



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 26, 2024 – 05:40 AM EDT

PDB ID : 6YFR  
Title : Virus-like particle of bacteriophage NT-391  
Authors : Rumnieks, J.; Kalnins, G.; Sisovs, M.; Lieknina, I.; Tars, K.  
Deposited on : 2020-03-26  
Resolution : 2.60 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                     | : | 4.02b-467  |
| Xtriage (Phenix)               | : | 1.13   |
| EDS                            | : | 2.37.1   |
| Percentile statistics          | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac                         | : | 5.8.0158   |
| CCP4                           | : | 7.0.044 (Gargrove)   |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)  |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)  |
| Validation Pipeline (wwPDB-VP) | : | 2.37.1   |

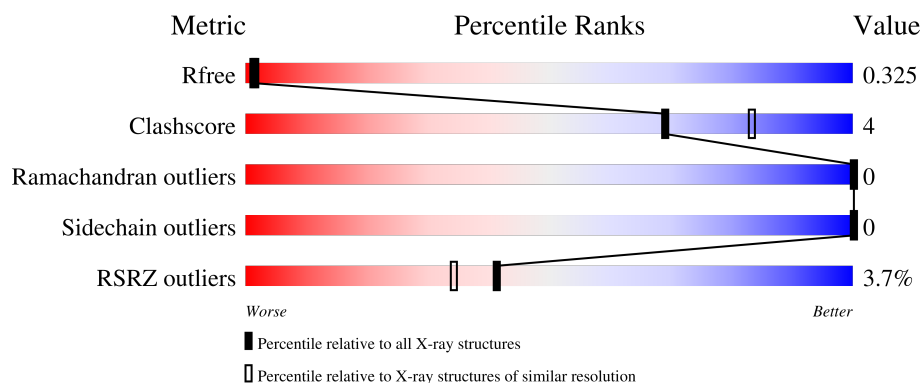
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 3163 (2.60-2.60)                                      |
| Clashscore            | 141614                      | 3518 (2.60-2.60)                                      |
| Ramachandran outliers | 138981                      | 3455 (2.60-2.60)                                      |
| Sidechain outliers    | 138945                      | 3455 (2.60-2.60)                                      |
| RSRZ outliers         | 127900                      | 3104 (2.60-2.60)                                      |

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   | AA    | 123    | <div> <div>2%</div> <div>91%</div> <div>9%</div> </div>  |
| 1   | AB    | 123    | <div> <div>3%</div> <div>86%</div> <div>14%</div> </div> |
| 1   | AC    | 123    | <div> <div>3%</div> <div>91%</div> <div>9%</div> </div>  |
| 1   | AD    | 123    | <div> <div>6%</div> <div>92%</div> <div>8%</div> </div>  |
| 1   | AE    | 123    | <div> <div>2%</div> <div>89%</div> <div>11%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | AF    | 123    |                  |
| 1   | AG    | 123    |                  |
| 1   | AH    | 123    |                  |
| 1   | AI    | 123    |                  |
| 1   | AJ    | 123    |                  |
| 1   | AK    | 123    |                  |
| 1   | AL    | 123    |                  |
| 1   | AM    | 123    |                  |
| 1   | AN    | 123    |                  |
| 1   | AO    | 123    |                  |
| 1   | AP    | 123    |                  |
| 1   | AQ    | 123    |                  |
| 1   | AR    | 123    |                  |
| 1   | AS    | 123    |                  |
| 1   | AT    | 123    |                  |
| 1   | AU    | 123    |                  |
| 1   | AV    | 123    |                  |
| 1   | AW    | 123    |                  |
| 1   | AX    | 123    |                  |
| 1   | AY    | 123    |                  |
| 1   | AZ    | 123    |                  |
| 1   | BA    | 123    |                  |
| 1   | BB    | 123    |                  |
| 1   | BC    | 123    |                  |
| 1   | BD    | 123    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | BE    | 123    |                  |
| 1   | BF    | 123    |                  |
| 1   | BG    | 123    |                  |
| 1   | BH    | 123    |                  |
| 1   | BI    | 123    |                  |
| 1   | BJ    | 123    |                  |
| 1   | BK    | 123    |                  |
| 1   | BL    | 123    |                  |
| 1   | BM    | 123    |                  |
| 1   | BN    | 123    |                  |
| 1   | BO    | 123    |                  |
| 1   | BP    | 123    |                  |
| 1   | BQ    | 123    |                  |
| 1   | BR    | 123    |                  |
| 1   | BS    | 123    |                  |
| 1   | BT    | 123    |                  |
| 1   | BU    | 123    |                  |
| 1   | BV    | 123    |                  |
| 1   | BW    | 123    |                  |
| 1   | BX    | 123    |                  |
| 1   | BY    | 123    |                  |
| 1   | BZ    | 123    |                  |
| 1   | CA    | 123    |                  |
| 1   | CB    | 123    |                  |
| 1   | CC    | 123    |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | CD    | 123    |  91% 9%  |
| 1   | CE    | 123    |  88% 12% |
| 1   | CF    | 123    |  89% 11% |
| 1   | CG    | 123    |  89% 11% |
| 1   | CH    | 123    |  89% 11% |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 56340 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 coat protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | AA    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | AB    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | AC    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | AD    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | AE    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | AF    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | AG    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | AH    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | AI    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | AJ    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | AK    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | AL    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | AM    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | AN    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | AO    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | AP    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms        |          |          |          |        | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|---------|-------|
| 1   | AQ    | 123      | Total<br>939 | C<br>591 | N<br>157 | O<br>186 | S<br>5 | 0       | 0       | 0     |
| 1   | AR    | 123      | Total<br>939 | C<br>591 | N<br>157 | O<br>186 | S<br>5 | 0       | 0       | 0     |
| 1   | AS    | 123      | Total<br>939 | C<br>591 | N<br>157 | O<br>186 | S<br>5 | 0       | 0       | 0     |
| 1   | AT    | 123      | Total<br>939 | C<br>591 | N<br>157 | O<br>186 | S<br>5 | 0       | 0       | 0     |
| 1   | AU    | 123      | Total<br>939 | C<br>591 | N<br>157 | O<br>186 | S<br>5 | 0       | 0       | 0     |
| 1   | AV    | 123      | Total<br>939 | C<br>591 | N<br>157 | O<br>186 | S<br>5 | 0       | 0       | 0     |
| 1   | AW    | 123      | Total<br>939 | C<br>591 | N<br>157 | O<br>186 | S<br>5 | 0       | 0       | 0     |
| 1   | AX    | 123      | Total<br>939 | C<br>591 | N<br>157 | O<br>186 | S<br>5 | 0       | 0       | 0     |
| 1   | AY    | 123      | Total<br>939 | C<br>591 | N<br>157 | O<br>186 | S<br>5 | 0       | 0       | 0     |
| 1   | AZ    | 123      | Total<br>939 | C<br>591 | N<br>157 | O<br>186 | S<br>5 | 0       | 0       | 0     |
| 1   | BA    | 123      | Total<br>939 | C<br>591 | N<br>157 | O<br>186 | S<br>5 | 0       | 0       | 0     |
| 1   | BB    | 123      | Total<br>939 | C<br>591 | N<br>157 | O<br>186 | S<br>5 | 0       | 0       | 0     |
| 1   | BC    | 123      | Total<br>939 | C<br>591 | N<br>157 | O<br>186 | S<br>5 | 0       | 0       | 0     |
| 1   | BD    | 123      | Total<br>939 | C<br>591 | N<br>157 | O<br>186 | S<br>5 | 0       | 0       | 0     |
| 1   | BE    | 123      | Total<br>939 | C<br>591 | N<br>157 | O<br>186 | S<br>5 | 0       | 0       | 0     |
| 1   | BF    | 123      | Total<br>939 | C<br>591 | N<br>157 | O<br>186 | S<br>5 | 0       | 0       | 0     |
| 1   | BG    | 123      | Total<br>939 | C<br>591 | N<br>157 | O<br>186 | S<br>5 | 0       | 0       | 0     |
| 1   | BH    | 123      | Total<br>939 | C<br>591 | N<br>157 | O<br>186 | S<br>5 | 0       | 0       | 0     |
| 1   | BI    | 123      | Total<br>939 | C<br>591 | N<br>157 | O<br>186 | S<br>5 | 0       | 0       | 0     |
| 1   | BJ    | 123      | Total<br>939 | C<br>591 | N<br>157 | O<br>186 | S<br>5 | 0       | 0       | 0     |
| 1   | BK    | 123      | Total<br>939 | C<br>591 | N<br>157 | O<br>186 | S<br>5 | 0       | 0       | 0     |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | BL    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | BM    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | BN    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | BO    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | BP    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | BQ    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | BR    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | BS    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | BT    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | BU    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | BV    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | BW    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | BX    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | BY    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | BZ    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | CA    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | CB    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | CC    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | CD    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | CE    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | CF    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | CG    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |
| 1   | CH    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 591 | 157 | 186 | 5 |         |         |       |

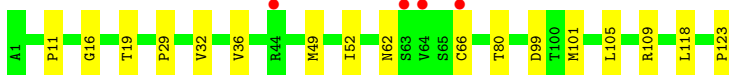
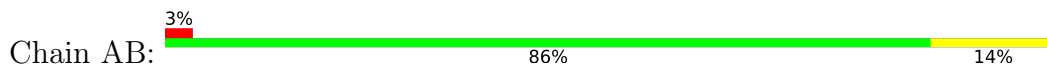
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

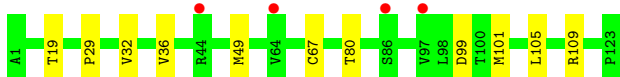
- Molecule 1: coat protein



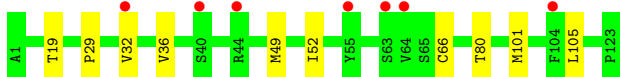
- Molecule 1: coat protein



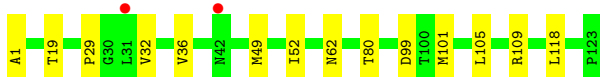
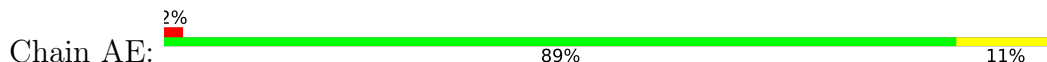
- Molecule 1: coat protein



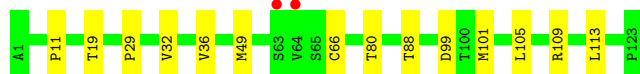
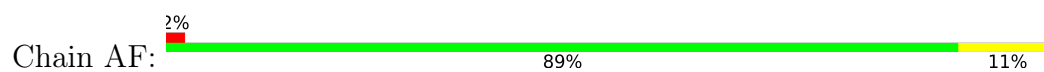
- Molecule 1: coat protein



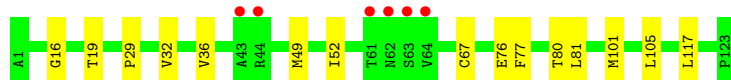
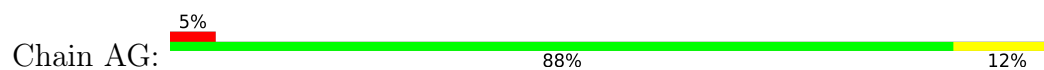
- Molecule 1: coat protein



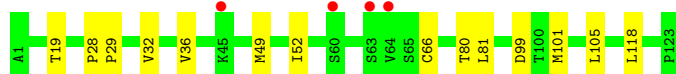
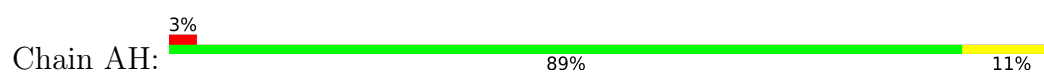
- Molecule 1: coat protein



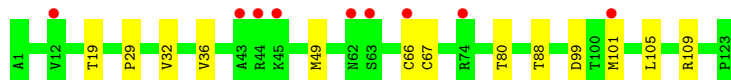
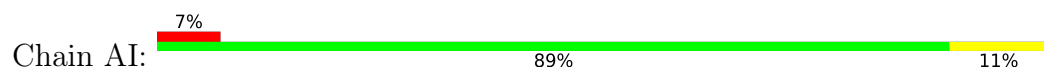
- Molecule 1: coat protein



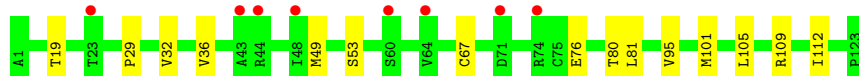
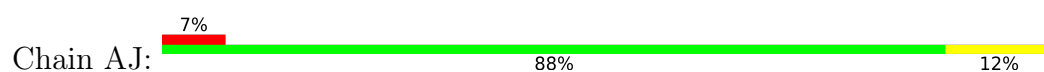
- Molecule 1: coat protein



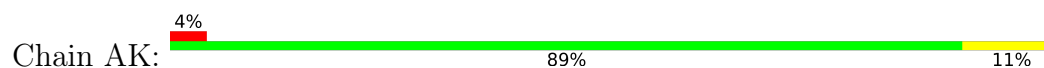
- Molecule 1: coat protein



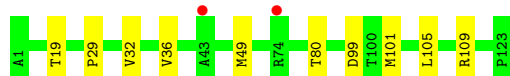
- Molecule 1: coat protein



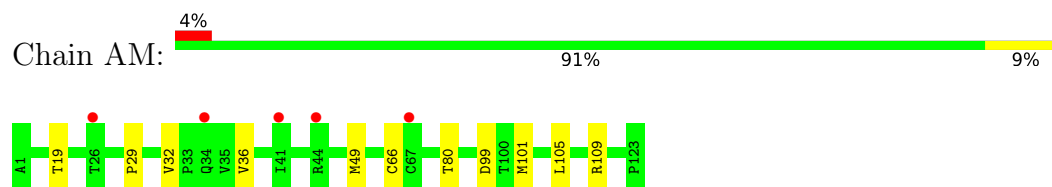
- Molecule 1: coat protein



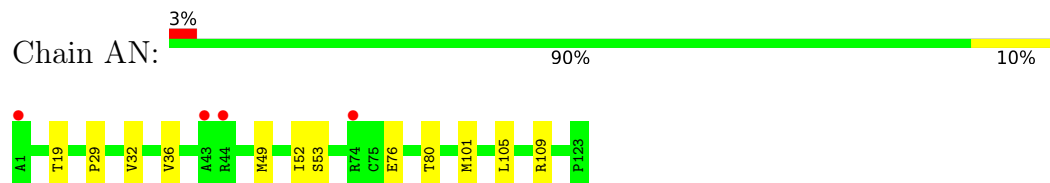
- Molecule 1: coat protein



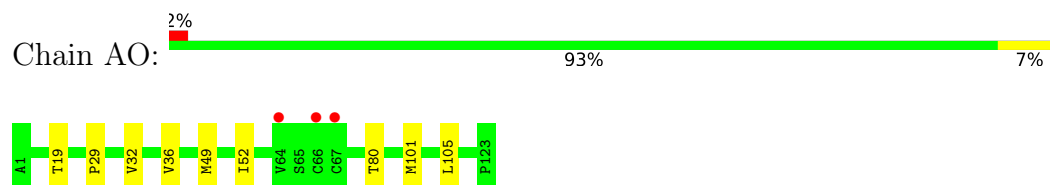
- Molecule 1: coat protein



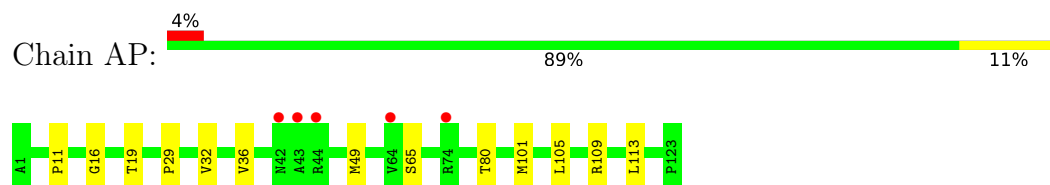
- Molecule 1: coat protein



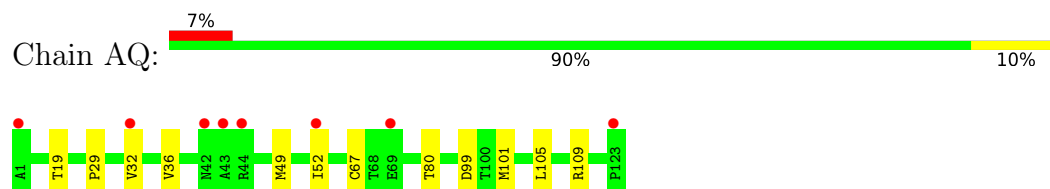
- Molecule 1: coat protein



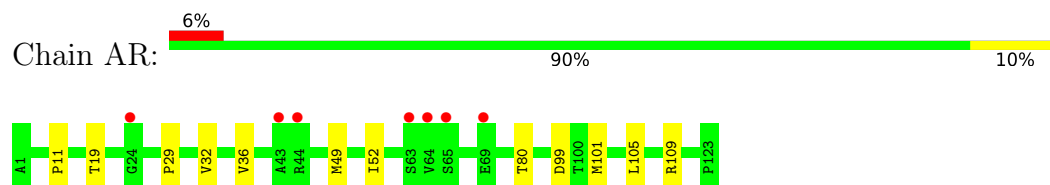
- Molecule 1: coat protein



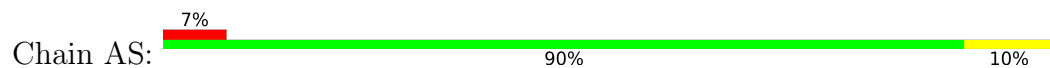
- Molecule 1: coat protein

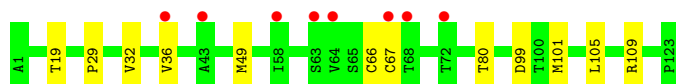


- Molecule 1: coat protein

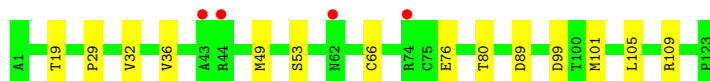
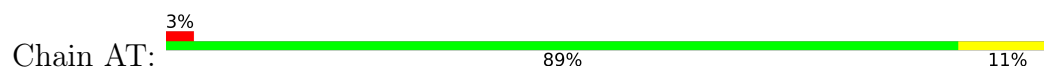


- Molecule 1: coat protein

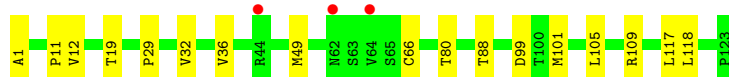
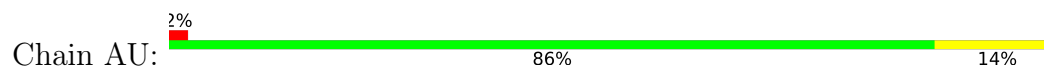




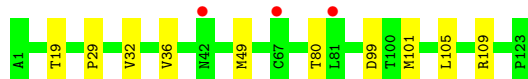
- Molecule 1: coat protein



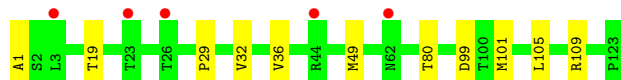
- Molecule 1: coat protein



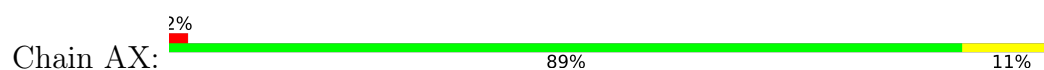
- Molecule 1: coat protein



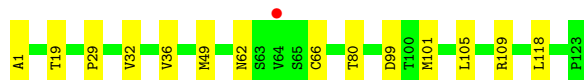
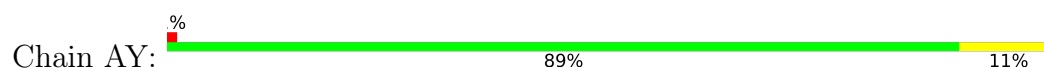
- Molecule 1: coat protein



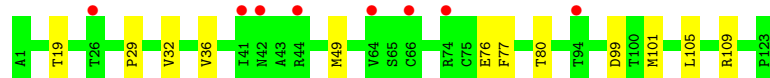
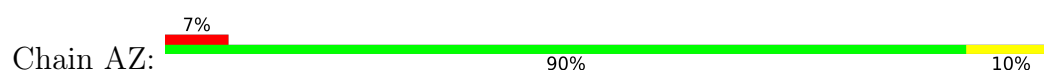
- Molecule 1: coat protein



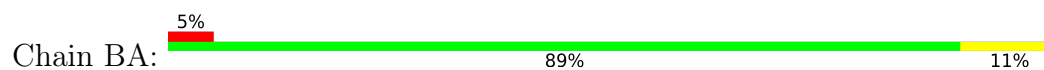
- Molecule 1: coat protein



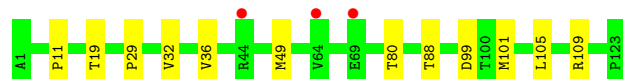
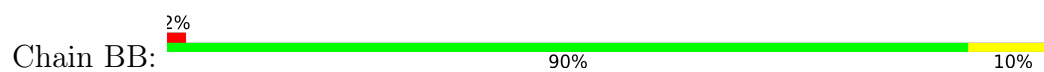
- Molecule 1: coat protein



- Molecule 1: coat protein



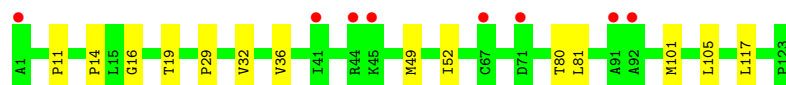
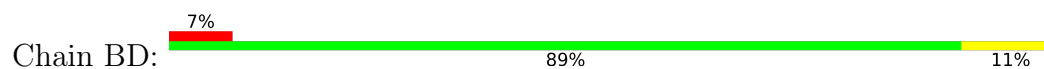
- Molecule 1: coat protein



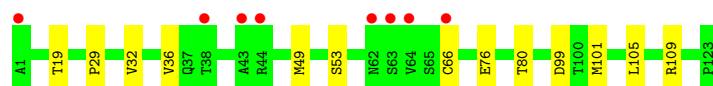
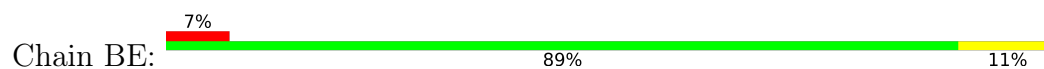
- Molecule 1: coat protein



- Molecule 1: coat protein



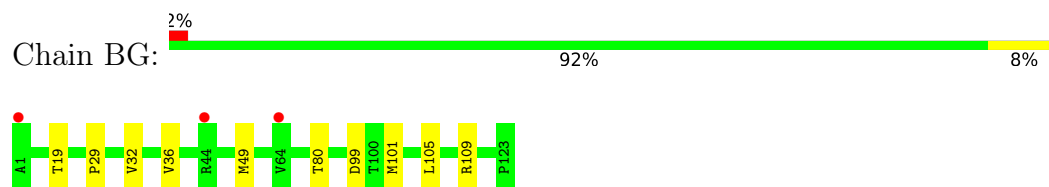
- Molecule 1: coat protein



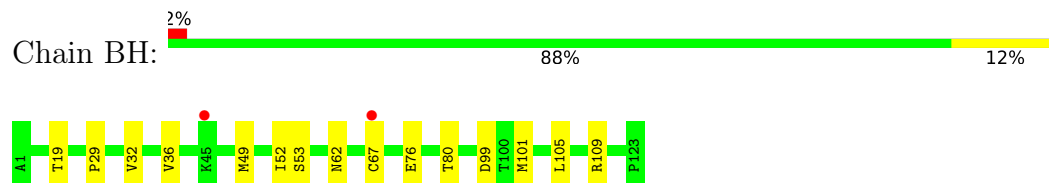
- Molecule 1: coat protein



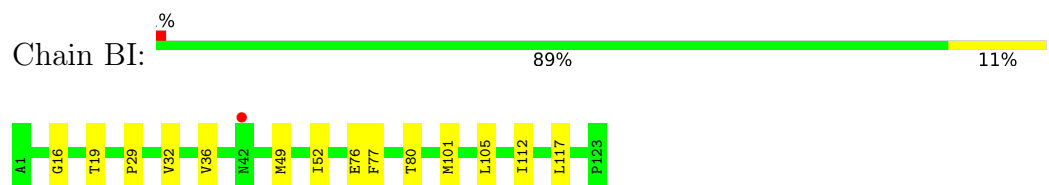
## ● Molecule 1: coat protein



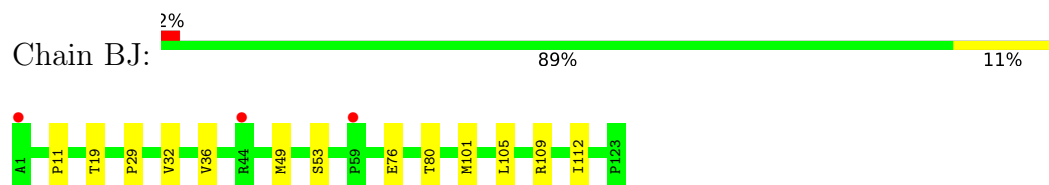
## ● Molecule 1: coat protein



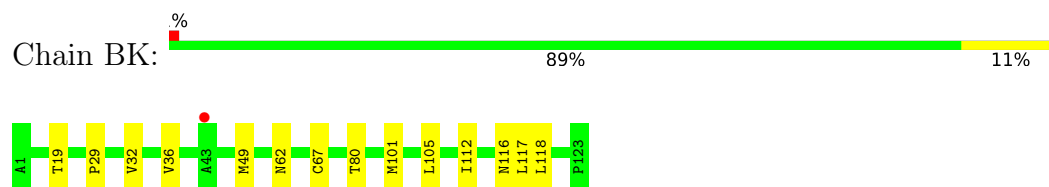
## ● Molecule 1: coat protein



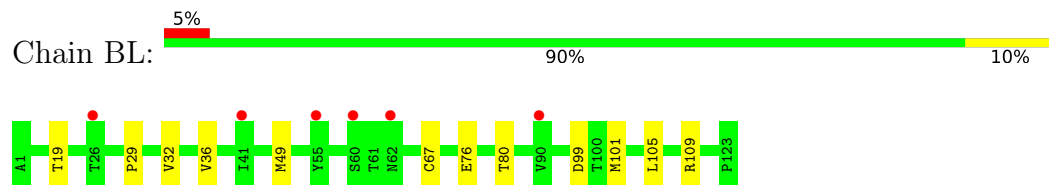
## ● Molecule 1: coat protein



## ● Molecule 1: coat protein



## ● Molecule 1: coat protein

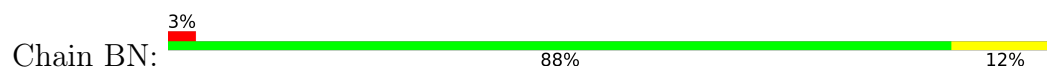


## ● Molecule 1: coat protein

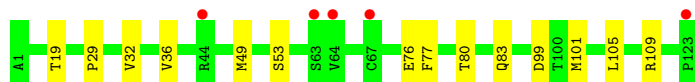
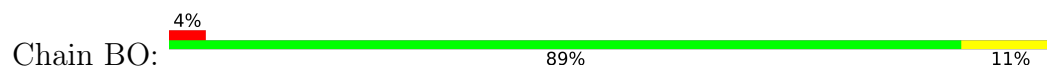




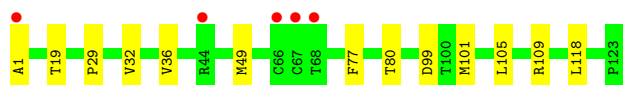
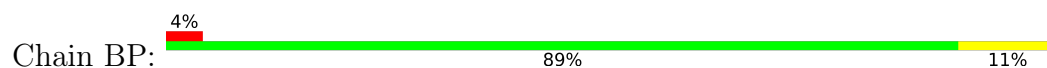
- Molecule 1: coat protein



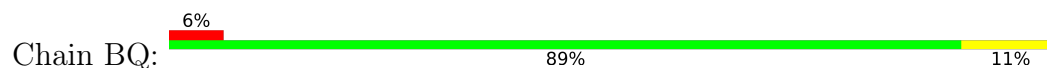
- Molecule 1: coat protein



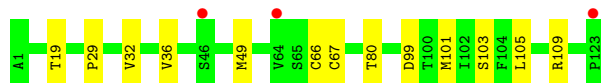
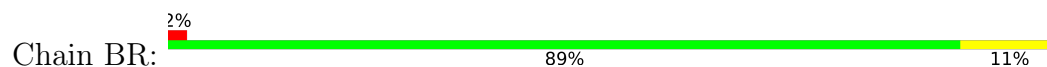
- Molecule 1: coat protein



- Molecule 1: coat protein



- Molecule 1: coat protein

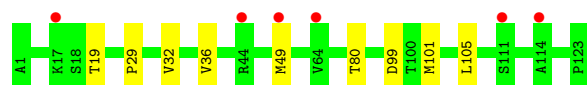


- Molecule 1: coat protein

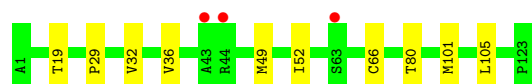


- Molecule 1: coat protein

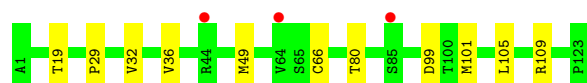
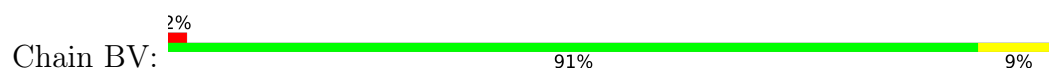




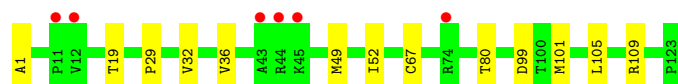
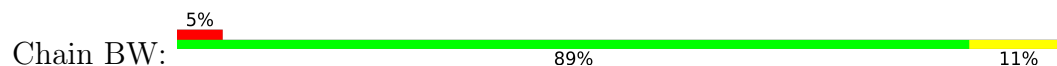
- Molecule 1: coat protein



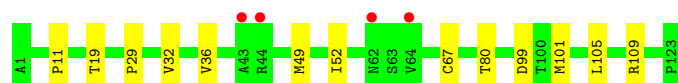
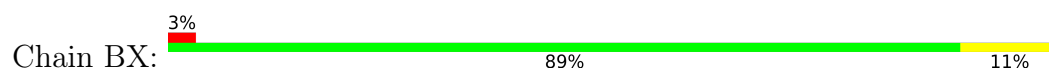
- Molecule 1: coat protein



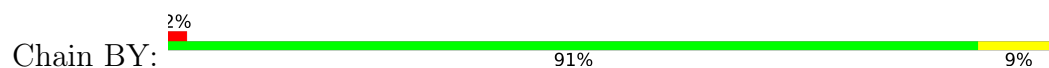
- Molecule 1: coat protein



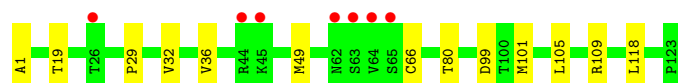
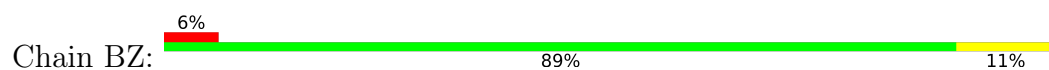
- Molecule 1: coat protein



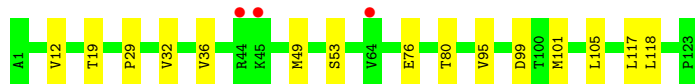
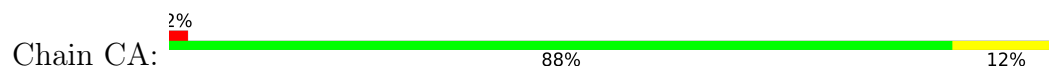
- Molecule 1: coat protein



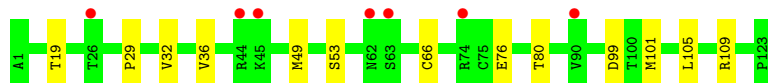
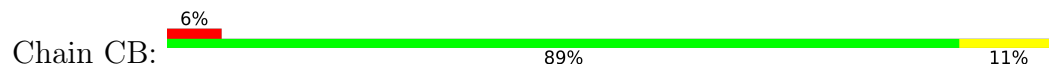
- Molecule 1: coat protein



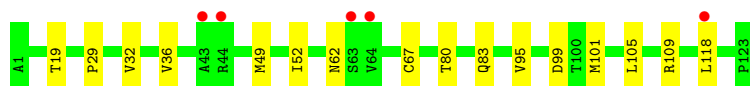
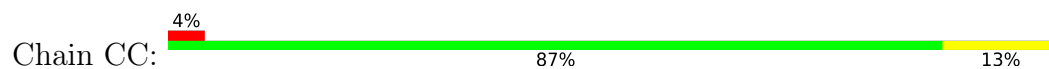
## ● Molecule 1: coat protein



## ● Molecule 1: coat protein



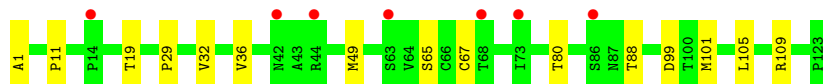
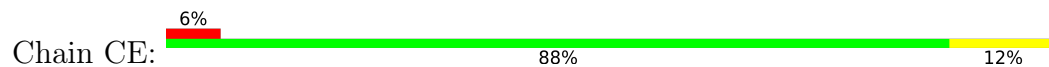
## ● Molecule 1: coat protein



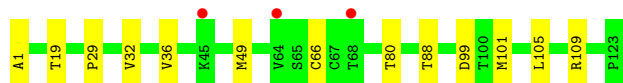
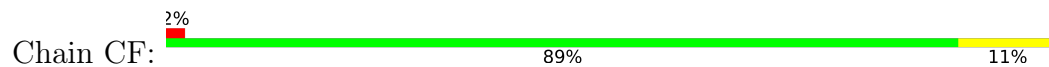
## ● Molecule 1: coat protein



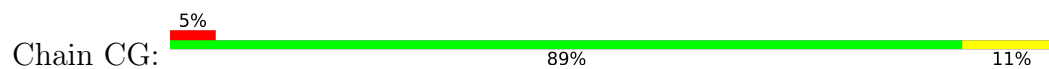
## ● Molecule 1: coat protein

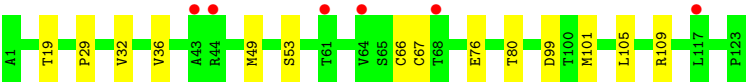


## ● Molecule 1: coat protein

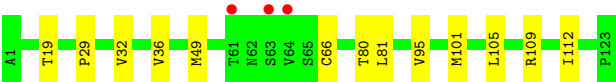
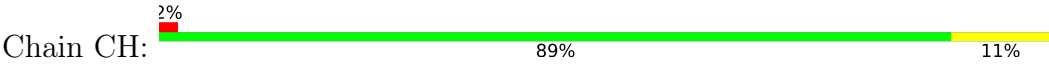


## ● Molecule 1: coat protein





● Molecule 1: coat protein



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 161.92Å 162.07Å 162.98Å<br>71.16° 66.67° 66.83°             | Depositor        |
| Resolution (Å)  | 51.88 – 2.60<br>51.88 – 2.60                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 68.0 (51.88-2.60)<br>69.4 (51.88-2.60)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | 0.24  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.22 (at 2.61Å)   | Xtriage          |
| Refinement program  | PHENIX 1.14 _3260   | Depositor        |
| R, $R_{free}$   | 0.318 , 0.323<br>0.319 , 0.325                              | Depositor<br>DCC |
| $R_{free}$ test set   | 9876 reflections (3.37%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 41.0  | Xtriage          |
| Anisotropy  | 0.467   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 43.0   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$ | Xtriage          |
| Estimated twinning fraction   | 0.028 for -h,-l,-k  | Xtriage          |
| $F_o, F_c$ correlation  | 0.81  | EDS              |
| Total number of atoms   | 56340   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 50.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.12% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 1   | AA    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | AB    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | AC    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | AD    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | AE    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | AF    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | AG    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | AH    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | AI    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | AJ    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | AK    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | AL    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | AM    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | AN    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | AO    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | AP    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | AQ    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | AR    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | AS    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | AT    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | AU    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | AV    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | AW    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | AX    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | AY    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | AZ    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | BA    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | BB    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | BC    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | BD    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | BE    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | BF    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | BG    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | BH    | 0.26         | 0/958   | 0.44        | 0/1313  |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 1   | BI    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | BJ    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | BK    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | BL    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | BM    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | BN    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | BO    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | BP    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | BQ    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | BR    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | BS    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | BT    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | BU    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | BV    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | BW    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | BX    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | BY    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | BZ    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | CA    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | CB    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | CC    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | CD    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | CE    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | CF    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | CG    | 0.26         | 0/958   | 0.44        | 0/1313  |
| 1   | CH    | 0.26         | 0/958   | 0.44        | 0/1313  |
| All | All   | 0.26         | 0/57480 | 0.44        | 0/78780 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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   | AA    | 939   | 0        | 950      | 7       | 0            |
| 1   | AB    | 939   | 0        | 950      | 13      | 1            |
| 1   | AC    | 939   | 0        | 950      | 9       | 0            |
| 1   | AD    | 939   | 0        | 950      | 7       | 0            |
| 1   | AE    | 939   | 0        | 950      | 11      | 0            |
| 1   | AF    | 939   | 0        | 950      | 11      | 0            |
| 1   | AG    | 939   | 0        | 950      | 12      | 0            |
| 1   | AH    | 939   | 0        | 951      | 10      | 0            |
| 1   | AI    | 939   | 0        | 951      | 12      | 0            |
| 1   | AJ    | 939   | 0        | 950      | 10      | 0            |
| 1   | AK    | 939   | 0        | 950      | 10      | 0            |
| 1   | AL    | 939   | 0        | 950      | 8       | 0            |
| 1   | AM    | 939   | 0        | 950      | 7       | 0            |
| 1   | AN    | 939   | 0        | 950      | 7       | 0            |
| 1   | AO    | 939   | 0        | 950      | 6       | 0            |
| 1   | AP    | 939   | 0        | 950      | 9       | 0            |
| 1   | AQ    | 939   | 0        | 950      | 8       | 0            |
| 1   | AR    | 939   | 0        | 950      | 8       | 0            |
| 1   | AS    | 939   | 0        | 950      | 8       | 0            |
| 1   | AT    | 939   | 0        | 951      | 12      | 1            |
| 1   | AU    | 939   | 0        | 950      | 14      | 0            |
| 1   | AV    | 939   | 0        | 950      | 6       | 0            |
| 1   | AW    | 939   | 0        | 950      | 8       | 0            |
| 1   | AX    | 939   | 0        | 951      | 10      | 0            |
| 1   | AY    | 939   | 0        | 950      | 10      | 0            |
| 1   | AZ    | 939   | 0        | 950      | 9       | 0            |
| 1   | BA    | 939   | 0        | 950      | 11      | 0            |
| 1   | BB    | 939   | 0        | 951      | 9       | 0            |
| 1   | BC    | 939   | 0        | 950      | 10      | 0            |
| 1   | BD    | 939   | 0        | 950      | 11      | 0            |
| 1   | BE    | 939   | 0        | 950      | 9       | 0            |
| 1   | BF    | 939   | 0        | 950      | 8       | 0            |
| 1   | BG    | 939   | 0        | 950      | 7       | 0            |
| 1   | BH    | 939   | 0        | 950      | 10      | 0            |
| 1   | BI    | 939   | 0        | 950      | 11      | 0            |
| 1   | BJ    | 939   | 0        | 950      | 9       | 0            |
| 1   | BK    | 939   | 0        | 950      | 11      | 0            |
| 1   | BL    | 939   | 0        | 951      | 9       | 0            |
| 1   | BM    | 939   | 0        | 950      | 9       | 0            |
| 1   | BN    | 939   | 0        | 950      | 11      | 0            |
| 1   | BO    | 939   | 0        | 950      | 9       | 0            |
| 1   | BP    | 939   | 0        | 950      | 9       | 0            |
| 1   | BQ    | 939   | 0        | 950      | 11      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | BR    | 939   | 0        | 950      | 8       | 1            |
| 1   | BS    | 939   | 0        | 951      | 7       | 0            |
| 1   | BT    | 939   | 0        | 950      | 6       | 0            |
| 1   | BU    | 939   | 0        | 950      | 7       | 0            |
| 1   | BV    | 939   | 0        | 950      | 7       | 0            |
| 1   | BW    | 939   | 0        | 950      | 9       | 1            |
| 1   | BX    | 939   | 0        | 950      | 10      | 0            |
| 1   | BY    | 939   | 0        | 950      | 8       | 0            |
| 1   | BZ    | 939   | 0        | 950      | 9       | 1            |
| 1   | CA    | 939   | 0        | 950      | 10      | 0            |
| 1   | CB    | 939   | 0        | 950      | 11      | 0            |
| 1   | CC    | 939   | 0        | 950      | 12      | 0            |
| 1   | CD    | 939   | 0        | 950      | 7       | 1            |
| 1   | CE    | 939   | 0        | 951      | 16      | 0            |
| 1   | CF    | 939   | 0        | 950      | 10      | 0            |
| 1   | CG    | 939   | 0        | 950      | 11      | 0            |
| 1   | CH    | 939   | 0        | 950      | 9       | 0            |
| All | All   | 56340 | 0        | 57008    | 407     | 3            |

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 4.

All (407) 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:AD:66:CYS:SG   | 1:AQ:67:CYS:N    | 2.45                     | 0.90              |
| 1:AC:67:CYS:SG   | 1:CB:66:CYS:HA   | 2.17                     | 0.85              |
| 1:AB:66:CYS:SG   | 1:AJ:67:CYS:N    | 2.62                     | 0.73              |
| 1:AF:66:CYS:SG   | 1:AP:65:SER:HB2  | 2.31                     | 0.70              |
| 1:AT:66:CYS:HA   | 1:CE:67:CYS:SG   | 2.32                     | 0.70              |
| 1:AI:66:CYS:HG   | 1:BL:67:CYS:HG   | 0.73                     | 0.68              |
| 1:AT:66:CYS:CB   | 1:CE:67:CYS:SG   | 2.84                     | 0.65              |
| 1:AT:66:CYS:SG   | 1:CE:65:SER:HB2  | 2.36                     | 0.65              |
| 1:AG:52:ILE:HB   | 1:BI:101:MET:HE1 | 1.79                     | 0.64              |
| 1:AY:99:ASP:OD1  | 1:BB:109:ARG:NH2 | 2.30                     | 0.64              |
| 1:AT:66:CYS:CB   | 1:CE:67:CYS:HG   | 2.11                     | 0.63              |
| 1:AC:67:CYS:SG   | 1:CB:66:CYS:CB   | 2.90                     | 0.60              |
| 1:AC:67:CYS:SG   | 1:CB:66:CYS:CA   | 2.89                     | 0.59              |
| 1:AR:101:MET:HE2 | 1:AR:105:LEU:HG  | 1.86                     | 0.58              |
| 1:AY:109:ARG:NH2 | 1:BB:99:ASP:OD1  | 2.36                     | 0.58              |
| 1:AB:101:MET:HE2 | 1:AB:105:LEU:HG  | 1.86                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:AL:109:ARG:NH2 | 1:CG:99:ASP:OD1  | 2.37                     | 0.58              |
| 1:AT:101:MET:HE2 | 1:AT:105:LEU:HG  | 1.87                     | 0.57              |
| 1:AG:67:CYS:N    | 1:BR:66:CYS:SG   | 2.77                     | 0.57              |
| 1:AH:101:MET:HE2 | 1:AH:105:LEU:HG  | 1.87                     | 0.57              |
| 1:AE:101:MET:HE2 | 1:AE:105:LEU:HG  | 1.87                     | 0.56              |
| 1:BM:109:ARG:NH2 | 1:BP:99:ASP:OD1  | 2.38                     | 0.56              |
| 1:AT:66:CYS:CA   | 1:CE:67:CYS:SG   | 2.94                     | 0.56              |
| 1:CG:101:MET:HE2 | 1:CG:105:LEU:HG  | 1.87                     | 0.56              |
| 1:BA:101:MET:HE1 | 1:BD:52:ILE:HB   | 1.88                     | 0.56              |
| 1:BW:101:MET:HE2 | 1:BW:105:LEU:HG  | 1.88                     | 0.56              |
| 1:BV:101:MET:HE2 | 1:BV:105:LEU:HG  | 1.87                     | 0.56              |
| 1:AA:101:MET:HE2 | 1:AA:105:LEU:HG  | 1.87                     | 0.56              |
| 1:AM:101:MET:HE2 | 1:AM:105:LEU:HG  | 1.87                     | 0.56              |
| 1:BX:67:CYS:SG   | 1:CF:66:CYS:HA   | 2.45                     | 0.56              |
| 1:AL:99:ASP:OD1  | 1:CG:109:ARG:NH2 | 2.38                     | 0.56              |
| 1:CA:101:MET:HE2 | 1:CA:105:LEU:HG  | 1.88                     | 0.56              |
| 1:CC:101:MET:HE2 | 1:CC:105:LEU:HG  | 1.87                     | 0.56              |
| 1:BM:101:MET:HE2 | 1:BM:105:LEU:HG  | 1.88                     | 0.56              |
| 1:BR:101:MET:HE2 | 1:BR:105:LEU:HG  | 1.87                     | 0.56              |
| 1:AN:101:MET:HE2 | 1:AN:105:LEU:HG  | 1.87                     | 0.56              |
| 1:AY:101:MET:HE2 | 1:AY:105:LEU:HG  | 1.87                     | 0.56              |
| 1:BC:101:MET:HE2 | 1:BC:105:LEU:HG  | 1.88                     | 0.55              |
| 1:BL:101:MET:HE2 | 1:BL:105:LEU:HG  | 1.88                     | 0.55              |
| 1:AJ:101:MET:HE2 | 1:AJ:105:LEU:HG  | 1.89                     | 0.55              |
| 1:BF:101:MET:HE2 | 1:BF:105:LEU:HG  | 1.89                     | 0.55              |
| 1:BB:101:MET:HE2 | 1:BB:105:LEU:HG  | 1.88                     | 0.55              |
| 1:AS:101:MET:HE2 | 1:AS:105:LEU:HG  | 1.89                     | 0.55              |
| 1:AF:109:ARG:NH2 | 1:CC:99:ASP:OD1  | 2.39                     | 0.55              |
| 1:AQ:109:ARG:NH2 | 1:CB:99:ASP:OD1  | 2.39                     | 0.55              |
| 1:AJ:112:ILE:O   | 1:CH:81:LEU:HD11 | 2.07                     | 0.55              |
| 1:AV:101:MET:HE2 | 1:AV:105:LEU:HG  | 1.90                     | 0.54              |
| 1:BU:101:MET:HE2 | 1:BU:105:LEU:HG  | 1.90                     | 0.54              |
| 1:AP:101:MET:HE2 | 1:AP:105:LEU:HG  | 1.89                     | 0.54              |
| 1:AL:101:MET:HE2 | 1:AL:105:LEU:HG  | 1.89                     | 0.54              |
| 1:BG:101:MET:HE2 | 1:BG:105:LEU:HG  | 1.90                     | 0.54              |
| 1:BP:101:MET:HE2 | 1:BP:105:LEU:HG  | 1.90                     | 0.54              |
| 1:AQ:101:MET:HE2 | 1:AQ:105:LEU:HG  | 1.88                     | 0.54              |
| 1:BY:101:MET:HE2 | 1:BY:105:LEU:HG  | 1.90                     | 0.54              |
| 1:AK:101:MET:HE2 | 1:AK:105:LEU:HG  | 1.90                     | 0.54              |
| 1:AW:101:MET:HE2 | 1:AW:105:LEU:HG  | 1.90                     | 0.54              |
| 1:BO:101:MET:HE2 | 1:BO:105:LEU:HG  | 1.90                     | 0.53              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:AU:101:MET:HE2  | 1:AU:105:LEU:HG  | 1.90                     | 0.53              |
| 1:AZ:101:MET:HE2  | 1:AZ:105:LEU:HG  | 1.90                     | 0.53              |
| 1:BT:101:MET:HE2  | 1:BT:105:LEU:HG  | 1.91                     | 0.53              |
| 1:BN:101:MET:HE2  | 1:BN:105:LEU:HG  | 1.90                     | 0.53              |
| 1:AG:101:MET:HE1  | 1:BI:52:ILE:HB   | 1.89                     | 0.53              |
| 1:BE:66:CYS:SG    | 1:CG:67:CYS:N    | 2.81                     | 0.53              |
| 1:CH:101:MET:HE2  | 1:CH:105:LEU:HG  | 1.89                     | 0.53              |
| 1:BH:101:MET:HE2  | 1:BH:105:LEU:HG  | 1.90                     | 0.53              |
| 1:AX:99:ASP:OD1   | 1:BX:109:ARG:NH2 | 2.41                     | 0.53              |
| 1:BK:117:LEU:HD11 | 1:BN:16:GLY:C    | 2.29                     | 0.53              |
| 1:BS:101:MET:HE2  | 1:BS:105:LEU:HG  | 1.91                     | 0.53              |
| 1:BX:101:MET:HE2  | 1:BX:105:LEU:HG  | 1.91                     | 0.53              |
| 1:BQ:101:MET:HE2  | 1:BQ:105:LEU:HG  | 1.91                     | 0.53              |
| 1:AO:101:MET:HE2  | 1:AO:105:LEU:HG  | 1.90                     | 0.52              |
| 1:AQ:99:ASP:OD1   | 1:CB:109:ARG:NH2 | 2.41                     | 0.52              |
| 1:BJ:101:MET:HE2  | 1:BJ:105:LEU:HG  | 1.91                     | 0.52              |
| 1:AC:101:MET:HE2  | 1:AC:105:LEU:HG  | 1.90                     | 0.52              |
| 1:AC:99:ASP:OD1   | 1:AS:109:ARG:NH2 | 2.42                     | 0.52              |
| 1:BK:101:MET:HE2  | 1:BK:105:LEU:HG  | 1.92                     | 0.52              |
| 1:AS:66:CYS:SG    | 1:CD:67:CYS:N    | 2.81                     | 0.52              |
| 1:BD:101:MET:HE2  | 1:BD:105:LEU:HG  | 1.92                     | 0.52              |
| 1:BE:101:MET:HE1  | 1:BS:52:ILE:HB   | 1.91                     | 0.52              |
| 1:BN:29:PRO:HA    | 1:BN:32:VAL:HG23 | 1.92                     | 0.52              |
| 1:BM:29:PRO:HA    | 1:BM:32:VAL:HG23 | 1.92                     | 0.52              |
| 1:BO:29:PRO:HA    | 1:BO:32:VAL:HG23 | 1.92                     | 0.52              |
| 1:AA:29:PRO:HA    | 1:AA:32:VAL:HG23 | 1.92                     | 0.52              |
| 1:BP:29:PRO:HA    | 1:BP:32:VAL:HG23 | 1.92                     | 0.52              |
| 1:BZ:29:PRO:HA    | 1:BZ:32:VAL:HG23 | 1.92                     | 0.52              |
| 1:BZ:101:MET:HE2  | 1:BZ:105:LEU:HG  | 1.90                     | 0.52              |
| 1:CD:101:MET:HE2  | 1:CD:105:LEU:HG  | 1.92                     | 0.52              |
| 1:AZ:29:PRO:HA    | 1:AZ:32:VAL:HG23 | 1.92                     | 0.52              |
| 1:BI:29:PRO:HA    | 1:BI:32:VAL:HG23 | 1.92                     | 0.52              |
| 1:BJ:29:PRO:HA    | 1:BJ:32:VAL:HG23 | 1.92                     | 0.52              |
| 1:BX:29:PRO:HA    | 1:BX:32:VAL:HG23 | 1.92                     | 0.52              |
| 1:AP:29:PRO:HA    | 1:AP:32:VAL:HG23 | 1.92                     | 0.51              |
| 1:CE:29:PRO:HA    | 1:CE:32:VAL:HG23 | 1.92                     | 0.51              |
| 1:AQ:29:PRO:HA    | 1:AQ:32:VAL:HG23 | 1.92                     | 0.51              |
| 1:CC:29:PRO:HA    | 1:CC:32:VAL:HG23 | 1.92                     | 0.51              |
| 1:CG:53:SER:OG    | 1:CG:76:GLU:OE1  | 2.27                     | 0.51              |
| 1:AC:29:PRO:HA    | 1:AC:32:VAL:HG23 | 1.92                     | 0.51              |
| 1:AD:101:MET:HE2  | 1:AD:105:LEU:HG  | 1.93                     | 0.51              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:BD:29:PRO:HA    | 1:BD:32:VAL:HG23 | 1.92                     | 0.51              |
| 1:CF:101:MET:HE2  | 1:CF:105:LEU:HG  | 1.91                     | 0.51              |
| 1:CH:29:PRO:HA    | 1:CH:32:VAL:HG23 | 1.92                     | 0.51              |
| 1:AN:29:PRO:HA    | 1:AN:32:VAL:HG23 | 1.92                     | 0.51              |
| 1:AO:29:PRO:HA    | 1:AO:32:VAL:HG23 | 1.92                     | 0.51              |
| 1:AU:29:PRO:HA    | 1:AU:32:VAL:HG23 | 1.92                     | 0.51              |
| 1:BW:29:PRO:HA    | 1:BW:32:VAL:HG23 | 1.92                     | 0.51              |
| 1:AB:29:PRO:HA    | 1:AB:32:VAL:HG23 | 1.92                     | 0.51              |
| 1:AD:29:PRO:HA    | 1:AD:32:VAL:HG23 | 1.92                     | 0.51              |
| 1:AI:29:PRO:HA    | 1:AI:32:VAL:HG23 | 1.92                     | 0.51              |
| 1:AP:109:ARG:NH2  | 1:CA:99:ASP:OD1  | 2.43                     | 0.51              |
| 1:BR:29:PRO:HA    | 1:BR:32:VAL:HG23 | 1.92                     | 0.51              |
| 1:AH:29:PRO:HA    | 1:AH:32:VAL:HG23 | 1.92                     | 0.51              |
| 1:AX:101:MET:HE2  | 1:AX:105:LEU:HG  | 1.92                     | 0.51              |
| 1:BV:29:PRO:HA    | 1:BV:32:VAL:HG23 | 1.92                     | 0.51              |
| 1:AA:109:ARG:NH2  | 1:AT:99:ASP:OD1  | 2.44                     | 0.51              |
| 1:BU:29:PRO:HA    | 1:BU:32:VAL:HG23 | 1.92                     | 0.51              |
| 1:BY:67:CYS:N     | 1:CG:66:CYS:SG   | 2.83                     | 0.51              |
| 1:AA:99:ASP:OD1   | 1:AT:109:ARG:NH2 | 2.42                     | 0.51              |
| 1:AF:29:PRO:HA    | 1:AF:32:VAL:HG23 | 1.92                     | 0.51              |
| 1:AR:109:ARG:NH2  | 1:BZ:99:ASP:OD1  | 2.44                     | 0.51              |
| 1:BC:29:PRO:HA    | 1:BC:32:VAL:HG23 | 1.92                     | 0.51              |
| 1:BK:29:PRO:HA    | 1:BK:32:VAL:HG23 | 1.92                     | 0.51              |
| 1:CA:29:PRO:HA    | 1:CA:32:VAL:HG23 | 1.92                     | 0.51              |
| 1:BA:117:LEU:HD11 | 1:BD:16:GLY:C    | 2.31                     | 0.51              |
| 1:CB:29:PRO:HA    | 1:CB:32:VAL:HG23 | 1.92                     | 0.51              |
| 1:AT:29:PRO:HA    | 1:AT:32:VAL:HG23 | 1.92                     | 0.50              |
| 1:BE:29:PRO:HA    | 1:BE:32:VAL:HG23 | 1.92                     | 0.50              |
| 1:CD:29:PRO:HA    | 1:CD:32:VAL:HG23 | 1.92                     | 0.50              |
| 1:CG:29:PRO:HA    | 1:CG:32:VAL:HG23 | 1.92                     | 0.50              |
| 1:AC:109:ARG:NH2  | 1:AS:99:ASP:OD1  | 2.45                     | 0.50              |
| 1:AG:101:MET:HE2  | 1:AG:105:LEU:HG  | 1.92                     | 0.50              |
| 1:AK:29:PRO:HA    | 1:AK:32:VAL:HG23 | 1.92                     | 0.50              |
| 1:AL:29:PRO:HA    | 1:AL:32:VAL:HG23 | 1.92                     | 0.50              |
| 1:AS:29:PRO:HA    | 1:AS:32:VAL:HG23 | 1.92                     | 0.50              |
| 1:BF:81:LEU:HD11  | 1:BQ:112:ILE:O   | 2.11                     | 0.50              |
| 1:AV:29:PRO:HA    | 1:AV:32:VAL:HG23 | 1.92                     | 0.50              |
| 1:AX:29:PRO:HA    | 1:AX:32:VAL:HG23 | 1.92                     | 0.50              |
| 1:BB:29:PRO:HA    | 1:BB:32:VAL:HG23 | 1.92                     | 0.50              |
| 1:AJ:29:PRO:HA    | 1:AJ:32:VAL:HG23 | 1.92                     | 0.50              |
| 1:AW:29:PRO:HA    | 1:AW:32:VAL:HG23 | 1.92                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:BY:29:PRO:HA    | 1:BY:32:VAL:HG23  | 1.92                     | 0.50              |
| 1:AE:29:PRO:HA    | 1:AE:32:VAL:HG23  | 1.92                     | 0.50              |
| 1:BT:29:PRO:HA    | 1:BT:32:VAL:HG23  | 1.92                     | 0.50              |
| 1:AG:29:PRO:HA    | 1:AG:32:VAL:HG23  | 1.92                     | 0.50              |
| 1:AJ:109:ARG:HH21 | 1:CH:95:VAL:HG13  | 1.77                     | 0.50              |
| 1:BH:29:PRO:HA    | 1:BH:32:VAL:HG23  | 1.92                     | 0.50              |
| 1:BL:29:PRO:HA    | 1:BL:32:VAL:HG23  | 1.92                     | 0.50              |
| 1:BQ:29:PRO:HA    | 1:BQ:32:VAL:HG23  | 1.92                     | 0.50              |
| 1:CF:29:PRO:HA    | 1:CF:32:VAL:HG23  | 1.92                     | 0.50              |
| 1:AP:11:PRO:HB2   | 1:CA:118:LEU:HD23 | 1.94                     | 0.50              |
| 1:AY:29:PRO:HA    | 1:AY:32:VAL:HG23  | 1.92                     | 0.50              |
| 1:BF:29:PRO:HA    | 1:BF:32:VAL:HG23  | 1.92                     | 0.50              |
| 1:BS:29:PRO:HA    | 1:BS:32:VAL:HG23  | 1.92                     | 0.50              |
| 1:AM:29:PRO:HA    | 1:AM:32:VAL:HG23  | 1.92                     | 0.49              |
| 1:BA:29:PRO:HA    | 1:BA:32:VAL:HG23  | 1.92                     | 0.49              |
| 1:BG:29:PRO:HA    | 1:BG:32:VAL:HG23  | 1.92                     | 0.49              |
| 1:AI:101:MET:HE1  | 1:BH:52:ILE:HB    | 1.93                     | 0.49              |
| 1:AR:29:PRO:HA    | 1:AR:32:VAL:HG23  | 1.92                     | 0.49              |
| 1:BG:19:THR:HG22  | 1:BG:36:VAL:HG22  | 1.95                     | 0.49              |
| 1:BY:19:THR:HG22  | 1:BY:36:VAL:HG22  | 1.95                     | 0.49              |
| 1:BX:19:THR:HG22  | 1:BX:36:VAL:HG22  | 1.95                     | 0.49              |
| 1:AI:19:THR:HG22  | 1:AI:36:VAL:HG22  | 1.95                     | 0.49              |
| 1:AM:19:THR:HG22  | 1:AM:36:VAL:HG22  | 1.95                     | 0.49              |
| 1:BC:19:THR:HG22  | 1:BC:36:VAL:HG22  | 1.95                     | 0.49              |
| 1:BW:19:THR:HG22  | 1:BW:36:VAL:HG22  | 1.95                     | 0.49              |
| 1:BZ:19:THR:HG22  | 1:BZ:36:VAL:HG22  | 1.95                     | 0.49              |
| 1:CB:19:THR:HG22  | 1:CB:36:VAL:HG22  | 1.95                     | 0.49              |
| 1:CB:101:MET:HE2  | 1:CB:105:LEU:HG   | 1.95                     | 0.49              |
| 1:BL:19:THR:HG22  | 1:BL:36:VAL:HG22  | 1.95                     | 0.49              |
| 1:CE:19:THR:HG22  | 1:CE:36:VAL:HG22  | 1.95                     | 0.49              |
| 1:AG:19:THR:HG22  | 1:AG:36:VAL:HG22  | 1.95                     | 0.49              |
| 1:CG:19:THR:HG22  | 1:CG:36:VAL:HG22  | 1.95                     | 0.49              |
| 1:AC:19:THR:HG22  | 1:AC:36:VAL:HG22  | 1.95                     | 0.49              |
| 1:AP:19:THR:HG22  | 1:AP:36:VAL:HG22  | 1.95                     | 0.49              |
| 1:AT:19:THR:HG22  | 1:AT:36:VAL:HG22  | 1.95                     | 0.49              |
| 1:BA:19:THR:HG22  | 1:BA:36:VAL:HG22  | 1.95                     | 0.49              |
| 1:BM:99:ASP:OD1   | 1:BP:109:ARG:NH2  | 2.44                     | 0.49              |
| 1:BP:19:THR:HG22  | 1:BP:36:VAL:HG22  | 1.95                     | 0.49              |
| 1:BQ:19:THR:HG22  | 1:BQ:36:VAL:HG22  | 1.95                     | 0.49              |
| 1:CD:19:THR:HG22  | 1:CD:36:VAL:HG22  | 1.95                     | 0.49              |
| 1:AD:101:MET:HE1  | 1:CD:52:ILE:HB    | 1.95                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:AJ:19:THR:HG22 | 1:AJ:36:VAL:HG22 | 1.95                     | 0.49              |
| 1:AM:99:ASP:OD1  | 1:BV:109:ARG:NH2 | 2.46                     | 0.49              |
| 1:AR:19:THR:HG22 | 1:AR:36:VAL:HG22 | 1.95                     | 0.49              |
| 1:AW:19:THR:HG22 | 1:AW:36:VAL:HG22 | 1.95                     | 0.49              |
| 1:AZ:19:THR:HG22 | 1:AZ:36:VAL:HG22 | 1.95                     | 0.49              |
| 1:BJ:19:THR:HG22 | 1:BJ:36:VAL:HG22 | 1.95                     | 0.49              |
| 1:BN:19:THR:HG22 | 1:BN:36:VAL:HG22 | 1.95                     | 0.49              |
| 1:CE:101:MET:HE2 | 1:CE:105:LEU:HG  | 1.94                     | 0.49              |
| 1:AB:19:THR:HG22 | 1:AB:36:VAL:HG22 | 1.95                     | 0.49              |
| 1:AQ:19:THR:HG22 | 1:AQ:36:VAL:HG22 | 1.95                     | 0.49              |
| 1:BA:101:MET:HE2 | 1:BA:105:LEU:HG  | 1.95                     | 0.49              |
| 1:BH:19:THR:HG22 | 1:BH:36:VAL:HG22 | 1.95                     | 0.49              |
| 1:AB:99:ASP:OD1  | 1:AU:109:ARG:NH2 | 2.45                     | 0.49              |
| 1:AE:52:ILE:HB   | 1:CE:101:MET:HE1 | 1.95                     | 0.49              |
| 1:AK:19:THR:HG22 | 1:AK:36:VAL:HG22 | 1.95                     | 0.49              |
| 1:AE:19:THR:HG22 | 1:AE:36:VAL:HG22 | 1.95                     | 0.48              |
| 1:AH:19:THR:HG22 | 1:AH:36:VAL:HG22 | 1.95                     | 0.48              |
| 1:AN:19:THR:HG22 | 1:AN:36:VAL:HG22 | 1.95                     | 0.48              |
| 1:AS:19:THR:HG22 | 1:AS:36:VAL:HG22 | 1.95                     | 0.48              |
| 1:AY:19:THR:HG22 | 1:AY:36:VAL:HG22 | 1.95                     | 0.48              |
| 1:CH:19:THR:HG22 | 1:CH:36:VAL:HG22 | 1.95                     | 0.48              |
| 1:AF:19:THR:HG22 | 1:AF:36:VAL:HG22 | 1.95                     | 0.48              |
| 1:AO:19:THR:HG22 | 1:AO:36:VAL:HG22 | 1.95                     | 0.48              |
| 1:AV:19:THR:HG22 | 1:AV:36:VAL:HG22 | 1.95                     | 0.48              |
| 1:BQ:67:CYS:N    | 1:BU:66:CYS:SG   | 2.86                     | 0.48              |
| 1:AD:52:ILE:HB   | 1:CD:101:MET:HE1 | 1.95                     | 0.48              |
| 1:AI:101:MET:HE2 | 1:AI:105:LEU:HG  | 1.95                     | 0.48              |
| 1:AX:1:ALA:N     | 1:BX:99:ASP:OD2  | 2.40                     | 0.48              |
| 1:BI:19:THR:HG22 | 1:BI:36:VAL:HG22 | 1.95                     | 0.48              |
| 1:AH:28:PRO:HB2  | 1:BN:83:GLN:O    | 2.12                     | 0.48              |
| 1:AU:19:THR:HG22 | 1:AU:36:VAL:HG22 | 1.95                     | 0.48              |
| 1:BV:19:THR:HG22 | 1:BV:36:VAL:HG22 | 1.95                     | 0.48              |
| 1:AF:101:MET:HE1 | 1:CC:52:ILE:HB   | 1.95                     | 0.48              |
| 1:AL:19:THR:HG22 | 1:AL:36:VAL:HG22 | 1.95                     | 0.48              |
| 1:BB:19:THR:HG22 | 1:BB:36:VAL:HG22 | 1.95                     | 0.48              |
| 1:BO:19:THR:HG22 | 1:BO:36:VAL:HG22 | 1.95                     | 0.48              |
| 1:CC:19:THR:HG22 | 1:CC:36:VAL:HG22 | 1.95                     | 0.48              |
| 1:AX:109:ARG:NH2 | 1:BX:99:ASP:OD1  | 2.46                     | 0.48              |
| 1:BE:19:THR:HG22 | 1:BE:36:VAL:HG22 | 1.95                     | 0.48              |
| 1:BF:19:THR:HG22 | 1:BF:36:VAL:HG22 | 1.95                     | 0.48              |
| 1:BK:19:THR:HG22 | 1:BK:36:VAL:HG22 | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:BM:19:THR:HG22  | 1:BM:36:VAL:HG22  | 1.95                     | 0.48              |
| 1:CF:19:THR:HG22  | 1:CF:36:VAL:HG22  | 1.95                     | 0.48              |
| 1:AB:109:ARG:NH2  | 1:AU:99:ASP:OD1   | 2.47                     | 0.48              |
| 1:BE:101:MET:HE2  | 1:BE:105:LEU:HG   | 1.94                     | 0.48              |
| 1:BS:19:THR:HG22  | 1:BS:36:VAL:HG22  | 1.95                     | 0.48              |
| 1:AH:66:CYS:SG    | 1:BK:67:CYS:N     | 2.87                     | 0.48              |
| 1:BL:109:ARG:NH2  | 1:BO:99:ASP:OD1   | 2.47                     | 0.48              |
| 1:AS:67:CYS:N     | 1:AX:66:CYS:SG    | 2.86                     | 0.48              |
| 1:AX:19:THR:HG22  | 1:AX:36:VAL:HG22  | 1.95                     | 0.48              |
| 1:BR:19:THR:HG22  | 1:BR:36:VAL:HG22  | 1.95                     | 0.48              |
| 1:BT:19:THR:HG22  | 1:BT:36:VAL:HG22  | 1.95                     | 0.48              |
| 1:AE:99:ASP:OD2   | 1:CE:1:ALA:N      | 2.37                     | 0.47              |
| 1:AK:52:ILE:HB    | 1:CF:101:MET:HE1  | 1.96                     | 0.47              |
| 1:CA:19:THR:HG22  | 1:CA:36:VAL:HG22  | 1.95                     | 0.47              |
| 1:AF:101:MET:HE2  | 1:AF:105:LEU:HG   | 1.96                     | 0.47              |
| 1:AI:109:ARG:NH2  | 1:BH:99:ASP:OD1   | 2.48                     | 0.47              |
| 1:BM:11:PRO:HB2   | 1:BP:118:LEU:HD23 | 1.97                     | 0.47              |
| 1:BK:101:MET:HE1  | 1:BN:52:ILE:HB    | 1.97                     | 0.47              |
| 1:AA:19:THR:HG22  | 1:AA:36:VAL:HG22  | 1.95                     | 0.47              |
| 1:AD:19:THR:HG22  | 1:AD:36:VAL:HG22  | 1.95                     | 0.47              |
| 1:BK:118:LEU:HD23 | 1:BN:11:PRO:HB2   | 1.96                     | 0.47              |
| 1:BM:99:ASP:OD2   | 1:BP:1:ALA:N      | 2.38                     | 0.47              |
| 1:AK:83:GLN:HA    | 1:BG:29:PRO:HG2   | 1.96                     | 0.47              |
| 1:BD:19:THR:HG22  | 1:BD:36:VAL:HG22  | 1.95                     | 0.47              |
| 1:AJ:95:VAL:HG13  | 1:CH:109:ARG:HH21 | 1.80                     | 0.47              |
| 1:BL:99:ASP:OD1   | 1:BO:109:ARG:NH2  | 2.48                     | 0.47              |
| 1:BU:19:THR:HG22  | 1:BU:36:VAL:HG22  | 1.95                     | 0.47              |
| 1:BH:53:SER:OG    | 1:BH:76:GLU:OE1   | 2.27                     | 0.47              |
| 1:AE:99:ASP:OD1   | 1:CE:109:ARG:NH2  | 2.45                     | 0.47              |
| 1:AQ:52:ILE:HB    | 1:CB:101:MET:HE1  | 1.97                     | 0.47              |
| 1:AI:66:CYS:SG    | 1:BL:67:CYS:CB    | 3.04                     | 0.46              |
| 1:AM:109:ARG:NH2  | 1:BV:99:ASP:OD1   | 2.47                     | 0.46              |
| 1:AP:113:LEU:HD13 | 1:CA:95:VAL:HG22  | 1.97                     | 0.46              |
| 1:BO:53:SER:OG    | 1:BO:76:GLU:OE1   | 2.27                     | 0.46              |
| 1:CB:53:SER:OG    | 1:CB:76:GLU:OE1   | 2.27                     | 0.46              |
| 1:BE:53:SER:OG    | 1:BE:76:GLU:OE1   | 2.27                     | 0.46              |
| 1:AE:118:LEU:HD23 | 1:CE:11:PRO:HB2   | 1.98                     | 0.46              |
| 1:BI:101:MET:HE2  | 1:BI:105:LEU:HG   | 1.97                     | 0.46              |
| 1:AI:99:ASP:OD1   | 1:BH:109:ARG:NH2  | 2.49                     | 0.46              |
| 1:BW:67:CYS:N     | 1:CH:66:CYS:SG    | 2.88                     | 0.46              |
| 1:AI:67:CYS:N     | 1:BQ:66:CYS:SG    | 2.82                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:BK:116:ASN:CG   | 1:BN:14:PRO:HB3   | 2.36                     | 0.46              |
| 1:BF:52:ILE:HB    | 1:BQ:101:MET:HE1  | 1.98                     | 0.46              |
| 1:BG:109:ARG:NH2  | 1:BR:99:ASP:OD1   | 2.49                     | 0.46              |
| 1:AF:88:THR:HG23  | 1:CC:62:ASN:HD21  | 1.80                     | 0.46              |
| 1:AY:118:LEU:HD23 | 1:BB:11:PRO:HB2   | 1.98                     | 0.45              |
| 1:AH:81:LEU:HD11  | 1:BJ:112:ILE:O    | 2.16                     | 0.45              |
| 1:AZ:99:ASP:OD1   | 1:BC:109:ARG:NH2  | 2.49                     | 0.45              |
| 1:AE:1:ALA:N      | 1:CE:99:ASP:OD2   | 2.34                     | 0.45              |
| 1:AH:52:ILE:HB    | 1:BJ:101:MET:HE1  | 1.99                     | 0.45              |
| 1:AE:62:ASN:HD21  | 1:CE:88:THR:HG23  | 1.81                     | 0.45              |
| 1:AR:99:ASP:OD1   | 1:BZ:109:ARG:NH2  | 2.50                     | 0.45              |
| 1:AX:118:LEU:HD23 | 1:BX:11:PRO:HB2   | 1.99                     | 0.45              |
| 1:AH:99:ASP:OD1   | 1:BJ:109:ARG:NH2  | 2.49                     | 0.45              |
| 1:AE:109:ARG:NH2  | 1:CE:99:ASP:OD1   | 2.50                     | 0.44              |
| 1:AW:99:ASP:OD1   | 1:BW:109:ARG:NH2  | 2.51                     | 0.44              |
| 1:AT:53:SER:OG    | 1:AT:76:GLU:OE1   | 2.27                     | 0.44              |
| 1:AV:99:ASP:OD1   | 1:BY:109:ARG:NH2  | 2.49                     | 0.44              |
| 1:AB:52:ILE:HB    | 1:AU:101:MET:HE1  | 1.99                     | 0.44              |
| 1:AP:16:GLY:C     | 1:CA:117:LEU:HD11 | 2.38                     | 0.44              |
| 1:AX:101:MET:HE1  | 1:BX:52:ILE:HB    | 2.00                     | 0.44              |
| 1:AZ:109:ARG:NH2  | 1:BC:99:ASP:OD1   | 2.50                     | 0.44              |
| 1:AK:99:ASP:OD1   | 1:CF:109:ARG:NH2  | 2.51                     | 0.44              |
| 1:BF:95:VAL:HG13  | 1:BQ:109:ARG:HH21 | 1.83                     | 0.44              |
| 1:AF:11:PRO:HB2   | 1:CC:118:LEU:HD23 | 2.00                     | 0.44              |
| 1:AK:99:ASP:OD2   | 1:CF:1:ALA:N      | 2.38                     | 0.44              |
| 1:AG:81:LEU:HD11  | 1:BI:112:ILE:O    | 2.17                     | 0.44              |
| 1:CH:49:MET:SD    | 1:CH:80:THR:HG22  | 2.58                     | 0.44              |
| 1:AJ:81:LEU:HD11  | 1:CH:112:ILE:O    | 2.18                     | 0.44              |
| 1:BR:49:MET:SD    | 1:BR:80:THR:HG22  | 2.58                     | 0.44              |
| 1:BT:49:MET:SD    | 1:BT:80:THR:HG22  | 2.58                     | 0.44              |
| 1:CA:49:MET:SD    | 1:CA:80:THR:HG22  | 2.58                     | 0.44              |
| 1:AO:52:ILE:HB    | 1:BU:101:MET:HE1  | 2.00                     | 0.43              |
| 1:AP:49:MET:SD    | 1:AP:80:THR:HG22  | 2.58                     | 0.43              |
| 1:AR:52:ILE:HB    | 1:BZ:101:MET:HE1  | 2.00                     | 0.43              |
| 1:AZ:49:MET:SD    | 1:AZ:80:THR:HG22  | 2.58                     | 0.43              |
| 1:BC:49:MET:SD    | 1:BC:80:THR:HG22  | 2.58                     | 0.43              |
| 1:BD:49:MET:SD    | 1:BD:80:THR:HG22  | 2.58                     | 0.43              |
| 1:BF:49:MET:SD    | 1:BF:80:THR:HG22  | 2.58                     | 0.43              |
| 1:BY:49:MET:SD    | 1:BY:80:THR:HG22  | 2.58                     | 0.43              |
| 1:BZ:49:MET:SD    | 1:BZ:80:THR:HG22  | 2.58                     | 0.43              |
| 1:AE:49:MET:SD    | 1:AE:80:THR:HG22  | 2.58                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:AF:113:LEU:HD13 | 1:CC:95:VAL:HG22 | 2.00                     | 0.43              |
| 1:AG:49:MET:SD    | 1:AG:80:THR:HG22 | 2.58                     | 0.43              |
| 1:AJ:49:MET:SD    | 1:AJ:80:THR:HG22 | 2.58                     | 0.43              |
| 1:AK:62:ASN:HD21  | 1:CF:88:THR:HG23 | 1.83                     | 0.43              |
| 1:AS:49:MET:SD    | 1:AS:80:THR:HG22 | 2.58                     | 0.43              |
| 1:BG:99:ASP:OD1   | 1:BR:109:ARG:NH2 | 2.50                     | 0.43              |
| 1:CD:49:MET:SD    | 1:CD:80:THR:HG22 | 2.58                     | 0.43              |
| 1:CF:49:MET:SD    | 1:CF:80:THR:HG22 | 2.58                     | 0.43              |
| 1:AB:49:MET:SD    | 1:AB:80:THR:HG22 | 2.58                     | 0.43              |
| 1:AN:49:MET:SD    | 1:AN:80:THR:HG22 | 2.58                     | 0.43              |
| 1:AO:49:MET:SD    | 1:AO:80:THR:HG22 | 2.58                     | 0.43              |
| 1:AU:49:MET:SD    | 1:AU:80:THR:HG22 | 2.58                     | 0.43              |
| 1:AV:49:MET:SD    | 1:AV:80:THR:HG22 | 2.58                     | 0.43              |
| 1:BX:49:MET:SD    | 1:BX:80:THR:HG22 | 2.58                     | 0.43              |
| 1:CC:49:MET:SD    | 1:CC:80:THR:HG22 | 2.58                     | 0.43              |
| 1:AL:49:MET:SD    | 1:AL:80:THR:HG22 | 2.58                     | 0.43              |
| 1:AR:49:MET:SD    | 1:AR:80:THR:HG22 | 2.58                     | 0.43              |
| 1:AW:49:MET:SD    | 1:AW:80:THR:HG22 | 2.58                     | 0.43              |
| 1:BA:49:MET:SD    | 1:BA:80:THR:HG22 | 2.58                     | 0.43              |
| 1:BU:49:MET:SD    | 1:BU:80:THR:HG22 | 2.58                     | 0.43              |
| 1:AA:49:MET:SD    | 1:AA:80:THR:HG22 | 2.58                     | 0.43              |
| 1:AD:49:MET:SD    | 1:AD:80:THR:HG22 | 2.58                     | 0.43              |
| 1:AH:49:MET:SD    | 1:AH:80:THR:HG22 | 2.58                     | 0.43              |
| 1:AT:49:MET:SD    | 1:AT:80:THR:HG22 | 2.58                     | 0.43              |
| 1:BK:49:MET:SD    | 1:BK:80:THR:HG22 | 2.58                     | 0.43              |
| 1:BL:49:MET:SD    | 1:BL:80:THR:HG22 | 2.58                     | 0.43              |
| 1:AF:49:MET:SD    | 1:AF:80:THR:HG22 | 2.58                     | 0.43              |
| 1:AF:99:ASP:OD1   | 1:CC:109:ARG:NH2 | 2.52                     | 0.43              |
| 1:AG:76:GLU:O     | 1:BI:77:PHE:HA   | 2.18                     | 0.43              |
| 1:AK:49:MET:SD    | 1:AK:80:THR:HG22 | 2.58                     | 0.43              |
| 1:AY:49:MET:SD    | 1:AY:80:THR:HG22 | 2.58                     | 0.43              |
| 1:BM:49:MET:SD    | 1:BM:80:THR:HG22 | 2.58                     | 0.43              |
| 1:CB:49:MET:SD    | 1:CB:80:THR:HG22 | 2.58                     | 0.43              |
| 1:CG:49:MET:SD    | 1:CG:80:THR:HG22 | 2.58                     | 0.43              |
| 1:AG:77:PHE:HA    | 1:BI:76:GLU:O    | 2.19                     | 0.43              |
| 1:AM:49:MET:SD    | 1:AM:80:THR:HG22 | 2.58                     | 0.43              |
| 1:BA:52:ILE:HB    | 1:BD:101:MET:HE1 | 2.00                     | 0.43              |
| 1:BQ:53:SER:OG    | 1:BQ:76:GLU:OE1  | 2.27                     | 0.43              |
| 1:BV:49:MET:SD    | 1:BV:80:THR:HG22 | 2.58                     | 0.43              |
| 1:BW:49:MET:SD    | 1:BW:80:THR:HG22 | 2.58                     | 0.43              |
| 1:CE:49:MET:SD    | 1:CE:80:THR:HG22 | 2.58                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:AC:49:MET:SD    | 1:AC:80:THR:HG22 | 2.58                     | 0.43              |
| 1:AV:109:ARG:NH2  | 1:BY:99:ASP:OD1  | 2.50                     | 0.43              |
| 1:BH:49:MET:SD    | 1:BH:80:THR:HG22 | 2.58                     | 0.43              |
| 1:AB:62:ASN:HD21  | 1:AU:88:THR:HG23 | 1.84                     | 0.43              |
| 1:AM:66:CYS:SG    | 1:BH:67:CYS:N    | 2.88                     | 0.43              |
| 1:AX:49:MET:SD    | 1:AX:80:THR:HG22 | 2.58                     | 0.43              |
| 1:BE:49:MET:SD    | 1:BE:80:THR:HG22 | 2.58                     | 0.43              |
| 1:BG:49:MET:SD    | 1:BG:80:THR:HG22 | 2.58                     | 0.43              |
| 1:AB:99:ASP:OD2   | 1:AU:1:ALA:N     | 2.38                     | 0.43              |
| 1:BK:62:ASN:OD1   | 1:BN:87:ASN:HA   | 2.18                     | 0.43              |
| 1:BN:49:MET:SD    | 1:BN:80:THR:HG22 | 2.58                     | 0.43              |
| 1:BO:49:MET:SD    | 1:BO:80:THR:HG22 | 2.58                     | 0.43              |
| 1:BS:49:MET:SD    | 1:BS:80:THR:HG22 | 2.58                     | 0.43              |
| 1:BB:49:MET:SD    | 1:BB:80:THR:HG22 | 2.58                     | 0.42              |
| 1:BI:49:MET:SD    | 1:BI:80:THR:HG22 | 2.58                     | 0.42              |
| 1:BQ:49:MET:SD    | 1:BQ:80:THR:HG22 | 2.58                     | 0.42              |
| 1:CA:53:SER:OG    | 1:CA:76:GLU:OE1  | 2.27                     | 0.42              |
| 1:AI:49:MET:SD    | 1:AI:80:THR:HG22 | 2.58                     | 0.42              |
| 1:AI:88:THR:HG23  | 1:BH:62:ASN:HD21 | 1.84                     | 0.42              |
| 1:AQ:49:MET:SD    | 1:AQ:80:THR:HG22 | 2.58                     | 0.42              |
| 1:BA:116:ASN:CG   | 1:BD:14:PRO:HB3  | 2.39                     | 0.42              |
| 1:BJ:49:MET:SD    | 1:BJ:80:THR:HG22 | 2.58                     | 0.42              |
| 1:BP:49:MET:SD    | 1:BP:80:THR:HG22 | 2.58                     | 0.42              |
| 1:AY:1:ALA:N      | 1:BB:99:ASP:OD2  | 2.44                     | 0.42              |
| 1:AZ:101:MET:HE1  | 1:BC:52:ILE:HB   | 2.02                     | 0.42              |
| 1:AK:109:ARG:NH2  | 1:CF:99:ASP:OD1  | 2.53                     | 0.42              |
| 1:BE:99:ASP:OD1   | 1:BS:109:ARG:NH2 | 2.52                     | 0.42              |
| 1:AY:62:ASN:HD21  | 1:BB:88:THR:HG23 | 1.85                     | 0.42              |
| 1:AW:101:MET:HE1  | 1:BW:52:ILE:HB   | 2.00                     | 0.41              |
| 1:AW:1:ALA:N      | 1:BW:99:ASP:OD2  | 2.39                     | 0.41              |
| 1:BF:99:ASP:OD1   | 1:BQ:109:ARG:NH2 | 2.53                     | 0.41              |
| 1:BY:29:PRO:HG2   | 1:CC:83:GLN:HA   | 2.01                     | 0.41              |
| 1:AN:52:ILE:HB    | 1:BT:101:MET:HE1 | 2.02                     | 0.41              |
| 1:BK:112:ILE:O    | 1:BN:81:LEU:HD11 | 2.20                     | 0.41              |
| 1:AJ:53:SER:OG    | 1:AJ:76:GLU:OE1  | 2.27                     | 0.41              |
| 1:AZ:77:PHE:HA    | 1:BC:76:GLU:O    | 2.21                     | 0.41              |
| 1:BA:112:ILE:O    | 1:BD:81:LEU:HD11 | 2.21                     | 0.41              |
| 1:AA:67:CYS:N     | 1:BZ:66:CYS:SG   | 2.93                     | 0.41              |
| 1:AH:118:LEU:HD23 | 1:BJ:11:PRO:HB2  | 2.02                     | 0.41              |
| 1:BE:109:ARG:NH2  | 1:BS:99:ASP:OD1  | 2.51                     | 0.41              |
| 1:AN:53:SER:OG    | 1:AN:76:GLU:OE1  | 2.27                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AN:109:ARG:NH2  | 1:BT:99:ASP:OD1   | 2.54                     | 0.41              |
| 1:AU:12:VAL:HG12  | 1:CA:12:VAL:HG21  | 2.01                     | 0.41              |
| 1:BR:67:CYS:N     | 1:BV:66:CYS:SG    | 2.87                     | 0.41              |
| 1:AB:118:LEU:HD23 | 1:AU:11:PRO:HB2   | 2.03                     | 0.41              |
| 1:AG:117:LEU:HD11 | 1:BI:16:GLY:C     | 2.41                     | 0.41              |
| 1:AL:99:ASP:CG    | 1:CG:109:ARG:HH22 | 2.23                     | 0.41              |
| 1:AR:11:PRO:HB2   | 1:BZ:118:LEU:HD23 | 2.03                     | 0.41              |
| 1:AU:66:CYS:SG    | 1:CC:67:CYS:N     | 2.93                     | 0.41              |
| 1:BL:76:GLU:O     | 1:BO:77:PHE:HA    | 2.21                     | 0.41              |
| 1:BM:76:GLU:O     | 1:BP:77:PHE:HA    | 2.21                     | 0.41              |
| 1:AB:16:GLY:C     | 1:AU:117:LEU:HD11 | 2.42                     | 0.40              |
| 1:AG:16:GLY:C     | 1:BI:117:LEU:HD11 | 2.42                     | 0.40              |
| 1:AL:109:ARG:HH22 | 1:CG:99:ASP:CG    | 2.24                     | 0.40              |
| 1:AZ:76:GLU:O     | 1:BC:77:PHE:HA    | 2.22                     | 0.40              |
| 1:AB:11:PRO:HB2   | 1:AU:118:LEU:HD23 | 2.02                     | 0.40              |
| 1:AY:66:CYS:SG    | 1:BC:67:CYS:N     | 2.94                     | 0.40              |
| 1:AI:29:PRO:HG2   | 1:BO:83:GLN:HA    | 2.04                     | 0.40              |
| 1:AW:109:ARG:NH2  | 1:BW:99:ASP:OD1   | 2.52                     | 0.40              |
| 1:BA:118:LEU:HD23 | 1:BD:11:PRO:HB2   | 2.03                     | 0.40              |
| 1:AO:101:MET:HE1  | 1:BU:52:ILE:HB    | 2.03                     | 0.40              |
| 1:BA:16:GLY:C     | 1:BD:117:LEU:HD11 | 2.42                     | 0.40              |
| 1:BJ:53:SER:OG    | 1:BJ:76:GLU:OE1   | 2.27                     | 0.40              |

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1           | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------------|--------------------------|-------------------|
| 1:AB:123:PRO:OXT | 1:BR:103:SER:OG[1_654] | 1.65                     | 0.55              |
| 1:AT:89:ASP:OD1  | 1:BW:1:ALA:CB[1_556]   | 2.06                     | 0.14              |
| 1:BZ:1:ALA:CB    | 1:CD:89:ASP:OD1[1_556] | 2.14                     | 0.06              |

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 1   | AA    | 121/123 (98%) | 121 (100%) | 0       | 0        | 100         | 100 |
| 1   | AB    | 121/123 (98%) | 121 (100%) | 0       | 0        | 100         | 100 |
| 1   | AC    | 121/123 (98%) | 121 (100%) | 0       | 0        | 100         | 100 |
| 1   | AD    | 121/123 (98%) | 121 (100%) | 0       | 0        | 100         | 100 |
| 1   | AE    | 121/123 (98%) | 121 (100%) | 0       | 0        | 100         | 100 |
| 1   | AF    | 121/123 (98%) | 121 (100%) | 0       | 0        | 100         | 100 |
| 1   | AG    | 121/123 (98%) | 121 (100%) | 0       | 0        | 100         | 100 |
| 1   | AH    | 121/123 (98%) | 121 (100%) | 0       | 0        | 100         | 100 |
| 1   | AI    | 121/123 (98%) | 121 (100%) | 0       | 0        | 100         | 100 |
| 1   | AJ    | 121/123 (98%) | 121 (100%) | 0       | 0        | 100         | 100 |
| 1   | AK    | 121/123 (98%) | 121 (100%) | 0       | 0        | 100         | 100 |
| 1   | AL    | 121/123 (98%) | 121 (100%) | 0       | 0        | 100         | 100 |
| 1   | AM    | 121/123 (98%) | 121 (100%) | 0       | 0        | 100         | 100 |
| 1   | AN    | 121/123 (98%) | 121 (100%) | 0       | 0        | 100         | 100 |
| 1   | AO    | 121/123 (98%) | 121 (100%) | 0       | 0        | 100         | 100 |
| 1   | AP    | 121/123 (98%) | 121 (100%) | 0       | 0        | 100         | 100 |
| 1   | AQ    | 121/123 (98%) | 121 (100%) | 0       | 0        | 100         | 100 |
| 1   | AR    | 121/123 (98%) | 121 (100%) | 0       | 0        | 100         | 100 |
| 1   | AS    | 121/123 (98%) | 121 (100%) | 0       | 0        | 100         | 100 |
| 1   | AT    | 121/123 (98%) | 121 (100%) | 0       | 0        | 100         | 100 |
| 1   | AU    | 121/123 (98%) | 121 (100%) | 0       | 0        | 100         | 100 |
| 1   | AV    | 121/123 (98%) | 121 (100%) | 0       | 0        | 100         | 100 |
| 1   | AW    | 121/123 (98%) | 121 (100%) | 0       | 0        | 100         | 100 |
| 1   | AX    | 121/123 (98%) | 121 (100%) | 0       | 0        | 100         | 100 |
| 1   | AY    | 121/123 (98%) | 121 (100%) | 0       | 0        | 100         | 100 |
| 1   | AZ    | 121/123 (98%) | 121 (100%) | 0       | 0        | 100         | 100 |
| 1   | BA    | 121/123 (98%) | 121 (100%) | 0       | 0        | 100         | 100 |
| 1   | BB    | 121/123 (98%) | 121 (100%) | 0       | 0        | 100         | 100 |
| 1   | BC    | 121/123 (98%) | 121 (100%) | 0       | 0        | 100         | 100 |
| 1   | BD    | 121/123 (98%) | 121 (100%) | 0       | 0        | 100         | 100 |
| 1   | BE    | 121/123 (98%) | 121 (100%) | 0       | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured    | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|---------|----------|-------------|-----|
| 1   | BF    | 121/123 (98%)   | 121 (100%)  | 0       | 0        | 100         | 100 |
| 1   | BG    | 121/123 (98%)   | 121 (100%)  | 0       | 0        | 100         | 100 |
| 1   | BH    | 121/123 (98%)   | 121 (100%)  | 0       | 0        | 100         | 100 |
| 1   | BI    | 121/123 (98%)   | 121 (100%)  | 0       | 0        | 100         | 100 |
| 1   | BJ    | 121/123 (98%)   | 121 (100%)  | 0       | 0        | 100         | 100 |
| 1   | BK    | 121/123 (98%)   | 121 (100%)  | 0       | 0        | 100         | 100 |
| 1   | BL    | 121/123 (98%)   | 121 (100%)  | 0       | 0        | 100         | 100 |
| 1   | BM    | 121/123 (98%)   | 121 (100%)  | 0       | 0        | 100         | 100 |
| 1   | BN    | 121/123 (98%)   | 121 (100%)  | 0       | 0        | 100         | 100 |
| 1   | BO    | 121/123 (98%)   | 121 (100%)  | 0       | 0        | 100         | 100 |
| 1   | BP    | 121/123 (98%)   | 121 (100%)  | 0       | 0        | 100         | 100 |
| 1   | BQ    | 121/123 (98%)   | 121 (100%)  | 0       | 0        | 100         | 100 |
| 1   | BR    | 121/123 (98%)   | 121 (100%)  | 0       | 0        | 100         | 100 |
| 1   | BS    | 121/123 (98%)   | 121 (100%)  | 0       | 0        | 100         | 100 |
| 1   | BT    | 121/123 (98%)   | 121 (100%)  | 0       | 0        | 100         | 100 |
| 1   | BU    | 121/123 (98%)   | 121 (100%)  | 0       | 0        | 100         | 100 |
| 1   | BV    | 121/123 (98%)   | 121 (100%)  | 0       | 0        | 100         | 100 |
| 1   | BW    | 121/123 (98%)   | 121 (100%)  | 0       | 0        | 100         | 100 |
| 1   | BX    | 121/123 (98%)   | 121 (100%)  | 0       | 0        | 100         | 100 |
| 1   | BY    | 121/123 (98%)   | 121 (100%)  | 0       | 0        | 100         | 100 |
| 1   | BZ    | 121/123 (98%)   | 121 (100%)  | 0       | 0        | 100         | 100 |
| 1   | CA    | 121/123 (98%)   | 121 (100%)  | 0       | 0        | 100         | 100 |
| 1   | CB    | 121/123 (98%)   | 121 (100%)  | 0       | 0        | 100         | 100 |
| 1   | CC    | 121/123 (98%)   | 121 (100%)  | 0       | 0        | 100         | 100 |
| 1   | CD    | 121/123 (98%)   | 121 (100%)  | 0       | 0        | 100         | 100 |
| 1   | CE    | 121/123 (98%)   | 121 (100%)  | 0       | 0        | 100         | 100 |
| 1   | CF    | 121/123 (98%)   | 121 (100%)  | 0       | 0        | 100         | 100 |
| 1   | CG    | 121/123 (98%)   | 121 (100%)  | 0       | 0        | 100         | 100 |
| 1   | CH    | 121/123 (98%)   | 121 (100%)  | 0       | 0        | 100         | 100 |
| All | All   | 7260/7380 (98%) | 7260 (100%) | 0       | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | AA    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | AB    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | AC    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | AD    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | AE    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | AF    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | AG    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | AH    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | AI    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | AJ    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | AK    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | AL    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | AM    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | AN    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | AO    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | AP    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | AQ    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | AR    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | AS    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | AT    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | AU    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | AV    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | AW    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | AX    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | AY    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | AZ    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | BA    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | BB    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | BC    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | BD    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | BE    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | BF    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | BG    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | BH    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | BI    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | BJ    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | BK    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | BL    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | BM    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | BN    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | BO    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | BP    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | BQ    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | BR    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | BS    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | BT    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | BU    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | BV    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | BW    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | BX    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | BY    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | BZ    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | CA    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | CB    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | CC    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | CD    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 1   | CE    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Rotameric   | Outliers | Percentiles |     |
|-----|-------|------------------|-------------|----------|-------------|-----|
| 1   | CF    | 113/113 (100%)   | 113 (100%)  | 0        | 100         | 100 |
| 1   | CG    | 113/113 (100%)   | 113 (100%)  | 0        | 100         | 100 |
| 1   | CH    | 113/113 (100%)   | 113 (100%)  | 0        | 100         | 100 |
| All | All   | 6780/6780 (100%) | 6780 (100%) | 0        | 100         | 100 |

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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   | AA    | 123/123 (100%) | 0.18   | 2 (1%) 72 68 | 29, 44, 98, 126       | 0     |
| 1   | AB    | 123/123 (100%) | 0.14   | 4 (3%) 46 39 | 29, 44, 98, 126       | 0     |
| 1   | AC    | 123/123 (100%) | 0.31   | 4 (3%) 46 39 | 29, 44, 98, 126       | 0     |
| 1   | AD    | 123/123 (100%) | 0.26   | 7 (5%) 23 18 | 29, 44, 98, 126       | 0     |
| 1   | AE    | 123/123 (100%) | 0.24   | 2 (1%) 72 68 | 29, 44, 98, 126       | 0     |
| 1   | AF    | 123/123 (100%) | 0.20   | 2 (1%) 72 68 | 29, 44, 98, 126       | 0     |
| 1   | AG    | 123/123 (100%) | 0.26   | 6 (4%) 29 23 | 29, 44, 98, 126       | 0     |
| 1   | AH    | 123/123 (100%) | 0.15   | 4 (3%) 46 39 | 29, 44, 98, 126       | 0     |
| 1   | AI    | 123/123 (100%) | 0.33   | 9 (7%) 15 11 | 29, 44, 98, 126       | 0     |
| 1   | AJ    | 123/123 (100%) | 0.34   | 8 (6%) 18 14 | 29, 44, 98, 126       | 0     |
| 1   | AK    | 123/123 (100%) | 0.19   | 5 (4%) 37 30 | 29, 44, 98, 126       | 0     |
| 1   | AL    | 123/123 (100%) | 0.29   | 2 (1%) 72 68 | 29, 44, 98, 126       | 0     |
| 1   | AM    | 123/123 (100%) | 0.18   | 5 (4%) 37 30 | 29, 44, 98, 126       | 0     |
| 1   | AN    | 123/123 (100%) | 0.11   | 4 (3%) 46 39 | 29, 44, 98, 126       | 0     |
| 1   | AO    | 123/123 (100%) | 0.17   | 3 (2%) 59 53 | 29, 44, 98, 126       | 0     |
| 1   | AP    | 123/123 (100%) | 0.20   | 5 (4%) 37 30 | 29, 44, 98, 126       | 0     |
| 1   | AQ    | 123/123 (100%) | 0.28   | 8 (6%) 18 14 | 29, 44, 98, 126       | 0     |
| 1   | AR    | 123/123 (100%) | 0.30   | 7 (5%) 23 18 | 29, 44, 98, 126       | 0     |
| 1   | AS    | 123/123 (100%) | 0.41   | 8 (6%) 18 14 | 29, 44, 98, 126       | 0     |
| 1   | AT    | 123/123 (100%) | 0.26   | 4 (3%) 46 39 | 29, 44, 98, 126       | 0     |
| 1   | AU    | 123/123 (100%) | 0.10   | 3 (2%) 59 53 | 29, 44, 98, 126       | 0     |
| 1   | AV    | 123/123 (100%) | 0.33   | 3 (2%) 59 53 | 29, 44, 98, 126       | 0     |
| 1   | AW    | 123/123 (100%) | 0.18   | 5 (4%) 37 30 | 29, 44, 98, 126       | 0     |
| 1   | AX    | 123/123 (100%) | 0.23   | 3 (2%) 59 53 | 29, 44, 98, 126       | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 1   | AY    | 123/123 (100%) | 0.10   | 1 (0%) 86 84 | 29, 44, 98, 126       | 0     |
| 1   | AZ    | 123/123 (100%) | 0.38   | 8 (6%) 18 14 | 29, 44, 98, 126       | 0     |
| 1   | BA    | 123/123 (100%) | 0.28   | 6 (4%) 29 23 | 29, 44, 98, 126       | 0     |
| 1   | BB    | 123/123 (100%) | 0.20   | 3 (2%) 59 53 | 29, 44, 98, 126       | 0     |
| 1   | BC    | 123/123 (100%) | 0.22   | 0 100 100    | 29, 44, 98, 126       | 0     |
| 1   | BD    | 123/123 (100%) | 0.17   | 8 (6%) 18 14 | 29, 44, 98, 126       | 0     |
| 1   | BE    | 123/123 (100%) | 0.39   | 8 (6%) 18 14 | 29, 44, 98, 126       | 0     |
| 1   | BF    | 123/123 (100%) | 0.11   | 5 (4%) 37 30 | 29, 44, 98, 126       | 0     |
| 1   | BG    | 123/123 (100%) | 0.19   | 3 (2%) 59 53 | 29, 44, 98, 126       | 0     |
| 1   | BH    | 123/123 (100%) | 0.30   | 2 (1%) 72 68 | 29, 44, 98, 126       | 0     |
| 1   | BI    | 123/123 (100%) | 0.00   | 1 (0%) 86 84 | 29, 44, 98, 126       | 0     |
| 1   | BJ    | 123/123 (100%) | 0.20   | 3 (2%) 59 53 | 29, 44, 98, 126       | 0     |
| 1   | BK    | 123/123 (100%) | 0.11   | 1 (0%) 86 84 | 29, 44, 98, 126       | 0     |
| 1   | BL    | 123/123 (100%) | 0.32   | 6 (4%) 29 23 | 29, 44, 98, 126       | 0     |
| 1   | BM    | 123/123 (100%) | 0.23   | 5 (4%) 37 30 | 29, 44, 98, 126       | 0     |
| 1   | BN    | 123/123 (100%) | 0.22   | 4 (3%) 46 39 | 29, 44, 98, 126       | 0     |
| 1   | BO    | 123/123 (100%) | 0.35   | 5 (4%) 37 30 | 29, 44, 98, 126       | 0     |
| 1   | BP    | 123/123 (100%) | 0.20   | 5 (4%) 37 30 | 29, 44, 98, 126       | 0     |
| 1   | BQ    | 123/123 (100%) | 0.25   | 7 (5%) 23 18 | 29, 44, 98, 126       | 0     |
| 1   | BR    | 123/123 (100%) | 0.25   | 3 (2%) 59 53 | 29, 44, 98, 126       | 0     |
| 1   | BS    | 123/123 (100%) | 0.26   | 4 (3%) 46 39 | 29, 44, 98, 126       | 0     |
| 1   | BT    | 123/123 (100%) | 0.39   | 6 (4%) 29 23 | 29, 44, 98, 126       | 0     |
| 1   | BU    | 123/123 (100%) | 0.14   | 3 (2%) 59 53 | 29, 44, 98, 126       | 0     |
| 1   | BV    | 123/123 (100%) | 0.25   | 3 (2%) 59 53 | 29, 44, 98, 126       | 0     |
| 1   | BW    | 123/123 (100%) | 0.21   | 6 (4%) 29 23 | 29, 44, 98, 126       | 0     |
| 1   | BX    | 123/123 (100%) | 0.13   | 4 (3%) 46 39 | 29, 44, 98, 126       | 0     |
| 1   | BY    | 123/123 (100%) | 0.20   | 3 (2%) 59 53 | 29, 44, 98, 126       | 0     |
| 1   | BZ    | 123/123 (100%) | 0.23   | 7 (5%) 23 18 | 29, 44, 98, 126       | 0     |
| 1   | CA    | 123/123 (100%) | 0.24   | 3 (2%) 59 53 | 29, 44, 98, 126       | 0     |
| 1   | CB    | 123/123 (100%) | 0.34   | 7 (5%) 23 18 | 29, 44, 98, 126       | 0     |
| 1   | CC    | 123/123 (100%) | 0.33   | 5 (4%) 37 30 | 29, 44, 98, 126       | 0     |

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| Mol | Chain | Analysed         | <RSRZ> | #RSRZ>2  |    |    | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|------------------|--------|----------|----|----|-----------------------|-------|
| 1   | CD    | 123/123 (100%)   | 0.24   | 3 (2%)   | 59 | 53 | 29, 44, 98, 126       | 0     |
| 1   | CE    | 123/123 (100%)   | 0.21   | 7 (5%)   | 23 | 18 | 29, 44, 98, 126       | 0     |
| 1   | CF    | 123/123 (100%)   | 0.32   | 3 (2%)   | 59 | 53 | 29, 44, 98, 126       | 0     |
| 1   | CG    | 123/123 (100%)   | 0.41   | 6 (4%)   | 29 | 23 | 29, 44, 98, 126       | 0     |
| 1   | CH    | 123/123 (100%)   | 0.25   | 3 (2%)   | 59 | 53 | 29, 44, 98, 126       | 0     |
| All | All   | 7380/7380 (100%) | 0.24   | 270 (3%) | 41 | 34 | 29, 44, 99, 126       | 0     |

All (270) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | AJ    | 44  | ARG  | 7.9  |
| 1   | AS    | 64  | VAL  | 7.6  |
| 1   | AR    | 44  | ARG  | 7.5  |
| 1   | BG    | 44  | ARG  | 7.3  |
| 1   | AU    | 64  | VAL  | 7.1  |
| 1   | AK    | 44  | ARG  | 7.0  |
| 1   | CC    | 43  | ALA  | 6.8  |
| 1   | BS    | 43  | ALA  | 6.6  |
| 1   | BM    | 44  | ARG  | 6.6  |
| 1   | BO    | 67  | CYS  | 6.2  |
| 1   | CG    | 43  | ALA  | 6.1  |
| 1   | AQ    | 43  | ALA  | 6.1  |
| 1   | AW    | 44  | ARG  | 5.9  |
| 1   | BW    | 44  | ARG  | 5.7  |
| 1   | BE    | 43  | ALA  | 5.6  |
| 1   | AX    | 67  | CYS  | 5.5  |
| 1   | BZ    | 64  | VAL  | 5.3  |
| 1   | BP    | 1   | ALA  | 5.3  |
| 1   | BD    | 1   | ALA  | 5.2  |
| 1   | CC    | 64  | VAL  | 5.1  |
| 1   | BJ    | 44  | ARG  | 5.0  |
| 1   | CG    | 44  | ARG  | 4.9  |
| 1   | AM    | 44  | ARG  | 4.9  |
| 1   | AD    | 44  | ARG  | 4.8  |
| 1   | CC    | 44  | ARG  | 4.8  |
| 1   | CF    | 64  | VAL  | 4.7  |
| 1   | BZ    | 62  | ASN  | 4.6  |
| 1   | BE    | 44  | ARG  | 4.5  |
| 1   | AR    | 64  | VAL  | 4.5  |
| 1   | AJ    | 64  | VAL  | 4.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | BT    | 64  | VAL  | 4.4  |
| 1   | BZ    | 44  | ARG  | 4.4  |
| 1   | AH    | 64  | VAL  | 4.3  |
| 1   | BV    | 64  | VAL  | 4.3  |
| 1   | AC    | 64  | VAL  | 4.2  |
| 1   | BR    | 64  | VAL  | 4.2  |
| 1   | AX    | 64  | VAL  | 4.2  |
| 1   | CD    | 43  | ALA  | 4.2  |
| 1   | AR    | 69  | GLU  | 4.2  |
| 1   | BE    | 64  | VAL  | 4.1  |
| 1   | BX    | 44  | ARG  | 4.1  |
| 1   | AR    | 63  | SER  | 4.1  |
| 1   | BT    | 114 | ALA  | 4.1  |
| 1   | BU    | 63  | SER  | 4.1  |
| 1   | AF    | 64  | VAL  | 4.0  |
| 1   | BX    | 62  | ASN  | 3.9  |
| 1   | AG    | 43  | ALA  | 3.8  |
| 1   | AJ    | 43  | ALA  | 3.8  |
| 1   | BW    | 43  | ALA  | 3.8  |
| 1   | BO    | 63  | SER  | 3.7  |
| 1   | AS    | 58  | ILE  | 3.7  |
| 1   | AJ    | 48  | ILE  | 3.7  |
| 1   | AD    | 64  | VAL  | 3.7  |
| 1   | BF    | 64  | VAL  | 3.7  |
| 1   | BG    | 1   | ALA  | 3.6  |
| 1   | AG    | 64  | VAL  | 3.6  |
| 1   | BS    | 44  | ARG  | 3.6  |
| 1   | BN    | 44  | ARG  | 3.6  |
| 1   | BV    | 44  | ARG  | 3.6  |
| 1   | AC    | 97  | VAL  | 3.6  |
| 1   | CA    | 45  | LYS  | 3.6  |
| 1   | AA    | 44  | ARG  | 3.5  |
| 1   | BP    | 66  | CYS  | 3.5  |
| 1   | BZ    | 63  | SER  | 3.5  |
| 1   | BF    | 44  | ARG  | 3.5  |
| 1   | BU    | 44  | ARG  | 3.5  |
| 1   | AP    | 64  | VAL  | 3.5  |
| 1   | AZ    | 66  | CYS  | 3.5  |
| 1   | AS    | 63  | SER  | 3.4  |
| 1   | CA    | 64  | VAL  | 3.4  |
| 1   | CF    | 68  | THR  | 3.4  |
| 1   | BA    | 3   | LEU  | 3.4  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | BM           | 26         | THR         | 3.4         |
| 1          | BE           | 63         | SER         | 3.4         |
| 1          | BW           | 74         | ARG         | 3.4         |
| 1          | CB           | 44         | ARG         | 3.4         |
| 1          | CC           | 118        | LEU         | 3.3         |
| 1          | AO           | 64         | VAL         | 3.3         |
| 1          | AF           | 63         | SER         | 3.3         |
| 1          | AX           | 85         | SER         | 3.3         |
| 1          | AP           | 44         | ARG         | 3.3         |
| 1          | CA           | 44         | ARG         | 3.3         |
| 1          | BN           | 68         | THR         | 3.3         |
| 1          | BP           | 67         | CYS         | 3.3         |
| 1          | AT           | 44         | ARG         | 3.2         |
| 1          | AG           | 63         | SER         | 3.2         |
| 1          | AB           | 63         | SER         | 3.2         |
| 1          | BD           | 71         | ASP         | 3.2         |
| 1          | AO           | 66         | CYS         | 3.2         |
| 1          | BQ           | 123        | PRO         | 3.2         |
| 1          | AG           | 44         | ARG         | 3.1         |
| 1          | AZ           | 44         | ARG         | 3.1         |
| 1          | BE           | 62         | ASN         | 3.1         |
| 1          | AH           | 45         | LYS         | 3.1         |
| 1          | AJ           | 71         | ASP         | 3.1         |
| 1          | AI           | 43         | ALA         | 3.1         |
| 1          | AB           | 64         | VAL         | 3.1         |
| 1          | AD           | 104        | PHE         | 3.1         |
| 1          | BX           | 43         | ALA         | 3.1         |
| 1          | BO           | 123        | PRO         | 3.1         |
| 1          | AV           | 67         | CYS         | 3.1         |
| 1          | AS           | 67         | CYS         | 3.0         |
| 1          | AI           | 63         | SER         | 3.0         |
| 1          | BD           | 44         | ARG         | 3.0         |
| 1          | AV           | 42         | ASN         | 3.0         |
| 1          | BJ           | 1          | ALA         | 3.0         |
| 1          | AA           | 123        | PRO         | 3.0         |
| 1          | BM           | 29         | PRO         | 3.0         |
| 1          | AY           | 64         | VAL         | 2.9         |
| 1          | BS           | 64         | VAL         | 2.9         |
| 1          | AK           | 63         | SER         | 2.9         |
| 1          | AM           | 26         | THR         | 2.9         |
| 1          | AS           | 43         | ALA         | 2.9         |
| 1          | CE           | 68         | THR         | 2.9         |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | BN    | 56  | TYR  | 2.9  |
| 1   | AN    | 43  | ALA  | 2.9  |
| 1   | AP    | 43  | ALA  | 2.9  |
| 1   | AQ    | 1   | ALA  | 2.9  |
| 1   | AK    | 64  | VAL  | 2.9  |
| 1   | AD    | 55  | TYR  | 2.9  |
| 1   | CE    | 14  | PRO  | 2.9  |
| 1   | BL    | 26  | THR  | 2.8  |
| 1   | BM    | 66  | CYS  | 2.8  |
| 1   | BB    | 44  | ARG  | 2.8  |
| 1   | AQ    | 42  | ASN  | 2.8  |
| 1   | BO    | 64  | VAL  | 2.8  |
| 1   | CG    | 68  | THR  | 2.8  |
| 1   | CE    | 42  | ASN  | 2.8  |
| 1   | AR    | 43  | ALA  | 2.8  |
| 1   | BA    | 26  | THR  | 2.8  |
| 1   | AI    | 62  | ASN  | 2.8  |
| 1   | AC    | 44  | ARG  | 2.8  |
| 1   | AP    | 42  | ASN  | 2.8  |
| 1   | BB    | 64  | VAL  | 2.7  |
| 1   | BD    | 91  | ALA  | 2.7  |
| 1   | BA    | 63  | SER  | 2.7  |
| 1   | AT    | 62  | ASN  | 2.7  |
| 1   | AS    | 68  | THR  | 2.7  |
| 1   | AZ    | 94  | THR  | 2.7  |
| 1   | AT    | 74  | ARG  | 2.7  |
| 1   | AQ    | 52  | ILE  | 2.7  |
| 1   | AZ    | 41  | ILE  | 2.7  |
| 1   | BG    | 64  | VAL  | 2.7  |
| 1   | CB    | 62  | ASN  | 2.7  |
| 1   | BF    | 45  | LYS  | 2.7  |
| 1   | AL    | 43  | ALA  | 2.7  |
| 1   | AG    | 62  | ASN  | 2.7  |
| 1   | AZ    | 64  | VAL  | 2.7  |
| 1   | BA    | 66  | CYS  | 2.7  |
| 1   | AS    | 72  | THR  | 2.7  |
| 1   | BV    | 85  | SER  | 2.7  |
| 1   | CG    | 61  | THR  | 2.6  |
| 1   | AT    | 43  | ALA  | 2.6  |
| 1   | BA    | 41  | ILE  | 2.6  |
| 1   | BD    | 67  | CYS  | 2.6  |
| 1   | BA    | 112 | ILE  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | AB    | 44  | ARG  | 2.6  |
| 1   | BQ    | 61  | THR  | 2.6  |
| 1   | AN    | 74  | ARG  | 2.6  |
| 1   | AE    | 31  | LEU  | 2.6  |
| 1   | AQ    | 69  | GLU  | 2.6  |
| 1   | AW    | 23  | THR  | 2.6  |
| 1   | BZ    | 26  | THR  | 2.6  |
| 1   | BD    | 45  | LYS  | 2.5  |
| 1   | BL    | 55  | TYR  | 2.5  |
| 1   | BE    | 1   | ALA  | 2.5  |
| 1   | AL    | 74  | ARG  | 2.5  |
| 1   | BZ    | 65  | SER  | 2.5  |
| 1   | BM    | 64  | VAL  | 2.5  |
| 1   | AQ    | 123 | PRO  | 2.5  |
| 1   | CH    | 61  | THR  | 2.5  |
| 1   | AZ    | 74  | ARG  | 2.5  |
| 1   | BY    | 44  | ARG  | 2.5  |
| 1   | AJ    | 60  | SER  | 2.5  |
| 1   | AI    | 101 | MET  | 2.5  |
| 1   | AP    | 74  | ARG  | 2.5  |
| 1   | BT    | 44  | ARG  | 2.5  |
| 1   | AO    | 67  | CYS  | 2.5  |
| 1   | BQ    | 67  | CYS  | 2.5  |
| 1   | AR    | 65  | SER  | 2.5  |
| 1   | BF    | 42  | ASN  | 2.5  |
| 1   | BE    | 38  | THR  | 2.4  |
| 1   | AB    | 66  | CYS  | 2.4  |
| 1   | AK    | 43  | ALA  | 2.4  |
| 1   | BL    | 41  | ILE  | 2.4  |
| 1   | AW    | 3   | LEU  | 2.4  |
| 1   | AD    | 63  | SER  | 2.4  |
| 1   | AS    | 36  | VAL  | 2.4  |
| 1   | BJ    | 59  | PRO  | 2.4  |
| 1   | BQ    | 43  | ALA  | 2.4  |
| 1   | BT    | 111 | SER  | 2.4  |
| 1   | AZ    | 42  | ASN  | 2.4  |
| 1   | BO    | 44  | ARG  | 2.4  |
| 1   | AJ    | 23  | THR  | 2.4  |
| 1   | CC    | 63  | SER  | 2.4  |
| 1   | BI    | 42  | ASN  | 2.4  |
| 1   | AG    | 61  | THR  | 2.3  |
| 1   | CE    | 63  | SER  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | CB    | 74  | ARG  | 2.3  |
| 1   | BB    | 69  | GLU  | 2.3  |
| 1   | CB    | 45  | LYS  | 2.3  |
| 1   | AK    | 59  | PRO  | 2.3  |
| 1   | AQ    | 44  | ARG  | 2.3  |
| 1   | BQ    | 65  | SER  | 2.3  |
| 1   | AW    | 26  | THR  | 2.3  |
| 1   | CD    | 44  | ARG  | 2.3  |
| 1   | AW    | 62  | ASN  | 2.3  |
| 1   | BZ    | 45  | LYS  | 2.3  |
| 1   | AI    | 44  | ARG  | 2.3  |
| 1   | BX    | 64  | VAL  | 2.3  |
| 1   | BF    | 74  | ARG  | 2.3  |
| 1   | BQ    | 118 | LEU  | 2.3  |
| 1   | CB    | 63  | SER  | 2.3  |
| 1   | AC    | 86  | SER  | 2.3  |
| 1   | AQ    | 32  | VAL  | 2.3  |
| 1   | BL    | 60  | SER  | 2.2  |
| 1   | AJ    | 74  | ARG  | 2.2  |
| 1   | AN    | 44  | ARG  | 2.2  |
| 1   | AM    | 67  | CYS  | 2.2  |
| 1   | BD    | 41  | ILE  | 2.2  |
| 1   | BQ    | 22  | VAL  | 2.2  |
| 1   | AM    | 34  | GLN  | 2.2  |
| 1   | BS    | 48  | ILE  | 2.2  |
| 1   | CE    | 73  | ILE  | 2.2  |
| 1   | AI    | 45  | LYS  | 2.2  |
| 1   | BE    | 66  | CYS  | 2.2  |
| 1   | BP    | 68  | THR  | 2.2  |
| 1   | BY    | 64  | VAL  | 2.2  |
| 1   | BP    | 44  | ARG  | 2.2  |
| 1   | BR    | 46  | SER  | 2.2  |
| 1   | CH    | 64  | VAL  | 2.2  |
| 1   | BN    | 67  | CYS  | 2.2  |
| 1   | AE    | 42  | ASN  | 2.1  |
| 1   | CG    | 64  | VAL  | 2.1  |
| 1   | AI    | 66  | CYS  | 2.1  |
| 1   | CB    | 26  | THR  | 2.1  |
| 1   | CF    | 45  | LYS  | 2.1  |
| 1   | AH    | 60  | SER  | 2.1  |
| 1   | AH    | 63  | SER  | 2.1  |
| 1   | BL    | 62  | ASN  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | CH    | 63  | SER  | 2.1  |
| 1   | CG    | 117 | LEU  | 2.1  |
| 1   | BY    | 58  | ILE  | 2.1  |
| 1   | BD    | 92  | ALA  | 2.1  |
| 1   | AR    | 24  | GLY  | 2.1  |
| 1   | CE    | 44  | ARG  | 2.1  |
| 1   | BH    | 45  | LYS  | 2.1  |
| 1   | BT    | 17  | LYS  | 2.1  |
| 1   | AD    | 32  | VAL  | 2.1  |
| 1   | CB    | 90  | VAL  | 2.1  |
| 1   | AN    | 1   | ALA  | 2.1  |
| 1   | BK    | 43  | ALA  | 2.1  |
| 1   | AZ    | 26  | THR  | 2.1  |
| 1   | AI    | 12  | VAL  | 2.1  |
| 1   | BR    | 123 | PRO  | 2.1  |
| 1   | AD    | 40  | SER  | 2.1  |
| 1   | AV    | 81  | LEU  | 2.0  |
| 1   | BL    | 90  | VAL  | 2.0  |
| 1   | AI    | 74  | ARG  | 2.0  |
| 1   | BH    | 67  | CYS  | 2.0  |
| 1   | BT    | 49  | MET  | 2.0  |
| 1   | AM    | 41  | ILE  | 2.0  |
| 1   | AU    | 44  | ARG  | 2.0  |
| 1   | BU    | 43  | ALA  | 2.0  |
| 1   | CE    | 86  | SER  | 2.0  |
| 1   | BW    | 11  | PRO  | 2.0  |
| 1   | BW    | 12  | VAL  | 2.0  |
| 1   | CD    | 64  | VAL  | 2.0  |
| 1   | AU    | 62  | ASN  | 2.0  |
| 1   | BW    | 45  | LYS  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.



## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.