



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:56 PM UTC

PDB ID : 7AE4 / pdb\_00007ae4  
Title : Structure of Sedimentibacter hydroxybenzoicus vanillic acid decarboxylase (ShVdcCD) in closed form  
Authors : Marshall, S.A.; Leys, D.  
Deposited on : 2020-09-17  
Resolution : 3.31 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

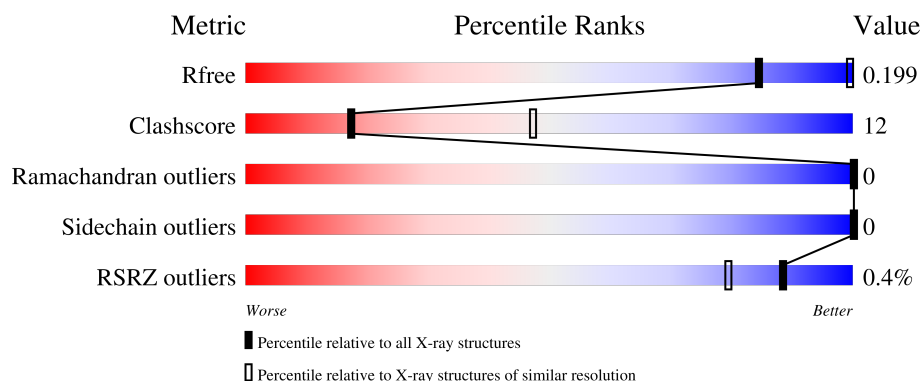
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

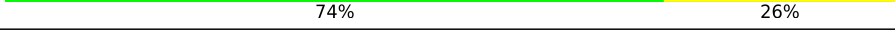
The reported resolution of this entry is 3.31 Å.

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                      | 1153 (3.34-3.30)                                      |
| Clashscore            | 190562                      | 1193 (3.34-3.30)                                      |
| Ramachandran outliers | 187476                      | 1172 (3.34-3.30)                                      |
| Sidechain outliers    | 187428                      | 1171 (3.34-3.30)                                      |
| RSRZ outliers         | 180081                      | 1153 (3.34-3.30)                                      |

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     | 480    |  |
| 1   | B     | 480    |  |
| 1   | C     | 480    |  |
| 1   | D     | 480    |  |
| 1   | E     | 480    |  |

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| Mol | Chain | Length | Quality of chain                                                                                 |
|-----|-------|--------|--------------------------------------------------------------------------------------------------|
| 1   | F     | 480    | <div><div><div>%</div><div><div></div><div>72%</div><div>28%</div></div><div></div></div></div>  |
| 2   | a     | 68     | <div><div><div></div><div>72%</div><div>26%</div><div></div></div></div>                         |
| 2   | b     | 68     | <div><div><div>%</div><div><div></div><div>72%</div><div>26%</div></div><div></div></div></div>  |
| 2   | c     | 68     | <div><div><div></div><div>81%</div><div>18%</div><div></div></div></div>                         |
| 2   | d     | 68     | <div><div><div>3%</div><div><div></div><div>76%</div><div>22%</div></div><div></div></div></div> |
| 2   | e     | 68     | <div><div><div>%</div><div><div></div><div>81%</div><div>18%</div></div><div></div></div></div>  |
| 2   | f     | 68     | <div><div><div>%</div><div><div></div><div>76%</div><div>22%</div></div><div></div></div></div>  |

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 25763 atoms, of which 66 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 Phenolic acid decarboxylase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 476      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3758  | 2406 | 628 | 709 | 15 |         |         |       |
| 1   | B     | 476      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3737  | 2393 | 625 | 704 | 15 |         |         |       |
| 1   | C     | 476      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3709  | 2373 | 621 | 700 | 15 |         |         |       |
| 1   | D     | 476      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3751  | 2403 | 628 | 705 | 15 |         |         |       |
| 1   | E     | 475      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3753  | 2403 | 627 | 708 | 15 |         |         |       |
| 1   | F     | 476      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3748  | 2399 | 627 | 707 | 15 |         |         |       |

- Molecule 2 is a protein called Protein ShdD.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 2   | a     | 67       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 522   | 329 | 90 | 94 | 9 |         |         |       |
| 2   | b     | 67       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 522   | 329 | 90 | 94 | 9 |         |         |       |
| 2   | c     | 67       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 522   | 329 | 90 | 94 | 9 |         |         |       |
| 2   | d     | 67       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 522   | 329 | 90 | 94 | 9 |         |         |       |
| 2   | e     | 67       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 522   | 329 | 90 | 94 | 9 |         |         |       |
| 2   | f     | 67       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 522   | 329 | 90 | 94 | 9 |         |         |       |

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



| Mol | Chain | Residues | Atoms |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---|---------|---------|
| 3   | A     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 3   | C     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 3   | D     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 3   | E     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 3   | E     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |
| 3   | F     | 1        | Total | C | H  | O | 0       | 0       |
|     |       |          | 17    | 4 | 10 | 3 |         |         |

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | A     | 3        | Total | Na | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 4   | B     | 3        | Total | Na | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 4   | C     | 2        | Total | Na | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 4   | D     | 2        | Total | Na | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 4   | E     | 3        | Total | Na | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 4   | F     | 2        | Total | Na | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula:  $\text{O}_4\text{P}$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 5   | A     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | B     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | C     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | D     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | E     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | F     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula:  $\text{Mg}$ ).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 6   | A     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 6   | B     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 6   | C     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 6   | D     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 6   | E     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

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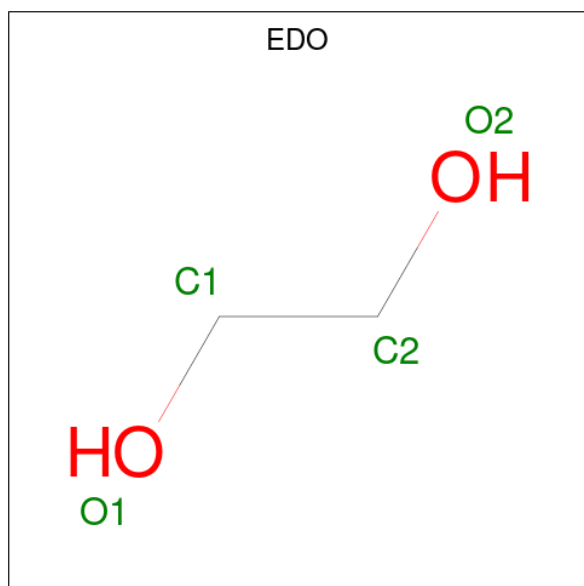
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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 6   | F     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 7   | A     | 2        | Total | Cl | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 7   | B     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 7   | C     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 7   | D     | 2        | Total | Cl | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 8   | E     | 1        | Total | C | H | O | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 2 |         |         |

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 9   | a     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

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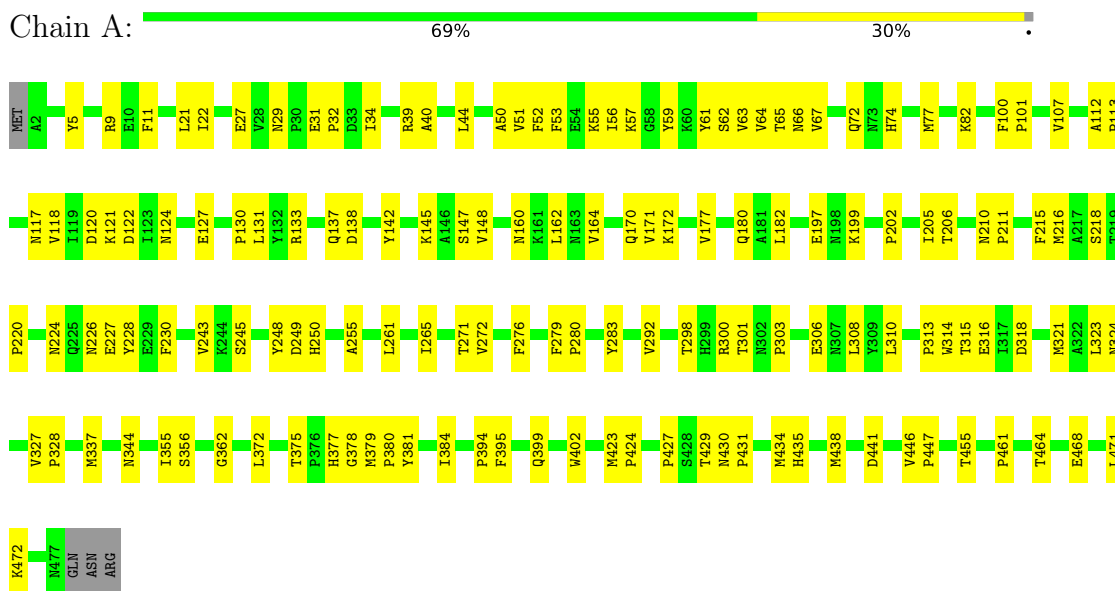
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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 9   | b     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 9   | c     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 9   | d     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 9   | e     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 9   | f     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |

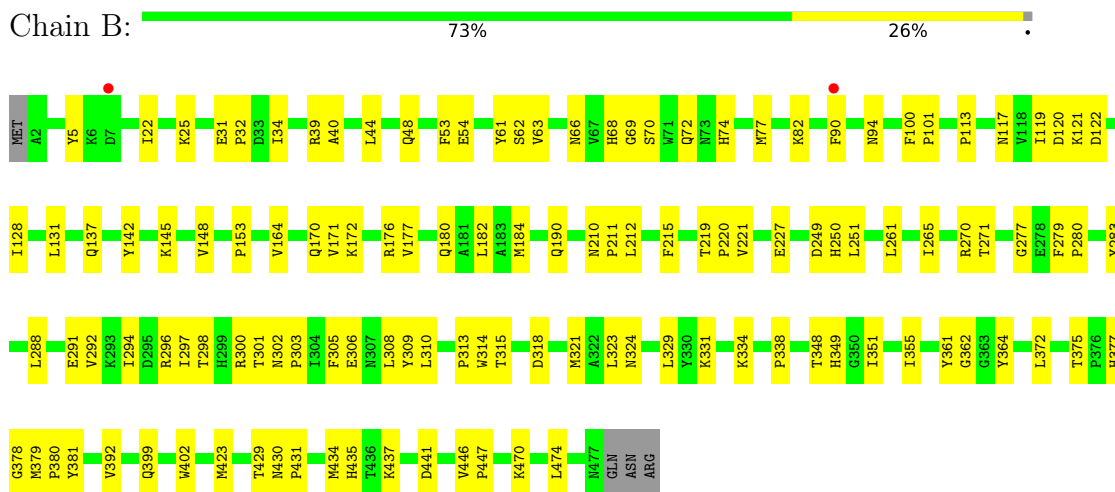
### 3 Residue-property plots

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

- Molecule 1: Phenolic acid decarboxylase

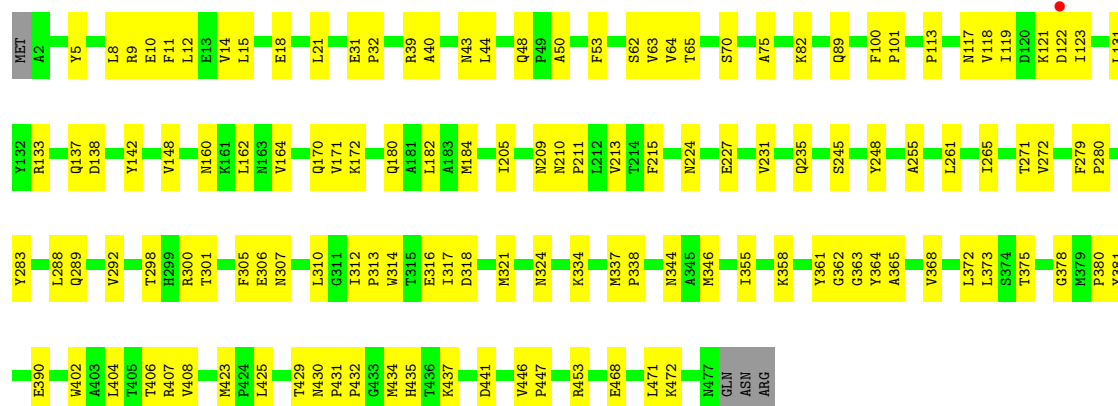


- Molecule 1: Phenolic acid decarboxylase



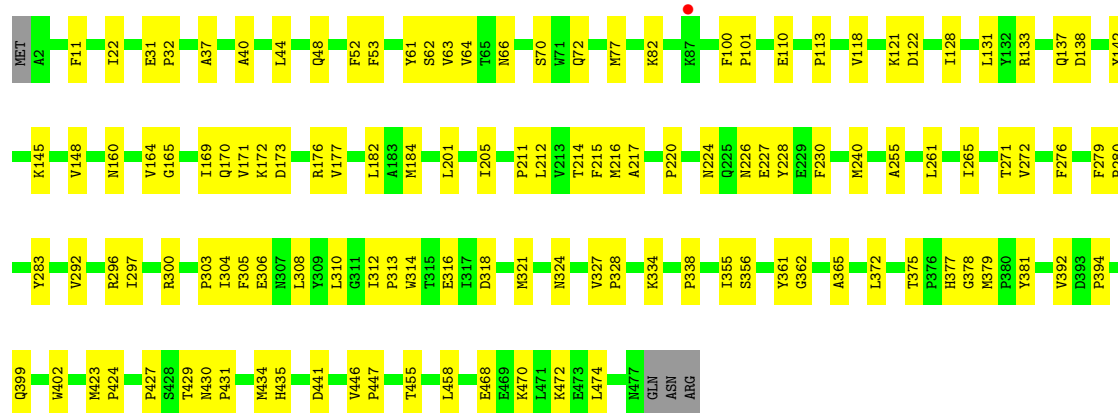
- Molecule 1: Phenolic acid decarboxylase

Chain C:  72% 27% .



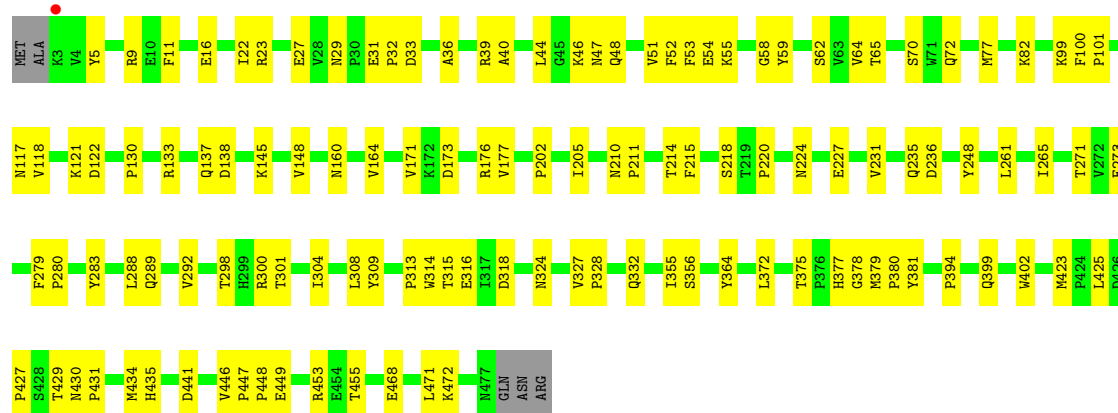
• Molecule 1: Phenolic acid decarboxylase

Chain D:  74% 26% .

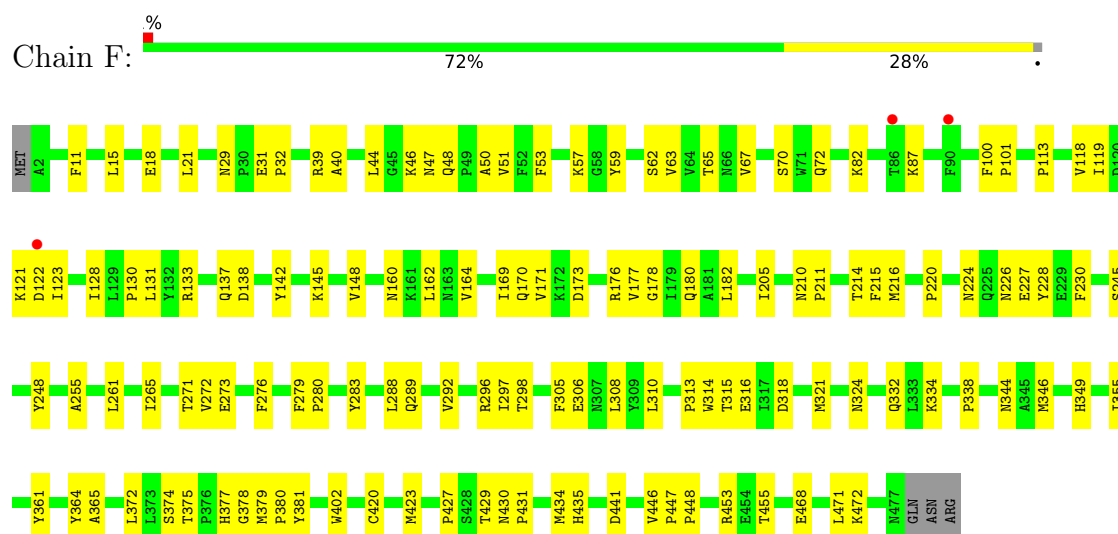


• Molecule 1: Phenolic acid decarboxylase

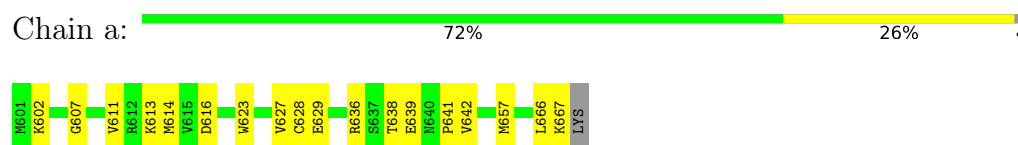
Chain E:  74% 25% .



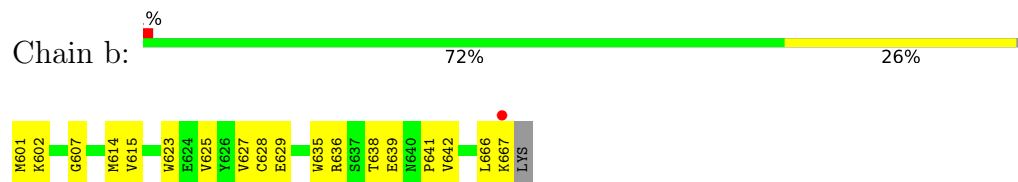
• Molecule 1: Phenolic acid decarboxylase



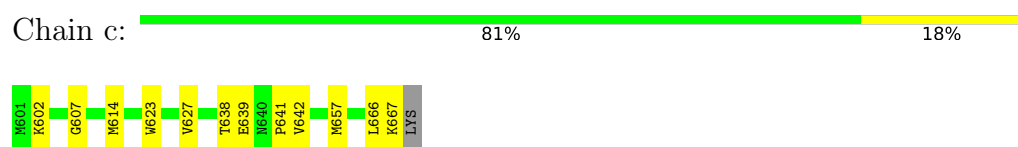
• Molecule 2: Protein ShdD



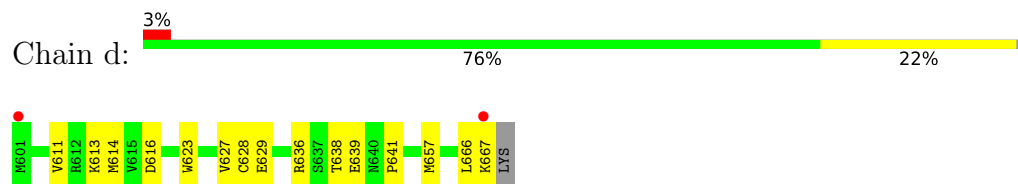
• Molecule 2: Protein ShdD



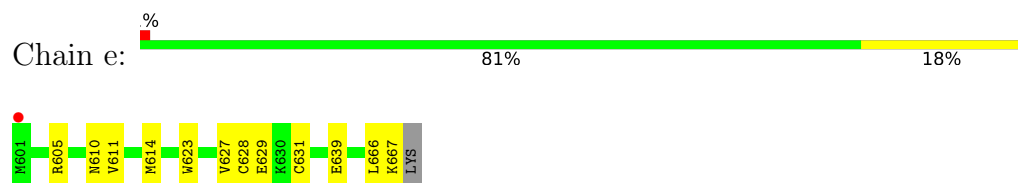
• Molecule 2: Protein ShdD



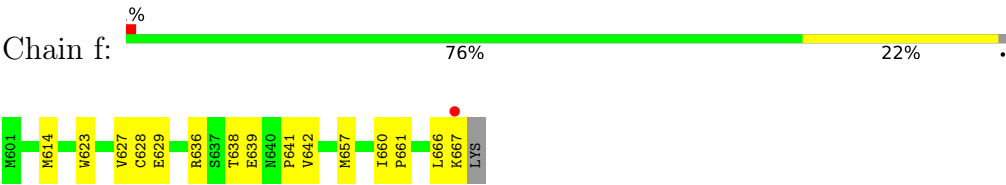
• Molecule 2: Protein ShdD



• Molecule 2: Protein ShdD



● Molecule 2: Protein ShdD



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | F 2 2 2                                                     | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 270.92Å 320.55Å 326.23Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 64.05 – 3.31<br>64.05 – 3.31                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 100.0 (64.05-3.31)<br>100.0 (64.05-3.31)                    | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.11                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.67 (at 3.33Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.19.2_4158                                          | Depositor        |
| R, $R_{free}$                                                           | 0.163 , 0.198<br>0.165 , 0.199                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 5121 reflections (4.89%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 125.3                                                       | Xtriage          |
| Anisotropy                                                              | 0.195                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.33 , 92.4                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | 0.002 for -h,l,k                                            | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.96                                                        | EDS              |
| Total number of atoms                                                   | 25763                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 130.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.00% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, PO4, MG, NA, EDO, ZN, CL

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

| Mol | Chain | Bond lengths |             | Bond angles |             |
|-----|-------|--------------|-------------|-------------|-------------|
|     |       | RMSZ         | # $ Z  > 5$ | RMSZ        | # $ Z  > 5$ |
| 1   | A     | 0.16         | 0/3852      | 0.34        | 0/5250      |
| 1   | B     | 0.17         | 0/3831      | 0.37        | 0/5226      |
| 1   | C     | 0.15         | 0/3802      | 0.36        | 0/5190      |
| 1   | D     | 0.17         | 0/3845      | 0.38        | 0/5241      |
| 1   | E     | 0.17         | 0/3847      | 0.35        | 0/5243      |
| 1   | F     | 0.16         | 0/3842      | 0.34        | 0/5238      |
| 2   | a     | 0.14         | 0/535       | 0.33        | 0/725       |
| 2   | b     | 0.17         | 0/535       | 0.38        | 0/725       |
| 2   | c     | 0.16         | 0/535       | 0.39        | 0/725       |
| 2   | d     | 0.15         | 0/535       | 0.35        | 0/725       |
| 2   | e     | 0.16         | 0/535       | 0.39        | 0/725       |
| 2   | f     | 0.13         | 0/535       | 0.31        | 0/725       |
| All | All   | 0.16         | 0/26229     | 0.36        | 0/35738     |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3758  | 0        | 3725     | 110     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | B     | 3737  | 0        | 3681     | 95      | 0            |
| 1   | C     | 3709  | 0        | 3633     | 119     | 0            |
| 1   | D     | 3751  | 0        | 3719     | 94      | 0            |
| 1   | E     | 3753  | 0        | 3720     | 86      | 0            |
| 1   | F     | 3748  | 0        | 3703     | 100     | 0            |
| 2   | a     | 522   | 0        | 508      | 13      | 0            |
| 2   | b     | 522   | 0        | 508      | 13      | 0            |
| 2   | c     | 522   | 0        | 508      | 11      | 0            |
| 2   | d     | 522   | 0        | 508      | 12      | 0            |
| 2   | e     | 522   | 0        | 508      | 12      | 0            |
| 2   | f     | 522   | 0        | 508      | 13      | 0            |
| 3   | A     | 7     | 10       | 10       | 1       | 0            |
| 3   | C     | 7     | 10       | 10       | 0       | 0            |
| 3   | D     | 7     | 10       | 10       | 1       | 0            |
| 3   | E     | 14    | 20       | 20       | 1       | 0            |
| 3   | F     | 7     | 10       | 10       | 0       | 0            |
| 4   | A     | 3     | 0        | 0        | 0       | 0            |
| 4   | B     | 3     | 0        | 0        | 0       | 0            |
| 4   | C     | 2     | 0        | 0        | 0       | 0            |
| 4   | D     | 2     | 0        | 0        | 0       | 0            |
| 4   | E     | 3     | 0        | 0        | 0       | 0            |
| 4   | F     | 2     | 0        | 0        | 0       | 0            |
| 5   | A     | 5     | 0        | 0        | 0       | 0            |
| 5   | B     | 5     | 0        | 0        | 0       | 0            |
| 5   | C     | 5     | 0        | 0        | 0       | 0            |
| 5   | D     | 5     | 0        | 0        | 0       | 0            |
| 5   | E     | 5     | 0        | 0        | 0       | 0            |
| 5   | F     | 5     | 0        | 0        | 0       | 0            |
| 6   | A     | 1     | 0        | 0        | 0       | 0            |
| 6   | B     | 1     | 0        | 0        | 0       | 0            |
| 6   | C     | 1     | 0        | 0        | 0       | 0            |
| 6   | D     | 1     | 0        | 0        | 0       | 0            |
| 6   | E     | 1     | 0        | 0        | 0       | 0            |
| 6   | F     | 1     | 0        | 0        | 0       | 0            |
| 7   | A     | 2     | 0        | 0        | 0       | 0            |
| 7   | B     | 1     | 0        | 0        | 0       | 0            |
| 7   | C     | 1     | 0        | 0        | 0       | 0            |
| 7   | D     | 2     | 0        | 0        | 0       | 0            |
| 8   | E     | 4     | 6        | 6        | 0       | 0            |
| 9   | a     | 1     | 0        | 0        | 0       | 0            |
| 9   | b     | 1     | 0        | 0        | 0       | 0            |
| 9   | c     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 9   | d     | 1     | 0        | 0        | 0       | 0            |
| 9   | e     | 1     | 0        | 0        | 0       | 0            |
| 9   | f     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 25697 | 66       | 25295    | 636     | 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 12.

All (636) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:429:THR:HG22 | 1:A:435:HIS:HB3  | 1.49                     | 0.95              |
| 1:A:375:THR:HG23 | 1:A:378:GLY:H    | 1.36                     | 0.89              |
| 1:C:430:ASN:HB3  | 1:C:431:PRO:HD3  | 1.57                     | 0.86              |
| 1:D:313:PRO:HG2  | 1:F:402:TRP:CD1  | 2.10                     | 0.86              |
| 1:B:131:LEU:HD21 | 1:B:171:VAL:HG21 | 1.58                     | 0.85              |
| 1:E:51:VAL:HG22  | 1:E:65:THR:HG22  | 1.58                     | 0.85              |
| 1:C:11:PHE:CD2   | 1:C:211:PRO:HG3  | 2.10                     | 0.84              |
| 1:B:375:THR:HG23 | 1:B:378:GLY:H    | 1.42                     | 0.84              |
| 1:A:313:PRO:HG2  | 1:E:402:TRP:CD1  | 2.15                     | 0.82              |
| 1:A:112:ALA:HB2  | 1:A:243:VAL:HG11 | 1.60                     | 0.82              |
| 1:F:63:VAL:HG12  | 1:F:305:PHE:HB3  | 1.62                     | 0.82              |
| 1:A:51:VAL:HG22  | 1:A:65:THR:HG22  | 1.60                     | 0.81              |
| 1:F:51:VAL:HG22  | 1:F:65:THR:HG22  | 1.62                     | 0.81              |
| 1:F:430:ASN:HB3  | 1:F:431:PRO:HD3  | 1.63                     | 0.80              |
| 1:A:430:ASN:HB3  | 1:A:431:PRO:HD3  | 1.64                     | 0.80              |
| 1:C:429:THR:HG22 | 1:C:435:HIS:HB3  | 1.64                     | 0.79              |
| 1:D:131:LEU:HD21 | 1:D:171:VAL:HG21 | 1.65                     | 0.78              |
| 1:A:402:TRP:CD1  | 1:E:313:PRO:HG2  | 2.19                     | 0.78              |
| 1:B:402:TRP:CD1  | 1:C:313:PRO:HG2  | 2.19                     | 0.78              |
| 1:F:321:MET:HE2  | 1:F:349:HIS:CE1  | 2.20                     | 0.77              |
| 1:A:381:TYR:CZ   | 1:A:423:MET:HE3  | 2.20                     | 0.77              |
| 1:B:313:PRO:HG2  | 1:C:402:TRP:CD1  | 2.20                     | 0.77              |
| 1:E:429:THR:HG22 | 1:E:435:HIS:HB3  | 1.66                     | 0.77              |
| 1:B:381:TYR:CZ   | 1:B:423:MET:HE3  | 2.19                     | 0.76              |
| 1:E:430:ASN:HB3  | 1:E:431:PRO:HD3  | 1.67                     | 0.76              |
| 1:B:429:THR:HG22 | 1:B:435:HIS:HB3  | 1.69                     | 0.75              |
| 1:C:12:LEU:HD21  | 1:C:64:VAL:HG11  | 1.67                     | 0.75              |
| 1:B:277:GLY:O    | 1:B:310:LEU:HD11 | 1.86                     | 0.74              |
| 1:C:378:GLY:H    | 1:C:380:PRO:HD2  | 1.51                     | 0.74              |
| 1:C:117:ASN:HD21 | 1:C:301:THR:HG23 | 1.53                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:377:HIS:O    | 1:F:381:TYR:HB2  | 1.88                     | 0.74              |
| 1:D:100:PHE:HB3  | 1:D:101:PRO:HD3  | 1.69                     | 0.73              |
| 1:D:375:THR:HG23 | 1:D:378:GLY:H    | 1.53                     | 0.73              |
| 1:B:39:ARG:NH1   | 1:B:315:THR:HG22 | 2.04                     | 0.73              |
| 1:C:372:LEU:O    | 1:C:375:THR:HG22 | 1.88                     | 0.73              |
| 1:D:402:TRP:CD1  | 1:F:313:PRO:HG2  | 2.23                     | 0.73              |
| 1:A:117:ASN:HD21 | 1:A:301:THR:HG23 | 1.54                     | 0.72              |
| 1:E:372:LEU:O    | 1:E:375:THR:HG22 | 1.89                     | 0.72              |
| 2:d:614:MET:HB2  | 2:d:627:VAL:HG23 | 1.72                     | 0.72              |
| 1:D:429:THR:HG22 | 1:D:435:HIS:HB3  | 1.72                     | 0.72              |
| 1:E:100:PHE:HB3  | 1:E:101:PRO:HD3  | 1.72                     | 0.72              |
| 1:B:321:MET:HE2  | 1:B:349:HIS:CE1  | 2.24                     | 0.71              |
| 2:e:614:MET:HE3  | 2:e:627:VAL:CG2  | 2.20                     | 0.71              |
| 1:D:430:ASN:HB3  | 1:D:431:PRO:HD3  | 1.71                     | 0.71              |
| 2:b:614:MET:HE3  | 2:b:627:VAL:CG2  | 2.21                     | 0.71              |
| 2:f:614:MET:HE3  | 2:f:627:VAL:CG2  | 2.20                     | 0.70              |
| 1:C:406:THR:HG23 | 1:C:407:ARG:HG2  | 1.72                     | 0.70              |
| 1:B:77:MET:HG3   | 1:B:211:PRO:HB2  | 1.74                     | 0.69              |
| 1:B:100:PHE:HB3  | 1:B:101:PRO:HD3  | 1.73                     | 0.69              |
| 1:C:11:PHE:CE2   | 1:C:211:PRO:HG3  | 2.27                     | 0.69              |
| 1:D:372:LEU:O    | 1:D:375:THR:HG22 | 1.91                     | 0.69              |
| 1:E:377:HIS:O    | 1:E:381:TYR:HB2  | 1.91                     | 0.69              |
| 1:D:446:VAL:HG13 | 1:D:447:PRO:HD2  | 1.75                     | 0.69              |
| 1:A:372:LEU:O    | 1:A:375:THR:HG22 | 1.92                     | 0.69              |
| 1:A:107:VAL:HG22 | 1:A:243:VAL:HG12 | 1.75                     | 0.69              |
| 1:C:100:PHE:HB3  | 1:C:101:PRO:HD3  | 1.73                     | 0.69              |
| 1:D:381:TYR:CZ   | 1:D:423:MET:HE3  | 2.28                     | 0.69              |
| 1:F:381:TYR:CZ   | 1:F:423:MET:HE3  | 2.29                     | 0.68              |
| 1:A:100:PHE:HB3  | 1:A:101:PRO:HD3  | 1.75                     | 0.68              |
| 1:C:5:TYR:HE2    | 1:C:14:VAL:HG21  | 1.59                     | 0.68              |
| 1:F:429:THR:HG22 | 1:F:435:HIS:HB3  | 1.74                     | 0.68              |
| 1:C:210:ASN:OD1  | 1:C:211:PRO:HD2  | 1.93                     | 0.67              |
| 1:C:5:TYR:O      | 1:C:210:ASN:ND2  | 2.27                     | 0.67              |
| 2:d:614:MET:HE3  | 2:d:627:VAL:CG2  | 2.24                     | 0.67              |
| 1:C:11:PHE:HD2   | 1:C:211:PRO:HG3  | 1.57                     | 0.67              |
| 2:c:614:MET:HE3  | 2:c:627:VAL:CG2  | 2.25                     | 0.67              |
| 1:A:22:ILE:HD11  | 1:E:471:LEU:HD22 | 1.77                     | 0.67              |
| 1:F:375:THR:HG23 | 1:F:378:GLY:H    | 1.60                     | 0.67              |
| 1:F:372:LEU:O    | 1:F:375:THR:HG22 | 1.96                     | 0.66              |
| 1:B:215:PHE:CZ   | 1:B:324:ASN:HB3  | 2.31                     | 0.66              |
| 1:B:265:ILE:HG12 | 1:B:292:VAL:HG12 | 1.78                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:f:614:MET:HB2  | 2:f:627:VAL:HG23 | 1.78                     | 0.65              |
| 1:B:362:GLY:C    | 1:E:434:MET:HE1  | 2.21                     | 0.65              |
| 1:A:424:PRO:O    | 1:E:453:ARG:NH2  | 2.30                     | 0.65              |
| 1:D:22:ILE:HD11  | 1:F:471:LEU:HG   | 1.79                     | 0.65              |
| 1:B:372:LEU:O    | 1:B:375:THR:HG22 | 1.97                     | 0.64              |
| 1:F:265:ILE:HG12 | 1:F:292:VAL:HG22 | 1.78                     | 0.64              |
| 1:D:172:LYS:NZ   | 1:D:271:THR:OG1  | 2.31                     | 0.64              |
| 1:B:430:ASN:HB3  | 1:B:431:PRO:HD3  | 1.80                     | 0.64              |
| 1:C:402:TRP:O    | 1:C:406:THR:HG22 | 1.98                     | 0.64              |
| 1:C:381:TYR:CZ   | 1:C:423:MET:HE1  | 2.33                     | 0.63              |
| 1:A:39:ARG:NH1   | 1:A:315:THR:HG22 | 2.14                     | 0.63              |
| 1:A:137:GLN:HB2  | 1:A:283:TYR:CZ   | 2.33                     | 0.63              |
| 1:C:265:ILE:HG12 | 1:C:292:VAL:HG22 | 1.81                     | 0.63              |
| 1:E:375:THR:HG23 | 1:E:378:GLY:H    | 1.65                     | 0.62              |
| 2:a:614:MET:HE3  | 2:a:627:VAL:CG2  | 2.29                     | 0.62              |
| 2:c:614:MET:HB2  | 2:c:627:VAL:HG23 | 1.81                     | 0.62              |
| 1:D:169:ILE:HD13 | 1:D:205:ILE:HD13 | 1.82                     | 0.62              |
| 1:B:362:GLY:O    | 1:E:434:MET:HE1  | 1.99                     | 0.61              |
| 2:a:614:MET:HB2  | 2:a:627:VAL:HG23 | 1.83                     | 0.61              |
| 1:A:51:VAL:CG2   | 1:A:65:THR:HG22  | 2.30                     | 0.61              |
| 1:F:40:ALA:O     | 1:F:44:LEU:HD13  | 2.00                     | 0.61              |
| 2:e:614:MET:HB2  | 2:e:627:VAL:HG23 | 1.82                     | 0.61              |
| 1:C:31:GLU:HB2   | 1:C:32:PRO:HD3   | 1.82                     | 0.61              |
| 1:C:205:ILE:HB   | 1:C:261:LEU:HB2  | 1.82                     | 0.60              |
| 1:C:118:VAL:HG22 | 1:C:298:THR:HG22 | 1.83                     | 0.60              |
| 1:E:39:ARG:NH1   | 1:E:315:THR:HG22 | 2.17                     | 0.60              |
| 1:A:172:LYS:NZ   | 1:A:271:THR:OG1  | 2.34                     | 0.60              |
| 1:B:77:MET:HG2   | 1:B:212:LEU:CD1  | 2.31                     | 0.60              |
| 1:B:40:ALA:O     | 1:B:44:LEU:HD13  | 2.01                     | 0.60              |
| 1:D:220:PRO:HB2  | 1:D:377:HIS:HB2  | 1.83                     | 0.60              |
| 1:C:12:LEU:CD2   | 1:C:64:VAL:HG11  | 2.32                     | 0.60              |
| 1:E:164:VAL:CG1  | 1:E:227:GLU:HB2  | 2.31                     | 0.59              |
| 1:F:31:GLU:HB2   | 1:F:32:PRO:HD3   | 1.84                     | 0.59              |
| 1:A:52:PHE:CD2   | 1:A:64:VAL:HG22  | 2.37                     | 0.59              |
| 1:D:31:GLU:HB2   | 1:D:32:PRO:HD3   | 1.82                     | 0.59              |
| 1:C:453:ARG:HG2  | 1:C:453:ARG:HH11 | 1.67                     | 0.59              |
| 1:F:272:VAL:HG13 | 2:f:657:MET:HE1  | 1.84                     | 0.59              |
| 1:E:31:GLU:HB2   | 1:E:32:PRO:HD3   | 1.85                     | 0.59              |
| 1:F:11:PHE:CE2   | 1:F:15:LEU:HD21  | 2.37                     | 0.59              |
| 1:A:131:LEU:HD21 | 1:A:171:VAL:HG21 | 1.85                     | 0.59              |
| 1:B:31:GLU:HB2   | 1:B:32:PRO:HD3   | 1.84                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:63:VAL:HG12  | 1:C:305:PHE:HB3  | 1.84                     | 0.58              |
| 1:A:5:TYR:O      | 1:A:210:ASN:ND2  | 2.36                     | 0.58              |
| 1:A:377:HIS:O    | 1:A:381:TYR:HB2  | 2.03                     | 0.58              |
| 1:E:52:PHE:CD2   | 1:E:64:VAL:HG22  | 2.38                     | 0.58              |
| 1:C:48:GLN:HB2   | 1:C:70:SER:HB3   | 1.84                     | 0.58              |
| 1:F:48:GLN:HB2   | 1:F:70:SER:HB3   | 1.85                     | 0.58              |
| 1:E:265:ILE:HG12 | 1:E:292:VAL:HG22 | 1.85                     | 0.58              |
| 1:C:210:ASN:O    | 1:C:213:VAL:HG22 | 2.04                     | 0.58              |
| 2:b:601:MET:HE2  | 2:b:635:TRP:HZ2  | 1.69                     | 0.58              |
| 1:A:272:VAL:HG13 | 2:a:657:MET:HE1  | 1.86                     | 0.57              |
| 1:B:137:GLN:HB2  | 1:B:283:TYR:CZ   | 2.39                     | 0.57              |
| 1:D:220:PRO:CB   | 1:D:377:HIS:HB2  | 2.34                     | 0.57              |
| 1:C:215:PHE:CZ   | 1:C:324:ASN:HB3  | 2.38                     | 0.57              |
| 1:D:48:GLN:HB2   | 1:D:70:SER:HB3   | 1.85                     | 0.57              |
| 1:F:67:VAL:HB    | 1:F:145:LYS:NZ   | 2.19                     | 0.57              |
| 1:B:220:PRO:HB2  | 1:B:377:HIS:HB2  | 1.86                     | 0.57              |
| 1:C:365:ALA:HB3  | 1:C:441:ASP:OD2  | 2.05                     | 0.57              |
| 1:B:63:VAL:HG12  | 1:B:305:PHE:HB3  | 1.87                     | 0.57              |
| 1:E:40:ALA:O     | 1:E:44:LEU:HD13  | 2.04                     | 0.57              |
| 1:F:131:LEU:HD21 | 1:F:171:VAL:HG21 | 1.87                     | 0.57              |
| 1:D:131:LEU:CD2  | 1:D:171:VAL:HG21 | 2.33                     | 0.57              |
| 1:B:131:LEU:CD2  | 1:B:171:VAL:HG21 | 2.32                     | 0.56              |
| 1:B:355:ILE:HD11 | 1:B:372:LEU:HG   | 1.87                     | 0.56              |
| 1:C:131:LEU:HD21 | 1:C:171:VAL:HG21 | 1.86                     | 0.56              |
| 1:A:31:GLU:HB2   | 1:A:32:PRO:HD3   | 1.86                     | 0.56              |
| 1:B:142:TYR:CZ   | 1:B:170:GLN:HB2  | 2.40                     | 0.56              |
| 1:C:137:GLN:HB2  | 1:C:283:TYR:CZ   | 2.40                     | 0.56              |
| 1:C:164:VAL:CG1  | 1:C:227:GLU:HB2  | 2.35                     | 0.56              |
| 1:D:164:VAL:CG1  | 1:D:227:GLU:HB2  | 2.35                     | 0.56              |
| 1:E:423:MET:HE3  | 1:E:425:LEU:HB2  | 1.86                     | 0.56              |
| 1:E:51:VAL:CG2   | 1:E:65:THR:HG22  | 2.31                     | 0.56              |
| 1:D:308:LEU:C    | 1:D:308:LEU:HD12 | 2.31                     | 0.56              |
| 1:C:310:LEU:HD21 | 1:C:317:ILE:HD12 | 1.87                     | 0.56              |
| 1:A:53:PHE:O     | 1:A:62:SER:HB2   | 2.05                     | 0.56              |
| 1:D:272:VAL:HG13 | 2:d:657:MET:HE1  | 1.87                     | 0.56              |
| 1:B:446:VAL:HG13 | 1:B:447:PRO:HD2  | 1.88                     | 0.56              |
| 2:b:614:MET:HB2  | 2:b:627:VAL:HG23 | 1.87                     | 0.56              |
| 1:D:128:ILE:HD13 | 1:D:297:ILE:HG21 | 1.88                     | 0.56              |
| 1:A:434:MET:HE1  | 1:D:362:GLY:O    | 2.06                     | 0.55              |
| 1:D:63:VAL:HG12  | 1:D:305:PHE:HB3  | 1.88                     | 0.55              |
| 1:C:8:LEU:HD13   | 1:C:209:ASN:O    | 2.06                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:215:PHE:CZ   | 1:F:324:ASN:HB3  | 2.40                     | 0.55              |
| 1:B:5:TYR:O      | 1:B:210:ASN:ND2  | 2.40                     | 0.55              |
| 1:A:118:VAL:HG12 | 1:A:298:THR:HG22 | 1.88                     | 0.55              |
| 1:F:314:TRP:HA   | 1:F:318:ASP:HB2  | 1.87                     | 0.55              |
| 1:A:77:MET:HG3   | 1:A:211:PRO:HB2  | 1.89                     | 0.55              |
| 1:C:10:GLU:O     | 1:C:14:VAL:HG23  | 2.07                     | 0.55              |
| 1:D:377:HIS:O    | 1:D:381:TYR:HB2  | 2.07                     | 0.55              |
| 1:E:308:LEU:HD12 | 1:E:308:LEU:C    | 2.32                     | 0.55              |
| 1:B:172:LYS:NZ   | 1:B:271:THR:OG1  | 2.35                     | 0.55              |
| 1:A:72:GLN:HG3   | 1:A:82:LYS:HG3   | 1.88                     | 0.55              |
| 1:E:100:PHE:CB   | 1:E:101:PRO:HD3  | 2.37                     | 0.55              |
| 1:F:51:VAL:CG2   | 1:F:65:THR:HG22  | 2.34                     | 0.55              |
| 1:F:148:VAL:O    | 1:F:164:VAL:HA   | 2.07                     | 0.55              |
| 1:A:9:ARG:NH2    | 1:A:300:ARG:HD2  | 2.22                     | 0.55              |
| 1:A:133:ARG:NH1  | 1:A:138:ASP:O    | 2.40                     | 0.55              |
| 1:B:94:ASN:OD1   | 1:B:331:LYS:HE2  | 2.07                     | 0.55              |
| 1:B:379:MET:HB3  | 1:B:380:PRO:HD3  | 1.89                     | 0.55              |
| 2:b:628:CYS:O    | 2:b:629:GLU:HB3  | 2.07                     | 0.55              |
| 2:d:614:MET:HE3  | 2:d:627:VAL:HG22 | 1.89                     | 0.54              |
| 1:A:164:VAL:CG1  | 1:A:227:GLU:HB2  | 2.37                     | 0.54              |
| 1:E:164:VAL:HG12 | 1:E:227:GLU:HB2  | 1.89                     | 0.54              |
| 1:C:53:PHE:O     | 1:C:62:SER:HB2   | 2.08                     | 0.54              |
| 1:C:310:LEU:HD21 | 1:C:317:ILE:CD1  | 2.37                     | 0.54              |
| 1:D:77:MET:HG3   | 1:D:211:PRO:HB2  | 1.89                     | 0.54              |
| 1:E:5:TYR:O      | 1:E:210:ASN:ND2  | 2.40                     | 0.54              |
| 1:E:9:ARG:NH2    | 1:E:300:ARG:HD2  | 2.22                     | 0.54              |
| 1:E:39:ARG:HD2   | 1:E:309:TYR:CE2  | 2.43                     | 0.54              |
| 1:A:34:ILE:HD11  | 1:A:56:ILE:HD12  | 1.89                     | 0.54              |
| 1:E:64:VAL:HG23  | 1:E:304:ILE:HG22 | 1.89                     | 0.54              |
| 1:A:355:ILE:HD11 | 1:A:372:LEU:HG   | 1.89                     | 0.54              |
| 1:E:220:PRO:HB2  | 1:E:377:HIS:HB2  | 1.90                     | 0.54              |
| 1:D:100:PHE:CB   | 1:D:101:PRO:HD3  | 2.38                     | 0.54              |
| 1:B:434:MET:HG3  | 1:E:448:PRO:HG2  | 1.90                     | 0.53              |
| 1:D:110:GLU:CD   | 1:D:110:GLU:H    | 2.16                     | 0.53              |
| 1:E:137:GLN:HB2  | 1:E:283:TYR:CZ   | 2.43                     | 0.53              |
| 1:C:164:VAL:HG12 | 1:C:227:GLU:HB2  | 1.89                     | 0.53              |
| 1:C:11:PHE:HD2   | 1:C:211:PRO:CG   | 2.21                     | 0.53              |
| 1:B:22:ILE:HD11  | 1:C:471:LEU:HG   | 1.90                     | 0.53              |
| 1:C:402:TRP:CE2  | 1:C:406:THR:HG21 | 2.44                     | 0.53              |
| 1:F:11:PHE:CD2   | 1:F:211:PRO:HG3  | 2.43                     | 0.53              |
| 2:e:611:VAL:HG23 | 2:e:627:VAL:O    | 2.09                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:277:GLY:O    | 1:B:310:LEU:CD1  | 2.55                     | 0.53              |
| 1:E:133:ARG:NH1  | 1:E:138:ASP:O    | 2.41                     | 0.53              |
| 1:C:321:MET:HA   | 1:C:324:ASN:OD1  | 2.09                     | 0.53              |
| 1:A:455:THR:HG22 | 1:E:427:PRO:HB2  | 1.90                     | 0.53              |
| 1:C:142:TYR:CZ   | 1:C:170:GLN:HB2  | 2.44                     | 0.53              |
| 1:D:455:THR:HG22 | 1:F:427:PRO:HB2  | 1.91                     | 0.52              |
| 1:E:48:GLN:HB2   | 1:E:70:SER:HB3   | 1.91                     | 0.52              |
| 2:b:642:VAL:O    | 2:b:642:VAL:HG13 | 2.09                     | 0.52              |
| 1:C:430:ASN:HB3  | 1:C:431:PRO:CD   | 2.35                     | 0.52              |
| 1:F:271:THR:O    | 1:F:288:LEU:HA   | 2.08                     | 0.52              |
| 1:B:100:PHE:CB   | 1:B:101:PRO:HD3  | 2.39                     | 0.52              |
| 1:B:279:PHE:CG   | 1:B:280:PRO:HD3  | 2.44                     | 0.52              |
| 1:D:314:TRP:HA   | 1:D:318:ASP:HB2  | 1.91                     | 0.52              |
| 1:A:308:LEU:HD12 | 1:A:308:LEU:C    | 2.34                     | 0.52              |
| 1:B:53:PHE:O     | 1:B:62:SER:HB2   | 2.09                     | 0.52              |
| 1:B:310:LEU:C    | 1:B:310:LEU:HD12 | 2.35                     | 0.52              |
| 1:E:99:LYS:NZ    | 1:E:236:ASP:OD1  | 2.43                     | 0.52              |
| 2:d:623:TRP:HB3  | 2:d:638:THR:HG23 | 1.91                     | 0.52              |
| 1:C:210:ASN:HB3  | 1:C:213:VAL:HG22 | 1.91                     | 0.52              |
| 1:E:16:GLU:OE2   | 1:E:23:ARG:NH1   | 2.42                     | 0.52              |
| 1:A:215:PHE:CZ   | 1:A:324:ASN:HB3  | 2.45                     | 0.52              |
| 1:A:379:MET:HE3  | 1:D:361:TYR:OH   | 2.10                     | 0.52              |
| 1:A:375:THR:CG2  | 1:A:378:GLY:H    | 2.15                     | 0.52              |
| 1:C:373:LEU:HD22 | 1:C:437:LYS:HE3  | 1.92                     | 0.52              |
| 1:F:53:PHE:O     | 1:F:62:SER:HB2   | 2.10                     | 0.52              |
| 1:D:171:VAL:HA   | 1:D:177:VAL:HG12 | 1.92                     | 0.51              |
| 1:F:220:PRO:HB2  | 1:F:377:HIS:HB2  | 1.92                     | 0.51              |
| 2:f:623:TRP:HB3  | 2:f:638:THR:HG23 | 1.92                     | 0.51              |
| 1:A:164:VAL:HG12 | 1:A:227:GLU:HB2  | 1.92                     | 0.51              |
| 1:E:160:ASN:HB3  | 1:E:224:ASN:O    | 2.10                     | 0.51              |
| 1:C:362:GLY:C    | 1:F:434:MET:HE1  | 2.36                     | 0.51              |
| 1:A:265:ILE:HG12 | 1:A:292:VAL:HG22 | 1.90                     | 0.51              |
| 1:A:314:TRP:HA   | 1:A:318:ASP:HB2  | 1.92                     | 0.51              |
| 1:A:344:ASN:HA   | 1:A:395:PHE:HE1  | 1.74                     | 0.51              |
| 1:B:148:VAL:O    | 1:B:164:VAL:HA   | 2.10                     | 0.51              |
| 1:C:133:ARG:NH1  | 1:C:138:ASP:O    | 2.43                     | 0.51              |
| 1:C:310:LEU:CD2  | 1:C:317:ILE:HG21 | 2.40                     | 0.51              |
| 1:D:137:GLN:HB2  | 1:D:283:TYR:CZ   | 2.45                     | 0.51              |
| 1:F:365:ALA:HB3  | 1:F:441:ASP:OD2  | 2.09                     | 0.51              |
| 1:C:180:GLN:HG2  | 1:C:182:LEU:HG   | 1.93                     | 0.51              |
| 2:e:666:LEU:O    | 2:e:667:LYS:CB   | 2.58                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:a:611:VAL:HG23 | 2:a:627:VAL:O    | 2.11                     | 0.51              |
| 1:C:148:VAL:O    | 1:C:164:VAL:HA   | 2.11                     | 0.51              |
| 1:C:381:TYR:CE2  | 1:C:423:MET:HE2  | 2.46                     | 0.51              |
| 1:F:355:ILE:HD11 | 1:F:372:LEU:HG   | 1.93                     | 0.51              |
| 1:F:446:VAL:HG13 | 1:F:447:PRO:HD2  | 1.92                     | 0.51              |
| 1:C:39:ARG:HD3   | 1:C:39:ARG:O     | 2.10                     | 0.50              |
| 1:C:215:PHE:CE1  | 1:C:324:ASN:HB3  | 2.47                     | 0.50              |
| 1:C:213:VAL:HG12 | 1:C:231:VAL:HG21 | 1.94                     | 0.50              |
| 1:C:310:LEU:HD21 | 1:C:317:ILE:HG21 | 1.93                     | 0.50              |
| 2:c:623:TRP:HB3  | 2:c:638:THR:HG23 | 1.94                     | 0.50              |
| 1:E:145:LYS:HD3  | 1:E:214:THR:HG21 | 1.92                     | 0.50              |
| 1:A:29:ASN:HA    | 1:A:57:LYS:HB2   | 1.94                     | 0.50              |
| 1:C:314:TRP:HA   | 1:C:318:ASP:HB2  | 1.94                     | 0.50              |
| 1:C:355:ILE:HD11 | 1:C:372:LEU:HG   | 1.94                     | 0.50              |
| 1:F:137:GLN:HB2  | 1:F:283:TYR:CZ   | 2.47                     | 0.50              |
| 1:A:27:GLU:HA    | 1:A:55:LYS:HB3   | 1.94                     | 0.49              |
| 1:A:381:TYR:CZ   | 1:A:423:MET:CE   | 2.95                     | 0.49              |
| 1:C:113:PRO:O    | 1:C:300:ARG:HG2  | 2.12                     | 0.49              |
| 1:C:468:GLU:O    | 1:C:472:LYS:HG3  | 2.12                     | 0.49              |
| 1:D:446:VAL:CG1  | 1:D:447:PRO:HD2  | 2.42                     | 0.49              |
| 1:A:379:MET:HB3  | 1:A:380:PRO:HD3  | 1.94                     | 0.49              |
| 1:A:399:GLN:HG2  | 3:A:501:PEG:H41  | 1.93                     | 0.49              |
| 2:d:613:LYS:HD2  | 2:d:616:ASP:OD1  | 2.11                     | 0.49              |
| 1:D:279:PHE:CG   | 1:D:280:PRO:HD3  | 2.47                     | 0.49              |
| 2:e:639:GLU:O    | 2:e:639:GLU:HG3  | 2.11                     | 0.49              |
| 1:B:377:HIS:O    | 1:B:380:PRO:HD2  | 2.13                     | 0.49              |
| 1:C:53:PHE:HB2   | 1:C:63:VAL:HG22  | 1.95                     | 0.49              |
| 1:C:162:LEU:C    | 1:C:162:LEU:HD23 | 2.37                     | 0.49              |
| 1:C:334:LYS:HD3  | 1:C:338:PRO:HA   | 1.95                     | 0.49              |
| 1:A:120:ASP:OD1  | 1:A:120:ASP:N    | 2.45                     | 0.49              |
| 2:a:623:TRP:HB3  | 2:a:638:THR:HG23 | 1.95                     | 0.49              |
| 1:B:375:THR:CG2  | 1:B:378:GLY:H    | 2.19                     | 0.49              |
| 1:C:381:TYR:CZ   | 1:C:423:MET:CE   | 2.95                     | 0.49              |
| 1:D:424:PRO:O    | 1:F:453:ARG:NH2  | 2.40                     | 0.49              |
| 1:E:446:VAL:HG13 | 1:E:447:PRO:HD2  | 1.94                     | 0.49              |
| 2:d:666:LEU:O    | 2:d:667:LYS:CB   | 2.60                     | 0.49              |
| 1:B:308:LEU:C    | 1:B:308:LEU:HD12 | 2.37                     | 0.49              |
| 1:C:337:MET:HE1  | 1:C:368:VAL:HA   | 1.94                     | 0.49              |
| 1:F:11:PHE:CG    | 1:F:211:PRO:HG3  | 2.48                     | 0.49              |
| 1:C:40:ALA:O     | 1:C:44:LEU:HD13  | 2.13                     | 0.49              |
| 1:C:272:VAL:HG13 | 2:c:657:MET:HE1  | 1.94                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:133:ARG:NH1  | 1:D:138:ASP:O    | 2.46                     | 0.49              |
| 1:F:133:ARG:NH1  | 1:F:138:ASP:O    | 2.45                     | 0.49              |
| 1:A:148:VAL:O    | 1:A:164:VAL:HA   | 2.13                     | 0.49              |
| 1:B:215:PHE:CE1  | 1:B:324:ASN:HB3  | 2.48                     | 0.49              |
| 2:f:614:MET:HE3  | 2:f:627:VAL:HG22 | 1.92                     | 0.49              |
| 1:E:117:ASN:OD1  | 1:E:301:THR:HG23 | 2.13                     | 0.48              |
| 1:F:100:PHE:HB3  | 1:F:101:PRO:HD3  | 1.94                     | 0.48              |
| 2:b:639:GLU:O    | 2:b:641:PRO:HD3  | 2.12                     | 0.48              |
| 2:c:666:LEU:O    | 2:c:667:LYS:CB   | 2.60                     | 0.48              |
| 1:A:220:PRO:HB2  | 1:A:377:HIS:HB2  | 1.94                     | 0.48              |
| 1:B:120:ASP:OD2  | 1:B:296:ARG:NH2  | 2.46                     | 0.48              |
| 1:B:270:ARG:HB3  | 1:B:288:LEU:HB3  | 1.95                     | 0.48              |
| 1:E:29:ASN:O     | 1:E:33:ASP:HB2   | 2.13                     | 0.48              |
| 1:F:118:VAL:HG22 | 1:F:298:THR:HG22 | 1.94                     | 0.48              |
| 1:B:171:VAL:HA   | 1:B:177:VAL:HG12 | 1.94                     | 0.48              |
| 1:C:381:TYR:CE2  | 1:C:423:MET:CE   | 2.97                     | 0.48              |
| 1:F:215:PHE:CE1  | 1:F:324:ASN:HB3  | 2.48                     | 0.48              |
| 1:B:182:LEU:HD13 | 1:B:423:MET:HE1  | 1.95                     | 0.48              |
| 1:A:202:PRO:HB3  | 1:A:248:TYR:CD1  | 2.49                     | 0.48              |
| 1:B:121:LYS:O    | 1:B:122:ASP:C    | 2.56                     | 0.48              |
| 1:C:210:ASN:O    | 1:C:213:VAL:CG2  | 2.62                     | 0.48              |
| 1:A:61:TYR:CD1   | 1:A:303:PRO:HD2  | 2.49                     | 0.48              |
| 1:C:160:ASN:HB3  | 1:C:224:ASN:O    | 2.14                     | 0.48              |
| 1:C:434:MET:HG3  | 1:F:448:PRO:HG2  | 1.95                     | 0.48              |
| 1:D:355:ILE:HD11 | 1:D:372:LEU:HG   | 1.94                     | 0.48              |
| 1:A:124:ASN:HB3  | 1:A:127:GLU:HG3  | 1.95                     | 0.48              |
| 1:D:279:PHE:N    | 1:D:280:PRO:CD   | 2.76                     | 0.48              |
| 1:D:334:LYS:HD3  | 1:D:338:PRO:HA   | 1.96                     | 0.48              |
| 1:A:100:PHE:CB   | 1:A:101:PRO:HD3  | 2.44                     | 0.48              |
| 1:F:430:ASN:HB3  | 1:F:431:PRO:CD   | 2.38                     | 0.48              |
| 2:e:605:ARG:NH2  | 2:e:631:CYS:O    | 2.47                     | 0.48              |
| 1:D:182:LEU:HD13 | 1:D:423:MET:HE1  | 1.96                     | 0.48              |
| 1:D:365:ALA:HB3  | 1:D:441:ASP:OD2  | 2.13                     | 0.48              |
| 1:E:279:PHE:N    | 1:E:280:PRO:CD   | 2.77                     | 0.48              |
| 2:b:623:TRP:HB3  | 2:b:638:THR:HG23 | 1.95                     | 0.48              |
| 1:B:128:ILE:HD13 | 1:B:297:ILE:HG21 | 1.96                     | 0.47              |
| 1:E:314:TRP:HA   | 1:E:318:ASP:HB2  | 1.95                     | 0.47              |
| 1:F:276:PHE:CZ   | 1:F:310:LEU:HD21 | 2.49                     | 0.47              |
| 1:F:279:PHE:CG   | 1:F:280:PRO:HD3  | 2.49                     | 0.47              |
| 2:e:628:CYS:O    | 2:e:629:GLU:HB3  | 2.14                     | 0.47              |
| 1:A:446:VAL:HG13 | 1:A:447:PRO:HD2  | 1.95                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:119:ILE:HG22 | 1:F:123:ILE:HD13 | 1.95                     | 0.47              |
| 2:f:666:LEU:O    | 2:f:667:LYS:CB   | 2.62                     | 0.47              |
| 1:A:430:ASN:HB3  | 1:A:431:PRO:CD   | 2.41                     | 0.47              |
| 1:C:9:ARG:HH21   | 1:C:300:ARG:NE   | 2.12                     | 0.47              |
| 1:D:145:LYS:HD3  | 1:D:214:THR:HG21 | 1.97                     | 0.47              |
| 1:E:11:PHE:CG    | 1:E:211:PRO:HG3  | 2.50                     | 0.47              |
| 1:E:227:GLU:N    | 1:E:227:GLU:OE1  | 2.48                     | 0.47              |
| 1:D:265:ILE:HG12 | 1:D:292:VAL:HG22 | 1.96                     | 0.47              |
| 1:F:308:LEU:C    | 1:F:308:LEU:HD12 | 2.39                     | 0.47              |
| 2:e:614:MET:HE3  | 2:e:627:VAL:HG22 | 1.94                     | 0.47              |
| 1:B:220:PRO:CB   | 1:B:377:HIS:HB2  | 2.43                     | 0.47              |
| 1:D:52:PHE:CD2   | 1:D:64:VAL:HG22  | 2.49                     | 0.47              |
| 2:a:666:LEU:O    | 2:a:667:LYS:CB   | 2.62                     | 0.47              |
| 2:b:602:LYS:HD2  | 2:b:607:GLY:O    | 2.14                     | 0.47              |
| 1:B:334:LYS:HD3  | 1:B:338:PRO:HA   | 1.96                     | 0.47              |
| 1:E:53:PHE:O     | 1:E:62:SER:HB2   | 2.14                     | 0.47              |
| 1:E:381:TYR:CZ   | 1:E:423:MET:HE2  | 2.49                     | 0.47              |
| 2:d:639:GLU:O    | 2:d:641:PRO:HD3  | 2.14                     | 0.47              |
| 1:A:362:GLY:O    | 1:D:434:MET:HE1  | 2.15                     | 0.47              |
| 1:C:39:ARG:HD2   | 1:C:43:ASN:ND2   | 2.29                     | 0.47              |
| 1:E:215:PHE:CZ   | 1:E:324:ASN:HB3  | 2.49                     | 0.47              |
| 1:F:11:PHE:CZ    | 1:F:15:LEU:HD21  | 2.50                     | 0.47              |
| 1:F:273:GLU:HB3  | 1:F:289:GLN:HG3  | 1.96                     | 0.47              |
| 1:B:72:GLN:HG3   | 1:B:82:LYS:HG3   | 1.97                     | 0.47              |
| 1:D:468:GLU:O    | 1:D:472:LYS:HG3  | 2.15                     | 0.47              |
| 1:F:334:LYS:HD3  | 1:F:338:PRO:HA   | 1.97                     | 0.47              |
| 2:d:611:VAL:HG23 | 2:d:627:VAL:O    | 2.15                     | 0.47              |
| 2:b:666:LEU:O    | 2:b:667:LYS:CB   | 2.63                     | 0.46              |
| 1:C:227:GLU:N    | 1:C:227:GLU:OE1  | 2.48                     | 0.46              |
| 1:A:40:ALA:O     | 1:A:44:LEU:HD13  | 2.15                     | 0.46              |
| 1:F:162:LEU:C    | 1:F:162:LEU:HD23 | 2.41                     | 0.46              |
| 2:a:613:LYS:HD2  | 2:a:616:ASP:OD1  | 2.16                     | 0.46              |
| 1:D:201:LEU:HD23 | 1:D:265:ILE:HD12 | 1.97                     | 0.46              |
| 2:a:602:LYS:HD2  | 2:a:607:GLY:O    | 2.16                     | 0.46              |
| 2:d:628:CYS:O    | 2:d:629:GLU:HB3  | 2.16                     | 0.46              |
| 1:A:464:THR:HG22 | 1:E:36:ALA:HA    | 1.96                     | 0.46              |
| 1:B:48:GLN:HB2   | 1:B:70:SER:HB3   | 1.97                     | 0.46              |
| 1:B:392:VAL:HG13 | 1:B:399:GLN:HB3  | 1.98                     | 0.46              |
| 1:C:100:PHE:CB   | 1:C:101:PRO:HD3  | 2.41                     | 0.46              |
| 1:D:121:LYS:O    | 1:D:122:ASP:C    | 2.59                     | 0.46              |
| 1:D:142:TYR:CZ   | 1:D:170:GLN:HB2  | 2.51                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:c:639:GLU:O    | 2:c:641:PRO:HD3  | 2.15                     | 0.46              |
| 1:D:470:LYS:O    | 1:D:474:LEU:HD13 | 2.16                     | 0.46              |
| 1:F:321:MET:HA   | 1:F:324:ASN:OD1  | 2.16                     | 0.46              |
| 1:C:279:PHE:CG   | 1:C:280:PRO:HD3  | 2.51                     | 0.46              |
| 1:F:205:ILE:HB   | 1:F:261:LEU:HB2  | 1.98                     | 0.46              |
| 2:a:639:GLU:O    | 2:a:641:PRO:HD3  | 2.15                     | 0.46              |
| 1:A:427:PRO:HB2  | 1:E:455:THR:HG22 | 1.98                     | 0.46              |
| 1:C:446:VAL:HG13 | 1:C:447:PRO:HD2  | 1.98                     | 0.46              |
| 1:E:46:LYS:HE2   | 1:E:47:ASN:HD21  | 1.79                     | 0.46              |
| 1:E:72:GLN:HG3   | 1:E:82:LYS:HG3   | 1.98                     | 0.46              |
| 1:F:279:PHE:N    | 1:F:280:PRO:CD   | 2.79                     | 0.46              |
| 2:f:639:GLU:O    | 2:f:641:PRO:HD3  | 2.15                     | 0.46              |
| 1:A:121:LYS:O    | 1:A:122:ASP:C    | 2.59                     | 0.46              |
| 1:A:215:PHE:CE1  | 1:A:324:ASN:HB3  | 2.51                     | 0.46              |
| 1:A:468:GLU:O    | 1:A:472:LYS:HG3  | 2.16                     | 0.46              |
| 1:C:113:PRO:HD2  | 1:C:255:ALA:O    | 2.15                     | 0.46              |
| 1:B:113:PRO:O    | 1:B:300:ARG:HG2  | 2.15                     | 0.45              |
| 1:F:72:GLN:HG3   | 1:F:82:LYS:HG3   | 1.97                     | 0.45              |
| 1:F:113:PRO:HD2  | 1:F:255:ALA:O    | 2.16                     | 0.45              |
| 2:c:614:MET:HE3  | 2:c:627:VAL:HG22 | 1.98                     | 0.45              |
| 1:A:67:VAL:HB    | 1:A:145:LYS:NZ   | 2.31                     | 0.45              |
| 1:E:273:GLU:HB3  | 1:E:289:GLN:HG3  | 1.98                     | 0.45              |
| 1:E:399:GLN:NE2  | 3:E:503:PEG:H42  | 2.31                     | 0.45              |
| 1:F:29:ASN:HB3   | 1:F:57:LYS:HD3   | 1.97                     | 0.45              |
| 1:F:288:LEU:HG   | 2:f:657:MET:HB3  | 1.98                     | 0.45              |
| 1:F:332:GLN:OE1  | 1:F:375:THR:OG1  | 2.34                     | 0.45              |
| 2:f:628:CYS:O    | 2:f:629:GLU:HB3  | 2.15                     | 0.45              |
| 1:A:313:PRO:HG2  | 1:E:402:TRP:NE1  | 2.30                     | 0.45              |
| 1:B:61:TYR:CD1   | 1:B:303:PRO:HD2  | 2.51                     | 0.45              |
| 1:B:153:PRO:HD3  | 1:B:190:GLN:HB3  | 1.99                     | 0.45              |
| 1:C:65:THR:HA    | 1:C:307:ASN:O    | 2.16                     | 0.45              |
| 1:C:381:TYR:OH   | 1:C:423:MET:HE1  | 2.15                     | 0.45              |
| 1:D:61:TYR:CD1   | 1:D:303:PRO:HD2  | 2.51                     | 0.45              |
| 1:F:180:GLN:HG2  | 1:F:182:LEU:HG   | 1.98                     | 0.45              |
| 1:D:53:PHE:O     | 1:D:62:SER:HB2   | 2.17                     | 0.45              |
| 1:D:148:VAL:O    | 1:D:164:VAL:HA   | 2.15                     | 0.45              |
| 1:D:226:ASN:OD1  | 1:D:228:TYR:HB2  | 2.17                     | 0.45              |
| 1:E:23:ARG:HD3   | 1:E:54:GLU:OE2   | 2.15                     | 0.45              |
| 1:E:220:PRO:CB   | 1:E:377:HIS:HB2  | 2.46                     | 0.45              |
| 1:E:355:ILE:HD11 | 1:E:372:LEU:HD22 | 1.99                     | 0.45              |
| 1:A:321:MET:HA   | 1:A:324:ASN:OD1  | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:423:MET:HG3  | 1:C:425:LEU:H    | 1.80                     | 0.45              |
| 1:E:218:SER:HB2  | 1:E:324:ASN:ND2  | 2.31                     | 0.45              |
| 1:A:147:SER:HB2  | 1:A:206:THR:OG1  | 2.17                     | 0.45              |
| 1:B:39:ARG:HD2   | 1:B:309:TYR:CE2  | 2.51                     | 0.45              |
| 1:F:31:GLU:OE2   | 2:f:636:ARG:NH2  | 2.44                     | 0.45              |
| 1:F:100:PHE:CB   | 1:F:101:PRO:HD3  | 2.45                     | 0.45              |
| 1:A:279:PHE:CG   | 1:A:280:PRO:HD3  | 2.52                     | 0.45              |
| 1:B:184:MET:HB2  | 1:B:380:PRO:HG3  | 1.99                     | 0.45              |
| 1:C:117:ASN:O    | 1:C:298:THR:HA   | 2.17                     | 0.45              |
| 1:D:427:PRO:HB2  | 1:F:455:THR:HG22 | 1.98                     | 0.45              |
| 2:e:667:LYS:HB2  | 2:e:667:LYS:HE3  | 1.65                     | 0.45              |
| 1:C:373:LEU:HD13 | 1:C:437:LYS:HD2  | 1.98                     | 0.45              |
| 1:F:361:TYR:O    | 1:F:364:TYR:HB2  | 2.17                     | 0.45              |
| 1:B:441:ASP:OD1  | 1:B:441:ASP:C    | 2.60                     | 0.45              |
| 1:D:215:PHE:CZ   | 1:D:324:ASN:HB3  | 2.51                     | 0.45              |
| 1:B:164:VAL:CG1  | 1:B:227:GLU:HB2  | 2.47                     | 0.45              |
| 1:C:21:LEU:HA    | 1:C:50:ALA:O     | 2.17                     | 0.45              |
| 1:A:461:PRO:HD2  | 1:A:464:THR:HG21 | 1.97                     | 0.44              |
| 1:B:279:PHE:N    | 1:B:280:PRO:CD   | 2.80                     | 0.44              |
| 1:B:377:HIS:O    | 1:B:381:TYR:HB2  | 2.17                     | 0.44              |
| 1:C:373:LEU:HD22 | 1:C:437:LYS:CD   | 2.47                     | 0.44              |
| 1:E:171:VAL:HA   | 1:E:177:VAL:HG12 | 1.99                     | 0.44              |
| 1:A:53:PHE:HB2   | 1:A:63:VAL:HG22  | 1.98                     | 0.44              |
| 1:B:39:ARG:HH12  | 1:B:315:THR:HG22 | 1.76                     | 0.44              |
| 1:B:261:LEU:HB3  | 1:B:294:ILE:HD12 | 1.99                     | 0.44              |
| 1:B:314:TRP:HA   | 1:B:318:ASP:HB2  | 1.98                     | 0.44              |
| 1:C:180:GLN:HE21 | 1:C:289:GLN:HE22 | 1.65                     | 0.44              |
| 1:C:404:LEU:O    | 1:C:408:VAL:HB   | 2.18                     | 0.44              |
| 1:D:66:ASN:HA    | 1:D:316:GLU:CD   | 2.42                     | 0.44              |
| 1:E:327:VAL:N    | 1:E:328:PRO:HD2  | 2.32                     | 0.44              |
| 1:F:379:MET:HB3  | 1:F:380:PRO:HD3  | 1.99                     | 0.44              |
| 2:a:667:LYS:HE3  | 2:a:667:LYS:HB2  | 1.85                     | 0.44              |
| 1:A:21:LEU:HA    | 1:A:50:ALA:O     | 2.17                     | 0.44              |
| 1:C:11:PHE:CD1   | 1:C:15:LEU:HG    | 2.53                     | 0.44              |
| 1:C:64:VAL:HG23  | 1:C:306:GLU:HA   | 1.98                     | 0.44              |
| 1:F:121:LYS:O    | 1:F:122:ASP:C    | 2.60                     | 0.44              |
| 1:F:344:ASN:OD1  | 1:F:346:MET:HG2  | 2.17                     | 0.44              |
| 1:A:137:GLN:HB2  | 1:A:283:TYR:CE2  | 2.51                     | 0.44              |
| 1:A:162:LEU:C    | 1:A:162:LEU:HD23 | 2.43                     | 0.44              |
| 1:B:219:THR:HG22 | 1:B:221:VAL:HG13 | 2.00                     | 0.44              |
| 1:D:72:GLN:HG3   | 1:D:82:LYS:HG3   | 1.98                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:429:THR:HG1  | 1:F:453:ARG:HH12 | 1.65                     | 0.44              |
| 1:E:279:PHE:CG   | 1:E:280:PRO:HD3  | 2.52                     | 0.44              |
| 1:F:18:GLU:HG3   | 1:F:82:LYS:HD2   | 1.99                     | 0.44              |
| 1:F:128:ILE:HD13 | 1:F:297:ILE:HG21 | 1.99                     | 0.44              |
| 1:A:107:VAL:CG2  | 1:A:243:VAL:HG12 | 2.45                     | 0.44              |
| 1:E:205:ILE:HB   | 1:E:261:LEU:HB2  | 2.00                     | 0.44              |
| 1:E:430:ASN:HB3  | 1:E:431:PRO:CD   | 2.44                     | 0.44              |
| 1:F:63:VAL:HG12  | 1:F:305:PHE:CB   | 2.42                     | 0.44              |
| 1:B:379:MET:HE1  | 1:E:364:TYR:CE1  | 2.52                     | 0.44              |
| 1:D:31:GLU:CB    | 1:D:32:PRO:HD3   | 2.46                     | 0.44              |
| 1:D:215:PHE:CE2  | 1:D:324:ASN:HB3  | 2.52                     | 0.44              |
| 1:E:173:ASP:CB   | 1:E:176:ARG:HG2  | 2.47                     | 0.44              |
| 1:F:145:LYS:HD2  | 1:F:306:GLU:HG2  | 1.99                     | 0.44              |
| 1:A:142:TYR:CZ   | 1:A:170:GLN:HB2  | 2.53                     | 0.44              |
| 1:A:356:SER:HB2  | 1:A:394:PRO:HD3  | 1.99                     | 0.44              |
| 1:B:279:PHE:CD1  | 1:B:280:PRO:HD3  | 2.53                     | 0.44              |
| 1:C:172:LYS:NZ   | 1:C:271:THR:OG1  | 2.44                     | 0.44              |
| 1:F:226:ASN:OD1  | 1:F:228:TYR:HB2  | 2.18                     | 0.44              |
| 1:B:176:ARG:HD2  | 1:B:291:GLU:OE1  | 2.17                     | 0.44              |
| 1:E:441:ASP:OD1  | 1:E:441:ASP:C    | 2.60                     | 0.43              |
| 1:F:142:TYR:CZ   | 1:F:170:GLN:HB2  | 2.53                     | 0.43              |
| 1:A:210:ASN:OD1  | 1:A:211:PRO:HD2  | 2.18                     | 0.43              |
| 1:B:301:THR:HG22 | 1:B:302:ASN:ND2  | 2.32                     | 0.43              |
| 1:D:441:ASP:C    | 1:D:441:ASP:OD1  | 2.61                     | 0.43              |
| 1:E:118:VAL:HG22 | 1:E:298:THR:HG22 | 2.01                     | 0.43              |
| 1:F:216:MET:HE2  | 1:F:230:PHE:CB   | 2.48                     | 0.43              |
| 1:C:18:GLU:O     | 1:C:82:LYS:NZ    | 2.46                     | 0.43              |
| 1:C:453:ARG:HG2  | 1:C:453:ARG:NH1  | 2.33                     | 0.43              |
| 1:E:145:LYS:NZ   | 1:E:316:GLU:OE2  | 2.42                     | 0.43              |
| 1:E:231:VAL:O    | 1:E:235:GLN:HG3  | 2.17                     | 0.43              |
| 2:c:602:LYS:HD2  | 2:c:607:GLY:O    | 2.18                     | 0.43              |
| 1:C:8:LEU:HB2    | 1:C:209:ASN:C    | 2.43                     | 0.43              |
| 1:C:231:VAL:O    | 1:C:235:GLN:HG3  | 2.19                     | 0.43              |
| 1:D:40:ALA:O     | 1:D:44:LEU:HD13  | 2.18                     | 0.43              |
| 1:F:164:VAL:CG1  | 1:F:227:GLU:HB2  | 2.49                     | 0.43              |
| 1:A:279:PHE:N    | 1:A:280:PRO:CD   | 2.82                     | 0.43              |
| 1:B:321:MET:HA   | 1:B:324:ASN:OD1  | 2.18                     | 0.43              |
| 1:A:441:ASP:C    | 1:A:441:ASP:OD1  | 2.62                     | 0.43              |
| 1:B:119:ILE:HB   | 1:B:297:ILE:HB   | 1.99                     | 0.43              |
| 1:B:434:MET:SD   | 1:E:449:GLU:HB2  | 2.58                     | 0.43              |
| 1:C:245:SER:HB3  | 1:C:248:TYR:O    | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:113:PRO:O    | 1:D:300:ARG:HG2  | 2.19                     | 0.43              |
| 1:D:392:VAL:HG13 | 1:D:399:GLN:HB3  | 2.01                     | 0.43              |
| 1:F:160:ASN:HB3  | 1:F:224:ASN:O    | 2.18                     | 0.43              |
| 2:f:660:ILE:HA   | 2:f:661:PRO:HA   | 1.85                     | 0.43              |
| 1:B:68:HIS:CD2   | 1:B:77:MET:HE2   | 2.54                     | 0.43              |
| 1:B:100:PHE:CD1  | 1:B:100:PHE:C    | 2.97                     | 0.43              |
| 1:D:77:MET:HG2   | 1:D:212:LEU:CD1  | 2.48                     | 0.43              |
| 1:D:118:VAL:HG11 | 1:D:296:ARG:NH1  | 2.33                     | 0.43              |
| 1:E:137:GLN:H    | 1:E:283:TYR:HH   | 1.64                     | 0.43              |
| 1:F:145:LYS:NZ   | 1:F:316:GLU:OE2  | 2.47                     | 0.43              |
| 1:A:276:PHE:CZ   | 1:A:310:LEU:HD21 | 2.54                     | 0.43              |
| 1:B:435:HIS:HE1  | 1:B:437:LYS:NZ   | 2.17                     | 0.43              |
| 1:C:11:PHE:CD2   | 1:C:211:PRO:CG   | 2.91                     | 0.43              |
| 1:C:121:LYS:O    | 1:C:122:ASP:C    | 2.61                     | 0.43              |
| 1:F:21:LEU:HA    | 1:F:50:ALA:O     | 2.18                     | 0.43              |
| 1:F:245:SER:HB3  | 1:F:248:TYR:O    | 2.18                     | 0.43              |
| 1:A:171:VAL:HA   | 1:A:177:VAL:HG12 | 2.01                     | 0.43              |
| 1:D:113:PRO:HD2  | 1:D:255:ALA:O    | 2.19                     | 0.43              |
| 1:D:458:LEU:H    | 1:D:458:LEU:HD23 | 1.84                     | 0.43              |
| 2:d:636:ARG:HB3  | 2:d:639:GLU:HG2  | 2.00                     | 0.43              |
| 1:B:227:GLU:OE1  | 1:B:227:GLU:N    | 2.52                     | 0.43              |
| 1:B:34:ILE:H     | 1:B:34:ILE:HG12  | 1.72                     | 0.42              |
| 1:F:131:LEU:CD2  | 1:F:171:VAL:HG21 | 2.50                     | 0.42              |
| 1:F:145:LYS:HD3  | 1:F:214:THR:HG21 | 2.01                     | 0.42              |
| 2:e:666:LEU:O    | 2:e:667:LYS:HB2  | 2.19                     | 0.42              |
| 1:B:249:ASP:C    | 1:B:251:LEU:H    | 2.27                     | 0.42              |
| 1:C:288:LEU:HG   | 2:c:657:MET:HB3  | 2.00                     | 0.42              |
| 1:D:356:SER:HB2  | 1:D:394:PRO:HD3  | 2.01                     | 0.42              |
| 1:A:11:PHE:CG    | 1:A:211:PRO:HG3  | 2.54                     | 0.42              |
| 1:B:329:LEU:HD11 | 1:B:377:HIS:HB3  | 2.01                     | 0.42              |
| 1:C:344:ASN:OD1  | 1:C:346:MET:HG2  | 2.19                     | 0.42              |
| 1:F:46:LYS:HG2   | 1:F:47:ASN:ND2   | 2.34                     | 0.42              |
| 1:A:112:ALA:CB   | 1:A:243:VAL:HG11 | 2.42                     | 0.42              |
| 1:C:131:LEU:CD2  | 1:C:171:VAL:HG21 | 2.49                     | 0.42              |
| 1:E:202:PRO:HB3  | 1:E:248:TYR:CD1  | 2.54                     | 0.42              |
| 2:b:614:MET:HE3  | 2:b:627:VAL:HG21 | 1.97                     | 0.42              |
| 2:b:636:ARG:HB3  | 2:b:639:GLU:HG2  | 2.01                     | 0.42              |
| 1:A:197:GLU:HB2  | 1:A:199:LYS:HE2  | 2.01                     | 0.42              |
| 1:A:245:SER:HB3  | 1:A:248:TYR:O    | 2.19                     | 0.42              |
| 1:B:180:GLN:HG2  | 1:B:182:LEU:HG   | 2.02                     | 0.42              |
| 1:D:160:ASN:HB3  | 1:D:224:ASN:O    | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:113:PRO:HD2  | 1:A:255:ALA:O    | 2.19                     | 0.42              |
| 1:D:173:ASP:CB   | 1:D:176:ARG:HG2  | 2.49                     | 0.42              |
| 1:D:327:VAL:N    | 1:D:328:PRO:HD2  | 2.34                     | 0.42              |
| 2:b:667:LYS:HE3  | 2:b:667:LYS:HB2  | 1.81                     | 0.42              |
| 1:C:279:PHE:N    | 1:C:280:PRO:CD   | 2.81                     | 0.42              |
| 1:C:361:TYR:O    | 1:C:364:TYR:HB2  | 2.20                     | 0.42              |
| 1:D:64:VAL:HG23  | 1:D:304:ILE:HG22 | 2.02                     | 0.42              |
| 1:E:332:GLN:OE1  | 1:E:375:THR:OG1  | 2.38                     | 0.42              |
| 2:a:642:VAL:HG13 | 2:a:642:VAL:O    | 2.19                     | 0.42              |
| 1:B:249:ASP:O    | 1:B:250:HIS:HB2  | 2.20                     | 0.42              |
| 1:E:271:THR:O    | 1:E:288:LEU:HA   | 2.20                     | 0.42              |
| 2:a:628:CYS:O    | 2:a:629:GLU:HB3  | 2.19                     | 0.42              |
| 1:A:51:VAL:HG22  | 1:A:65:THR:CG2   | 2.42                     | 0.42              |
| 1:C:39:ARG:HD2   | 1:C:43:ASN:HD21  | 1.84                     | 0.42              |
| 1:F:87:LYS:HB2   | 1:F:87:LYS:HE2   | 1.94                     | 0.42              |
| 1:C:271:THR:O    | 1:C:288:LEU:HA   | 2.20                     | 0.42              |
| 1:C:363:GLY:HA3  | 1:F:434:MET:HE1  | 2.01                     | 0.42              |
| 1:D:128:ILE:CD1  | 1:D:297:ILE:HG21 | 2.50                     | 0.42              |
| 2:b:615:VAL:HG12 | 2:b:625:VAL:HB   | 2.01                     | 0.42              |
| 1:A:74:HIS:CE1   | 1:A:323:LEU:HD12 | 2.55                     | 0.41              |
| 1:B:361:TYR:O    | 1:B:364:TYR:HB2  | 2.20                     | 0.41              |
| 1:D:145:LYS:HD2  | 1:D:306:GLU:HG2  | 2.02                     | 0.41              |
| 1:E:121:LYS:O    | 1:E:122:ASP:C    | 2.63                     | 0.41              |
| 1:E:379:MET:HB3  | 1:E:380:PRO:HD3  | 2.02                     | 0.41              |
| 1:C:65:THR:O     | 1:C:316:GLU:OE1  | 2.38                     | 0.41              |
| 1:C:119:ILE:HG22 | 1:C:123:ILE:HD13 | 2.01                     | 0.41              |
| 1:F:227:GLU:OE1  | 1:F:227:GLU:N    | 2.53                     | 0.41              |
| 1:A:59:TYR:CD1   | 1:A:130:PRO:HA   | 2.56                     | 0.41              |
| 1:B:66:ASN:ND2   | 1:B:69:GLY:HA3   | 2.36                     | 0.41              |
| 1:B:470:LYS:O    | 1:B:474:LEU:HD13 | 2.20                     | 0.41              |
| 1:D:314:TRP:H    | 1:D:318:ASP:CG   | 2.28                     | 0.41              |
| 1:E:356:SER:HB2  | 1:E:394:PRO:HD3  | 2.02                     | 0.41              |
| 1:F:39:ARG:NH2   | 1:F:315:THR:HG22 | 2.35                     | 0.41              |
| 1:F:169:ILE:HA   | 1:F:178:GLY:O    | 2.20                     | 0.41              |
| 1:F:220:PRO:CB   | 1:F:377:HIS:HB2  | 2.50                     | 0.41              |
| 1:A:362:GLY:C    | 1:D:434:MET:HE1  | 2.46                     | 0.41              |
| 1:B:219:THR:OG1  | 1:B:324:ASN:HB2  | 2.21                     | 0.41              |
| 1:D:312:ILE:HA   | 1:D:313:PRO:HD3  | 1.88                     | 0.41              |
| 1:F:420:CYS:O    | 1:F:434:MET:HE3  | 2.20                     | 0.41              |
| 2:c:667:LYS:HB2  | 2:c:667:LYS:HE3  | 1.58                     | 0.41              |
| 1:A:423:MET:SD   | 1:A:424:PRO:HD2  | 2.60                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:184:MET:HE3  | 1:C:184:MET:HB3  | 1.93                     | 0.41              |
| 1:D:216:MET:HE2  | 1:D:230:PHE:CB   | 2.50                     | 0.41              |
| 1:D:227:GLU:OE1  | 1:D:227:GLU:N    | 2.52                     | 0.41              |
| 1:D:455:THR:CG2  | 1:F:427:PRO:HB2  | 2.49                     | 0.41              |
| 1:E:51:VAL:HG22  | 1:E:65:THR:CG2   | 2.40                     | 0.41              |
| 1:A:61:TYR:CE1   | 1:A:303:PRO:HD2  | 2.55                     | 0.41              |
| 1:C:441:ASP:OD1  | 1:C:441:ASP:C    | 2.64                     | 0.41              |
| 1:E:77:MET:HG3   | 1:E:211:PRO:HB2  | 2.01                     | 0.41              |
| 2:f:667:LYS:HB2  | 2:f:667:LYS:HE3  | 1.76                     | 0.41              |
| 1:A:218:SER:HB2  | 1:A:324:ASN:ND2  | 2.35                     | 0.41              |
| 1:A:249:ASP:O    | 1:A:250:HIS:HB2  | 2.21                     | 0.41              |
| 1:A:471:LEU:HG   | 1:E:22:ILE:HD11  | 2.02                     | 0.41              |
| 1:D:11:PHE:CG    | 1:D:211:PRO:HG3  | 2.55                     | 0.41              |
| 1:D:173:ASP:HB3  | 1:D:176:ARG:HG2  | 2.02                     | 0.41              |
| 2:c:642:VAL:O    | 2:c:642:VAL:HG13 | 2.21                     | 0.41              |
| 2:e:610:ASN:O    | 2:e:628:CYS:O    | 2.38                     | 0.41              |
| 1:A:197:GLU:CB   | 1:A:199:LYS:HE2  | 2.49                     | 0.41              |
| 1:A:205:ILE:HB   | 1:A:261:LEU:HB2  | 2.01                     | 0.41              |
| 1:B:113:PRO:C    | 1:B:300:ARG:HG2  | 2.46                     | 0.41              |
| 1:E:468:GLU:O    | 1:E:472:LYS:HG3  | 2.21                     | 0.41              |
| 1:B:74:HIS:CE1   | 1:B:323:LEU:HD12 | 2.56                     | 0.41              |
| 1:B:117:ASN:O    | 1:B:298:THR:HA   | 2.20                     | 0.41              |
| 1:C:31:GLU:CB    | 1:C:32:PRO:HD3   | 2.50                     | 0.41              |
| 1:C:312:ILE:HA   | 1:C:313:PRO:HD3  | 1.96                     | 0.41              |
| 1:C:358:LYS:HA   | 1:C:390:GLU:HG3  | 2.02                     | 0.41              |
| 1:C:434:MET:HE2  | 1:C:434:MET:HB3  | 1.99                     | 0.41              |
| 1:E:59:TYR:CD1   | 1:E:130:PRO:HA   | 2.55                     | 0.41              |
| 1:E:148:VAL:O    | 1:E:164:VAL:HA   | 2.20                     | 0.41              |
| 1:F:118:VAL:HG11 | 1:F:296:ARG:NH1  | 2.36                     | 0.41              |
| 1:F:171:VAL:HA   | 1:F:177:VAL:HG12 | 2.03                     | 0.41              |
| 1:F:431:PRO:HB2  | 1:F:434:MET:HB3  | 2.02                     | 0.41              |
| 1:F:441:ASP:OD1  | 1:F:441:ASP:C    | 2.64                     | 0.41              |
| 1:A:59:TYR:CG    | 1:A:130:PRO:HA   | 2.55                     | 0.41              |
| 1:A:216:MET:HE2  | 1:A:230:PHE:CB   | 2.51                     | 0.41              |
| 1:B:145:LYS:HD2  | 1:B:306:GLU:HG2  | 2.02                     | 0.41              |
| 1:B:429:THR:O    | 1:C:453:ARG:HD3  | 2.21                     | 0.41              |
| 1:C:113:PRO:C    | 1:C:300:ARG:HG2  | 2.46                     | 0.41              |
| 1:C:430:ASN:O    | 1:C:432:PRO:HD3  | 2.21                     | 0.41              |
| 1:D:165:GLY:HA2  | 1:D:217:ALA:O    | 2.21                     | 0.41              |
| 1:E:27:GLU:HA    | 1:E:55:LYS:HB3   | 2.01                     | 0.41              |
| 1:A:9:ARG:CZ     | 1:A:300:ARG:HD2  | 2.51                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:31:GLU:CB    | 1:A:32:PRO:HD3   | 2.51                     | 0.40              |
| 1:A:145:LYS:HD2  | 1:A:306:GLU:HG2  | 2.02                     | 0.40              |
| 1:A:180:GLN:HG2  | 1:A:182:LEU:HG   | 2.03                     | 0.40              |
| 1:A:384:ILE:HG12 | 1:A:438:MET:HE2  | 2.02                     | 0.40              |
| 1:B:348:THR:HG22 | 1:B:351:ILE:HD12 | 2.03                     | 0.40              |
| 1:D:205:ILE:HB   | 1:D:261:LEU:HB2  | 2.03                     | 0.40              |
| 1:F:59:TYR:CD1   | 1:F:130:PRO:HA   | 2.57                     | 0.40              |
| 1:F:349:HIS:O    | 1:F:349:HIS:ND1  | 2.55                     | 0.40              |
| 1:C:75:ALA:HB2   | 1:C:89:GLN:NE2   | 2.37                     | 0.40              |
| 1:A:66:ASN:HA    | 1:A:316:GLU:CD   | 2.45                     | 0.40              |
| 1:A:160:ASN:HB3  | 1:A:224:ASN:O    | 2.20                     | 0.40              |
| 1:A:327:VAL:N    | 1:A:328:PRO:HD2  | 2.36                     | 0.40              |
| 1:A:337:MET:HE2  | 1:D:379:MET:HE1  | 2.03                     | 0.40              |
| 1:B:25:LYS:HD3   | 1:B:54:GLU:OE1   | 2.20                     | 0.40              |
| 1:D:276:PHE:CZ   | 1:D:310:LEU:HD21 | 2.56                     | 0.40              |
| 1:D:399:GLN:NE2  | 3:D:501:PEG:H32  | 2.37                     | 0.40              |
| 1:F:210:ASN:OD1  | 1:F:211:PRO:HD2  | 2.22                     | 0.40              |
| 1:C:11:PHE:HE1   | 1:C:15:LEU:HD21  | 1.87                     | 0.40              |
| 1:E:58:GLY:HA3   | 2:e:623:TRP:NE1  | 2.36                     | 0.40              |
| 1:F:173:ASP:CB   | 1:F:176:ARG:HG2  | 2.52                     | 0.40              |
| 1:F:468:GLU:O    | 1:F:472:LYS:HG3  | 2.20                     | 0.40              |
| 2:d:667:LYS:HE3  | 2:d:667:LYS:HB2  | 1.84                     | 0.40              |
| 1:A:226:ASN:OD1  | 1:A:228:TYR:HB2  | 2.21                     | 0.40              |
| 1:B:90:PHE:HD1   | 1:B:323:LEU:HD22 | 1.87                     | 0.40              |
| 1:C:435:HIS:CE1  | 1:C:437:LYS:NZ   | 2.90                     | 0.40              |
| 1:D:37:ALA:CB    | 1:D:53:PHE:HZ    | 2.34                     | 0.40              |
| 1:D:184:MET:HE3  | 1:D:184:MET:HB3  | 1.97                     | 0.40              |
| 1:D:240:MET:HE3  | 1:D:240:MET:HB2  | 1.88                     | 0.40              |
| 1:D:321:MET:HA   | 1:D:324:ASN:OD1  | 2.22                     | 0.40              |
| 1:F:374:SER:HA   | 1:F:379:MET:HE3  | 2.04                     | 0.40              |
| 2:a:636:ARG:HB3  | 2:a:639:GLU:HG2  | 2.04                     | 0.40              |
| 2:f:642:VAL:O    | 2:f:642:VAL:HG13 | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

of similar resolution.

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 474/480 (99%)   | 456 (96%)  | 18 (4%)  | 0        | 100         | 100 |
| 1   | B     | 474/480 (99%)   | 453 (96%)  | 21 (4%)  | 0        | 100         | 100 |
| 1   | C     | 474/480 (99%)   | 452 (95%)  | 22 (5%)  | 0        | 100         | 100 |
| 1   | D     | 474/480 (99%)   | 451 (95%)  | 23 (5%)  | 0        | 100         | 100 |
| 1   | E     | 473/480 (98%)   | 454 (96%)  | 19 (4%)  | 0        | 100         | 100 |
| 1   | F     | 474/480 (99%)   | 453 (96%)  | 21 (4%)  | 0        | 100         | 100 |
| 2   | a     | 65/68 (96%)     | 61 (94%)   | 4 (6%)   | 0        | 100         | 100 |
| 2   | b     | 65/68 (96%)     | 61 (94%)   | 4 (6%)   | 0        | 100         | 100 |
| 2   | c     | 65/68 (96%)     | 61 (94%)   | 4 (6%)   | 0        | 100         | 100 |
| 2   | d     | 65/68 (96%)     | 61 (94%)   | 4 (6%)   | 0        | 100         | 100 |
| 2   | e     | 65/68 (96%)     | 62 (95%)   | 3 (5%)   | 0        | 100         | 100 |
| 2   | f     | 65/68 (96%)     | 62 (95%)   | 3 (5%)   | 0        | 100         | 100 |
| All | All   | 3233/3288 (98%) | 3087 (96%) | 146 (4%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | A     | 413/419 (99%) | 413 (100%) | 0        | 100         | 100 |
| 1   | B     | 407/419 (97%) | 407 (100%) | 0        | 100         | 100 |
| 1   | C     | 401/419 (96%) | 401 (100%) | 0        | 100         | 100 |
| 1   | D     | 411/419 (98%) | 411 (100%) | 0        | 100         | 100 |
| 1   | E     | 413/419 (99%) | 413 (100%) | 0        | 100         | 100 |
| 1   | F     | 410/419 (98%) | 410 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 2   | a     | 60/63 (95%)     | 60 (100%)   | 0        | 100         | 100 |
| 2   | b     | 60/63 (95%)     | 60 (100%)   | 0        | 100         | 100 |
| 2   | c     | 60/63 (95%)     | 60 (100%)   | 0        | 100         | 100 |
| 2   | d     | 60/63 (95%)     | 60 (100%)   | 0        | 100         | 100 |
| 2   | e     | 60/63 (95%)     | 60 (100%)   | 0        | 100         | 100 |
| 2   | f     | 60/63 (95%)     | 60 (100%)   | 0        | 100         | 100 |
| All | All   | 2815/2892 (97%) | 2815 (100%) | 0        | 100         | 100 |

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 20  | GLN  |
| 1   | A     | 68  | HIS  |
| 1   | A     | 83  | ASN  |
| 1   | A     | 89  | GLN  |
| 1   | A     | 117 | ASN  |
| 1   | A     | 135 | ASN  |
| 1   | B     | 20  | GLN  |
| 1   | B     | 68  | HIS  |
| 1   | B     | 135 | ASN  |
| 1   | B     | 224 | ASN  |
| 1   | B     | 302 | ASN  |
| 1   | B     | 430 | ASN  |
| 1   | B     | 435 | HIS  |
| 1   | B     | 456 | GLN  |
| 1   | C     | 20  | GLN  |
| 1   | C     | 89  | GLN  |
| 1   | C     | 117 | ASN  |
| 1   | C     | 124 | ASN  |
| 1   | C     | 180 | GLN  |
| 1   | C     | 224 | ASN  |
| 1   | C     | 235 | GLN  |
| 1   | C     | 435 | HIS  |
| 1   | D     | 20  | GLN  |
| 1   | D     | 68  | HIS  |
| 1   | D     | 180 | GLN  |
| 1   | D     | 224 | ASN  |
| 1   | E     | 20  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 47  | ASN  |
| 1   | E     | 180 | GLN  |
| 1   | E     | 224 | ASN  |
| 1   | E     | 235 | GLN  |
| 1   | E     | 349 | HIS  |
| 1   | F     | 20  | GLN  |
| 1   | F     | 47  | ASN  |
| 1   | F     | 68  | HIS  |
| 1   | F     | 135 | ASN  |
| 1   | F     | 185 | HIS  |
| 1   | F     | 224 | ASN  |
| 1   | F     | 235 | GLN  |
| 2   | a     | 610 | ASN  |
| 2   | a     | 656 | ASN  |
| 2   | b     | 656 | ASN  |
| 2   | c     | 604 | HIS  |
| 2   | d     | 610 | ASN  |
| 2   | e     | 656 | ASN  |
| 2   | f     | 656 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 46 ligands modelled in this entry, 33 are monoatomic - leaving 13 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 5   | PO4  | E     | 507 | 6,4  | 4,4,4        | 0.98 | 0           | 6,6,6       | 0.41 | 0           |
| 3   | PEG  | E     | 501 | -    | 6,6,6        | 0.19 | 0           | 5,5,5       | 0.06 | 0           |
| 3   | PEG  | C     | 501 | -    | 6,6,6        | 0.22 | 0           | 5,5,5       | 0.10 | 0           |
| 3   | PEG  | A     | 501 | -    | 6,6,6        | 0.20 | 0           | 5,5,5       | 0.09 | 0           |
| 5   | PO4  | C     | 504 | 6,4  | 4,4,4        | 0.94 | 0           | 6,6,6       | 0.54 | 0           |
| 3   | PEG  | F     | 501 | -    | 6,6,6        | 0.20 | 0           | 5,5,5       | 0.05 | 0           |
| 5   | PO4  | B     | 504 | 6,4  | 4,4,4        | 0.92 | 0           | 6,6,6       | 0.55 | 0           |
| 5   | PO4  | F     | 504 | 6,4  | 4,4,4        | 0.90 | 0           | 6,6,6       | 0.64 | 0           |
| 3   | PEG  | E     | 503 | -    | 6,6,6        | 0.24 | 0           | 5,5,5       | 0.06 | 0           |
| 5   | PO4  | A     | 505 | 6,4  | 4,4,4        | 0.96 | 0           | 6,6,6       | 0.45 | 0           |
| 8   | EDO  | E     | 502 | -    | 3,3,3        | 0.56 | 0           | 2,2,2       | 0.20 | 0           |
| 5   | PO4  | D     | 504 | 6,4  | 4,4,4        | 0.91 | 0           | 6,6,6       | 0.52 | 0           |
| 3   | PEG  | D     | 501 | -    | 6,6,6        | 0.23 | 0           | 5,5,5       | 0.06 | 0           |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 3   | PEG  | E     | 501 | -    | -       | 0/4/4/4  | -     |
| 3   | PEG  | C     | 501 | -    | -       | 0/4/4/4  | -     |
| 3   | PEG  | A     | 501 | -    | -       | 3/4/4/4  | -     |
| 3   | PEG  | F     | 501 | -    | -       | 1/4/4/4  | -     |
| 3   | PEG  | E     | 503 | -    | -       | 3/4/4/4  | -     |
| 8   | EDO  | E     | 502 | -    | -       | 0/1/1/1  | -     |
| 3   | PEG  | D     | 501 | -    | -       | 3/4/4/4  | -     |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 3   | F     | 501 | PEG  | O1-C1-C2-O2 |
| 3   | E     | 503 | PEG  | O1-C1-C2-O2 |
| 3   | D     | 501 | PEG  | O2-C3-C4-O4 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 3   | A     | 501 | PEG  | C4-C3-O2-C2 |
| 3   | A     | 501 | PEG  | O1-C1-C2-O2 |
| 3   | D     | 501 | PEG  | C1-C2-O2-C3 |
| 3   | D     | 501 | PEG  | O1-C1-C2-O2 |
| 3   | E     | 503 | PEG  | O2-C3-C4-O4 |
| 3   | A     | 501 | PEG  | C1-C2-O2-C3 |
| 3   | E     | 503 | PEG  | C4-C3-O2-C2 |

There are no ring outliers.

3 monomers are involved in 3 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | A     | 501 | PEG  | 1       | 0            |
| 3   | E     | 503 | PEG  | 1       | 0            |
| 3   | D     | 501 | PEG  | 1       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ > 2                               | OWAB(Å <sup>2</sup> ) | Q < 0.9 |
|-----|-------|-----------------|--------|-----------------------------------------|-----------------------|---------|
| 1   | A     | 476/480 (99%)   | -0.60  | 0 <span>100</span> <span>100</span>     | 85, 128, 163, 179     | 0       |
| 1   | B     | 476/480 (99%)   | -0.59  | 2 (0%) <span>88</span> <span>79</span>  | 86, 114, 152, 195     | 0       |
| 1   | C     | 476/480 (99%)   | -0.52  | 1 (0%) <span>91</span> <span>86</span>  | 93, 142, 178, 199     | 0       |
| 1   | D     | 476/480 (99%)   | -0.49  | 1 (0%) <span>91</span> <span>86</span>  | 88, 127, 158, 188     | 0       |
| 1   | E     | 475/480 (98%)   | -0.64  | 1 (0%) <span>91</span> <span>86</span>  | 82, 114, 150, 172     | 0       |
| 1   | F     | 476/480 (99%)   | -0.58  | 3 (0%) <span>85</span> <span>73</span>  | 94, 135, 170, 194     | 0       |
| 2   | a     | 67/68 (98%)     | -0.44  | 0 <span>100</span> <span>100</span>     | 113, 142, 167, 179    | 0       |
| 2   | b     | 67/68 (98%)     | -0.46  | 1 (1%) <span>72</span> <span>53</span>  | 99, 127, 158, 188     | 0       |
| 2   | c     | 67/68 (98%)     | -0.42  | 0 <span>100</span> <span>100</span>     | 117, 156, 185, 205    | 0       |
| 2   | d     | 67/68 (98%)     | -0.46  | 2 (2%) <span>52</span> <span>35</span>  | 116, 142, 174, 193    | 0       |
| 2   | e     | 67/68 (98%)     | -0.32  | 1 (1%) <span>72</span> <span>53</span>  | 108, 128, 167, 179    | 0       |
| 2   | f     | 67/68 (98%)     | -0.56  | 1 (1%) <span>72</span> <span>53</span>  | 119, 148, 174, 193    | 0       |
| All | All   | 3257/3288 (99%) | -0.55  | 13 (0%) <span>88</span> <span>79</span> | 82, 128, 169, 205     | 0       |

All (13) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 122 | ASP  | 3.1  |
| 2   | b     | 667 | LYS  | 3.0  |
| 2   | d     | 601 | MET  | 3.0  |
| 1   | B     | 7   | ASP  | 2.9  |
| 1   | B     | 90  | PHE  | 2.7  |
| 1   | F     | 90  | PHE  | 2.5  |
| 2   | e     | 601 | MET  | 2.4  |
| 1   | F     | 86  | THR  | 2.2  |
| 1   | D     | 87  | LYS  | 2.2  |
| 1   | C     | 122 | ASP  | 2.1  |
| 1   | E     | 3   | LYS  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | d     | 667 | LYS  | 2.1  |
| 2   | f     | 667 | LYS  | 2.1  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 8   | EDO  | E     | 502 | 4/4   | 0.81 | 0.56 | 134,164,202,202            | 0     |
| 6   | MG   | E     | 508 | 1/1   | 0.85 | 0.11 | 127,127,127,127            | 0     |
| 5   | PO4  | B     | 504 | 5/5   | 0.87 | 0.07 | 122,122,152,153            | 0     |
| 6   | MG   | D     | 505 | 1/1   | 0.89 | 0.10 | 136,136,136,136            | 0     |
| 5   | PO4  | A     | 505 | 5/5   | 0.89 | 0.06 | 164,168,176,190            | 0     |
| 3   | PEG  | E     | 501 | 7/7   | 0.89 | 0.11 | 120,150,191,191            | 0     |
| 5   | PO4  | E     | 507 | 5/5   | 0.91 | 0.08 | 151,152,159,175            | 0     |
| 5   | PO4  | C     | 504 | 5/5   | 0.91 | 0.06 | 154,155,189,200            | 0     |
| 5   | PO4  | D     | 504 | 5/5   | 0.92 | 0.05 | 142,154,172,174            | 0     |
| 4   | NA   | E     | 506 | 1/1   | 0.92 | 0.05 | 139,139,139,139            | 0     |
| 5   | PO4  | F     | 504 | 5/5   | 0.92 | 0.06 | 158,171,189,200            | 0     |
| 3   | PEG  | E     | 503 | 7/7   | 0.93 | 0.14 | 116,140,167,167            | 0     |
| 3   | PEG  | C     | 501 | 7/7   | 0.93 | 0.14 | 109,132,147,174            | 0     |
| 6   | MG   | A     | 506 | 1/1   | 0.93 | 0.07 | 136,136,136,136            | 0     |
| 6   | MG   | C     | 505 | 1/1   | 0.94 | 0.12 | 151,151,151,151            | 0     |
| 4   | NA   | F     | 503 | 1/1   | 0.94 | 0.10 | 79,79,79,79                | 0     |
| 4   | NA   | A     | 503 | 1/1   | 0.95 | 0.07 | 89,89,89,89                | 0     |
| 6   | MG   | B     | 505 | 1/1   | 0.95 | 0.12 | 118,118,118,118            | 0     |
| 7   | CL   | A     | 508 | 1/1   | 0.95 | 0.17 | 110,110,110,110            | 0     |
| 4   | NA   | B     | 503 | 1/1   | 0.95 | 0.05 | 132,132,132,132            | 0     |
| 3   | PEG  | F     | 501 | 7/7   | 0.96 | 0.11 | 131,157,166,188            | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | PEG  | A     | 501 | 7/7   | 0.96 | 0.12 | 124,149,172,172             | 0     |
| 4   | NA   | B     | 502 | 1/1   | 0.96 | 0.09 | 85,85,85,85                 | 0     |
| 6   | MG   | F     | 505 | 1/1   | 0.96 | 0.09 | 139,139,139,139             | 0     |
| 7   | CL   | A     | 507 | 1/1   | 0.96 | 0.14 | 99,99,99,99                 | 0     |
| 3   | PEG  | D     | 501 | 7/7   | 0.96 | 0.12 | 124,148,177,177             | 0     |
| 4   | NA   | E     | 504 | 1/1   | 0.96 | 0.07 | 81,81,81,81                 | 0     |
| 4   | NA   | E     | 505 | 1/1   | 0.97 | 0.09 | 87,87,87,87                 | 0     |
| 4   | NA   | C     | 503 | 1/1   | 0.97 | 0.05 | 86,86,86,86                 | 0     |
| 7   | CL   | B     | 506 | 1/1   | 0.97 | 0.16 | 88,88,88,88                 | 0     |
| 7   | CL   | C     | 506 | 1/1   | 0.97 | 0.25 | 111,111,111,111             | 0     |
| 7   | CL   | D     | 506 | 1/1   | 0.97 | 0.19 | 115,115,115,115             | 0     |
| 7   | CL   | D     | 507 | 1/1   | 0.97 | 0.23 | 108,108,108,108             | 0     |
| 4   | NA   | A     | 504 | 1/1   | 0.97 | 0.03 | 155,155,155,155             | 0     |
| 4   | NA   | C     | 502 | 1/1   | 0.98 | 0.05 | 117,117,117,117             | 0     |
| 4   | NA   | D     | 502 | 1/1   | 0.98 | 0.05 | 110,110,110,110             | 0     |
| 4   | NA   | D     | 503 | 1/1   | 0.98 | 0.06 | 93,93,93,93                 | 0     |
| 4   | NA   | F     | 502 | 1/1   | 0.98 | 0.07 | 116,116,116,116             | 0     |
| 4   | NA   | A     | 502 | 1/1   | 0.99 | 0.03 | 103,103,103,103             | 0     |
| 4   | NA   | B     | 501 | 1/1   | 0.99 | 0.07 | 88,88,88,88                 | 0     |
| 9   | ZN   | b     | 701 | 1/1   | 0.99 | 0.04 | 148,148,148,148             | 0     |
| 9   | ZN   | d     | 701 | 1/1   | 0.99 | 0.04 | 176,176,176,176             | 0     |
| 9   | ZN   | c     | 701 | 1/1   | 1.00 | 0.05 | 173,173,173,173             | 0     |
| 9   | ZN   | a     | 701 | 1/1   | 1.00 | 0.05 | 163,163,163,163             | 0     |
| 9   | ZN   | e     | 701 | 1/1   | 1.00 | 0.04 | 145,145,145,145             | 0     |
| 9   | ZN   | f     | 701 | 1/1   | 1.00 | 0.04 | 151,151,151,151             | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.