



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:27 PM UTC

PDB ID : 4ATP / pdb\_00004atp  
Title : Structure of GABA-transaminase A1R958 from *Arthrobacter aureescens* in complex with PLP  
Authors : Bruce, H.; Tuan, A.N.; Mangas Sanchez, J.; Hart, S.; Turkenburg, J.P.; Grogan, G.  
Deposited on : 2012-05-09  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

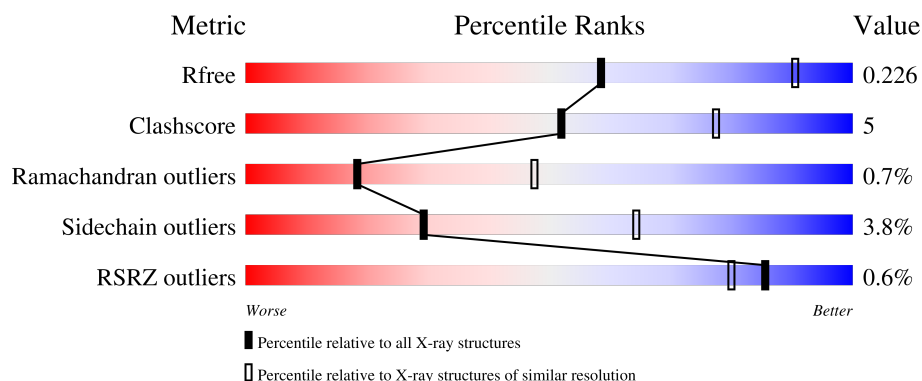
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 3866 (2.80-2.80)                                      |
| Clashscore            | 190562                      | 4276 (2.80-2.80)                                      |
| Ramachandran outliers | 187476                      | 4196 (2.80-2.80)                                      |
| Sidechain outliers    | 187428                      | 4198 (2.80-2.80)                                      |
| RSRZ outliers         | 180081                      | 3869 (2.80-2.80)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                                                     |
|-----|-------|--------|------------------------------------------------------------------------------------------------------|
| 1   | A     | 456    | <br>87% 8% . .   |
| 1   | B     | 456    | <br>87% 8% . . . |
| 1   | C     | 456    | <br>85% 11% . .  |
| 1   | D     | 456    | <br>85% 10% . .  |
| 1   | E     | 456    | <br>86% 9% . .   |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | F     | 456    | <div><div></div><div>85%</div><div>9%</div><div></div><div></div></div>              |
| 1   | G     | 456    | <div>%<div><div></div><div>84%</div><div>11%</div><div></div><div></div></div></div> |
| 1   | H     | 456    | <div>%<div><div></div><div>85%</div><div>10%</div><div></div><div></div></div></div> |
| 1   | I     | 456    | <div><div></div><div>86%</div><div>9%</div><div></div><div></div></div>              |
| 1   | J     | 456    | <div>%<div><div></div><div>85%</div><div>10%</div><div></div><div></div></div></div> |
| 1   | K     | 456    | <div>3%<div><div></div><div>85%</div><div>9%</div><div></div><div></div></div></div> |
| 1   | L     | 456    | <div><div></div><div>84%</div><div>10%</div><div></div><div></div></div>             |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 39107 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 4-AMINO BUTYRATE TRANSAMINASE.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 442      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 3242  | 2056 | 565 | 607 | 14 |         |         |       |
| 1   | B     | 442      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3217  | 2045 | 557 | 601 | 14 |         |         |       |
| 1   | C     | 442      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3225  | 2046 | 561 | 604 | 14 |         |         |       |
| 1   | D     | 439      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3205  | 2030 | 559 | 602 | 14 |         |         |       |
| 1   | E     | 442      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3226  | 2044 | 563 | 605 | 14 |         |         |       |
| 1   | F     | 439      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 3206  | 2035 | 560 | 597 | 14 |         |         |       |
| 1   | G     | 440      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3130  | 1984 | 542 | 590 | 14 |         |         |       |
| 1   | H     | 440      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3161  | 2006 | 549 | 592 | 14 |         |         |       |
| 1   | I     | 441      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3190  | 2023 | 556 | 597 | 14 |         |         |       |
| 1   | J     | 438      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3152  | 2000 | 553 | 585 | 14 |         |         |       |
| 1   | K     | 439      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3130  | 1980 | 543 | 593 | 14 |         |         |       |
| 1   | L     | 436      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3097  | 1964 | 536 | 583 | 14 |         |         |       |

There are 12 discrepancies between the modelled and reference sequences:

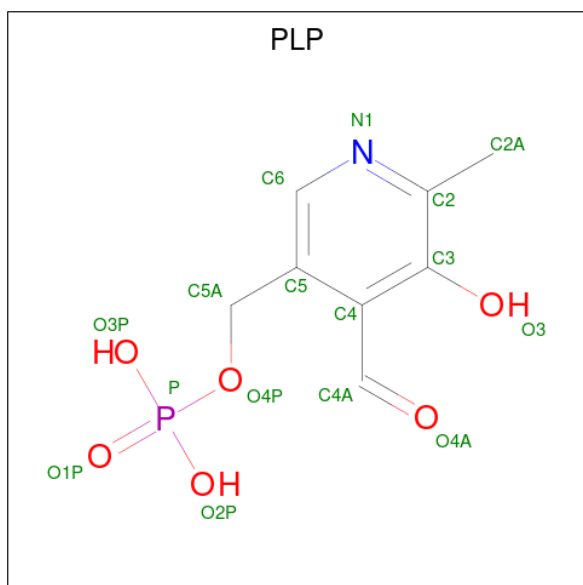
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 113     | THR      | ALA    | SEE REMARK 999 | UNP A1R958 |
| B     | 113     | THR      | ALA    | SEE REMARK 999 | UNP A1R958 |
| C     | 113     | THR      | ALA    | SEE REMARK 999 | UNP A1R958 |
| D     | 113     | THR      | ALA    | SEE REMARK 999 | UNP A1R958 |
| E     | 113     | THR      | ALA    | SEE REMARK 999 | UNP A1R958 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| F     | 113     | THR      | ALA    | SEE REMARK 999 | UNP A1R958 |
| G     | 113     | THR      | ALA    | SEE REMARK 999 | UNP A1R958 |
| H     | 113     | THR      | ALA    | SEE REMARK 999 | UNP A1R958 |
| I     | 113     | THR      | ALA    | SEE REMARK 999 | UNP A1R958 |
| J     | 113     | THR      | ALA    | SEE REMARK 999 | UNP A1R958 |
| K     | 113     | THR      | ALA    | SEE REMARK 999 | UNP A1R958 |
| L     | 113     | THR      | ALA    | SEE REMARK 999 | UNP A1R958 |

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula:  $C_8H_{10}NO_6P$ ).



| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 2   | A     | 1        | Total | C | N | O | P | 0       | 0       |
|     |       |          | 15    | 8 | 1 | 5 | 1 |         |         |
| 2   | B     | 1        | Total | C | N | O | P | 0       | 0       |
|     |       |          | 15    | 8 | 1 | 5 | 1 |         |         |
| 2   | C     | 1        | Total | C | N | O | P | 0       | 0       |
|     |       |          | 15    | 8 | 1 | 5 | 1 |         |         |
| 2   | D     | 1        | Total | C | N | O | P | 0       | 0       |
|     |       |          | 15    | 8 | 1 | 5 | 1 |         |         |
| 2   | E     | 1        | Total | C | N | O | P | 0       | 0       |
|     |       |          | 15    | 8 | 1 | 5 | 1 |         |         |
| 2   | F     | 1        | Total | C | N | O | P | 0       | 0       |
|     |       |          | 15    | 8 | 1 | 5 | 1 |         |         |
| 2   | G     | 1        | Total | C | N | O | P | 0       | 0       |
|     |       |          | 15    | 8 | 1 | 5 | 1 |         |         |
| 2   | H     | 1        | Total | C | N | O | P | 0       | 0       |
|     |       |          | 15    | 8 | 1 | 5 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 2   | I     | 1        | Total | C | N | O | P | 0       | 0       |
|     |       |          | 15    | 8 | 1 | 5 | 1 |         |         |
| 2   | J     | 1        | Total | C | N | O | P | 0       | 0       |
|     |       |          | 15    | 8 | 1 | 5 | 1 |         |         |
| 2   | K     | 1        | Total | C | N | O | P | 0       | 0       |
|     |       |          | 15    | 8 | 1 | 5 | 1 |         |         |
| 2   | L     | 1        | Total | C | N | O | P | 0       | 0       |
|     |       |          | 15    | 8 | 1 | 5 | 1 |         |         |

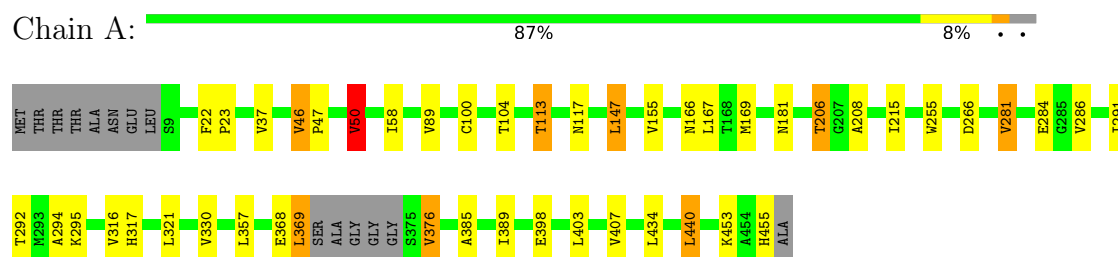
- Molecule 3 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 3   | A     | 120      | Total | O   | 0       | 0       |
|     |       |          | 120   | 120 |         |         |
| 3   | B     | 105      | Total | O   | 0       | 0       |
|     |       |          | 105   | 105 |         |         |
| 3   | C     | 95       | Total | O   | 0       | 0       |
|     |       |          | 95    | 95  |         |         |
| 3   | D     | 63       | Total | O   | 0       | 0       |
|     |       |          | 63    | 63  |         |         |
| 3   | E     | 110      | Total | O   | 0       | 0       |
|     |       |          | 110   | 110 |         |         |
| 3   | F     | 85       | Total | O   | 0       | 0       |
|     |       |          | 85    | 85  |         |         |
| 3   | G     | 38       | Total | O   | 0       | 0       |
|     |       |          | 38    | 38  |         |         |
| 3   | H     | 28       | Total | O   | 0       | 0       |
|     |       |          | 28    | 28  |         |         |
| 3   | I     | 32       | Total | O   | 0       | 0       |
|     |       |          | 32    | 32  |         |         |
| 3   | J     | 24       | Total | O   | 0       | 0       |
|     |       |          | 24    | 24  |         |         |
| 3   | K     | 25       | Total | O   | 0       | 0       |
|     |       |          | 25    | 25  |         |         |
| 3   | L     | 21       | Total | O   | 0       | 0       |
|     |       |          | 21    | 21  |         |         |

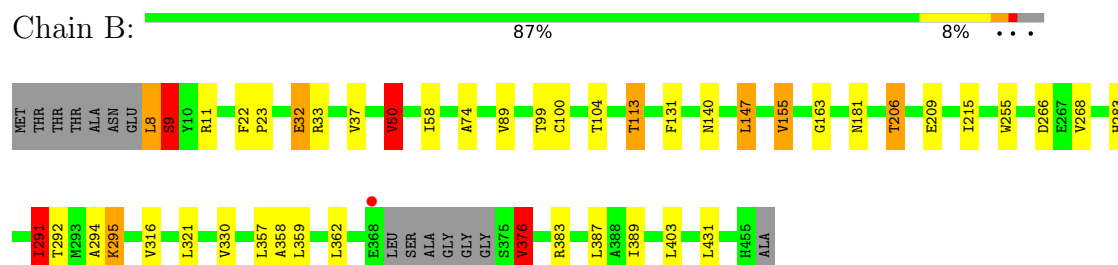
### 3 Residue-property plots

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

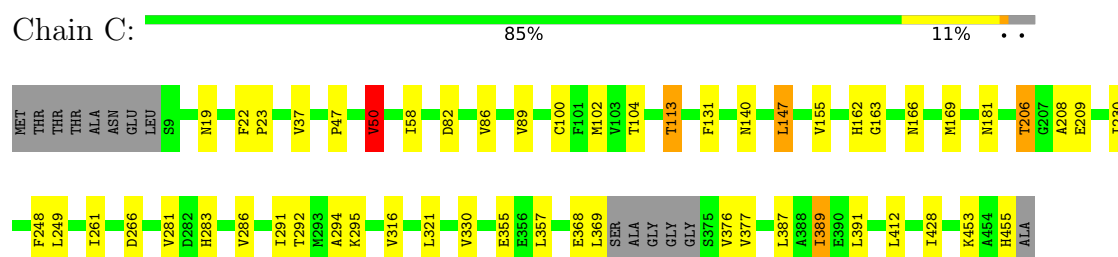
#### • Molecule 1: 4-AMINOBUTYRATE TRANSAMINASE



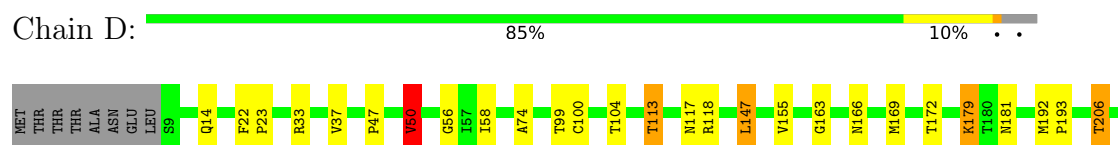
#### • Molecule 1: 4-AMINOBUTYRATE TRANSAMINASE

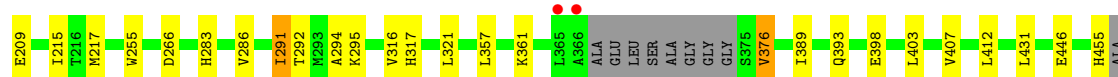


#### • Molecule 1: 4-AMINOBUTYRATE TRANSAMINASE



#### • Molecule 1: 4-AMINOBUTYRATE TRANSAMINASE





• Molecule 1: 4-AMINOBUTYRATE TRANSAMINASE

Chain E: 86% 9% . .



• Molecule 1: 4-AMINOBUTYRATE TRANSAMINASE

Chain F: 85% 9% . .



• Molecule 1: 4-AMINOBUTYRATE TRANSAMINASE

Chain G: 84% 11% . .



• Molecule 1: 4-AMINOBUTYRATE TRANSAMINASE

Chain H: 85% 10% . .

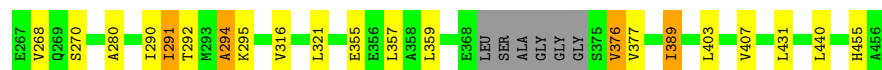






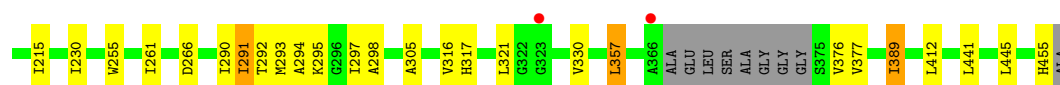
• Molecule 1: 4-AMINOBUTYRATE TRANSAMINASE

Chain I: 86% 9% . .



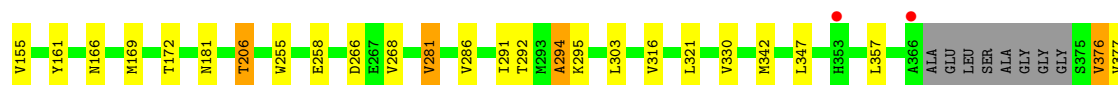
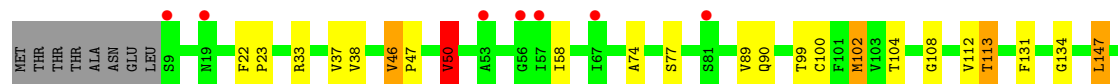
• Molecule 1: 4-AMINOBUTYRATE TRANSAMINASE

Chain J: 85% 10% . .



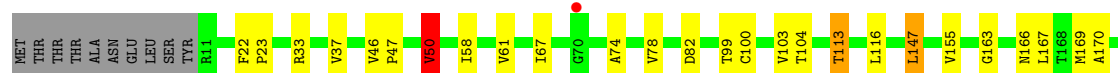
• Molecule 1: 4-AMINOBUTYRATE TRANSAMINASE

Chain K: 85% 9% . . 3%



• Molecule 1: 4-AMINOBUTYRATE TRANSAMINASE

Chain L: 84% 10% . .



RES  
ALA

## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 2 <sub>1</sub> 2 <sub>1</sub> 2                           | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 175.70Å 290.99Å 104.54Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 89.84 – 2.80<br>89.84 – 2.80                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 100.0 (89.84-2.80)<br>100.0 (89.84-2.80)                    | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.18                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.71 (at 2.82Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.6.0119                                             | Depositor        |
| R, $R_{free}$                                                           | 0.193 , 0.229<br>0.193 , 0.226                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 6667 reflections (5.04%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 34.7                                                        | Xtriage          |
| Anisotropy                                                              | 0.205                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 37.9                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                        | EDS              |
| Total number of atoms                                                   | 39107                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 28.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PLP

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

| Mol | Chain | Bond lengths |                 | Bond angles |                 |
|-----|-------|--------------|-----------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 5$     | RMSZ        | $\# Z  > 5$     |
| 1   | A     | 0.91         | 4/3305 (0.1%)   | 0.91        | 2/4492 (0.0%)   |
| 1   | B     | 0.95         | 0/3275          | 0.94        | 7/4452 (0.2%)   |
| 1   | C     | 0.92         | 3/3283 (0.1%)   | 0.93        | 2/4462 (0.0%)   |
| 1   | D     | 0.92         | 2/3264 (0.1%)   | 0.91        | 4/4439 (0.1%)   |
| 1   | E     | 0.92         | 0/3285          | 0.93        | 3/4468 (0.1%)   |
| 1   | F     | 0.92         | 3/3268 (0.1%)   | 0.90        | 1/4445 (0.0%)   |
| 1   | G     | 0.87         | 2/3188 (0.1%)   | 0.91        | 2/4351 (0.0%)   |
| 1   | H     | 0.85         | 1/3220 (0.0%)   | 0.90        | 1/4387 (0.0%)   |
| 1   | I     | 0.84         | 2/3249 (0.1%)   | 0.89        | 1/4425 (0.0%)   |
| 1   | J     | 0.85         | 1/3211 (0.0%)   | 0.89        | 1/4376 (0.0%)   |
| 1   | K     | 0.85         | 0/3188          | 0.90        | 3/4349 (0.1%)   |
| 1   | L     | 0.83         | 0/3155          | 0.89        | 2/4306 (0.0%)   |
| All | All   | 0.89         | 18/38891 (0.0%) | 0.91        | 29/52952 (0.1%) |

All (18) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | F     | 283 | HIS  | CG-CD2  | 7.05  | 1.43        | 1.35     |
| 1   | A     | 455 | HIS  | CG-CD2  | 6.41  | 1.43        | 1.35     |
| 1   | C     | 455 | HIS  | CG-CD2  | 6.13  | 1.42        | 1.35     |
| 1   | D     | 455 | HIS  | ND1-CE1 | 5.89  | 1.38        | 1.32     |
| 1   | A     | 455 | HIS  | ND1-CE1 | 5.78  | 1.38        | 1.32     |
| 1   | I     | 455 | HIS  | CG-CD2  | 5.68  | 1.42        | 1.35     |
| 1   | A     | 317 | HIS  | ND1-CE1 | 5.38  | 1.38        | 1.32     |
| 1   | C     | 162 | HIS  | CG-ND1  | -5.34 | 1.32        | 1.38     |
| 1   | F     | 317 | HIS  | CG-CD2  | 5.30  | 1.41        | 1.35     |
| 1   | C     | 283 | HIS  | CG-CD2  | 5.21  | 1.41        | 1.35     |
| 1   | D     | 317 | HIS  | CG-ND1  | -5.18 | 1.32        | 1.38     |
| 1   | F     | 455 | HIS  | CG-CD2  | 5.14  | 1.41        | 1.35     |
| 1   | A     | 317 | HIS  | CG-CD2  | 5.12  | 1.41        | 1.35     |
| 1   | H     | 455 | HIS  | CG-CD2  | 5.11  | 1.41        | 1.35     |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | I     | 95  | HIS  | CG-CD2 | 5.09 | 1.41        | 1.35     |
| 1   | J     | 317 | HIS  | CG-CD2 | 5.08 | 1.41        | 1.35     |
| 1   | G     | 98  | HIS  | CG-CD2 | 5.05 | 1.41        | 1.35     |
| 1   | G     | 366 | ALA  | CA-C   | 5.02 | 1.59        | 1.52     |

All (29) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 50  | VAL  | CB-CA-C    | -7.05 | 100.54      | 111.26   |
| 1   | A     | 376 | VAL  | CB-CA-C    | -6.92 | 102.19      | 110.84   |
| 1   | D     | 50  | VAL  | CB-CA-C    | -6.69 | 101.08      | 111.26   |
| 1   | A     | 50  | VAL  | CB-CA-C    | -6.57 | 101.28      | 111.26   |
| 1   | J     | 50  | VAL  | CB-CA-C    | -6.36 | 101.59      | 111.26   |
| 1   | F     | 50  | VAL  | CB-CA-C    | -6.34 | 101.62      | 111.26   |
| 1   | B     | 50  | VAL  | CB-CA-C    | -6.30 | 101.69      | 111.26   |
| 1   | K     | 50  | VAL  | CB-CA-C    | -6.11 | 101.98      | 111.26   |
| 1   | B     | 32  | GLU  | CA-CB-CG   | 5.98  | 126.06      | 114.10   |
| 1   | H     | 50  | VAL  | CB-CA-C    | -5.97 | 102.18      | 111.26   |
| 1   | L     | 50  | VAL  | CB-CA-C    | -5.85 | 102.37      | 111.26   |
| 1   | C     | 163 | GLY  | N-CA-C     | 5.79  | 118.29      | 111.63   |
| 1   | E     | 50  | VAL  | CB-CA-C    | -5.73 | 102.55      | 111.26   |
| 1   | B     | 163 | GLY  | N-CA-C     | 5.68  | 118.16      | 111.63   |
| 1   | B     | 9   | SER  | N-CA-C     | 5.57  | 118.30      | 109.50   |
| 1   | D     | 179 | LYS  | CB-CG-CD   | -5.54 | 98.55       | 111.30   |
| 1   | G     | 155 | VAL  | N-CA-CB    | 5.53  | 117.62      | 110.99   |
| 1   | G     | 50  | VAL  | CB-CA-C    | -5.52 | 102.87      | 111.26   |
| 1   | D     | 163 | GLY  | N-CA-C     | 5.44  | 117.88      | 111.63   |
| 1   | I     | 50  | VAL  | CB-CA-C    | -5.41 | 103.04      | 111.26   |
| 1   | L     | 163 | GLY  | N-CA-C     | 5.29  | 117.71      | 111.63   |
| 1   | K     | 376 | VAL  | N-CA-CB    | -5.25 | 106.43      | 112.21   |
| 1   | K     | 206 | THR  | N-CA-CB    | 5.25  | 118.75      | 110.56   |
| 1   | B     | 291 | ILE  | CB-CG1-CD1 | -5.20 | 102.87      | 113.80   |
| 1   | B     | 155 | VAL  | N-CA-CB    | 5.18  | 117.20      | 110.99   |
| 1   | E     | 377 | VAL  | N-CA-CB    | 5.17  | 117.80      | 111.60   |
| 1   | D     | 376 | VAL  | N-CA-CB    | -5.11 | 106.58      | 112.21   |
| 1   | E     | 376 | VAL  | N-CA-CB    | -5.03 | 106.68      | 112.21   |
| 1   | B     | 376 | VAL  | N-CA-CB    | -5.00 | 106.71      | 112.21   |

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   | A     | 3242  | 0        | 3239     | 31      | 0            |
| 1   | B     | 3217  | 0        | 3214     | 33      | 0            |
| 1   | C     | 3225  | 0        | 3218     | 33      | 0            |
| 1   | D     | 3205  | 0        | 3188     | 39      | 0            |
| 1   | E     | 3226  | 0        | 3218     | 46      | 0            |
| 1   | F     | 3206  | 0        | 3191     | 46      | 0            |
| 1   | G     | 3130  | 0        | 3047     | 46      | 0            |
| 1   | H     | 3161  | 0        | 3114     | 44      | 0            |
| 1   | I     | 3190  | 0        | 3157     | 42      | 0            |
| 1   | J     | 3152  | 0        | 3117     | 45      | 0            |
| 1   | K     | 3130  | 0        | 3036     | 40      | 0            |
| 1   | L     | 3097  | 0        | 3017     | 42      | 0            |
| 2   | A     | 15    | 0        | 7        | 0       | 0            |
| 2   | B     | 15    | 0        | 6        | 0       | 0            |
| 2   | C     | 15    | 0        | 6        | 0       | 0            |
| 2   | D     | 15    | 0        | 6        | 0       | 0            |
| 2   | E     | 15    | 0        | 6        | 0       | 0            |
| 2   | F     | 15    | 0        | 6        | 0       | 0            |
| 2   | G     | 15    | 0        | 6        | 2       | 0            |
| 2   | H     | 15    | 0        | 6        | 0       | 0            |
| 2   | I     | 15    | 0        | 6        | 2       | 0            |
| 2   | J     | 15    | 0        | 6        | 0       | 0            |
| 2   | K     | 15    | 0        | 6        | 1       | 0            |
| 2   | L     | 15    | 0        | 6        | 0       | 0            |
| 3   | A     | 120   | 0        | 0        | 3       | 0            |
| 3   | B     | 105   | 0        | 0        | 1       | 0            |
| 3   | C     | 95    | 0        | 0        | 2       | 0            |
| 3   | D     | 63    | 0        | 0        | 3       | 0            |
| 3   | E     | 110   | 0        | 0        | 1       | 0            |
| 3   | F     | 85    | 0        | 0        | 2       | 0            |
| 3   | G     | 38    | 0        | 0        | 3       | 0            |
| 3   | H     | 28    | 0        | 0        | 2       | 0            |
| 3   | I     | 32    | 0        | 0        | 0       | 0            |
| 3   | J     | 24    | 0        | 0        | 1       | 0            |
| 3   | K     | 25    | 0        | 0        | 1       | 0            |
| 3   | L     | 21    | 0        | 0        | 4       | 0            |
| All | All   | 39107 | 0        | 37829    | 389     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (389) 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:E:281:VAL:HG22 | 1:E:286:VAL:HG22 | 1.34                     | 1.09              |
| 1:C:248:PHE:C    | 1:C:249:LEU:CA   | 2.33                     | 1.01              |
| 1:F:14:GLN:HE22  | 1:F:56:GLY:H     | 1.12                     | 0.96              |
| 1:D:14:GLN:HE22  | 1:D:56:GLY:H     | 1.12                     | 0.96              |
| 1:E:281:VAL:CG2  | 1:E:286:VAL:HG22 | 1.98                     | 0.93              |
| 1:A:440:LEU:HD12 | 3:A:2003:HOH:O   | 1.69                     | 0.90              |
| 1:D:169:MET:O    | 1:D:179:LYS:HE2  | 1.72                     | 0.89              |
| 1:G:192:MET:SD   | 1:G:217:MET:HE2  | 2.13                     | 0.88              |
| 1:K:281:VAL:HG22 | 1:K:286:VAL:HB   | 1.55                     | 0.87              |
| 1:B:50:VAL:HG13  | 1:B:58:ILE:HG23  | 1.57                     | 0.86              |
| 1:G:50:VAL:HG13  | 1:G:58:ILE:HG23  | 1.59                     | 0.84              |
| 1:F:50:VAL:HG13  | 1:F:58:ILE:HG23  | 1.57                     | 0.84              |
| 1:A:50:VAL:HG13  | 1:A:58:ILE:HG23  | 1.60                     | 0.83              |
| 1:H:50:VAL:HG13  | 1:H:58:ILE:HG23  | 1.61                     | 0.83              |
| 1:G:104:THR:CG2  | 1:H:50:VAL:HG22  | 2.09                     | 0.82              |
| 1:E:50:VAL:HG13  | 1:E:58:ILE:HG23  | 1.64                     | 0.79              |
| 1:H:281:VAL:HG22 | 1:H:286:VAL:HB   | 1.63                     | 0.79              |
| 1:G:134:GLY:N    | 2:G:500:PLP:O1P  | 2.17                     | 0.78              |
| 1:A:281:VAL:HG22 | 1:A:286:VAL:HB   | 1.65                     | 0.78              |
| 3:G:2007:HOH:O   | 1:H:99:THR:HA    | 1.84                     | 0.77              |
| 1:D:192:MET:SD   | 1:D:217:MET:HE2  | 2.26                     | 0.76              |
| 1:G:50:VAL:HG22  | 1:H:104:THR:HG22 | 1.68                     | 0.75              |
| 1:E:37:VAL:HB    | 1:F:113:THR:HG23 | 1.69                     | 0.75              |
| 1:J:37:VAL:HB    | 1:K:113:THR:HG23 | 1.68                     | 0.75              |
| 1:J:104:THR:HG21 | 1:K:50:VAL:HG22  | 1.69                     | 0.74              |
| 1:D:172:THR:O    | 1:D:179:LYS:HE3  | 1.87                     | 0.73              |
| 1:G:104:THR:HG22 | 1:H:50:VAL:HG22  | 1.68                     | 0.73              |
| 1:C:377:VAL:HG13 | 1:C:389:ILE:HD11 | 1.70                     | 0.73              |
| 1:K:147:LEU:C    | 1:K:147:LEU:HD12 | 2.13                     | 0.73              |
| 1:D:50:VAL:HG13  | 1:D:58:ILE:HG23  | 1.70                     | 0.72              |
| 3:E:2020:HOH:O   | 1:F:117:ASN:HB2  | 1.88                     | 0.72              |
| 1:I:104:THR:HG22 | 1:L:50:VAL:HG22  | 1.70                     | 0.72              |
| 1:I:50:VAL:HG22  | 1:L:104:THR:HG21 | 1.72                     | 0.72              |
| 1:J:50:VAL:HG13  | 1:J:58:ILE:HG23  | 1.70                     | 0.72              |
| 1:A:113:THR:HG23 | 1:B:37:VAL:HB    | 1.72                     | 0.71              |
| 1:I:266:ASP:OD2  | 2:I:500:PLP:H2A3 | 1.91                     | 0.71              |
| 1:I:377:VAL:HG22 | 1:I:389:ILE:HD11 | 1.72                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:104:THR:HG22 | 1:D:50:VAL:HG22  | 1.71                     | 0.71              |
| 1:E:104:THR:HG22 | 1:F:50:VAL:HG22  | 1.72                     | 0.71              |
| 1:H:116:LEU:HD13 | 1:H:293:MET:HE1  | 1.72                     | 0.70              |
| 1:G:113:THR:HG23 | 1:H:37:VAL:HB    | 1.72                     | 0.70              |
| 1:L:50:VAL:HG13  | 1:L:58:ILE:HG23  | 1.72                     | 0.70              |
| 1:I:50:VAL:HG22  | 1:L:104:THR:CG2  | 2.22                     | 0.69              |
| 1:L:403:LEU:O    | 1:L:407:VAL:HG23 | 1.91                     | 0.69              |
| 1:H:293:MET:HE3  | 1:H:305:ALA:HB3  | 1.75                     | 0.69              |
| 1:A:50:VAL:HG22  | 1:B:104:THR:HG22 | 1.75                     | 0.69              |
| 1:J:104:THR:CG2  | 1:K:50:VAL:HG22  | 2.22                     | 0.69              |
| 1:L:78:VAL:O     | 3:L:2008:HOH:O   | 2.10                     | 0.69              |
| 1:J:37:VAL:HB    | 1:K:113:THR:CG2  | 2.21                     | 0.68              |
| 1:J:99:THR:HG21  | 1:K:50:VAL:HG21  | 1.74                     | 0.68              |
| 1:G:37:VAL:HB    | 1:H:113:THR:HG23 | 1.76                     | 0.68              |
| 1:I:50:VAL:HG13  | 1:I:58:ILE:HG23  | 1.75                     | 0.68              |
| 1:E:366:ALA:O    | 1:E:368:GLU:N    | 2.26                     | 0.68              |
| 1:H:147:LEU:CD1  | 1:H:147:LEU:C    | 2.66                     | 0.68              |
| 1:K:268:VAL:HG13 | 1:K:294:ALA:HB3  | 1.76                     | 0.67              |
| 1:E:50:VAL:HG22  | 1:F:104:THR:HG22 | 1.77                     | 0.67              |
| 1:D:316:VAL:HG11 | 1:D:321:LEU:HG   | 1.77                     | 0.67              |
| 1:C:50:VAL:HG22  | 1:D:104:THR:CG2  | 2.25                     | 0.67              |
| 1:E:37:VAL:CG2   | 1:F:113:THR:CG2  | 2.73                     | 0.67              |
| 1:G:104:THR:HG21 | 1:H:50:VAL:HG22  | 1.77                     | 0.66              |
| 1:I:74:ALA:HB2   | 1:I:431:LEU:HD13 | 1.77                     | 0.66              |
| 1:L:246:GLU:O    | 3:L:2013:HOH:O   | 2.12                     | 0.66              |
| 1:A:104:THR:HG22 | 1:B:50:VAL:HG22  | 1.77                     | 0.65              |
| 3:G:2008:HOH:O   | 1:H:51:GLU:O     | 2.13                     | 0.65              |
| 1:J:85:VAL:O     | 1:J:89:VAL:HG23  | 1.96                     | 0.65              |
| 1:K:50:VAL:HG13  | 1:K:58:ILE:HG23  | 1.78                     | 0.65              |
| 1:H:147:LEU:C    | 1:H:147:LEU:HD12 | 2.22                     | 0.65              |
| 1:K:147:LEU:C    | 1:K:147:LEU:CD1  | 2.69                     | 0.65              |
| 1:E:147:LEU:CD1  | 1:E:147:LEU:C    | 2.70                     | 0.64              |
| 1:I:37:VAL:HB    | 1:L:113:THR:HG23 | 1.78                     | 0.64              |
| 1:J:316:VAL:HG11 | 1:J:321:LEU:HG   | 1.80                     | 0.64              |
| 1:A:50:VAL:HG22  | 1:B:104:THR:CG2  | 2.28                     | 0.64              |
| 1:D:74:ALA:HB2   | 1:D:431:LEU:HD22 | 1.80                     | 0.64              |
| 1:G:50:VAL:HG22  | 1:H:104:THR:CG2  | 2.28                     | 0.64              |
| 1:I:113:THR:CG2  | 1:L:37:VAL:HB    | 2.28                     | 0.64              |
| 1:I:113:THR:HG23 | 1:L:37:VAL:HB    | 1.80                     | 0.63              |
| 1:C:113:THR:HG23 | 1:D:37:VAL:HB    | 1.80                     | 0.63              |
| 1:E:113:THR:HG23 | 1:F:37:VAL:HB    | 1.80                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:316:VAL:HG11 | 1:G:321:LEU:HG   | 1.80                     | 0.63              |
| 1:I:206:THR:HG22 | 1:I:209:GLU:H    | 1.64                     | 0.63              |
| 1:A:113:THR:CG2  | 1:B:37:VAL:HB    | 2.29                     | 0.63              |
| 1:I:403:LEU:O    | 1:I:407:VAL:HG23 | 1.99                     | 0.62              |
| 1:J:113:THR:HG23 | 1:K:37:VAL:HB    | 1.79                     | 0.62              |
| 1:I:50:VAL:HG21  | 1:L:99:THR:HG21  | 1.80                     | 0.62              |
| 1:C:37:VAL:HB    | 1:D:113:THR:HG23 | 1.81                     | 0.62              |
| 1:E:403:LEU:O    | 1:E:407:VAL:HG23 | 2.00                     | 0.62              |
| 1:G:376:VAL:HG11 | 1:G:403:LEU:HD21 | 1.81                     | 0.62              |
| 1:C:281:VAL:HG22 | 1:C:286:VAL:HB   | 1.81                     | 0.61              |
| 1:I:37:VAL:HB    | 1:L:113:THR:CG2  | 2.31                     | 0.61              |
| 1:L:82:ASP:HB2   | 3:L:2008:HOH:O   | 1.98                     | 0.60              |
| 1:J:147:LEU:HD22 | 1:K:181:ASN:HB2  | 1.83                     | 0.60              |
| 1:A:147:LEU:C    | 1:A:147:LEU:CD1  | 2.75                     | 0.60              |
| 1:F:283:HIS:CD2  | 1:F:383:ARG:HH11 | 2.19                     | 0.60              |
| 1:G:235:ILE:HG12 | 1:G:243:VAL:HG22 | 1.82                     | 0.60              |
| 1:A:369:LEU:HD22 | 1:A:376:VAL:HG22 | 1.82                     | 0.60              |
| 1:C:206:THR:HG22 | 1:C:209:GLU:H    | 1.66                     | 0.60              |
| 1:H:74:ALA:HB2   | 1:H:431:LEU:HD22 | 1.83                     | 0.60              |
| 1:L:74:ALA:HB2   | 1:L:431:LEU:HD13 | 1.83                     | 0.59              |
| 1:G:37:VAL:HB    | 1:H:113:THR:CG2  | 2.32                     | 0.59              |
| 1:B:316:VAL:HG11 | 1:B:321:LEU:HG   | 1.83                     | 0.59              |
| 1:C:50:VAL:HG22  | 1:D:104:THR:HG22 | 1.85                     | 0.59              |
| 1:C:181:ASN:HB2  | 1:D:147:LEU:HD22 | 1.83                     | 0.59              |
| 1:L:443:ASP:O    | 1:L:447:VAL:HG23 | 2.01                     | 0.59              |
| 1:C:37:VAL:HB    | 1:D:113:THR:CG2  | 2.33                     | 0.58              |
| 1:C:377:VAL:HG13 | 1:C:389:ILE:CD1  | 2.32                     | 0.58              |
| 1:F:283:HIS:CD2  | 1:F:383:ARG:NH1  | 2.71                     | 0.58              |
| 1:I:147:LEU:CD1  | 1:I:147:LEU:C    | 2.76                     | 0.58              |
| 1:H:269:GLN:HG2  | 1:H:386:MET:HE3  | 1.84                     | 0.58              |
| 1:J:113:THR:CG2  | 1:K:37:VAL:HB    | 2.32                     | 0.58              |
| 1:E:37:VAL:HG23  | 1:F:113:THR:CG2  | 2.34                     | 0.58              |
| 1:J:441:LEU:HG   | 1:J:445:LEU:HD11 | 1.86                     | 0.58              |
| 1:L:166:ASN:HA   | 1:L:169:MET:HE3  | 1.86                     | 0.58              |
| 1:A:104:THR:CG2  | 1:B:50:VAL:HG22  | 2.34                     | 0.58              |
| 1:E:37:VAL:HG23  | 1:F:113:THR:HG21 | 1.85                     | 0.58              |
| 1:I:147:LEU:C    | 1:I:147:LEU:HD12 | 2.28                     | 0.58              |
| 1:D:166:ASN:HA   | 1:D:169:MET:HE3  | 1.85                     | 0.57              |
| 1:H:166:ASN:HA   | 1:H:169:MET:HE3  | 1.85                     | 0.57              |
| 1:H:215:ILE:HG23 | 1:H:255:TRP:CE2  | 2.39                     | 0.57              |
| 1:A:368:GLU:OE1  | 1:A:453:LYS:HE2  | 2.04                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:316:VAL:HG11 | 1:C:321:LEU:HG   | 1.86                     | 0.57              |
| 1:G:147:LEU:HD12 | 1:G:147:LEU:C    | 2.30                     | 0.57              |
| 1:I:316:VAL:HG11 | 1:I:321:LEU:HG   | 1.85                     | 0.57              |
| 1:J:147:LEU:CD1  | 1:J:147:LEU:C    | 2.78                     | 0.57              |
| 1:K:108:GLY:O    | 1:K:112:VAL:HG23 | 2.04                     | 0.57              |
| 1:L:377:VAL:HG22 | 1:L:389:ILE:HD11 | 1.86                     | 0.57              |
| 1:J:50:VAL:HG22  | 1:K:104:THR:HG22 | 1.86                     | 0.57              |
| 1:L:316:VAL:HG11 | 1:L:321:LEU:HG   | 1.87                     | 0.56              |
| 1:G:147:LEU:C    | 1:G:147:LEU:CD1  | 2.78                     | 0.56              |
| 1:A:117:ASN:HB2  | 3:A:2040:HOH:O   | 2.05                     | 0.55              |
| 1:D:403:LEU:O    | 1:D:407:VAL:HG23 | 2.06                     | 0.55              |
| 1:E:37:VAL:HB    | 1:F:113:THR:CG2  | 2.35                     | 0.55              |
| 1:E:50:VAL:HG22  | 1:F:104:THR:CG2  | 2.36                     | 0.55              |
| 1:E:104:THR:CG2  | 1:F:50:VAL:HG22  | 2.35                     | 0.55              |
| 1:H:140:ASN:OD1  | 3:H:2011:HOH:O   | 2.18                     | 0.55              |
| 1:K:342:MET:HA   | 1:K:347:LEU:HD13 | 1.89                     | 0.55              |
| 1:B:283:HIS:HB2  | 3:B:2083:HOH:O   | 2.06                     | 0.55              |
| 1:G:113:THR:CG2  | 1:H:37:VAL:HB    | 2.37                     | 0.55              |
| 1:F:22:PHE:HA    | 1:F:23:PRO:C     | 2.31                     | 0.55              |
| 1:G:166:ASN:HA   | 1:G:169:MET:HE3  | 1.89                     | 0.54              |
| 1:I:166:ASN:HA   | 1:I:169:MET:HE3  | 1.90                     | 0.54              |
| 1:H:116:LEU:HD13 | 1:H:293:MET:CE   | 2.36                     | 0.54              |
| 1:J:166:ASN:HA   | 1:J:169:MET:HE3  | 1.89                     | 0.54              |
| 1:C:50:VAL:HG21  | 1:D:99:THR:HG21  | 1.88                     | 0.54              |
| 1:B:22:PHE:HA    | 1:B:23:PRO:C     | 2.33                     | 0.54              |
| 1:A:284:GLU:OE1  | 3:A:2098:HOH:O   | 2.19                     | 0.53              |
| 1:E:147:LEU:C    | 1:E:147:LEU:HD12 | 2.33                     | 0.53              |
| 1:J:50:VAL:HG22  | 1:K:104:THR:CG2  | 2.38                     | 0.53              |
| 1:F:147:LEU:C    | 1:F:147:LEU:HD12 | 2.33                     | 0.53              |
| 1:F:166:ASN:HA   | 1:F:169:MET:HE3  | 1.90                     | 0.53              |
| 1:K:347:LEU:HD23 | 1:K:434:LEU:HB2  | 1.90                     | 0.53              |
| 1:K:166:ASN:HA   | 1:K:169:MET:HE3  | 1.90                     | 0.53              |
| 1:D:361:LYS:NZ   | 1:D:446:GLU:HG3  | 2.23                     | 0.53              |
| 1:F:206:THR:HG22 | 1:F:208:ALA:N    | 2.24                     | 0.53              |
| 1:E:113:THR:CG2  | 1:F:37:VAL:HB    | 2.39                     | 0.53              |
| 1:I:22:PHE:HA    | 1:I:23:PRO:C     | 2.34                     | 0.53              |
| 1:C:50:VAL:HG22  | 1:D:104:THR:HG21 | 1.89                     | 0.53              |
| 1:H:141:ALA:HB1  | 1:H:264:ILE:HD13 | 1.91                     | 0.53              |
| 1:H:206:THR:HG22 | 1:H:208:ALA:N    | 2.24                     | 0.53              |
| 1:K:316:VAL:HG11 | 1:K:321:LEU:HG   | 1.91                     | 0.53              |
| 1:J:82:ASP:OD2   | 1:J:85:VAL:HG23  | 2.08                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:368:GLU:OE1  | 1:C:453:LYS:HE2  | 2.09                     | 0.53              |
| 1:J:104:THR:HG22 | 1:K:50:VAL:CG2   | 2.38                     | 0.53              |
| 1:G:403:LEU:O    | 1:G:407:VAL:HG23 | 2.10                     | 0.52              |
| 1:H:22:PHE:HA    | 1:H:23:PRO:C     | 2.34                     | 0.52              |
| 1:I:268:VAL:HG13 | 1:I:294:ALA:HB3  | 1.90                     | 0.52              |
| 1:E:194:MET:HE3  | 1:E:195:SER:O    | 2.08                     | 0.52              |
| 1:H:376:VAL:HG11 | 1:H:403:LEU:HD21 | 1.91                     | 0.52              |
| 1:D:361:LYS:HZ1  | 1:D:446:GLU:HG3  | 1.74                     | 0.52              |
| 1:L:22:PHE:HA    | 1:L:23:PRO:C     | 2.35                     | 0.52              |
| 1:G:22:PHE:HA    | 1:G:23:PRO:C     | 2.35                     | 0.52              |
| 1:A:22:PHE:HA    | 1:A:23:PRO:C     | 2.34                     | 0.52              |
| 1:C:22:PHE:HA    | 1:C:23:PRO:C     | 2.34                     | 0.52              |
| 1:E:22:PHE:HA    | 1:E:23:PRO:C     | 2.34                     | 0.52              |
| 1:D:22:PHE:HA    | 1:D:23:PRO:C     | 2.36                     | 0.51              |
| 1:D:193:PRO:HD3  | 1:D:217:MET:CE   | 2.41                     | 0.51              |
| 1:F:147:LEU:C    | 1:F:147:LEU:CD1  | 2.83                     | 0.51              |
| 1:J:22:PHE:HA    | 1:J:23:PRO:C     | 2.35                     | 0.51              |
| 1:J:441:LEU:HG   | 1:J:445:LEU:CD1  | 2.41                     | 0.51              |
| 1:G:104:THR:HG22 | 1:H:50:VAL:CG2   | 2.39                     | 0.51              |
| 1:A:166:ASN:HA   | 1:A:169:MET:HE3  | 1.93                     | 0.51              |
| 1:A:37:VAL:HB    | 1:B:113:THR:HG23 | 1.93                     | 0.51              |
| 1:G:99:THR:HG21  | 1:H:50:VAL:HG21  | 1.93                     | 0.51              |
| 1:D:147:LEU:C    | 1:D:147:LEU:HD12 | 2.36                     | 0.50              |
| 1:D:147:LEU:C    | 1:D:147:LEU:CD1  | 2.85                     | 0.50              |
| 1:I:140:ASN:O    | 1:I:144:VAL:HG23 | 2.11                     | 0.50              |
| 1:H:377:VAL:HG22 | 1:H:389:ILE:HD11 | 1.93                     | 0.50              |
| 1:I:38:VAL:CG2   | 1:L:113:THR:HG21 | 2.40                     | 0.50              |
| 1:F:212:LYS:HE3  | 3:F:2056:HOH:O   | 2.11                     | 0.50              |
| 1:K:22:PHE:HA    | 1:K:23:PRO:C     | 2.36                     | 0.50              |
| 1:G:206:THR:HG22 | 1:G:208:ALA:N    | 2.27                     | 0.50              |
| 1:G:391:LEU:HD11 | 1:G:428:ILE:HD12 | 1.92                     | 0.50              |
| 1:A:37:VAL:HB    | 1:B:113:THR:CG2  | 2.41                     | 0.50              |
| 3:C:2012:HOH:O   | 1:D:117:ASN:HB2  | 2.12                     | 0.50              |
| 1:F:215:ILE:HG23 | 1:F:255:TRP:CE2  | 2.46                     | 0.50              |
| 1:F:316:VAL:HG11 | 1:F:321:LEU:HG   | 1.93                     | 0.50              |
| 1:A:206:THR:HG22 | 1:A:208:ALA:N    | 2.26                     | 0.50              |
| 1:I:82:ASP:OD2   | 1:I:85:VAL:HG23  | 2.12                     | 0.49              |
| 1:K:134:GLY:N    | 2:K:500:PLP:O1P  | 2.44                     | 0.49              |
| 1:A:147:LEU:C    | 1:A:147:LEU:HD12 | 2.37                     | 0.49              |
| 1:C:50:VAL:HG13  | 1:C:58:ILE:HG23  | 1.93                     | 0.49              |
| 1:G:377:VAL:HG13 | 1:G:389:ILE:HD11 | 1.93                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:377:VAL:HG13 | 1:G:389:ILE:CD1  | 2.41                     | 0.49              |
| 1:K:77:SER:HB3   | 1:K:434:LEU:HD13 | 1.95                     | 0.49              |
| 1:L:215:ILE:HG23 | 1:L:255:TRP:CE2  | 2.48                     | 0.49              |
| 1:D:283:HIS:HB2  | 3:D:2052:HOH:O   | 2.12                     | 0.49              |
| 1:K:161:TYR:HA   | 1:K:172:THR:HG23 | 1.95                     | 0.49              |
| 1:L:147:LEU:CD1  | 1:L:147:LEU:C    | 2.85                     | 0.49              |
| 1:E:50:VAL:HG21  | 1:F:99:THR:HG21  | 1.95                     | 0.49              |
| 1:D:206:THR:HG22 | 1:D:209:GLU:H    | 1.77                     | 0.49              |
| 1:H:292:THR:HG22 | 1:H:306:ILE:HG22 | 1.95                     | 0.49              |
| 1:B:147:LEU:CD1  | 1:B:147:LEU:C    | 2.86                     | 0.49              |
| 1:B:74:ALA:HB2   | 1:B:431:LEU:HD13 | 1.94                     | 0.49              |
| 1:E:281:VAL:HG22 | 1:E:286:VAL:CG2  | 2.25                     | 0.48              |
| 1:J:377:VAL:HG13 | 1:J:389:ILE:CD1  | 2.43                     | 0.48              |
| 1:J:104:THR:CG2  | 1:K:50:VAL:CG2   | 2.88                     | 0.48              |
| 1:B:147:LEU:C    | 1:B:147:LEU:HD12 | 2.39                     | 0.48              |
| 1:I:50:VAL:CG2   | 1:L:104:THR:HG22 | 2.43                     | 0.48              |
| 1:D:193:PRO:HD3  | 1:D:217:MET:HE1  | 1.96                     | 0.48              |
| 1:I:57:ILE:HD11  | 1:I:440:LEU:HD21 | 1.95                     | 0.48              |
| 1:D:215:ILE:HG23 | 1:D:255:TRP:CE2  | 2.48                     | 0.48              |
| 1:E:147:LEU:HD22 | 1:F:181:ASN:HB2  | 1.96                     | 0.48              |
| 1:C:355:GLU:HA   | 1:C:387:LEU:HD11 | 1.95                     | 0.47              |
| 1:J:176:MET:HE1  | 3:K:2023:HOH:O   | 2.14                     | 0.47              |
| 1:C:166:ASN:HA   | 1:C:169:MET:HE3  | 1.96                     | 0.47              |
| 1:E:316:VAL:HG11 | 1:E:321:LEU:HG   | 1.97                     | 0.47              |
| 1:G:82:ASP:O     | 1:G:86:VAL:HG23  | 2.15                     | 0.47              |
| 1:E:113:THR:HG21 | 1:F:38:VAL:HG23  | 1.96                     | 0.47              |
| 1:C:19:ASN:HB2   | 3:C:2004:HOH:O   | 2.14                     | 0.47              |
| 1:F:33:ARG:O     | 1:F:37:VAL:HG22  | 2.14                     | 0.47              |
| 1:H:293:MET:HE3  | 1:H:293:MET:HB2  | 1.86                     | 0.47              |
| 1:B:358:ALA:HB3  | 1:B:387:LEU:CD1  | 2.45                     | 0.47              |
| 1:G:235:ILE:CG2  | 1:G:386:MET:HE2  | 2.45                     | 0.47              |
| 1:J:147:LEU:C    | 1:J:147:LEU:HD12 | 2.40                     | 0.46              |
| 1:L:67:ILE:HG12  | 1:L:440:LEU:HD22 | 1.98                     | 0.46              |
| 1:C:206:THR:HG22 | 1:C:208:ALA:N    | 2.30                     | 0.46              |
| 1:B:266:ASP:HA   | 1:B:292:THR:OG1  | 2.15                     | 0.46              |
| 1:E:37:VAL:CG2   | 1:F:113:THR:HG22 | 2.43                     | 0.46              |
| 1:G:89:VAL:HG13  | 1:G:330:VAL:CG1  | 2.46                     | 0.46              |
| 1:J:206:THR:HG22 | 1:J:208:ALA:N    | 2.29                     | 0.46              |
| 1:J:377:VAL:HG13 | 1:J:389:ILE:HD11 | 1.98                     | 0.46              |
| 1:J:455:HIS:O    | 3:J:2024:HOH:O   | 2.20                     | 0.46              |
| 1:C:113:THR:CG2  | 1:D:37:VAL:HB    | 2.42                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:297:ILE:HG23 | 1:G:298:ALA:N    | 2.31                     | 0.46              |
| 1:L:33:ARG:O     | 1:L:37:VAL:HG22  | 2.16                     | 0.46              |
| 1:F:266:ASP:HA   | 1:F:292:THR:OG1  | 2.16                     | 0.46              |
| 1:I:266:ASP:HA   | 1:I:292:THR:OG1  | 2.16                     | 0.46              |
| 1:E:46:VAL:CG1   | 1:E:48:VAL:HG22  | 2.46                     | 0.46              |
| 1:E:166:ASN:HA   | 1:E:169:MET:HE3  | 1.96                     | 0.46              |
| 1:E:206:THR:HG22 | 1:E:208:ALA:N    | 2.31                     | 0.46              |
| 1:G:215:ILE:HG23 | 1:G:255:TRP:CE2  | 2.51                     | 0.46              |
| 1:J:37:VAL:CG2   | 1:K:113:THR:CG2  | 2.94                     | 0.46              |
| 1:J:181:ASN:HB2  | 1:K:147:LEU:HD22 | 1.98                     | 0.46              |
| 1:E:44:SER:HA    | 1:F:102:MET:O    | 2.15                     | 0.45              |
| 1:G:376:VAL:HG11 | 1:G:403:LEU:CD2  | 2.46                     | 0.45              |
| 1:F:50:VAL:CG1   | 1:F:58:ILE:HG23  | 2.38                     | 0.45              |
| 1:H:85:VAL:O     | 1:H:89:VAL:HG23  | 2.17                     | 0.45              |
| 1:B:206:THR:HG22 | 1:B:209:GLU:H    | 1.82                     | 0.45              |
| 1:I:50:VAL:HG22  | 1:L:104:THR:HG22 | 1.97                     | 0.45              |
| 1:H:403:LEU:O    | 1:H:407:VAL:HG23 | 2.17                     | 0.45              |
| 1:A:266:ASP:HA   | 1:A:292:THR:OG1  | 2.16                     | 0.45              |
| 1:G:67:ILE:HG12  | 1:G:440:LEU:HD22 | 1.98                     | 0.45              |
| 1:J:266:ASP:HA   | 1:J:292:THR:OG1  | 2.17                     | 0.45              |
| 1:B:11:ARG:O     | 1:E:59:ARG:NH1   | 2.49                     | 0.45              |
| 1:B:33:ARG:O     | 1:B:37:VAL:HG22  | 2.17                     | 0.45              |
| 1:E:36:ALA:HA    | 1:I:258:GLU:CG   | 2.47                     | 0.45              |
| 1:E:37:VAL:HG21  | 1:F:113:THR:HG22 | 1.99                     | 0.45              |
| 1:F:283:HIS:CG   | 1:F:383:ARG:NH1  | 2.84                     | 0.45              |
| 1:B:215:ILE:HG23 | 1:B:255:TRP:CE2  | 2.52                     | 0.45              |
| 1:F:206:THR:HG22 | 1:F:209:GLU:H    | 1.81                     | 0.45              |
| 1:J:290:ILE:HG22 | 1:J:291:ILE:N    | 2.31                     | 0.45              |
| 1:G:33:ARG:O     | 1:G:37:VAL:HG22  | 2.17                     | 0.44              |
| 1:E:266:ASP:HA   | 1:E:292:THR:OG1  | 2.18                     | 0.44              |
| 1:I:106:TYR:HB3  | 1:L:50:VAL:HG23  | 2.00                     | 0.44              |
| 1:I:147:LEU:HD22 | 1:L:181:ASN:HB2  | 1.98                     | 0.44              |
| 1:I:376:VAL:HG21 | 1:I:403:LEU:HD22 | 1.99                     | 0.44              |
| 1:J:44:SER:HA    | 1:K:102:MET:O    | 2.17                     | 0.44              |
| 1:L:147:LEU:C    | 1:L:147:LEU:HD12 | 2.42                     | 0.44              |
| 1:L:266:ASP:HA   | 1:L:292:THR:OG1  | 2.18                     | 0.44              |
| 1:C:104:THR:CG2  | 1:D:50:VAL:HG22  | 2.42                     | 0.44              |
| 1:G:235:ILE:HG22 | 1:G:386:MET:HE2  | 1.99                     | 0.44              |
| 1:J:90:GLN:HG2   | 1:K:90:GLN:HG2   | 2.00                     | 0.44              |
| 1:J:293:MET:HE3  | 1:J:305:ALA:HB3  | 1.99                     | 0.44              |
| 1:G:266:ASP:HA   | 1:G:292:THR:OG1  | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:218:ILE:HG23 | 1:H:222:ILE:HD12 | 2.00                     | 0.44              |
| 1:I:355:GLU:HG2  | 1:I:359:LEU:HD12 | 1.98                     | 0.44              |
| 1:L:206:THR:HG22 | 1:L:208:ALA:N    | 2.32                     | 0.44              |
| 1:G:134:GLY:CA   | 2:G:500:PLP:O1P  | 2.65                     | 0.44              |
| 1:B:268:VAL:HG12 | 1:B:295:LYS:HD2  | 2.00                     | 0.44              |
| 1:E:37:VAL:CB    | 1:F:113:THR:CG2  | 2.96                     | 0.44              |
| 1:J:206:THR:HG22 | 1:J:209:GLU:H    | 1.83                     | 0.44              |
| 1:A:181:ASN:HB2  | 1:B:147:LEU:HD22 | 1.99                     | 0.44              |
| 1:B:291:ILE:HG21 | 1:B:291:ILE:HD13 | 1.69                     | 0.44              |
| 1:L:167:LEU:O    | 1:L:170:ALA:HB3  | 2.18                     | 0.44              |
| 1:E:215:ILE:HG23 | 1:E:255:TRP:CE2  | 2.52                     | 0.44              |
| 1:I:104:THR:CG2  | 1:L:50:VAL:HG22  | 2.45                     | 0.44              |
| 1:F:377:VAL:HG22 | 1:F:377:VAL:O    | 2.17                     | 0.43              |
| 1:J:357:LEU:HA   | 1:J:357:LEU:HD12 | 1.81                     | 0.43              |
| 1:K:266:ASP:HA   | 1:K:292:THR:OG1  | 2.17                     | 0.43              |
| 1:B:8:LEU:HD23   | 1:B:9:SER:H      | 1.83                     | 0.43              |
| 1:F:323:GLY:HA3  | 3:F:2035:HOH:O   | 2.16                     | 0.43              |
| 1:I:46:VAL:HB    | 1:L:103:VAL:O    | 2.18                     | 0.43              |
| 1:I:50:VAL:CG2   | 1:L:104:THR:CG2  | 2.93                     | 0.43              |
| 1:L:338:ALA:C    | 1:L:342:MET:HE3  | 2.43                     | 0.43              |
| 1:F:89:VAL:HG13  | 1:F:330:VAL:CG1  | 2.48                     | 0.43              |
| 1:H:316:VAL:HG11 | 1:H:321:LEU:HG   | 2.00                     | 0.43              |
| 1:G:249:LEU:HA   | 1:G:249:LEU:HD23 | 1.67                     | 0.43              |
| 1:I:266:ASP:OD2  | 2:I:500:PLP:C2A  | 2.64                     | 0.43              |
| 1:K:33:ARG:O     | 1:K:37:VAL:HG22  | 2.19                     | 0.43              |
| 1:L:279:PHE:CD1  | 1:L:291:ILE:HD11 | 2.53                     | 0.43              |
| 1:I:38:VAL:HG23  | 1:L:113:THR:HG21 | 2.00                     | 0.43              |
| 1:H:266:ASP:HA   | 1:H:292:THR:OG1  | 2.18                     | 0.43              |
| 1:C:266:ASP:HA   | 1:C:292:THR:OG1  | 2.18                     | 0.43              |
| 1:E:90:GLN:HG2   | 1:F:90:GLN:HG2   | 2.01                     | 0.43              |
| 1:E:276:GLY:O    | 1:E:352:ARG:NH1  | 2.51                     | 0.43              |
| 1:G:147:LEU:HD22 | 1:H:181:ASN:HB2  | 2.01                     | 0.43              |
| 1:G:167:LEU:O    | 1:G:170:ALA:HB3  | 2.18                     | 0.43              |
| 1:G:375:SER:HB3  | 3:G:2036:HOH:O   | 2.19                     | 0.43              |
| 1:K:131:PHE:O    | 1:K:303:LEU:HD12 | 2.19                     | 0.43              |
| 1:C:47:PRO:HD3   | 1:C:412:LEU:HD21 | 2.01                     | 0.42              |
| 1:E:89:VAL:HG13  | 1:E:330:VAL:CG1  | 2.49                     | 0.42              |
| 1:H:281:VAL:HG13 | 1:H:286:VAL:O    | 2.19                     | 0.42              |
| 1:D:266:ASP:HA   | 1:D:292:THR:OG1  | 2.20                     | 0.42              |
| 1:D:286:VAL:HA   | 3:D:2047:HOH:O   | 2.19                     | 0.42              |
| 1:B:11:ARG:HG3   | 1:E:59:ARG:NH1   | 2.34                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:269:GLN:HG2  | 1:H:386:MET:CE   | 2.49                     | 0.42              |
| 1:J:89:VAL:HG13  | 1:J:330:VAL:CG1  | 2.48                     | 0.42              |
| 1:B:89:VAL:HG13  | 1:B:330:VAL:CG1  | 2.49                     | 0.42              |
| 1:H:364:GLU:HG3  | 3:H:2026:HOH:O   | 2.19                     | 0.42              |
| 1:G:108:GLY:O    | 1:G:112:VAL:HG23 | 2.19                     | 0.42              |
| 1:J:37:VAL:CB    | 1:K:113:THR:CG2  | 2.96                     | 0.42              |
| 1:E:279:PHE:CD1  | 1:E:291:ILE:HD11 | 2.55                     | 0.42              |
| 1:B:362:LEU:HD23 | 1:B:362:LEU:HA   | 1.87                     | 0.42              |
| 1:C:147:LEU:HD22 | 1:D:181:ASN:HB2  | 2.00                     | 0.42              |
| 1:G:279:PHE:CD1  | 1:G:291:ILE:HD11 | 2.55                     | 0.42              |
| 1:G:377:VAL:HG22 | 1:G:389:ILE:HD11 | 2.01                     | 0.42              |
| 1:K:255:TRP:O    | 1:K:258:GLU:HB2  | 2.19                     | 0.42              |
| 1:E:206:THR:HG22 | 1:E:209:GLU:H    | 1.84                     | 0.42              |
| 1:A:403:LEU:O    | 1:A:407:VAL:HG23 | 2.20                     | 0.42              |
| 1:D:291:ILE:HG21 | 1:D:291:ILE:HD13 | 1.64                     | 0.42              |
| 1:I:290:ILE:HG22 | 1:I:291:ILE:N    | 2.34                     | 0.42              |
| 1:A:316:VAL:HG11 | 1:A:321:LEU:HG   | 2.02                     | 0.42              |
| 1:C:131:PHE:CZ   | 1:C:140:ASN:CG   | 2.98                     | 0.42              |
| 1:A:281:VAL:HG13 | 1:A:286:VAL:O    | 2.20                     | 0.41              |
| 1:B:376:VAL:HG11 | 1:B:403:LEU:HD21 | 2.02                     | 0.41              |
| 1:C:230:ILE:HG13 | 1:C:261:ILE:HG21 | 2.01                     | 0.41              |
| 1:D:47:PRO:HD3   | 1:D:412:LEU:HD21 | 2.00                     | 0.41              |
| 1:D:118:ARG:HB2  | 3:D:2020:HOH:O   | 2.20                     | 0.41              |
| 1:F:291:ILE:HG21 | 1:F:291:ILE:HD13 | 1.63                     | 0.41              |
| 1:H:355:GLU:HG2  | 1:H:359:LEU:HD12 | 2.02                     | 0.41              |
| 1:A:46:VAL:HA    | 1:A:47:PRO:HD3   | 1.95                     | 0.41              |
| 1:A:385:ALA:CB   | 1:A:434:LEU:CD2  | 2.98                     | 0.41              |
| 1:C:89:VAL:HG13  | 1:C:330:VAL:CG1  | 2.50                     | 0.41              |
| 1:L:82:ASP:CG    | 3:L:2008:HOH:O   | 2.63                     | 0.41              |
| 1:I:270:SER:HB2  | 1:I:280:ALA:HB2  | 2.01                     | 0.41              |
| 1:K:89:VAL:HG13  | 1:K:330:VAL:CG1  | 2.50                     | 0.41              |
| 1:A:147:LEU:HD22 | 1:B:181:ASN:HB2  | 2.03                     | 0.41              |
| 1:F:46:VAL:HA    | 1:F:47:PRO:HD3   | 1.97                     | 0.41              |
| 1:I:99:THR:HG21  | 1:L:50:VAL:HG11  | 2.02                     | 0.41              |
| 1:A:89:VAL:HG13  | 1:A:330:VAL:CG1  | 2.50                     | 0.41              |
| 1:B:131:PHE:CZ   | 1:B:140:ASN:CG   | 2.98                     | 0.41              |
| 1:C:391:LEU:HD11 | 1:C:428:ILE:HD12 | 2.03                     | 0.41              |
| 1:A:50:VAL:HG21  | 1:B:99:THR:HG21  | 2.02                     | 0.41              |
| 1:E:36:ALA:HA    | 1:I:258:GLU:HG3  | 2.03                     | 0.41              |
| 1:H:376:VAL:HG11 | 1:H:403:LEU:CD2  | 2.51                     | 0.41              |
| 1:I:38:VAL:HG22  | 1:L:113:THR:HG21 | 2.03                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:113:THR:HG21 | 1:K:38:VAL:HG23  | 2.02                     | 0.41              |
| 1:L:46:VAL:HA    | 1:L:47:PRO:HD3   | 1.97                     | 0.41              |
| 1:E:147:LEU:C    | 1:E:147:LEU:HD13 | 2.46                     | 0.41              |
| 1:F:155:VAL:HG22 | 1:F:230:ILE:HG12 | 2.03                     | 0.41              |
| 1:G:293:MET:HE3  | 1:G:293:MET:HB2  | 1.98                     | 0.41              |
| 1:J:50:VAL:HG21  | 1:K:99:THR:HG21  | 2.02                     | 0.41              |
| 1:K:46:VAL:HA    | 1:K:47:PRO:HD3   | 1.97                     | 0.41              |
| 1:A:215:ILE:HG23 | 1:A:255:TRP:CE2  | 2.56                     | 0.40              |
| 1:B:359:LEU:HD23 | 1:B:359:LEU:HA   | 1.89                     | 0.40              |
| 1:C:50:VAL:CG2   | 1:D:104:THR:HG22 | 2.50                     | 0.40              |
| 1:J:297:ILE:HG23 | 1:J:298:ALA:N    | 2.37                     | 0.40              |
| 1:D:33:ARG:O     | 1:D:37:VAL:HG22  | 2.20                     | 0.40              |
| 1:E:42:VAL:HG21  | 1:F:129:VAL:HG13 | 2.02                     | 0.40              |
| 1:J:215:ILE:HG23 | 1:J:255:TRP:CE2  | 2.57                     | 0.40              |
| 1:E:268:VAL:HG13 | 1:E:294:ALA:HB3  | 2.01                     | 0.40              |
| 1:F:82:ASP:OD2   | 1:F:85:VAL:HG23  | 2.21                     | 0.40              |
| 1:H:47:PRO:HD3   | 1:H:412:LEU:HD21 | 2.03                     | 0.40              |
| 1:J:167:LEU:O    | 1:J:170:ALA:HB3  | 2.21                     | 0.40              |
| 1:C:82:ASP:O     | 1:C:86:VAL:HG23  | 2.21                     | 0.40              |
| 1:G:292:THR:HG22 | 1:G:306:ILE:HG22 | 2.02                     | 0.40              |
| 1:J:166:ASN:HA   | 1:J:169:MET:CE   | 2.52                     | 0.40              |
| 1:J:230:ILE:HG13 | 1:J:261:ILE:HG21 | 2.04                     | 0.40              |
| 1:F:50:VAL:HG13  | 1:F:58:ILE:CG2   | 2.41                     | 0.40              |
| 1:K:74:ALA:HB2   | 1:K:431:LEU:HD13 | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |
|-----|-------|---------------|-----------|---------|----------|-------------|
| 1   | A     | 439/456 (96%) | 417 (95%) | 19 (4%) | 3 (1%)   | 18 47       |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1   | B     | 438/456 (96%)   | 417 (95%)  | 18 (4%)  | 3 (1%)   | 18          | 47 |
| 1   | C     | 436/456 (96%)   | 415 (95%)  | 18 (4%)  | 3 (1%)   | 18          | 47 |
| 1   | D     | 435/456 (95%)   | 414 (95%)  | 18 (4%)  | 3 (1%)   | 18          | 47 |
| 1   | E     | 438/456 (96%)   | 417 (95%)  | 17 (4%)  | 4 (1%)   | 14          | 41 |
| 1   | F     | 436/456 (96%)   | 415 (95%)  | 18 (4%)  | 3 (1%)   | 18          | 47 |
| 1   | G     | 436/456 (96%)   | 413 (95%)  | 20 (5%)  | 3 (1%)   | 18          | 47 |
| 1   | H     | 436/456 (96%)   | 414 (95%)  | 19 (4%)  | 3 (1%)   | 18          | 47 |
| 1   | I     | 437/456 (96%)   | 414 (95%)  | 20 (5%)  | 3 (1%)   | 18          | 47 |
| 1   | J     | 434/456 (95%)   | 412 (95%)  | 19 (4%)  | 3 (1%)   | 18          | 47 |
| 1   | K     | 435/456 (95%)   | 413 (95%)  | 19 (4%)  | 3 (1%)   | 18          | 47 |
| 1   | L     | 432/456 (95%)   | 411 (95%)  | 18 (4%)  | 3 (1%)   | 18          | 47 |
| All | All   | 5232/5472 (96%) | 4972 (95%) | 223 (4%) | 37 (1%)  | 18          | 47 |

All (37) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 367 | ALA  |
| 1   | A     | 295 | LYS  |
| 1   | B     | 294 | ALA  |
| 1   | B     | 295 | LYS  |
| 1   | C     | 294 | ALA  |
| 1   | C     | 295 | LYS  |
| 1   | D     | 295 | LYS  |
| 1   | E     | 295 | LYS  |
| 1   | F     | 294 | ALA  |
| 1   | F     | 295 | LYS  |
| 1   | G     | 295 | LYS  |
| 1   | H     | 295 | LYS  |
| 1   | I     | 295 | LYS  |
| 1   | J     | 294 | ALA  |
| 1   | J     | 295 | LYS  |
| 1   | K     | 295 | LYS  |
| 1   | L     | 294 | ALA  |
| 1   | L     | 295 | LYS  |
| 1   | A     | 294 | ALA  |
| 1   | D     | 294 | ALA  |
| 1   | E     | 294 | ALA  |
| 1   | G     | 294 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 294 | ALA  |
| 1   | I     | 294 | ALA  |
| 1   | K     | 294 | ALA  |
| 1   | B     | 100 | CYS  |
| 1   | C     | 100 | CYS  |
| 1   | D     | 100 | CYS  |
| 1   | E     | 100 | CYS  |
| 1   | G     | 100 | CYS  |
| 1   | H     | 100 | CYS  |
| 1   | I     | 100 | CYS  |
| 1   | J     | 100 | CYS  |
| 1   | K     | 100 | CYS  |
| 1   | L     | 100 | CYS  |
| 1   | A     | 100 | CYS  |
| 1   | F     | 100 | CYS  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A     | 321/336 (96%) | 307 (96%) | 14 (4%)  | 25          | 59 |
| 1   | B     | 314/336 (94%) | 301 (96%) | 13 (4%)  | 27          | 62 |
| 1   | C     | 316/336 (94%) | 305 (96%) | 11 (4%)  | 32          | 67 |
| 1   | D     | 315/336 (94%) | 304 (96%) | 11 (4%)  | 32          | 67 |
| 1   | E     | 318/336 (95%) | 303 (95%) | 15 (5%)  | 23          | 57 |
| 1   | F     | 312/336 (93%) | 302 (97%) | 10 (3%)  | 34          | 70 |
| 1   | G     | 297/336 (88%) | 286 (96%) | 11 (4%)  | 30          | 65 |
| 1   | H     | 304/336 (90%) | 294 (97%) | 10 (3%)  | 33          | 69 |
| 1   | I     | 309/336 (92%) | 299 (97%) | 10 (3%)  | 34          | 70 |
| 1   | J     | 305/336 (91%) | 294 (96%) | 11 (4%)  | 31          | 66 |
| 1   | K     | 297/336 (88%) | 284 (96%) | 13 (4%)  | 25          | 59 |
| 1   | L     | 295/336 (88%) | 284 (96%) | 11 (4%)  | 30          | 65 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |
|-----|-------|-----------------|------------|----------|-------------|
| All | All   | 3703/4032 (92%) | 3563 (96%) | 140 (4%) | 29 64       |

All (140) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 46  | VAL  |
| 1   | A     | 50  | VAL  |
| 1   | A     | 113 | THR  |
| 1   | A     | 147 | LEU  |
| 1   | A     | 155 | VAL  |
| 1   | A     | 167 | LEU  |
| 1   | A     | 206 | THR  |
| 1   | A     | 281 | VAL  |
| 1   | A     | 291 | ILE  |
| 1   | A     | 357 | LEU  |
| 1   | A     | 369 | LEU  |
| 1   | A     | 389 | ILE  |
| 1   | A     | 398 | GLU  |
| 1   | A     | 440 | LEU  |
| 1   | B     | 8   | LEU  |
| 1   | B     | 9   | SER  |
| 1   | B     | 32  | GLU  |
| 1   | B     | 50  | VAL  |
| 1   | B     | 113 | THR  |
| 1   | B     | 147 | LEU  |
| 1   | B     | 155 | VAL  |
| 1   | B     | 206 | THR  |
| 1   | B     | 291 | ILE  |
| 1   | B     | 357 | LEU  |
| 1   | B     | 376 | VAL  |
| 1   | B     | 383 | ARG  |
| 1   | B     | 389 | ILE  |
| 1   | C     | 50  | VAL  |
| 1   | C     | 102 | MET  |
| 1   | C     | 113 | THR  |
| 1   | C     | 147 | LEU  |
| 1   | C     | 155 | VAL  |
| 1   | C     | 206 | THR  |
| 1   | C     | 291 | ILE  |
| 1   | C     | 357 | LEU  |
| 1   | C     | 369 | LEU  |
| 1   | C     | 376 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 389 | ILE  |
| 1   | D     | 50  | VAL  |
| 1   | D     | 113 | THR  |
| 1   | D     | 147 | LEU  |
| 1   | D     | 155 | VAL  |
| 1   | D     | 206 | THR  |
| 1   | D     | 291 | ILE  |
| 1   | D     | 357 | LEU  |
| 1   | D     | 376 | VAL  |
| 1   | D     | 389 | ILE  |
| 1   | D     | 393 | GLN  |
| 1   | D     | 398 | GLU  |
| 1   | E     | 46  | VAL  |
| 1   | E     | 50  | VAL  |
| 1   | E     | 102 | MET  |
| 1   | E     | 113 | THR  |
| 1   | E     | 147 | LEU  |
| 1   | E     | 155 | VAL  |
| 1   | E     | 206 | THR  |
| 1   | E     | 281 | VAL  |
| 1   | E     | 286 | VAL  |
| 1   | E     | 291 | ILE  |
| 1   | E     | 352 | ARG  |
| 1   | E     | 357 | LEU  |
| 1   | E     | 376 | VAL  |
| 1   | E     | 377 | VAL  |
| 1   | E     | 389 | ILE  |
| 1   | F     | 50  | VAL  |
| 1   | F     | 113 | THR  |
| 1   | F     | 147 | LEU  |
| 1   | F     | 155 | VAL  |
| 1   | F     | 206 | THR  |
| 1   | F     | 291 | ILE  |
| 1   | F     | 357 | LEU  |
| 1   | F     | 376 | VAL  |
| 1   | F     | 377 | VAL  |
| 1   | F     | 389 | ILE  |
| 1   | G     | 37  | VAL  |
| 1   | G     | 50  | VAL  |
| 1   | G     | 102 | MET  |
| 1   | G     | 113 | THR  |
| 1   | G     | 147 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 155 | VAL  |
| 1   | G     | 206 | THR  |
| 1   | G     | 291 | ILE  |
| 1   | G     | 357 | LEU  |
| 1   | G     | 376 | VAL  |
| 1   | G     | 389 | ILE  |
| 1   | H     | 37  | VAL  |
| 1   | H     | 50  | VAL  |
| 1   | H     | 113 | THR  |
| 1   | H     | 147 | LEU  |
| 1   | H     | 155 | VAL  |
| 1   | H     | 206 | THR  |
| 1   | H     | 281 | VAL  |
| 1   | H     | 291 | ILE  |
| 1   | H     | 376 | VAL  |
| 1   | H     | 389 | ILE  |
| 1   | I     | 46  | VAL  |
| 1   | I     | 50  | VAL  |
| 1   | I     | 113 | THR  |
| 1   | I     | 147 | LEU  |
| 1   | I     | 155 | VAL  |
| 1   | I     | 206 | THR  |
| 1   | I     | 291 | ILE  |
| 1   | I     | 357 | LEU  |
| 1   | I     | 376 | VAL  |
| 1   | I     | 389 | ILE  |
| 1   | J     | 46  | VAL  |
| 1   | J     | 50  | VAL  |
| 1   | J     | 113 | THR  |
| 1   | J     | 147 | LEU  |
| 1   | J     | 155 | VAL  |
| 1   | J     | 206 | THR  |
| 1   | J     | 291 | ILE  |
| 1   | J     | 357 | LEU  |
| 1   | J     | 376 | VAL  |
| 1   | J     | 389 | ILE  |
| 1   | J     | 412 | LEU  |
| 1   | K     | 46  | VAL  |
| 1   | K     | 50  | VAL  |
| 1   | K     | 102 | MET  |
| 1   | K     | 113 | THR  |
| 1   | K     | 147 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 155 | VAL  |
| 1   | K     | 206 | THR  |
| 1   | K     | 281 | VAL  |
| 1   | K     | 291 | ILE  |
| 1   | K     | 357 | LEU  |
| 1   | K     | 376 | VAL  |
| 1   | K     | 377 | VAL  |
| 1   | K     | 389 | ILE  |
| 1   | L     | 50  | VAL  |
| 1   | L     | 61  | VAL  |
| 1   | L     | 113 | THR  |
| 1   | L     | 116 | LEU  |
| 1   | L     | 147 | LEU  |
| 1   | L     | 155 | VAL  |
| 1   | L     | 206 | THR  |
| 1   | L     | 291 | ILE  |
| 1   | L     | 357 | LEU  |
| 1   | L     | 376 | VAL  |
| 1   | L     | 389 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 269 | GLN  |
| 1   | B     | 181 | ASN  |
| 1   | B     | 269 | GLN  |
| 1   | C     | 269 | GLN  |
| 1   | D     | 14  | GLN  |
| 1   | D     | 90  | GLN  |
| 1   | D     | 269 | GLN  |
| 1   | D     | 283 | HIS  |
| 1   | E     | 17  | ASN  |
| 1   | E     | 19  | ASN  |
| 1   | E     | 269 | GLN  |
| 1   | E     | 283 | HIS  |
| 1   | E     | 345 | HIS  |
| 1   | E     | 393 | GLN  |
| 1   | F     | 14  | GLN  |
| 1   | F     | 17  | ASN  |
| 1   | F     | 19  | ASN  |
| 1   | F     | 132 | ASN  |
| 1   | F     | 221 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 269 | GLN  |
| 1   | F     | 345 | HIS  |
| 1   | G     | 269 | GLN  |
| 1   | H     | 140 | ASN  |
| 1   | H     | 181 | ASN  |
| 1   | H     | 269 | GLN  |
| 1   | H     | 283 | HIS  |
| 1   | H     | 345 | HIS  |
| 1   | I     | 19  | ASN  |
| 1   | I     | 283 | HIS  |
| 1   | J     | 19  | ASN  |
| 1   | J     | 283 | HIS  |
| 1   | K     | 345 | HIS  |
| 1   | K     | 353 | HIS  |
| 1   | L     | 283 | HIS  |
| 1   | L     | 345 | HIS  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | PLP  | J     | 500 | 1    | 15,15,16     | 3.39 | 4 (26%)  | 21,22,23    | 1.84 | 7 (33%)  |
| 2   | PLP  | F     | 500 | 1    | 15,15,16     | 2.85 | 3 (20%)  | 21,22,23    | 2.08 | 7 (33%)  |
| 2   | PLP  | K     | 500 | 1    | 15,15,16     | 3.43 | 3 (20%)  | 21,22,23    | 2.12 | 6 (28%)  |
| 2   | PLP  | G     | 500 | 1    | 15,15,16     | 3.07 | 4 (26%)  | 21,22,23    | 2.08 | 9 (42%)  |
| 2   | PLP  | C     | 500 | 1    | 15,15,16     | 2.81 | 3 (20%)  | 21,22,23    | 1.88 | 6 (28%)  |
| 2   | PLP  | E     | 500 | 1    | 15,15,16     | 3.42 | 3 (20%)  | 21,22,23    | 1.92 | 7 (33%)  |
| 2   | PLP  | H     | 500 | 1    | 15,15,16     | 3.70 | 4 (26%)  | 21,22,23    | 1.95 | 8 (38%)  |
| 2   | PLP  | L     | 500 | 1    | 15,15,16     | 2.82 | 3 (20%)  | 21,22,23    | 1.48 | 4 (19%)  |
| 2   | PLP  | A     | 500 | 1    | 15,15,16     | 2.93 | 3 (20%)  | 21,22,23    | 1.56 | 3 (14%)  |
| 2   | PLP  | I     | 500 | 1    | 15,15,16     | 2.75 | 3 (20%)  | 21,22,23    | 3.64 | 8 (38%)  |
| 2   | PLP  | D     | 500 | 1    | 15,15,16     | 3.69 | 5 (33%)  | 21,22,23    | 1.97 | 7 (33%)  |
| 2   | PLP  | B     | 500 | 1    | 15,15,16     | 3.27 | 4 (26%)  | 21,22,23    | 2.31 | 8 (38%)  |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 2   | PLP  | J     | 500 | 1    | -       | 0/6/6/8  | 0/1/1/1 |
| 2   | PLP  | F     | 500 | 1    | -       | 3/6/6/8  | 0/1/1/1 |
| 2   | PLP  | K     | 500 | 1    | -       | 2/6/6/8  | 0/1/1/1 |
| 2   | PLP  | G     | 500 | 1    | -       | 2/6/6/8  | 0/1/1/1 |
| 2   | PLP  | C     | 500 | 1    | -       | 0/6/6/8  | 0/1/1/1 |
| 2   | PLP  | E     | 500 | 1    | -       | 5/6/6/8  | 0/1/1/1 |
| 2   | PLP  | H     | 500 | 1    | -       | 0/6/6/8  | 0/1/1/1 |
| 2   | PLP  | L     | 500 | 1    | -       | 2/6/6/8  | 0/1/1/1 |
| 2   | PLP  | A     | 500 | 1    | -       | 0/6/6/8  | 0/1/1/1 |
| 2   | PLP  | I     | 500 | 1    | -       | 3/6/6/8  | 0/1/1/1 |
| 2   | PLP  | D     | 500 | 1    | -       | 0/6/6/8  | 0/1/1/1 |
| 2   | PLP  | B     | 500 | 1    | -       | 0/6/6/8  | 0/1/1/1 |

All (42) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | H     | 500 | PLP  | C3-C2 | 10.40 | 1.51        | 1.41     |
| 2   | D     | 500 | PLP  | C3-C2 | 9.81  | 1.51        | 1.41     |
| 2   | J     | 500 | PLP  | C5-C4 | 9.73  | 1.51        | 1.40     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | E     | 500 | PLP  | C3-C2  | 9.67  | 1.51        | 1.41     |
| 2   | K     | 500 | PLP  | C5-C4  | 9.41  | 1.51        | 1.40     |
| 2   | H     | 500 | PLP  | C5-C4  | 8.69  | 1.50        | 1.40     |
| 2   | D     | 500 | PLP  | C5-C4  | 8.57  | 1.50        | 1.40     |
| 2   | B     | 500 | PLP  | C5-C4  | 8.47  | 1.50        | 1.40     |
| 2   | F     | 500 | PLP  | C3-C2  | 8.44  | 1.49        | 1.41     |
| 2   | G     | 500 | PLP  | C5-C4  | 8.01  | 1.49        | 1.40     |
| 2   | K     | 500 | PLP  | C3-C2  | 7.99  | 1.49        | 1.41     |
| 2   | I     | 500 | PLP  | C5-C4  | 7.87  | 1.49        | 1.40     |
| 2   | E     | 500 | PLP  | C5-C4  | 7.79  | 1.49        | 1.40     |
| 2   | L     | 500 | PLP  | C3-C2  | 7.66  | 1.48        | 1.41     |
| 2   | J     | 500 | PLP  | C3-C2  | 7.33  | 1.48        | 1.41     |
| 2   | B     | 500 | PLP  | C3-C2  | 7.32  | 1.48        | 1.41     |
| 2   | A     | 500 | PLP  | C3-C2  | 7.30  | 1.48        | 1.41     |
| 2   | C     | 500 | PLP  | C5-C4  | 7.17  | 1.48        | 1.40     |
| 2   | A     | 500 | PLP  | C5-C4  | 7.06  | 1.48        | 1.40     |
| 2   | G     | 500 | PLP  | C3-C2  | 6.51  | 1.47        | 1.41     |
| 2   | C     | 500 | PLP  | C3-C2  | 6.23  | 1.47        | 1.41     |
| 2   | L     | 500 | PLP  | C5-C4  | 5.89  | 1.47        | 1.40     |
| 2   | I     | 500 | PLP  | C3-C2  | 5.68  | 1.46        | 1.41     |
| 2   | F     | 500 | PLP  | C5-C4  | 5.24  | 1.46        | 1.40     |
| 2   | G     | 500 | PLP  | C3-C4  | 5.23  | 1.50        | 1.40     |
| 2   | C     | 500 | PLP  | C3-C4  | 4.97  | 1.49        | 1.40     |
| 2   | B     | 500 | PLP  | C3-C4  | 4.92  | 1.49        | 1.40     |
| 2   | D     | 500 | PLP  | C3-C4  | 4.57  | 1.48        | 1.40     |
| 2   | L     | 500 | PLP  | C3-C4  | 4.44  | 1.48        | 1.40     |
| 2   | K     | 500 | PLP  | C3-C4  | 4.38  | 1.48        | 1.40     |
| 2   | A     | 500 | PLP  | C3-C4  | 4.33  | 1.48        | 1.40     |
| 2   | F     | 500 | PLP  | C3-C4  | 3.81  | 1.47        | 1.40     |
| 2   | H     | 500 | PLP  | C3-C4  | 3.43  | 1.46        | 1.40     |
| 2   | E     | 500 | PLP  | C3-C4  | 3.41  | 1.46        | 1.40     |
| 2   | I     | 500 | PLP  | C3-C4  | 3.24  | 1.46        | 1.40     |
| 2   | J     | 500 | PLP  | C3-C4  | 3.15  | 1.46        | 1.40     |
| 2   | B     | 500 | PLP  | C4A-C4 | -2.40 | 1.46        | 1.51     |
| 2   | G     | 500 | PLP  | C4A-C4 | -2.28 | 1.47        | 1.51     |
| 2   | J     | 500 | PLP  | C4A-C4 | -2.27 | 1.47        | 1.51     |
| 2   | D     | 500 | PLP  | C2-N1  | 2.17  | 1.37        | 1.33     |
| 2   | H     | 500 | PLP  | C4A-C4 | -2.12 | 1.47        | 1.51     |
| 2   | D     | 500 | PLP  | C6-C5  | 2.08  | 1.41        | 1.37     |

All (80) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | I     | 500 | PLP  | C4A-C4-C5  | 12.68 | 134.01      | 120.94   |
| 2   | I     | 500 | PLP  | C3-C4-C5   | -5.46 | 112.03      | 118.59   |
| 2   | F     | 500 | PLP  | C3-C4-C5   | -5.01 | 112.58      | 118.59   |
| 2   | D     | 500 | PLP  | C6-C5-C4   | 4.83  | 122.06      | 118.10   |
| 2   | I     | 500 | PLP  | C6-C5-C4   | 4.57  | 121.85      | 118.10   |
| 2   | B     | 500 | PLP  | C4A-C4-C5  | -4.57 | 116.23      | 120.94   |
| 2   | I     | 500 | PLP  | C4A-C4-C3  | -4.47 | 113.07      | 120.52   |
| 2   | A     | 500 | PLP  | C3-C4-C5   | -4.41 | 113.29      | 118.59   |
| 2   | C     | 500 | PLP  | C3-C4-C5   | -4.30 | 113.43      | 118.59   |
| 2   | G     | 500 | PLP  | O4P-C5A-C5 | 4.20  | 117.22      | 109.36   |
| 2   | G     | 500 | PLP  | C4A-C4-C5  | -4.19 | 116.62      | 120.94   |
| 2   | C     | 500 | PLP  | C4A-C4-C5  | 4.18  | 125.25      | 120.94   |
| 2   | K     | 500 | PLP  | C5A-C5-C6  | -4.07 | 112.73      | 119.36   |
| 2   | H     | 500 | PLP  | O3-C3-C2   | 4.00  | 125.87      | 117.58   |
| 2   | F     | 500 | PLP  | O3P-P-O4P  | -3.86 | 96.61       | 106.67   |
| 2   | K     | 500 | PLP  | C3-C4-C5   | -3.84 | 113.98      | 118.59   |
| 2   | K     | 500 | PLP  | C6-C5-C4   | 3.78  | 121.19      | 118.10   |
| 2   | B     | 500 | PLP  | C6-N1-C2   | 3.65  | 125.82      | 119.20   |
| 2   | B     | 500 | PLP  | O3P-P-O2P  | 3.65  | 121.48      | 107.80   |
| 2   | E     | 500 | PLP  | O3P-P-O4P  | -3.51 | 97.52       | 106.67   |
| 2   | B     | 500 | PLP  | O3P-P-O4P  | -3.50 | 97.54       | 106.67   |
| 2   | B     | 500 | PLP  | C4A-C4-C3  | 3.44  | 126.26      | 120.52   |
| 2   | B     | 500 | PLP  | O4P-C5A-C5 | 3.42  | 115.76      | 109.36   |
| 2   | E     | 500 | PLP  | C2A-C2-C3  | 3.38  | 124.76      | 120.80   |
| 2   | I     | 500 | PLP  | O3P-P-O1P  | 3.30  | 123.69      | 110.83   |
| 2   | D     | 500 | PLP  | O3-C3-C2   | 3.28  | 124.37      | 117.58   |
| 2   | F     | 500 | PLP  | C6-C5-C4   | 3.27  | 120.78      | 118.10   |
| 2   | H     | 500 | PLP  | C2A-C2-C3  | 3.25  | 124.61      | 120.80   |
| 2   | K     | 500 | PLP  | C4A-C4-C3  | 3.24  | 125.92      | 120.52   |
| 2   | I     | 500 | PLP  | O4P-P-O1P  | -3.19 | 97.81       | 106.44   |
| 2   | D     | 500 | PLP  | C3-C4-C5   | -3.17 | 114.79      | 118.59   |
| 2   | K     | 500 | PLP  | O4P-C5A-C5 | 3.12  | 115.20      | 109.36   |
| 2   | L     | 500 | PLP  | O3P-P-O4P  | -3.12 | 98.55       | 106.67   |
| 2   | E     | 500 | PLP  | O3P-P-O2P  | 3.10  | 119.44      | 107.80   |
| 2   | F     | 500 | PLP  | O3P-P-O2P  | 3.05  | 119.24      | 107.80   |
| 2   | G     | 500 | PLP  | C6-N1-C2   | 2.97  | 124.59      | 119.20   |
| 2   | L     | 500 | PLP  | C6-C5-C4   | 2.97  | 120.53      | 118.10   |
| 2   | K     | 500 | PLP  | O3P-P-O4P  | -2.96 | 98.95       | 106.67   |
| 2   | D     | 500 | PLP  | O4P-C5A-C5 | 2.91  | 114.81      | 109.36   |
| 2   | J     | 500 | PLP  | O3-C3-C2   | 2.90  | 123.59      | 117.58   |
| 2   | J     | 500 | PLP  | C4A-C4-C5  | -2.90 | 117.95      | 120.94   |
| 2   | C     | 500 | PLP  | C6-C5-C4   | 2.89  | 120.47      | 118.10   |
| 2   | A     | 500 | PLP  | O4P-P-O1P  | -2.88 | 98.67       | 106.44   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | J     | 500 | PLP  | C6-N1-C2   | 2.85  | 124.36      | 119.20   |
| 2   | E     | 500 | PLP  | C5A-C5-C6  | -2.84 | 114.74      | 119.36   |
| 2   | G     | 500 | PLP  | C4A-C4-C3  | 2.83  | 125.25      | 120.52   |
| 2   | F     | 500 | PLP  | C4A-C4-C5  | 2.83  | 123.86      | 120.94   |
| 2   | J     | 500 | PLP  | O4P-C5A-C5 | 2.81  | 114.62      | 109.36   |
| 2   | C     | 500 | PLP  | O3P-P-O2P  | 2.78  | 118.21      | 107.80   |
| 2   | I     | 500 | PLP  | C2A-C2-C3  | -2.74 | 117.58      | 120.80   |
| 2   | G     | 500 | PLP  | C5A-C5-C6  | -2.71 | 114.94      | 119.36   |
| 2   | J     | 500 | PLP  | C4-C3-C2   | -2.68 | 115.88      | 119.89   |
| 2   | F     | 500 | PLP  | O4P-C5A-C5 | 2.62  | 114.26      | 109.36   |
| 2   | H     | 500 | PLP  | O4P-C5A-C5 | 2.60  | 114.24      | 109.36   |
| 2   | E     | 500 | PLP  | O2P-P-O4P  | 2.60  | 113.46      | 106.67   |
| 2   | C     | 500 | PLP  | O4P-C5A-C5 | 2.60  | 114.22      | 109.36   |
| 2   | H     | 500 | PLP  | C3-C4-C5   | -2.58 | 115.50      | 118.59   |
| 2   | E     | 500 | PLP  | O3-C3-C2   | 2.56  | 122.89      | 117.58   |
| 2   | H     | 500 | PLP  | O2P-P-O4P  | -2.53 | 100.08      | 106.67   |
| 2   | J     | 500 | PLP  | O3P-P-O1P  | 2.51  | 120.60      | 110.83   |
| 2   | D     | 500 | PLP  | C5A-C5-C4  | -2.50 | 117.71      | 122.64   |
| 2   | D     | 500 | PLP  | C6-N1-C2   | 2.50  | 123.73      | 119.20   |
| 2   | A     | 500 | PLP  | C4A-C4-C5  | 2.47  | 123.49      | 120.94   |
| 2   | H     | 500 | PLP  | C4A-C4-C3  | 2.45  | 124.61      | 120.52   |
| 2   | L     | 500 | PLP  | C3-C4-C5   | -2.38 | 115.73      | 118.59   |
| 2   | J     | 500 | PLP  | C6-C5-C4   | 2.38  | 120.05      | 118.10   |
| 2   | H     | 500 | PLP  | C6-C5-C4   | 2.38  | 120.05      | 118.10   |
| 2   | G     | 500 | PLP  | O3P-P-O2P  | 2.36  | 116.66      | 107.80   |
| 2   | G     | 500 | PLP  | O3-C3-C4   | 2.31  | 124.13      | 118.10   |
| 2   | D     | 500 | PLP  | O3P-P-O2P  | 2.28  | 116.36      | 107.80   |
| 2   | B     | 500 | PLP  | C3-C2-N1   | -2.28 | 118.09      | 120.96   |
| 2   | G     | 500 | PLP  | O3P-P-O4P  | 2.24  | 112.51      | 106.67   |
| 2   | L     | 500 | PLP  | C6-N1-C2   | 2.17  | 123.14      | 119.20   |
| 2   | E     | 500 | PLP  | C3-C4-C5   | -2.12 | 116.04      | 118.59   |
| 2   | I     | 500 | PLP  | C2A-C2-N1  | 2.11  | 121.61      | 117.64   |
| 2   | C     | 500 | PLP  | C6-N1-C2   | 2.08  | 122.97      | 119.20   |
| 2   | H     | 500 | PLP  | O2P-P-O1P  | 2.06  | 118.87      | 110.83   |
| 2   | G     | 500 | PLP  | C5A-C5-C4  | 2.02  | 126.63      | 122.64   |
| 2   | B     | 500 | PLP  | C2A-C2-C3  | 2.01  | 123.14      | 120.80   |
| 2   | F     | 500 | PLP  | C3-C2-N1   | -2.00 | 118.43      | 120.96   |

There are no chirality outliers.

All (17) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 2   | E     | 500 | PLP  | C4-C5-C5A-O4P |
| 2   | E     | 500 | PLP  | C6-C5-C5A-O4P |
| 2   | E     | 500 | PLP  | C5A-O4P-P-O1P |
| 2   | E     | 500 | PLP  | C5A-O4P-P-O2P |
| 2   | E     | 500 | PLP  | C5A-O4P-P-O3P |
| 2   | F     | 500 | PLP  | C5A-O4P-P-O1P |
| 2   | F     | 500 | PLP  | C5A-O4P-P-O2P |
| 2   | F     | 500 | PLP  | C5A-O4P-P-O3P |
| 2   | G     | 500 | PLP  | C4-C5-C5A-O4P |
| 2   | G     | 500 | PLP  | C6-C5-C5A-O4P |
| 2   | I     | 500 | PLP  | C5A-O4P-P-O1P |
| 2   | I     | 500 | PLP  | C5A-O4P-P-O2P |
| 2   | I     | 500 | PLP  | C5A-O4P-P-O3P |
| 2   | K     | 500 | PLP  | C4-C5-C5A-O4P |
| 2   | K     | 500 | PLP  | C6-C5-C5A-O4P |
| 2   | L     | 500 | PLP  | C4-C5-C5A-O4P |
| 2   | L     | 500 | PLP  | C6-C5-C5A-O4P |

There are no ring outliers.

3 monomers are involved in 5 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | K     | 500 | PLP  | 1       | 0            |
| 2   | G     | 500 | PLP  | 2       | 0            |
| 2   | I     | 500 | PLP  | 2       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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   | A     | 442/456 (96%)   | -0.58  | 0 100 100     | 9, 17, 35, 59         | 1 (0%) |
| 1   | B     | 442/456 (96%)   | -0.56  | 1 (0%) 91 88  | 7, 16, 28, 47         | 0      |
| 1   | C     | 442/456 (96%)   | -0.61  | 0 100 100     | 9, 17, 32, 48         | 0      |
| 1   | D     | 439/456 (96%)   | -0.47  | 2 (0%) 87 82  | 9, 20, 35, 64         | 0      |
| 1   | E     | 442/456 (96%)   | -0.49  | 1 (0%) 91 88  | 10, 19, 33, 50        | 0      |
| 1   | F     | 439/456 (96%)   | -0.47  | 1 (0%) 91 88  | 9, 20, 35, 56         | 1 (0%) |
| 1   | G     | 440/456 (96%)   | 0.15   | 6 (1%) 73 64  | 15, 36, 54, 65        | 0      |
| 1   | H     | 440/456 (96%)   | 0.12   | 5 (1%) 78 70  | 16, 36, 57, 69        | 0      |
| 1   | I     | 441/456 (96%)   | -0.20  | 0 100 100     | 14, 31, 51, 72        | 0      |
| 1   | J     | 438/456 (96%)   | -0.07  | 4 (0%) 81 74  | 14, 33, 50, 67        | 0      |
| 1   | K     | 439/456 (96%)   | 0.25   | 12 (2%) 56 46 | 20, 39, 63, 87        | 0      |
| 1   | L     | 436/456 (95%)   | 0.21   | 2 (0%) 87 82  | 20, 41, 62, 72        | 0      |
| All | All   | 5280/5472 (96%) | -0.23  | 34 (0%) 85 80 | 7, 26, 53, 87         | 2 (0%) |

All (34) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 367 | ALA  | 5.2  |
| 1   | K     | 366 | ALA  | 4.2  |
| 1   | J     | 366 | ALA  | 3.5  |
| 1   | J     | 93  | ALA  | 3.3  |
| 1   | D     | 366 | ALA  | 3.1  |
| 1   | F     | 366 | ALA  | 3.1  |
| 1   | K     | 19  | ASN  | 3.1  |
| 1   | B     | 368 | GLU  | 2.6  |
| 1   | H     | 367 | ALA  | 2.6  |
| 1   | G     | 63  | GLY  | 2.6  |
| 1   | G     | 62  | ASP  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | J     | 323 | GLY  | 2.5  |
| 1   | G     | 25  | PRO  | 2.5  |
| 1   | D     | 365 | LEU  | 2.4  |
| 1   | H     | 19  | ASN  | 2.4  |
| 1   | K     | 57  | ILE  | 2.3  |
| 1   | K     | 67  | ILE  | 2.3  |
| 1   | K     | 81  | SER  | 2.3  |
| 1   | H     | 17  | ASN  | 2.3  |
| 1   | K     | 53  | ALA  | 2.2  |
| 1   | H     | 363 | ARG  | 2.2  |
| 1   | K     | 438 | ASP  | 2.2  |
| 1   | K     | 455 | HIS  | 2.2  |
| 1   | L     | 365 | LEU  | 2.2  |
| 1   | J     | 20  | GLY  | 2.2  |
| 1   | G     | 9   | SER  | 2.1  |
| 1   | G     | 27  | SER  | 2.1  |
| 1   | H     | 442 | ILE  | 2.1  |
| 1   | K     | 9   | SER  | 2.0  |
| 1   | K     | 396 | SER  | 2.0  |
| 1   | K     | 353 | HIS  | 2.0  |
| 1   | K     | 56  | GLY  | 2.0  |
| 1   | L     | 70  | GLY  | 2.0  |
| 1   | E     | 367 | ALA  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|-----|-----------------------------|-------|
|-----|------|-------|-----|-------|------|-----|-----------------------------|-------|

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | PLP  | I     | 500 | 15/16 | 0.94 | 0.09 | 30,34,36,39                 | 0     |
| 2   | PLP  | G     | 500 | 15/16 | 0.95 | 0.09 | 25,27,37,39                 | 0     |
| 2   | PLP  | L     | 500 | 15/16 | 0.95 | 0.09 | 33,36,38,44                 | 0     |
| 2   | PLP  | K     | 500 | 15/16 | 0.96 | 0.08 | 35,40,44,48                 | 0     |
| 2   | PLP  | J     | 500 | 15/16 | 0.96 | 0.08 | 22,24,27,28                 | 0     |
| 2   | PLP  | C     | 500 | 15/16 | 0.97 | 0.07 | 16,17,19,21                 | 0     |
| 2   | PLP  | H     | 500 | 15/16 | 0.97 | 0.07 | 22,25,30,33                 | 0     |
| 2   | PLP  | D     | 500 | 15/16 | 0.97 | 0.07 | 15,16,17,18                 | 0     |
| 2   | PLP  | E     | 500 | 15/16 | 0.98 | 0.06 | 12,13,14,15                 | 0     |
| 2   | PLP  | F     | 500 | 15/16 | 0.98 | 0.06 | 13,14,15,16                 | 0     |
| 2   | PLP  | A     | 500 | 15/16 | 0.98 | 0.06 | 15,16,19,20                 | 0     |
| 2   | PLP  | B     | 500 | 15/16 | 0.98 | 0.06 | 11,13,14,15                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.