ARG:NH1  | 1:C:189:PRO:O      | 2.54                     | 0.41              |
| 1:C:240:THR:HG22 | 1:C:475:VAL:HG22   | 2.02                     | 0.41              |
| 1:C:283:LEU:HD21 | 1:C:352:LEU:HD11   | 2.00                     | 0.41              |
| 1:C:434:GLU:OE1  | 1:C:453:ASP:OD2    | 2.39                     | 0.41              |
| 1:A:72:LYS:HG2   | 8:A:592:HOH:O      | 2.21                     | 0.41              |
| 1:A:342:ILE:O    | 1:A:371:VAL:HA     | 2.21                     | 0.41              |
| 1:B:465:LEU:C    | 1:B:465:LEU:CD2    | 2.94                     | 0.41              |
| 1:C:395:HIS:O    | 1:C:396[B]:ARG:HG3 | 2.21                     | 0.41              |
| 1:B:217:LEU:HA   | 3:B:507:ACT:CH3    | 2.51                     | 0.40              |
| 1:B:240:THR:HG22 | 1:B:475:VAL:HG22   | 2.03                     | 0.40              |
| 1:B:292:THR:O    | 1:B:293:LEU:C      | 2.65                     | 0.40              |
| 1:C:38:VAL:HG21  | 1:C:46:VAL:CG1     | 2.50                     | 0.40              |
| 1:C:92:LEU:C     | 1:C:94:ASN:N       | 2.78                     | 0.40              |
| 1:A:331:ASP:HB3  | 1:A:365:ARG:NH1    | 2.35                     | 0.40              |
| 1:B:27:MET:HG3   | 8:B:624:HOH:O      | 2.21                     | 0.40              |
| 1:A:175:TYR:HA   | 1:A:196:PHE:O      | 2.22                     | 0.40              |
| 1:B:165:TRP:HH2  | 1:B:191:ILE:HB     | 1.87                     | 0.40              |
| 1:C:221:GLU:HA   | 1:C:473[B]:MET:SD  | 2.62                     | 0.40              |

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     | 511/502 (102%)   | 473 (93%)  | 33 (6%) | 5 (1%)   | 12          | 24 |
| 1   | B     | 510/502 (102%)   | 478 (94%)  | 30 (6%) | 2 (0%)   | 30          | 49 |
| 1   | C     | 505/502 (101%)   | 467 (92%)  | 31 (6%) | 7 (1%)   | 9           | 17 |
| All | All   | 1526/1506 (101%) | 1418 (93%) | 94 (6%) | 14 (1%)  | 14          | 27 |

All (14) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 67  | LEU  |
| 1   | A     | 74  | SER  |
| 1   | C     | 59  | ASP  |
| 1   | C     | 282 | ALA  |
| 1   | A     | 113 | LEU  |
| 1   | B     | 286 | THR  |
| 1   | C     | 17  | LEU  |
| 1   | C     | 95  | ARG  |
| 1   | A     | 347 | ILE  |
| 1   | B     | 340 | LEU  |
| 1   | A     | 145 | SER  |
| 1   | C     | 220 | ASN  |
| 1   | C     | 415 | SER  |
| 1   | A     | 493 | PRO  |

### 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     | 435/425 (102%)   | 384 (88%)  | 51 (12%)  | 5           | 11 |
| 1   | B     | 440/425 (104%)   | 397 (90%)  | 43 (10%)  | 7           | 16 |
| 1   | C     | 432/425 (102%)   | 380 (88%)  | 52 (12%)  | 5           | 10 |
| All | All   | 1307/1275 (102%) | 1161 (89%) | 146 (11%) | 6           | 12 |

All (146) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 4      | ASP  |
| 1   | A     | 17     | LEU  |
| 1   | A     | 23     | THR  |
| 1   | A     | 38     | VAL  |
| 1   | A     | 46     | VAL  |
| 1   | A     | 52     | LYS  |
| 1   | A     | 53     | SER  |
| 1   | A     | 58     | GLU  |
| 1   | A     | 64     | THR  |
| 1   | A     | 86     | GLU  |
| 1   | A     | 95     | ARG  |
| 1   | A     | 101    | LEU  |
| 1   | A     | 103    | LEU  |
| 1   | A     | 107    | ILE  |
| 1   | A     | 113    | LEU  |
| 1   | A     | 120    | ILE  |
| 1   | A     | 121    | THR  |
| 1   | A     | 131[A] | GLN  |
| 1   | A     | 131[B] | GLN  |
| 1   | A     | 145    | SER  |
| 1   | A     | 156    | ILE  |
| 1   | A     | 167    | LEU  |
| 1   | A     | 171    | LYS  |
| 1   | A     | 172    | LEU  |
| 1   | A     | 173    | ASN  |
| 1   | A     | 181    | ASN  |
| 1   | A     | 182    | GLU  |
| 1   | A     | 191    | ILE  |
| 1   | A     | 216    | LEU  |
| 1   | A     | 221    | GLU  |
| 1   | A     | 224    | LEU  |
| 1   | A     | 242    | LEU  |
| 1   | A     | 244    | GLN  |
| 1   | A     | 248    | THR  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 250    | MET  |
| 1   | A     | 254    | ASN  |
| 1   | A     | 279    | ILE  |
| 1   | A     | 316    | LYS  |
| 1   | A     | 319    | LEU  |
| 1   | A     | 321    | LYS  |
| 1   | A     | 325    | THR  |
| 1   | A     | 331    | ASP  |
| 1   | A     | 371    | VAL  |
| 1   | A     | 373    | LEU  |
| 1   | A     | 387    | ASP  |
| 1   | A     | 416    | HIS  |
| 1   | A     | 438    | VAL  |
| 1   | A     | 439    | LEU  |
| 1   | A     | 452    | ARG  |
| 1   | A     | 479    | GLU  |
| 1   | A     | 482    | ASN  |
| 1   | B     | 4      | ASP  |
| 1   | B     | 6      | ILE  |
| 1   | B     | 7      | THR  |
| 1   | B     | 12     | VAL  |
| 1   | B     | 38     | VAL  |
| 1   | B     | 46     | VAL  |
| 1   | B     | 71     | VAL  |
| 1   | B     | 82[A]  | GLU  |
| 1   | B     | 82[B]  | GLU  |
| 1   | B     | 101    | LEU  |
| 1   | B     | 103    | LEU  |
| 1   | B     | 114    | SER  |
| 1   | B     | 131    | GLN  |
| 1   | B     | 150    | HIS  |
| 1   | B     | 167    | LEU  |
| 1   | B     | 168    | GLN  |
| 1   | B     | 179    | VAL  |
| 1   | B     | 181    | ASN  |
| 1   | B     | 214[A] | ILE  |
| 1   | B     | 214[B] | ILE  |
| 1   | B     | 216    | LEU  |
| 1   | B     | 224    | LEU  |
| 1   | B     | 250    | MET  |
| 1   | B     | 253    | LEU  |
| 1   | B     | 283    | LEU  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | B     | 288[A] | GLN  |
| 1   | B     | 288[B] | GLN  |
| 1   | B     | 309[A] | GLN  |
| 1   | B     | 309[B] | GLN  |
| 1   | B     | 319    | LEU  |
| 1   | B     | 345    | SER  |
| 1   | B     | 355    | SER  |
| 1   | B     | 364    | MET  |
| 1   | B     | 371    | VAL  |
| 1   | B     | 373    | LEU  |
| 1   | B     | 374    | ILE  |
| 1   | B     | 380    | SER  |
| 1   | B     | 392    | MET  |
| 1   | B     | 410    | SER  |
| 1   | B     | 413    | VAL  |
| 1   | B     | 439    | LEU  |
| 1   | B     | 450    | LEU  |
| 1   | B     | 490    | THR  |
| 1   | C     | 8      | THR  |
| 1   | C     | 12     | VAL  |
| 1   | C     | 17     | LEU  |
| 1   | C     | 27     | MET  |
| 1   | C     | 46     | VAL  |
| 1   | C     | 53     | SER  |
| 1   | C     | 58     | GLU  |
| 1   | C     | 64     | THR  |
| 1   | C     | 77     | GLU  |
| 1   | C     | 95     | ARG  |
| 1   | C     | 96     | GLN  |
| 1   | C     | 101    | LEU  |
| 1   | C     | 103    | LEU  |
| 1   | C     | 115    | LYS  |
| 1   | C     | 116    | THR  |
| 1   | C     | 123    | LYS  |
| 1   | C     | 130    | LEU  |
| 1   | C     | 131    | GLN  |
| 1   | C     | 148    | LYS  |
| 1   | C     | 156    | ILE  |
| 1   | C     | 160    | ILE  |
| 1   | C     | 167    | LEU  |
| 1   | C     | 169    | GLU  |
| 1   | C     | 179    | VAL  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | C     | 182    | GLU  |
| 1   | C     | 213    | ASP  |
| 1   | C     | 216    | LEU  |
| 1   | C     | 224    | LEU  |
| 1   | C     | 246    | ILE  |
| 1   | C     | 249    | VAL  |
| 1   | C     | 250    | MET  |
| 1   | C     | 276    | LYS  |
| 1   | C     | 303    | LEU  |
| 1   | C     | 306    | LYS  |
| 1   | C     | 320[A] | GLU  |
| 1   | C     | 320[B] | GLU  |
| 1   | C     | 341    | ARG  |
| 1   | C     | 371    | VAL  |
| 1   | C     | 373    | LEU  |
| 1   | C     | 380    | SER  |
| 1   | C     | 386    | ARG  |
| 1   | C     | 387    | ASP  |
| 1   | C     | 438    | VAL  |
| 1   | C     | 439    | LEU  |
| 1   | C     | 441    | THR  |
| 1   | C     | 450    | LEU  |
| 1   | C     | 473[A] | MET  |
| 1   | C     | 473[B] | MET  |
| 1   | C     | 475    | VAL  |
| 1   | C     | 490    | THR  |
| 1   | C     | 495    | GLU  |
| 1   | C     | 498    | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 13  | ASN  |
| 1   | A     | 26  | GLN  |
| 1   | A     | 87  | ASN  |
| 1   | A     | 94  | ASN  |
| 1   | A     | 106 | GLN  |
| 1   | A     | 119 | GLN  |
| 1   | A     | 146 | GLN  |
| 1   | A     | 181 | ASN  |
| 1   | A     | 244 | GLN  |
| 1   | A     | 254 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 338 | GLN  |
| 1   | A     | 361 | GLN  |
| 1   | A     | 405 | HIS  |
| 1   | A     | 442 | HIS  |
| 1   | A     | 459 | HIS  |
| 1   | A     | 496 | GLN  |
| 1   | B     | 13  | ASN  |
| 1   | B     | 20  | HIS  |
| 1   | B     | 26  | GLN  |
| 1   | B     | 87  | ASN  |
| 1   | B     | 94  | ASN  |
| 1   | B     | 146 | GLN  |
| 1   | B     | 149 | ASN  |
| 1   | B     | 150 | HIS  |
| 1   | B     | 174 | GLN  |
| 1   | B     | 181 | ASN  |
| 1   | B     | 235 | ASN  |
| 1   | B     | 244 | GLN  |
| 1   | B     | 420 | GLN  |
| 1   | B     | 448 | GLN  |
| 1   | B     | 496 | GLN  |
| 1   | C     | 13  | ASN  |
| 1   | C     | 20  | HIS  |
| 1   | C     | 26  | GLN  |
| 1   | C     | 56  | HIS  |
| 1   | C     | 87  | ASN  |
| 1   | C     | 106 | GLN  |
| 1   | C     | 149 | ASN  |
| 1   | C     | 173 | ASN  |
| 1   | C     | 181 | ASN  |
| 1   | C     | 220 | ASN  |
| 1   | C     | 239 | HIS  |
| 1   | C     | 270 | ASN  |
| 1   | C     | 274 | ASN  |
| 1   | C     | 338 | GLN  |
| 1   | C     | 416 | HIS  |
| 1   | C     | 420 | GLN  |
| 1   | C     | 482 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 33 ligands modelled in this entry, 10 are monoatomic - leaving 23 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 3   | ACT  | C     | 504 | -    | 3,3,3        | 1.68 | 1 (33%)     | 3,3,3       | 3.87 | 2 (66%)     |
| 7   | GOL  | A     | 514 | -    | 5,5,5        | 0.43 | 0           | 5,5,5       | 0.41 | 0           |
| 3   | ACT  | A     | 504 | -    | 3,3,3        | 0.94 | 0           | 3,3,3       | 0.69 | 0           |
| 3   | ACT  | A     | 506 | -    | 3,3,3        | 0.78 | 0           | 3,3,3       | 1.49 | 0           |
| 7   | GOL  | A     | 513 | -    | 5,5,5        | 0.45 | 0           | 5,5,5       | 0.62 | 0           |
| 3   | ACT  | C     | 505 | -    | 3,3,3        | 0.88 | 0           | 3,3,3       | 1.83 | 2 (66%)     |
| 3   | ACT  | B     | 504 | -    | 3,3,3        | 0.83 | 0           | 3,3,3       | 1.21 | 0           |
| 7   | GOL  | B     | 512 | -    | 5,5,5        | 0.40 | 0           | 5,5,5       | 0.55 | 0           |
| 7   | GOL  | A     | 515 | -    | 5,5,5        | 0.45 | 0           | 5,5,5       | 0.36 | 0           |
| 3   | ACT  | B     | 507 | -    | 3,3,3        | 0.97 | 0           | 3,3,3       | 0.34 | 0           |
| 6   | HCT  | B     | 511 | 2    | 12,12,12     | 2.78 | 3 (25%)     | 14,15,15    | 2.97 | 6 (42%)     |
| 3   | ACT  | B     | 505 | -    | 3,3,3        | 0.99 | 0           | 3,3,3       | 1.15 | 0           |
| 4   | SO4  | A     | 508 | -    | 4,4,4        | 0.25 | 0           | 6,6,6       | 0.37 | 0           |
| 7   | GOL  | B     | 513 | -    | 5,5,5        | 0.26 | 0           | 5,5,5       | 0.85 | 0           |
| 6   | HCT  | A     | 511 | 2    | 12,12,12     | 1.94 | 3 (25%)     | 14,15,15    | 2.64 | 6 (42%)     |
| 3   | ACT  | A     | 507 | -    | 3,3,3        | 0.82 | 0           | 3,3,3       | 1.49 | 0           |
| 6   | HCT  | C     | 509 | 2    | 12,12,12     | 2.07 | 2 (16%)     | 14,15,15    | 2.41 | 2 (14%)     |
| 7   | GOL  | B     | 514 | -    | 5,5,5        | 0.33 | 0           | 5,5,5       | 0.35 | 0           |
| 7   | GOL  | B     | 515 | -    | 5,5,5        | 0.61 | 0           | 5,5,5       | 0.97 | 0           |
| 7   | GOL  | A     | 512 | -    | 5,5,5        | 0.29 | 0           | 5,5,5       | 0.51 | 0           |
| 3   | ACT  | B     | 506 | -    | 3,3,3        | 0.86 | 0           | 3,3,3       | 1.36 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | ACT  | C     | 506 | -    | 3,3,3        | 1.13 | 0        | 3,3,3       | 0.75 | 0        |
| 3   | ACT  | A     | 505 | -    | 3,3,3        | 0.91 | 0        | 3,3,3       | 1.18 | 0        |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings |
|-----|------|-------|-----|------|---------|------------|-------|
| 6   | HCT  | B     | 511 | 2    | -       | 4/13/13/13 | -     |
| 7   | GOL  | A     | 514 | -    | -       | 2/4/4/4    | -     |
| 6   | HCT  | C     | 509 | 2    | -       | 7/13/13/13 | -     |
| 7   | GOL  | B     | 514 | -    | -       | 4/4/4/4    | -     |
| 7   | GOL  | B     | 515 | -    | -       | 3/4/4/4    | -     |
| 7   | GOL  | A     | 512 | -    | -       | 2/4/4/4    | -     |
| 7   | GOL  | B     | 513 | -    | -       | 4/4/4/4    | -     |
| 7   | GOL  | B     | 512 | -    | -       | 2/4/4/4    | -     |
| 7   | GOL  | A     | 513 | -    | -       | 0/4/4/4    | -     |
| 6   | HCT  | A     | 511 | 2    | -       | 5/13/13/13 | -     |
| 7   | GOL  | A     | 515 | -    | -       | 1/4/4/4    | -     |

All (9) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 6   | B     | 511 | HCT  | C2-C1 | 5.62 | 1.65        | 1.51     |
| 6   | B     | 511 | HCT  | C2-C3 | 5.24 | 1.64        | 1.53     |
| 6   | C     | 509 | HCT  | C2-C1 | 4.44 | 1.62        | 1.51     |
| 6   | B     | 511 | HCT  | C5-C6 | 4.36 | 1.60        | 1.50     |
| 6   | C     | 509 | HCT  | C2-C3 | 3.86 | 1.61        | 1.53     |
| 6   | A     | 511 | HCT  | C2-C1 | 3.82 | 1.61        | 1.51     |
| 6   | A     | 511 | HCT  | C2-C3 | 3.67 | 1.61        | 1.53     |
| 6   | A     | 511 | HCT  | C3-C7 | 2.37 | 1.55        | 1.51     |
| 3   | C     | 504 | ACT  | CH3-C | 2.20 | 1.57        | 1.49     |

All (18) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 6   | C     | 509 | HCT  | C3-C2-C1 | 6.73 | 129.14      | 113.92   |
| 6   | B     | 511 | HCT  | C3-C2-C1 | 6.72 | 129.11      | 113.92   |
| 6   | A     | 511 | HCT  | C3-C2-C1 | 5.90 | 127.25      | 113.92   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 3   | C     | 504 | ACT  | OXT-C-O   | -5.55 | 101.43      | 122.03   |
| 6   | B     | 511 | HCT  | C5-C4-C3  | 5.49  | 123.19      | 113.45   |
| 6   | C     | 509 | HCT  | C2-C3-C7  | 4.54  | 122.78      | 110.18   |
| 6   | A     | 511 | HCT  | C2-C3-C7  | 4.35  | 122.26      | 110.18   |
| 6   | B     | 511 | HCT  | O6-C7-C3  | -4.06 | 112.08      | 122.86   |
| 3   | C     | 504 | ACT  | OXT-C-CH3 | 3.37  | 129.17      | 115.05   |
| 6   | A     | 511 | HCT  | O6-C7-C3  | -3.11 | 114.61      | 122.86   |
| 6   | A     | 511 | HCT  | C5-C4-C3  | -2.82 | 108.44      | 113.45   |
| 6   | A     | 511 | HCT  | C4-C5-C6  | 2.76  | 119.84      | 112.49   |
| 6   | B     | 511 | HCT  | O5-C7-C3  | 2.66  | 121.05      | 114.16   |
| 6   | A     | 511 | HCT  | O3-C6-C5  | -2.51 | 115.14      | 123.09   |
| 6   | B     | 511 | HCT  | C2-C3-C7  | 2.44  | 116.97      | 110.18   |
| 3   | C     | 505 | ACT  | OXT-C-O   | -2.38 | 113.20      | 122.03   |
| 6   | B     | 511 | HCT  | O4-C6-C5  | 2.23  | 121.04      | 114.00   |
| 3   | C     | 505 | ACT  | OXT-C-CH3 | 2.09  | 123.82      | 115.05   |

There are no chirality outliers.

All (34) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 6   | B     | 511 | HCT  | C1-C2-C3-C4 |
| 6   | B     | 511 | HCT  | C1-C2-C3-C7 |
| 6   | C     | 509 | HCT  | C1-C2-C3-C7 |
| 7   | A     | 512 | GOL  | O1-C1-C2-C3 |
| 7   | B     | 512 | GOL  | O1-C1-C2-O2 |
| 7   | B     | 512 | GOL  | O1-C1-C2-C3 |
| 7   | B     | 513 | GOL  | O1-C1-C2-C3 |
| 7   | B     | 514 | GOL  | C1-C2-C3-O3 |
| 7   | B     | 515 | GOL  | C1-C2-C3-O3 |
| 6   | C     | 509 | HCT  | C3-C4-C5-C6 |
| 7   | A     | 514 | GOL  | O1-C1-C2-C3 |
| 7   | B     | 513 | GOL  | C1-C2-C3-O3 |
| 7   | B     | 514 | GOL  | O1-C1-C2-C3 |
| 7   | B     | 515 | GOL  | O1-C1-C2-C3 |
| 7   | B     | 513 | GOL  | O2-C2-C3-O3 |
| 7   | B     | 514 | GOL  | O2-C2-C3-O3 |
| 7   | B     | 515 | GOL  | O2-C2-C3-O3 |
| 6   | B     | 511 | HCT  | C2-C3-C4-C5 |
| 7   | A     | 512 | GOL  | O1-C1-C2-O2 |
| 6   | A     | 511 | HCT  | C3-C4-C5-C6 |
| 6   | C     | 509 | HCT  | O1-C1-C2-C3 |
| 6   | A     | 511 | HCT  | O1-C1-C2-C3 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 6   | A     | 511 | HCT  | O2-C1-C2-C3 |
| 6   | C     | 509 | HCT  | O2-C1-C2-C3 |
| 7   | A     | 514 | GOL  | O1-C1-C2-O2 |
| 7   | B     | 513 | GOL  | O1-C1-C2-O2 |
| 6   | B     | 511 | HCT  | C3-C4-C5-C6 |
| 7   | B     | 514 | GOL  | O1-C1-C2-O2 |
| 6   | C     | 509 | HCT  | C4-C5-C6-O4 |
| 6   | C     | 509 | HCT  | C4-C5-C6-O3 |
| 6   | A     | 511 | HCT  | C4-C5-C6-O3 |
| 6   | C     | 509 | HCT  | C1-C2-C3-C4 |
| 6   | A     | 511 | HCT  | C4-C5-C6-O4 |
| 7   | A     | 515 | GOL  | O2-C2-C3-O3 |

There are no ring outliers.

11 monomers are involved in 44 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | C     | 504 | ACT  | 3       | 0            |
| 7   | A     | 514 | GOL  | 10      | 0            |
| 3   | A     | 506 | ACT  | 1       | 0            |
| 7   | A     | 513 | GOL  | 1       | 0            |
| 3   | B     | 504 | ACT  | 1       | 0            |
| 3   | B     | 507 | ACT  | 15      | 0            |
| 7   | B     | 513 | GOL  | 4       | 0            |
| 6   | A     | 511 | HCT  | 1       | 0            |
| 3   | A     | 507 | ACT  | 2       | 0            |
| 7   | B     | 515 | GOL  | 5       | 0            |
| 7   | A     | 512 | GOL  | 1       | 0            |

## 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     | 498/502 (99%)   | -0.33  | 3 (0%) 85 83 | 20, 46, 66, 76        | 15 (3%) |
| 1   | B     | 497/502 (99%)   | -0.41  | 0 100 100    | 20, 44, 63, 83        | 19 (3%) |
| 1   | C     | 496/502 (98%)   | -0.05  | 4 (0%) 82 80 | 24, 59, 87, 99        | 12 (2%) |
| All | All   | 1491/1506 (99%) | -0.26  | 7 (0%) 87 85 | 20, 48, 79, 99        | 46 (3%) |

All (7) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 382 | TYR  | 4.9  |
| 1   | C     | 67  | LEU  | 4.0  |
| 1   | A     | 3   | PRO  | 2.9  |
| 1   | A     | 183 | ASN  | 2.6  |
| 1   | C     | 60  | GLY  | 2.6  |
| 1   | C     | 499 | PRO  | 2.2  |
| 1   | A     | 2   | ALA  | 2.0  |

### 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 3   | ACT  | A     | 505 | 4/4   | 0.48 | 0.39 | 45,45,45,46                | 4     |
| 3   | ACT  | B     | 506 | 4/4   | 0.51 | 0.23 | 41,43,43,43                | 4     |
| 7   | GOL  | A     | 512 | 6/6   | 0.53 | 0.26 | 57,59,61,63                | 6     |
| 7   | GOL  | B     | 514 | 6/6   | 0.58 | 0.31 | 51,52,53,55                | 6     |
| 3   | ACT  | A     | 507 | 4/4   | 0.60 | 0.21 | 48,49,49,50                | 4     |
| 7   | GOL  | A     | 515 | 6/6   | 0.62 | 0.20 | 51,54,55,55                | 6     |
| 3   | ACT  | B     | 504 | 4/4   | 0.66 | 0.28 | 41,41,41,42                | 4     |
| 3   | ACT  | A     | 506 | 4/4   | 0.68 | 0.23 | 57,58,58,58                | 4     |
| 7   | GOL  | B     | 515 | 6/6   | 0.69 | 0.20 | 29,40,42,42                | 6     |
| 7   | GOL  | B     | 512 | 6/6   | 0.70 | 0.31 | 46,49,50,51                | 6     |
| 3   | ACT  | C     | 505 | 4/4   | 0.71 | 0.32 | 40,40,40,40                | 4     |
| 7   | GOL  | A     | 514 | 6/6   | 0.71 | 0.22 | 39,42,44,45                | 6     |
| 5   | CL   | B     | 510 | 1/1   | 0.71 | 0.35 | 50,50,50,50                | 1     |
| 3   | ACT  | C     | 506 | 4/4   | 0.72 | 0.22 | 34,34,35,35                | 4     |
| 7   | GOL  | A     | 513 | 6/6   | 0.77 | 0.35 | 45,49,50,51                | 6     |
| 7   | GOL  | B     | 513 | 6/6   | 0.79 | 0.20 | 28,30,31,33                | 6     |
| 5   | CL   | A     | 510 | 1/1   | 0.85 | 0.09 | 90,90,90,90                | 0     |
| 4   | SO4  | A     | 508 | 5/5   | 0.85 | 0.16 | 47,48,52,52                | 5     |
| 3   | ACT  | C     | 504 | 4/4   | 0.87 | 0.16 | 37,38,38,39                | 0     |
| 6   | HCT  | C     | 509 | 13/13 | 0.88 | 0.11 | 48,58,65,67                | 0     |
| 3   | ACT  | B     | 505 | 4/4   | 0.88 | 0.09 | 65,66,66,66                | 0     |
| 3   | ACT  | B     | 507 | 4/4   | 0.88 | 0.11 | 36,37,37,37                | 4     |
| 3   | ACT  | A     | 504 | 4/4   | 0.90 | 0.11 | 66,66,66,66                | 0     |
| 5   | CL   | B     | 508 | 1/1   | 0.90 | 0.36 | 44,44,44,44                | 1     |
| 6   | HCT  | A     | 511 | 13/13 | 0.93 | 0.09 | 33,53,61,61                | 0     |
| 6   | HCT  | B     | 511 | 13/13 | 0.94 | 0.08 | 35,47,52,53                | 0     |
| 5   | CL   | C     | 508 | 1/1   | 0.97 | 0.04 | 58,58,58,58                | 0     |
| 2   | NI   | A     | 503 | 1/1   | 0.97 | 0.05 | 78,78,78,78                | 0     |
| 2   | NI   | C     | 503 | 1/1   | 0.97 | 0.04 | 66,66,66,66                | 0     |
| 5   | CL   | A     | 509 | 1/1   | 0.97 | 0.13 | 61,61,61,61                | 0     |
| 5   | CL   | C     | 507 | 1/1   | 0.98 | 0.15 | 57,57,57,57                | 0     |
| 2   | NI   | B     | 503 | 1/1   | 0.99 | 0.03 | 53,53,53,53                | 0     |
| 5   | CL   | B     | 509 | 1/1   | 0.99 | 0.04 | 40,40,40,40                | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.