



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:25 PM GMT

PDB ID : 4RJK  
Title : Acetolactate synthase from Bacillus subtilis bound to LThDP - crystal form II  
Authors : Sommer, B.; von Moeller, H.; Haack, M.; Qoura, F.; Langner, C.; Bourenkov, G.; Garbe, D.; Brueck, T.; Loll, B.  
Deposited on : 2014-10-09  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

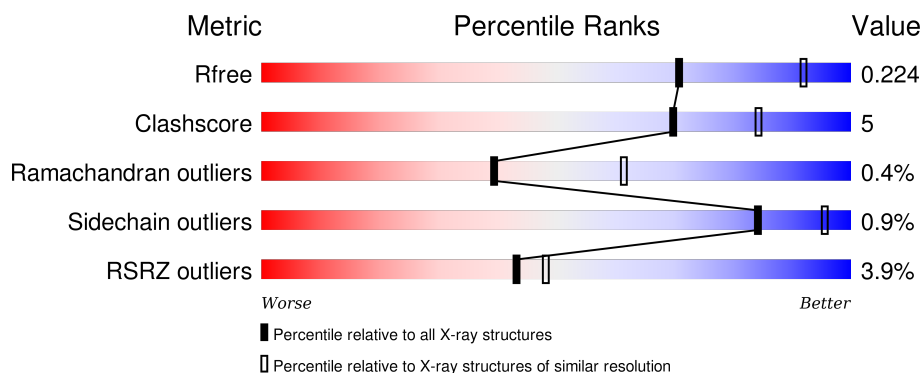
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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






| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 91344                       | 3553 (2.50-2.50)                                      |
| Clashscore            | 102246                      | 4242 (2.50-2.50)                                      |
| Ramachandran outliers | 100387                      | 4156 (2.50-2.50)                                      |
| Sidechain outliers    | 100360                      | 4158 (2.50-2.50)                                      |
| RSRZ outliers         | 91569                       | 3562 (2.50-2.50)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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     | 571    | <div> <div>5%</div> <div>84%</div> <div>12%</div> <div>••</div> </div> |
| 1   | B     | 571    | <div> <div>5%</div> <div>85%</div> <div>11%</div> <div>•</div> </div>  |
| 1   | C     | 571    | <div> <div>4%</div> <div>87%</div> <div>10%</div> <div>•</div> </div>  |
| 1   | D     | 571    | <div> <div>3%</div> <div>85%</div> <div>11%</div> <div>•</div> </div>  |
| 1   | E     | 571    | <div> <div>3%</div> <div>87%</div> <div>9%</div> <div>••</div> </div>  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | F     | 571    |  |
| 1   | G     | 571    |  |
| 1   | H     | 571    |  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 4   | PG4  | A     | 605 | -         | -        | -       | X                |
| 4   | PG4  | A     | 606 | -         | -        | -       | X                |
| 4   | PG4  | A     | 608 | -         | -        | -       | X                |
| 4   | PG4  | B     | 605 | -         | -        | -       | X                |
| 4   | PG4  | B     | 606 | -         | -        | -       | X                |
| 4   | PG4  | B     | 607 | -         | -        | -       | X                |
| 4   | PG4  | C     | 603 | -         | -        | -       | X                |
| 4   | PG4  | C     | 604 | -         | -        | -       | X                |
| 4   | PG4  | C     | 605 | -         | -        | -       | X                |
| 4   | PG4  | D     | 603 | -         | -        | -       | X                |
| 4   | PG4  | D     | 606 | -         | -        | -       | X                |
| 4   | PG4  | D     | 608 | -         | -        | -       | X                |
| 4   | PG4  | E     | 603 | -         | -        | -       | X                |
| 4   | PG4  | E     | 605 | -         | -        | -       | X                |
| 4   | PG4  | E     | 606 | -         | -        | -       | X                |
| 4   | PG4  | E     | 608 | -         | -        | -       | X                |
| 4   | PG4  | F     | 603 | -         | -        | -       | X                |
| 4   | PG4  | F     | 606 | -         | -        | -       | X                |
| 4   | PG4  | F     | 607 | -         | -        | -       | X                |
| 4   | PG4  | G     | 604 | -         | -        | -       | X                |
| 4   | PG4  | G     | 605 | -         | -        | -       | X                |
| 4   | PG4  | G     | 606 | -         | -        | -       | X                |
| 4   | PG4  | H     | 603 | -         | -        | -       | X                |
| 5   | PYR  | F     | 610 | -         | -        | -       | X                |
| 5   | PYR  | G     | 607 | -         | -        | -       | X                |

## 2 Entry composition

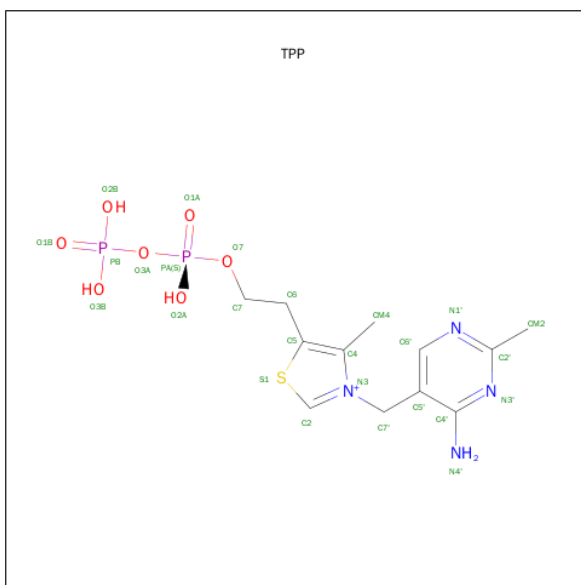
There are 7 unique types of molecules in this entry. The entry contains 35447 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Acetolactate synthase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 552      | Total | C    | N   | O   | S  | 0       | 2       | 0     |
|     |       |          | 4236  | 2688 | 727 | 809 | 12 |         |         |       |
| 1   | B     | 550      | Total | C    | N   | O   | S  | 0       | 4       | 0     |
|     |       |          | 4231  | 2685 | 724 | 810 | 12 |         |         |       |
| 1   | C     | 553      | Total | C    | N   | O   | S  | 0       | 4       | 0     |
|     |       |          | 4257  | 2702 | 730 | 812 | 13 |         |         |       |
| 1   | D     | 550      | Total | C    | N   | O   | S  | 0       | 7       | 0     |
|     |       |          | 4246  | 2702 | 724 | 808 | 12 |         |         |       |
| 1   | E     | 552      | Total | C    | N   | O   | S  | 0       | 4       | 0     |
|     |       |          | 4247  | 2699 | 726 | 810 | 12 |         |         |       |
| 1   | F     | 552      | Total | C    | N   | O   | S  | 0       | 2       | 0     |
|     |       |          | 4239  | 2689 | 729 | 809 | 12 |         |         |       |
| 1   | G     | 553      | Total | C    | N   | O   | S  | 0       | 4       | 0     |
|     |       |          | 4252  | 2697 | 730 | 813 | 12 |         |         |       |
| 1   | H     | 548      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 4201  | 2665 | 723 | 802 | 11 |         |         |       |

- Molecule 2 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C<sub>12</sub>H<sub>19</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).



| Mol | Chain | Residues | Atoms       |         |        |        |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|--------|--------|---------|---------|
| 2   | A     | 1        | Total<br>26 | C<br>12 | N<br>4 | O<br>7 | P<br>2 | S<br>1 | 0       | 0       |
| 2   | B     | 1        | Total<br>26 | C<br>12 | N<br>4 | O<br>7 | P<br>2 | S<br>1 | 0       | 0       |
| 2   | C     | 1        | Total<br>26 | C<br>12 | N<br>4 | O<br>7 | P<br>2 | S<br>1 | 0       | 0       |
| 2   | D     | 1        | Total<br>26 | C<br>12 | N<br>4 | O<br>7 | P<br>2 | S<br>1 | 0       | 0       |
| 2   | E     | 1        | Total<br>26 | C<br>12 | N<br>4 | O<br>7 | P<br>2 | S<br>1 | 0       | 0       |
| 2   | F     | 1        | Total<br>26 | C<br>12 | N<br>4 | O<br>7 | P<br>2 | S<br>1 | 0       | 0       |
| 2   | G     | 1        | Total<br>26 | C<br>12 | N<br>4 | O<br>7 | P<br>2 | S<br>1 | 0       | 0       |

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

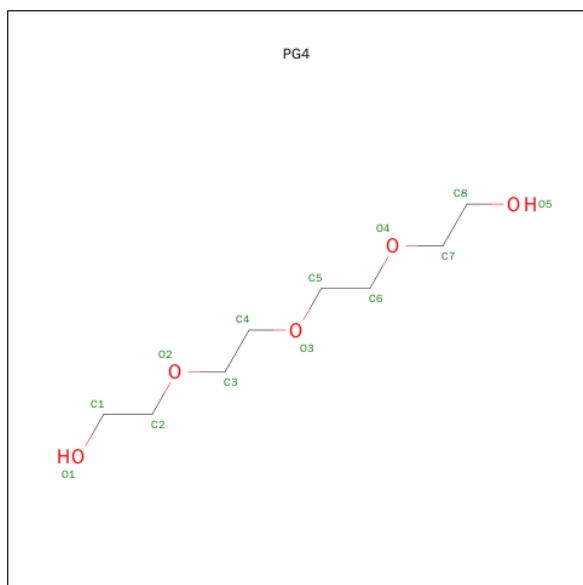
| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 3   | G     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 3   | D     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 3   | E     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 3   | H     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 3   | B     | 1        | Total Mg<br>1 1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | C     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | A     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | F     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 8 | 5 |         |         |
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 8 | 5 |         |         |
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 8 | 5 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 8 | 5 |         |         |
| 4   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 8 | 5 |         |         |
| 4   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 8 | 5 |         |         |
| 4   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 4   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 4   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 7     | 4 | 3 |         |         |
| 4   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 8 | 5 |         |         |
| 4   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 7 | 4 |         |         |
| 4   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 8 | 5 |         |         |
| 4   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 4   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 4   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 7     | 4 | 3 |         |         |
| 4   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 7     | 4 | 3 |         |         |
| 4   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 4   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 8 | 5 |         |         |
| 4   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 5 | 3 |         |         |
| 4   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 8 | 5 |         |         |
| 4   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 5 | 3 |         |         |
| 4   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |

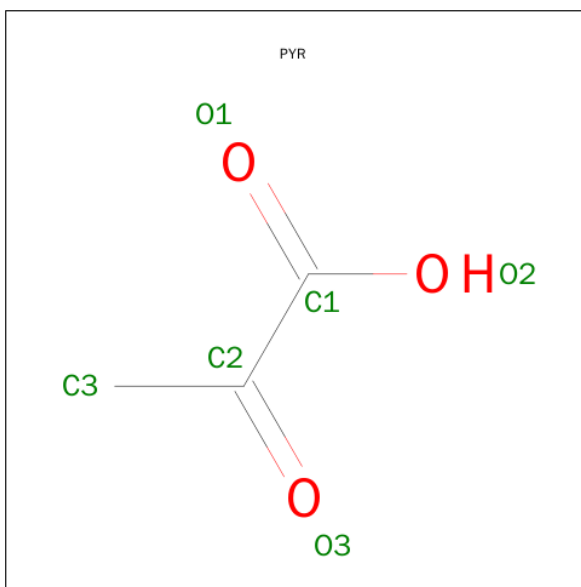
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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 4   | F     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 8 | 5 |         |         |
| 4   | F     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 7     | 4 | 3 |         |         |
| 4   | F     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 4   | F     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 4   | F     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 4   | F     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 8 | 5 |         |         |
| 4   | G     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 4   | G     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 8 | 5 |         |         |
| 4   | G     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 7 | 4 |         |         |
| 4   | G     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 5 | 3 |         |         |
| 4   | H     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 8 | 5 |         |         |
| 4   | H     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 8 | 5 |         |         |

- Molecule 5 is PYRUVIC ACID (three-letter code: PYR) (formula:  $C_3H_4O_3$ ).





| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 5   | F     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 5   | F     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 5   | G     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 5   | G     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 5   | H     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |

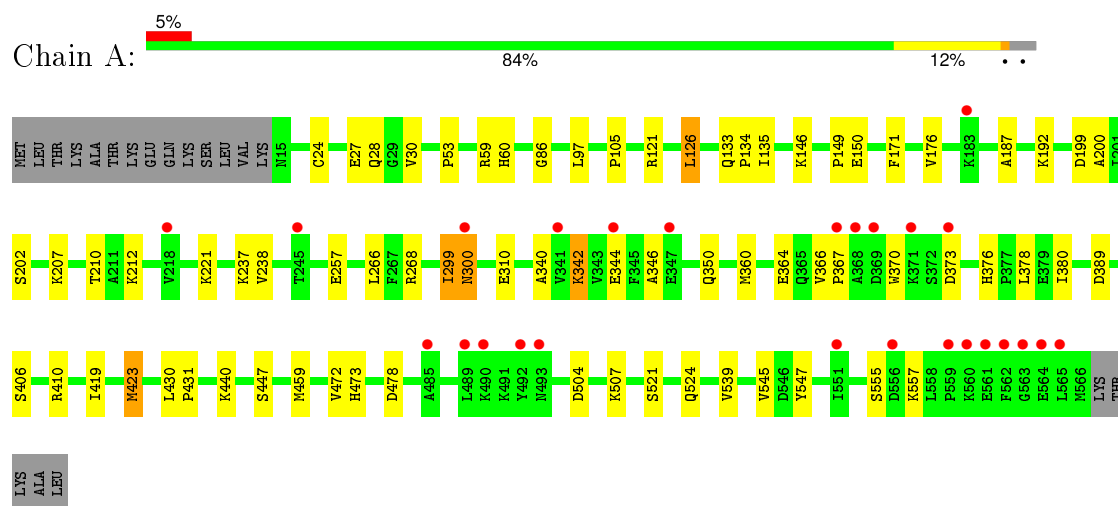
- Molecule 6 is 3-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-2-(1-CARBOXY-1-HYDROXYETHYL)-5-(2-{[HYDROXY(PHOSPHONOOXY)PHOSPHORYL]OXY}ETHYL)-4-METHYL-1,3-THIAZOL-3-IUM (three-letter code: TDL) (formula: C<sub>15</sub>H<sub>23</sub>N<sub>4</sub>O<sub>10</sub>P<sub>2</sub>S).



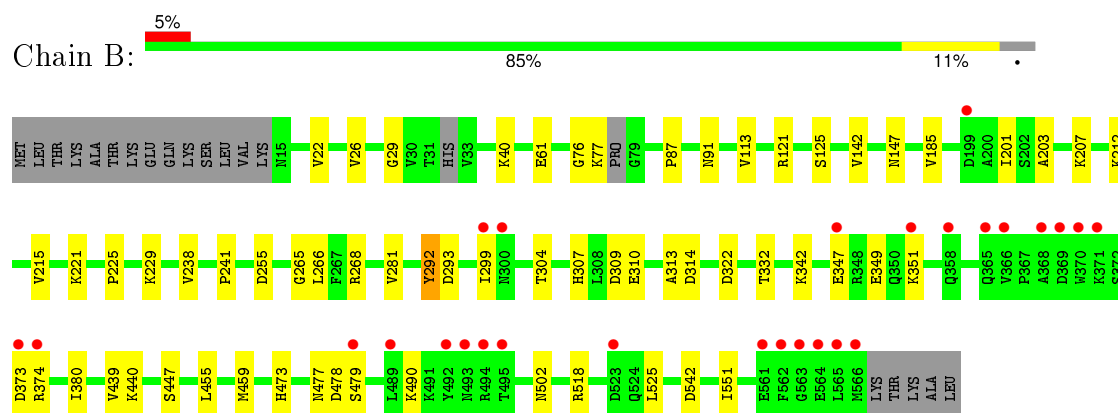
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

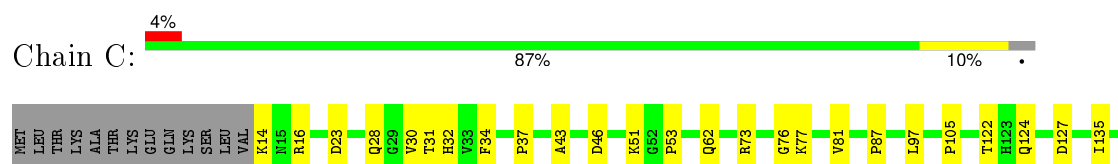
#### • Molecule 1: Acetolactate synthase

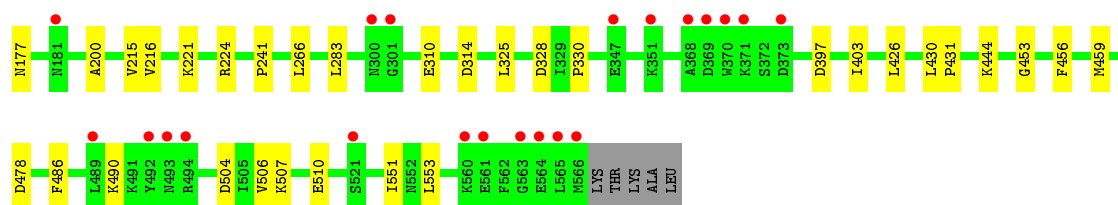


#### • Molecule 1: Acetolactate synthase

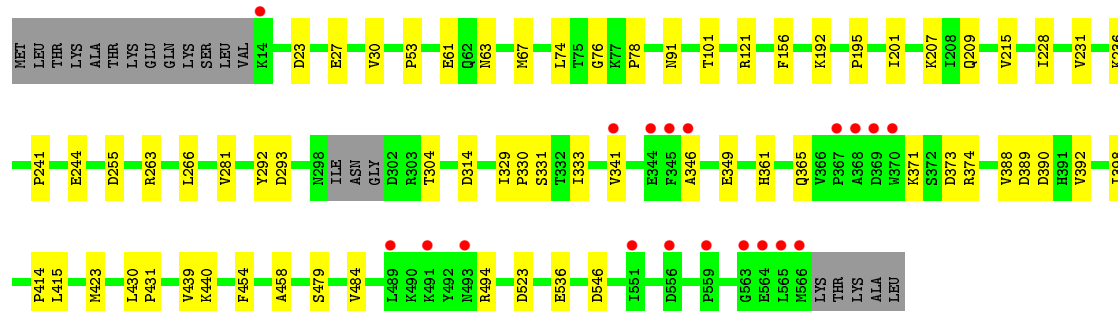
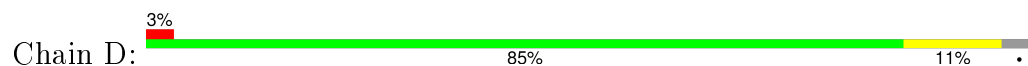


#### • Molecule 1: Acetolactate synthase

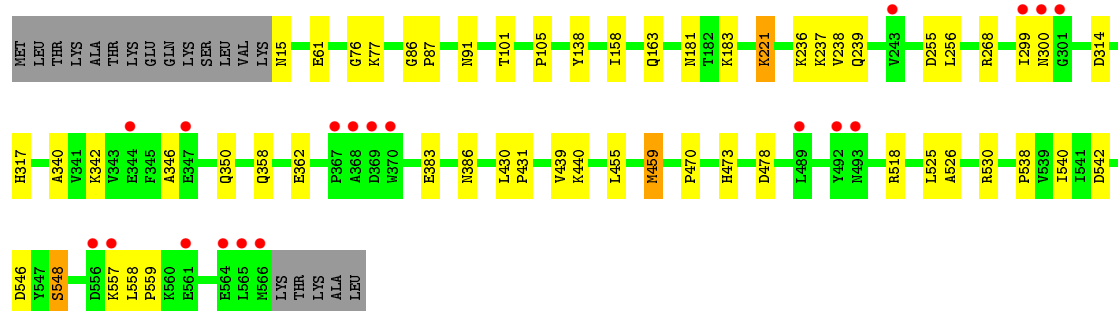
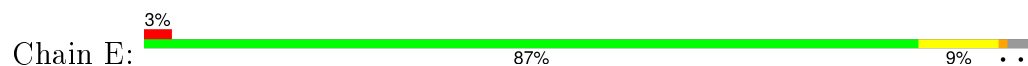




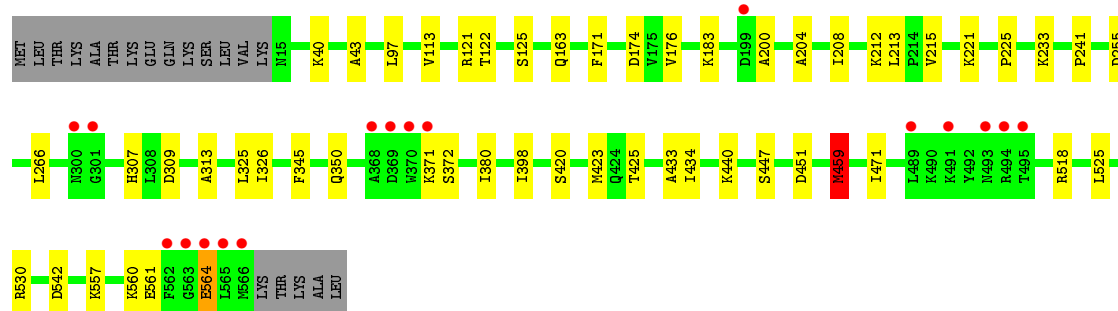
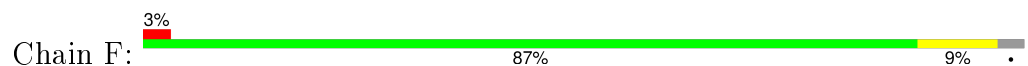
• Molecule 1: Acetolactate synthase



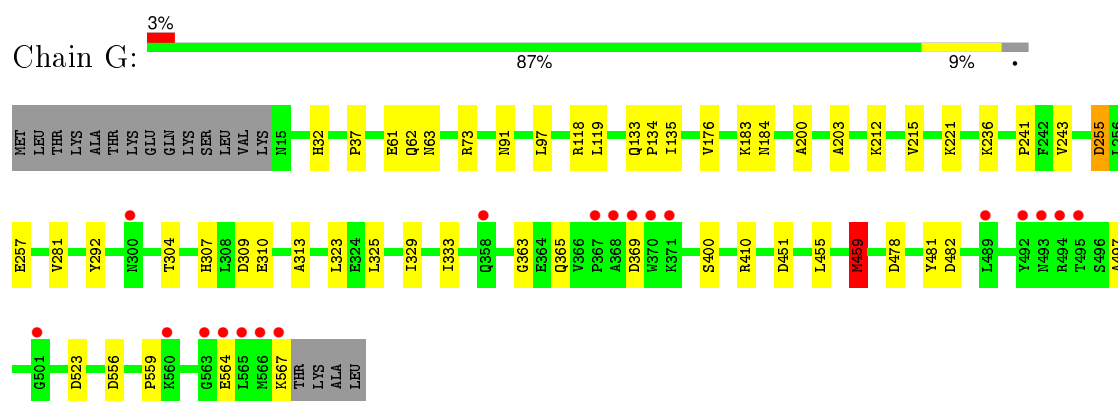
• Molecule 1: Acetolactate synthase



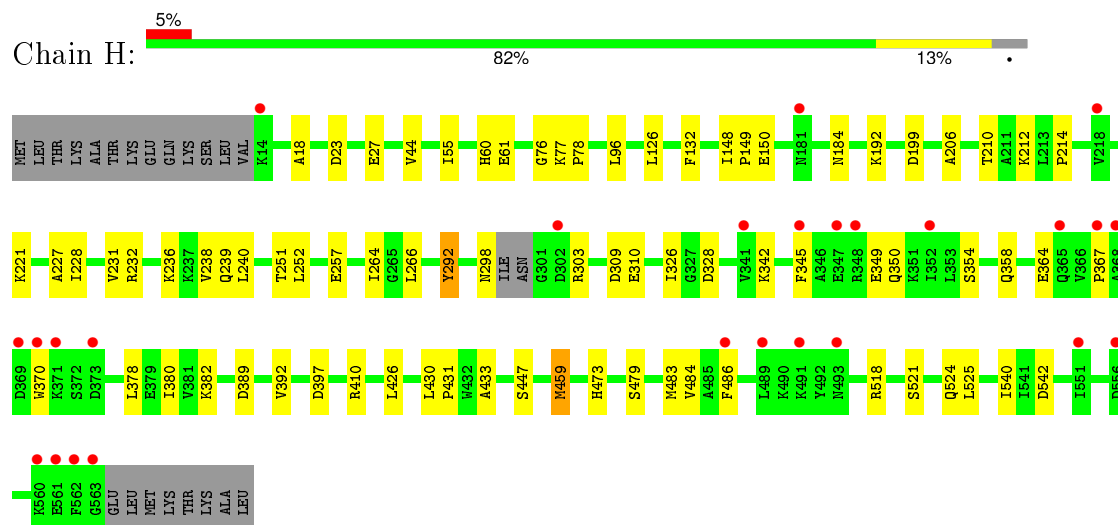
• Molecule 1: Acetolactate synthase



• Molecule 1: Acetolactate synthase



- Molecule 1: Acetolactate synthase



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 2 21   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 111.51Å 170.75Å 342.59Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 30.00 – 2.50<br>30.00 – 2.50                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.9 (30.00-2.50)<br>99.9 (30.00-2.50)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.17 (at 2.51Å)   | Xtriage          |
| Refinement program  | PHENIX (phenix.refine: 1.8.4_1496)                          | Depositor        |
| R, $R_{free}$   | 0.166 , 0.217<br>0.179 , 0.224                              | Depositor<br>DCC |
| $R_{free}$ test set   | 11235 reflections (5.24%)                                   | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 47.7  | Xtriage          |
| Anisotropy  | 0.217   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.37 , 63.6   | EDS              |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$ | Xtriage          |
| Outliers  | 0 of 225450 reflections                                     | Xtriage          |
| $F_o, F_c$ correlation  | 0.96  | EDS              |
| Total number of atoms   | 35447   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 50.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.75 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.6146e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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: PG4, MG, TPP, PYR, TDL

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     | 0.43         | 0/4323      | 0.58        | 1/5880 (0.0%)  |
| 1   | B     | 0.42         | 0/4321      | 0.57        | 0/5873         |
| 1   | C     | 0.43         | 0/4347      | 0.56        | 1/5911 (0.0%)  |
| 1   | D     | 0.44         | 0/4347      | 0.58        | 0/5911         |
| 1   | E     | 0.44         | 0/4340      | 0.58        | 2/5903 (0.0%)  |
| 1   | F     | 0.44         | 0/4327      | 0.58        | 1/5885 (0.0%)  |
| 1   | G     | 0.42         | 0/4345      | 0.57        | 1/5908 (0.0%)  |
| 1   | H     | 0.42         | 0/4284      | 0.57        | 1/5824 (0.0%)  |
| All | All   | 0.43         | 0/34634     | 0.57        | 7/47095 (0.0%) |

There are no bond length outliers.

All (7) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | G     | 459 | MET  | CG-SD-CE | -7.11 | 88.83       | 100.20   |
| 1   | A     | 423 | MET  | CG-SD-CE | -6.46 | 89.86       | 100.20   |
| 1   | E     | 459 | MET  | CA-CB-CG | -6.29 | 102.61      | 113.30   |
| 1   | F     | 459 | MET  | CA-CB-CG | -5.96 | 103.16      | 113.30   |
| 1   | C     | 459 | MET  | CA-CB-CG | -5.92 | 103.24      | 113.30   |
| 1   | H     | 459 | MET  | CA-CB-CG | -5.84 | 103.37      | 113.30   |
| 1   | E     | 459 | MET  | CB-CG-SD | 5.66  | 129.38      | 112.40   |

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     | 4236  | 0        | 4247     | 48      | 0            |
| 1   | B     | 4231  | 0        | 4240     | 39      | 0            |
| 1   | C     | 4257  | 0        | 4275     | 32      | 0            |
| 1   | D     | 4246  | 0        | 4282     | 45      | 0            |
| 1   | E     | 4247  | 0        | 4269     | 37      | 0            |
| 1   | F     | 4239  | 0        | 4245     | 38      | 0            |
| 1   | G     | 4252  | 0        | 4267     | 40      | 0            |
| 1   | H     | 4201  | 0        | 4209     | 44      | 0            |
| 2   | A     | 26    | 0        | 16       | 0       | 0            |
| 2   | B     | 26    | 0        | 16       | 0       | 0            |
| 2   | C     | 26    | 0        | 16       | 3       | 0            |
| 2   | D     | 26    | 0        | 16       | 2       | 0            |
| 2   | E     | 26    | 0        | 16       | 0       | 0            |
| 2   | F     | 26    | 0        | 16       | 1       | 0            |
| 2   | G     | 26    | 0        | 16       | 2       | 0            |
| 3   | A     | 1     | 0        | 0        | 0       | 0            |
| 3   | B     | 1     | 0        | 0        | 0       | 0            |
| 3   | C     | 1     | 0        | 0        | 0       | 0            |
| 3   | D     | 1     | 0        | 0        | 0       | 0            |
| 3   | E     | 1     | 0        | 0        | 0       | 0            |
| 3   | F     | 1     | 0        | 0        | 0       | 0            |
| 3   | G     | 1     | 0        | 0        | 0       | 0            |
| 3   | H     | 1     | 0        | 0        | 0       | 0            |
| 4   | A     | 66    | 0        | 88       | 7       | 0            |
| 4   | B     | 56    | 0        | 75       | 8       | 0            |
| 4   | C     | 53    | 0        | 71       | 4       | 0            |
| 4   | D     | 71    | 0        | 93       | 9       | 0            |
| 4   | E     | 72    | 0        | 92       | 7       | 0            |
| 4   | F     | 63    | 0        | 84       | 6       | 0            |
| 4   | G     | 42    | 0        | 53       | 0       | 0            |
| 4   | H     | 26    | 0        | 36       | 1       | 0            |
| 5   | F     | 12    | 0        | 6        | 0       | 0            |
| 5   | G     | 12    | 0        | 6        | 2       | 0            |
| 5   | H     | 6     | 0        | 3        | 0       | 0            |
| 6   | H     | 32    | 0        | 19       | 3       | 0            |
| 7   | A     | 91    | 0        | 0        | 1       | 0            |
| 7   | B     | 112   | 0        | 0        | 1       | 0            |
| 7   | C     | 117   | 0        | 0        | 1       | 0            |
| 7   | D     | 109   | 0        | 0        | 1       | 0            |
| 7   | E     | 133   | 0        | 0        | 5       | 0            |
| 7   | F     | 119   | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 7   | G     | 96    | 0        | 0        | 2       | 0            |
| 7   | H     | 60    | 0        | 0        | 2       | 0            |
| All | All   | 35447 | 0        | 34772    | 315     | 0            |

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

All (315) 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:D:76:GLY:HA2   | 4:D:607:PG4:H31  | 1.52                     | 0.88              |
| 1:B:76:GLY:HA2   | 4:B:603:PG4:H51  | 1.53                     | 0.87              |
| 1:C:28:GLN:O     | 1:C:77:LYS:NZ    | 2.09                     | 0.85              |
| 1:F:398:ILE:HD11 | 1:F:420:SER:HB3  | 1.63                     | 0.81              |
| 1:H:367:PRO:HG2  | 1:H:370:TRP:HB2  | 1.63                     | 0.80              |
| 1:A:342:LYS:HE3  | 1:A:344:GLU:HG2  | 1.64                     | 0.80              |
| 1:F:225:PRO:HG2  | 4:F:603:PG4:H21  | 1.67                     | 0.77              |
| 1:D:390:ASP:H    | 4:D:603:PG4:H12  | 1.48                     | 0.77              |
| 1:B:477:ASN:HD21 | 1:B:502:ASN:HD21 | 1.33                     | 0.75              |
| 1:G:63:ASN:ND2   | 1:G:459:MET:HE1  | 2.01                     | 0.75              |
| 1:B:322:ASP:HB3  | 4:B:607:PG4:H81  | 1.68                     | 0.74              |
| 1:B:518:ARG:NH1  | 1:B:542:ASP:OD2  | 2.21                     | 0.74              |
| 1:D:192:LYS:NZ   | 7:D:790:HOH:O    | 2.22                     | 0.72              |
| 1:A:207:LYS:HG2  | 4:E:603:PG4:H41  | 1.72                     | 0.71              |
| 1:H:27:GLU:OE2   | 1:H:184:ASN:ND2  | 2.24                     | 0.70              |
| 1:A:299:ILE:HG13 | 1:A:300:ASN:H    | 1.58                     | 0.67              |
| 1:B:373:ASP:OD2  | 1:B:374:ARG:NH1  | 2.28                     | 0.67              |
| 1:F:371:LYS:HD2  | 1:F:372:SER:N    | 2.10                     | 0.67              |
| 1:B:439:VAL:HG12 | 1:B:440:LYS:HG3  | 1.77                     | 0.66              |
| 1:B:40:LYS:NZ    | 7:B:782:HOH:O    | 2.28                     | 0.66              |
| 1:B:490:LYS:HG3  | 1:B:551:ILE:HD11 | 1.78                     | 0.66              |
| 1:D:209:GLN:NE2  | 1:D:341[A]:VAL:H | 1.94                     | 0.65              |
| 1:C:87:PRO:HD3   | 1:D:423:MET:HE3  | 1.77                     | 0.65              |
| 1:D:209:GLN:NE2  | 1:D:341[B]:VAL:H | 1.95                     | 0.65              |
| 1:G:183:LYS:HD2  | 1:G:184:ASN:H    | 1.61                     | 0.65              |
| 1:G:32:HIS:ND1   | 7:G:764:HOH:O    | 2.30                     | 0.64              |
| 1:B:215:VAL:HG12 | 1:B:241:PRO:HG2  | 1.78                     | 0.64              |
| 1:A:268:ARG:CZ   | 1:A:299:ILE:HD11 | 2.27                     | 0.64              |
| 1:C:73:ARG:NH1   | 7:C:761:HOH:O    | 2.31                     | 0.64              |
| 1:E:87:PRO:HD3   | 1:F:423:MET:HG3  | 1.80                     | 0.63              |
| 1:E:76:GLY:HA2   | 4:E:609:PG4:H42  | 1.79                     | 0.63              |

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| Atom-1              | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|------------------|--------------------------|-------------------|
| 1:B:113[A]:VAL:HG21 | 1:B:125:SER:HB2  | 1.81                     | 0.63              |
| 1:B:347:GLU:HG2     | 1:B:351:LYS:HE2  | 1.81                     | 0.62              |
| 1:H:345:PHE:O       | 1:H:350:GLN:NE2  | 2.33                     | 0.62              |
| 1:E:358:GLN:O       | 1:E:362:GLU:HG2  | 1.99                     | 0.62              |
| 1:H:364:GLU:OE2     | 1:H:410:ARG:NH2  | 2.33                     | 0.62              |
| 6:H:601:TDL:OL1     | 6:H:601:TDL:N4'  | 2.31                     | 0.61              |
| 1:B:61:GLU:HB2      | 1:B:91:ASN:HB3   | 1.82                     | 0.61              |
| 1:G:281:VAL:HG22    | 1:G:304:THR:HB   | 1.82                     | 0.61              |
| 1:A:423:MET:HE3     | 1:B:87:PRO:HD3   | 1.83                     | 0.60              |
| 1:A:60:HIS:HB2      | 1:A:459:MET:HE1  | 1.81                     | 0.60              |
| 1:D:207:LYS:HD3     | 4:D:605:PG4:H32  | 1.84                     | 0.59              |
| 1:H:192:LYS:HE2     | 1:H:328:ASP:OD1  | 2.03                     | 0.58              |
| 1:E:105:PRO:HG3     | 4:E:609:PG4:H61  | 1.86                     | 0.58              |
| 1:H:518:ARG:NH1     | 1:H:542:ASP:OD2  | 2.32                     | 0.58              |
| 1:C:490:LYS:HG2     | 1:C:551:ILE:HD11 | 1.86                     | 0.58              |
| 1:E:518:ARG:HD3     | 1:E:542:ASP:OD2  | 2.05                     | 0.57              |
| 1:H:221:LYS:HD2     | 1:H:310:GLU:OE2  | 2.04                     | 0.57              |
| 1:B:447:SER:OG      | 1:B:473:HIS:ND1  | 2.38                     | 0.57              |
| 1:A:504:ASP:OD2     | 1:A:507:LYS:HE2  | 2.05                     | 0.56              |
| 1:E:546:ASP:OD1     | 1:E:548:SER:OG   | 2.21                     | 0.56              |
| 1:G:63:ASN:HD21     | 1:G:459:MET:HE1  | 1.67                     | 0.56              |
| 1:H:150:GLU:OE2     | 7:H:740:HOH:O    | 2.18                     | 0.56              |
| 1:D:281:VAL:HG22    | 1:D:304:THR:HB   | 1.88                     | 0.56              |
| 1:G:37:PRO:HB2      | 1:H:484:VAL:HG11 | 1.87                     | 0.56              |
| 1:H:257:GLU:OE1     | 1:H:410:ARG:NH1  | 2.38                     | 0.56              |
| 4:E:606:PG4:H12     | 1:F:121:ARG:HG2  | 1.87                     | 0.56              |
| 1:F:307:HIS:CD2     | 1:F:313:ALA:HB2  | 2.41                     | 0.56              |
| 1:F:440:LYS:HG2     | 4:F:606:PG4:H21  | 1.87                     | 0.56              |
| 1:E:221:LYS:NZ      | 7:E:728:HOH:O    | 2.40                     | 0.55              |
| 1:E:455:LEU:O       | 1:F:459:MET:HE2  | 2.07                     | 0.55              |
| 1:C:105:PRO:HG3     | 4:C:605:PG4:H21  | 1.88                     | 0.55              |
| 1:F:163:GLN:HG3     | 1:F:221:LYS:HD3  | 1.87                     | 0.55              |
| 1:G:257:GLU:OE2     | 1:G:410:ARG:NH1  | 2.40                     | 0.55              |
| 1:A:150:GLU:OE2     | 7:A:749:HOH:O    | 2.18                     | 0.54              |
| 1:A:367:PRO:HG2     | 1:A:370:TRP:HB2  | 1.90                     | 0.54              |
| 4:D:604:PG4:H81     | 1:E:470:PRO:HB3  | 1.90                     | 0.54              |
| 1:A:210:THR:HB      | 1:E:386:ASN:ND2  | 2.23                     | 0.53              |
| 1:A:221:LYS:HD2     | 1:A:310:GLU:OE1  | 2.08                     | 0.53              |
| 1:G:221:LYS:HD2     | 1:G:310:GLU:OE1  | 2.08                     | 0.53              |
| 1:D:439:VAL:HG12    | 1:D:440:LYS:HG3  | 1.89                     | 0.53              |
| 1:D:373:ASP:N       | 1:D:373:ASP:OD1  | 2.38                     | 0.53              |

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| Atom-1           | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|---------------------|--------------------------|-------------------|
| 1:F:518:ARG:HD3  | 1:F:542:ASP:OD2     | 2.08                     | 0.53              |
| 1:D:536:GLU:HG2  | 4:E:604:PG4:H72     | 1.90                     | 0.53              |
| 1:A:364:GLU:OE2  | 1:A:410:ARG:NH2     | 2.41                     | 0.53              |
| 1:A:440:LYS:HE3  | 4:A:606:PG4:O1      | 2.08                     | 0.53              |
| 1:B:29:GLY:O     | 1:B:77:LYS:NZ       | 2.38                     | 0.53              |
| 1:A:389:ASP:HB2  | 4:A:604:PG4:H12     | 1.90                     | 0.53              |
| 1:C:215:VAL:HG12 | 1:C:241:PRO:HG2     | 1.89                     | 0.53              |
| 1:E:76:GLY:HA2   | 4:E:609:PG4:H62     | 1.91                     | 0.53              |
| 1:H:228:ILE:HG23 | 1:H:251:THR:HA      | 1.91                     | 0.53              |
| 1:H:76:GLY:HA2   | 4:H:604:PG4:H61     | 1.90                     | 0.53              |
| 1:D:195:PRO:HB3  | 1:D:331:SER:HB3     | 1.91                     | 0.52              |
| 1:F:122:THR:HG23 | 1:F:125:SER:HB2     | 1.91                     | 0.52              |
| 1:B:203:ALA:HB1  | 4:B:607:PG4:H41     | 1.91                     | 0.52              |
| 1:A:504:ASP:CG   | 1:A:507:LYS:HG3     | 2.30                     | 0.52              |
| 1:H:264:ILE:HD12 | 1:H:292:TYR:HD2     | 1.75                     | 0.52              |
| 1:D:523:ASP:OD1  | 1:D:523:ASP:N       | 2.40                     | 0.52              |
| 1:B:281:VAL:HG22 | 1:B:304:THR:HB      | 1.92                     | 0.52              |
| 1:E:101:THR:HG22 | 4:E:606:PG4:H22     | 1.92                     | 0.52              |
| 1:G:215:VAL:HG12 | 1:G:241:PRO:HG2     | 1.90                     | 0.52              |
| 1:G:481:TYR:HB3  | 2:G:601:TPP:H61     | 1.92                     | 0.51              |
| 1:H:430:LEU:HB3  | 1:H:431:PRO:HD3     | 1.91                     | 0.51              |
| 1:H:232:ARG:NH2  | 1:H:252:LEU:O       | 2.43                     | 0.51              |
| 1:C:403:ILE:HG21 | 1:C:553:LEU:HD13    | 1.92                     | 0.51              |
| 1:H:236:LYS:O    | 1:H:239[B]:GLN:NE2  | 2.35                     | 0.51              |
| 7:E:784:HOH:O    | 1:F:459:MET:HE3     | 2.11                     | 0.51              |
| 1:E:86:GLY:HA2   | 1:F:423:MET:HE3     | 1.93                     | 0.51              |
| 1:A:380:ILE:HD11 | 1:A:545[B]:VAL:HG12 | 1.91                     | 0.51              |
| 1:G:307:HIS:CD2  | 1:G:313:ALA:HB2     | 2.45                     | 0.51              |
| 1:B:221:LYS:HD3  | 1:B:310:GLU:OE1     | 2.10                     | 0.51              |
| 1:E:163:GLN:OE1  | 1:E:221:LYS:HE3     | 2.11                     | 0.51              |
| 1:D:430:LEU:HB3  | 1:D:431:PRO:HD3     | 1.93                     | 0.51              |
| 1:D:74:LEU:HD23  | 1:D:415:LEU:HB3     | 1.93                     | 0.50              |
| 1:B:201:ILE:HD11 | 1:B:332:THR:HG23    | 1.93                     | 0.50              |
| 1:A:121:ARG:HD3  | 1:B:314:ASP:OD2     | 2.12                     | 0.50              |
| 1:A:238:VAL:HA   | 1:A:342:LYS:HA      | 1.94                     | 0.50              |
| 1:G:97:LEU:HD13  | 1:G:135:ILE:HG22    | 1.94                     | 0.50              |
| 1:A:105:PRO:HG3  | 4:A:603:PG4:H11     | 1.93                     | 0.50              |
| 1:G:63:ASN:ND2   | 1:G:459:MET:CE      | 2.74                     | 0.50              |
| 1:H:309:ASP:O    | 1:H:326:ILE:HA      | 2.12                     | 0.50              |
| 1:A:447:SER:HG   | 1:A:473:HIS:HD1     | 1.60                     | 0.49              |
| 1:F:215:VAL:HG12 | 1:F:241:PRO:HG2     | 1.93                     | 0.49              |

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| Atom-1              | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|------------------|--------------------------|-------------------|
| 1:B:447:SER:HG      | 1:B:473:HIS:HD1  | 1.55                     | 0.49              |
| 1:H:378:LEU:O       | 1:H:382:LYS:HG2  | 2.12                     | 0.49              |
| 1:H:380:ILE:HA      | 1:H:525:LEU:HD21 | 1.95                     | 0.49              |
| 1:D:63:ASN:O        | 1:D:67:MET:HG3   | 2.13                     | 0.49              |
| 1:B:347:GLU:O       | 1:B:351:LYS:HG2  | 2.12                     | 0.49              |
| 1:F:345:PHE:O       | 1:F:350:GLN:NE2  | 2.39                     | 0.49              |
| 4:A:605:PG4:H82     | 4:A:608:PG4:H21  | 1.94                     | 0.49              |
| 1:C:76:GLY:HA2      | 4:C:605:PG4:H31  | 1.94                     | 0.49              |
| 1:E:61:GLU:HB2      | 1:E:91:ASN:HB3   | 1.95                     | 0.49              |
| 1:D:236:LYS:HE2     | 1:D:255:ASP:OD2  | 2.12                     | 0.49              |
| 1:H:238:VAL:HA      | 1:H:342:LYS:HA   | 1.94                     | 0.49              |
| 1:A:521:SER:O       | 1:A:524:GLN:HG2  | 2.13                     | 0.49              |
| 1:A:346:ALA:O       | 1:A:350:GLN:HG3  | 2.13                     | 0.48              |
| 1:A:86:GLY:HA2      | 1:A:126:LEU:HD23 | 1.95                     | 0.48              |
| 1:C:14:LYS:HD2      | 1:C:16:ARG:CZ    | 2.44                     | 0.48              |
| 1:C:221:LYS:HD2     | 1:C:310:GLU:OE1  | 2.13                     | 0.48              |
| 1:B:76:GLY:HA2      | 4:B:603:PG4:H31  | 1.96                     | 0.48              |
| 4:D:603:PG4:H52     | 4:D:603:PG4:H72  | 1.69                     | 0.48              |
| 1:D:101:THR:OG1     | 1:D:423:MET:HG2  | 2.14                     | 0.48              |
| 1:F:233:LYS:HG3     | 4:F:604:PG4:H42  | 1.95                     | 0.48              |
| 1:F:40:LYS:HE2      | 1:F:113:VAL:HG12 | 1.96                     | 0.48              |
| 1:C:506:VAL:O       | 1:C:510:GLU:HG3  | 2.14                     | 0.48              |
| 1:C:46:ASP:OD1      | 1:D:494:ARG:NE   | 2.46                     | 0.48              |
| 1:B:265:GLY:HA2     | 1:B:292:TYR:CD1  | 2.48                     | 0.48              |
| 1:D:209:GLN:HE22    | 1:D:341[A]:VAL:H | 1.61                     | 0.48              |
| 1:E:237:LYS:HE2     | 1:E:340:ALA:O    | 2.14                     | 0.48              |
| 1:A:60:HIS:HB2      | 1:A:459:MET:CE   | 2.43                     | 0.48              |
| 1:F:380:ILE:HA      | 1:F:525:LEU:HD21 | 1.94                     | 0.48              |
| 1:C:87:PRO:HD3      | 1:C:124:GLN:HG2  | 1.96                     | 0.47              |
| 1:C:23:ASP:OD1      | 1:C:51:LYS:NZ    | 2.39                     | 0.47              |
| 1:C:122[B]:THR:HG22 | 1:D:293:ASP:OD1  | 2.15                     | 0.47              |
| 1:H:199:ASP:N       | 1:H:199:ASP:OD1  | 2.39                     | 0.47              |
| 1:D:209:GLN:HE22    | 1:D:341[B]:VAL:H | 1.62                     | 0.47              |
| 1:E:268:ARG:CZ      | 1:E:299:ILE:HD11 | 2.45                     | 0.47              |
| 1:A:555:SER:OG      | 1:A:557:LYS:HG3  | 2.14                     | 0.47              |
| 1:C:37:PRO:HB2      | 1:D:484:VAL:HG11 | 1.96                     | 0.47              |
| 1:F:97:LEU:HD11     | 1:F:423:MET:HE1  | 1.97                     | 0.47              |
| 1:H:227:ALA:O       | 1:H:231:VAL:HG23 | 2.15                     | 0.47              |
| 1:F:561:GLU:O       | 1:F:564:GLU:HB3  | 2.15                     | 0.46              |
| 1:H:521:SER:O       | 1:H:524:GLN:HG2  | 2.15                     | 0.46              |
| 1:G:556:ASP:C       | 1:G:559:PRO:HD2  | 2.36                     | 0.46              |

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| Atom-1              | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|------------------|--------------------------|-------------------|
| 1:F:434:ILE:HA      | 1:F:471:ILE:HD11 | 1.97                     | 0.46              |
| 1:E:346:ALA:O       | 1:E:350:GLN:HG3  | 2.14                     | 0.46              |
| 1:G:309:ASP:OD1     | 1:G:310:GLU:N    | 2.40                     | 0.46              |
| 1:A:30:VAL:O        | 1:A:53:PRO:HB3   | 2.16                     | 0.46              |
| 1:C:453:GLY:O       | 1:C:456:PHE:HB2  | 2.15                     | 0.46              |
| 1:E:538:PRO:HD2     | 7:E:806:HOH:O    | 2.15                     | 0.46              |
| 1:F:233:LYS:NZ      | 4:F:604:PG4:H21  | 2.31                     | 0.46              |
| 1:E:236:LYS:HE2     | 1:E:255:ASP:OD2  | 2.16                     | 0.46              |
| 1:C:34:PHE:O        | 1:C:81:VAL:HA    | 2.15                     | 0.46              |
| 1:G:451:ASP:N       | 1:G:451:ASP:OD1  | 2.47                     | 0.46              |
| 1:A:237:LYS:HE2     | 1:A:340:ALA:O    | 2.16                     | 0.46              |
| 1:A:59:ARG:CZ       | 1:B:455:LEU:HD12 | 2.46                     | 0.46              |
| 1:A:430:LEU:HB3     | 1:A:431:PRO:HD3  | 1.98                     | 0.46              |
| 1:H:212:LYS:O       | 1:H:349:GLU:HG2  | 2.15                     | 0.46              |
| 1:D:371:LYS:HE3     | 1:D:371:LYS:HB2  | 1.72                     | 0.46              |
| 1:F:212:LYS:HG2     | 1:F:213:LEU:N    | 2.31                     | 0.46              |
| 1:A:360:MET:O       | 1:A:364:GLU:HG3  | 2.16                     | 0.45              |
| 1:A:366:VAL:HG22    | 1:A:378:LEU:HB2  | 1.98                     | 0.45              |
| 1:H:483:MET:SD      | 6:H:601:TDL:HLB3 | 2.57                     | 0.45              |
| 1:A:406:SER:OG      | 1:A:419:ILE:HD13 | 2.16                     | 0.45              |
| 1:A:472:VAL:HG13    | 1:A:539:VAL:HG13 | 1.98                     | 0.45              |
| 1:E:459:MET:H       | 1:E:459:MET:HG2  | 1.39                     | 0.45              |
| 1:A:97:LEU:HD13     | 1:A:135:ILE:HG22 | 1.98                     | 0.45              |
| 1:G:400:SER:OG      | 1:G:482:ASP:OD2  | 2.30                     | 0.45              |
| 1:B:309:ASP:OD1     | 1:B:310:GLU:N    | 2.45                     | 0.45              |
| 1:E:473:HIS:HB3     | 1:E:540:ILE:HD13 | 1.99                     | 0.45              |
| 1:E:362:GLU:H       | 1:E:362:GLU:HG2  | 1.56                     | 0.45              |
| 1:C:486:PHE:HB2     | 1:C:551:ILE:HD12 | 1.99                     | 0.45              |
| 1:G:118:ARG:HG3     | 1:G:119:LEU:HD23 | 1.99                     | 0.45              |
| 1:E:238:VAL:HA      | 1:E:342:LYS:HA   | 1.99                     | 0.45              |
| 1:D:23:ASP:O        | 1:D:27:GLU:HG2   | 2.17                     | 0.45              |
| 1:F:371:LYS:C       | 1:F:371:LYS:HD2  | 2.37                     | 0.45              |
| 1:D:215[B]:VAL:HG22 | 1:D:241:PRO:HG2  | 1.97                     | 0.45              |
| 1:E:138:TYR:CD2     | 1:E:158:ILE:HD12 | 2.52                     | 0.45              |
| 4:A:605:PG4:H31     | 1:B:121:ARG:HD2  | 1.98                     | 0.45              |
| 1:G:564:GLU:HA      | 1:G:567:LYS:HZ2  | 1.82                     | 0.45              |
| 1:G:183:LYS:HD2     | 1:G:184:ASN:N    | 2.31                     | 0.45              |
| 1:H:192:LYS:HA      | 1:H:192:LYS:HD2  | 1.60                     | 0.45              |
| 1:F:557:LYS:O       | 1:F:561:GLU:HG3  | 2.17                     | 0.45              |
| 1:H:473:HIS:HB3     | 1:H:540:ILE:HD13 | 1.99                     | 0.45              |
| 1:F:174:ASP:OD1     | 1:F:174:ASP:N    | 2.50                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:23:ASP:HB3   | 1:H:184:ASN:ND2  | 2.32                     | 0.44              |
| 2:D:601:TPP:C2   | 2:D:601:TPP:HN42 | 2.31                     | 0.44              |
| 1:F:530:ARG:HG2  | 1:G:255:ASP:HA   | 1.99                     | 0.44              |
| 1:D:30:VAL:O     | 1:D:53:PRO:HB3   | 2.17                     | 0.44              |
| 1:C:314:ASP:OD2  | 1:D:121:ARG:HD3  | 2.17                     | 0.44              |
| 1:A:171:PHE:HB3  | 1:A:176:VAL:HG13 | 1.99                     | 0.44              |
| 1:E:430:LEU:HB3  | 1:E:431:PRO:HD3  | 1.99                     | 0.44              |
| 1:F:43:ALA:HB3   | 1:F:176:VAL:HG23 | 1.98                     | 0.44              |
| 1:D:244:GLU:O    | 1:D:263:ARG:HA   | 2.17                     | 0.44              |
| 1:F:560:LYS:HD3  | 1:F:560:LYS:HA   | 1.53                     | 0.44              |
| 1:E:439:VAL:HG12 | 1:E:440:LYS:HG3  | 1.98                     | 0.44              |
| 1:G:200:ALA:HB1  | 1:G:325:LEU:HD22 | 1.98                     | 0.44              |
| 4:B:606:PG4:H72  | 4:B:606:PG4:O1   | 2.17                     | 0.44              |
| 1:E:383:GLU:OE2  | 1:E:526:ALA:HB2  | 2.18                     | 0.44              |
| 1:G:133:GLN:HB3  | 1:G:134:PRO:HD3  | 1.99                     | 0.44              |
| 1:D:389:ASP:OD2  | 4:D:603:PG4:H11  | 2.17                     | 0.43              |
| 1:B:440:LYS:HG2  | 4:B:606:PG4:H41  | 1.99                     | 0.43              |
| 1:H:459:MET:H    | 1:H:459:MET:HG2  | 1.29                     | 0.43              |
| 1:G:459:MET:HE3  | 1:G:459:MET:HB2  | 1.42                     | 0.43              |
| 1:G:62:GLN:HE22  | 1:H:60:HIS:HE2   | 1.66                     | 0.43              |
| 1:H:206:ALA:O    | 1:H:210:THR:HG23 | 2.18                     | 0.43              |
| 1:H:214:PRO:HG2  | 1:H:240:LEU:HD22 | 2.01                     | 0.43              |
| 1:C:216:VAL:HG22 | 1:C:283:LEU:HD23 | 1.99                     | 0.43              |
| 1:A:440:LYS:HG2  | 4:A:606:PG4:H52  | 1.99                     | 0.43              |
| 1:B:380:ILE:HA   | 1:B:525:LEU:HD21 | 2.00                     | 0.43              |
| 1:G:63:ASN:HD21  | 1:G:459:MET:CE   | 2.32                     | 0.43              |
| 1:H:426:LEU:HD11 | 6:H:601:TDL:HM43 | 2.01                     | 0.43              |
| 1:D:78:PRO:HG2   | 1:D:156:PHE:CD2  | 2.53                     | 0.43              |
| 1:D:361:HIS:O    | 1:D:365:GLN:HG2  | 2.18                     | 0.43              |
| 1:A:212:LYS:NZ   | 1:E:530:ARG:NH2  | 2.67                     | 0.43              |
| 4:F:605:PG4:H31  | 1:G:236:LYS:HD3  | 2.01                     | 0.43              |
| 1:A:423:MET:HE3  | 1:B:87:PRO:CD    | 2.47                     | 0.43              |
| 1:D:536:GLU:OE2  | 1:E:183:LYS:HE3  | 2.19                     | 0.43              |
| 1:A:257:GLU:OE1  | 1:A:410:ARG:NH1  | 2.52                     | 0.43              |
| 1:A:27:GLU:HB3   | 1:A:187:ALA:HB2  | 2.01                     | 0.43              |
| 1:H:433:ALA:HB2  | 1:H:447:SER:HB3  | 2.01                     | 0.43              |
| 1:F:433:ALA:HB2  | 1:F:447:SER:HB3  | 2.00                     | 0.43              |
| 1:D:454:PHE:O    | 1:D:458:ALA:HB2  | 2.19                     | 0.43              |
| 1:B:225:PRO:O    | 1:B:229:LYS:HD3  | 2.19                     | 0.43              |
| 1:F:309:ASP:O    | 1:F:326:ILE:HA   | 2.18                     | 0.42              |
| 1:D:346:ALA:HB3  | 1:D:349:GLU:OE1  | 2.18                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:459:MET:H    | 1:B:459:MET:HG2  | 1.43                     | 0.42              |
| 2:D:601:TPP:HN42 | 2:D:601:TPP:H2   | 1.83                     | 0.42              |
| 1:C:97:LEU:HD13  | 1:C:135:ILE:HG22 | 2.00                     | 0.42              |
| 1:C:43:ALA:HB2   | 1:C:177:ASN:OD1  | 2.20                     | 0.42              |
| 1:C:504:ASP:OD2  | 1:C:507:LYS:HD2  | 2.19                     | 0.42              |
| 2:C:601:TPP:N1'  | 1:D:61:GLU:OE2   | 2.52                     | 0.42              |
| 1:B:268:ARG:NE   | 1:B:299:ILE:HD11 | 2.35                     | 0.42              |
| 1:F:183:LYS:HD3  | 1:F:183:LYS:HA   | 1.84                     | 0.42              |
| 1:E:268:ARG:NE   | 1:E:299:ILE:HD11 | 2.35                     | 0.42              |
| 1:B:22:VAL:O     | 1:B:26:VAL:HG23  | 2.20                     | 0.42              |
| 1:H:354:SER:O    | 1:H:358:GLN:HG3  | 2.20                     | 0.42              |
| 1:H:298:ASN:OD1  | 1:H:303:ARG:NH2  | 2.52                     | 0.42              |
| 1:G:329:ILE:O    | 1:G:333:ILE:HG13 | 2.20                     | 0.42              |
| 1:H:518:ARG:HD3  | 1:H:542:ASP:OD2  | 2.19                     | 0.42              |
| 4:A:608:PG4:H32  | 4:A:608:PG4:H51  | 1.45                     | 0.42              |
| 1:B:207:LYS:HZ2  | 4:B:607:PG4:H12  | 1.85                     | 0.42              |
| 1:C:30:VAL:O     | 1:C:53:PRO:HB3   | 2.19                     | 0.42              |
| 1:G:203:ALA:HB3  | 1:G:323:LEU:HD21 | 2.00                     | 0.42              |
| 1:C:31:THR:OG1   | 1:C:32:HIS:ND1   | 2.46                     | 0.42              |
| 1:E:256:LEU:HA   | 1:E:256:LEU:HD23 | 1.87                     | 0.42              |
| 1:H:389:ASP:HB3  | 1:H:392:VAL:HG23 | 2.00                     | 0.42              |
| 1:E:314:ASP:OD2  | 1:F:121:ARG:HD3  | 2.20                     | 0.42              |
| 1:H:18:ALA:HB1   | 1:H:44:VAL:HA    | 2.02                     | 0.42              |
| 1:B:142:VAL:HG13 | 1:B:147:ASN:HB3  | 2.01                     | 0.42              |
| 1:A:24:CYS:O     | 1:A:28:GLN:HG2   | 2.20                     | 0.41              |
| 1:D:398:ILE:HD13 | 1:D:398:ILE:HA   | 1.91                     | 0.41              |
| 1:E:77:LYS:HA    | 1:E:77:LYS:HD3   | 1.83                     | 0.41              |
| 1:D:374:ARG:HB2  | 1:D:546:ASP:HB2  | 2.01                     | 0.41              |
| 1:F:171:PHE:HB3  | 1:F:176:VAL:CG1  | 2.50                     | 0.41              |
| 1:G:212:LYS:HE2  | 1:G:212:LYS:HB2  | 1.88                     | 0.41              |
| 1:A:146:LYS:O    | 1:A:149:PRO:HD2  | 2.20                     | 0.41              |
| 1:D:76:GLY:HA2   | 4:D:607:PG4:H12  | 2.02                     | 0.41              |
| 1:A:370:TRP:CE2  | 1:A:376:HIS:HB2  | 2.55                     | 0.41              |
| 2:G:601:TPP:N1'  | 1:H:61:GLU:OE2   | 2.53                     | 0.41              |
| 2:C:601:TPP:HN42 | 2:C:601:TPP:C2   | 2.34                     | 0.41              |
| 1:G:459:MET:HG3  | 1:G:459:MET:H    | 1.03                     | 0.41              |
| 4:F:606:PG4:H12  | 4:F:606:PG4:H32  | 1.75                     | 0.41              |
| 1:B:212:LYS:O    | 1:B:349:GLU:HG2  | 2.21                     | 0.41              |
| 2:F:601:TPP:HN42 | 2:F:601:TPP:C2   | 2.34                     | 0.41              |
| 1:G:455:LEU:HA   | 1:G:455:LEU:HD23 | 1.83                     | 0.41              |
| 1:A:199:ASP:OD1  | 1:A:200:ALA:N    | 2.54                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:61:GLU:HB2   | 1:G:91:ASN:HB3   | 2.03                     | 0.41              |
| 1:G:523:ASP:N    | 1:G:523:ASP:OD1  | 2.51                     | 0.41              |
| 1:F:451:ASP:OD1  | 1:F:451:ASP:N    | 2.54                     | 0.41              |
| 1:A:373:ASP:OD1  | 1:A:373:ASP:N    | 2.51                     | 0.41              |
| 1:G:365:GLN:O    | 5:G:608:PYR:H31  | 2.20                     | 0.41              |
| 1:B:238:VAL:HA   | 1:B:342:LYS:HA   | 2.03                     | 0.41              |
| 1:C:328:ASP:OD2  | 1:C:330:PRO:HD2  | 2.21                     | 0.41              |
| 1:F:204:ALA:O    | 1:F:208:ILE:HG13 | 2.20                     | 0.41              |
| 4:D:606:PG4:H31  | 4:D:606:PG4:H11  | 1.85                     | 0.41              |
| 1:E:558:LEU:HB3  | 1:E:559:PRO:HD3  | 2.03                     | 0.41              |
| 1:F:200:ALA:HB1  | 1:F:325:LEU:HD22 | 2.03                     | 0.41              |
| 1:E:317:HIS:HB2  | 7:E:810:HOH:O    | 2.20                     | 0.41              |
| 1:D:329:ILE:HB   | 1:D:330:PRO:HD3  | 2.02                     | 0.41              |
| 1:E:557:LYS:HG2  | 7:E:762:HOH:O    | 2.20                     | 0.41              |
| 1:H:148:ILE:HB   | 1:H:149:PRO:HD3  | 2.03                     | 0.41              |
| 1:F:423:MET:HB3  | 1:F:425:THR:OG1  | 2.21                     | 0.40              |
| 1:C:224:ARG:HG3  | 4:C:605:PG4:H42  | 2.03                     | 0.40              |
| 1:A:28:GLN:HB2   | 1:A:30:VAL:HG23  | 2.03                     | 0.40              |
| 1:D:228:ILE:HD12 | 1:D:414:PRO:HB3  | 2.03                     | 0.40              |
| 1:G:497:ALA:HB2  | 1:H:55:ILE:HG21  | 2.02                     | 0.40              |
| 1:A:192:LYS:HD3  | 1:A:192:LYS:HA   | 1.89                     | 0.40              |
| 1:D:388:VAL:HG13 | 1:D:392:VAL:HB   | 2.03                     | 0.40              |
| 4:B:603:PG4:H51  | 4:B:603:PG4:H31  | 1.77                     | 0.40              |
| 1:C:444:LYS:HE3  | 4:C:606:PG4:H42  | 2.03                     | 0.40              |
| 1:B:307:HIS:CD2  | 1:B:313:ALA:HB2  | 2.56                     | 0.40              |
| 1:G:459:MET:HG2  | 7:H:730:HOH:O    | 2.21                     | 0.40              |
| 1:C:426:LEU:HD12 | 2:C:601:TPP:C2'  | 2.52                     | 0.40              |
| 1:D:61:GLU:HB2   | 1:D:91:ASN:HB3   | 2.03                     | 0.40              |
| 1:C:200:ALA:HB1  | 1:C:325:LEU:HD22 | 2.02                     | 0.40              |
| 1:C:430:LEU:HB3  | 1:C:431:PRO:HD3  | 2.03                     | 0.40              |
| 1:D:231:VAL:HG23 | 1:D:333:ILE:HD13 | 2.03                     | 0.40              |
| 1:G:369:ASP:OD1  | 1:G:369:ASP:N    | 2.55                     | 0.40              |
| 1:D:440:LYS:HG2  | 4:D:606:PG4:H11  | 2.03                     | 0.40              |
| 1:G:363:GLY:O    | 5:G:608:PYR:H33  | 2.22                     | 0.40              |
| 1:G:73:ARG:NH1   | 7:G:773:HOH:O    | 2.49                     | 0.40              |
| 1:A:133:GLN:HB3  | 1:A:134:PRO:HD3  | 2.04                     | 0.40              |
| 1:H:77:LYS:HA    | 1:H:78:PRO:HD3   | 1.98                     | 0.40              |
| 1:H:96:LEU:HD12  | 1:H:132:PHE:CE1  | 2.57                     | 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     | 552/571 (97%)   | 537 (97%)  | 12 (2%)  | 3 (0%)   | 34          | 55 |
| 1   | B     | 548/571 (96%)   | 530 (97%)  | 16 (3%)  | 2 (0%)   | 39          | 61 |
| 1   | C     | 555/571 (97%)   | 534 (96%)  | 19 (3%)  | 2 (0%)   | 39          | 61 |
| 1   | D     | 553/571 (97%)   | 534 (97%)  | 16 (3%)  | 3 (0%)   | 34          | 55 |
| 1   | E     | 554/571 (97%)   | 538 (97%)  | 15 (3%)  | 1 (0%)   | 52          | 75 |
| 1   | F     | 552/571 (97%)   | 534 (97%)  | 16 (3%)  | 2 (0%)   | 39          | 61 |
| 1   | G     | 555/571 (97%)   | 535 (96%)  | 19 (3%)  | 1 (0%)   | 52          | 75 |
| 1   | H     | 545/571 (95%)   | 531 (97%)  | 11 (2%)  | 3 (1%)   | 30          | 50 |
| All | All   | 4414/4568 (97%) | 4273 (97%) | 124 (3%) | 17 (0%)  | 39          | 61 |

All (17) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 266 | LEU  |
| 1   | D     | 479 | SER  |
| 1   | A     | 300 | ASN  |
| 1   | E     | 300 | ASN  |
| 1   | F     | 564 | GLU  |
| 1   | D     | 292 | TYR  |
| 1   | H     | 292 | TYR  |
| 1   | B     | 266 | LEU  |
| 1   | B     | 292 | TYR  |
| 1   | C     | 266 | LEU  |
| 1   | D     | 266 | LEU  |
| 1   | F     | 266 | LEU  |
| 1   | G     | 292 | TYR  |
| 1   | H     | 266 | LEU  |
| 1   | C     | 127 | ASP  |
| 1   | H     | 126 | LEU  |
| 1   | A     | 299 | ILE  |

### 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     | 453/468 (97%)   | 448 (99%)  | 5 (1%)   | 80          | 94 |
| 1   | B     | 453/468 (97%)   | 448 (99%)  | 5 (1%)   | 80          | 94 |
| 1   | C     | 456/468 (97%)   | 453 (99%)  | 3 (1%)   | 88          | 97 |
| 1   | D     | 457/468 (98%)   | 455 (100%) | 2 (0%)   | 93          | 98 |
| 1   | E     | 455/468 (97%)   | 448 (98%)  | 7 (2%)   | 72          | 91 |
| 1   | F     | 453/468 (97%)   | 451 (100%) | 2 (0%)   | 93          | 98 |
| 1   | G     | 456/468 (97%)   | 451 (99%)  | 5 (1%)   | 80          | 94 |
| 1   | H     | 448/468 (96%)   | 445 (99%)  | 3 (1%)   | 88          | 97 |
| All | All   | 3631/3744 (97%) | 3599 (99%) | 32 (1%)  | 84          | 95 |

All (32) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 126 | LEU  |
| 1   | A     | 202 | SER  |
| 1   | A     | 342 | LYS  |
| 1   | A     | 478 | ASP  |
| 1   | A     | 547 | TYR  |
| 1   | B     | 185 | VAL  |
| 1   | B     | 255 | ASP  |
| 1   | B     | 293 | ASP  |
| 1   | B     | 478 | ASP  |
| 1   | B     | 479 | SER  |
| 1   | C     | 62  | GLN  |
| 1   | C     | 397 | ASP  |
| 1   | C     | 478 | ASP  |
| 1   | D     | 201 | ILE  |
| 1   | D     | 314 | ASP  |
| 1   | E     | 15  | ASN  |
| 1   | E     | 181 | ASN  |
| 1   | E     | 221 | LYS  |
| 1   | E     | 239 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 478 | ASP  |
| 1   | E     | 525 | LEU  |
| 1   | E     | 548 | SER  |
| 1   | F     | 255 | ASP  |
| 1   | F     | 459 | MET  |
| 1   | G     | 176 | VAL  |
| 1   | G     | 243 | VAL  |
| 1   | G     | 255 | ASP  |
| 1   | G     | 459 | MET  |
| 1   | G     | 478 | ASP  |
| 1   | H     | 397 | ASP  |
| 1   | H     | 479 | SER  |
| 1   | H     | 486 | PHE  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 502 | ASN  |
| 1   | C     | 124 | GLN  |
| 1   | D     | 209 | GLN  |
| 1   | E     | 239 | GLN  |
| 1   | F     | 15  | ASN  |
| 1   | G     | 62  | GLN  |
| 1   | G     | 63  | ASN  |
| 1   | G     | 123 | HIS  |
| 1   | H     | 534 | 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 63 ligands modelled in this entry, 8 are monoatomic - leaving 55 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$ |
| 2   | TPP  | A     | 601 | 3    | 20,27,27     | 1.44 | 6 (30%)     | 31,40,40    | 1.78 | 9 (29%)     |
| 4   | PG4  | A     | 603 | -    | 9,9,12       | 0.63 | 0           | 8,8,11      | 0.63 | 0           |
| 4   | PG4  | A     | 604 | -    | 12,12,12     | 0.60 | 0           | 11,11,11    | 1.10 | 2 (18%)     |
| 4   | PG4  | A     | 605 | -    | 9,9,12       | 0.59 | 0           | 8,8,11      | 0.96 | 0           |
| 4   | PG4  | A     | 606 | -    | 9,9,12       | 0.63 | 0           | 8,8,11      | 0.75 | 0           |
| 4   | PG4  | A     | 607 | -    | 12,12,12     | 0.52 | 0           | 11,11,11    | 1.03 | 0           |
| 4   | PG4  | A     | 608 | -    | 9,9,12       | 0.68 | 0           | 8,8,11      | 0.84 | 0           |
| 2   | TPP  | B     | 601 | 3    | 20,27,27     | 1.40 | 5 (25%)     | 31,40,40    | 1.71 | 8 (25%)     |
| 4   | PG4  | B     | 603 | -    | 9,9,12       | 0.77 | 0           | 8,8,11      | 0.85 | 0           |
| 4   | PG4  | B     | 604 | -    | 9,9,12       | 0.52 | 0           | 8,8,11      | 0.77 | 0           |
| 4   | PG4  | B     | 605 | -    | 9,9,12       | 0.52 | 0           | 8,8,11      | 0.88 | 0           |
| 4   | PG4  | B     | 606 | -    | 12,12,12     | 0.60 | 0           | 11,11,11    | 0.90 | 0           |
| 4   | PG4  | B     | 607 | -    | 12,12,12     | 0.66 | 0           | 11,11,11    | 0.69 | 0           |
| 2   | TPP  | C     | 601 | 3    | 20,27,27     | 1.45 | 5 (25%)     | 31,40,40    | 1.87 | 10 (32%)    |
| 4   | PG4  | C     | 603 | -    | 12,12,12     | 0.64 | 0           | 11,11,11    | 0.68 | 0           |
| 4   | PG4  | C     | 604 | -    | 12,12,12     | 0.64 | 0           | 11,11,11    | 0.70 | 0           |
| 4   | PG4  | C     | 605 | -    | 9,9,12       | 0.65 | 0           | 8,8,11      | 0.67 | 0           |
| 4   | PG4  | C     | 606 | -    | 9,9,12       | 0.62 | 0           | 8,8,11      | 0.96 | 0           |
| 4   | PG4  | C     | 607 | -    | 6,6,12       | 0.57 | 0           | 5,5,11      | 0.77 | 0           |
| 2   | TPP  | D     | 601 | 3    | 20,27,27     | 1.45 | 5 (25%)     | 31,40,40    | 1.75 | 10 (32%)    |
| 4   | PG4  | D     | 603 | -    | 12,12,12     | 0.82 | 0           | 11,11,11    | 0.90 | 0           |
| 4   | PG4  | D     | 604 | -    | 10,10,12     | 0.64 | 0           | 9,9,11      | 0.91 | 0           |
| 4   | PG4  | D     | 605 | -    | 12,12,12     | 0.65 | 0           | 11,11,11    | 0.87 | 0           |
| 4   | PG4  | D     | 606 | -    | 9,9,12       | 0.54 | 0           | 8,8,11      | 0.96 | 1 (12%)     |
| 4   | PG4  | D     | 607 | -    | 9,9,12       | 0.67 | 0           | 8,8,11      | 0.77 | 0           |
| 4   | PG4  | D     | 608 | -    | 6,6,12       | 0.59 | 0           | 5,5,11      | 0.67 | 0           |
| 4   | PG4  | D     | 609 | -    | 6,6,12       | 0.61 | 0           | 5,5,11      | 0.67 | 0           |
| 2   | TPP  | E     | 601 | 3    | 20,27,27     | 1.41 | 4 (20%)     | 31,40,40    | 1.80 | 12 (38%)    |
| 4   | PG4  | E     | 603 | -    | 9,9,12       | 0.81 | 0           | 8,8,11      | 1.10 | 0           |
| 4   | PG4  | E     | 604 | -    | 12,12,12     | 0.71 | 0           | 11,11,11    | 0.94 | 1 (9%)      |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | PG4  | E     | 605 | -    | 7,7,12       | 0.59 | 0        | 6,6,11      | 0.69 | 0        |
| 4   | PG4  | E     | 606 | -    | 12,12,12     | 0.55 | 0        | 11,11,11    | 0.94 | 1 (9%)   |
| 4   | PG4  | E     | 607 | -    | 7,7,12       | 0.55 | 0        | 6,6,11      | 0.83 | 0        |
| 4   | PG4  | E     | 608 | -    | 9,9,12       | 0.54 | 0        | 8,8,11      | 1.09 | 2 (25%)  |
| 4   | PG4  | E     | 609 | -    | 9,9,12       | 0.66 | 0        | 8,8,11      | 0.74 | 0        |
| 2   | TPP  | F     | 601 | 3    | 20,27,27     | 1.56 | 5 (25%)  | 31,40,40    | 1.77 | 8 (25%)  |
| 4   | PG4  | F     | 603 | -    | 12,12,12     | 0.68 | 0        | 11,11,11    | 1.00 | 0        |
| 4   | PG4  | F     | 604 | -    | 6,6,12       | 0.49 | 0        | 5,5,11      | 0.75 | 0        |
| 4   | PG4  | F     | 605 | -    | 9,9,12       | 0.52 | 0        | 8,8,11      | 0.85 | 0        |
| 4   | PG4  | F     | 606 | -    | 9,9,12       | 0.64 | 0        | 8,8,11      | 0.90 | 0        |
| 4   | PG4  | F     | 607 | -    | 9,9,12       | 0.48 | 0        | 8,8,11      | 1.16 | 1 (12%)  |
| 4   | PG4  | F     | 608 | -    | 12,12,12     | 0.62 | 0        | 11,11,11    | 0.78 | 0        |
| 5   | PYR  | F     | 609 | -    | 2,5,5        | 1.96 | 1 (50%)  | 2,6,6       | 0.51 | 0        |
| 5   | PYR  | F     | 610 | -    | 2,5,5        | 1.89 | 1 (50%)  | 2,6,6       | 0.36 | 0        |
| 2   | TPP  | G     | 601 | 3    | 20,27,27     | 1.49 | 5 (25%)  | 31,40,40    | 1.79 | 10 (32%) |
| 4   | PG4  | G     | 603 | -    | 9,9,12       | 0.69 | 0        | 8,8,11      | 1.09 | 0        |
| 4   | PG4  | G     | 604 | -    | 12,12,12     | 0.65 | 0        | 11,11,11    | 0.62 | 0        |
| 4   | PG4  | G     | 605 | -    | 10,10,12     | 0.58 | 0        | 9,9,11      | 0.88 | 0        |
| 4   | PG4  | G     | 606 | -    | 7,7,12       | 0.54 | 0        | 6,6,11      | 0.82 | 0        |
| 5   | PYR  | G     | 607 | -    | 2,5,5        | 1.91 | 1 (50%)  | 2,6,6       | 0.07 | 0        |
| 5   | PYR  | G     | 608 | -    | 2,5,5        | 1.87 | 1 (50%)  | 2,6,6       | 0.33 | 0        |
| 6   | TDL  | H     | 601 | 3    | 23,33,33     | 3.26 | 6 (26%)  | 31,51,51    | 1.85 | 8 (25%)  |
| 4   | PG4  | H     | 603 | -    | 12,12,12     | 0.51 | 0        | 11,11,11    | 1.10 | 1 (9%)   |
| 4   | PG4  | H     | 604 | -    | 12,12,12     | 0.69 | 0        | 11,11,11    | 0.76 | 0        |
| 5   | PYR  | H     | 605 | -    | 2,5,5        | 1.80 | 1 (50%)  | 2,6,6       | 0.10 | 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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 2   | TPP  | A     | 601 | 3    | -       | 0/16/17/17 | 0/2/2/2 |
| 4   | PG4  | A     | 603 | -    | -       | 0/7/7/10   | 0/0/0/0 |
| 4   | PG4  | A     | 604 | -    | -       | 0/10/10/10 | 0/0/0/0 |
| 4   | PG4  | A     | 605 | -    | -       | 0/7/7/10   | 0/0/0/0 |
| 4   | PG4  | A     | 606 | -    | -       | 0/7/7/10   | 0/0/0/0 |
| 4   | PG4  | A     | 607 | -    | -       | 0/10/10/10 | 0/0/0/0 |
| 4   | PG4  | A     | 608 | -    | -       | 0/7/7/10   | 0/0/0/0 |
| 2   | TPP  | B     | 601 | 3    | -       | 0/16/17/17 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 4   | PG4  | B     | 603 | -    | -       | 0/7/7/10   | 0/0/0/0 |
| 4   | PG4  | B     | 604 | -    | -       | 0/7/7/10   | 0/0/0/0 |
| 4   | PG4  | B     | 605 | -    | -       | 0/7/7/10   | 0/0/0/0 |
| 4   | PG4  | B     | 606 | -    | -       | 0/10/10/10 | 0/0/0/0 |
| 4   | PG4  | B     | 607 | -    | -       | 0/10/10/10 | 0/0/0/0 |
| 2   | TPP  | C     | 601 | 3    | -       | 0/16/17/17 | 0/2/2/2 |
| 4   | PG4  | C     | 603 | -    | -       | 0/10/10/10 | 0/0/0/0 |
| 4   | PG4  | C     | 604 | -    | -       | 0/10/10/10 | 0/0/0/0 |
| 4   | PG4  | C     | 605 | -    | -       | 0/7/7/10   | 0/0/0/0 |
| 4   | PG4  | C     | 606 | -    | -       | 0/7/7/10   | 0/0/0/0 |
| 4   | PG4  | C     | 607 | -    | -       | 0/4/4/10   | 0/0/0/0 |
| 2   | TPP  | D     | 601 | 3    | -       | 0/16/17/17 | 0/2/2/2 |
| 4   | PG4  | D     | 603 | -    | -       | 0/10/10/10 | 0/0/0/0 |
| 4   | PG4  | D     | 604 | -    | -       | 0/8/8/10   | 0/0/0/0 |
| 4   | PG4  | D     | 605 | -    | -       | 0/10/10/10 | 0/0/0/0 |
| 4   | PG4  | D     | 606 | -    | -       | 0/7/7/10   | 0/0/0/0 |
| 4   | PG4  | D     | 607 | -    | -       | 0/7/7/10   | 0/0/0/0 |
| 4   | PG4  | D     | 608 | -    | -       | 0/4/4/10   | 0/0/0/0 |
| 4   | PG4  | D     | 609 | -    | -       | 0/4/4/10   | 0/0/0/0 |
| 2   | TPP  | E     | 601 | 3    | -       | 0/16/17/17 | 0/2/2/2 |
| 4   | PG4  | E     | 603 | -    | -       | 0/7/7/10   | 0/0/0/0 |
| 4   | PG4  | E     | 604 | -    | -       | 0/10/10/10 | 0/0/0/0 |
| 4   | PG4  | E     | 605 | -    | -       | 0/5/5/10   | 0/0/0/0 |
| 4   | PG4  | E     | 606 | -    | -       | 0/10/10/10 | 0/0/0/0 |
| 4   | PG4  | E     | 607 | -    | -       | 0/5/5/10   | 0/0/0/0 |
| 4   | PG4  | E     | 608 | -    | -       | 0/7/7/10   | 0/0/0/0 |
| 4   | PG4  | E     | 609 | -    | -       | 0/7/7/10   | 0/0/0/0 |
| 2   | TPP  | F     | 601 | 3    | -       | 0/16/17/17 | 0/2/2/2 |
| 4   | PG4  | F     | 603 | -    | -       | 0/10/10/10 | 0/0/0/0 |
| 4   | PG4  | F     | 604 | -    | -       | 0/4/4/10   | 0/0/0/0 |
| 4   | PG4  | F     | 605 | -    | -       | 0/7/7/10   | 0/0/0/0 |
| 4   | PG4  | F     | 606 | -    | -       | 0/7/7/10   | 0/0/0/0 |
| 4   | PG4  | F     | 607 | -    | -       | 0/7/7/10   | 0/0/0/0 |
| 4   | PG4  | F     | 608 | -    | -       | 0/10/10/10 | 0/0/0/0 |
| 5   | PYR  | F     | 609 | -    | -       | 0/0/4/4    | 0/0/0/0 |
| 5   | PYR  | F     | 610 | -    | -       | 0/0/4/4    | 0/0/0/0 |
| 2   | TPP  | G     | 601 | 3    | -       | 0/16/17/17 | 0/2/2/2 |
| 4   | PG4  | G     | 603 | -    | -       | 0/7/7/10   | 0/0/0/0 |
| 4   | PG4  | G     | 604 | -    | -       | 0/10/10/10 | 0/0/0/0 |
| 4   | PG4  | G     | 605 | -    | -       | 0/8/8/10   | 0/0/0/0 |
| 4   | PG4  | G     | 606 | -    | -       | 0/5/5/10   | 0/0/0/0 |
| 5   | PYR  | G     | 607 | -    | -       | 0/0/4/4    | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 5   | PYR  | G     | 608 | -    | -       | 0/0/4/4    | 0/0/0/0 |
| 6   | TDL  | H     | 601 | 3    | -       | 0/16/29/29 | 0/2/2/2 |
| 4   | PG4  | H     | 603 | -    | -       | 0/10/10/10 | 0/0/0/0 |
| 4   | PG4  | H     | 604 | -    | -       | 0/10/10/10 | 0/0/0/0 |
| 5   | PYR  | H     | 605 | -    | -       | 0/0/4/4    | 0/0/0/0 |

All (46) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 6   | H     | 601 | TDL  | C5-S1   | -10.47 | 1.54        | 1.74     |
| 2   | F     | 601 | TPP  | C4-N3   | -3.75  | 1.36        | 1.39     |
| 2   | G     | 601 | TPP  | C4-N3   | -3.26  | 1.36        | 1.39     |
| 2   | B     | 601 | TPP  | C4-N3   | -3.13  | 1.37        | 1.39     |
| 2   | E     | 601 | TPP  | C4-N3   | -3.11  | 1.37        | 1.39     |
| 2   | D     | 601 | TPP  | C4-N3   | -3.06  | 1.37        | 1.39     |
| 6   | H     | 601 | TDL  | OL1-CLA | -2.90  | 1.41        | 1.43     |
| 2   | A     | 601 | TPP  | C4-N3   | -2.86  | 1.37        | 1.39     |
| 2   | C     | 601 | TPP  | C4-N3   | -2.72  | 1.37        | 1.39     |
| 2   | A     | 601 | TPP  | C7'-N3  | -2.02  | 1.45        | 1.48     |
| 2   | B     | 601 | TPP  | C6'-N1' | 2.01   | 1.38        | 1.34     |
| 2   | E     | 601 | TPP  | C6'-N1' | 2.12   | 1.39        | 1.34     |
| 2   | G     | 601 | TPP  | C4'-N3' | 2.13   | 1.38        | 1.35     |
| 2   | E     | 601 | TPP  | C4'-N3' | 2.14   | 1.38        | 1.35     |
| 2   | B     | 601 | TPP  | C2'-N3' | 2.15   | 1.38        | 1.34     |
| 2   | D     | 601 | TPP  | C4'-N3' | 2.19   | 1.38        | 1.35     |
| 2   | A     | 601 | TPP  | C6'-N1' | 2.21   | 1.39        | 1.34     |
| 6   | H     | 601 | TDL  | C7'-C5' | 2.21   | 1.56        | 1.51     |
| 2   | D     | 601 | TPP  | C6'-N1' | 2.21   | 1.39        | 1.34     |
| 2   | B     | 601 | TPP  | C4'-N3' | 2.22   | 1.38        | 1.35     |
| 2   | A     | 601 | TPP  | C2'-N1' | 2.23   | 1.38        | 1.34     |
| 2   | G     | 601 | TPP  | C2'-N3' | 2.27   | 1.38        | 1.34     |
| 2   | C     | 601 | TPP  | C6'-N1' | 2.29   | 1.39        | 1.34     |
| 2   | D     | 601 | TPP  | C2'-N3' | 2.34   | 1.38        | 1.34     |
| 2   | G     | 601 | TPP  | C6'-N1' | 2.35   | 1.39        | 1.34     |
| 2   | B     | 601 | TPP  | C2'-N1' | 2.41   | 1.38        | 1.34     |
| 2   | A     | 601 | TPP  | C4'-N3' | 2.42   | 1.38        | 1.35     |
| 2   | C     | 601 | TPP  | C4'-N3' | 2.44   | 1.38        | 1.35     |
| 2   | F     | 601 | TPP  | C4'-N3' | 2.45   | 1.38        | 1.35     |
| 2   | D     | 601 | TPP  | C2'-N1' | 2.45   | 1.38        | 1.34     |
| 2   | F     | 601 | TPP  | C6'-N1' | 2.45   | 1.39        | 1.34     |
| 2   | F     | 601 | TPP  | C2'-N3' | 2.47   | 1.38        | 1.34     |
| 2   | A     | 601 | TPP  | C2'-N3' | 2.50   | 1.38        | 1.34     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 5   | H     | 605 | PYR  | O3-C2   | 2.53 | 1.31        | 1.22     |
| 5   | F     | 610 | PYR  | O3-C2   | 2.61 | 1.31        | 1.22     |
| 2   | C     | 601 | TPP  | C2'-N3' | 2.61 | 1.39        | 1.34     |
| 5   | G     | 608 | PYR  | O3-C2   | 2.63 | 1.31        | 1.22     |
| 5   | G     | 607 | PYR  | O3-C2   | 2.66 | 1.32        | 1.22     |
| 5   | F     | 609 | PYR  | O3-C2   | 2.68 | 1.32        | 1.22     |
| 2   | C     | 601 | TPP  | C2'-N1' | 2.74 | 1.39        | 1.34     |
| 2   | E     | 601 | TPP  | C2'-N1' | 2.98 | 1.39        | 1.34     |
| 2   | F     | 601 | TPP  | C2'-N1' | 3.04 | 1.39        | 1.34     |
| 2   | G     | 601 | TPP  | C2'-N1' | 3.07 | 1.39        | 1.34     |
| 6   | H     | 601 | TDL  | C4'-N4' | 3.32 | 1.42        | 1.34     |
| 6   | H     | 601 | TDL  | C2-N3   | 4.81 | 1.46        | 1.35     |
| 6   | H     | 601 | TDL  | C4-N3   | 8.75 | 1.58        | 1.39     |

All (84) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | F     | 601 | TPP  | C6-C5-S1    | -3.82 | 114.90      | 120.24   |
| 6   | H     | 601 | TDL  | N1'-C2'-N3' | -3.71 | 118.74      | 125.60   |
| 2   | B     | 601 | TPP  | C6-C5-S1    | -3.66 | 115.11      | 120.24   |
| 2   | G     | 601 | TPP  | C6-C5-S1    | -3.66 | 115.11      | 120.24   |
| 2   | F     | 601 | TPP  | PA-O3A-PB   | -3.56 | 120.72      | 132.67   |
| 2   | A     | 601 | TPP  | N1'-C2'-N3' | -3.47 | 119.19      | 125.60   |
| 2   | C     | 601 | TPP  | CM4-C4-C5   | -3.44 | 121.17      | 128.90   |
| 2   | C     | 601 | TPP  | N1'-C2'-N3' | -3.43 | 119.25      | 125.60   |
| 2   | D     | 601 | TPP  | N1'-C2'-N3' | -3.33 | 119.44      | 125.60   |
| 2   | B     | 601 | TPP  | PA-O3A-PB   | -3.26 | 121.75      | 132.67   |
| 2   | G     | 601 | TPP  | PA-O3A-PB   | -3.08 | 122.34      | 132.67   |
| 2   | D     | 601 | TPP  | C6-C5-S1    | -3.03 | 116.00      | 120.24   |
| 2   | A     | 601 | TPP  | PA-O3A-PB   | -3.00 | 122.60      | 132.67   |
| 2   | B     | 601 | TPP  | N1'-C2'-N3' | -2.98 | 120.08      | 125.60   |
| 2   | G     | 601 | TPP  | N1'-C2'-N3' | -2.90 | 120.23      | 125.60   |
| 2   | E     | 601 | TPP  | C6-C5-S1    | -2.89 | 116.19      | 120.24   |
| 2   | E     | 601 | TPP  | C5'-C7'-N3  | -2.84 | 108.57      | 113.33   |
| 2   | F     | 601 | TPP  | N1'-C2'-N3' | -2.84 | 120.35      | 125.60   |
| 6   | H     | 601 | TDL  | C6-C5-C4    | -2.83 | 125.03      | 127.56   |
| 2   | E     | 601 | TPP  | N1'-C2'-N3' | -2.83 | 120.37      | 125.60   |
| 2   | E     | 601 | TPP  | CM4-C4-C5   | -2.72 | 122.78      | 128.90   |
| 2   | C     | 601 | TPP  | PA-O3A-PB   | -2.55 | 124.11      | 132.67   |
| 2   | A     | 601 | TPP  | CM4-C4-C5   | -2.54 | 123.19      | 128.90   |
| 2   | C     | 601 | TPP  | C5'-C7'-N3  | -2.47 | 109.20      | 113.33   |
| 2   | A     | 601 | TPP  | C6-C5-S1    | -2.44 | 116.82      | 120.24   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | D     | 601 | TPP  | PA-O3A-PB   | -2.32 | 124.88      | 132.67   |
| 2   | E     | 601 | TPP  | PA-O3A-PB   | -2.30 | 124.96      | 132.67   |
| 2   | B     | 601 | TPP  | C5'-C6'-N1' | -2.30 | 119.87      | 123.86   |
| 2   | D     | 601 | TPP  | C5'-C7'-N3  | -2.22 | 109.61      | 113.33   |
| 2   | D     | 601 | TPP  | CM4-C4-C5   | -2.19 | 123.98      | 128.90   |
| 2   | G     | 601 | TPP  | CM4-C4-C5   | -2.15 | 124.08      | 128.90   |
| 2   | G     | 601 | TPP  | C5'-C6'-N1' | -2.13 | 120.16      | 123.86   |
| 2   | F     | 601 | TPP  | C5'-C6'-N1' | -2.08 | 120.25      | 123.86   |
| 2   | E     | 601 | TPP  | C5'-C6'-N1' | -2.05 | 120.30      | 123.86   |
| 2   | C     | 601 | TPP  | C5'-C4'-N4' | -2.01 | 119.30      | 122.25   |
| 6   | H     | 601 | TDL  | PA-O3A-PB   | -2.00 | 125.95      | 132.67   |
| 4   | A     | 604 | PG4  | C5-O3-C4    | 2.00  | 121.92      | 113.31   |
| 2   | D     | 601 | TPP  | O3A-PA-O7   | 2.02  | 108.30      | 102.94   |
| 4   | E     | 604 | PG4  | C3-O2-C2    | 2.09  | 122.28      | 113.31   |
| 4   | A     | 604 | PG4  | C7-O4-C6    | 2.10  | 122.33      | 113.31   |
| 4   | E     | 608 | PG4  | C5-O3-C4    | 2.11  | 122.38      | 113.31   |
| 2   | E     | 601 | TPP  | O2A-PA-O3A  | 2.12  | 114.69      | 105.09   |
| 2   | C     | 601 | TPP  | C6'-C5'-C4' | 2.12  | 118.76      | 115.72   |
| 2   | E     | 601 | TPP  | C6-C5-C4    | 2.15  | 129.50      | 127.56   |
| 4   | E     | 606 | PG4  | C3-O2-C2    | 2.16  | 122.61      | 113.31   |
| 2   | C     | 601 | TPP  | C6'-N1'-C2' | 2.19  | 119.61      | 115.77   |
| 2   | G     | 601 | TPP  | C6'-N1'-C2' | 2.20  | 119.61      | 115.77   |
| 4   | D     | 606 | PG4  | C3-O2-C2    | 2.22  | 122.84      | 113.31   |
| 4   | E     | 608 | PG4  | C3-O2-C2    | 2.22  | 122.85      | 113.31   |
| 2   | D     | 601 | TPP  | C6'-N1'-C2' | 2.22  | 119.65      | 115.77   |
| 2   | E     | 601 | TPP  | C6'-N1'-C2' | 2.26  | 119.71      | 115.77   |
| 2   | A     | 601 | TPP  | C6'-C5'-C4' | 2.27  | 118.97      | 115.72   |
| 2   | E     | 601 | TPP  | C6'-C5'-C4' | 2.28  | 119.00      | 115.72   |
| 2   | G     | 601 | TPP  | CM4-C4-N3   | 2.29  | 125.64      | 122.59   |
| 2   | F     | 601 | TPP  | C6'-C5'-C4' | 2.34  | 119.08      | 115.72   |
| 6   | H     | 601 | TDL  | CM4-C4-N3   | 2.35  | 125.94      | 122.82   |
| 2   | F     | 601 | TPP  | C6'-N1'-C2' | 2.36  | 119.90      | 115.77   |
| 2   | G     | 601 | TPP  | C6'-C5'-C4' | 2.40  | 119.16      | 115.72   |
| 4   | F     | 607 | PG4  | C3-O2-C2    | 2.40  | 123.63      | 113.31   |
| 4   | H     | 603 | PG4  | C7-O4-C6    | 2.41  | 123.67      | 113.31   |
| 2   | D     | 601 | TPP  | C6-C5-C4    | 2.47  | 129.78      | 127.56   |
| 2   | B     | 601 | TPP  | C6'-C5'-C4' | 2.50  | 119.31      | 115.72   |
| 2   | A     | 601 | TPP  | O3A-PA-O7   | 2.53  | 109.65      | 102.94   |
| 2   | D     | 601 | TPP  | CM4-C4-N3   | 2.57  | 126.01      | 122.59   |
| 2   | A     | 601 | TPP  | C6'-N1'-C2' | 2.57  | 120.26      | 115.77   |
| 2   | B     | 601 | TPP  | C6'-N1'-C2' | 2.62  | 120.35      | 115.77   |
| 2   | A     | 601 | TPP  | CM2-C2'-N1' | 2.68  | 120.24      | 117.03   |

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| Mol | Chain | Res | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 2   | B     | 601 | TPP  | CM2-C2'-N1' | 2.72 | 120.29      | 117.03   |
| 2   | C     | 601 | TPP  | N4'-C4'-N3' | 2.73 | 120.90      | 116.95   |
| 6   | H     | 601 | TDL  | O3A-PA-O7   | 3.06 | 111.04      | 102.94   |
| 2   | E     | 601 | TPP  | CM4-C4-N3   | 3.15 | 126.79      | 122.59   |
| 6   | H     | 601 | TDL  | CM2-C2'-N1' | 3.27 | 120.95      | 117.03   |
| 6   | H     | 601 | TDL  | C6'-N1'-C2' | 3.27 | 121.49      | 115.77   |
| 2   | G     | 601 | TPP  | C6-C5-C4    | 3.37 | 130.58      | 127.56   |
| 2   | B     | 601 | TPP  | C6-C5-C4    | 3.50 | 130.71      | 127.56   |
| 2   | A     | 601 | TPP  | CM4-C4-N3   | 3.62 | 127.42      | 122.59   |
| 2   | C     | 601 | TPP  | CM2-C2'-N1' | 3.66 | 121.42      | 117.03   |
| 2   | F     | 601 | TPP  | C6-C5-C4    | 3.66 | 130.84      | 127.56   |
| 2   | F     | 601 | TPP  | CM2-C2'-N1' | 3.78 | 121.57      | 117.03   |
| 2   | D     | 601 | TPP  | CM2-C2'-N1' | 3.83 | 121.62      | 117.03   |
| 2   | G     | 601 | TPP  | CM2-C2'-N1' | 3.89 | 121.70      | 117.03   |
| 6   | H     | 601 | TDL  | C6-C5-S1    | 4.13 | 126.02      | 120.24   |
| 2   | E     | 601 | TPP  | CM2-C2'-N1' | 4.16 | 122.02      | 117.03   |
| 2   | C     | 601 | TPP  | CM4-C4-N3   | 4.21 | 128.21      | 122.59   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

30 monomers are involved in 55 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | A     | 603 | PG4  | 1       | 0            |
| 4   | A     | 604 | PG4  | 1       | 0            |
| 4   | A     | 605 | PG4  | 2       | 0            |
| 4   | A     | 606 | PG4  | 2       | 0            |
| 4   | A     | 608 | PG4  | 2       | 0            |
| 4   | B     | 603 | PG4  | 3       | 0            |
| 4   | B     | 606 | PG4  | 2       | 0            |
| 4   | B     | 607 | PG4  | 3       | 0            |
| 2   | C     | 601 | TPP  | 3       | 0            |
| 4   | C     | 605 | PG4  | 3       | 0            |
| 4   | C     | 606 | PG4  | 1       | 0            |
| 2   | D     | 601 | TPP  | 2       | 0            |
| 4   | D     | 603 | PG4  | 3       | 0            |
| 4   | D     | 604 | PG4  | 1       | 0            |
| 4   | D     | 605 | PG4  | 1       | 0            |
| 4   | D     | 606 | PG4  | 2       | 0            |
| 4   | D     | 607 | PG4  | 2       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | E     | 603 | PG4  | 1       | 0            |
| 4   | E     | 604 | PG4  | 1       | 0            |
| 4   | E     | 606 | PG4  | 2       | 0            |
| 4   | E     | 609 | PG4  | 3       | 0            |
| 2   | F     | 601 | TPP  | 1       | 0            |
| 4   | F     | 603 | PG4  | 1       | 0            |
| 4   | F     | 604 | PG4  | 2       | 0            |
| 4   | F     | 605 | PG4  | 1       | 0            |
| 4   | F     | 606 | PG4  | 2       | 0            |
| 2   | G     | 601 | TPP  | 2       | 0            |
| 5   | G     | 608 | PYR  | 2       | 0            |
| 6   | H     | 601 | TDL  | 3       | 0            |
| 4   | H     | 604 | PG4  | 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2  |    |    | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------|----|----|-----------------------|-------|
| 1   | A     | 552/571 (96%)   | -0.10  | 26 (4%)  | 35 | 40 | 34, 49, 73, 104       | 0     |
| 1   | B     | 550/571 (96%)   | -0.15  | 27 (4%)  | 33 | 38 | 34, 47, 73, 101       | 0     |
| 1   | C     | 553/571 (96%)   | -0.20  | 21 (3%)  | 44 | 49 | 32, 46, 70, 96        | 0     |
| 1   | D     | 550/571 (96%)   | -0.19  | 19 (3%)  | 48 | 53 | 32, 45, 70, 101       | 0     |
| 1   | E     | 552/571 (96%)   | -0.22  | 19 (3%)  | 49 | 54 | 33, 44, 69, 98        | 0     |
| 1   | F     | 552/571 (96%)   | -0.22  | 17 (3%)  | 52 | 57 | 32, 46, 72, 104       | 0     |
| 1   | G     | 553/571 (96%)   | -0.23  | 19 (3%)  | 49 | 54 | 34, 46, 72, 96        | 0     |
| 1   | H     | 548/571 (95%)   | -0.10  | 26 (4%)  | 35 | 40 | 36, 49, 73, 100       | 0     |
| All | All   | 4410/4568 (96%) | -0.17  | 174 (3%) | 43 | 48 | 32, 47, 72, 104       | 0     |

All (174) RSRZ outliers are listed below:

| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | B     | 368    | ALA  | 5.9  |
| 1   | A     | 565    | LEU  | 5.8  |
| 1   | F     | 564    | GLU  | 5.6  |
| 1   | D     | 565    | LEU  | 5.4  |
| 1   | G     | 368    | ALA  | 5.1  |
| 1   | F     | 368    | ALA  | 4.9  |
| 1   | C     | 493[A] | ASN  | 4.8  |
| 1   | F     | 563    | GLY  | 4.8  |
| 1   | G     | 565    | LEU  | 4.8  |
| 1   | C     | 300    | ASN  | 4.7  |
| 1   | E     | 368    | ALA  | 4.6  |
| 1   | A     | 493    | ASN  | 4.5  |
| 1   | G     | 563    | GLY  | 4.5  |
| 1   | F     | 565    | LEU  | 4.4  |
| 1   | D     | 368    | ALA  | 4.4  |
| 1   | A     | 368    | ALA  | 4.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 564 | GLU  | 4.3  |
| 1   | B     | 300 | ASN  | 4.2  |
| 1   | G     | 369 | ASP  | 4.2  |
| 1   | B     | 489 | LEU  | 4.1  |
| 1   | B     | 565 | LEU  | 4.1  |
| 1   | G     | 564 | GLU  | 4.1  |
| 1   | E     | 300 | ASN  | 4.1  |
| 1   | G     | 567 | LYS  | 4.0  |
| 1   | A     | 367 | PRO  | 4.0  |
| 1   | H     | 493 | ASN  | 4.0  |
| 1   | F     | 300 | ASN  | 4.0  |
| 1   | F     | 494 | ARG  | 4.0  |
| 1   | F     | 493 | ASN  | 3.9  |
| 1   | E     | 369 | ASP  | 3.9  |
| 1   | H     | 368 | ALA  | 3.8  |
| 1   | A     | 300 | ASN  | 3.8  |
| 1   | B     | 564 | GLU  | 3.8  |
| 1   | G     | 501 | GLY  | 3.8  |
| 1   | B     | 371 | LYS  | 3.8  |
| 1   | E     | 489 | LEU  | 3.8  |
| 1   | C     | 492 | TYR  | 3.7  |
| 1   | D     | 369 | ASP  | 3.7  |
| 1   | G     | 493 | ASN  | 3.7  |
| 1   | E     | 565 | LEU  | 3.6  |
| 1   | D     | 489 | LEU  | 3.6  |
| 1   | C     | 566 | MET  | 3.6  |
| 1   | F     | 489 | LEU  | 3.6  |
| 1   | G     | 300 | ASN  | 3.6  |
| 1   | F     | 495 | THR  | 3.6  |
| 1   | B     | 369 | ASP  | 3.5  |
| 1   | B     | 562 | PHE  | 3.5  |
| 1   | C     | 368 | ALA  | 3.5  |
| 1   | H     | 370 | TRP  | 3.5  |
| 1   | D     | 493 | ASN  | 3.4  |
| 1   | E     | 564 | GLU  | 3.4  |
| 1   | E     | 493 | ASN  | 3.4  |
| 1   | C     | 564 | GLU  | 3.4  |
| 1   | A     | 564 | GLU  | 3.4  |
| 1   | D     | 367 | PRO  | 3.3  |
| 1   | H     | 369 | ASP  | 3.3  |
| 1   | B     | 492 | TYR  | 3.3  |
| 1   | B     | 493 | ASN  | 3.3  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | C     | 489    | LEU  | 3.2  |
| 1   | C     | 563    | GLY  | 3.2  |
| 1   | E     | 556[A] | ASP  | 3.2  |
| 1   | A     | 560    | LYS  | 3.2  |
| 1   | G     | 370    | TRP  | 3.2  |
| 1   | C     | 369    | ASP  | 3.2  |
| 1   | H     | 562    | PHE  | 3.2  |
| 1   | A     | 369    | ASP  | 3.1  |
| 1   | B     | 494    | ARG  | 3.1  |
| 1   | C     | 494    | ARG  | 3.1  |
| 1   | A     | 347    | GLU  | 3.0  |
| 1   | H     | 489    | LEU  | 3.0  |
| 1   | F     | 199    | ASP  | 2.9  |
| 1   | F     | 369    | ASP  | 2.9  |
| 1   | C     | 181    | ASN  | 2.9  |
| 1   | C     | 565    | LEU  | 2.9  |
| 1   | C     | 373    | ASP  | 2.9  |
| 1   | A     | 344    | GLU  | 2.8  |
| 1   | E     | 561    | GLU  | 2.8  |
| 1   | G     | 492    | TYR  | 2.8  |
| 1   | H     | 302    | ASP  | 2.8  |
| 1   | H     | 345    | PHE  | 2.8  |
| 1   | C     | 370    | TRP  | 2.8  |
| 1   | B     | 365    | GLN  | 2.8  |
| 1   | B     | 347    | GLU  | 2.8  |
| 1   | A     | 489    | LEU  | 2.7  |
| 1   | G     | 495    | THR  | 2.7  |
| 1   | H     | 556    | ASP  | 2.7  |
| 1   | E     | 557    | LYS  | 2.7  |
| 1   | E     | 370    | TRP  | 2.7  |
| 1   | B     | 566    | MET  | 2.7  |
| 1   | A     | 559    | PRO  | 2.7  |
| 1   | D     | 563    | GLY  | 2.7  |
| 1   | E     | 566    | MET  | 2.7  |
| 1   | B     | 370    | TRP  | 2.7  |
| 1   | H     | 14     | LYS  | 2.7  |
| 1   | G     | 566    | MET  | 2.6  |
| 1   | C     | 301    | GLY  | 2.6  |
| 1   | A     | 490    | LYS  | 2.6  |
| 1   | D     | 14     | LYS  | 2.6  |
| 1   | A     | 218    | VAL  | 2.6  |
| 1   | C     | 521    | SER  | 2.6  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | E     | 367    | PRO  | 2.6  |
| 1   | A     | 551    | ILE  | 2.6  |
| 1   | H     | 367    | PRO  | 2.5  |
| 1   | B     | 358    | GLN  | 2.5  |
| 1   | E     | 347    | GLU  | 2.5  |
| 1   | G     | 371    | LYS  | 2.5  |
| 1   | D     | 370    | TRP  | 2.5  |
| 1   | D     | 491    | LYS  | 2.5  |
| 1   | C     | 560    | LYS  | 2.4  |
| 1   | D     | 559    | PRO  | 2.4  |
| 1   | B     | 495    | THR  | 2.4  |
| 1   | C     | 351    | LYS  | 2.4  |
| 1   | C     | 371    | LYS  | 2.4  |
| 1   | F     | 371    | LYS  | 2.4  |
| 1   | A     | 563    | GLY  | 2.4  |
| 1   | F     | 301    | GLY  | 2.4  |
| 1   | E     | 492    | TYR  | 2.4  |
| 1   | E     | 301    | GLY  | 2.4  |
| 1   | A     | 371    | LYS  | 2.4  |
| 1   | A     | 561    | GLU  | 2.4  |
| 1   | H     | 347    | GLU  | 2.4  |
| 1   | H     | 563    | GLY  | 2.4  |
| 1   | A     | 373    | ASP  | 2.4  |
| 1   | D     | 551    | ILE  | 2.4  |
| 1   | E     | 344    | GLU  | 2.4  |
| 1   | A     | 562    | PHE  | 2.3  |
| 1   | H     | 218    | VAL  | 2.3  |
| 1   | H     | 341    | VAL  | 2.3  |
| 1   | B     | 563    | GLY  | 2.3  |
| 1   | D     | 341[A] | VAL  | 2.3  |
| 1   | F     | 566    | MET  | 2.3  |
| 1   | F     | 370    | TRP  | 2.3  |
| 1   | H     | 373    | ASP  | 2.3  |
| 1   | A     | 485    | ALA  | 2.3  |
| 1   | H     | 551    | ILE  | 2.3  |
| 1   | D     | 556[A] | ASP  | 2.3  |
| 1   | B     | 561    | GLU  | 2.2  |
| 1   | A     | 183    | LYS  | 2.2  |
| 1   | H     | 486    | PHE  | 2.2  |
| 1   | C     | 347    | GLU  | 2.2  |
| 1   | E     | 243    | VAL  | 2.2  |
| 1   | B     | 523    | ASP  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 346 | ALA  | 2.2  |
| 1   | H     | 371 | LYS  | 2.2  |
| 1   | A     | 341 | VAL  | 2.2  |
| 1   | A     | 492 | TYR  | 2.2  |
| 1   | C     | 561 | GLU  | 2.2  |
| 1   | H     | 181 | ASN  | 2.2  |
| 1   | D     | 566 | MET  | 2.1  |
| 1   | H     | 560 | LYS  | 2.1  |
| 1   | H     | 365 | GLN  | 2.1  |
| 1   | B     | 374 | ARG  | 2.1  |
| 1   | G     | 494 | ARG  | 2.1  |
| 1   | G     | 367 | PRO  | 2.1  |
| 1   | B     | 351 | LYS  | 2.1  |
| 1   | B     | 366 | VAL  | 2.1  |
| 1   | B     | 373 | ASP  | 2.1  |
| 1   | B     | 299 | ILE  | 2.1  |
| 1   | H     | 491 | LYS  | 2.1  |
| 1   | A     | 556 | ASP  | 2.1  |
| 1   | B     | 479 | SER  | 2.1  |
| 1   | G     | 560 | LYS  | 2.1  |
| 1   | E     | 299 | ILE  | 2.0  |
| 1   | H     | 561 | GLU  | 2.0  |
| 1   | F     | 491 | LYS  | 2.0  |
| 1   | B     | 199 | ASP  | 2.0  |
| 1   | G     | 489 | LEU  | 2.0  |
| 1   | A     | 245 | THR  | 2.0  |
| 1   | D     | 344 | GLU  | 2.0  |
| 1   | G     | 358 | GLN  | 2.0  |
| 1   | H     | 352 | ILE  | 2.0  |
| 1   | H     | 348 | ARG  | 2.0  |
| 1   | D     | 345 | PHE  | 2.0  |
| 1   | F     | 562 | PHE  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|----------------------------|-------|
| 4   | PG4  | A     | 605 | 10/13 | 0.87 | 0.22 | 15.99 | 56,63,70,72                | 0     |
| 4   | PG4  | B     | 606 | 13/13 | 0.82 | 0.37 | 14.18 | 55,66,74,74                | 0     |
| 4   | PG4  | E     | 605 | 8/13  | 0.87 | 0.36 | 11.22 | 59,66,74,78                | 0     |
| 4   | PG4  | C     | 604 | 13/13 | 0.93 | 0.29 | 10.91 | 56,63,71,74                | 0     |
| 4   | PG4  | D     | 606 | 10/13 | 0.89 | 0.34 | 9.26  | 64,71,75,77                | 0     |
| 4   | PG4  | B     | 607 | 13/13 | 0.93 | 0.26 | 8.24  | 50,57,63,65                | 0     |
| 4   | PG4  | A     | 608 | 10/13 | 0.93 | 0.22 | 7.49  | 45,62,72,73                | 0     |
| 4   | PG4  | F     | 606 | 10/13 | 0.87 | 0.26 | 7.15  | 52,65,69,78                | 0     |
| 4   | PG4  | C     | 603 | 13/13 | 0.92 | 0.19 | 6.70  | 52,58,63,65                | 0     |
| 4   | PG4  | E     | 606 | 13/13 | 0.88 | 0.18 | 6.18  | 40,57,64,66                | 0     |
| 4   | PG4  | F     | 603 | 13/13 | 0.88 | 0.17 | 5.20  | 38,50,66,70                | 0     |
| 4   | PG4  | G     | 605 | 11/13 | 0.88 | 0.26 | 5.02  | 64,69,78,78                | 0     |
| 5   | PYR  | F     | 610 | 6/6   | 0.88 | 0.30 | 4.81  | 54,65,75,76                | 0     |
| 4   | PG4  | G     | 604 | 13/13 | 0.95 | 0.24 | 4.30  | 41,57,65,71                | 0     |
| 4   | PG4  | F     | 607 | 10/13 | 0.80 | 0.22 | 4.22  | 51,61,64,66                | 0     |
| 4   | PG4  | H     | 603 | 13/13 | 0.84 | 0.19 | 3.89  | 42,62,69,69                | 0     |
| 4   | PG4  | D     | 603 | 13/13 | 0.92 | 0.17 | 3.87  | 43,52,63,66                | 0     |
| 4   | PG4  | E     | 603 | 10/13 | 0.95 | 0.15 | 3.36  | 45,52,58,60                | 0     |
| 4   | PG4  | E     | 608 | 10/13 | 0.89 | 0.19 | 3.36  | 55,61,67,75                | 0     |
| 4   | PG4  | A     | 606 | 10/13 | 0.83 | 0.29 | 3.32  | 59,69,76,77                | 0     |
| 5   | PYR  | G     | 607 | 6/6   | 0.91 | 0.24 | 2.76  | 53,70,72,72                | 0     |
| 4   | PG4  | B     | 605 | 10/13 | 0.77 | 0.22 | 2.43  | 58,64,73,74                | 0     |
| 4   | PG4  | D     | 608 | 7/13  | 0.92 | 0.14 | 2.34  | 46,48,56,58                | 0     |
| 4   | PG4  | C     | 605 | 10/13 | 0.95 | 0.13 | 2.26  | 35,48,55,56                | 0     |
| 4   | PG4  | G     | 606 | 8/13  | 0.91 | 0.27 | 2.13  | 68,78,81,82                | 0     |
| 4   | PG4  | E     | 604 | 13/13 | 0.91 | 0.21 | 2.00  | 40,53,74,74                | 0     |
| 4   | PG4  | H     | 604 | 13/13 | 0.93 | 0.24 | 1.91  | 48,53,65,73                | 0     |
| 4   | PG4  | D     | 609 | 7/13  | 0.92 | 0.23 | 1.88  | 50,52,67,71                | 0     |
| 4   | PG4  | A     | 603 | 10/13 | 0.94 | 0.19 | 1.87  | 46,56,59,59                | 0     |
| 4   | PG4  | F     | 608 | 13/13 | 0.94 | 0.16 | 1.77  | 48,55,60,64                | 0     |
| 4   | PG4  | E     | 609 | 10/13 | 0.96 | 0.17 | 1.65  | 43,49,54,64                | 0     |
| 4   | PG4  | F     | 604 | 7/13  | 0.85 | 0.16 | 1.54  | 55,60,64,64                | 0     |
| 4   | PG4  | G     | 603 | 10/13 | 0.96 | 0.12 | 1.44  | 36,46,55,66                | 0     |
| 4   | PG4  | B     | 604 | 10/13 | 0.92 | 0.15 | 1.33  | 54,57,65,66                | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|-----------------------------|-------|
| 4   | PG4  | D     | 604 | 11/13 | 0.93 | 0.17 | 1.22  | 47,50,64,65                 | 0     |
| 4   | PG4  | C     | 607 | 7/13  | 0.96 | 0.10 | 1.15  | 46,52,62,62                 | 0     |
| 4   | PG4  | D     | 605 | 13/13 | 0.94 | 0.16 | 1.00  | 54,65,70,74                 | 0     |
| 4   | PG4  | F     | 605 | 10/13 | 0.93 | 0.14 | 0.78  | 48,53,60,63                 | 0     |
| 4   | PG4  | C     | 606 | 10/13 | 0.93 | 0.15 | 0.70  | 55,59,63,66                 | 0     |
| 4   | PG4  | A     | 607 | 13/13 | 0.91 | 0.12 | 0.35  | 50,56,67,67                 | 0     |
| 4   | PG4  | B     | 603 | 10/13 | 0.97 | 0.12 | 0.23  | 43,46,60,63                 | 0     |
| 4   | PG4  | A     | 604 | 13/13 | 0.94 | 0.13 | 0.20  | 52,59,64,66                 | 0     |
| 4   | PG4  | E     | 607 | 8/13  | 0.91 | 0.17 | 0.17  | 62,70,72,73                 | 0     |
| 4   | PG4  | D     | 607 | 10/13 | 0.97 | 0.10 | -0.04 | 42,47,53,58                 | 0     |
| 6   | TDL  | H     | 601 | 32/32 | 0.95 | 0.15 | -0.15 | 38,57,69,72                 | 0     |
| 2   | TPP  | A     | 601 | 26/26 | 0.95 | 0.13 | -0.51 | 42,56,63,66                 | 0     |
| 2   | TPP  | G     | 601 | 26/26 | 0.97 | 0.12 | -0.71 | 37,49,60,63                 | 0     |
| 2   | TPP  | E     | 601 | 26/26 | 0.97 | 0.13 | -0.73 | 39,54,59,62                 | 0     |
| 2   | TPP  | D     | 601 | 26/26 | 0.96 | 0.13 | -0.85 | 29,52,62,64                 | 0     |
| 5   | PYR  | G     | 608 | 6/6   | 0.95 | 0.11 | -0.88 | 65,72,75,77                 | 0     |
| 2   | TPP  | B     | 601 | 26/26 | 0.97 | 0.12 | -0.98 | 42,55,64,66                 | 0     |
| 3   | MG   | C     | 602 | 1/1   | 0.97 | 0.12 | -0.99 | 54,54,54,54                 | 0     |
| 2   | TPP  | C     | 601 | 26/26 | 0.97 | 0.12 | -1.06 | 38,50,59,60                 | 0     |
| 2   | TPP  | F     | 601 | 26/26 | 0.97 | 0.12 | -1.15 | 42,51,59,60                 | 0     |
| 3   | MG   | B     | 602 | 1/1   | 0.97 | 0.10 | -1.36 | 57,57,57,57                 | 0     |
| 3   | MG   | G     | 602 | 1/1   | 0.97 | 0.09 | -1.80 | 49,49,49,49                 | 0     |
| 3   | MG   | D     | 602 | 1/1   | 0.99 | 0.11 | -1.91 | 50,50,50,50                 | 0     |
| 3   | MG   | H     | 602 | 1/1   | 0.98 | 0.08 | -2.21 | 55,55,55,55                 | 0     |
| 3   | MG   | F     | 602 | 1/1   | 0.99 | 0.07 | -2.26 | 53,53,53,53                 | 0     |
| 3   | MG   | E     | 602 | 1/1   | 0.94 | 0.03 | -3.89 | 59,59,59,59                 | 0     |
| 3   | MG   | A     | 602 | 1/1   | 0.94 | 0.05 | -5.56 | 56,56,56,56                 | 0     |
| 5   | PYR  | H     | 605 | 6/6   | 0.92 | 0.39 | -     | 75,83,84,85                 | 0     |
| 5   | PYR  | F     | 609 | 6/6   | 0.71 | 0.40 | -     | 63,67,72,75                 | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.