



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:39 AM GMT

PDB ID : 1RCX  
Title : NON-ACTIVATED SPINACH RUBISCO IN COMPLEX WITH ITS SUB-  
STRATE RIBULOSE-1,5-BISPHOSPHATE  
Authors : Taylor, T.C.; Andersson, I.  
Deposited on : 1996-12-06  
Resolution : 2.40 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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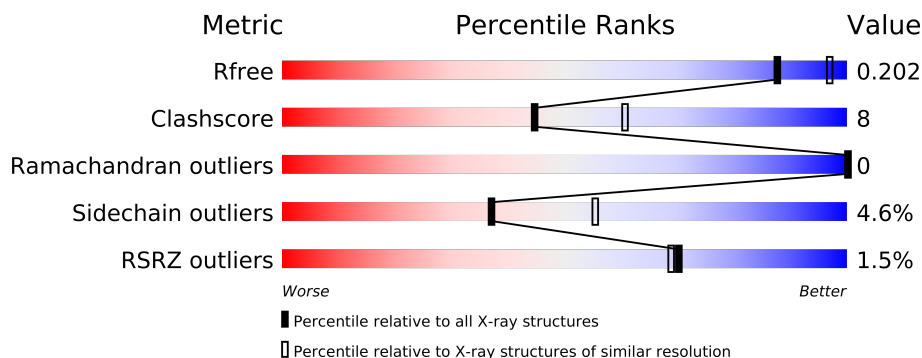
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.40 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 66092                       | 2207 (2.40-2.40)                                      |
| Clashscore            | 79885                       | 2789 (2.40-2.40)                                      |
| Ramachandran outliers | 78287                       | 2736 (2.40-2.40)                                      |
| Sidechain outliers    | 78261                       | 2737 (2.40-2.40)                                      |
| RSRZ outliers         | 66119                       | 2210 (2.40-2.40)                                      |

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | B     | 475    |                  |
| 1   | E     | 475    |                  |
| 1   | H     | 475    |                  |
| 1   | K     | 475    |                  |
| 1   | L     | 475    |                  |
| 1   | O     | 475    |                  |
| 1   | R     | 475    |                  |
| 1   | V     | 475    |                  |
| 2   | C     | 123    |                  |
| 2   | F     | 123    |                  |
| 2   | I     | 123    |                  |
| 2   | M     | 123    |                  |
| 2   | P     | 123    |                  |
| 2   | S     | 123    |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 2   | T     | 123    |  |
| 2   | W     | 123    |  |

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Geometry | Electron density |
|-----|------|-------|-----|----------|------------------|
| 3   | RUB  | B     | 476 | -        | X                |
| 3   | RUB  | E     | 476 | -        | X                |
| 3   | RUB  | H     | 476 | -        | X                |
| 3   | RUB  | K     | 476 | -        | X                |
| 3   | RUB  | L     | 476 | -        | X                |
| 3   | RUB  | O     | 476 | -        | X                |
| 3   | RUB  | R     | 476 | -        | X                |
| 3   | RUB  | V     | 476 | -        | X                |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 39368 atoms, of which 0 are hydrogen and 0 are deuterium.

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 RIBULOSE BISPHOSPHATE CARBOXYLASE/OXYGEN ASE.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | L     | 467      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3649  | 2315 | 640 | 676 | 18 |         |         |       |
| 1   | B     | 467      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3649  | 2315 | 640 | 676 | 18 |         |         |       |
| 1   | E     | 467      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3649  | 2315 | 640 | 676 | 18 |         |         |       |
| 1   | H     | 467      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3649  | 2315 | 640 | 676 | 18 |         |         |       |
| 1   | K     | 467      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3649  | 2315 | 640 | 676 | 18 |         |         |       |
| 1   | O     | 467      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3649  | 2315 | 640 | 676 | 18 |         |         |       |
| 1   | R     | 467      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3649  | 2315 | 640 | 676 | 18 |         |         |       |
| 1   | V     | 467      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3649  | 2315 | 640 | 676 | 18 |         |         |       |

- Molecule 2 is a protein called RIBULOSE BISPHOSPHATE CARBOXYLASE/OXYGEN ASE.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | S     | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1033  | 673 | 167 | 186 | 7 |         |         |       |
| 2   | C     | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1033  | 673 | 167 | 186 | 7 |         |         |       |
| 2   | F     | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1033  | 673 | 167 | 186 | 7 |         |         |       |
| 2   | I     | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1033  | 673 | 167 | 186 | 7 |         |         |       |
| 2   | M     | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1033  | 673 | 167 | 186 | 7 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | P     | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1033  | 673 | 167 | 186 | 7 |         |         |       |
| 2   | T     | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1033  | 673 | 167 | 186 | 7 |         |         |       |
| 2   | W     | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1033  | 673 | 167 | 186 | 7 |         |         |       |

There are 56 discrepancies between the modelled and reference sequences:

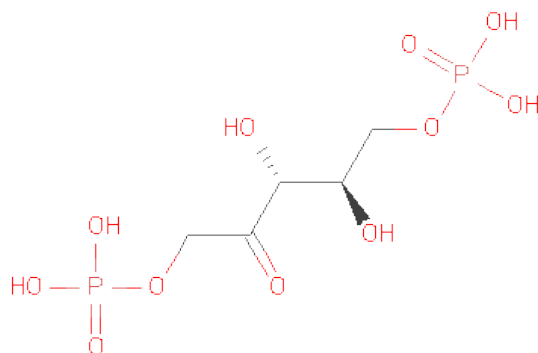
| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| S     | 2       | GLN      | LYS    | CONFLICT | UNP P00870 |
| S     | 6       | ILE      | THR    | CONFLICT | UNP P00870 |
| S     | 7       | LEU      | GLN    | CONFLICT | UNP P00870 |
| S     | 9       | LEU      | MET    | CONFLICT | UNP P00870 |
| S     | 11      | LYS      | ARG    | CONFLICT | UNP P00870 |
| S     | 109     | GLU      | GLN    | CONFLICT | UNP P00870 |
| S     | 113     | ILE      | VAL    | CONFLICT | UNP P00870 |
| C     | 2       | GLN      | LYS    | CONFLICT | UNP P00870 |
| C     | 6       | ILE      | THR    | CONFLICT | UNP P00870 |
| C     | 7       | LEU      | GLN    | CONFLICT | UNP P00870 |
| C     | 9       | LEU      | MET    | CONFLICT | UNP P00870 |
| C     | 11      | LYS      | ARG    | CONFLICT | UNP P00870 |
| C     | 109     | GLU      | GLN    | CONFLICT | UNP P00870 |
| C     | 113     | ILE      | VAL    | CONFLICT | UNP P00870 |
| F     | 2       | GLN      | LYS    | CONFLICT | UNP P00870 |
| F     | 6       | ILE      | THR    | CONFLICT | UNP P00870 |
| F     | 7       | LEU      | GLN    | CONFLICT | UNP P00870 |
| F     | 9       | LEU      | MET    | CONFLICT | UNP P00870 |
| F     | 11      | LYS      | ARG    | CONFLICT | UNP P00870 |
| F     | 109     | GLU      | GLN    | CONFLICT | UNP P00870 |
| F     | 113     | ILE      | VAL    | CONFLICT | UNP P00870 |
| I     | 2       | GLN      | LYS    | CONFLICT | UNP P00870 |
| I     | 6       | ILE      | THR    | CONFLICT | UNP P00870 |
| I     | 7       | LEU      | GLN    | CONFLICT | UNP P00870 |
| I     | 9       | LEU      | MET    | CONFLICT | UNP P00870 |
| I     | 11      | LYS      | ARG    | CONFLICT | UNP P00870 |
| I     | 109     | GLU      | GLN    | CONFLICT | UNP P00870 |
| I     | 113     | ILE      | VAL    | CONFLICT | UNP P00870 |
| M     | 2       | GLN      | LYS    | CONFLICT | UNP P00870 |
| M     | 6       | ILE      | THR    | CONFLICT | UNP P00870 |
| M     | 7       | LEU      | GLN    | CONFLICT | UNP P00870 |
| M     | 9       | LEU      | MET    | CONFLICT | UNP P00870 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| M     | 11      | LYS      | ARG    | CONFLICT | UNP P00870 |
| M     | 109     | GLU      | GLN    | CONFLICT | UNP P00870 |
| M     | 113     | ILE      | VAL    | CONFLICT | UNP P00870 |
| P     | 2       | GLN      | LYS    | CONFLICT | UNP P00870 |
| P     | 6       | ILE      | THR    | CONFLICT | UNP P00870 |
| P     | 7       | LEU      | GLN    | CONFLICT | UNP P00870 |
| P     | 9       | LEU      | MET    | CONFLICT | UNP P00870 |
| P     | 11      | LYS      | ARG    | CONFLICT | UNP P00870 |
| P     | 109     | GLU      | GLN    | CONFLICT | UNP P00870 |
| P     | 113     | ILE      | VAL    | CONFLICT | UNP P00870 |
| T     | 2       | GLN      | LYS    | CONFLICT | UNP P00870 |
| T     | 6       | ILE      | THR    | CONFLICT | UNP P00870 |
| T     | 7       | LEU      | GLN    | CONFLICT | UNP P00870 |
| T     | 9       | LEU      | MET    | CONFLICT | UNP P00870 |
| T     | 11      | LYS      | ARG    | CONFLICT | UNP P00870 |
| T     | 109     | GLU      | GLN    | CONFLICT | UNP P00870 |
| T     | 113     | ILE      | VAL    | CONFLICT | UNP P00870 |
| W     | 2       | GLN      | LYS    | CONFLICT | UNP P00870 |
| W     | 6       | ILE      | THR    | CONFLICT | UNP P00870 |
| W     | 7       | LEU      | GLN    | CONFLICT | UNP P00870 |
| W     | 9       | LEU      | MET    | CONFLICT | UNP P00870 |
| W     | 11      | LYS      | ARG    | CONFLICT | UNP P00870 |
| W     | 109     | GLU      | GLN    | CONFLICT | UNP P00870 |
| W     | 113     | ILE      | VAL    | CONFLICT | UNP P00870 |

- Molecule 3 is SUGAR (RIBULOSE-1,5-DIPHOSPHATE) (three-letter code: RUB) (formula:  $C_5H_{12}O_{11}P_2$ ).



| Mol | Chain | Residues | Atoms                    | ZeroOcc | AltConf |
|-----|-------|----------|--------------------------|---------|---------|
| 3   | L     | 1        | Total C O P<br>18 5 11 2 | 0       | 0       |
| 3   | B     | 1        | Total C O P<br>18 5 11 2 | 0       | 0       |
| 3   | E     | 1        | Total C O P<br>18 5 11 2 | 0       | 0       |
| 3   | H     | 1        | Total C O P<br>18 5 11 2 | 0       | 0       |
| 3   | K     | 1        | Total C O P<br>18 5 11 2 | 0       | 0       |
| 3   | O     | 1        | Total C O P<br>18 5 11 2 | 0       | 0       |
| 3   | R     | 1        | Total C O P<br>18 5 11 2 | 0       | 0       |
| 3   | V     | 1        | Total C O P<br>18 5 11 2 | 0       | 0       |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 4   | B     | 174      | Total O<br>174 174 | 0       | 0       |
| 4   | C     | 48       | Total O<br>48 48   | 0       | 0       |
| 4   | E     | 175      | Total O<br>175 175 | 0       | 0       |
| 4   | F     | 46       | Total O<br>46 46   | 0       | 0       |
| 4   | H     | 173      | Total O<br>173 173 | 0       | 0       |
| 4   | I     | 48       | Total O<br>48 48   | 0       | 0       |
| 4   | K     | 175      | Total O<br>175 175 | 0       | 0       |
| 4   | L     | 173      | Total O<br>173 173 | 0       | 0       |
| 4   | M     | 48       | Total O<br>48 48   | 0       | 0       |
| 4   | O     | 172      | Total O<br>172 172 | 0       | 0       |
| 4   | P     | 46       | Total O<br>46 46   | 0       | 0       |
| 4   | R     | 171      | Total O<br>171 171 | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 4   | S     | 52       | Total<br>52  | O<br>52  | 0       | 0       |
| 4   | T     | 48       | Total<br>48  | O<br>48  | 0       | 0       |
| 4   | V     | 171      | Total<br>171 | O<br>171 | 0       | 0       |
| 4   | W     | 48       | Total<br>48  | O<br>48  | 0       | 0       |

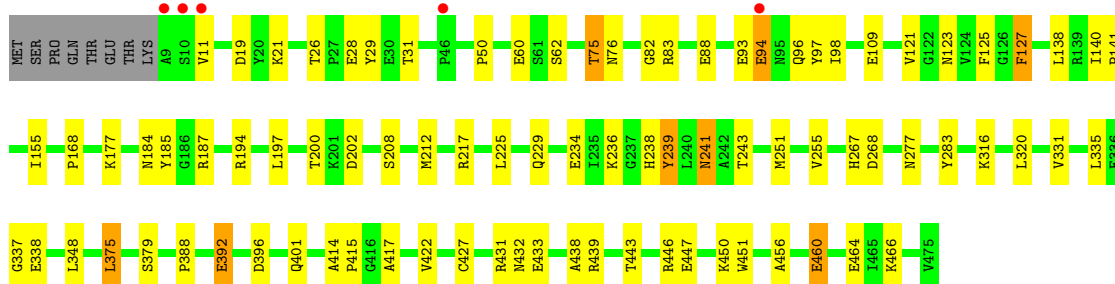


### 3 Residue-property plots

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.

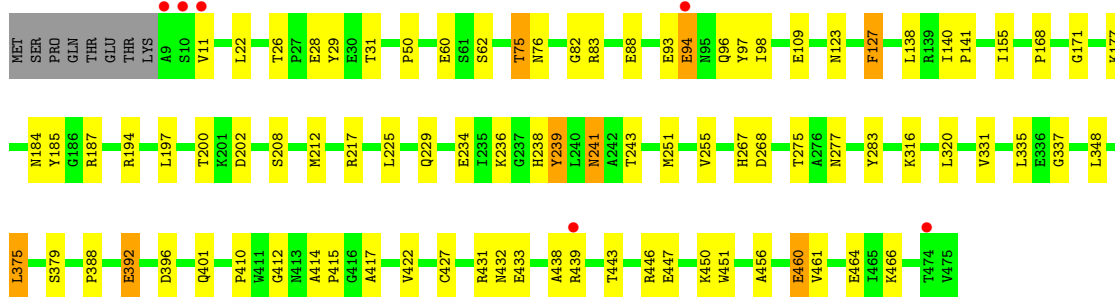
#### • Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE/OXYGENASE

Chain L: 



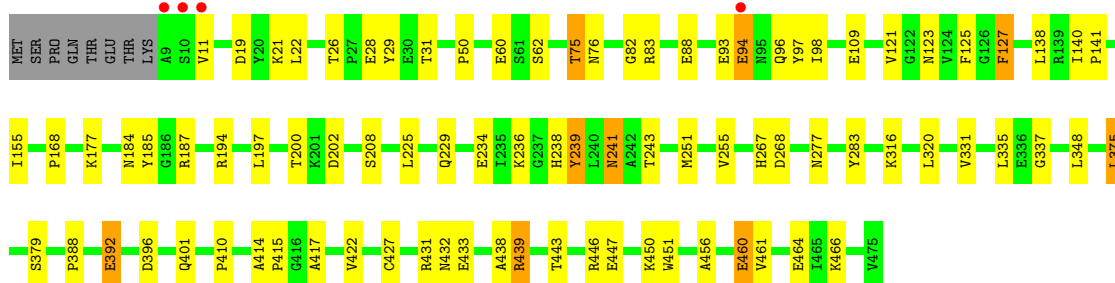
#### • Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE/OXYGENASE

Chain B: 



#### • Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE/OXYGENASE

Chain E: 



#### • Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE/OXYGENASE



| Age Group | Percentage |
|-----------|------------|
| 18-24     | 10%        |
| 25-34     | 45%        |
| 35-44     | 30%        |
| 45-54     | 10%        |
| 55-64     | 5%         |
| 65-74     | 2%         |
| 75-84     | 1%         |
| 85+       | 1%         |



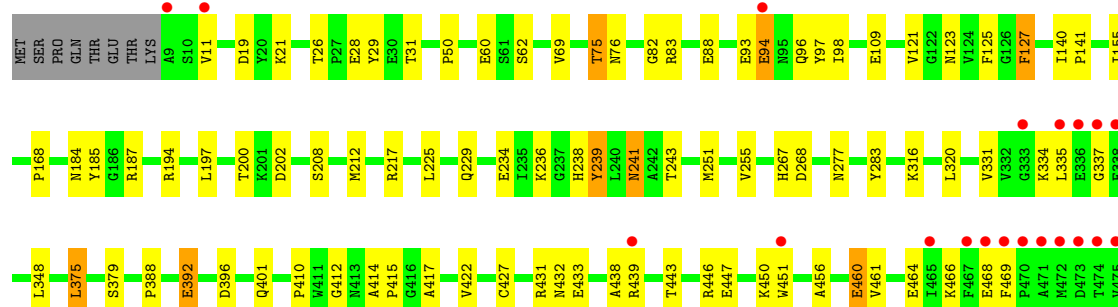
| Age Group | Percentage |
|-----------|------------|
| 18-24     | 10%        |
| 25-34     | 45%        |
| 35-44     | 30%        |
| 45-54     | 10%        |
| 55-64     | 5%         |
| 65-74     | 2%         |
| 75-84     | 1%         |
| 85+       | 1%         |





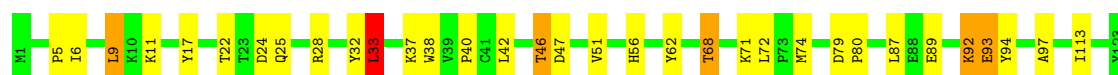
- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE/OXYGENASE

Chain V:



- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE/OXYGENASE

Chain S:



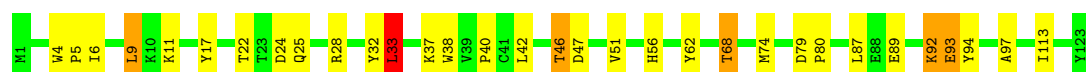
- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE/OXYGENASE

Chain C:



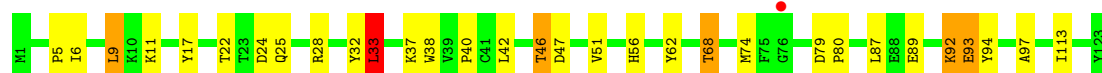
- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE/OXYGENASE

Chain F:



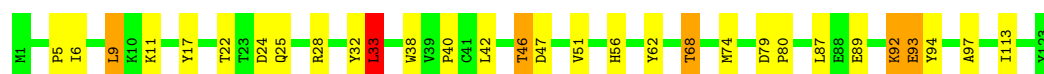
- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE/OXYGENASE

Chain I:



- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE/OXYGENASE

Chain M:



- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE/OXYGENASE

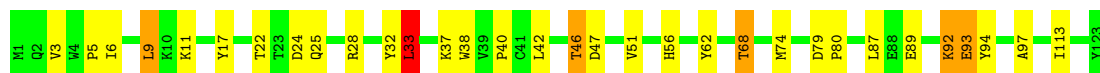
Chain P:





- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE/OXYGENASE

Chain T:



- Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE/OXYGENASE

Chain W:



Y123

## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 2   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 218.30Å 219.00Å 113.50Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 7.00 – 2.40<br>19.89 – 2.40                                 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 63.0 (7.00-2.40)<br>70.4 (19.89-2.40)                       | Depositor<br>EDS |
| $R_{merge}$   | 0.10  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.51 (at 2.41Å)   | Xtriage          |
| Refinement program  | X-PLOR 3.1  | Depositor        |
| R, $R_{free}$   | 0.224 , 0.237<br>0.208 , 0.202                              | Depositor<br>DCC |
| $R_{free}$ test set   | 6184 reflections (4.30%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 22.8  | Xtriage          |
| Anisotropy  | 0.478   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 21.6   | EDS              |
| Estimated twinning fraction   | 0.013 for k,h,-l  | Xtriage          |
| L-test for twinning   | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Outliers  | 0 of 149426 reflections                                     | Xtriage          |
| $F_o, F_c$ correlation  | 0.93  | EDS              |
| Total number of atoms   | 39368   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 19.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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   | B     | 0.56         | 1/3739 (0.0%)  | 0.80        | 2/5071 (0.0%)   |
| 1   | E     | 0.56         | 1/3739 (0.0%)  | 0.80        | 2/5071 (0.0%)   |
| 1   | H     | 0.56         | 1/3739 (0.0%)  | 0.80        | 2/5071 (0.0%)   |
| 1   | K     | 0.56         | 1/3739 (0.0%)  | 0.80        | 2/5071 (0.0%)   |
| 1   | L     | 0.56         | 1/3739 (0.0%)  | 0.80        | 2/5071 (0.0%)   |
| 1   | O     | 0.56         | 1/3739 (0.0%)  | 0.80        | 2/5071 (0.0%)   |
| 1   | R     | 0.56         | 1/3739 (0.0%)  | 0.80        | 2/5071 (0.0%)   |
| 1   | V     | 0.56         | 1/3739 (0.0%)  | 0.80        | 2/5071 (0.0%)   |
| 2   | C     | 0.59         | 0/1068         | 0.79        | 1/1453 (0.1%)   |
| 2   | F     | 0.59         | 0/1068         | 0.79        | 1/1453 (0.1%)   |
| 2   | I     | 0.59         | 0/1068         | 0.79        | 1/1453 (0.1%)   |
| 2   | M     | 0.59         | 0/1068         | 0.79        | 1/1453 (0.1%)   |
| 2   | P     | 0.59         | 0/1068         | 0.79        | 1/1453 (0.1%)   |
| 2   | S     | 0.59         | 0/1068         | 0.79        | 1/1453 (0.1%)   |
| 2   | T     | 0.59         | 0/1068         | 0.79        | 1/1453 (0.1%)   |
| 2   | W     | 0.59         | 0/1068         | 0.79        | 1/1453 (0.1%)   |
| All | All   | 0.57         | 8/38456 (0.0%) | 0.80        | 24/52192 (0.0%) |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | K     | 460 | GLU  | CG-CD | 6.49 | 1.61        | 1.51     |
| 1   | H     | 460 | GLU  | CG-CD | 6.47 | 1.61        | 1.51     |
| 1   | R     | 460 | GLU  | CG-CD | 6.46 | 1.61        | 1.51     |
| 1   | L     | 460 | GLU  | CG-CD | 6.46 | 1.61        | 1.51     |
| 1   | V     | 460 | GLU  | CG-CD | 6.46 | 1.61        | 1.51     |
| 1   | E     | 460 | GLU  | CG-CD | 6.45 | 1.61        | 1.51     |
| 1   | B     | 460 | GLU  | CG-CD | 6.45 | 1.61        | 1.51     |
| 1   | O     | 460 | GLU  | CG-CD | 6.43 | 1.61        | 1.51     |

All (24) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | P     | 33  | LEU  | CA-CB-CG | 6.83  | 131.02      | 115.30   |
| 2   | F     | 33  | LEU  | CA-CB-CG | 6.83  | 131.01      | 115.30   |
| 2   | T     | 33  | LEU  | CA-CB-CG | 6.83  | 131.01      | 115.30   |
| 2   | W     | 33  | LEU  | CA-CB-CG | 6.82  | 130.99      | 115.30   |
| 2   | S     | 33  | LEU  | CA-CB-CG | 6.82  | 130.97      | 115.30   |
| 2   | I     | 33  | LEU  | CA-CB-CG | 6.82  | 130.97      | 115.30   |
| 2   | C     | 33  | LEU  | CA-CB-CG | 6.81  | 130.96      | 115.30   |
| 2   | M     | 33  | LEU  | CA-CB-CG | 6.79  | 130.93      | 115.30   |
| 1   | K     | 375 | LEU  | CA-CB-CG | 5.81  | 128.66      | 115.30   |
| 1   | V     | 375 | LEU  | CA-CB-CG | 5.81  | 128.65      | 115.30   |
| 1   | E     | 375 | LEU  | CA-CB-CG | 5.80  | 128.65      | 115.30   |
| 1   | H     | 375 | LEU  | CA-CB-CG | 5.80  | 128.64      | 115.30   |
| 1   | B     | 375 | LEU  | CA-CB-CG | 5.80  | 128.64      | 115.30   |
| 1   | L     | 375 | LEU  | CA-CB-CG | 5.80  | 128.63      | 115.30   |
| 1   | R     | 375 | LEU  | CA-CB-CG | 5.80  | 128.63      | 115.30   |
| 1   | O     | 375 | LEU  | CA-CB-CG | 5.79  | 128.62      | 115.30   |
| 1   | H     | 82  | GLY  | N-CA-C   | -5.33 | 99.77       | 113.10   |
| 1   | O     | 82  | GLY  | N-CA-C   | -5.32 | 99.79       | 113.10   |
| 1   | R     | 82  | GLY  | N-CA-C   | -5.32 | 99.79       | 113.10   |
| 1   | B     | 82  | GLY  | N-CA-C   | -5.32 | 99.79       | 113.10   |
| 1   | L     | 82  | GLY  | N-CA-C   | -5.32 | 99.81       | 113.10   |
| 1   | E     | 82  | GLY  | N-CA-C   | -5.32 | 99.81       | 113.10   |
| 1   | V     | 82  | GLY  | N-CA-C   | -5.32 | 99.81       | 113.10   |
| 1   | K     | 82  | GLY  | N-CA-C   | -5.32 | 99.81       | 113.10   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | B     | 3649  | 0        | 3564     | 65      | 0            |
| 1   | E     | 3649  | 0        | 3564     | 63      | 1            |
| 1   | H     | 3649  | 0        | 3564     | 62      | 5            |
| 1   | K     | 3649  | 0        | 3564     | 64      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | L     | 3649  | 0        | 3564     | 63      | 1            |
| 1   | O     | 3649  | 0        | 3564     | 61      | 0            |
| 1   | R     | 3649  | 0        | 3564     | 64      | 1            |
| 1   | V     | 3649  | 0        | 3564     | 61      | 10           |
| 2   | C     | 1033  | 0        | 990      | 22      | 0            |
| 2   | F     | 1033  | 0        | 990      | 22      | 0            |
| 2   | I     | 1033  | 0        | 990      | 21      | 0            |
| 2   | M     | 1033  | 0        | 990      | 21      | 0            |
| 2   | P     | 1033  | 0        | 990      | 21      | 0            |
| 2   | S     | 1033  | 0        | 990      | 22      | 0            |
| 2   | T     | 1033  | 0        | 990      | 21      | 0            |
| 2   | W     | 1033  | 0        | 990      | 22      | 0            |
| 3   | B     | 18    | 0        | 8        | 1       | 0            |
| 3   | E     | 18    | 0        | 8        | 1       | 0            |
| 3   | H     | 18    | 0        | 8        | 1       | 0            |
| 3   | K     | 18    | 0        | 8        | 1       | 0            |
| 3   | L     | 18    | 0        | 8        | 1       | 0            |
| 3   | O     | 18    | 0        | 8        | 1       | 0            |
| 3   | R     | 18    | 0        | 8        | 1       | 0            |
| 3   | V     | 18    | 0        | 8        | 0       | 0            |
| 4   | B     | 174   | 0        | 0        | 3       | 0            |
| 4   | C     | 48    | 0        | 0        | 0       | 0            |
| 4   | E     | 175   | 0        | 0        | 2       | 0            |
| 4   | F     | 46    | 0        | 0        | 0       | 0            |
| 4   | H     | 173   | 0        | 0        | 2       | 5            |
| 4   | I     | 48    | 0        | 0        | 0       | 0            |
| 4   | K     | 175   | 0        | 0        | 3       | 1            |
| 4   | L     | 173   | 0        | 0        | 3       | 0            |
| 4   | M     | 48    | 0        | 0        | 0       | 0            |
| 4   | O     | 172   | 0        | 0        | 3       | 0            |
| 4   | P     | 46    | 0        | 0        | 0       | 0            |
| 4   | R     | 171   | 0        | 0        | 2       | 0            |
| 4   | S     | 52    | 0        | 0        | 0       | 0            |
| 4   | T     | 48    | 0        | 0        | 0       | 0            |
| 4   | V     | 171   | 0        | 0        | 3       | 0            |
| 4   | W     | 48    | 0        | 0        | 0       | 0            |
| All | All   | 39368 | 0        | 36496    | 626     | 12           |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (626) close contacts within the same asymmetric unit are listed below.



| Atom-1          | Atom-2           | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 1:E:267:HIS:HD2 | 1:E:277:ASN:HD22 | 1.14        | 0.96     |
| 1:H:267:HIS:HD2 | 1:H:277:ASN:HD22 | 1.14        | 0.95     |
| 1:O:267:HIS:HD2 | 1:O:277:ASN:HD22 | 1.14        | 0.94     |
| 1:L:267:HIS:HD2 | 1:L:277:ASN:HD22 | 1.14        | 0.93     |
| 1:B:267:HIS:HD2 | 1:B:277:ASN:HD22 | 1.14        | 0.93     |
| 1:K:267:HIS:HD2 | 1:K:277:ASN:HD22 | 1.14        | 0.91     |
| 2:P:33:LEU:HB2  | 2:P:113:ILE:HD12 | 1.54        | 0.90     |
| 1:R:267:HIS:HD2 | 1:R:277:ASN:HD22 | 1.14        | 0.90     |
| 2:M:33:LEU:HB2  | 2:M:113:ILE:HD12 | 1.54        | 0.90     |
| 2:S:33:LEU:HB2  | 2:S:113:ILE:HD12 | 1.54        | 0.89     |
| 1:V:267:HIS:HD2 | 1:V:277:ASN:HD22 | 1.14        | 0.89     |
| 2:C:33:LEU:HB2  | 2:C:113:ILE:HD12 | 1.54        | 0.88     |
| 2:W:33:LEU:HB2  | 2:W:113:ILE:HD12 | 1.54        | 0.88     |
| 2:T:33:LEU:HB2  | 2:T:113:ILE:HD12 | 1.54        | 0.87     |
| 2:I:33:LEU:HB2  | 2:I:113:ILE:HD12 | 1.54        | 0.87     |
| 2:F:33:LEU:HB2  | 2:F:113:ILE:HD12 | 1.54        | 0.86     |
| 1:R:26:THR:CG2  | 1:R:29:TYR:HB2   | 2.06        | 0.85     |
| 1:V:26:THR:CG2  | 1:V:29:TYR:HB2   | 2.06        | 0.85     |
| 1:E:26:THR:CG2  | 1:E:29:TYR:HB2   | 2.06        | 0.85     |
| 1:H:26:THR:CG2  | 1:H:29:TYR:HB2   | 2.06        | 0.85     |
| 1:K:26:THR:CG2  | 1:K:29:TYR:HB2   | 2.06        | 0.85     |
| 1:L:26:THR:CG2  | 1:L:29:TYR:HB2   | 2.06        | 0.85     |
| 1:B:26:THR:CG2  | 1:B:29:TYR:HB2   | 2.06        | 0.85     |
| 1:O:26:THR:CG2  | 1:O:29:TYR:HB2   | 2.06        | 0.85     |
| 1:L:60:GLU:HG3  | 1:L:127:PHE:HZ   | 1.44        | 0.82     |
| 1:R:26:THR:HG22 | 1:R:29:TYR:HB2   | 1.62        | 0.82     |
| 1:V:26:THR:HG22 | 1:V:29:TYR:HB2   | 1.62        | 0.82     |
| 1:O:26:THR:HG22 | 1:O:29:TYR:HB2   | 1.62        | 0.82     |
| 1:L:26:THR:HG22 | 1:L:29:TYR:HB2   | 1.62        | 0.82     |
| 1:V:60:GLU:HG3  | 1:V:127:PHE:HZ   | 1.44        | 0.82     |
| 1:R:60:GLU:HG3  | 1:R:127:PHE:HZ   | 1.44        | 0.82     |
| 1:O:60:GLU:HG3  | 1:O:127:PHE:HZ   | 1.44        | 0.81     |
| 1:H:60:GLU:HG3  | 1:H:127:PHE:HZ   | 1.44        | 0.81     |
| 1:K:26:THR:HG22 | 1:K:29:TYR:HB2   | 1.62        | 0.81     |
| 1:B:26:THR:HG22 | 1:B:29:TYR:HB2   | 1.62        | 0.80     |
| 2:P:92:LYS:HE2  | 2:P:93:GLU:HB2   | 1.64        | 0.80     |
| 1:B:60:GLU:HG3  | 1:B:127:PHE:HZ   | 1.44        | 0.80     |
| 2:F:92:LYS:HE2  | 2:F:93:GLU:HB2   | 1.64        | 0.80     |
| 2:I:92:LYS:HE2  | 2:I:93:GLU:HB2   | 1.64        | 0.80     |
| 2:S:92:LYS:HE2  | 2:S:93:GLU:HB2   | 1.64        | 0.80     |
| 1:E:26:THR:HG22 | 1:E:29:TYR:HB2   | 1.62        | 0.80     |
| 2:M:92:LYS:HE2  | 2:M:93:GLU:HB2   | 1.64        | 0.79     |
| 1:H:26:THR:HG22 | 1:H:29:TYR:HB2   | 1.62        | 0.79     |

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| Atom-1           | Atom-2          | Distance(Å) | Clash(Å) |
|------------------|-----------------|-------------|----------|
| 2:W:92:LYS:HE2   | 2:W:93:GLU:HB2  | 1.64        | 0.79     |
| 2:T:92:LYS:HE2   | 2:T:93:GLU:HB2  | 1.64        | 0.79     |
| 1:E:60:GLU:HG3   | 1:E:127:PHE:HZ  | 1.44        | 0.79     |
| 2:C:92:LYS:HE2   | 2:C:93:GLU:HB2  | 1.64        | 0.79     |
| 1:K:60:GLU:HG3   | 1:K:127:PHE:HZ  | 1.45        | 0.79     |
| 2:M:22:THR:H     | 2:M:25:GLN:HE21 | 1.33        | 0.77     |
| 2:F:22:THR:H     | 2:F:25:GLN:HE21 | 1.34        | 0.76     |
| 2:I:22:THR:H     | 2:I:25:GLN:HE21 | 1.33        | 0.76     |
| 2:C:22:THR:H     | 2:C:25:GLN:HE21 | 1.34        | 0.76     |
| 1:R:60:GLU:HG3   | 1:R:127:PHE:CZ  | 2.21        | 0.76     |
| 1:V:60:GLU:HG3   | 1:V:127:PHE:CZ  | 2.22        | 0.75     |
| 1:O:60:GLU:HG3   | 1:O:127:PHE:CZ  | 2.22        | 0.75     |
| 1:L:60:GLU:HG3   | 1:L:127:PHE:CZ  | 2.22        | 0.75     |
| 1:H:60:GLU:HG3   | 1:H:127:PHE:CZ  | 2.21        | 0.75     |
| 1:E:60:GLU:HG3   | 1:E:127:PHE:CZ  | 2.22        | 0.75     |
| 2:P:22:THR:H     | 2:P:25:GLN:HE21 | 1.33        | 0.75     |
| 1:K:60:GLU:HG3   | 1:K:127:PHE:CZ  | 2.22        | 0.75     |
| 1:B:60:GLU:HG3   | 1:B:127:PHE:CZ  | 2.21        | 0.75     |
| 2:W:22:THR:H     | 2:W:25:GLN:HE21 | 1.34        | 0.75     |
| 2:S:22:THR:H     | 2:S:25:GLN:HE21 | 1.34        | 0.74     |
| 2:T:22:THR:H     | 2:T:25:GLN:HE21 | 1.34        | 0.74     |
| 1:B:26:THR:HG22  | 1:B:26:THR:O    | 1.89        | 0.73     |
| 1:R:94:GLU:H     | 1:R:94:GLU:CD   | 1.92        | 0.73     |
| 1:K:26:THR:HG22  | 1:K:26:THR:O    | 1.89        | 0.73     |
| 1:V:94:GLU:CD    | 1:V:94:GLU:H    | 1.92        | 0.73     |
| 1:H:94:GLU:CD    | 1:H:94:GLU:H    | 1.92        | 0.73     |
| 1:L:26:THR:O     | 1:L:26:THR:HG22 | 1.89        | 0.72     |
| 1:O:94:GLU:CD    | 1:O:94:GLU:H    | 1.92        | 0.72     |
| 1:B:94:GLU:CD    | 1:B:94:GLU:H    | 1.92        | 0.72     |
| 1:E:94:GLU:H     | 1:E:94:GLU:CD   | 1.92        | 0.72     |
| 1:L:94:GLU:H     | 1:L:94:GLU:CD   | 1.92        | 0.72     |
| 1:V:26:THR:O     | 1:V:26:THR:HG22 | 1.89        | 0.72     |
| 1:K:94:GLU:CD    | 1:K:94:GLU:H    | 1.92        | 0.71     |
| 1:R:26:THR:O     | 1:R:26:THR:HG22 | 1.89        | 0.71     |
| 1:O:26:THR:HG22  | 1:O:26:THR:O    | 1.89        | 0.71     |
| 1:H:26:THR:HG22  | 1:H:26:THR:O    | 1.89        | 0.71     |
| 1:E:26:THR:HG22  | 1:E:26:THR:O    | 1.89        | 0.70     |
| 2:S:68:THR:HG21  | 2:T:6:ILE:HG12  | 1.73        | 0.69     |
| 1:V:229:GLN:HE21 | 1:V:236:LYS:H   | 1.43        | 0.66     |
| 2:F:6:ILE:HG12   | 2:M:68:THR:HG21 | 1.78        | 0.66     |
| 1:E:229:GLN:HE21 | 1:E:236:LYS:H   | 1.42        | 0.66     |
| 1:O:229:GLN:HE21 | 1:O:236:LYS:H   | 1.42        | 0.66     |

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| Atom-1           | Atom-2          | Distance(Å) | Clash(Å) |
|------------------|-----------------|-------------|----------|
| 2:C:6:ILE:HG12   | 2:W:68:THR:HG21 | 1.78        | 0.66     |
| 1:R:229:GLN:HE21 | 1:R:236:LYS:H   | 1.43        | 0.65     |
| 1:H:229:GLN:HE21 | 1:H:236:LYS:H   | 1.43        | 0.65     |
| 1:B:229:GLN:HE21 | 1:B:236:LYS:H   | 1.42        | 0.65     |
| 1:L:229:GLN:HE21 | 1:L:236:LYS:H   | 1.42        | 0.65     |
| 1:K:229:GLN:HE21 | 1:K:236:LYS:H   | 1.43        | 0.65     |
| 1:K:267:HIS:HE1  | 4:O:1157:HOH:O  | 1.81        | 0.64     |
| 1:E:267:HIS:HE1  | 4:H:529:HOH:O   | 1.81        | 0.63     |
| 1:K:88:GLU:HG2   | 1:K:98:ILE:HB   | 1.80        | 0.63     |
| 1:O:88:GLU:HG2   | 1:O:98:ILE:HB   | 1.81        | 0.63     |
| 1:B:88:GLU:HG2   | 1:B:98:ILE:HB   | 1.81        | 0.63     |
| 1:L:88:GLU:HG2   | 1:L:98:ILE:HB   | 1.81        | 0.63     |
| 1:L:267:HIS:HE1  | 4:B:517:HOH:O   | 1.82        | 0.63     |
| 1:R:50:PRO:HG3   | 1:R:97:TYR:CZ   | 2.34        | 0.63     |
| 1:H:50:PRO:HG3   | 1:H:97:TYR:CZ   | 2.34        | 0.63     |
| 1:R:88:GLU:HG2   | 1:R:98:ILE:HB   | 1.80        | 0.63     |
| 1:O:50:PRO:HG3   | 1:O:97:TYR:CZ   | 2.34        | 0.62     |
| 1:V:88:GLU:HG2   | 1:V:98:ILE:HB   | 1.80        | 0.62     |
| 1:H:88:GLU:HG2   | 1:H:98:ILE:HB   | 1.81        | 0.62     |
| 1:R:200:THR:OG1  | 1:R:238:HIS:HD2 | 1.82        | 0.62     |
| 1:L:50:PRO:HG3   | 1:L:97:TYR:CZ   | 2.34        | 0.62     |
| 1:K:50:PRO:HG3   | 1:K:97:TYR:CZ   | 2.34        | 0.62     |
| 1:E:88:GLU:HG2   | 1:E:98:ILE:HB   | 1.81        | 0.62     |
| 4:L:508:HOH:O    | 1:B:267:HIS:HE1 | 1.82        | 0.62     |
| 1:B:50:PRO:HG3   | 1:B:97:TYR:CZ   | 2.34        | 0.62     |
| 1:K:200:THR:OG1  | 1:K:238:HIS:HD2 | 1.82        | 0.62     |
| 2:F:46:THR:HG22  | 2:F:97:ALA:HB2  | 1.82        | 0.62     |
| 1:V:50:PRO:HG3   | 1:V:97:TYR:CZ   | 2.34        | 0.62     |
| 1:B:200:THR:OG1  | 1:B:238:HIS:HD2 | 1.82        | 0.62     |
| 2:I:46:THR:HG22  | 2:I:97:ALA:HB2  | 1.82        | 0.62     |
| 2:W:46:THR:HG22  | 2:W:97:ALA:HB2  | 1.82        | 0.62     |
| 4:K:513:HOH:O    | 1:O:267:HIS:HE1 | 1.83        | 0.62     |
| 1:E:50:PRO:HG3   | 1:E:97:TYR:CZ   | 2.34        | 0.62     |
| 1:L:200:THR:OG1  | 1:L:238:HIS:HD2 | 1.82        | 0.62     |
| 4:E:513:HOH:O    | 1:H:267:HIS:HE1 | 1.82        | 0.62     |
| 1:V:200:THR:OG1  | 1:V:238:HIS:HD2 | 1.82        | 0.62     |
| 1:O:200:THR:OG1  | 1:O:238:HIS:HD2 | 1.83        | 0.62     |
| 2:T:46:THR:HG22  | 2:T:97:ALA:HB2  | 1.82        | 0.61     |
| 2:M:46:THR:HG22  | 2:M:97:ALA:HB2  | 1.82        | 0.61     |
| 1:R:267:HIS:HE1  | 4:V:530:HOH:O   | 1.84        | 0.61     |
| 2:C:46:THR:HG22  | 2:C:97:ALA:HB2  | 1.82        | 0.61     |
| 2:S:46:THR:HG22  | 2:S:97:ALA:HB2  | 1.82        | 0.61     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:R:267:HIS:CD2  | 1:R:277:ASN:HD22 | 2.06        | 0.61     |
| 2:P:46:THR:HG22  | 2:P:97:ALA:HB2   | 1.82        | 0.61     |
| 1:E:200:THR:OG1  | 1:E:238:HIS:HD2  | 1.82        | 0.60     |
| 1:H:200:THR:OG1  | 1:H:238:HIS:HD2  | 1.83        | 0.60     |
| 1:B:267:HIS:CD2  | 1:B:277:ASN:HD22 | 2.07        | 0.59     |
| 1:H:443:THR:O    | 1:H:447:GLU:HG3  | 2.03        | 0.59     |
| 1:K:443:THR:O    | 1:K:447:GLU:HG3  | 2.03        | 0.59     |
| 1:B:443:THR:O    | 1:B:447:GLU:HG3  | 2.03        | 0.59     |
| 1:E:443:THR:O    | 1:E:447:GLU:HG3  | 2.03        | 0.59     |
| 2:W:89:GLU:O     | 2:W:92:LYS:HG3   | 2.03        | 0.59     |
| 2:T:89:GLU:O     | 2:T:92:LYS:HG3   | 2.03        | 0.59     |
| 2:P:89:GLU:O     | 2:P:92:LYS:HG3   | 2.03        | 0.59     |
| 1:E:267:HIS:CD2  | 1:E:277:ASN:HD22 | 2.07        | 0.59     |
| 2:S:89:GLU:O     | 2:S:92:LYS:HG3   | 2.03        | 0.59     |
| 1:O:443:THR:O    | 1:O:447:GLU:HG3  | 2.03        | 0.58     |
| 1:K:267:HIS:CD2  | 1:K:277:ASN:HD22 | 2.07        | 0.58     |
| 2:M:89:GLU:O     | 2:M:92:LYS:HG3   | 2.03        | 0.58     |
| 1:R:443:THR:O    | 1:R:447:GLU:HG3  | 2.03        | 0.58     |
| 1:B:431:ARG:HH21 | 1:B:432:ASN:HD21 | 1.51        | 0.58     |
| 1:O:431:ARG:HH21 | 1:O:432:ASN:HD21 | 1.51        | 0.58     |
| 2:M:6:ILE:HG12   | 2:T:68:THR:HG21  | 1.83        | 0.58     |
| 1:O:26:THR:HG22  | 1:O:29:TYR:CB    | 2.33        | 0.58     |
| 2:C:89:GLU:O     | 2:C:92:LYS:HG3   | 2.03        | 0.58     |
| 1:K:431:ARG:HH21 | 1:K:432:ASN:HD21 | 1.51        | 0.58     |
| 1:H:431:ARG:HH21 | 1:H:432:ASN:HD21 | 1.51        | 0.58     |
| 1:E:431:ARG:HH21 | 1:E:432:ASN:HD21 | 1.51        | 0.58     |
| 1:L:26:THR:HG22  | 1:L:29:TYR:CB    | 2.33        | 0.58     |
| 2:F:89:GLU:O     | 2:F:92:LYS:HG3   | 2.03        | 0.58     |
| 2:I:89:GLU:O     | 2:I:92:LYS:HG3   | 2.03        | 0.58     |
| 1:L:431:ARG:HH21 | 1:L:432:ASN:HD21 | 1.51        | 0.58     |
| 1:R:431:ARG:HH21 | 1:R:432:ASN:HD21 | 1.51        | 0.58     |
| 1:L:267:HIS:CD2  | 1:L:277:ASN:HD22 | 2.07        | 0.58     |
| 1:V:431:ARG:HH21 | 1:V:432:ASN:HD21 | 1.51        | 0.58     |
| 1:V:26:THR:HG22  | 1:V:29:TYR:CB    | 2.33        | 0.58     |
| 1:B:414:ALA:HB3  | 1:B:415:PRO:HD3  | 1.86        | 0.58     |
| 1:K:414:ALA:HB3  | 1:K:415:PRO:HD3  | 1.86        | 0.58     |
| 1:O:414:ALA:HB3  | 1:O:415:PRO:HD3  | 1.86        | 0.57     |
| 1:E:155:ILE:HG12 | 1:E:375:LEU:HD13 | 1.86        | 0.57     |
| 1:V:184:ASN:ND2  | 1:V:187:ARG:HH11 | 2.03        | 0.57     |
| 1:H:155:ILE:HG12 | 1:H:375:LEU:HD13 | 1.86        | 0.57     |
| 1:V:443:THR:O    | 1:V:447:GLU:HG3  | 2.03        | 0.57     |
| 1:V:464:GLU:HA   | 1:V:466:LYS:HZ2  | 1.69        | 0.57     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:L:414:ALA:HB3  | 1:L:415:PRO:HD3  | 1.86        | 0.57     |
| 1:L:443:THR:O    | 1:L:447:GLU:HG3  | 2.03        | 0.57     |
| 1:R:155:ILE:HG12 | 1:R:375:LEU:HD13 | 1.86        | 0.57     |
| 1:V:155:ILE:HG12 | 1:V:375:LEU:HD13 | 1.86        | 0.57     |
| 1:R:26:THR:HG22  | 1:R:29:TYR:CB    | 2.33        | 0.57     |
| 1:E:414:ALA:HB3  | 1:E:415:PRO:HD3  | 1.86        | 0.57     |
| 1:K:155:ILE:HG12 | 1:K:375:LEU:HD13 | 1.86        | 0.57     |
| 1:L:184:ASN:ND2  | 1:L:187:ARG:HH11 | 2.03        | 0.57     |
| 1:B:155:ILE:HG12 | 1:B:375:LEU:HD13 | 1.86        | 0.57     |
| 1:R:184:ASN:ND2  | 1:R:187:ARG:HH11 | 2.03        | 0.57     |
| 1:V:414:ALA:HB3  | 1:V:415:PRO:HD3  | 1.86        | 0.57     |
| 1:H:184:ASN:ND2  | 1:H:187:ARG:HH11 | 2.03        | 0.57     |
| 1:B:26:THR:HG22  | 1:B:29:TYR:CB    | 2.33        | 0.57     |
| 1:H:414:ALA:HB3  | 1:H:415:PRO:HD3  | 1.86        | 0.57     |
| 1:R:414:ALA:HB3  | 1:R:415:PRO:HD3  | 1.86        | 0.57     |
| 1:E:141:PRO:HB2  | 4:E:547:HOH:O    | 2.05        | 0.56     |
| 1:O:184:ASN:ND2  | 1:O:187:ARG:HH11 | 2.03        | 0.56     |
| 1:V:422:VAL:HG13 | 1:V:451:TRP:CH2  | 2.40        | 0.56     |
| 1:H:141:PRO:HB2  | 4:H:563:HOH:O    | 2.05        | 0.56     |
| 1:L:155:ILE:HG12 | 1:L:375:LEU:HD13 | 1.86        | 0.56     |
| 1:O:155:ILE:HG12 | 1:O:375:LEU:HD13 | 1.86        | 0.56     |
| 1:K:184:ASN:ND2  | 1:K:187:ARG:HH11 | 2.03        | 0.56     |
| 1:H:267:HIS:CD2  | 1:H:277:ASN:HD22 | 2.07        | 0.56     |
| 1:O:267:HIS:CD2  | 1:O:277:ASN:HD22 | 2.07        | 0.56     |
| 2:P:93:GLU:HG2   | 2:P:94:TYR:CE2   | 2.40        | 0.56     |
| 2:F:93:GLU:HG2   | 2:F:94:TYR:CE2   | 2.40        | 0.56     |
| 2:C:93:GLU:HG2   | 2:C:94:TYR:CE2   | 2.40        | 0.56     |
| 1:E:184:ASN:ND2  | 1:E:187:ARG:HH11 | 2.03        | 0.56     |
| 1:R:422:VAL:HG13 | 1:R:451:TRP:CH2  | 2.41        | 0.56     |
| 1:L:422:VAL:HG13 | 1:L:451:TRP:CH2  | 2.40        | 0.56     |
| 1:B:422:VAL:HG13 | 1:B:451:TRP:CH2  | 2.40        | 0.56     |
| 1:E:422:VAL:HG13 | 1:E:451:TRP:CH2  | 2.40        | 0.56     |
| 2:S:93:GLU:HG2   | 2:S:94:TYR:CE2   | 2.40        | 0.56     |
| 2:M:93:GLU:HG2   | 2:M:94:TYR:CE2   | 2.40        | 0.56     |
| 1:V:251:MET:O    | 1:V:255:VAL:HG23 | 2.06        | 0.56     |
| 2:I:68:THR:HG21  | 2:P:6:ILE:HG12   | 1.87        | 0.56     |
| 1:B:251:MET:HE1  | 1:B:283:TYR:CD1  | 2.40        | 0.56     |
| 2:I:93:GLU:HG2   | 2:I:94:TYR:CE2   | 2.40        | 0.56     |
| 1:L:251:MET:O    | 1:L:255:VAL:HG23 | 2.06        | 0.56     |
| 1:V:141:PRO:HB2  | 4:V:565:HOH:O    | 2.05        | 0.56     |
| 1:O:251:MET:O    | 1:O:255:VAL:HG23 | 2.06        | 0.56     |
| 1:O:422:VAL:HG13 | 1:O:451:TRP:CH2  | 2.40        | 0.56     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:W:93:GLU:HG2   | 2:W:94:TYR:CE2   | 2.40        | 0.56     |
| 1:V:202:ASP:OD1  | 1:V:238:HIS:HE1  | 1.89        | 0.56     |
| 1:K:422:VAL:HG13 | 1:K:451:TRP:CH2  | 2.40        | 0.56     |
| 1:O:202:ASP:OD1  | 1:O:238:HIS:HE1  | 1.89        | 0.56     |
| 1:B:141:PRO:HB2  | 4:B:552:HOH:O    | 2.05        | 0.56     |
| 1:H:422:VAL:HG13 | 1:H:451:TRP:CH2  | 2.40        | 0.56     |
| 1:K:141:PRO:HB2  | 4:K:548:HOH:O    | 2.05        | 0.56     |
| 1:E:251:MET:O    | 1:E:255:VAL:HG23 | 2.06        | 0.56     |
| 2:T:93:GLU:HG2   | 2:T:94:TYR:CE2   | 2.40        | 0.56     |
| 1:L:202:ASP:OD1  | 1:L:238:HIS:HE1  | 1.89        | 0.56     |
| 1:R:141:PRO:HB2  | 4:R:556:HOH:O    | 2.05        | 0.56     |
| 1:E:29:TYR:CE2   | 1:E:31:THR:HA    | 2.42        | 0.55     |
| 1:H:29:TYR:CE2   | 1:H:31:THR:HA    | 2.42        | 0.55     |
| 1:O:141:PRO:HB2  | 4:O:1201:HOH:O   | 2.05        | 0.55     |
| 1:R:202:ASP:OD1  | 1:R:238:HIS:HE1  | 1.89        | 0.55     |
| 1:K:251:MET:O    | 1:K:255:VAL:HG23 | 2.06        | 0.55     |
| 2:C:68:THR:HG21  | 2:I:6:ILE:HG12   | 1.88        | 0.55     |
| 1:K:29:TYR:CE2   | 1:K:31:THR:HA    | 2.41        | 0.55     |
| 1:B:251:MET:O    | 1:B:255:VAL:HG23 | 2.06        | 0.55     |
| 1:L:141:PRO:HB2  | 4:L:543:HOH:O    | 2.05        | 0.55     |
| 1:B:184:ASN:ND2  | 1:B:187:ARG:HH11 | 2.03        | 0.55     |
| 1:H:202:ASP:OD1  | 1:H:238:HIS:HE1  | 1.89        | 0.55     |
| 1:H:251:MET:O    | 1:H:255:VAL:HG23 | 2.06        | 0.55     |
| 1:E:177:LYS:HB2  | 1:H:62:SER:O     | 2.06        | 0.55     |
| 1:B:94:GLU:CD    | 1:B:94:GLU:N     | 2.60        | 0.55     |
| 1:K:464:GLU:HA   | 1:K:466:LYS:HZ2  | 1.72        | 0.55     |
| 1:H:140:ILE:HD13 | 1:H:320:LEU:HD11 | 1.89        | 0.55     |
| 1:R:251:MET:O    | 1:R:255:VAL:HG23 | 2.06        | 0.55     |
| 1:K:140:ILE:HD13 | 1:K:320:LEU:HD11 | 1.88        | 0.55     |
| 1:R:140:ILE:HD13 | 1:R:320:LEU:HD11 | 1.89        | 0.55     |
| 1:K:26:THR:HG22  | 1:K:29:TYR:CB    | 2.33        | 0.55     |
| 1:V:140:ILE:HD13 | 1:V:320:LEU:HD11 | 1.89        | 0.55     |
| 2:S:6:ILE:HG12   | 2:F:68:THR:HG21  | 1.89        | 0.55     |
| 1:E:140:ILE:HD13 | 1:E:320:LEU:HD11 | 1.89        | 0.55     |
| 1:R:29:TYR:CE2   | 1:R:31:THR:HA    | 2.42        | 0.55     |
| 1:B:140:ILE:HD13 | 1:B:320:LEU:HD11 | 1.89        | 0.55     |
| 1:V:29:TYR:CE2   | 1:V:31:THR:HA    | 2.42        | 0.55     |
| 1:O:94:GLU:CD    | 1:O:94:GLU:N     | 2.60        | 0.55     |
| 1:E:202:ASP:OD1  | 1:E:238:HIS:HE1  | 1.89        | 0.55     |
| 1:O:140:ILE:HD13 | 1:O:320:LEU:HD11 | 1.89        | 0.55     |
| 1:L:140:ILE:HD13 | 1:L:320:LEU:HD11 | 1.89        | 0.55     |
| 1:H:26:THR:HG22  | 1:H:29:TYR:CB    | 2.33        | 0.55     |

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| Atom-1          | Atom-2           | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 1:B:29:TYR:CE2  | 1:B:31:THR:HA    | 2.42        | 0.55     |
| 1:K:202:ASP:OD1 | 1:K:238:HIS:HE1  | 1.89        | 0.55     |
| 1:E:26:THR:HG22 | 1:E:29:TYR:CB    | 2.33        | 0.54     |
| 1:V:94:GLU:N    | 1:V:94:GLU:CD    | 2.60        | 0.54     |
| 1:H:94:GLU:N    | 1:H:94:GLU:CD    | 2.60        | 0.54     |
| 1:E:94:GLU:CD   | 1:E:94:GLU:N     | 2.60        | 0.54     |
| 1:B:202:ASP:OD1 | 1:B:238:HIS:HE1  | 1.89        | 0.54     |
| 1:E:456:ALA:O   | 1:E:460:GLU:HG3  | 2.08        | 0.54     |
| 1:K:94:GLU:N    | 1:K:94:GLU:CD    | 2.60        | 0.54     |
| 1:O:251:MET:HE1 | 1:O:283:TYR:CD1  | 2.42        | 0.54     |
| 1:R:177:LYS:HB2 | 1:V:62:SER:O     | 2.06        | 0.54     |
| 2:F:51:VAL:CG2  | 2:F:62:TYR:HB3   | 2.38        | 0.54     |
| 1:K:177:LYS:HB2 | 1:O:62:SER:O     | 2.08        | 0.54     |
| 1:K:456:ALA:O   | 1:K:460:GLU:HG3  | 2.08        | 0.54     |
| 1:E:26:THR:CG2  | 1:E:26:THR:O     | 2.56        | 0.54     |
| 1:L:29:TYR:CE2  | 1:L:31:THR:HA    | 2.41        | 0.54     |
| 1:O:29:TYR:CE2  | 1:O:31:THR:HA    | 2.42        | 0.54     |
| 2:C:51:VAL:CG2  | 2:C:62:TYR:HB3   | 2.38        | 0.54     |
| 1:R:26:THR:O    | 1:R:26:THR:CG2   | 2.56        | 0.54     |
| 1:E:251:MET:HE1 | 1:E:283:TYR:CD1  | 2.43        | 0.54     |
| 1:H:251:MET:HE1 | 1:H:283:TYR:CD1  | 2.43        | 0.54     |
| 1:B:456:ALA:O   | 1:B:460:GLU:HG3  | 2.08        | 0.54     |
| 1:V:456:ALA:O   | 1:V:460:GLU:HG3  | 2.08        | 0.54     |
| 2:M:51:VAL:CG2  | 2:M:62:TYR:HB3   | 2.38        | 0.54     |
| 1:O:456:ALA:O   | 1:O:460:GLU:HG3  | 2.08        | 0.54     |
| 2:I:51:VAL:CG2  | 2:I:62:TYR:HB3   | 2.38        | 0.54     |
| 1:V:26:THR:O    | 1:V:26:THR:CG2   | 2.56        | 0.54     |
| 1:B:26:THR:CG2  | 1:B:26:THR:O     | 2.56        | 0.54     |
| 1:R:251:MET:HE1 | 1:R:283:TYR:CD1  | 2.42        | 0.54     |
| 1:H:456:ALA:O   | 1:H:460:GLU:HG3  | 2.08        | 0.54     |
| 1:L:94:GLU:CD   | 1:L:94:GLU:N     | 2.60        | 0.53     |
| 1:R:94:GLU:N    | 1:R:94:GLU:CD    | 2.60        | 0.53     |
| 1:V:267:HIS:CD2 | 1:V:277:ASN:HD22 | 2.06        | 0.53     |
| 1:H:26:THR:CG2  | 1:H:26:THR:O     | 2.56        | 0.53     |
| 2:T:51:VAL:CG2  | 2:T:62:TYR:HB3   | 2.38        | 0.53     |
| 1:K:26:THR:O    | 1:K:26:THR:CG2   | 2.56        | 0.53     |
| 2:W:51:VAL:CG2  | 2:W:62:TYR:HB3   | 2.38        | 0.53     |
| 1:K:251:MET:HE1 | 1:K:283:TYR:CD1  | 2.43        | 0.53     |
| 2:S:51:VAL:CG2  | 2:S:62:TYR:HB3   | 2.38        | 0.53     |
| 2:P:51:VAL:CG2  | 2:P:62:TYR:HB3   | 2.38        | 0.53     |
| 1:L:26:THR:O    | 1:L:26:THR:CG2   | 2.56        | 0.53     |
| 1:R:456:ALA:O   | 1:R:460:GLU:HG3  | 2.08        | 0.53     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:E:62:SER:O     | 1:H:177:LYS:HB2  | 2.08        | 0.52     |
| 4:R:521:HOH:O    | 1:V:267:HIS:HE1  | 1.92        | 0.52     |
| 1:O:26:THR:CG2   | 1:O:26:THR:O     | 2.56        | 0.52     |
| 1:E:123:ASN:ND2  | 3:H:476:RUB:O4   | 2.43        | 0.52     |
| 1:R:433:GLU:HG2  | 2:T:28:ARG:HD2   | 1.92        | 0.52     |
| 1:L:456:ALA:O    | 1:L:460:GLU:HG3  | 2.08        | 0.52     |
| 1:K:433:GLU:HG2  | 2:M:28:ARG:HD2   | 1.92        | 0.52     |
| 1:V:433:GLU:HG2  | 2:W:28:ARG:HD2   | 1.92        | 0.52     |
| 3:E:476:RUB:O4   | 1:H:123:ASN:ND2  | 2.42        | 0.52     |
| 1:B:433:GLU:HG2  | 2:C:28:ARG:HD2   | 1.92        | 0.52     |
| 1:E:464:GLU:HA   | 1:E:466:LYS:HZ2  | 1.74        | 0.51     |
| 1:L:251:MET:HE1  | 1:L:283:TYR:CD1  | 2.45        | 0.51     |
| 1:O:433:GLU:HG2  | 2:P:28:ARG:HD2   | 1.92        | 0.51     |
| 1:L:184:ASN:HD22 | 1:L:187:ARG:HH11 | 1.59        | 0.51     |
| 1:V:251:MET:HE1  | 1:V:283:TYR:CD1  | 2.45        | 0.51     |
| 3:K:476:RUB:O4   | 1:O:123:ASN:ND2  | 2.44        | 0.51     |
| 1:O:184:ASN:HD22 | 1:O:187:ARG:HH11 | 1.59        | 0.50     |
| 1:L:177:LYS:HB2  | 1:B:62:SER:O     | 2.11        | 0.50     |
| 1:L:433:GLU:HG2  | 2:S:28:ARG:HD2   | 1.92        | 0.50     |
| 1:L:62:SER:O     | 1:B:177:LYS:HB2  | 2.11        | 0.50     |
| 1:H:433:GLU:HG2  | 2:I:28:ARG:HD2   | 1.92        | 0.50     |
| 1:O:464:GLU:HA   | 1:O:466:LYS:HZ2  | 1.76        | 0.50     |
| 1:E:184:ASN:HD22 | 1:E:187:ARG:HH11 | 1.59        | 0.50     |
| 1:E:433:GLU:HG2  | 2:F:28:ARG:HD2   | 1.92        | 0.50     |
| 1:H:184:ASN:HD22 | 1:H:187:ARG:HH11 | 1.59        | 0.50     |
| 1:B:184:ASN:HD22 | 1:B:187:ARG:HH11 | 1.59        | 0.49     |
| 1:B:412:GLY:HA2  | 2:W:72:LEU:HD21  | 1.95        | 0.49     |
| 1:L:123:ASN:ND2  | 3:B:476:RUB:O4   | 2.46        | 0.49     |
| 2:P:70:TRP:CE3   | 2:W:3:VAL:HG21   | 2.48        | 0.49     |
| 1:R:184:ASN:HD22 | 1:R:187:ARG:HH11 | 1.59        | 0.49     |
| 1:V:184:ASN:HD22 | 1:V:187:ARG:HH11 | 1.59        | 0.48     |
| 1:B:431:ARG:HE   | 1:B:432:ASN:ND2  | 2.12        | 0.48     |
| 1:H:464:GLU:HA   | 1:H:466:LYS:HZ2  | 1.77        | 0.48     |
| 2:P:32:TYR:CD2   | 2:P:113:ILE:HD11 | 2.49        | 0.48     |
| 2:S:32:TYR:CD2   | 2:S:113:ILE:HD11 | 2.49        | 0.48     |
| 1:R:464:GLU:HA   | 1:R:466:LYS:HZ2  | 1.79        | 0.48     |
| 1:K:168:PRO:HA   | 1:K:396:ASP:O    | 2.14        | 0.48     |
| 2:M:32:TYR:CD2   | 2:M:113:ILE:HD11 | 2.49        | 0.48     |
| 1:K:431:ARG:HE   | 1:K:432:ASN:ND2  | 2.12        | 0.48     |
| 1:L:431:ARG:HE   | 1:L:432:ASN:ND2  | 2.12        | 0.48     |
| 1:H:168:PRO:HA   | 1:H:396:ASP:O    | 2.14        | 0.48     |
| 1:L:168:PRO:HA   | 1:L:396:ASP:O    | 2.14        | 0.48     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:E:109:GLU:HB2  | 1:H:208:SER:O    | 2.14        | 0.48     |
| 2:F:32:TYR:CD2   | 2:F:113:ILE:HD11 | 2.49        | 0.48     |
| 3:L:476:RUB:O4   | 1:B:123:ASN:ND2  | 2.46        | 0.48     |
| 2:I:32:TYR:CD2   | 2:I:113:ILE:HD11 | 2.49        | 0.48     |
| 1:E:431:ARG:HE   | 1:E:432:ASN:ND2  | 2.12        | 0.48     |
| 1:H:464:GLU:OE1  | 1:H:466:LYS:NZ   | 2.47        | 0.48     |
| 1:V:168:PRO:HA   | 1:V:396:ASP:O    | 2.14        | 0.48     |
| 2:W:32:TYR:CD2   | 2:W:113:ILE:HD11 | 2.49        | 0.47     |
| 2:C:22:THR:N     | 2:C:25:GLN:HE21  | 2.08        | 0.47     |
| 1:K:464:GLU:OE1  | 1:K:466:LYS:NZ   | 2.47        | 0.47     |
| 2:T:32:TYR:CD2   | 2:T:113:ILE:HD11 | 2.49        | 0.47     |
| 1:V:431:ARG:HE   | 1:V:432:ASN:ND2  | 2.12        | 0.47     |
| 1:K:388:PRO:HG3  | 1:K:427:CYS:SG   | 2.55        | 0.47     |
| 1:E:388:PRO:HG3  | 1:E:427:CYS:SG   | 2.55        | 0.47     |
| 3:R:476:RUB:O4   | 1:V:123:ASN:ND2  | 2.47        | 0.47     |
| 1:H:431:ARG:HE   | 1:H:432:ASN:ND2  | 2.12        | 0.47     |
| 1:E:208:SER:O    | 1:H:109:GLU:HB2  | 2.15        | 0.47     |
| 1:V:388:PRO:HG3  | 1:V:427:CYS:SG   | 2.54        | 0.47     |
| 1:B:168:PRO:HA   | 1:B:396:ASP:O    | 2.14        | 0.47     |
| 1:E:168:PRO:HA   | 1:E:396:ASP:O    | 2.14        | 0.47     |
| 1:K:184:ASN:HD22 | 1:K:187:ARG:HH11 | 1.59        | 0.47     |
| 1:E:464:GLU:OE1  | 1:E:466:LYS:NZ   | 2.47        | 0.47     |
| 1:R:168:PRO:HA   | 1:R:396:ASP:O    | 2.14        | 0.47     |
| 2:C:33:LEU:HD13  | 2:C:38:TRP:HB2   | 1.96        | 0.47     |
| 2:T:33:LEU:HD13  | 2:T:38:TRP:HB2   | 1.96        | 0.47     |
| 1:B:388:PRO:HG3  | 1:B:427:CYS:SG   | 2.55        | 0.47     |
| 2:S:33:LEU:HD13  | 2:S:38:TRP:HB2   | 1.96        | 0.47     |
| 2:C:32:TYR:CD2   | 2:C:113:ILE:HD11 | 2.49        | 0.47     |
| 1:V:464:GLU:OE1  | 1:V:466:LYS:NZ   | 2.47        | 0.47     |
| 1:O:464:GLU:OE1  | 1:O:466:LYS:NZ   | 2.47        | 0.47     |
| 2:P:33:LEU:HD13  | 2:P:38:TRP:HB2   | 1.96        | 0.47     |
| 2:I:33:LEU:HD13  | 2:I:38:TRP:HB2   | 1.96        | 0.47     |
| 2:M:22:THR:N     | 2:M:25:GLN:HE21  | 2.08        | 0.47     |
| 1:H:392:GLU:OE2  | 1:H:438:ALA:HB2  | 2.15        | 0.47     |
| 1:R:388:PRO:HG3  | 1:R:427:CYS:SG   | 2.54        | 0.47     |
| 1:L:388:PRO:HG3  | 1:L:427:CYS:SG   | 2.54        | 0.47     |
| 1:O:431:ARG:HE   | 1:O:432:ASN:ND2  | 2.12        | 0.47     |
| 1:B:392:GLU:OE2  | 1:B:438:ALA:HB2  | 2.15        | 0.47     |
| 1:O:392:GLU:OE2  | 1:O:438:ALA:HB2  | 2.15        | 0.47     |
| 2:F:33:LEU:HD13  | 2:F:38:TRP:HB2   | 1.96        | 0.47     |
| 1:R:431:ARG:HE   | 1:R:432:ASN:ND2  | 2.12        | 0.47     |
| 1:H:93:GLU:HB3   | 1:H:96:GLN:HB3   | 1.97        | 0.47     |

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| Atom-1           | Atom-2          | Distance(Å) | Clash(Å) |
|------------------|-----------------|-------------|----------|
| 1:O:388:PRO:HG3  | 1:O:427:CYS:SG  | 2.54        | 0.47     |
| 1:O:168:PRO:HA   | 1:O:396:ASP:O   | 2.14        | 0.47     |
| 1:V:93:GLU:HB3   | 1:V:96:GLN:HB3  | 1.97        | 0.47     |
| 1:B:464:GLU:OE1  | 1:B:466:LYS:NZ  | 2.47        | 0.47     |
| 1:H:388:PRO:HG3  | 1:H:427:CYS:SG  | 2.55        | 0.47     |
| 1:R:93:GLU:HB3   | 1:R:96:GLN:HB3  | 1.97        | 0.47     |
| 1:E:93:GLU:HB3   | 1:E:96:GLN:HB3  | 1.97        | 0.46     |
| 1:R:446:ARG:HE   | 1:R:450:LYS:NZ  | 2.14        | 0.46     |
| 2:S:42:LEU:HD21  | 2:S:87:LEU:HA   | 1.98        | 0.46     |
| 1:E:446:ARG:HE   | 1:E:450:LYS:NZ  | 2.14        | 0.46     |
| 1:L:392:GLU:OE2  | 1:L:438:ALA:HB2 | 2.15        | 0.46     |
| 1:V:392:GLU:OE2  | 1:V:438:ALA:HB2 | 2.15        | 0.46     |
| 1:L:93:GLU:HB3   | 1:L:96:GLN:HB3  | 1.97        | 0.46     |
| 1:O:93:GLU:HB3   | 1:O:96:GLN:HB3  | 1.97        | 0.46     |
| 1:L:464:GLU:OE1  | 1:L:466:LYS:NZ  | 2.47        | 0.46     |
| 1:R:392:GLU:OE2  | 1:R:438:ALA:HB2 | 2.15        | 0.46     |
| 1:V:446:ARG:HE   | 1:V:450:LYS:NZ  | 2.14        | 0.46     |
| 2:M:33:LEU:HD13  | 2:M:38:TRP:HB2  | 1.96        | 0.46     |
| 1:K:392:GLU:OE2  | 1:K:438:ALA:HB2 | 2.15        | 0.46     |
| 1:V:412:GLY:HA3  | 4:V:484:HOH:O   | 2.16        | 0.46     |
| 1:E:138:LEU:O    | 1:E:316:LYS:NZ  | 2.49        | 0.46     |
| 1:E:331:VAL:HA   | 1:E:337:GLY:O   | 2.16        | 0.46     |
| 2:P:42:LEU:HD21  | 2:P:87:LEU:HA   | 1.98        | 0.46     |
| 1:O:464:GLU:HA   | 1:O:466:LYS:NZ  | 2.30        | 0.46     |
| 1:R:446:ARG:HH21 | 1:R:450:LYS:NZ  | 2.14        | 0.46     |
| 1:E:446:ARG:HH21 | 1:E:450:LYS:NZ  | 2.14        | 0.46     |
| 1:K:446:ARG:HE   | 1:K:450:LYS:NZ  | 2.14        | 0.46     |
| 2:C:5:PRO:HB2    | 2:C:9:LEU:HG    | 1.98        | 0.46     |
| 1:R:464:GLU:OE1  | 1:R:466:LYS:NZ  | 2.47        | 0.46     |
| 1:H:331:VAL:HA   | 1:H:337:GLY:O   | 2.16        | 0.46     |
| 2:M:5:PRO:HB2    | 2:M:9:LEU:HG    | 1.98        | 0.46     |
| 1:K:331:VAL:HA   | 1:K:337:GLY:O   | 2.16        | 0.46     |
| 1:L:464:GLU:HA   | 1:L:466:LYS:NZ  | 2.31        | 0.46     |
| 2:I:42:LEU:HD21  | 2:I:87:LEU:HA   | 1.97        | 0.46     |
| 2:C:42:LEU:HD21  | 2:C:87:LEU:HA   | 1.98        | 0.46     |
| 1:V:446:ARG:HH21 | 1:V:450:LYS:NZ  | 2.14        | 0.46     |
| 2:W:42:LEU:HD21  | 2:W:87:LEU:HA   | 1.98        | 0.46     |
| 2:S:11:LYS:HG3   | 2:S:17:TYR:CZ   | 2.51        | 0.46     |
| 1:H:446:ARG:HH21 | 1:H:450:LYS:NZ  | 2.14        | 0.46     |
| 1:B:93:GLU:HB3   | 1:B:96:GLN:HB3  | 1.97        | 0.46     |
| 1:B:331:VAL:HA   | 1:B:337:GLY:O   | 2.16        | 0.46     |
| 2:T:11:LYS:HG3   | 2:T:17:TYR:CE1  | 2.51        | 0.46     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:446:ARG:HE   | 1:B:450:LYS:NZ   | 2.14        | 0.46     |
| 2:S:5:PRO:HB2    | 2:S:9:LEU:HG     | 1.98        | 0.46     |
| 1:K:93:GLU:HB3   | 1:K:96:GLN:HB3   | 1.97        | 0.46     |
| 2:T:5:PRO:HB2    | 2:T:9:LEU:HG     | 1.98        | 0.46     |
| 2:W:33:LEU:HD13  | 2:W:38:TRP:HB2   | 1.96        | 0.46     |
| 1:H:446:ARG:HE   | 1:H:450:LYS:NZ   | 2.14        | 0.46     |
| 2:P:5:PRO:HB2    | 2:P:9:LEU:HG     | 1.98        | 0.46     |
| 1:R:208:SER:O    | 1:V:109:GLU:HB2  | 2.16        | 0.46     |
| 2:T:42:LEU:HD21  | 2:T:87:LEU:HA    | 1.98        | 0.46     |
| 2:I:5:PRO:HB2    | 2:I:9:LEU:HG     | 1.98        | 0.46     |
| 2:F:11:LYS:HG3   | 2:F:17:TYR:CE1   | 2.51        | 0.46     |
| 1:V:464:GLU:HA   | 1:V:466:LYS:NZ   | 2.31        | 0.45     |
| 1:H:464:GLU:HA   | 1:H:466:LYS:NZ   | 2.30        | 0.45     |
| 2:W:11:LYS:HG3   | 2:W:17:TYR:CZ    | 2.51        | 0.45     |
| 1:L:446:ARG:HE   | 1:L:450:LYS:NZ   | 2.14        | 0.45     |
| 2:F:5:PRO:HB2    | 2:F:9:LEU:HG     | 1.98        | 0.45     |
| 1:V:331:VAL:HA   | 1:V:337:GLY:O    | 2.16        | 0.45     |
| 1:E:392:GLU:OE2  | 1:E:438:ALA:HB2  | 2.15        | 0.45     |
| 2:P:11:LYS:HG3   | 2:P:17:TYR:CZ    | 2.51        | 0.45     |
| 1:B:464:GLU:HA   | 1:B:466:LYS:NZ   | 2.30        | 0.45     |
| 2:T:11:LYS:HG3   | 2:T:17:TYR:CZ    | 2.51        | 0.45     |
| 1:K:197:LEU:HG   | 1:K:417:ALA:HB1  | 1.99        | 0.45     |
| 2:W:5:PRO:HB2    | 2:W:9:LEU:HG     | 1.98        | 0.45     |
| 1:L:331:VAL:HA   | 1:L:337:GLY:O    | 2.16        | 0.45     |
| 1:E:464:GLU:HA   | 1:E:466:LYS:NZ   | 2.30        | 0.45     |
| 2:F:42:LEU:HD21  | 2:F:87:LEU:HA    | 1.98        | 0.45     |
| 1:O:331:VAL:HA   | 1:O:337:GLY:O    | 2.16        | 0.45     |
| 2:C:11:LYS:HG3   | 2:C:17:TYR:CZ    | 2.51        | 0.45     |
| 2:C:11:LYS:HG3   | 2:C:17:TYR:CE1   | 2.51        | 0.45     |
| 1:R:331:VAL:HA   | 1:R:337:GLY:O    | 2.16        | 0.45     |
| 1:K:464:GLU:HA   | 1:K:466:LYS:NZ   | 2.31        | 0.45     |
| 1:O:197:LEU:HG   | 1:O:417:ALA:HB1  | 1.99        | 0.45     |
| 2:I:11:LYS:HG3   | 2:I:17:TYR:CE1   | 2.51        | 0.45     |
| 1:R:464:GLU:HA   | 1:R:466:LYS:NZ   | 2.30        | 0.45     |
| 2:S:11:LYS:HG3   | 2:S:17:TYR:CE1   | 2.51        | 0.45     |
| 2:M:11:LYS:HG3   | 2:M:17:TYR:CE1   | 2.51        | 0.45     |
| 2:M:42:LEU:HD21  | 2:M:87:LEU:HA    | 1.98        | 0.45     |
| 1:R:138:LEU:O    | 1:R:316:LYS:NZ   | 2.49        | 0.45     |
| 1:E:127:PHE:HA   | 1:H:335:LEU:HD23 | 1.98        | 0.45     |
| 1:K:446:ARG:HH21 | 1:K:450:LYS:NZ   | 2.14        | 0.45     |
| 2:W:11:LYS:HG3   | 2:W:17:TYR:CE1   | 2.51        | 0.45     |
| 1:L:446:ARG:HH21 | 1:L:450:LYS:NZ   | 2.14        | 0.45     |

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| Atom-1           | Atom-2          | Distance(Å) | Clash(Å) |
|------------------|-----------------|-------------|----------|
| 1:O:446:ARG:HE   | 1:O:450:LYS:NZ  | 2.14        | 0.45     |
| 2:F:11:LYS:HG3   | 2:F:17:TYR:CZ   | 2.51        | 0.45     |
| 2:M:11:LYS:HG3   | 2:M:17:TYR:CZ   | 2.51        | 0.45     |
| 2:W:22:THR:N     | 2:W:25:GLN:HE21 | 2.08        | 0.45     |
| 1:O:446:ARG:HH21 | 1:O:450:LYS:NZ  | 2.14        | 0.45     |
| 1:E:197:LEU:HG   | 1:E:417:ALA:HB1 | 1.99        | 0.45     |
| 2:S:71:LYS:H     | 2:T:3:VAL:HG22  | 1.81        | 0.45     |
| 1:K:75:THR:HG22  | 1:K:76:ASN:H    | 1.82        | 0.45     |
| 1:B:75:THR:HG22  | 1:B:76:ASN:H    | 1.82        | 0.45     |
| 1:V:75:THR:HG22  | 1:V:76:ASN:H    | 1.82        | 0.45     |
| 1:H:197:LEU:HG   | 1:H:417:ALA:HB1 | 1.99        | 0.44     |
| 1:R:75:THR:HG22  | 1:R:76:ASN:H    | 1.82        | 0.44     |
| 1:L:464:GLU:HA   | 1:L:466:LYS:HZ2 | 1.81        | 0.44     |
| 1:B:446:ARG:HH21 | 1:B:450:LYS:NZ  | 2.14        | 0.44     |
| 2:P:11:LYS:HG3   | 2:P:17:TYR:CE1  | 2.51        | 0.44     |
| 2:I:11:LYS:HG3   | 2:I:17:TYR:CZ   | 2.51        | 0.44     |
| 1:K:208:SER:O    | 1:O:109:GLU:HB2 | 2.17        | 0.44     |
| 1:R:197:LEU:HG   | 1:R:417:ALA:HB1 | 1.99        | 0.44     |
| 2:P:68:THR:HG21  | 2:W:6:ILE:HG12  | 1.98        | 0.44     |
| 2:C:3:VAL:HG21   | 2:W:70:TRP:CE3  | 2.52        | 0.44     |
| 1:L:138:LEU:O    | 1:L:316:LYS:NZ  | 2.49        | 0.44     |
| 2:P:22:THR:N     | 2:P:25:GLN:HE21 | 2.08        | 0.44     |
| 1:L:197:LEU:HG   | 1:L:417:ALA:HB1 | 1.99        | 0.44     |
| 2:P:40:PRO:HG2   | 2:P:74:MET:HB2  | 2.00        | 0.44     |
| 1:B:197:LEU:HG   | 1:B:417:ALA:HB1 | 1.99        | 0.44     |
| 2:S:40:PRO:HG2   | 2:S:74:MET:HB2  | 2.00        | 0.44     |
| 1:K:241:ASN:ND2  | 1:K:243:THR:H   | 2.16        | 0.44     |
| 1:V:197:LEU:HG   | 1:V:417:ALA:HB1 | 1.99        | 0.44     |
| 2:I:79:ASP:HA    | 2:I:80:PRO:HD2  | 1.89        | 0.44     |
| 1:H:241:ASN:ND2  | 1:H:243:THR:H   | 2.16        | 0.44     |
| 2:T:79:ASP:HA    | 2:T:80:PRO:HD2  | 1.88        | 0.44     |
| 1:O:138:LEU:O    | 1:O:316:LYS:NZ  | 2.49        | 0.44     |
| 2:W:40:PRO:HG2   | 2:W:74:MET:HB2  | 2.00        | 0.44     |
| 1:O:241:ASN:ND2  | 1:O:243:THR:H   | 2.16        | 0.44     |
| 1:E:241:ASN:ND2  | 1:E:243:THR:H   | 2.16        | 0.43     |
| 2:T:40:PRO:HG2   | 2:T:74:MET:HB2  | 2.00        | 0.43     |
| 1:L:241:ASN:ND2  | 1:L:243:THR:H   | 2.16        | 0.43     |
| 1:B:138:LEU:O    | 1:B:316:LYS:NZ  | 2.49        | 0.43     |
| 2:P:79:ASP:HA    | 2:P:80:PRO:HD2  | 1.89        | 0.43     |
| 1:K:138:LEU:O    | 1:K:316:LYS:NZ  | 2.49        | 0.43     |
| 1:V:241:ASN:ND2  | 1:V:243:THR:H   | 2.16        | 0.43     |
| 1:O:75:THR:HG22  | 1:O:76:ASN:H    | 1.82        | 0.43     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:F:79:ASP:HA    | 2:F:80:PRO:HD2   | 1.89        | 0.43     |
| 2:S:79:ASP:HA    | 2:S:80:PRO:HD2   | 1.89        | 0.43     |
| 1:K:62:SER:O     | 1:O:177:LYS:HB2  | 2.18        | 0.43     |
| 2:M:33:LEU:HB2   | 2:M:113:ILE:CD1  | 2.38        | 0.43     |
| 1:R:241:ASN:ND2  | 1:R:243:THR:H    | 2.16        | 0.43     |
| 1:L:316:LYS:HE3  | 1:L:348:LEU:HD13 | 2.01        | 0.43     |
| 1:E:75:THR:HG22  | 1:E:76:ASN:H     | 1.82        | 0.43     |
| 1:H:75:THR:HG22  | 1:H:76:ASN:H     | 1.82        | 0.43     |
| 1:R:200:THR:OG1  | 1:R:238:HIS:CD2  | 2.69        | 0.43     |
| 1:O:316:LYS:HE3  | 1:O:348:LEU:HD13 | 2.01        | 0.43     |
| 2:C:33:LEU:HB2   | 2:C:113:ILE:CD1  | 2.38        | 0.43     |
| 1:R:316:LYS:HE3  | 1:R:348:LEU:HD13 | 2.01        | 0.43     |
| 2:C:40:PRO:HG2   | 2:C:74:MET:HB2   | 2.00        | 0.43     |
| 1:L:75:THR:HG22  | 1:L:76:ASN:H     | 1.82        | 0.43     |
| 1:K:123:ASN:ND2  | 3:O:476:RUB:O4   | 2.52        | 0.43     |
| 2:M:40:PRO:HG2   | 2:M:74:MET:HB2   | 2.00        | 0.43     |
| 1:E:335:LEU:HD23 | 1:H:127:PHE:HA   | 2.00        | 0.43     |
| 2:T:22:THR:N     | 2:T:25:GLN:HE21  | 2.08        | 0.43     |
| 1:B:241:ASN:ND2  | 1:B:243:THR:H    | 2.16        | 0.43     |
| 1:O:379:SER:HB2  | 1:O:401:GLN:HB2  | 2.01        | 0.42     |
| 1:L:379:SER:HB2  | 1:L:401:GLN:HB2  | 2.01        | 0.42     |
| 1:K:151:PRO:HA   | 1:K:152:PRO:HD3  | 1.95        | 0.42     |
| 1:K:316:LYS:HE3  | 1:K:348:LEU:HD13 | 2.01        | 0.42     |
| 1:L:109:GLU:HB2  | 1:B:208:SER:O    | 2.20        | 0.42     |
| 1:B:379:SER:HB2  | 1:B:401:GLN:HB2  | 2.01        | 0.42     |
| 1:B:316:LYS:HE3  | 1:B:348:LEU:HD13 | 2.01        | 0.42     |
| 1:R:239:TYR:HE2  | 1:R:401:GLN:HE22 | 1.68        | 0.42     |
| 2:I:40:PRO:HG2   | 2:I:74:MET:HB2   | 2.00        | 0.42     |
| 1:H:239:TYR:HE2  | 1:H:401:GLN:HE22 | 1.68        | 0.42     |
| 2:F:40:PRO:HG2   | 2:F:74:MET:HB2   | 2.00        | 0.42     |
| 1:E:239:TYR:HE2  | 1:E:401:GLN:HE22 | 1.68        | 0.42     |
| 1:H:200:THR:OG1  | 1:H:238:HIS:CD2  | 2.69        | 0.42     |
| 1:E:316:LYS:HE3  | 1:E:348:LEU:HD13 | 2.01        | 0.42     |
| 1:H:151:PRO:HA   | 1:H:152:PRO:HD3  | 1.95        | 0.42     |
| 1:V:239:TYR:HE2  | 1:V:401:GLN:HE22 | 1.68        | 0.42     |
| 1:K:335:LEU:HD23 | 1:O:127:PHE:HA   | 2.02        | 0.42     |
| 1:K:200:THR:OG1  | 1:K:238:HIS:CD2  | 2.69        | 0.42     |
| 1:L:239:TYR:HE2  | 1:L:401:GLN:HE22 | 1.68        | 0.42     |
| 1:H:316:LYS:HE3  | 1:H:348:LEU:HD13 | 2.01        | 0.42     |
| 1:L:127:PHE:HA   | 1:B:335:LEU:HD23 | 2.01        | 0.42     |
| 2:I:22:THR:N     | 2:I:25:GLN:HE21  | 2.08        | 0.42     |
| 1:H:379:SER:HB2  | 1:H:401:GLN:HB2  | 2.01        | 0.42     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:E:379:SER:HB2  | 1:E:401:GLN:HB2  | 2.01        | 0.42     |
| 1:E:200:THR:OG1  | 1:E:238:HIS:CD2  | 2.69        | 0.42     |
| 1:O:239:TYR:HE2  | 1:O:401:GLN:HE22 | 1.68        | 0.42     |
| 1:K:239:TYR:HE2  | 1:K:401:GLN:HE22 | 1.68        | 0.42     |
| 1:V:316:LYS:HE3  | 1:V:348:LEU:HD13 | 2.01        | 0.42     |
| 2:S:72:LEU:HD21  | 1:R:412:GLY:HA2  | 2.01        | 0.42     |
| 1:E:194:ARG:NH1  | 2:F:6:ILE:HD12   | 2.35        | 0.41     |
| 1:L:194:ARG:NH1  | 2:S:6:ILE:HD12   | 2.35        | 0.41     |
| 1:H:19:ASP:HB3   | 1:H:21:LYS:HG2   | 2.02        | 0.41     |
| 1:O:151:PRO:HA   | 1:O:152:PRO:HD3  | 1.95        | 0.41     |
| 1:E:19:ASP:HB3   | 1:E:21:LYS:HG2   | 2.02        | 0.41     |
| 1:H:194:ARG:NH1  | 2:I:6:ILE:HD12   | 2.35        | 0.41     |
| 1:B:464:GLU:HA   | 1:B:466:LYS:HZ2  | 1.84        | 0.41     |
| 1:L:335:LEU:HD23 | 1:B:127:PHE:HA   | 2.02        | 0.41     |
| 1:R:194:ARG:NH1  | 2:T:6:ILE:HD12   | 2.35        | 0.41     |
| 1:K:229:GLN:HG3  | 1:K:234:GLU:O    | 2.21        | 0.41     |
| 1:O:194:ARG:NH1  | 2:P:6:ILE:HD12   | 2.35        | 0.41     |
| 1:V:194:ARG:NH1  | 2:W:6:ILE:HD12   | 2.35        | 0.41     |
| 1:R:379:SER:HB2  | 1:R:401:GLN:HB2  | 2.01        | 0.41     |
| 1:L:19:ASP:HB3   | 1:L:21:LYS:HG2   | 2.03        | 0.41     |
| 1:K:410:PRO:HD3  | 1:K:461:VAL:HG21 | 2.03        | 0.41     |
| 1:B:410:PRO:HD3  | 1:B:461:VAL:HG21 | 2.03        | 0.41     |
| 2:C:79:ASP:HA    | 2:C:80:PRO:HD2   | 1.89        | 0.41     |
| 1:L:208:SER:O    | 1:B:109:GLU:HB2  | 2.20        | 0.41     |
| 1:B:194:ARG:NH1  | 2:C:6:ILE:HD12   | 2.35        | 0.41     |
| 1:B:239:TYR:HE2  | 1:B:401:GLN:HE22 | 1.68        | 0.41     |
| 1:O:19:ASP:HB3   | 1:O:21:LYS:HG2   | 2.02        | 0.41     |
| 2:I:33:LEU:HB2   | 2:I:113:ILE:CD1  | 2.38        | 0.41     |
| 1:R:184:ASN:HA   | 1:R:184:ASN:HD22 | 1.75        | 0.41     |
| 1:H:138:LEU:O    | 1:H:316:LYS:NZ   | 2.49        | 0.41     |
| 1:B:22:LEU:HD23  | 1:B:22:LEU:HA    | 1.90        | 0.41     |
| 2:F:4:TRP:HA     | 2:F:5:PRO:HD3    | 1.92        | 0.41     |
| 1:O:212:MET:SD   | 1:O:217:ARG:HD3  | 2.61        | 0.41     |
| 1:R:410:PRO:HD3  | 1:R:461:VAL:HG21 | 2.03        | 0.41     |
| 1:V:121:VAL:HG22 | 1:V:125:PHE:CE1  | 2.56        | 0.41     |
| 2:M:79:ASP:HA    | 2:M:80:PRO:HD2   | 1.89        | 0.41     |
| 1:H:410:PRO:HD3  | 1:H:461:VAL:HG21 | 2.03        | 0.41     |
| 2:F:33:LEU:HB2   | 2:F:113:ILE:CD1  | 2.38        | 0.41     |
| 2:S:22:THR:N     | 2:S:25:GLN:HE21  | 2.08        | 0.41     |
| 1:V:229:GLN:HG3  | 1:V:234:GLU:O    | 2.21        | 0.41     |
| 1:K:194:ARG:NH1  | 2:M:6:ILE:HD12   | 2.35        | 0.41     |
| 1:O:121:VAL:HG22 | 1:O:125:PHE:CE1  | 2.56        | 0.41     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:V:212:MET:SD   | 1:V:217:ARG:HD3  | 2.61        | 0.41     |
| 1:K:212:MET:SD   | 1:K:217:ARG:HD3  | 2.61        | 0.41     |
| 1:R:212:MET:SD   | 1:R:217:ARG:HD3  | 2.61        | 0.41     |
| 1:L:212:MET:SD   | 1:L:217:ARG:HD3  | 2.61        | 0.41     |
| 1:V:19:ASP:HB3   | 1:V:21:LYS:HG2   | 2.02        | 0.41     |
| 1:E:22:LEU:HA    | 1:E:22:LEU:HD23  | 1.90        | 0.41     |
| 1:O:229:GLN:HG3  | 1:O:234:GLU:O    | 2.21        | 0.41     |
| 1:R:229:GLN:HG3  | 1:R:234:GLU:O    | 2.21        | 0.41     |
| 1:L:229:GLN:HG3  | 1:L:234:GLU:O    | 2.21        | 0.41     |
| 1:V:379:SER:HB2  | 1:V:401:GLN:HB2  | 2.01        | 0.41     |
| 1:K:379:SER:HB2  | 1:K:401:GLN:HB2  | 2.01        | 0.41     |
| 1:E:410:PRO:HD3  | 1:E:461:VAL:HG21 | 2.03        | 0.41     |
| 1:V:410:PRO:HD3  | 1:V:461:VAL:HG21 | 2.03        | 0.41     |
| 1:R:121:VAL:HG22 | 1:R:125:PHE:CE1  | 2.56        | 0.41     |
| 1:B:212:MET:SD   | 1:B:217:ARG:HD3  | 2.61        | 0.41     |
| 1:B:177:LYS:HE3  | 4:B:495:HOH:O    | 2.21        | 0.41     |
| 1:E:121:VAL:HG22 | 1:E:125:PHE:CE1  | 2.56        | 0.41     |
| 1:H:121:VAL:HG22 | 1:H:125:PHE:CE1  | 2.56        | 0.41     |
| 1:L:200:THR:OG1  | 1:L:238:HIS:CD2  | 2.69        | 0.40     |
| 1:R:109:GLU:HB2  | 1:V:208:SER:O    | 2.21        | 0.40     |
| 1:L:121:VAL:HG22 | 1:L:125:PHE:CE1  | 2.56        | 0.40     |
| 1:R:19:ASP:HB3   | 1:R:21:LYS:HG2   | 2.02        | 0.40     |
| 1:K:296:ALA:O    | 1:K:297:MET:HB3  | 2.22        | 0.40     |
| 1:V:334:LYS:HG3  | 1:V:335:LEU:HG   | 2.04        | 0.40     |
| 2:F:22:THR:N     | 2:F:25:GLN:HE21  | 2.09        | 0.40     |
| 1:B:229:GLN:HG3  | 1:B:234:GLU:O    | 2.21        | 0.40     |
| 1:K:177:LYS:HE3  | 4:K:490:HOH:O    | 2.21        | 0.40     |
| 1:B:171:GLY:HA3  | 1:B:401:GLN:HG2  | 2.04        | 0.40     |
| 4:L:507:HOH:O    | 1:B:275:THR:HB   | 2.22        | 0.40     |
| 1:R:334:LYS:HG3  | 1:R:335:LEU:HG   | 2.04        | 0.40     |
| 1:K:275:THR:HB   | 4:O:1156:HOH:O   | 2.22        | 0.40     |
| 1:R:407:LEU:O    | 1:V:69:VAL:HA    | 2.22        | 0.40     |
| 1:R:296:ALA:O    | 1:R:297:MET:HB3  | 2.22        | 0.40     |
| 1:E:229:GLN:HG3  | 1:E:234:GLU:O    | 2.21        | 0.40     |
| 1:L:251:MET:HE2  | 1:L:251:MET:HB3  | 1.88        | 0.40     |
| 1:O:334:LYS:HG3  | 1:O:335:LEU:HG   | 2.04        | 0.40     |
| 1:K:121:VAL:HG22 | 1:K:125:PHE:CE1  | 2.56        | 0.40     |

All (12) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

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| Atom-1          | Atom-2                 | Distance(Å) | Clash(Å) |
|-----------------|------------------------|-------------|----------|
| 1:H:464:GLU:CD  | 1:V:468:GLU:OE1[3_446] | 1.11        | 1.09     |
| 1:H:464:GLU:OE1 | 1:V:468:GLU:OE1[3_446] | 1.37        | 0.83     |
| 1:V:469:PHE:CA  | 4:H:634:HOH:O[3_456]   | 1.39        | 0.81     |
| 1:V:469:PHE:N   | 4:H:634:HOH:O[3_456]   | 1.62        | 0.58     |
| 1:H:464:GLU:CG  | 1:V:468:GLU:OE1[3_446] | 1.85        | 0.35     |
| 1:V:468:GLU:C   | 4:H:634:HOH:O[3_456]   | 1.86        | 0.34     |
| 1:V:468:GLU:O   | 4:H:634:HOH:O[3_456]   | 1.92        | 0.28     |
| 1:H:464:GLU:OE2 | 1:V:468:GLU:OE1[3_446] | 2.00        | 0.20     |
| 1:H:464:GLU:OE2 | 1:V:468:GLU:CB[3_446]  | 2.01        | 0.19     |
| 1:L:338:GLU:OE2 | 4:K:619:HOH:O[4_455]   | 2.15        | 0.05     |
| 1:V:469:PHE:C   | 4:H:634:HOH:O[3_456]   | 2.18        | 0.02     |
| 1:E:439:ARG:NH1 | 1:R:469:PHE:O[3_445]   | 2.19        | 0.01     |

## 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   | B     | 465/475 (98%) | 449 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | E     | 465/475 (98%) | 449 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | H     | 465/475 (98%) | 449 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | K     | 465/475 (98%) | 449 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | L     | 465/475 (98%) | 449 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | O     | 465/475 (98%) | 449 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | R     | 465/475 (98%) | 449 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | V     | 465/475 (98%) | 449 (97%) | 16 (3%) | 0        | 100         | 100 |
| 2   | C     | 121/123 (98%) | 117 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 2   | F     | 121/123 (98%) | 117 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 2   | I     | 121/123 (98%) | 117 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 2   | M     | 121/123 (98%) | 117 (97%) | 4 (3%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 2   | P     | 121/123 (98%)   | 117 (97%)  | 4 (3%)   | 0        | 100         | 100 |
| 2   | S     | 121/123 (98%)   | 117 (97%)  | 4 (3%)   | 0        | 100         | 100 |
| 2   | T     | 121/123 (98%)   | 117 (97%)  | 4 (3%)   | 0        | 100         | 100 |
| 2   | W     | 121/123 (98%)   | 117 (97%)  | 4 (3%)   | 0        | 100         | 100 |
| All | All   | 4688/4784 (98%) | 4528 (97%) | 160 (3%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | B     | 378/386 (98%)   | 365 (97%)  | 13 (3%)  | 49          | 70 |
| 1   | E     | 378/386 (98%)   | 365 (97%)  | 13 (3%)  | 49          | 70 |
| 1   | H     | 378/386 (98%)   | 365 (97%)  | 13 (3%)  | 49          | 70 |
| 1   | K     | 378/386 (98%)   | 365 (97%)  | 13 (3%)  | 49          | 70 |
| 1   | L     | 378/386 (98%)   | 365 (97%)  | 13 (3%)  | 49          | 70 |
| 1   | O     | 378/386 (98%)   | 365 (97%)  | 13 (3%)  | 49          | 70 |
| 1   | R     | 378/386 (98%)   | 365 (97%)  | 13 (3%)  | 49          | 70 |
| 1   | V     | 378/386 (98%)   | 365 (97%)  | 13 (3%)  | 49          | 70 |
| 2   | C     | 112/112 (100%)  | 103 (92%)  | 9 (8%)   | 17          | 26 |
| 2   | F     | 112/112 (100%)  | 102 (91%)  | 10 (9%)  | 14          | 21 |
| 2   | I     | 112/112 (100%)  | 102 (91%)  | 10 (9%)  | 14          | 21 |
| 2   | M     | 112/112 (100%)  | 103 (92%)  | 9 (8%)   | 17          | 26 |
| 2   | P     | 112/112 (100%)  | 102 (91%)  | 10 (9%)  | 14          | 21 |
| 2   | S     | 112/112 (100%)  | 102 (91%)  | 10 (9%)  | 14          | 21 |
| 2   | T     | 112/112 (100%)  | 102 (91%)  | 10 (9%)  | 14          | 21 |
| 2   | W     | 112/112 (100%)  | 103 (92%)  | 9 (8%)   | 17          | 26 |
| All | All   | 3920/3984 (98%) | 3739 (95%) | 181 (5%) | 37          | 55 |

All (181) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 11  | VAL  |
| 1   | L     | 28  | GLU  |
| 1   | L     | 75  | THR  |
| 1   | L     | 83  | ARG  |
| 1   | L     | 94  | GLU  |
| 1   | L     | 127 | PHE  |
| 1   | L     | 185 | TYR  |
| 1   | L     | 225 | LEU  |
| 1   | L     | 239 | TYR  |
| 1   | L     | 241 | ASN  |
| 1   | L     | 268 | ASP  |
| 1   | L     | 392 | GLU  |
| 1   | L     | 439 | ARG  |
| 2   | S     | 9   | LEU  |
| 2   | S     | 24  | ASP  |
| 2   | S     | 33  | LEU  |
| 2   | S     | 37  | LYS  |
| 2   | S     | 46  | THR  |
| 2   | S     | 47  | ASP  |
| 2   | S     | 56  | HIS  |
| 2   | S     | 68  | THR  |
| 2   | S     | 92  | LYS  |
| 2   | S     | 93  | GLU  |
| 1   | B     | 11  | VAL  |
| 1   | B     | 28  | GLU  |
| 1   | B     | 75  | THR  |
| 1   | B     | 83  | ARG  |
| 1   | B     | 94  | GLU  |
| 1   | B     | 127 | PHE  |
| 1   | B     | 185 | TYR  |
| 1   | B     | 225 | LEU  |
| 1   | B     | 239 | TYR  |
| 1   | B     | 241 | ASN  |
| 1   | B     | 268 | ASP  |
| 1   | B     | 392 | GLU  |
| 1   | B     | 439 | ARG  |
| 2   | C     | 9   | LEU  |
| 2   | C     | 24  | ASP  |
| 2   | C     | 33  | LEU  |
| 2   | C     | 46  | THR  |
| 2   | C     | 47  | ASP  |
| 2   | C     | 56  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 68  | THR  |
| 2   | C     | 92  | LYS  |
| 2   | C     | 93  | GLU  |
| 1   | E     | 11  | VAL  |
| 1   | E     | 28  | GLU  |
| 1   | E     | 75  | THR  |
| 1   | E     | 83  | ARG  |
| 1   | E     | 94  | GLU  |
| 1   | E     | 127 | PHE  |
| 1   | E     | 185 | TYR  |
| 1   | E     | 225 | LEU  |
| 1   | E     | 239 | TYR  |
| 1   | E     | 241 | ASN  |
| 1   | E     | 268 | ASP  |
| 1   | E     | 392 | GLU  |
| 1   | E     | 439 | ARG  |
| 2   | F     | 9   | LEU  |
| 2   | F     | 24  | ASP  |
| 2   | F     | 33  | LEU  |
| 2   | F     | 37  | LYS  |
| 2   | F     | 46  | THR  |
| 2   | F     | 47  | ASP  |
| 2   | F     | 56  | HIS  |
| 2   | F     | 68  | THR  |
| 2   | F     | 92  | LYS  |
| 2   | F     | 93  | GLU  |
| 1   | H     | 11  | VAL  |
| 1   | H     | 28  | GLU  |
| 1   | H     | 75  | THR  |
| 1   | H     | 83  | ARG  |
| 1   | H     | 94  | GLU  |
| 1   | H     | 127 | PHE  |
| 1   | H     | 185 | TYR  |
| 1   | H     | 225 | LEU  |
| 1   | H     | 239 | TYR  |
| 1   | H     | 241 | ASN  |
| 1   | H     | 268 | ASP  |
| 1   | H     | 392 | GLU  |
| 1   | H     | 439 | ARG  |
| 2   | I     | 9   | LEU  |
| 2   | I     | 24  | ASP  |
| 2   | I     | 33  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | I     | 37  | LYS  |
| 2   | I     | 46  | THR  |
| 2   | I     | 47  | ASP  |
| 2   | I     | 56  | HIS  |
| 2   | I     | 68  | THR  |
| 2   | I     | 92  | LYS  |
| 2   | I     | 93  | GLU  |
| 1   | K     | 11  | VAL  |
| 1   | K     | 28  | GLU  |
| 1   | K     | 75  | THR  |
| 1   | K     | 83  | ARG  |
| 1   | K     | 94  | GLU  |
| 1   | K     | 127 | PHE  |
| 1   | K     | 185 | TYR  |
| 1   | K     | 225 | LEU  |
| 1   | K     | 239 | TYR  |
| 1   | K     | 241 | ASN  |
| 1   | K     | 268 | ASP  |
| 1   | K     | 392 | GLU  |
| 1   | K     | 439 | ARG  |
| 2   | M     | 9   | LEU  |
| 2   | M     | 24  | ASP  |
| 2   | M     | 33  | LEU  |
| 2   | M     | 46  | THR  |
| 2   | M     | 47  | ASP  |
| 2   | M     | 56  | HIS  |
| 2   | M     | 68  | THR  |
| 2   | M     | 92  | LYS  |
| 2   | M     | 93  | GLU  |
| 1   | O     | 11  | VAL  |
| 1   | O     | 28  | GLU  |
| 1   | O     | 75  | THR  |
| 1   | O     | 83  | ARG  |
| 1   | O     | 94  | GLU  |
| 1   | O     | 127 | PHE  |
| 1   | O     | 185 | TYR  |
| 1   | O     | 225 | LEU  |
| 1   | O     | 239 | TYR  |
| 1   | O     | 241 | ASN  |
| 1   | O     | 268 | ASP  |
| 1   | O     | 392 | GLU  |
| 1   | O     | 439 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | P     | 9   | LEU  |
| 2   | P     | 24  | ASP  |
| 2   | P     | 33  | LEU  |
| 2   | P     | 37  | LYS  |
| 2   | P     | 46  | THR  |
| 2   | P     | 47  | ASP  |
| 2   | P     | 56  | HIS  |
| 2   | P     | 68  | THR  |
| 2   | P     | 92  | LYS  |
| 2   | P     | 93  | GLU  |
| 1   | R     | 11  | VAL  |
| 1   | R     | 28  | GLU  |
| 1   | R     | 75  | THR  |
| 1   | R     | 83  | ARG  |
| 1   | R     | 94  | GLU  |
| 1   | R     | 127 | PHE  |
| 1   | R     | 185 | TYR  |
| 1   | R     | 225 | LEU  |
| 1   | R     | 239 | TYR  |
| 1   | R     | 241 | ASN  |
| 1   | R     | 268 | ASP  |
| 1   | R     | 392 | GLU  |
| 1   | R     | 439 | ARG  |
| 2   | T     | 9   | LEU  |
| 2   | T     | 24  | ASP  |
| 2   | T     | 33  | LEU  |
| 2   | T     | 37  | LYS  |
| 2   | T     | 46  | THR  |
| 2   | T     | 47  | ASP  |
| 2   | T     | 56  | HIS  |
| 2   | T     | 68  | THR  |
| 2   | T     | 92  | LYS  |
| 2   | T     | 93  | GLU  |
| 1   | V     | 11  | VAL  |
| 1   | V     | 28  | GLU  |
| 1   | V     | 75  | THR  |
| 1   | V     | 83  | ARG  |
| 1   | V     | 94  | GLU  |
| 1   | V     | 127 | PHE  |
| 1   | V     | 185 | TYR  |
| 1   | V     | 225 | LEU  |
| 1   | V     | 239 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | V     | 241 | ASN  |
| 1   | V     | 268 | ASP  |
| 1   | V     | 392 | GLU  |
| 1   | V     | 439 | ARG  |
| 2   | W     | 9   | LEU  |
| 2   | W     | 24  | ASP  |
| 2   | W     | 33  | LEU  |
| 2   | W     | 46  | THR  |
| 2   | W     | 47  | ASP  |
| 2   | W     | 56  | HIS  |
| 2   | W     | 68  | THR  |
| 2   | W     | 92  | LYS  |
| 2   | W     | 93  | GLU  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 184 | ASN  |
| 1   | L     | 229 | GLN  |
| 1   | L     | 238 | HIS  |
| 1   | L     | 241 | ASN  |
| 1   | L     | 267 | HIS  |
| 1   | L     | 277 | ASN  |
| 1   | L     | 282 | HIS  |
| 1   | L     | 304 | GLN  |
| 1   | L     | 401 | GLN  |
| 1   | L     | 432 | ASN  |
| 1   | L     | 442 | ASN  |
| 2   | S     | 25  | GLN  |
| 2   | S     | 29  | GLN  |
| 1   | B     | 184 | ASN  |
| 1   | B     | 229 | GLN  |
| 1   | B     | 238 | HIS  |
| 1   | B     | 241 | ASN  |
| 1   | B     | 267 | HIS  |
| 1   | B     | 277 | ASN  |
| 1   | B     | 282 | HIS  |
| 1   | B     | 304 | GLN  |
| 1   | B     | 401 | GLN  |
| 1   | B     | 432 | ASN  |
| 1   | B     | 442 | ASN  |
| 2   | C     | 25  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 29  | GLN  |
| 1   | E     | 184 | ASN  |
| 1   | E     | 229 | GLN  |
| 1   | E     | 238 | HIS  |
| 1   | E     | 241 | ASN  |
| 1   | E     | 267 | HIS  |
| 1   | E     | 277 | ASN  |
| 1   | E     | 282 | HIS  |
| 1   | E     | 294 | HIS  |
| 1   | E     | 304 | GLN  |
| 1   | E     | 401 | GLN  |
| 1   | E     | 432 | ASN  |
| 1   | E     | 442 | ASN  |
| 2   | F     | 25  | GLN  |
| 2   | F     | 29  | GLN  |
| 1   | H     | 184 | ASN  |
| 1   | H     | 229 | GLN  |
| 1   | H     | 238 | HIS  |
| 1   | H     | 241 | ASN  |
| 1   | H     | 267 | HIS  |
| 1   | H     | 277 | ASN  |
| 1   | H     | 282 | HIS  |
| 1   | H     | 304 | GLN  |
| 1   | H     | 401 | GLN  |
| 1   | H     | 432 | ASN  |
| 1   | H     | 442 | ASN  |
| 2   | I     | 25  | GLN  |
| 2   | I     | 29  | GLN  |
| 1   | K     | 184 | ASN  |
| 1   | K     | 229 | GLN  |
| 1   | K     | 238 | HIS  |
| 1   | K     | 241 | ASN  |
| 1   | K     | 267 | HIS  |
| 1   | K     | 277 | ASN  |
| 1   | K     | 282 | HIS  |
| 1   | K     | 304 | GLN  |
| 1   | K     | 401 | GLN  |
| 1   | K     | 432 | ASN  |
| 1   | K     | 442 | ASN  |
| 2   | M     | 25  | GLN  |
| 2   | M     | 29  | GLN  |
| 1   | O     | 184 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 229 | GLN  |
| 1   | O     | 238 | HIS  |
| 1   | O     | 241 | ASN  |
| 1   | O     | 267 | HIS  |
| 1   | O     | 277 | ASN  |
| 1   | O     | 282 | HIS  |
| 1   | O     | 304 | GLN  |
| 1   | O     | 401 | GLN  |
| 1   | O     | 432 | ASN  |
| 1   | O     | 442 | ASN  |
| 2   | P     | 25  | GLN  |
| 2   | P     | 29  | GLN  |
| 1   | R     | 184 | ASN  |
| 1   | R     | 229 | GLN  |
| 1   | R     | 238 | HIS  |
| 1   | R     | 241 | ASN  |
| 1   | R     | 267 | HIS  |
| 1   | R     | 277 | ASN  |
| 1   | R     | 282 | HIS  |
| 1   | R     | 304 | GLN  |
| 1   | R     | 401 | GLN  |
| 1   | R     | 432 | ASN  |
| 1   | R     | 442 | ASN  |
| 2   | T     | 25  | GLN  |
| 2   | T     | 29  | GLN  |
| 1   | V     | 184 | ASN  |
| 1   | V     | 229 | GLN  |
| 1   | V     | 238 | HIS  |
| 1   | V     | 241 | ASN  |
| 1   | V     | 267 | HIS  |
| 1   | V     | 277 | ASN  |
| 1   | V     | 282 | HIS  |
| 1   | V     | 304 | GLN  |
| 1   | V     | 401 | GLN  |
| 1   | V     | 432 | ASN  |
| 1   | V     | 442 | ASN  |
| 2   | W     | 25  | GLN  |
| 2   | W     | 29  | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.



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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 3   | RUB  | B     | 476 | -    | 17,17,17     | 2.04 | 6 (35%)     | 25,25,25    | 1.72 | 5 (20%)     |
| 3   | RUB  | E     | 476 | -    | 17,17,17     | 2.04 | 5 (29%)     | 25,25,25    | 1.72 | 5 (20%)     |
| 3   | RUB  | H     | 476 | -    | 17,17,17     | 2.04 | 5 (29%)     | 25,25,25    | 1.72 | 5 (20%)     |
| 3   | RUB  | K     | 476 | -    | 17,17,17     | 2.04 | 6 (35%)     | 25,25,25    | 1.72 | 5 (20%)     |
| 3   | RUB  | L     | 476 | -    | 17,17,17     | 2.04 | 6 (35%)     | 25,25,25    | 1.72 | 5 (20%)     |
| 3   | RUB  | O     | 476 | -    | 17,17,17     | 2.05 | 6 (35%)     | 25,25,25    | 1.71 | 5 (20%)     |
| 3   | RUB  | R     | 476 | -    | 17,17,17     | 2.04 | 5 (29%)     | 25,25,25    | 1.72 | 5 (20%)     |
| 3   | RUB  | V     | 476 | -    | 17,17,17     | 2.06 | 6 (35%)     | 25,25,25    | 1.72 | 5 (20%)     |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 3   | RUB  | B     | 476 | -    | -       | 0/20/20/20 | 0/0/0/0 |
| 3   | RUB  | E     | 476 | -    | -       | 0/20/20/20 | 0/0/0/0 |
| 3   | RUB  | H     | 476 | -    | -       | 0/20/20/20 | 0/0/0/0 |
| 3   | RUB  | K     | 476 | -    | -       | 0/20/20/20 | 0/0/0/0 |
| 3   | RUB  | L     | 476 | -    | -       | 0/20/20/20 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 3   | RUB  | O     | 476 | -    | -       | 0/20/20/20 | 0/0/0/0 |
| 3   | RUB  | R     | 476 | -    | -       | 0/20/20/20 | 0/0/0/0 |
| 3   | RUB  | V     | 476 | -    | -       | 0/20/20/20 | 0/0/0/0 |

All (45) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 3   | B     | 476 | RUB  | C3-C2  | 3.89 | 1.58        | 1.52     |
| 3   | E     | 476 | RUB  | C3-C2  | 3.89 | 1.58        | 1.52     |
| 3   | O     | 476 | RUB  | C3-C2  | 3.89 | 1.58        | 1.52     |
| 3   | L     | 476 | RUB  | C3-C2  | 3.86 | 1.58        | 1.52     |
| 3   | K     | 476 | RUB  | C3-C2  | 3.86 | 1.58        | 1.52     |
| 3   | R     | 476 | RUB  | C3-C2  | 3.82 | 1.58        | 1.52     |
| 3   | V     | 476 | RUB  | C3-C2  | 3.82 | 1.58        | 1.52     |
| 3   | H     | 476 | RUB  | C3-C2  | 3.80 | 1.58        | 1.52     |
| 3   | V     | 476 | RUB  | C5-C4  | 3.33 | 1.57        | 1.51     |
| 3   | H     | 476 | RUB  | C5-C4  | 3.32 | 1.56        | 1.51     |
| 3   | R     | 476 | RUB  | C5-C4  | 3.32 | 1.56        | 1.51     |
| 3   | K     | 476 | RUB  | C5-C4  | 3.31 | 1.56        | 1.51     |
| 3   | O     | 476 | RUB  | C5-C4  | 3.30 | 1.56        | 1.51     |
| 3   | L     | 476 | RUB  | C5-C4  | 3.29 | 1.56        | 1.51     |
| 3   | E     | 476 | RUB  | C5-C4  | 3.29 | 1.56        | 1.51     |
| 3   | B     | 476 | RUB  | C5-C4  | 3.24 | 1.56        | 1.51     |
| 3   | O     | 476 | RUB  | C4-C3  | 3.05 | 1.56        | 1.53     |
| 3   | V     | 476 | RUB  | C4-C3  | 3.04 | 1.56        | 1.53     |
| 3   | H     | 476 | RUB  | C4-C3  | 3.04 | 1.56        | 1.53     |
| 3   | E     | 476 | RUB  | C4-C3  | 3.00 | 1.56        | 1.53     |
| 3   | R     | 476 | RUB  | C4-C3  | 2.97 | 1.56        | 1.53     |
| 3   | L     | 476 | RUB  | C4-C3  | 2.97 | 1.56        | 1.53     |
| 3   | K     | 476 | RUB  | P2-O5P | 2.97 | 1.65        | 1.54     |
| 3   | V     | 476 | RUB  | P2-O5P | 2.97 | 1.65        | 1.54     |
| 3   | B     | 476 | RUB  | P2-O5P | 2.96 | 1.65        | 1.54     |
| 3   | B     | 476 | RUB  | C4-C3  | 2.95 | 1.56        | 1.53     |
| 3   | L     | 476 | RUB  | P2-O5P | 2.94 | 1.65        | 1.54     |
| 3   | O     | 476 | RUB  | P2-O5P | 2.94 | 1.65        | 1.54     |
| 3   | E     | 476 | RUB  | P2-O5P | 2.94 | 1.65        | 1.54     |
| 3   | R     | 476 | RUB  | P2-O5P | 2.93 | 1.65        | 1.54     |
| 3   | H     | 476 | RUB  | P2-O5P | 2.93 | 1.65        | 1.54     |
| 3   | K     | 476 | RUB  | C4-C3  | 2.91 | 1.56        | 1.53     |
| 3   | B     | 476 | RUB  | P2-O5  | 2.69 | 1.69        | 1.60     |
| 3   | H     | 476 | RUB  | P2-O5  | 2.69 | 1.69        | 1.60     |
| 3   | L     | 476 | RUB  | P2-O5  | 2.69 | 1.69        | 1.60     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | V     | 476 | RUB  | P2-O5 | 2.69  | 1.69        | 1.60     |
| 3   | E     | 476 | RUB  | P2-O5 | 2.68  | 1.69        | 1.60     |
| 3   | R     | 476 | RUB  | P2-O5 | 2.68  | 1.69        | 1.60     |
| 3   | O     | 476 | RUB  | P2-O5 | 2.67  | 1.69        | 1.60     |
| 3   | K     | 476 | RUB  | P2-O5 | 2.67  | 1.69        | 1.60     |
| 3   | B     | 476 | RUB  | O4-C4 | -2.05 | 1.38        | 1.43     |
| 3   | V     | 476 | RUB  | O4-C4 | -2.03 | 1.38        | 1.43     |
| 3   | O     | 476 | RUB  | O4-C4 | -2.01 | 1.38        | 1.43     |
| 3   | K     | 476 | RUB  | O4-C4 | -2.01 | 1.38        | 1.43     |
| 3   | L     | 476 | RUB  | O4-C4 | -2.00 | 1.38        | 1.43     |

All (40) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 3   | V     | 476 | RUB  | O1-C1-C2   | 5.33 | 118.79      | 110.31   |
| 3   | E     | 476 | RUB  | O1-C1-C2   | 5.32 | 118.77      | 110.31   |
| 3   | H     | 476 | RUB  | O1-C1-C2   | 5.31 | 118.76      | 110.31   |
| 3   | L     | 476 | RUB  | O1-C1-C2   | 5.30 | 118.74      | 110.31   |
| 3   | B     | 476 | RUB  | O1-C1-C2   | 5.30 | 118.74      | 110.31   |
| 3   | R     | 476 | RUB  | O1-C1-C2   | 5.30 | 118.74      | 110.31   |
| 3   | K     | 476 | RUB  | O1-C1-C2   | 5.29 | 118.72      | 110.31   |
| 3   | O     | 476 | RUB  | O1-C1-C2   | 5.27 | 118.69      | 110.31   |
| 3   | K     | 476 | RUB  | C4-C3-C2   | 3.31 | 115.05      | 110.77   |
| 3   | H     | 476 | RUB  | C4-C3-C2   | 3.30 | 115.04      | 110.77   |
| 3   | L     | 476 | RUB  | C4-C3-C2   | 3.29 | 115.02      | 110.77   |
| 3   | E     | 476 | RUB  | C4-C3-C2   | 3.29 | 115.02      | 110.77   |
| 3   | V     | 476 | RUB  | C4-C3-C2   | 3.28 | 115.00      | 110.77   |
| 3   | B     | 476 | RUB  | C4-C3-C2   | 3.27 | 115.00      | 110.77   |
| 3   | O     | 476 | RUB  | C4-C3-C2   | 3.27 | 114.99      | 110.77   |
| 3   | R     | 476 | RUB  | C4-C3-C2   | 3.26 | 114.98      | 110.77   |
| 3   | V     | 476 | RUB  | O3P-P1-O1P | 2.79 | 119.55      | 110.44   |
| 3   | R     | 476 | RUB  | O3P-P1-O1P | 2.78 | 119.53      | 110.44   |
| 3   | H     | 476 | RUB  | O3P-P1-O1P | 2.78 | 119.52      | 110.44   |
| 3   | L     | 476 | RUB  | O3P-P1-O1P | 2.78 | 119.52      | 110.44   |
| 3   | E     | 476 | RUB  | O3P-P1-O1P | 2.77 | 119.50      | 110.44   |
| 3   | B     | 476 | RUB  | O3P-P1-O1P | 2.77 | 119.50      | 110.44   |
| 3   | O     | 476 | RUB  | O3P-P1-O1P | 2.77 | 119.49      | 110.44   |
| 3   | K     | 476 | RUB  | O3P-P1-O1P | 2.77 | 119.49      | 110.44   |
| 3   | K     | 476 | RUB  | C5-C4-C3   | 2.40 | 115.90      | 111.84   |
| 3   | R     | 476 | RUB  | C5-C4-C3   | 2.40 | 115.91      | 111.84   |
| 3   | L     | 476 | RUB  | C5-C4-C3   | 2.40 | 115.90      | 111.84   |
| 3   | B     | 476 | RUB  | C5-C4-C3   | 2.40 | 115.90      | 111.84   |

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| Mol | Chain | Res | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 3   | E     | 476 | RUB  | C5-C4-C3   | 2.40 | 115.89      | 111.84   |
| 3   | H     | 476 | RUB  | C5-C4-C3   | 2.39 | 115.88      | 111.84   |
| 3   | V     | 476 | RUB  | C5-C4-C3   | 2.39 | 115.87      | 111.84   |
| 3   | O     | 476 | RUB  | C5-C4-C3   | 2.38 | 115.87      | 111.84   |
| 3   | B     | 476 | RUB  | O6P-P2-O4P | 2.26 | 117.84      | 110.44   |
| 3   | H     | 476 | RUB  | O6P-P2-O4P | 2.26 | 117.83      | 110.44   |
| 3   | K     | 476 | RUB  | O6P-P2-O4P | 2.26 | 117.82      | 110.44   |
| 3   | O     | 476 | RUB  | O6P-P2-O4P | 2.26 | 117.81      | 110.44   |
| 3   | L     | 476 | RUB  | O6P-P2-O4P | 2.25 | 117.81      | 110.44   |
| 3   | V     | 476 | RUB  | O6P-P2-O4P | 2.25 | 117.81      | 110.44   |
| 3   | R     | 476 | RUB  | O6P-P2-O4P | 2.25 | 117.78      | 110.44   |
| 3   | E     | 476 | RUB  | O6P-P2-O4P | 2.24 | 117.78      | 110.44   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | B     | 467/475 (98%)   | -0.65  | 6 (1%) 74 73  | 6, 15, 36, 56         | 0     |
| 1   | E     | 467/475 (98%)   | -0.66  | 4 (0%) 81 81  | 6, 15, 36, 56         | 0     |
| 1   | H     | 467/475 (98%)   | -0.60  | 8 (1%) 67 65  | 6, 15, 36, 56         | 0     |
| 1   | K     | 467/475 (98%)   | -0.57  | 5 (1%) 77 77  | 6, 15, 36, 56         | 0     |
| 1   | L     | 467/475 (98%)   | -0.58  | 5 (1%) 77 77  | 6, 15, 36, 56         | 0     |
| 1   | O     | 467/475 (98%)   | -0.56  | 5 (1%) 77 77  | 6, 15, 36, 56         | 0     |
| 1   | R     | 467/475 (98%)   | -0.43  | 14 (2%) 48 45 | 6, 15, 36, 56         | 0     |
| 1   | V     | 467/475 (98%)   | -0.45  | 20 (4%) 34 32 | 6, 15, 36, 56         | 0     |
| 2   | C     | 123/123 (100%)  | -0.40  | 1 (0%) 83 82  | 9, 21, 37, 45         | 0     |
| 2   | F     | 123/123 (100%)  | -0.49  | 0 100 100     | 9, 21, 37, 45         | 0     |
| 2   | I     | 123/123 (100%)  | -0.24  | 1 (0%) 83 82  | 9, 21, 37, 45         | 0     |
| 2   | M     | 123/123 (100%)  | -0.57  | 0 100 100     | 9, 21, 37, 45         | 0     |
| 2   | P     | 123/123 (100%)  | -0.07  | 2 (1%) 68 67  | 9, 21, 37, 45         | 0     |
| 2   | S     | 123/123 (100%)  | -0.39  | 0 100 100     | 9, 21, 37, 45         | 0     |
| 2   | T     | 123/123 (100%)  | -0.58  | 0 100 100     | 9, 21, 37, 45         | 0     |
| 2   | W     | 123/123 (100%)  | -0.32  | 1 (0%) 83 82  | 9, 21, 37, 45         | 0     |
| All | All   | 4720/4784 (98%) | -0.53  | 72 (1%) 70 69 | 6, 17, 37, 56         | 0     |

All (72) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | V     | 475 | VAL  | 6.3  |
| 1   | K     | 9   | ALA  | 5.9  |
| 1   | H     | 9   | ALA  | 5.3  |
| 1   | R     | 11  | VAL  | 5.2  |
| 1   | V     | 474 | THR  | 5.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 9   | ALA  | 4.9  |
| 1   | O     | 9   | ALA  | 4.9  |
| 1   | R     | 9   | ALA  | 4.8  |
| 1   | L     | 9   | ALA  | 4.8  |
| 1   | H     | 474 | THR  | 4.0  |
| 1   | V     | 471 | ALA  | 4.0  |
| 1   | R     | 46  | PRO  | 3.9  |
| 1   | R     | 47  | GLY  | 3.6  |
| 1   | V     | 467 | PHE  | 3.5  |
| 1   | E     | 9   | ALA  | 3.5  |
| 1   | R     | 10  | SER  | 3.4  |
| 1   | B     | 474 | THR  | 3.3  |
| 1   | R     | 94  | GLU  | 3.3  |
| 1   | V     | 465 | ILE  | 3.2  |
| 1   | R     | 22  | LEU  | 3.2  |
| 1   | V     | 337 | GLY  | 3.2  |
| 1   | E     | 11  | VAL  | 3.1  |
| 1   | H     | 439 | ARG  | 3.1  |
| 1   | H     | 94  | GLU  | 3.0  |
| 1   | E     | 94  | GLU  | 3.0  |
| 1   | R     | 439 | ARG  | 3.0  |
| 1   | O     | 439 | ARG  | 3.0  |
| 1   | V     | 338 | GLU  | 3.0  |
| 1   | V     | 439 | ARG  | 3.0  |
| 1   | V     | 470 | PRO  | 3.0  |
| 1   | V     | 333 | GLY  | 2.9  |
| 1   | K     | 11  | VAL  | 2.9  |
| 1   | R     | 92  | GLY  | 2.8  |
| 1   | R     | 48  | VAL  | 2.8  |
| 1   | L     | 94  | GLU  | 2.8  |
| 1   | R     | 90  | VAL  | 2.8  |
| 1   | B     | 439 | ARG  | 2.7  |
| 1   | V     | 473 | ASP  | 2.7  |
| 1   | H     | 11  | VAL  | 2.6  |
| 1   | B     | 10  | SER  | 2.6  |
| 1   | V     | 468 | GLU  | 2.6  |
| 1   | K     | 439 | ARG  | 2.6  |
| 1   | V     | 472 | MET  | 2.5  |
| 1   | L     | 10  | SER  | 2.5  |
| 2   | W     | 121 | ALA  | 2.5  |
| 1   | V     | 9   | ALA  | 2.5  |
| 2   | I     | 76  | GLY  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | P     | 37  | LYS  | 2.4  |
| 1   | K     | 92  | GLY  | 2.4  |
| 1   | R     | 89  | PRO  | 2.4  |
| 1   | O     | 474 | THR  | 2.4  |
| 1   | B     | 94  | GLU  | 2.4  |
| 1   | H     | 468 | GLU  | 2.4  |
| 1   | H     | 475 | VAL  | 2.3  |
| 2   | P     | 78  | THR  | 2.3  |
| 1   | R     | 20  | TYR  | 2.3  |
| 1   | K     | 94  | GLU  | 2.3  |
| 1   | L     | 11  | VAL  | 2.3  |
| 1   | B     | 11  | VAL  | 2.3  |
| 1   | E     | 10  | SER  | 2.3  |
| 1   | O     | 91  | ALA  | 2.2  |
| 1   | V     | 336 | GLU  | 2.2  |
| 1   | H     | 467 | PHE  | 2.2  |
| 1   | V     | 451 | TRP  | 2.1  |
| 1   | V     | 469 | PHE  | 2.1  |
| 1   | L     | 46  | PRO  | 2.1  |
| 1   | V     | 94  | GLU  | 2.1  |
| 1   | R     | 97  | TYR  | 2.0  |
| 1   | O     | 469 | PHE  | 2.0  |
| 1   | V     | 11  | VAL  | 2.0  |
| 2   | C     | 78  | THR  | 2.0  |
| 1   | V     | 335 | LEU  | 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 | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | RUB  | O     | 476 | 18/18 | 0.28 | 6.92 | 22,46,58,58                 | 0     |
| 3   | RUB  | H     | 476 | 18/18 | 0.26 | 6.44 | 22,46,58,58                 | 0     |
| 3   | RUB  | L     | 476 | 18/18 | 0.21 | 4.80 | 22,46,58,58                 | 0     |
| 3   | RUB  | B     | 476 | 18/18 | 0.22 | 4.52 | 22,46,58,58                 | 0     |
| 3   | RUB  | K     | 476 | 18/18 | 0.20 | 4.42 | 22,46,58,58                 | 0     |
| 3   | RUB  | E     | 476 | 18/18 | 0.20 | 3.62 | 22,46,58,58                 | 0     |
| 3   | RUB  | V     | 476 | 18/18 | 0.35 | 3.37 | 22,46,58,58                 | 0     |
| 3   | RUB  | R     | 476 | 18/18 | 0.19 | 2.38 | 22,46,58,58                 | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.