



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:42 PM UTC

PDB ID : 2XRX / pdb\_00002xrx  
Title : CRYSTAL STRUCTURE OF BIPHENYL DIOXYGENASE IN COMPLEX  
WITH BIPHENYL FROM BURKHOLDERIA XENOVORANS LB400  
Authors : Kumar, P.; Bolin, J.T.  
Deposited on : 2010-09-23  
Resolution : 2.42 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

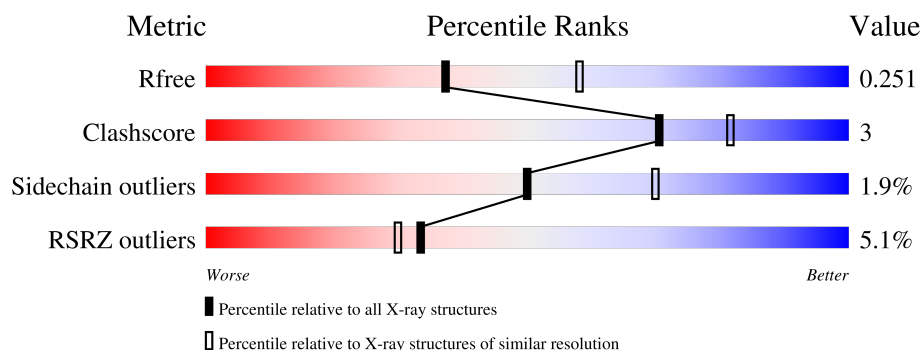
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.42 Å.

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



| Metric             | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|--------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$         | 180053                      | 6062 (2.44-2.40)                                      |
| Clashscore         | 190562                      | 6562 (2.44-2.40)                                      |
| Sidechain outliers | 187428                      | 6482 (2.44-2.40)                                      |
| RSRZ outliers      | 180081                      | 6066 (2.44-2.40)                                      |

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

| Mol | Chain | Length | Quality of chain                                 |
|-----|-------|--------|--------------------------------------------------|
| 1   | A     | 459    | <div> <div>2%</div> <div>85% 9% 6%</div> </div>  |
| 1   | C     | 459    | <div> <div>4%</div> <div>85% 9% 6%</div> </div>  |
| 1   | E     | 459    | <div> <div>2%</div> <div>86% 7% 6%</div> </div>  |
| 1   | G     | 459    | <div> <div>3%</div> <div>84% 10% 6%</div> </div> |
| 1   | I     | 459    | <div> <div>7%</div> <div>86% 8% 6%</div> </div>  |
| 1   | K     | 459    | <div> <div>6%</div> <div>85% 8% 6%</div> </div>  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | M     | 459    |                  |
| 1   | O     | 459    |                  |
| 1   | Q     | 459    |                  |
| 1   | S     | 459    |                  |
| 1   | U     | 459    |                  |
| 1   | W     | 459    |                  |
| 2   | B     | 188    |                  |
| 2   | D     | 188    |                  |
| 2   | F     | 188    |                  |
| 2   | H     | 188    |                  |
| 2   | J     | 188    |                  |
| 2   | L     | 188    |                  |
| 2   | N     | 188    |                  |
| 2   | P     | 188    |                  |
| 2   | R     | 188    |                  |
| 2   | T     | 188    |                  |
| 2   | V     | 188    |                  |
| 2   | X     | 188    |                  |

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 59977 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called BIPHENYL DIOXYGENASE SUBUNIT ALPHA.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 432      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3421  | 2175 | 601 | 622 | 23 |         |         |       |
| 1   | C     | 432      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3421  | 2175 | 601 | 622 | 23 |         |         |       |
| 1   | E     | 432      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3421  | 2175 | 601 | 622 | 23 |         |         |       |
| 1   | G     | 432      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3416  | 2172 | 600 | 621 | 23 |         |         |       |
| 1   | I     | 432      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3416  | 2172 | 600 | 621 | 23 |         |         |       |
| 1   | K     | 432      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3416  | 2172 | 600 | 621 | 23 |         |         |       |
| 1   | M     | 432      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3421  | 2175 | 601 | 622 | 23 |         |         |       |
| 1   | O     | 432      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3421  | 2175 | 601 | 622 | 23 |         |         |       |
| 1   | Q     | 432      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3421  | 2175 | 601 | 622 | 23 |         |         |       |
| 1   | S     | 432      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3417  | 2172 | 600 | 622 | 23 |         |         |       |
| 1   | U     | 432      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3417  | 2172 | 600 | 622 | 23 |         |         |       |
| 1   | W     | 432      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3417  | 2172 | 600 | 622 | 23 |         |         |       |

- Molecule 2 is a protein called BIPHENYL DIOXYGENASE SUBUNIT BETA.

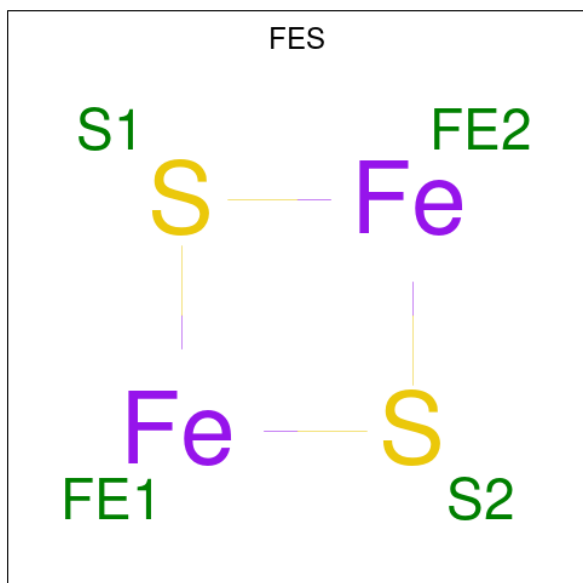
| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | B     | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1497  | 952 | 263 | 278 | 4 |         |         |       |
| 2   | D     | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1497  | 952 | 263 | 278 | 4 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | F     | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1497  | 952 | 263 | 278 | 4 |         |         |       |
| 2   | H     | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1507  | 957 | 266 | 280 | 4 |         |         |       |
| 2   | J     | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1507  | 957 | 266 | 280 | 4 |         |         |       |
| 2   | L     | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1507  | 957 | 266 | 280 | 4 |         |         |       |
| 2   | N     | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1507  | 957 | 266 | 280 | 4 |         |         |       |
| 2   | P     | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1507  | 957 | 266 | 280 | 4 |         |         |       |
| 2   | R     | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1507  | 957 | 266 | 280 | 4 |         |         |       |
| 2   | T     | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1507  | 957 | 266 | 280 | 4 |         |         |       |
| 2   | V     | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1507  | 957 | 266 | 280 | 4 |         |         |       |
| 2   | X     | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1507  | 957 | 266 | 280 | 4 |         |         |       |

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 3   | A     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 4     | 2  | 2 |         |         |

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| Mol | Chain | Residues | Atoms      |         |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|--------|---------|---------|
| 3   | C     | 1        | Total<br>4 | Fe<br>2 | S<br>2 | 0       | 0       |
| 3   | E     | 1        | Total<br>4 | Fe<br>2 | S<br>2 | 0       | 0       |
| 3   | G     | 1        | Total<br>4 | Fe<br>2 | S<br>2 | 0       | 0       |
| 3   | I     | 1        | Total<br>4 | Fe<br>2 | S<br>2 | 0       | 0       |
| 3   | K     | 1        | Total<br>4 | Fe<br>2 | S<br>2 | 0       | 0       |
| 3   | M     | 1        | Total<br>4 | Fe<br>2 | S<br>2 | 0       | 0       |
| 3   | O     | 1        | Total<br>4 | Fe<br>2 | S<br>2 | 0       | 0       |
| 3   | Q     | 1        | Total<br>4 | Fe<br>2 | S<br>2 | 0       | 0       |
| 3   | S     | 1        | Total<br>4 | Fe<br>2 | S<br>2 | 0       | 0       |
| 3   | U     | 1        | Total<br>4 | Fe<br>2 | S<br>2 | 0       | 0       |
| 3   | W     | 1        | Total<br>4 | Fe<br>2 | S<br>2 | 0       | 0       |

- Molecule 4 is FE (II) ION (CCD ID: FE2) (formula: Fe).

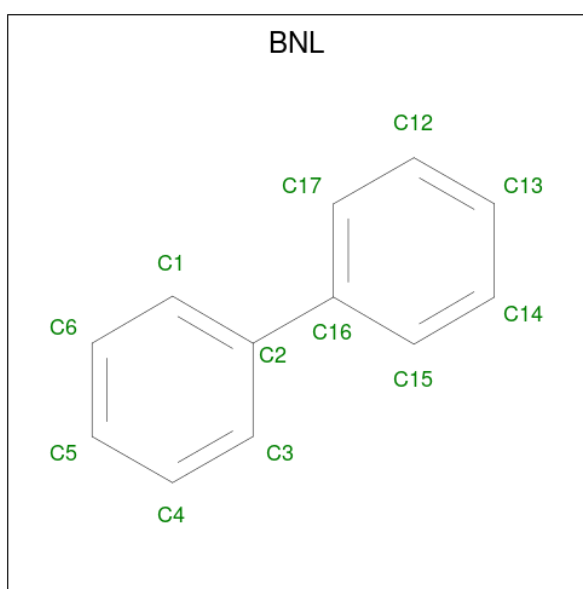
| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 4   | A     | 1        | Total<br>1 | Fe<br>1 | 0       | 0       |
| 4   | C     | 1        | Total<br>1 | Fe<br>1 | 0       | 0       |
| 4   | E     | 1        | Total<br>1 | Fe<br>1 | 0       | 0       |
| 4   | G     | 1        | Total<br>1 | Fe<br>1 | 0       | 0       |
| 4   | I     | 1        | Total<br>1 | Fe<br>1 | 0       | 0       |
| 4   | K     | 1        | Total<br>1 | Fe<br>1 | 0       | 0       |
| 4   | M     | 1        | Total<br>1 | Fe<br>1 | 0       | 0       |
| 4   | O     | 1        | Total<br>1 | Fe<br>1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 4   | Q     | 1        | Total<br>1 | Fe<br>1 | 0       | 0       |
| 4   | S     | 1        | Total<br>1 | Fe<br>1 | 0       | 0       |
| 4   | U     | 1        | Total<br>1 | Fe<br>1 | 0       | 0       |
| 4   | W     | 1        | Total<br>1 | Fe<br>1 | 0       | 0       |

- Molecule 5 is BIPHENYL (CCD ID: BNL) (formula:  $C_{12}H_{10}$ ).



| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 5   | A     | 1        | Total<br>12 | C<br>12 | 0       | 0       |
| 5   | C     | 1        | Total<br>12 | C<br>12 | 0       | 0       |
| 5   | E     | 1        | Total<br>12 | C<br>12 | 0       | 0       |
| 5   | G     | 1        | Total<br>12 | C<br>12 | 0       | 0       |
| 5   | I     | 1        | Total<br>12 | C<br>12 | 0       | 0       |
| 5   | K     | 1        | Total<br>12 | C<br>12 | 0       | 0       |
| 5   | M     | 1        | Total<br>12 | C<br>12 | 0       | 0       |

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| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 5   | O     | 1        | Total C<br>12 12 | 0       | 0       |
| 5   | Q     | 1        | Total C<br>12 12 | 0       | 0       |
| 5   | S     | 1        | Total C<br>12 12 | 0       | 0       |
| 5   | U     | 1        | Total C<br>12 12 | 0       | 0       |
| 5   | W     | 1        | Total C<br>12 12 | 0       | 0       |

- Molecule 6 is water.

| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 6   | A     | 44       | Total O<br>44 44 | 0       | 0       |
| 6   | B     | 19       | Total O<br>19 19 | 0       | 0       |
| 6   | C     | 31       | Total O<br>31 31 | 0       | 0       |
| 6   | D     | 21       | Total O<br>21 21 | 0       | 0       |
| 6   | E     | 50       | Total O<br>50 50 | 0       | 0       |
| 6   | F     | 35       | Total O<br>35 35 | 0       | 0       |
| 6   | G     | 24       | Total O<br>24 24 | 0       | 0       |
| 6   | H     | 12       | Total O<br>12 12 | 0       | 0       |
| 6   | I     | 25       | Total O<br>25 25 | 0       | 0       |
| 6   | J     | 7        | Total O<br>7 7   | 0       | 0       |
| 6   | K     | 16       | Total O<br>16 16 | 0       | 0       |
| 6   | L     | 12       | Total O<br>12 12 | 0       | 0       |
| 6   | M     | 38       | Total O<br>38 38 | 0       | 0       |
| 6   | N     | 25       | Total O<br>25 25 | 0       | 0       |

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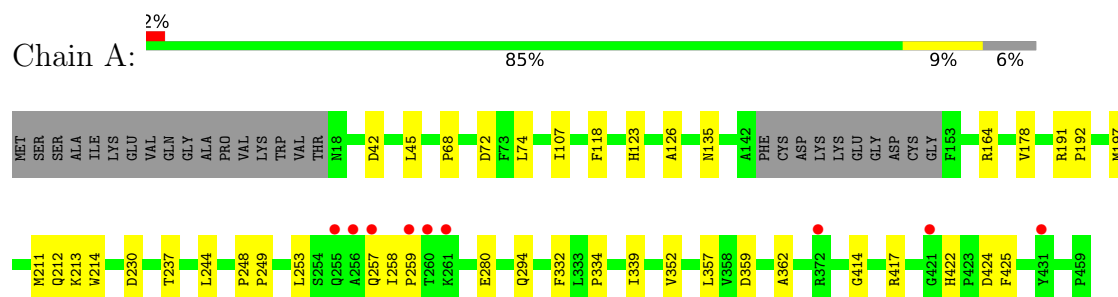
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| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 6   | O     | 65       | Total<br>65 | O<br>65 | 0       | 0       |
| 6   | P     | 26       | Total<br>26 | O<br>26 | 0       | 0       |
| 6   | Q     | 83       | Total<br>83 | O<br>83 | 0       | 0       |
| 6   | R     | 30       | Total<br>30 | O<br>30 | 0       | 0       |
| 6   | S     | 33       | Total<br>33 | O<br>33 | 0       | 0       |
| 6   | T     | 18       | Total<br>18 | O<br>18 | 0       | 0       |
| 6   | U     | 25       | Total<br>25 | O<br>25 | 0       | 0       |
| 6   | V     | 11       | Total<br>11 | O<br>11 | 0       | 0       |
| 6   | W     | 30       | Total<br>30 | O<br>30 | 0       | 0       |
| 6   | X     | 14       | Total<br>14 | O<br>14 | 0       | 0       |

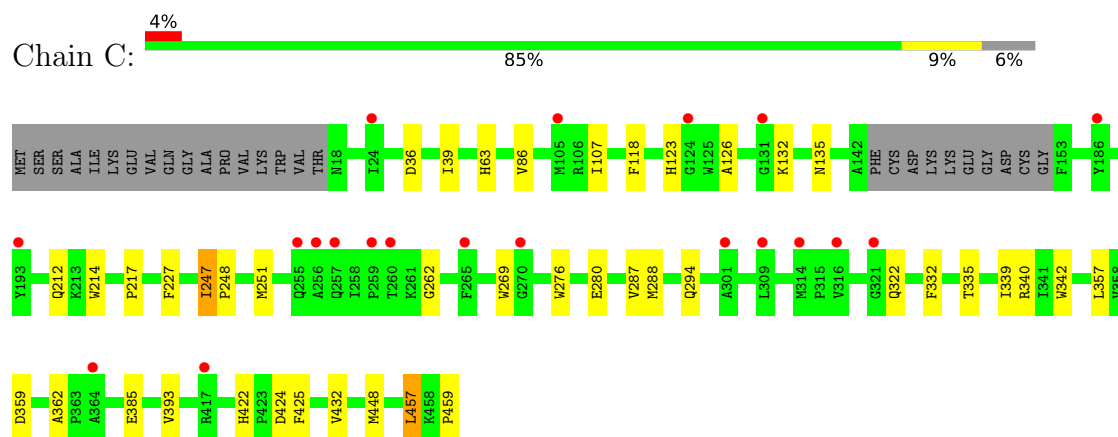
### 3 Residue-property plots [i](#)

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

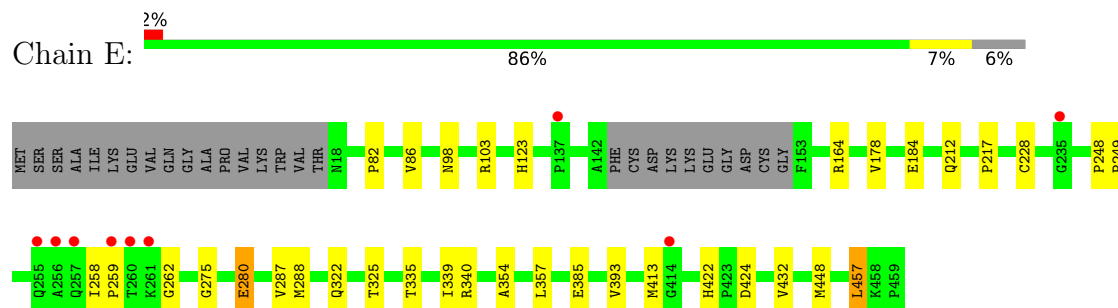
- Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



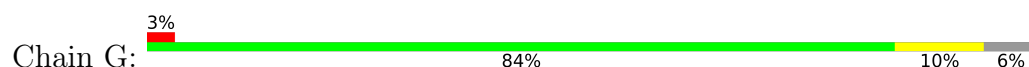
- Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

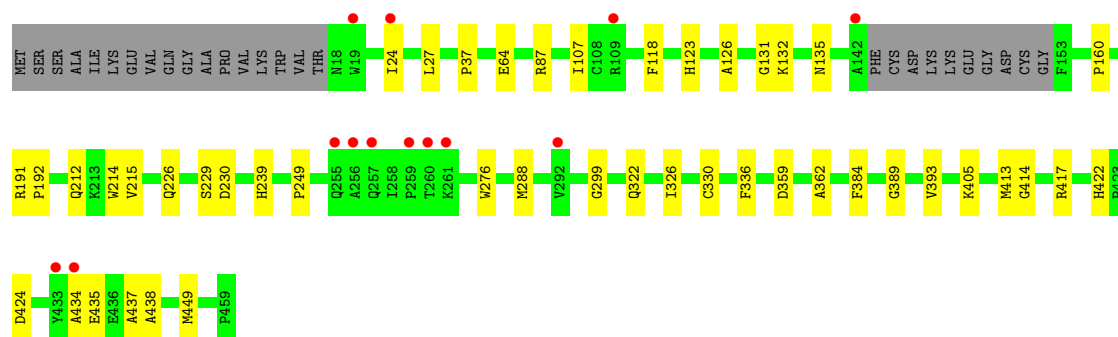


- Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

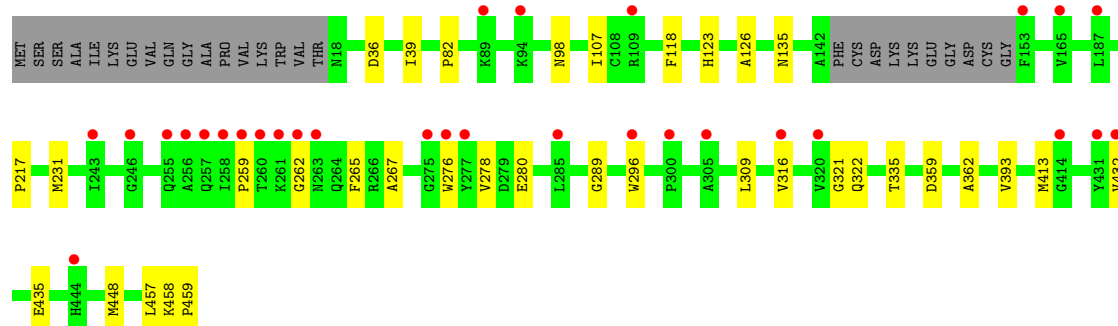
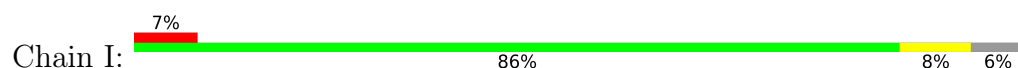


- Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

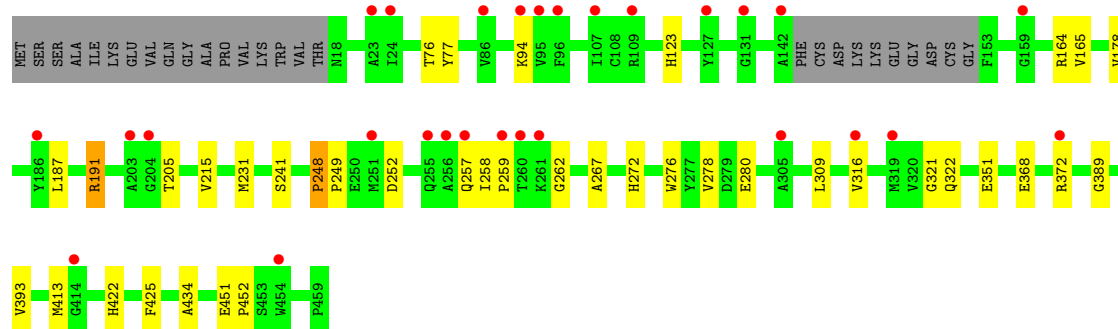
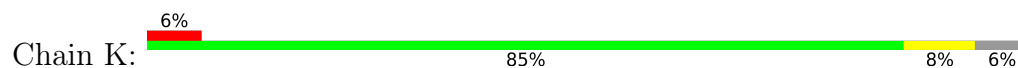




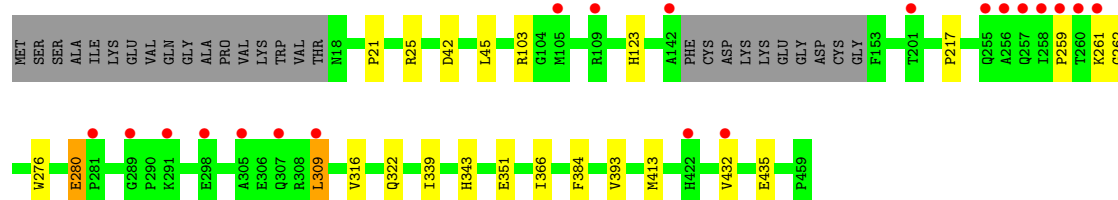
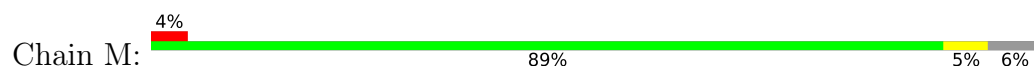
• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



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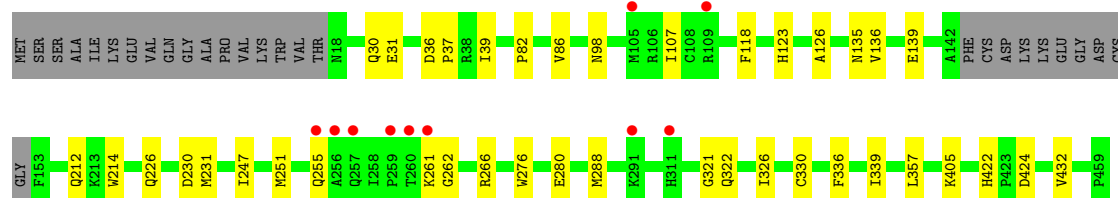


• Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



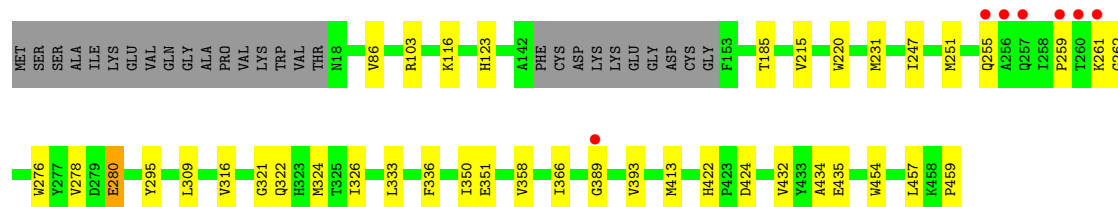
● Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain O: 



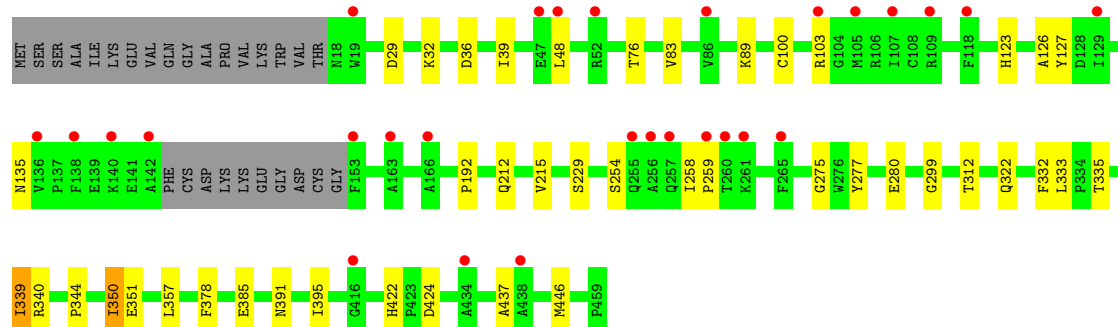
● Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain Q: 



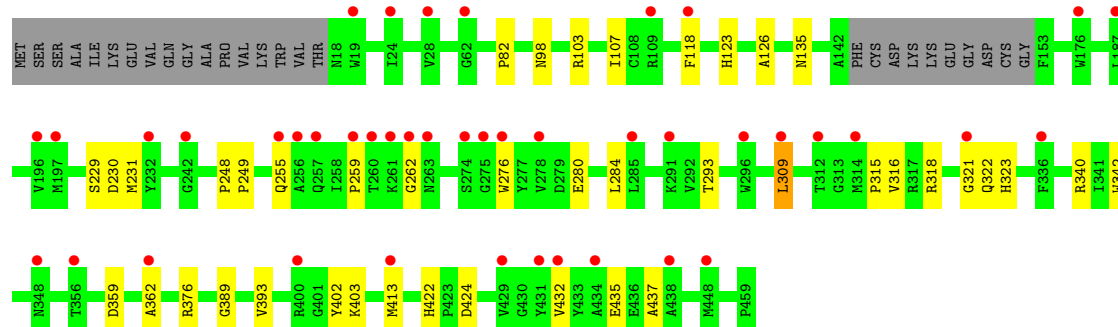
● Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

Chain S: 

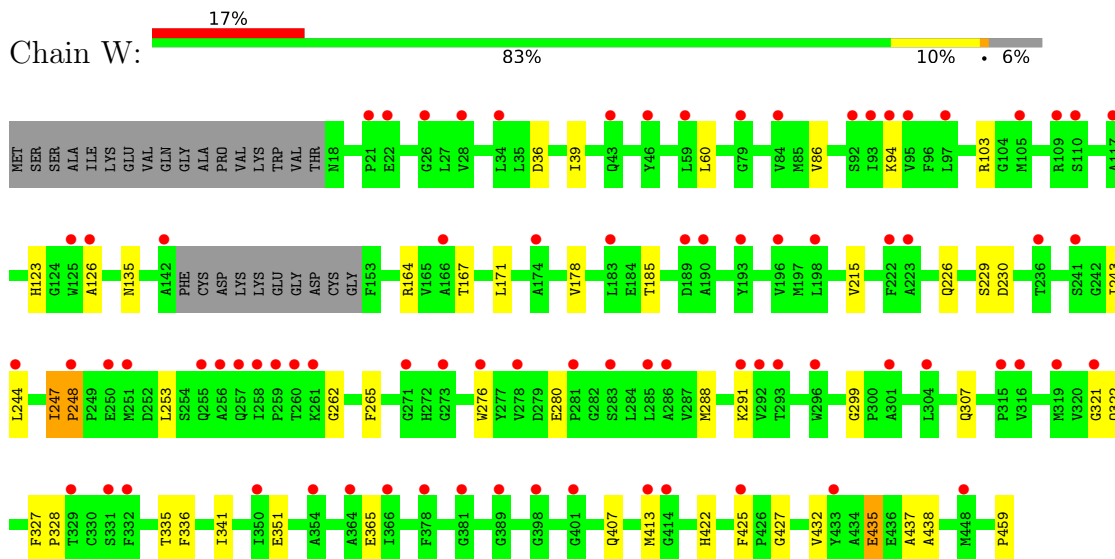


● Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA

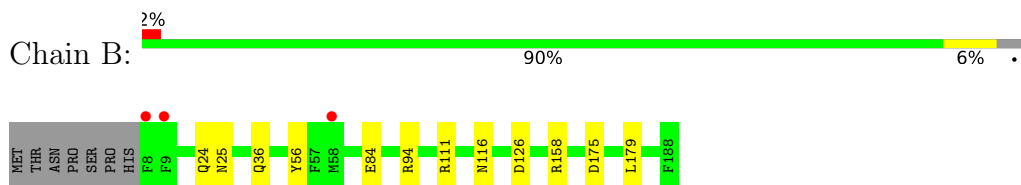
Chain U: 



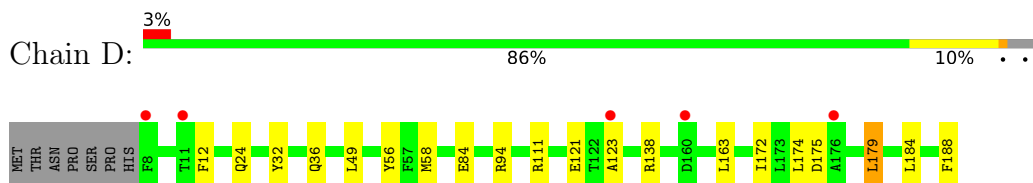
## ● Molecule 1: BIPHENYL DIOXYGENASE SUBUNIT ALPHA



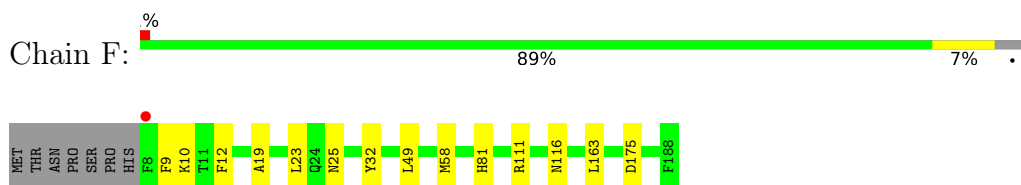
## ● Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



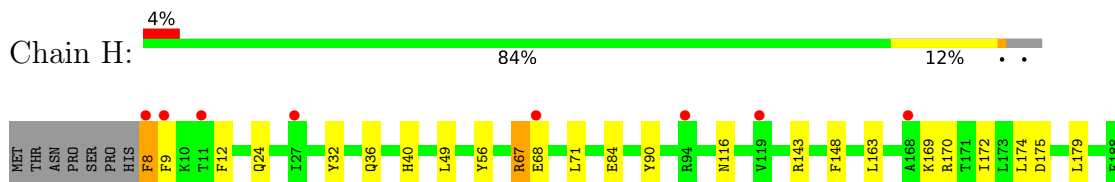
## ● Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



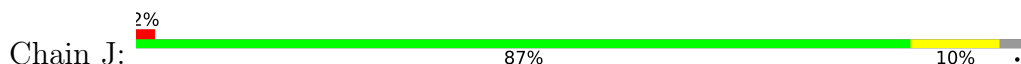
## ● Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

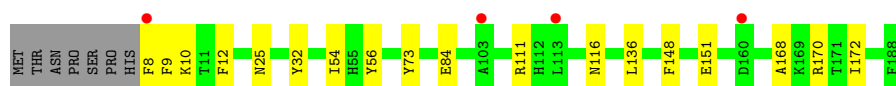


## ● Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

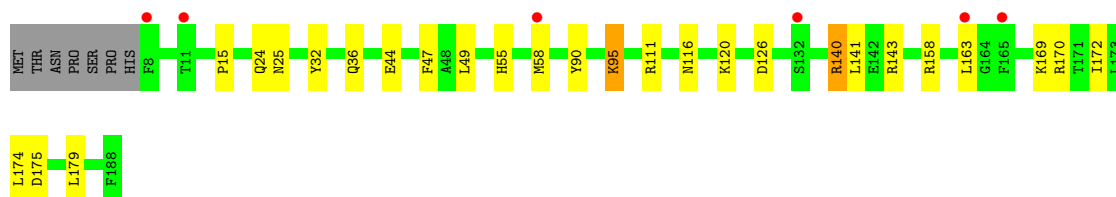
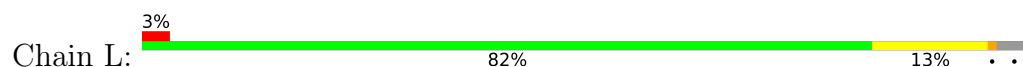


## ● Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

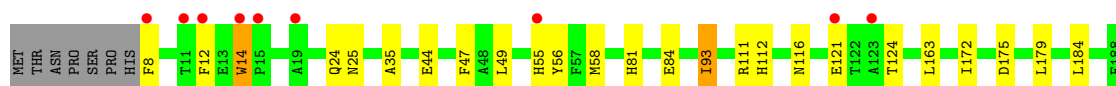
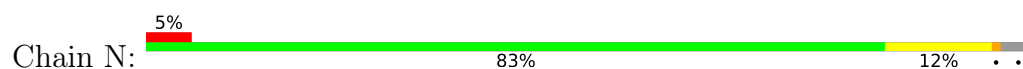




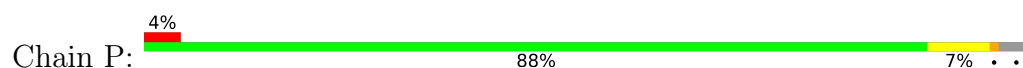
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



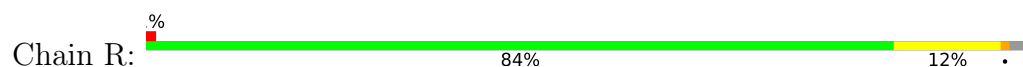
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



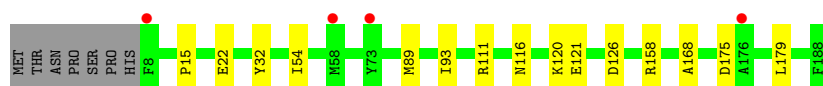
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



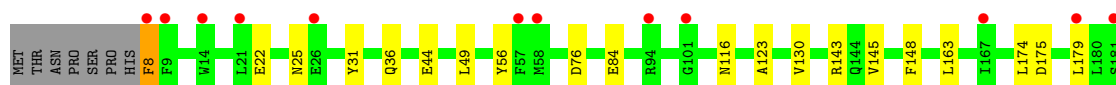
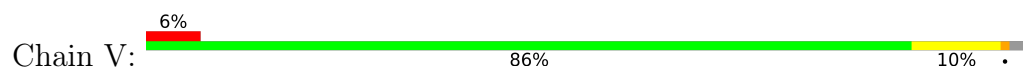
• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA

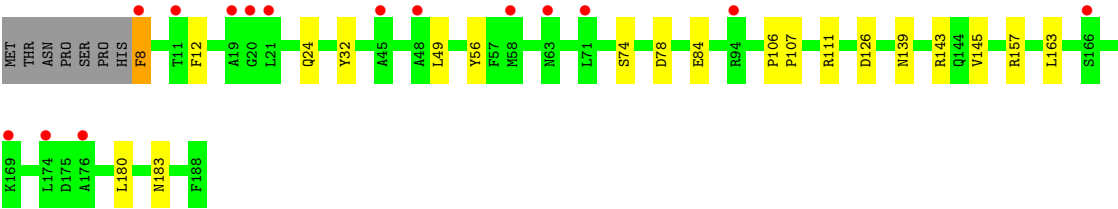
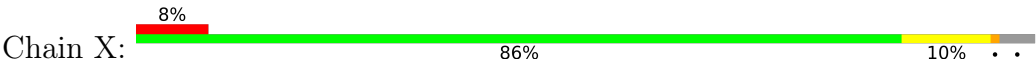


• Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA





● Molecule 2: BIPHENYL DIOXYGENASE SUBUNIT BETA



## 4 Data and refinement statistics

| Property                                                                | Value                                                                                                | Source           |
|-------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------|------------------|
| Space group                                                             | P 1                                                                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 132.82Å 132.65Å 130.42Å<br>102.65° 101.11° 105.31°                                                   | Depositor        |
| Resolution (Å)                                                          | 119.52 – 2.42<br>119.52 – 2.42                                                                       | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 95.0 (119.52-2.42)<br>82.8 (119.52-2.42)                                                             | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.06                                                                                                 | Depositor        |
| $R_{sym}$                                                               | (Not available)                                                                                      | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.43 (at 2.42Å)                                                                                      | Xtriage          |
| Refinement program                                                      | REFMAC 5.2.0019                                                                                      | Depositor        |
| R, $R_{free}$                                                           | 0.233 , 0.270<br>(Not available) , 0.251                                                             | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2612 reflections (0.97%)                                                                             | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 41.6                                                                                                 | Xtriage          |
| Anisotropy                                                              | 0.231                                                                                                | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.33 , 44.1                                                                                          | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$                                          | Xtriage          |
| Estimated twinning fraction                                             | 0.007 for l,h,k<br>0.007 for k,l,h<br>0.010 for -h,-l,-k<br>0.008 for -l,-k,-h<br>0.010 for -k,-h,-l | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                                                                 | EDS              |
| Total number of atoms                                                   | 59977                                                                                                | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 44.0                                                                                                 | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.26% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, BNL, FE2

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

| Mol | Chain | Bond lengths |         | Bond angles |                 |
|-----|-------|--------------|---------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5         |
| 1   | A     | 0.43         | 0/3523  | 0.77        | 0/4784          |
| 1   | C     | 0.42         | 0/3523  | 0.77        | 0/4784          |
| 1   | E     | 0.42         | 0/3523  | 0.79        | 0/4784          |
| 1   | G     | 0.43         | 0/3518  | 0.78        | 2/4777 (0.0%)   |
| 1   | I     | 0.42         | 0/3518  | 0.78        | 2/4777 (0.0%)   |
| 1   | K     | 0.42         | 0/3518  | 0.78        | 2/4777 (0.0%)   |
| 1   | M     | 0.42         | 0/3523  | 0.78        | 0/4784          |
| 1   | O     | 0.42         | 0/3523  | 0.77        | 0/4784          |
| 1   | Q     | 0.43         | 0/3523  | 0.77        | 0/4784          |
| 1   | S     | 0.42         | 0/3519  | 0.77        | 4/4780 (0.1%)   |
| 1   | U     | 0.44         | 0/3519  | 0.76        | 0/4780          |
| 1   | W     | 0.46         | 0/3519  | 0.79        | 6/4780 (0.1%)   |
| 2   | B     | 0.40         | 0/1532  | 0.68        | 0/2072          |
| 2   | D     | 0.40         | 0/1532  | 0.72        | 0/2072          |
| 2   | F     | 0.41         | 0/1532  | 0.70        | 0/2072          |
| 2   | H     | 0.40         | 0/1542  | 0.73        | 2/2084 (0.1%)   |
| 2   | J     | 0.41         | 0/1542  | 0.72        | 0/2084          |
| 2   | L     | 0.40         | 0/1542  | 0.70        | 0/2084          |
| 2   | N     | 0.41         | 0/1542  | 0.74        | 2/2084 (0.1%)   |
| 2   | P     | 0.41         | 0/1542  | 0.74        | 0/2084          |
| 2   | R     | 0.40         | 0/1542  | 0.75        | 2/2084 (0.1%)   |
| 2   | T     | 0.41         | 0/1542  | 0.70        | 0/2084          |
| 2   | V     | 0.42         | 0/1542  | 0.70        | 0/2084          |
| 2   | X     | 0.41         | 0/1542  | 0.73        | 0/2084          |
| All | All   | 0.42         | 0/60723 | 0.76        | 22/82347 (0.0%) |

There are no bond length outliers.

All (22) bond angle outliers are listed below:

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | S     | 299 | GLY  | CA-C-N | 6.62 | 126.12      | 119.24   |
| 1   | S     | 299 | GLY  | C-N-CA | 6.62 | 126.12      | 119.24   |
| 2   | N     | 14  | TRP  | CA-C-N | 6.36 | 127.79      | 119.84   |
| 2   | N     | 14  | TRP  | C-N-CA | 6.36 | 127.79      | 119.84   |
| 1   | G     | 299 | GLY  | CA-C-N | 6.35 | 125.84      | 119.24   |
| 1   | G     | 299 | GLY  | C-N-CA | 6.35 | 125.84      | 119.24   |
| 1   | W     | 248 | PRO  | CA-C-N | 6.21 | 125.89      | 119.56   |
| 1   | W     | 248 | PRO  | C-N-CA | 6.21 | 125.89      | 119.56   |
| 2   | R     | 8   | PHE  | CA-C-N | 5.47 | 131.55      | 121.70   |
| 2   | R     | 8   | PHE  | C-N-CA | 5.47 | 131.55      | 121.70   |
| 2   | H     | 8   | PHE  | CA-C-N | 5.46 | 131.53      | 121.70   |
| 2   | H     | 8   | PHE  | C-N-CA | 5.46 | 131.53      | 121.70   |
| 1   | W     | 247 | ILE  | CA-C-N | 5.29 | 125.83      | 120.38   |
| 1   | W     | 247 | ILE  | C-N-CA | 5.29 | 125.83      | 120.38   |
| 1   | S     | 333 | LEU  | CA-C-N | 5.07 | 125.10      | 119.32   |
| 1   | S     | 333 | LEU  | C-N-CA | 5.07 | 125.10      | 119.32   |
| 1   | K     | 248 | PRO  | CA-C-N | 5.03 | 125.31      | 119.47   |
| 1   | K     | 248 | PRO  | C-N-CA | 5.03 | 125.31      | 119.47   |
| 1   | W     | 299 | GLY  | CA-C-N | 5.03 | 124.52      | 119.19   |
| 1   | W     | 299 | GLY  | C-N-CA | 5.03 | 124.52      | 119.19   |
| 1   | I     | 289 | GLY  | CA-C-N | 5.01 | 124.31      | 118.85   |
| 1   | I     | 289 | GLY  | C-N-CA | 5.01 | 124.31      | 118.85   |

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3421  | 0        | 3269     | 27      | 0            |
| 1   | C     | 3421  | 0        | 3269     | 23      | 0            |
| 1   | E     | 3421  | 0        | 3269     | 18      | 0            |
| 1   | G     | 3416  | 0        | 3262     | 28      | 0            |
| 1   | I     | 3416  | 0        | 3262     | 19      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | K     | 3416  | 0        | 3262     | 22      | 0            |
| 1   | M     | 3421  | 0        | 3269     | 11      | 0            |
| 1   | O     | 3421  | 0        | 3269     | 18      | 0            |
| 1   | Q     | 3421  | 0        | 3269     | 20      | 0            |
| 1   | S     | 3417  | 0        | 3258     | 22      | 0            |
| 1   | U     | 3417  | 0        | 3258     | 23      | 0            |
| 1   | W     | 3417  | 0        | 3258     | 24      | 0            |
| 2   | B     | 1497  | 0        | 1441     | 13      | 0            |
| 2   | D     | 1497  | 0        | 1441     | 17      | 0            |
| 2   | F     | 1497  | 0        | 1441     | 12      | 0            |
| 2   | H     | 1507  | 0        | 1456     | 19      | 0            |
| 2   | J     | 1507  | 0        | 1456     | 17      | 0            |
| 2   | L     | 1507  | 0        | 1456     | 21      | 0            |
| 2   | N     | 1507  | 0        | 1456     | 18      | 0            |
| 2   | P     | 1507  | 0        | 1456     | 17      | 0            |
| 2   | R     | 1507  | 0        | 1456     | 20      | 0            |
| 2   | T     | 1507  | 0        | 1456     | 11      | 0            |
| 2   | V     | 1507  | 0        | 1456     | 16      | 0            |
| 2   | X     | 1507  | 0        | 1456     | 16      | 0            |
| 3   | A     | 4     | 0        | 0        | 1       | 0            |
| 3   | C     | 4     | 0        | 0        | 1       | 0            |
| 3   | E     | 4     | 0        | 0        | 1       | 0            |
| 3   | G     | 4     | 0        | 0        | 1       | 0            |
| 3   | I     | 4     | 0        | 0        | 1       | 0            |
| 3   | K     | 4     | 0        | 0        | 1       | 0            |
| 3   | M     | 4     | 0        | 0        | 1       | 0            |
| 3   | O     | 4     | 0        | 0        | 1       | 0            |
| 3   | Q     | 4     | 0        | 0        | 1       | 0            |
| 3   | S     | 4     | 0        | 0        | 1       | 0            |
| 3   | U     | 4     | 0        | 0        | 1       | 0            |
| 3   | W     | 4     | 0        | 0        | 1       | 0            |
| 4   | A     | 1     | 0        | 0        | 0       | 0            |
| 4   | C     | 1     | 0        | 0        | 0       | 0            |
| 4   | E     | 1     | 0        | 0        | 0       | 0            |
| 4   | G     | 1     | 0        | 0        | 0       | 0            |
| 4   | I     | 1     | 0        | 0        | 0       | 0            |
| 4   | K     | 1     | 0        | 0        | 0       | 0            |
| 4   | M     | 1     | 0        | 0        | 0       | 0            |
| 4   | O     | 1     | 0        | 0        | 0       | 0            |
| 4   | Q     | 1     | 0        | 0        | 0       | 0            |
| 4   | S     | 1     | 0        | 0        | 0       | 0            |
| 4   | U     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | W     | 1     | 0        | 0        | 0       | 0            |
| 5   | A     | 12    | 0        | 10       | 0       | 0            |
| 5   | C     | 12    | 0        | 10       | 0       | 0            |
| 5   | E     | 12    | 0        | 10       | 0       | 0            |
| 5   | G     | 12    | 0        | 10       | 0       | 0            |
| 5   | I     | 12    | 0        | 10       | 0       | 0            |
| 5   | K     | 12    | 0        | 10       | 0       | 0            |
| 5   | M     | 12    | 0        | 10       | 1       | 0            |
| 5   | O     | 12    | 0        | 10       | 0       | 0            |
| 5   | Q     | 12    | 0        | 10       | 0       | 0            |
| 5   | S     | 12    | 0        | 10       | 0       | 0            |
| 5   | U     | 12    | 0        | 10       | 0       | 0            |
| 5   | W     | 12    | 0        | 10       | 0       | 0            |
| 6   | A     | 44    | 0        | 0        | 1       | 0            |
| 6   | B     | 19    | 0        | 0        | 0       | 0            |
| 6   | C     | 31    | 0        | 0        | 0       | 0            |
| 6   | D     | 21    | 0        | 0        | 0       | 0            |
| 6   | E     | 50    | 0        | 0        | 1       | 0            |
| 6   | F     | 35    | 0        | 0        | 0       | 0            |
| 6   | G     | 24    | 0        | 0        | 0       | 0            |
| 6   | H     | 12    | 0        | 0        | 0       | 0            |
| 6   | I     | 25    | 0        | 0        | 0       | 0            |
| 6   | J     | 7     | 0        | 0        | 0       | 0            |
| 6   | K     | 16    | 0        | 0        | 0       | 0            |
| 6   | L     | 12    | 0        | 0        | 0       | 0            |
| 6   | M     | 38    | 0        | 0        | 0       | 0            |
| 6   | N     | 25    | 0        | 0        | 1       | 0            |
| 6   | O     | 65    | 0        | 0        | 0       | 0            |
| 6   | P     | 26    | 0        | 0        | 0       | 0            |
| 6   | Q     | 83    | 0        | 0        | 0       | 0            |
| 6   | R     | 30    | 0        | 0        | 0       | 0            |
| 6   | S     | 33    | 0        | 0        | 0       | 0            |
| 6   | T     | 18    | 0        | 0        | 0       | 0            |
| 6   | U     | 25    | 0        | 0        | 0       | 0            |
| 6   | V     | 11    | 0        | 0        | 1       | 0            |
| 6   | W     | 30    | 0        | 0        | 1       | 0            |
| 6   | X     | 14    | 0        | 0        | 0       | 0            |
| All | All   | 59977 | 0        | 56721    | 389     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (389) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:8:PHE:HA     | 2:H:9:PHE:HB2    | 1.28                     | 1.16              |
| 2:X:8:PHE:HD1    | 2:X:8:PHE:O      | 1.54                     | 0.90              |
| 2:P:94:ARG:HG2   | 2:P:94:ARG:HH11  | 1.36                     | 0.89              |
| 2:J:8:PHE:HA     | 2:J:73:TYR:HD2   | 1.37                     | 0.88              |
| 2:R:8:PHE:N      | 2:R:9:PHE:HB2    | 1.87                     | 0.88              |
| 1:S:123:HIS:HB2  | 3:S:1460:FES:S2  | 2.14                     | 0.88              |
| 1:M:123:HIS:HB2  | 3:M:1460:FES:S2  | 2.16                     | 0.86              |
| 1:I:123:HIS:HB2  | 3:I:1460:FES:S2  | 2.21                     | 0.80              |
| 2:H:8:PHE:HA     | 2:H:9:PHE:CB     | 2.10                     | 0.78              |
| 1:W:123:HIS:HB2  | 3:W:1460:FES:S2  | 2.24                     | 0.77              |
| 1:E:339:ILE:CD1  | 1:E:357:LEU:HG   | 2.15                     | 0.76              |
| 1:A:259:PRO:HB3  | 1:A:280:GLU:HG2  | 1.67                     | 0.75              |
| 1:K:259:PRO:HB3  | 1:K:280:GLU:HG2  | 1.69                     | 0.75              |
| 1:C:123:HIS:HB2  | 3:C:1460:FES:S2  | 2.27                     | 0.74              |
| 1:Q:259:PRO:HB3  | 1:Q:280:GLU:HG2  | 1.68                     | 0.74              |
| 1:Q:123:HIS:HB2  | 3:Q:1460:FES:S2  | 2.27                     | 0.74              |
| 1:W:413:MET:HB2  | 1:W:435:GLU:HB2  | 1.69                     | 0.73              |
| 1:E:339:ILE:HD11 | 1:E:357:LEU:HG   | 1.72                     | 0.71              |
| 1:A:123:HIS:HB2  | 3:A:1460:FES:S2  | 2.31                     | 0.70              |
| 1:Q:422:HIS:HD2  | 1:Q:424:ASP:H    | 1.41                     | 0.69              |
| 2:R:8:PHE:N      | 2:R:9:PHE:CB     | 2.56                     | 0.68              |
| 2:N:58:MET:HE2   | 2:N:81:HIS:HB2   | 1.75                     | 0.68              |
| 2:P:94:ARG:HG2   | 2:P:94:ARG:NH1   | 2.07                     | 0.67              |
| 2:B:94:ARG:HH11  | 2:B:94:ARG:HG2   | 1.61                     | 0.66              |
| 1:S:339:ILE:HD11 | 1:S:357:LEU:HG   | 1.77                     | 0.66              |
| 2:J:56:TYR:HB3   | 2:J:84:GLU:HB2   | 1.78                     | 0.65              |
| 1:M:309:LEU:HD13 | 1:M:316:VAL:HG11 | 1.78                     | 0.65              |
| 1:W:288:MET:HE3  | 1:W:336:PHE:HB3  | 1.77                     | 0.65              |
| 1:G:123:HIS:HB2  | 3:G:1460:FES:S2  | 2.37                     | 0.64              |
| 2:N:175:ASP:OD2  | 2:R:111:ARG:HB2  | 1.98                     | 0.64              |
| 2:V:8:PHE:CD1    | 2:V:8:PHE:N      | 2.66                     | 0.64              |
| 1:C:247:ILE:HG13 | 1:C:248:PRO:HD2  | 1.79                     | 0.64              |
| 1:W:291:LYS:HE2  | 1:W:365:GLU:HG2  | 1.80                     | 0.63              |
| 2:H:148:PHE:HB3  | 2:H:174:LEU:HD11 | 1.80                     | 0.63              |
| 2:V:143:ARG:HD3  | 1:W:215:VAL:HG21 | 1.80                     | 0.63              |
| 2:X:8:PHE:O      | 2:X:8:PHE:CD1    | 2.44                     | 0.63              |
| 1:S:339:ILE:CD1  | 1:S:357:LEU:HG   | 2.29                     | 0.61              |
| 2:T:111:ARG:HB2  | 2:V:175:ASP:OD2  | 1.99                     | 0.61              |
| 2:J:8:PHE:HA     | 2:J:73:TYR:CD2   | 2.29                     | 0.61              |
| 2:D:58:MET:HE3   | 2:D:174:LEU:HD22 | 1.82                     | 0.61              |
| 1:I:413:MET:HE2  | 1:I:435:GLU:HG3  | 1.83                     | 0.60              |
| 1:I:448:MET:HG2  | 1:I:457:LEU:HD21 | 1.82                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:217:PRO:HD2  | 1:I:393:VAL:HG22 | 1.83                     | 0.60              |
| 2:P:10:LYS:HG2   | 2:P:10:LYS:O     | 2.02                     | 0.60              |
| 1:G:229:SER:OG   | 1:G:438:ALA:HB2  | 2.01                     | 0.60              |
| 2:N:58:MET:HE2   | 2:N:81:HIS:CB    | 2.32                     | 0.60              |
| 1:K:123:HIS:HB2  | 3:K:1460:FES:S2  | 2.42                     | 0.59              |
| 2:V:56:TYR:HB3   | 2:V:84:GLU:HB2   | 1.84                     | 0.59              |
| 1:E:339:ILE:HD13 | 1:E:357:LEU:HG   | 1.84                     | 0.59              |
| 1:S:215:VAL:HG22 | 1:S:351:GLU:HG2  | 1.84                     | 0.59              |
| 2:D:58:MET:CE    | 2:D:174:LEU:HD22 | 2.33                     | 0.59              |
| 1:S:340:ARG:HH12 | 1:S:385:GLU:CD   | 2.10                     | 0.58              |
| 2:V:25:ASN:HD21  | 2:X:24:GLN:HG2   | 1.68                     | 0.58              |
| 1:A:339:ILE:HD13 | 1:A:357:LEU:HG   | 1.85                     | 0.58              |
| 1:A:258:ILE:HD11 | 2:N:8:PHE:C      | 2.29                     | 0.58              |
| 1:E:259:PRO:HB3  | 1:E:280:GLU:HG2  | 1.85                     | 0.57              |
| 1:G:413:MET:HE2  | 1:G:435:GLU:HG3  | 1.86                     | 0.57              |
| 1:K:257:GLN:NE2  | 2:P:8:PHE:HB3    | 2.18                     | 0.57              |
| 2:V:8:PHE:N      | 2:V:8:PHE:HD1    | 2.01                     | 0.57              |
| 1:E:123:HIS:HB2  | 3:E:1460:FES:S2  | 2.45                     | 0.57              |
| 2:N:25:ASN:HD21  | 2:P:24:GLN:HG2   | 1.68                     | 0.57              |
| 2:D:56:TYR:HB3   | 2:D:84:GLU:HB2   | 1.87                     | 0.57              |
| 1:K:94:LYS:HA    | 1:K:165:VAL:HG21 | 1.86                     | 0.57              |
| 2:P:58:MET:HE2   | 2:P:81:HIS:HB2   | 1.86                     | 0.57              |
| 1:S:229:SER:HB2  | 1:S:437:ALA:HB3  | 1.87                     | 0.56              |
| 2:R:58:MET:HE3   | 2:R:174:LEU:HD22 | 1.88                     | 0.56              |
| 2:R:58:MET:CE    | 2:R:174:LEU:HD22 | 2.36                     | 0.55              |
| 2:H:24:GLN:HG2   | 2:L:25:ASN:HD21  | 1.71                     | 0.55              |
| 1:O:123:HIS:HB2  | 3:O:1460:FES:S2  | 2.46                     | 0.55              |
| 1:I:448:MET:HA   | 1:I:457:LEU:HD11 | 1.87                     | 0.55              |
| 1:Q:185:THR:HG22 | 1:Q:459:PRO:HG2  | 1.89                     | 0.55              |
| 1:I:259:PRO:HB3  | 1:I:280:GLU:HG2  | 1.89                     | 0.55              |
| 1:A:107:ILE:HG22 | 1:A:118:PHE:HB3  | 1.88                     | 0.55              |
| 2:B:111:ARG:HB2  | 2:D:175:ASP:OD2  | 2.07                     | 0.55              |
| 1:C:340:ARG:HH12 | 1:C:385:GLU:CD   | 2.15                     | 0.55              |
| 2:T:126:ASP:HB3  | 2:T:158:ARG:HB2  | 1.87                     | 0.55              |
| 2:L:140:ARG:HG3  | 2:L:141:LEU:HG   | 1.89                     | 0.55              |
| 1:K:413:MET:HG2  | 1:K:434:ALA:HA   | 1.88                     | 0.55              |
| 2:N:56:TYR:HB3   | 2:N:84:GLU:HB2   | 1.88                     | 0.55              |
| 1:U:123:HIS:HB2  | 3:U:1460:FES:S2  | 2.47                     | 0.55              |
| 1:U:359:ASP:HB2  | 1:U:362:ALA:HB2  | 1.89                     | 0.55              |
| 1:W:226:GLN:HA   | 1:W:230:ASP:HB2  | 1.88                     | 0.55              |
| 2:L:55:HIS:HB3   | 2:L:169:LYS:HG3  | 1.90                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:W:229:SER:HB3  | 1:W:437:ALA:HB3  | 1.89                     | 0.54              |
| 2:B:94:ARG:HG2   | 2:B:94:ARG:NH1   | 2.18                     | 0.54              |
| 1:O:107:ILE:HG22 | 1:O:118:PHE:HB3  | 1.89                     | 0.54              |
| 2:X:56:TYR:HB3   | 2:X:84:GLU:HB2   | 1.88                     | 0.54              |
| 1:C:269:TRP:CD2  | 1:C:459:PRO:HG3  | 2.43                     | 0.54              |
| 1:E:340:ARG:HH12 | 1:E:385:GLU:CD   | 2.16                     | 0.54              |
| 2:P:58:MET:HE2   | 2:P:81:HIS:CB    | 2.38                     | 0.54              |
| 2:D:111:ARG:HB2  | 2:F:175:ASP:OD2  | 2.08                     | 0.54              |
| 1:Q:324:MET:HE2  | 1:Q:326:ILE:HD11 | 1.89                     | 0.53              |
| 1:I:359:ASP:HB2  | 1:I:362:ALA:HB2  | 1.90                     | 0.53              |
| 1:W:226:GLN:HA   | 1:W:230:ASP:CB   | 2.39                     | 0.53              |
| 1:I:262:GLY:HA2  | 1:I:278:VAL:HG23 | 1.88                     | 0.53              |
| 1:Q:413:MET:HG2  | 1:Q:434:ALA:HA   | 1.91                     | 0.53              |
| 2:B:175:ASP:OD2  | 2:F:111:ARG:HB2  | 2.08                     | 0.53              |
| 2:D:49:LEU:HD21  | 2:D:163:LEU:HD13 | 1.91                     | 0.53              |
| 1:G:24:ILE:HD11  | 1:G:449:MET:HB3  | 1.91                     | 0.53              |
| 2:H:175:ASP:OD2  | 2:L:111:ARG:HB2  | 2.09                     | 0.53              |
| 1:U:309:LEU:HD13 | 1:U:316:VAL:HG11 | 1.89                     | 0.53              |
| 2:J:8:PHE:CD1    | 2:J:8:PHE:C      | 2.87                     | 0.53              |
| 2:N:24:GLN:HG2   | 2:R:25:ASN:HD21  | 1.74                     | 0.53              |
| 1:W:215:VAL:HG22 | 1:W:351:GLU:HG2  | 1.89                     | 0.53              |
| 1:E:448:MET:HA   | 1:E:457:LEU:HD11 | 1.90                     | 0.52              |
| 2:P:25:ASN:HD21  | 2:R:24:GLN:HG2   | 1.74                     | 0.52              |
| 1:W:422:HIS:HD2  | 1:W:425:PHE:H    | 1.56                     | 0.52              |
| 1:G:249:PRO:HB3  | 2:H:90:TYR:CE2   | 2.45                     | 0.52              |
| 1:K:164:ARG:HD2  | 1:K:178:VAL:HA   | 1.91                     | 0.52              |
| 2:H:56:TYR:HB3   | 2:H:84:GLU:HB2   | 1.90                     | 0.52              |
| 1:C:227:PHE:CZ   | 1:C:340:ARG:HD2  | 2.45                     | 0.52              |
| 1:G:64:GLU:HG2   | 1:G:87:ARG:HH22  | 1.73                     | 0.52              |
| 1:A:359:ASP:HB2  | 1:A:362:ALA:HB2  | 1.91                     | 0.52              |
| 2:D:123:ALA:HA   | 1:G:132:LYS:HD3  | 1.92                     | 0.52              |
| 2:V:148:PHE:HB3  | 2:V:174:LEU:HD11 | 1.92                     | 0.52              |
| 2:B:36:GLN:HE21  | 2:D:12:PHE:H     | 1.58                     | 0.52              |
| 1:G:413:MET:HG2  | 1:G:434:ALA:HA   | 1.92                     | 0.52              |
| 2:H:32:TYR:CD1   | 2:J:116:ASN:HA   | 2.44                     | 0.52              |
| 2:N:49:LEU:HD21  | 2:N:163:LEU:HD13 | 1.92                     | 0.52              |
| 2:J:9:PHE:O      | 2:J:10:LYS:HG2   | 2.10                     | 0.52              |
| 1:A:126:ALA:HB3  | 1:A:135:ASN:HB3  | 1.91                     | 0.52              |
| 2:H:36:GLN:HE21  | 2:J:12:PHE:H     | 1.57                     | 0.51              |
| 1:I:309:LEU:HD13 | 1:I:316:VAL:HG11 | 1.91                     | 0.51              |
| 1:K:262:GLY:HA2  | 1:K:278:VAL:HG23 | 1.92                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:259:PRO:HB3  | 1:M:280:GLU:HG2  | 1.92                     | 0.51              |
| 1:K:241:SER:HB2  | 2:L:95:LYS:HG2   | 1.92                     | 0.51              |
| 2:J:25:ASN:HD21  | 2:L:24:GLN:HG2   | 1.75                     | 0.51              |
| 1:A:237:THR:HG22 | 2:N:12:PHE:HB3   | 1.93                     | 0.51              |
| 1:I:82:PRO:HB2   | 1:I:98:ASN:HB3   | 1.93                     | 0.51              |
| 2:H:12:PHE:H     | 2:L:36:GLN:HE21  | 1.57                     | 0.51              |
| 1:A:422:HIS:CD2  | 1:A:424:ASP:H    | 2.28                     | 0.51              |
| 1:O:276:TRP:HB3  | 1:O:322:GLN:HG3  | 1.92                     | 0.51              |
| 1:E:217:PRO:HD2  | 1:E:393:VAL:HG22 | 1.93                     | 0.50              |
| 2:B:25:ASN:HD21  | 2:D:24:GLN:HG2   | 1.76                     | 0.50              |
| 1:G:131:GLY:O    | 1:G:160:PRO:HD2  | 2.12                     | 0.50              |
| 1:Q:309:LEU:HD22 | 1:Q:316:VAL:HG11 | 1.94                     | 0.50              |
| 2:J:32:TYR:CD1   | 2:L:116:ASN:HA   | 2.46                     | 0.50              |
| 2:L:58:MET:HE3   | 2:L:174:LEU:HD22 | 1.94                     | 0.50              |
| 1:A:414:GLY:HA2  | 1:A:417:ARG:HD2  | 1.94                     | 0.50              |
| 1:G:229:SER:HB3  | 1:G:437:ALA:HB3  | 1.92                     | 0.50              |
| 1:C:422:HIS:HD2  | 1:C:425:PHE:H    | 1.60                     | 0.49              |
| 1:G:215:VAL:HG21 | 2:L:143:ARG:HD3  | 1.93                     | 0.49              |
| 1:K:231:MET:HE1  | 1:K:321:GLY:O    | 2.12                     | 0.49              |
| 2:J:170:ARG:HD3  | 2:J:172:ILE:HD11 | 1.94                     | 0.49              |
| 1:G:126:ALA:HB3  | 1:G:135:ASN:HB3  | 1.93                     | 0.49              |
| 1:Q:276:TRP:HB3  | 1:Q:322:GLN:HG3  | 1.94                     | 0.49              |
| 1:G:288:MET:HE3  | 1:G:336:PHE:HB3  | 1.94                     | 0.49              |
| 2:X:49:LEU:HD21  | 2:X:163:LEU:HD13 | 1.95                     | 0.49              |
| 2:B:116:ASN:HA   | 2:F:32:TYR:CD1   | 2.48                     | 0.49              |
| 1:E:262:GLY:C    | 1:E:432:VAL:HB   | 2.38                     | 0.49              |
| 2:N:111:ARG:HB2  | 2:P:175:ASP:OD2  | 2.12                     | 0.49              |
| 1:I:265:PHE:CZ   | 1:I:267:ALA:HA   | 2.48                     | 0.48              |
| 2:T:22:GLU:H     | 2:T:22:GLU:CD    | 2.21                     | 0.48              |
| 1:S:422:HIS:HD2  | 1:S:424:ASP:H    | 1.60                     | 0.48              |
| 2:F:49:LEU:HD21  | 2:F:163:LEU:HD13 | 1.94                     | 0.48              |
| 2:N:116:ASN:HA   | 2:R:32:TYR:CD1   | 2.48                     | 0.48              |
| 1:W:36:ASP:O     | 1:W:39:ILE:HG12  | 2.13                     | 0.48              |
| 1:M:413:MET:HE2  | 1:M:435:GLU:HG3  | 1.95                     | 0.48              |
| 2:N:35:ALA:HB1   | 2:N:112:HIS:HB2  | 1.95                     | 0.48              |
| 1:Q:422:HIS:CD2  | 1:Q:424:ASP:H    | 2.26                     | 0.48              |
| 1:U:259:PRO:HB3  | 1:U:280:GLU:HG2  | 1.94                     | 0.48              |
| 1:S:332:PHE:HB3  | 1:S:339:ILE:HG23 | 1.96                     | 0.48              |
| 1:E:422:HIS:HD2  | 1:E:424:ASP:H    | 1.60                     | 0.48              |
| 1:K:309:LEU:HD13 | 1:K:316:VAL:HG11 | 1.95                     | 0.48              |
| 1:M:262:GLY:C    | 1:M:432:VAL:HB   | 2.38                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:54:ILE:HA    | 2:J:168:ALA:O    | 2.14                     | 0.48              |
| 1:O:37:PRO:HG2   | 1:O:405:LYS:HA   | 1.94                     | 0.48              |
| 1:A:422:HIS:HD2  | 1:A:424:ASP:H    | 1.62                     | 0.47              |
| 1:C:36:ASP:O     | 1:C:39:ILE:HG12  | 2.13                     | 0.47              |
| 1:A:258:ILE:HD11 | 2:N:8:PHE:O      | 2.13                     | 0.47              |
| 2:H:68:GLU:HB3   | 2:H:71:LEU:HD12  | 1.96                     | 0.47              |
| 1:M:42:ASP:HB3   | 1:M:45:LEU:HB2   | 1.96                     | 0.47              |
| 1:O:82:PRO:HB2   | 1:O:98:ASN:HB3   | 1.96                     | 0.47              |
| 2:P:40:HIS:HE1   | 2:R:151:GLU:OE2  | 1.97                     | 0.47              |
| 1:S:126:ALA:HB3  | 1:S:135:ASN:HB3  | 1.96                     | 0.47              |
| 1:U:389:GLY:O    | 1:U:393:VAL:HG23 | 2.15                     | 0.47              |
| 1:U:402:TYR:CE2  | 1:U:403:LYS:HE3  | 2.49                     | 0.47              |
| 1:C:359:ASP:HB2  | 1:C:362:ALA:HB2  | 1.95                     | 0.47              |
| 2:N:47:PHE:HB2   | 2:N:93:ILE:HD13  | 1.97                     | 0.47              |
| 2:T:116:ASN:HA   | 2:X:32:TYR:CD1   | 2.49                     | 0.47              |
| 1:C:262:GLY:C    | 1:C:432:VAL:HB   | 2.40                     | 0.47              |
| 1:G:359:ASP:HB2  | 1:G:362:ALA:HB2  | 1.97                     | 0.47              |
| 1:M:217:PRO:HG2  | 1:M:393:VAL:HG22 | 1.96                     | 0.47              |
| 2:N:55:HIS:HB3   | 6:N:2014:HOH:O   | 2.14                     | 0.47              |
| 2:R:56:TYR:HB3   | 2:R:84:GLU:HB2   | 1.96                     | 0.47              |
| 1:W:126:ALA:HB3  | 1:W:135:ASN:HB3  | 1.96                     | 0.47              |
| 1:G:107:ILE:HG22 | 1:G:118:PHE:HB3  | 1.95                     | 0.47              |
| 1:S:36:ASP:O     | 1:S:39:ILE:HG12  | 2.14                     | 0.47              |
| 2:B:116:ASN:HA   | 2:F:32:TYR:CG    | 2.50                     | 0.47              |
| 1:S:259:PRO:HB2  | 1:S:277:TYR:CE2  | 2.50                     | 0.47              |
| 1:A:332:PHE:HB3  | 1:A:339:ILE:HG13 | 1.97                     | 0.47              |
| 1:C:448:MET:HA   | 1:C:457:LEU:HD11 | 1.97                     | 0.47              |
| 2:P:90:TYR:CE2   | 2:P:94:ARG:HD2   | 2.50                     | 0.46              |
| 1:S:192:PRO:HB3  | 1:S:312:THR:HG21 | 1.97                     | 0.46              |
| 1:U:82:PRO:HB2   | 1:U:98:ASN:HB3   | 1.98                     | 0.46              |
| 2:X:106:PRO:HA   | 2:X:107:PRO:HD3  | 1.83                     | 0.46              |
| 1:G:24:ILE:HG13  | 1:G:27:LEU:HD12  | 1.97                     | 0.46              |
| 1:I:126:ALA:HB3  | 1:I:135:ASN:HB3  | 1.97                     | 0.46              |
| 2:L:47:PHE:CZ    | 2:L:90:TYR:HB2   | 2.50                     | 0.46              |
| 1:O:247:ILE:HD12 | 1:O:251:MET:HB3  | 1.96                     | 0.46              |
| 1:U:284:LEU:HD23 | 1:U:293:THR:HG23 | 1.98                     | 0.46              |
| 1:Q:215:VAL:HG22 | 1:Q:351:GLU:HG2  | 1.97                     | 0.46              |
| 1:W:276:TRP:HB3  | 1:W:322:GLN:HG3  | 1.95                     | 0.46              |
| 1:I:231:MET:HE1  | 1:I:321:GLY:O    | 2.16                     | 0.46              |
| 1:C:107:ILE:HG22 | 1:C:118:PHE:HB3  | 1.97                     | 0.46              |
| 2:X:74:SER:HB2   | 2:X:78:ASP:HB2   | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:191:ARG:N    | 1:A:192:PRO:HD2  | 2.31                     | 0.45              |
| 1:O:36:ASP:O     | 1:O:39:ILE:HG12  | 2.16                     | 0.45              |
| 1:E:164:ARG:HD2  | 1:E:178:VAL:HA   | 1.97                     | 0.45              |
| 2:R:49:LEU:HD21  | 2:R:163:LEU:HD13 | 1.97                     | 0.45              |
| 2:T:175:ASP:OD2  | 2:X:111:ARG:HB2  | 2.16                     | 0.45              |
| 1:E:82:PRO:HB2   | 1:E:98:ASN:HB3   | 1.98                     | 0.45              |
| 1:O:136:VAL:O    | 1:O:139:GLU:HB2  | 2.17                     | 0.45              |
| 2:T:32:TYR:CD1   | 2:V:116:ASN:HA   | 2.51                     | 0.45              |
| 1:G:24:ILE:CD1   | 1:G:449:MET:HB3  | 2.47                     | 0.45              |
| 1:U:276:TRP:HB3  | 1:U:322:GLN:HG3  | 1.98                     | 0.45              |
| 6:W:2026:HOH:O   | 2:X:183:ASN:HB3  | 2.16                     | 0.45              |
| 2:X:126:ASP:O    | 2:X:157:ARG:HA   | 2.17                     | 0.45              |
| 2:J:111:ARG:HB2  | 2:L:175:ASP:OD2  | 2.16                     | 0.45              |
| 1:Q:413:MET:HE2  | 1:Q:435:GLU:HG3  | 1.98                     | 0.45              |
| 2:R:126:ASP:HB3  | 2:R:158:ARG:HB2  | 1.98                     | 0.45              |
| 2:T:89:MET:O     | 2:T:93:ILE:HG12  | 2.16                     | 0.45              |
| 2:V:145:VAL:HG21 | 2:X:180:LEU:HD11 | 1.99                     | 0.45              |
| 2:P:32:TYR:CD1   | 2:R:116:ASN:HA   | 2.52                     | 0.45              |
| 2:T:15:PRO:HD3   | 2:T:120:LYS:HG3  | 1.99                     | 0.45              |
| 1:W:244:LEU:HD13 | 1:W:253:LEU:HG   | 1.99                     | 0.45              |
| 1:K:187:LEU:HB2  | 1:K:191:ARG:HD3  | 1.99                     | 0.44              |
| 2:L:58:MET:CE    | 2:L:174:LEU:HD22 | 2.46                     | 0.44              |
| 2:N:116:ASN:HA   | 2:R:32:TYR:CG    | 2.52                     | 0.44              |
| 2:B:24:GLN:HG2   | 2:F:25:ASN:HD21  | 1.82                     | 0.44              |
| 1:E:287:VAL:HG12 | 1:E:288:MET:HE2  | 1.99                     | 0.44              |
| 1:Q:454:TRP:HA   | 1:Q:457:LEU:HB2  | 1.99                     | 0.44              |
| 1:W:164:ARG:HD2  | 1:W:178:VAL:HA   | 1.99                     | 0.44              |
| 2:H:170:ARG:HD3  | 2:H:172:ILE:HD11 | 1.99                     | 0.44              |
| 2:N:58:MET:HG3   | 2:N:172:ILE:HB   | 1.99                     | 0.44              |
| 1:A:213:LYS:HA   | 1:A:352:VAL:O    | 2.17                     | 0.44              |
| 1:M:384:PHE:CE2  | 5:M:1462:BNL:H12 | 2.53                     | 0.44              |
| 1:Q:262:GLY:HA2  | 1:Q:278:VAL:HG23 | 1.99                     | 0.44              |
| 1:I:262:GLY:C    | 1:I:432:VAL:HB   | 2.43                     | 0.44              |
| 1:E:212:GLN:HG3  | 1:E:354:ALA:HB3  | 2.00                     | 0.44              |
| 1:G:37:PRO:HG2   | 1:G:405:LYS:HA   | 1.99                     | 0.44              |
| 1:G:422:HIS:HD2  | 1:G:424:ASP:H    | 1.65                     | 0.44              |
| 1:S:76:THR:HG23  | 1:S:83:VAL:HG23  | 1.99                     | 0.44              |
| 1:U:422:HIS:CD2  | 1:U:424:ASP:H    | 2.36                     | 0.44              |
| 1:G:276:TRP:HB3  | 1:G:322:GLN:HG3  | 1.98                     | 0.44              |
| 1:U:422:HIS:HD2  | 1:U:424:ASP:H    | 1.66                     | 0.44              |
| 1:M:343:HIS:HB2  | 1:M:351:GLU:HB2  | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:9:PHE:H      | 1:S:258:ILE:HD11 | 1.83                     | 0.43              |
| 2:D:172:ILE:HD13 | 2:D:188:PHE:HB2  | 2.00                     | 0.43              |
| 1:E:248:PRO:HA   | 1:E:249:PRO:HD3  | 1.93                     | 0.43              |
| 2:L:44:GLU:HG2   | 2:P:155:VAL:HG21 | 2.00                     | 0.43              |
| 2:T:54:ILE:HA    | 2:T:168:ALA:O    | 2.18                     | 0.43              |
| 2:T:116:ASN:HA   | 2:X:32:TYR:CG    | 2.54                     | 0.43              |
| 1:W:262:GLY:C    | 1:W:432:VAL:HB   | 2.43                     | 0.43              |
| 1:C:212:GLN:HG3  | 1:C:214:TRP:HZ3  | 1.82                     | 0.43              |
| 1:C:251:MET:O    | 2:D:94:ARG:NH2   | 2.50                     | 0.43              |
| 2:H:49:LEU:HD21  | 2:H:163:LEU:HD13 | 1.99                     | 0.43              |
| 1:C:217:PRO:HG2  | 1:C:393:VAL:HG22 | 2.00                     | 0.43              |
| 1:K:389:GLY:O    | 1:K:393:VAL:HG23 | 2.19                     | 0.43              |
| 1:K:422:HIS:HD2  | 1:K:425:PHE:H    | 1.64                     | 0.43              |
| 2:L:49:LEU:HD21  | 2:L:163:LEU:HD13 | 2.01                     | 0.43              |
| 1:U:107:ILE:HG22 | 1:U:118:PHE:HB3  | 2.00                     | 0.43              |
| 2:V:36:GLN:NE2   | 2:X:12:PHE:H     | 2.16                     | 0.43              |
| 1:Q:262:GLY:C    | 1:Q:432:VAL:HB   | 2.44                     | 0.43              |
| 2:R:10:LYS:HG3   | 1:S:254:SER:HB3  | 2.01                     | 0.43              |
| 2:V:49:LEU:HD21  | 2:V:163:LEU:HD13 | 2.01                     | 0.43              |
| 1:A:244:LEU:HD13 | 1:A:253:LEU:HG   | 1.99                     | 0.43              |
| 2:B:94:ARG:HH11  | 2:B:94:ARG:CG    | 2.29                     | 0.43              |
| 1:C:63:HIS:CD2   | 1:C:357:LEU:HD21 | 2.53                     | 0.43              |
| 1:I:107:ILE:HG22 | 1:I:118:PHE:HB3  | 2.01                     | 0.43              |
| 2:L:170:ARG:HD3  | 2:L:172:ILE:HD11 | 2.01                     | 0.43              |
| 2:P:179:LEU:HD21 | 2:P:184:LEU:HD11 | 2.01                     | 0.43              |
| 1:S:344:PRO:HA   | 1:S:350:ILE:HG22 | 1.99                     | 0.43              |
| 1:U:315:PRO:HB2  | 1:U:318:ARG:HD3  | 2.01                     | 0.43              |
| 2:H:116:ASN:HA   | 2:L:32:TYR:CD1   | 2.54                     | 0.43              |
| 1:A:294:GLN:HE21 | 1:A:294:GLN:HA   | 1.84                     | 0.43              |
| 1:E:184:GLU:HB2  | 6:E:2022:HOH:O   | 2.19                     | 0.43              |
| 1:G:414:GLY:HA2  | 1:G:417:ARG:HD2  | 2.01                     | 0.43              |
| 1:K:215:VAL:HG22 | 1:K:351:GLU:HG2  | 1.99                     | 0.43              |
| 1:U:229:SER:HB2  | 1:U:437:ALA:HB3  | 2.00                     | 0.43              |
| 1:W:185:THR:HG22 | 1:W:459:PRO:HG2  | 2.00                     | 0.43              |
| 1:C:132:LYS:HD2  | 2:V:123:ALA:HA   | 2.01                     | 0.43              |
| 1:I:276:TRP:HB3  | 1:I:322:GLN:HG3  | 2.01                     | 0.43              |
| 2:L:126:ASP:HB3  | 2:L:158:ARG:HB2  | 2.00                     | 0.43              |
| 1:O:226:GLN:HA   | 1:O:230:ASP:HB3  | 2.01                     | 0.43              |
| 1:A:74:LEU:HD21  | 1:A:211:MET:HE1  | 2.01                     | 0.42              |
| 2:B:126:ASP:HB3  | 2:B:158:ARG:HB2  | 2.00                     | 0.42              |
| 1:E:228:CYS:HB2  | 1:E:325:THR:HB   | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:126:ALA:HB3  | 1:U:135:ASN:HB3  | 2.00                     | 0.42              |
| 1:W:229:SER:OG   | 1:W:438:ALA:HB2  | 2.18                     | 0.42              |
| 1:C:276:TRP:HB3  | 1:C:322:GLN:HG3  | 2.01                     | 0.42              |
| 2:D:32:TYR:CD1   | 2:F:116:ASN:HA   | 2.54                     | 0.42              |
| 1:G:389:GLY:O    | 1:G:393:VAL:HG23 | 2.19                     | 0.42              |
| 1:K:451:GLU:HA   | 1:K:452:PRO:HD3  | 1.79                     | 0.42              |
| 2:P:111:ARG:HB2  | 2:R:175:ASP:OD2  | 2.20                     | 0.42              |
| 1:Q:220:TRP:HA   | 1:Q:350:ILE:HG21 | 2.02                     | 0.42              |
| 2:P:32:TYR:CG    | 2:R:116:ASN:HA   | 2.54                     | 0.42              |
| 1:A:164:ARG:HD2  | 1:A:178:VAL:HA   | 2.01                     | 0.42              |
| 2:H:40:HIS:NE2   | 2:J:151:GLU:OE2  | 2.48                     | 0.42              |
| 1:Q:247:ILE:HD12 | 1:Q:251:MET:HB3  | 2.02                     | 0.42              |
| 1:C:126:ALA:HB3  | 1:C:135:ASN:HB3  | 2.01                     | 0.42              |
| 1:G:212:GLN:HG3  | 1:G:214:TRP:HZ3  | 1.85                     | 0.42              |
| 1:K:257:GLN:HE22 | 2:P:8:PHE:HB3    | 1.81                     | 0.42              |
| 1:K:368:GLU:O    | 1:K:372:ARG:HG3  | 2.20                     | 0.42              |
| 1:Q:231:MET:HE1  | 1:Q:321:GLY:O    | 2.19                     | 0.42              |
| 1:W:247:ILE:HG13 | 1:W:248:PRO:HD2  | 2.00                     | 0.42              |
| 1:A:42:ASP:HB3   | 1:A:45:LEU:HB2   | 2.01                     | 0.42              |
| 2:B:36:GLN:NE2   | 2:D:12:PHE:H     | 2.18                     | 0.42              |
| 1:G:191:ARG:N    | 1:G:192:PRO:HD2  | 2.35                     | 0.42              |
| 1:O:231:MET:HE1  | 1:O:321:GLY:O    | 2.20                     | 0.42              |
| 1:Q:333:LEU:HD13 | 1:Q:336:PHE:HD1  | 1.84                     | 0.42              |
| 2:V:143:ARG:NH2  | 6:V:2011:HOH:O   | 2.53                     | 0.42              |
| 1:A:257:GLN:HB2  | 6:A:2030:HOH:O   | 2.19                     | 0.42              |
| 1:Q:295:TYR:CD1  | 1:Q:366:ILE:HD13 | 2.54                     | 0.42              |
| 2:L:15:PRO:HG3   | 2:L:120:LYS:HG3  | 2.01                     | 0.42              |
| 1:O:126:ALA:HB3  | 1:O:135:ASN:HB3  | 2.02                     | 0.42              |
| 1:S:100:CYS:SG   | 1:S:127:TYR:OH   | 2.78                     | 0.42              |
| 1:U:248:PRO:HA   | 1:U:249:PRO:HD3  | 1.90                     | 0.42              |
| 1:I:296:TRP:CE2  | 1:I:335:THR:HG23 | 2.55                     | 0.42              |
| 1:I:458:LYS:HB2  | 1:I:459:PRO:HD2  | 2.00                     | 0.42              |
| 1:M:276:TRP:HB3  | 1:M:322:GLN:HG3  | 2.02                     | 0.42              |
| 1:G:422:HIS:CD2  | 1:G:424:ASP:H    | 2.37                     | 0.41              |
| 2:H:36:GLN:NE2   | 2:J:12:PHE:H     | 2.17                     | 0.41              |
| 2:T:32:TYR:CG    | 2:V:116:ASN:HA   | 2.55                     | 0.41              |
| 1:U:231:MET:HE1  | 1:U:321:GLY:O    | 2.19                     | 0.41              |
| 1:A:422:HIS:HD2  | 1:A:425:PHE:H    | 1.67                     | 0.41              |
| 1:C:340:ARG:HD3  | 1:C:342:TRP:CH2  | 2.55                     | 0.41              |
| 2:D:138:ARG:HD2  | 2:D:138:ARG:C    | 2.45                     | 0.41              |
| 2:J:32:TYR:CG    | 2:L:116:ASN:HA   | 2.55                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:340:ARG:HD3  | 1:U:342:TRP:CH2  | 2.55                     | 0.41              |
| 1:W:265:PHE:HE1  | 1:W:427:GLY:HA3  | 1.84                     | 0.41              |
| 1:K:267:ALA:HB2  | 1:K:272:HIS:HB2  | 2.02                     | 0.41              |
| 2:F:58:MET:HE2   | 2:F:81:HIS:CB    | 2.50                     | 0.41              |
| 1:I:36:ASP:O     | 1:I:39:ILE:HG12  | 2.20                     | 0.41              |
| 1:M:21:PRO:O     | 1:M:25:ARG:HG3   | 2.20                     | 0.41              |
| 1:O:30:GLN:OE1   | 1:O:266:ARG:NH2  | 2.44                     | 0.41              |
| 2:R:58:MET:HE2   | 2:R:81:HIS:CD2   | 2.56                     | 0.41              |
| 2:V:22:GLU:H     | 2:V:22:GLU:CD    | 2.27                     | 0.41              |
| 2:B:56:TYR:HB3   | 2:B:84:GLU:HB2   | 2.02                     | 0.41              |
| 2:R:54:ILE:HA    | 2:R:168:ALA:O    | 2.20                     | 0.41              |
| 1:S:212:GLN:HE21 | 1:S:212:GLN:HB2  | 1.67                     | 0.41              |
| 1:U:413:MET:HE2  | 1:U:435:GLU:HG3  | 2.02                     | 0.41              |
| 1:A:248:PRO:HA   | 1:A:249:PRO:HD3  | 1.94                     | 0.41              |
| 1:O:339:ILE:HD11 | 1:O:357:LEU:HD11 | 2.03                     | 0.41              |
| 1:K:276:TRP:HB3  | 1:K:322:GLN:HG3  | 2.01                     | 0.41              |
| 1:A:212:GLN:HG3  | 1:A:214:TRP:HZ3  | 1.85                     | 0.41              |
| 1:K:76:THR:OG1   | 1:K:77:TYR:N     | 2.53                     | 0.41              |
| 1:U:231:MET:HB2  | 1:U:323:HIS:NE2  | 2.35                     | 0.41              |
| 1:A:197:MET:HB2  | 1:A:334:PRO:HB3  | 2.03                     | 0.41              |
| 2:D:36:GLN:HE21  | 2:F:12:PHE:H     | 1.68                     | 0.41              |
| 1:E:275:GLY:O    | 1:E:322:GLN:HA   | 2.21                     | 0.41              |
| 1:G:226:GLN:HA   | 1:G:230:ASP:HB3  | 2.03                     | 0.41              |
| 2:H:32:TYR:CG    | 2:J:116:ASN:HA   | 2.56                     | 0.41              |
| 1:O:326:ILE:HB   | 1:O:330:CYS:HB3  | 2.03                     | 0.41              |
| 2:V:31:TYR:HE2   | 2:V:130:VAL:HG11 | 1.86                     | 0.41              |
| 1:W:60:LEU:HD11  | 1:W:171:LEU:HD22 | 2.02                     | 0.41              |
| 1:W:321:GLY:HA2  | 1:W:336:PHE:CZ   | 2.56                     | 0.41              |
| 2:X:8:PHE:CD1    | 2:X:8:PHE:C      | 2.98                     | 0.41              |
| 1:K:248:PRO:HA   | 1:K:249:PRO:HD3  | 1.93                     | 0.41              |
| 1:S:340:ARG:NH2  | 1:S:378:PHE:HB3  | 2.36                     | 0.41              |
| 1:U:230:ASP:CG   | 1:W:123:HIS:HE2  | 2.28                     | 0.41              |
| 1:W:327:PHE:CG   | 1:W:328:PRO:HA   | 2.56                     | 0.41              |
| 2:X:139:ASN:HD22 | 2:X:145:VAL:HG22 | 1.85                     | 0.41              |
| 1:C:422:HIS:CD2  | 1:C:424:ASP:H    | 2.38                     | 0.40              |
| 2:H:24:GLN:HG2   | 2:L:25:ASN:ND2   | 2.35                     | 0.40              |
| 1:O:262:GLY:C    | 1:O:432:VAL:HB   | 2.46                     | 0.40              |
| 1:O:422:HIS:CD2  | 1:O:424:ASP:H    | 2.40                     | 0.40              |
| 1:A:230:ASP:CG   | 1:C:123:HIS:HE2  | 2.28                     | 0.40              |
| 1:C:332:PHE:HB3  | 1:C:339:ILE:HG23 | 2.03                     | 0.40              |
| 2:F:19:ALA:HB1   | 2:F:23:LEU:HD23  | 2.03                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:275:GLY:O    | 1:S:322:GLN:HA   | 2.22                     | 0.40              |
| 1:A:68:PRO:HD2   | 1:A:72:ASP:OD2   | 2.21                     | 0.40              |
| 2:D:179:LEU:HD21 | 2:D:184:LEU:HD11 | 2.03                     | 0.40              |
| 2:J:136:LEU:HB3  | 2:J:148:PHE:HB2  | 2.03                     | 0.40              |
| 1:K:258:ILE:HA   | 1:K:259:PRO:HD2  | 1.93                     | 0.40              |
| 2:N:179:LEU:HD21 | 2:N:184:LEU:HD11 | 2.03                     | 0.40              |
| 1:Q:389:GLY:O    | 1:Q:393:VAL:HG23 | 2.22                     | 0.40              |
| 1:C:287:VAL:HG12 | 1:C:288:MET:HE3  | 2.03                     | 0.40              |
| 1:G:326:ILE:HB   | 1:G:330:CYS:HB3  | 2.04                     | 0.40              |
| 2:H:67:ARG:HG2   | 2:H:68:GLU:HG3   | 2.03                     | 0.40              |
| 1:O:288:MET:HE3  | 1:O:336:PHE:HB3  | 2.03                     | 0.40              |
| 1:S:391:ASN:O    | 1:S:395:ILE:HG13 | 2.22                     | 0.40              |
| 2:D:36:GLN:NE2   | 2:F:12:PHE:H     | 2.19                     | 0.40              |
| 2:F:9:PHE:O      | 2:F:10:LYS:HG3   | 2.22                     | 0.40              |
| 1:G:239:HIS:CE1  | 1:G:384:PHE:O    | 2.74                     | 0.40              |
| 1:O:212:GLN:HG3  | 1:O:214:TRP:HZ3  | 1.87                     | 0.40              |
| 1:S:29:ASP:OD1   | 1:S:32:LYS:HE3   | 2.21                     | 0.40              |
| 1:U:107:ILE:CG2  | 1:U:118:PHE:HB3  | 2.52                     | 0.40              |
| 1:U:262:GLY:C    | 1:U:432:VAL:HB   | 2.47                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

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   | C     | 350/373 (94%) | 344 (98%) | 6 (2%)   | 53 73       |
| 1   | E     | 350/373 (94%) | 343 (98%) | 7 (2%)   | 48 68       |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 1   | I     | 82/373 (22%)    | 82 (100%)  | 0        | 100         | 100 |
| 1   | K     | 254/373 (68%)   | 251 (99%)  | 3 (1%)   | 63          | 79  |
| 1   | M     | 350/373 (94%)   | 344 (98%)  | 6 (2%)   | 53          | 73  |
| 1   | O     | 210/373 (56%)   | 205 (98%)  | 5 (2%)   | 43          | 63  |
| 1   | Q     | 350/373 (94%)   | 343 (98%)  | 7 (2%)   | 48          | 68  |
| 1   | S     | 349/373 (94%)   | 341 (98%)  | 8 (2%)   | 44          | 64  |
| 1   | U     | 349/373 (94%)   | 345 (99%)  | 4 (1%)   | 65          | 81  |
| 1   | W     | 349/373 (94%)   | 338 (97%)  | 11 (3%)  | 34          | 54  |
| 2   | B     | 84/167 (50%)    | 83 (99%)   | 1 (1%)   | 63          | 79  |
| 2   | D     | 158/167 (95%)   | 156 (99%)  | 2 (1%)   | 61          | 78  |
| 2   | H     | 127/167 (76%)   | 123 (97%)  | 4 (3%)   | 35          | 55  |
| 2   | L     | 160/167 (96%)   | 157 (98%)  | 3 (2%)   | 50          | 70  |
| 2   | N     | 160/167 (96%)   | 155 (97%)  | 5 (3%)   | 35          | 55  |
| 2   | P     | 104/167 (62%)   | 101 (97%)  | 3 (3%)   | 37          | 57  |
| 2   | R     | 160/167 (96%)   | 157 (98%)  | 3 (2%)   | 50          | 70  |
| 2   | T     | 160/167 (96%)   | 158 (99%)  | 2 (1%)   | 61          | 78  |
| 2   | V     | 160/167 (96%)   | 156 (98%)  | 4 (2%)   | 42          | 62  |
| 2   | X     | 160/167 (96%)   | 158 (99%)  | 2 (1%)   | 61          | 78  |
| All | All   | 4426/5400 (82%) | 4340 (98%) | 86 (2%)  | 50          | 70  |

All (86) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 179 | LEU  |
| 1   | C     | 86  | VAL  |
| 1   | C     | 247 | ILE  |
| 1   | C     | 280 | GLU  |
| 1   | C     | 294 | GLN  |
| 1   | C     | 335 | THR  |
| 1   | C     | 457 | LEU  |
| 2   | D     | 121 | GLU  |
| 2   | D     | 179 | LEU  |
| 1   | E     | 86  | VAL  |
| 1   | E     | 103 | ARG  |
| 1   | E     | 258 | ILE  |
| 1   | E     | 280 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 335 | THR  |
| 1   | E     | 413 | MET  |
| 1   | E     | 457 | LEU  |
| 2   | H     | 67  | ARG  |
| 2   | H     | 143 | ARG  |
| 2   | H     | 169 | LYS  |
| 2   | H     | 179 | LEU  |
| 1   | K     | 191 | ARG  |
| 1   | K     | 205 | THR  |
| 1   | K     | 252 | ASP  |
| 2   | L     | 95  | LYS  |
| 2   | L     | 140 | ARG  |
| 2   | L     | 179 | LEU  |
| 1   | M     | 103 | ARG  |
| 1   | M     | 261 | LYS  |
| 1   | M     | 280 | GLU  |
| 1   | M     | 309 | LEU  |
| 1   | M     | 339 | ILE  |
| 1   | M     | 366 | ILE  |
| 2   | N     | 14  | TRP  |
| 2   | N     | 44  | GLU  |
| 2   | N     | 93  | ILE  |
| 2   | N     | 121 | GLU  |
| 2   | N     | 124 | THR  |
| 1   | O     | 31  | GLU  |
| 1   | O     | 86  | VAL  |
| 1   | O     | 255 | GLN  |
| 1   | O     | 261 | LYS  |
| 1   | O     | 280 | GLU  |
| 2   | P     | 93  | ILE  |
| 2   | P     | 94  | ARG  |
| 2   | P     | 179 | LEU  |
| 1   | Q     | 86  | VAL  |
| 1   | Q     | 103 | ARG  |
| 1   | Q     | 116 | LYS  |
| 1   | Q     | 255 | GLN  |
| 1   | Q     | 261 | LYS  |
| 1   | Q     | 280 | GLU  |
| 1   | Q     | 358 | VAL  |
| 2   | R     | 93  | ILE  |
| 2   | R     | 94  | ARG  |
| 2   | R     | 179 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | S     | 48  | LEU  |
| 1   | S     | 89  | LYS  |
| 1   | S     | 103 | ARG  |
| 1   | S     | 280 | GLU  |
| 1   | S     | 335 | THR  |
| 1   | S     | 339 | ILE  |
| 1   | S     | 350 | ILE  |
| 1   | S     | 446 | MET  |
| 2   | T     | 121 | GLU  |
| 2   | T     | 179 | LEU  |
| 1   | U     | 103 | ARG  |
| 1   | U     | 255 | GLN  |
| 1   | U     | 309 | LEU  |
| 1   | U     | 376 | ARG  |
| 2   | V     | 8   | PHE  |
| 2   | V     | 44  | GLU  |
| 2   | V     | 76  | ASP  |
| 2   | V     | 179 | LEU  |
| 1   | W     | 86  | VAL  |
| 1   | W     | 94  | LYS  |
| 1   | W     | 103 | ARG  |
| 1   | W     | 167 | THR  |
| 1   | W     | 243 | ILE  |
| 1   | W     | 280 | GLU  |
| 1   | W     | 307 | GLN  |
| 1   | W     | 335 | THR  |
| 1   | W     | 341 | ILE  |
| 1   | W     | 407 | GLN  |
| 1   | W     | 435 | GLU  |
| 2   | X     | 8   | PHE  |
| 2   | X     | 143 | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 144 | GLN  |
| 2   | B     | 162 | ASN  |
| 1   | C     | 43  | GLN  |
| 1   | C     | 294 | GLN  |
| 1   | C     | 386 | GLN  |
| 1   | C     | 391 | ASN  |
| 1   | C     | 410 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 412 | GLN  |
| 1   | C     | 422 | HIS  |
| 1   | C     | 443 | HIS  |
| 1   | C     | 444 | HIS  |
| 2   | D     | 36  | GLN  |
| 2   | D     | 162 | ASN  |
| 1   | E     | 18  | ASN  |
| 1   | E     | 43  | GLN  |
| 1   | E     | 257 | GLN  |
| 1   | E     | 294 | GLN  |
| 1   | E     | 391 | ASN  |
| 1   | E     | 410 | ASN  |
| 1   | E     | 412 | GLN  |
| 1   | E     | 422 | HIS  |
| 1   | E     | 443 | HIS  |
| 1   | I     | 43  | GLN  |
| 1   | I     | 88  | GLN  |
| 1   | I     | 99  | GLN  |
| 1   | K     | 88  | GLN  |
| 1   | K     | 212 | GLN  |
| 1   | K     | 264 | GLN  |
| 1   | K     | 322 | GLN  |
| 1   | K     | 343 | HIS  |
| 1   | K     | 377 | ASN  |
| 1   | K     | 386 | GLN  |
| 1   | K     | 391 | ASN  |
| 1   | K     | 410 | ASN  |
| 1   | K     | 422 | HIS  |
| 1   | K     | 443 | HIS  |
| 2   | L     | 25  | ASN  |
| 2   | L     | 36  | GLN  |
| 2   | L     | 81  | HIS  |
| 2   | L     | 131 | ASN  |
| 1   | M     | 43  | GLN  |
| 1   | M     | 88  | GLN  |
| 1   | M     | 212 | GLN  |
| 1   | M     | 257 | GLN  |
| 1   | M     | 263 | ASN  |
| 1   | M     | 311 | HIS  |
| 1   | M     | 322 | GLN  |
| 1   | M     | 391 | ASN  |
| 1   | M     | 410 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | N     | 25  | ASN  |
| 2   | N     | 77  | GLN  |
| 2   | N     | 131 | ASN  |
| 1   | O     | 43  | GLN  |
| 1   | O     | 226 | GLN  |
| 1   | O     | 257 | GLN  |
| 2   | P     | 77  | GLN  |
| 2   | P     | 86  | HIS  |
| 1   | Q     | 255 | GLN  |
| 1   | Q     | 377 | ASN  |
| 1   | Q     | 391 | ASN  |
| 1   | Q     | 410 | ASN  |
| 1   | Q     | 422 | HIS  |
| 2   | R     | 25  | ASN  |
| 2   | R     | 40  | HIS  |
| 2   | R     | 77  | GLN  |
| 1   | S     | 43  | GLN  |
| 1   | S     | 212 | GLN  |
| 1   | S     | 343 | HIS  |
| 1   | S     | 377 | ASN  |
| 1   | S     | 386 | GLN  |
| 1   | S     | 391 | ASN  |
| 1   | S     | 410 | ASN  |
| 1   | S     | 422 | HIS  |
| 1   | S     | 428 | ASN  |
| 1   | S     | 443 | HIS  |
| 1   | S     | 444 | HIS  |
| 2   | T     | 25  | ASN  |
| 2   | T     | 36  | GLN  |
| 1   | U     | 43  | GLN  |
| 1   | U     | 212 | GLN  |
| 1   | U     | 226 | GLN  |
| 1   | U     | 255 | GLN  |
| 1   | U     | 264 | GLN  |
| 1   | U     | 322 | GLN  |
| 1   | U     | 343 | HIS  |
| 1   | U     | 386 | GLN  |
| 1   | U     | 410 | ASN  |
| 1   | U     | 422 | HIS  |
| 1   | U     | 443 | HIS  |
| 2   | V     | 25  | ASN  |
| 2   | V     | 36  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | V     | 81  | HIS  |
| 1   | W     | 212 | GLN  |
| 1   | W     | 264 | GLN  |
| 1   | W     | 386 | GLN  |
| 1   | W     | 391 | ASN  |
| 1   | W     | 410 | ASN  |
| 1   | W     | 422 | HIS  |
| 1   | W     | 443 | HIS  |
| 2   | X     | 25  | ASN  |
| 2   | X     | 86  | HIS  |
| 2   | X     | 131 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 3   | FES  | C     | 1460 | 1    | 0,4,4        | -    | -           | -           |      |             |
| 5   | BNL  | O     | 1462 | -    | 13,13,13     | 0.60 | 0           | 16,16,16    | 0.50 | 0           |
| 3   | FES  | S     | 1460 | 1    | 0,4,4        | -    | -           | -           |      |             |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | FES  | K     | 1460 | 1    | 0,4,4        | -    | -        | -           |      |          |
| 3   | FES  | I     | 1460 | 1    | 0,4,4        | -    | -        | -           |      |          |
| 5   | BNL  | W     | 1462 | -    | 13,13,13     | 0.60 | 0        | 16,16,16    | 0.57 | 0        |
| 3   | FES  | Q     | 1460 | 1    | 0,4,4        | -    | -        | -           |      |          |
| 5   | BNL  | U     | 1462 | -    | 13,13,13     | 0.57 | 0        | 16,16,16    | 0.55 | 0        |
| 3   | FES  | A     | 1460 | 1    | 0,4,4        | -    | -        | -           |      |          |
| 5   | BNL  | M     | 1462 | -    | 13,13,13     | 0.58 | 0        | 16,16,16    | 0.51 | 0        |
| 5   | BNL  | G     | 1462 | -    | 13,13,13     | 0.58 | 0        | 16,16,16    | 0.51 | 0        |
| 3   | FES  | W     | 1460 | 1    | 0,4,4        | -    | -        | -           |      |          |
| 3   | FES  | E     | 1460 | 1    | 0,4,4        | -    | -        | -           |      |          |
| 3   | FES  | M     | 1460 | 1    | 0,4,4        | -    | -        | -           |      |          |
| 3   | FES  | G     | 1460 | 1    | 0,4,4        | -    | -        | -           |      |          |
| 5   | BNL  | K     | 1462 | -    | 13,13,13     | 0.61 | 0        | 16,16,16    | 0.43 | 0        |
| 5   | BNL  | C     | 1462 | -    | 13,13,13     | 0.59 | 0        | 16,16,16    | 0.46 | 0        |
| 5   | BNL  | S     | 1462 | -    | 13,13,13     | 0.59 | 0        | 16,16,16    | 0.58 | 0        |
| 3   | FES  | U     | 1460 | 1    | 0,4,4        | -    | -        | -           |      |          |
| 3   | FES  | O     | 1460 | 1    | 0,4,4        | -    | -        | -           |      |          |
| 5   | BNL  | I     | 1462 | -    | 13,13,13     | 0.57 | 0        | 16,16,16    | 0.63 | 0        |
| 5   | BNL  | E     | 1462 | -    | 13,13,13     | 0.60 | 0        | 16,16,16    | 0.53 | 0        |
| 5   | BNL  | Q     | 1462 | -    | 13,13,13     | 0.66 | 0        | 16,16,16    | 0.45 | 0        |
| 5   | BNL  | A     | 1462 | -    | 13,13,13     | 0.59 | 0        | 16,16,16    | 0.58 | 0        |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 3   | FES  | C     | 1460 | 1    | -       | -        | 0/1/1/1 |
| 5   | BNL  | O     | 1462 | -    | -       | 0/4/4/4  | 0/2/2/2 |
| 3   | FES  | S     | 1460 | 1    | -       | -        | 0/1/1/1 |
| 3   | FES  | I     | 1460 | 1    | -       | -        | 0/1/1/1 |
| 3   | FES  | K     | 1460 | 1    | -       | -        | 0/1/1/1 |
| 5   | BNL  | W     | 1462 | -    | -       | 2/4/4/4  | 0/2/2/2 |
| 3   | FES  | Q     | 1460 | 1    | -       | -        | 0/1/1/1 |
| 5   | BNL  | U     | 1462 | -    | -       | 0/4/4/4  | 0/2/2/2 |
| 3   | FES  | A     | 1460 | 1    | -       | -        | 0/1/1/1 |
| 5   | BNL  | M     | 1462 | -    | -       | 0/4/4/4  | 0/2/2/2 |
| 5   | BNL  | G     | 1462 | -    | -       | 0/4/4/4  | 0/2/2/2 |
| 3   | FES  | W     | 1460 | 1    | -       | -        | 0/1/1/1 |
| 3   | FES  | E     | 1460 | 1    | -       | -        | 0/1/1/1 |
| 3   | FES  | M     | 1460 | 1    | -       | -        | 0/1/1/1 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 3   | FES  | G     | 1460 | 1    | -       | -        | 0/1/1/1 |
| 5   | BNL  | K     | 1462 | -    | -       | 0/4/4/4  | 0/2/2/2 |
| 5   | BNL  | C     | 1462 | -    | -       | 0/4/4/4  | 0/2/2/2 |
| 5   | BNL  | S     | 1462 | -    | -       | 0/4/4/4  | 0/2/2/2 |
| 3   | FES  | U     | 1460 | 1    | -       | -        | 0/1/1/1 |
| 3   | FES  | O     | 1460 | 1    | -       | -        | 0/1/1/1 |
| 5   | BNL  | I     | 1462 | -    | -       | 4/4/4/4  | 0/2/2/2 |
| 5   | BNL  | E     | 1462 | -    | -       | 0/4/4/4  | 0/2/2/2 |
| 5   | BNL  | Q     | 1462 | -    | -       | 0/4/4/4  | 0/2/2/2 |
| 5   | BNL  | A     | 1462 | -    | -       | 4/4/4/4  | 0/2/2/2 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms         |
|-----|-------|------|------|---------------|
| 5   | I     | 1462 | BNL  | C15-C16-C2-C1 |
| 5   | I     | 1462 | BNL  | C17-C16-C2-C3 |
| 5   | I     | 1462 | BNL  | C17-C16-C2-C1 |
| 5   | I     | 1462 | BNL  | C15-C16-C2-C3 |
| 5   | A     | 1462 | BNL  | C15-C16-C2-C1 |
| 5   | A     | 1462 | BNL  | C17-C16-C2-C3 |
| 5   | A     | 1462 | BNL  | C17-C16-C2-C1 |
| 5   | A     | 1462 | BNL  | C15-C16-C2-C3 |
| 5   | W     | 1462 | BNL  | C15-C16-C2-C1 |
| 5   | W     | 1462 | BNL  | C17-C16-C2-C3 |

There are no ring outliers.

13 monomers are involved in 13 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | C     | 1460 | FES  | 1       | 0            |
| 3   | S     | 1460 | FES  | 1       | 0            |
| 3   | K     | 1460 | FES  | 1       | 0            |
| 3   | I     | 1460 | FES  | 1       | 0            |
| 3   | Q     | 1460 | FES  | 1       | 0            |
| 3   | A     | 1460 | FES  | 1       | 0            |
| 5   | M     | 1462 | BNL  | 1       | 0            |
| 3   | W     | 1460 | FES  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | E     | 1460 | FES  | 1       | 0            |
| 3   | M     | 1460 | FES  | 1       | 0            |
| 3   | G     | 1460 | FES  | 1       | 0            |
| 3   | U     | 1460 | FES  | 1       | 0            |
| 3   | O     | 1460 | FES  | 1       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9   |
|-----|-------|---------------|--------|---------------|-----------------------|---------|
| 1   | A     | 432/459 (94%) | 0.34   | 9 (2%) 63 60  | 22, 40, 55, 61        | 17 (3%) |
| 1   | C     | 432/459 (94%) | 0.45   | 20 (4%) 37 33 | 25, 43, 54, 58        | 17 (3%) |
| 1   | E     | 432/459 (94%) | 0.15   | 9 (2%) 63 60  | 21, 35, 46, 55        | 17 (3%) |
| 1   | G     | 432/459 (94%) | 0.53   | 13 (3%) 52 49 | 29, 47, 60, 66        | 17 (3%) |
| 1   | I     | 432/459 (94%) | 0.74   | 30 (6%) 23 19 | 29, 51, 63, 69        | 17 (3%) |
| 1   | K     | 432/459 (94%) | 0.92   | 28 (6%) 25 21 | 27, 54, 65, 68        | 17 (3%) |
| 1   | M     | 432/459 (94%) | 0.33   | 20 (4%) 37 33 | 22, 38, 58, 62        | 17 (3%) |
| 1   | O     | 432/459 (94%) | 0.16   | 10 (2%) 61 57 | 20, 34, 49, 57        | 17 (3%) |
| 1   | Q     | 432/459 (94%) | -0.05  | 7 (1%) 70 67  | 17, 31, 42, 61        | 17 (3%) |
| 1   | S     | 432/459 (94%) | 0.70   | 28 (6%) 25 21 | 19, 47, 58, 67        | 17 (3%) |
| 1   | U     | 432/459 (94%) | 1.02   | 43 (9%) 12 9  | 31, 56, 72, 74        | 17 (3%) |
| 1   | W     | 432/459 (94%) | 1.37   | 80 (18%) 3 3  | 34, 59, 70, 74        | 17 (3%) |
| 2   | B     | 181/188 (96%) | 0.26   | 3 (1%) 69 66  | 26, 38, 47, 58        | 4 (2%)  |
| 2   | D     | 181/188 (96%) | 0.22   | 5 (2%) 55 51  | 28, 39, 51, 56        | 4 (2%)  |
| 2   | F     | 181/188 (96%) | 0.02   | 1 (0%) 85 84  | 23, 33, 47, 60        | 4 (2%)  |
| 2   | H     | 181/188 (96%) | 0.53   | 8 (4%) 39 34  | 32, 45, 60, 66        | 4 (2%)  |
| 2   | J     | 181/188 (96%) | 0.60   | 4 (2%) 62 59  | 35, 49, 57, 63        | 4 (2%)  |
| 2   | L     | 181/188 (96%) | 0.66   | 6 (3%) 49 45  | 35, 48, 63, 70        | 4 (2%)  |
| 2   | N     | 181/188 (96%) | 0.32   | 9 (4%) 34 30  | 25, 37, 61, 75        | 4 (2%)  |
| 2   | P     | 181/188 (96%) | 0.22   | 8 (4%) 39 34  | 24, 36, 64, 79        | 4 (2%)  |
| 2   | R     | 181/188 (96%) | 0.04   | 2 (1%) 78 75  | 21, 32, 52, 62        | 4 (2%)  |
| 2   | T     | 181/188 (96%) | 0.23   | 4 (2%) 62 59  | 28, 39, 55, 65        | 4 (2%)  |
| 2   | V     | 181/188 (96%) | 0.80   | 12 (6%) 24 20 | 40, 53, 59, 64        | 4 (2%)  |
| 2   | X     | 181/188 (96%) | 1.07   | 15 (8%) 17 14 | 37, 52, 59, 62        | 4 (2%)  |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2  |    |    | OWAB(Å <sup>2</sup> ) | Q<0.9    |
|-----|-------|-----------------|--------|----------|----|----|-----------------------|----------|
| All | All   | 7356/7764 (94%) | 0.51   | 374 (5%) | 33 | 30 | 17, 44, 63, 79        | 252 (3%) |

All (374) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 256 | ALA  | 10.0 |
| 1   | K     | 256 | ALA  | 8.9  |
| 1   | W     | 256 | ALA  | 8.4  |
| 1   | M     | 256 | ALA  | 8.3  |
| 1   | Q     | 260 | THR  | 7.8  |
| 1   | I     | 256 | ALA  | 7.6  |
| 1   | K     | 255 | GLN  | 7.4  |
| 1   | E     | 256 | ALA  | 6.8  |
| 1   | G     | 256 | ALA  | 6.7  |
| 1   | U     | 260 | THR  | 6.6  |
| 1   | O     | 256 | ALA  | 6.5  |
| 1   | S     | 256 | ALA  | 6.5  |
| 1   | W     | 260 | THR  | 5.8  |
| 1   | A     | 255 | GLN  | 5.8  |
| 1   | I     | 260 | THR  | 5.6  |
| 1   | A     | 421 | GLY  | 5.3  |
| 1   | M     | 255 | GLN  | 5.3  |
| 1   | U     | 256 | ALA  | 5.2  |
| 1   | E     | 259 | PRO  | 5.1  |
| 1   | I     | 246 | GLY  | 5.1  |
| 1   | Q     | 256 | ALA  | 5.1  |
| 1   | W     | 257 | GLN  | 4.9  |
| 1   | K     | 142 | ALA  | 4.9  |
| 1   | S     | 255 | GLN  | 4.9  |
| 1   | O     | 255 | GLN  | 4.8  |
| 1   | G     | 259 | PRO  | 4.8  |
| 1   | S     | 259 | PRO  | 4.7  |
| 1   | K     | 260 | THR  | 4.7  |
| 1   | E     | 255 | GLN  | 4.7  |
| 1   | U     | 255 | GLN  | 4.7  |
| 1   | S     | 105 | MET  | 4.6  |
| 1   | Q     | 259 | PRO  | 4.5  |
| 1   | C     | 257 | GLN  | 4.5  |
| 1   | C     | 256 | ALA  | 4.4  |
| 2   | X     | 11  | THR  | 4.4  |
| 1   | M     | 260 | THR  | 4.4  |
| 1   | A     | 260 | THR  | 4.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | W     | 292 | VAL  | 4.3  |
| 1   | M     | 259 | PRO  | 4.2  |
| 1   | O     | 261 | LYS  | 4.2  |
| 2   | F     | 8   | PHE  | 4.2  |
| 1   | S     | 142 | ALA  | 4.2  |
| 1   | U     | 259 | PRO  | 4.1  |
| 2   | N     | 14  | TRP  | 4.1  |
| 1   | C     | 260 | THR  | 4.0  |
| 1   | S     | 257 | GLN  | 4.0  |
| 2   | N     | 12  | PHE  | 3.9  |
| 1   | W     | 389 | GLY  | 3.9  |
| 1   | S     | 260 | THR  | 3.9  |
| 1   | W     | 94  | LYS  | 3.9  |
| 1   | I     | 262 | GLY  | 3.9  |
| 1   | I     | 259 | PRO  | 3.8  |
| 1   | K     | 259 | PRO  | 3.8  |
| 1   | W     | 261 | LYS  | 3.8  |
| 1   | O     | 311 | HIS  | 3.8  |
| 1   | W     | 255 | GLN  | 3.8  |
| 1   | G     | 260 | THR  | 3.7  |
| 1   | C     | 259 | PRO  | 3.7  |
| 1   | W     | 259 | PRO  | 3.7  |
| 1   | G     | 261 | LYS  | 3.7  |
| 1   | G     | 24  | ILE  | 3.7  |
| 2   | N     | 19  | ALA  | 3.6  |
| 2   | H     | 9   | PHE  | 3.6  |
| 1   | A     | 259 | PRO  | 3.6  |
| 1   | E     | 260 | THR  | 3.6  |
| 1   | W     | 125 | TRP  | 3.6  |
| 1   | M     | 257 | GLN  | 3.6  |
| 1   | A     | 257 | GLN  | 3.5  |
| 1   | U     | 257 | GLN  | 3.5  |
| 2   | J     | 103 | ALA  | 3.5  |
| 1   | S     | 138 | PHE  | 3.5  |
| 1   | U     | 356 | THR  | 3.5  |
| 1   | U     | 285 | LEU  | 3.5  |
| 1   | K     | 316 | VAL  | 3.5  |
| 1   | Q     | 261 | LYS  | 3.5  |
| 1   | K     | 257 | GLN  | 3.4  |
| 1   | I     | 320 | VAL  | 3.4  |
| 1   | I     | 255 | GLN  | 3.4  |
| 1   | M     | 261 | LYS  | 3.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | X     | 63  | ASN  | 3.4  |
| 1   | W     | 79  | GLY  | 3.4  |
| 1   | G     | 142 | ALA  | 3.4  |
| 1   | E     | 261 | LYS  | 3.3  |
| 1   | I     | 257 | GLN  | 3.3  |
| 1   | Q     | 257 | GLN  | 3.3  |
| 2   | P     | 14  | TRP  | 3.3  |
| 1   | G     | 292 | VAL  | 3.3  |
| 1   | U     | 262 | GLY  | 3.3  |
| 1   | G     | 257 | GLN  | 3.3  |
| 1   | O     | 259 | PRO  | 3.3  |
| 1   | W     | 286 | ALA  | 3.3  |
| 2   | J     | 8   | PHE  | 3.2  |
| 1   | K     | 186 | TYR  | 3.2  |
| 1   | K     | 131 | GLY  | 3.2  |
| 2   | N     | 8   | PHE  | 3.2  |
| 1   | S     | 261 | LYS  | 3.2  |
| 1   | M     | 142 | ALA  | 3.2  |
| 1   | W     | 250 | GLU  | 3.2  |
| 1   | S     | 129 | ILE  | 3.2  |
| 1   | Q     | 255 | GLN  | 3.1  |
| 2   | B     | 9   | PHE  | 3.1  |
| 1   | W     | 22  | GLU  | 3.1  |
| 1   | W     | 414 | GLY  | 3.1  |
| 1   | U     | 109 | ARG  | 3.1  |
| 1   | W     | 110 | SER  | 3.1  |
| 1   | W     | 316 | VAL  | 3.1  |
| 1   | E     | 257 | GLN  | 3.1  |
| 2   | V     | 9   | PHE  | 3.1  |
| 1   | U     | 187 | LEU  | 3.1  |
| 2   | X     | 174 | LEU  | 3.1  |
| 1   | I     | 275 | GLY  | 3.1  |
| 1   | U     | 400 | ARG  | 3.1  |
| 2   | D     | 123 | ALA  | 3.1  |
| 1   | W     | 285 | LEU  | 3.1  |
| 2   | J     | 113 | LEU  | 3.1  |
| 1   | S     | 109 | ARG  | 3.1  |
| 1   | W     | 196 | VAL  | 3.1  |
| 1   | W     | 236 | THR  | 3.0  |
| 1   | K     | 261 | LYS  | 3.0  |
| 1   | W     | 329 | THR  | 3.0  |
| 1   | I     | 261 | LYS  | 3.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | I     | 276 | TRP  | 3.0  |
| 2   | X     | 176 | ALA  | 3.0  |
| 1   | U     | 28  | VAL  | 3.0  |
| 1   | W     | 142 | ALA  | 3.0  |
| 1   | W     | 433 | TYR  | 3.0  |
| 1   | W     | 34  | LEU  | 3.0  |
| 1   | W     | 244 | LEU  | 3.0  |
| 1   | U     | 314 | MET  | 2.9  |
| 1   | W     | 291 | LYS  | 2.9  |
| 1   | K     | 372 | ARG  | 2.9  |
| 2   | P     | 12  | PHE  | 2.9  |
| 1   | M     | 258 | ILE  | 2.9  |
| 1   | S     | 103 | ARG  | 2.9  |
| 2   | N     | 11  | THR  | 2.9  |
| 1   | W     | 183 | LEU  | 2.9  |
| 1   | C     | 105 | MET  | 2.9  |
| 1   | K     | 24  | ILE  | 2.9  |
| 2   | L     | 163 | LEU  | 2.9  |
| 1   | G     | 433 | TYR  | 2.9  |
| 1   | W     | 425 | PHE  | 2.8  |
| 1   | U     | 232 | TYR  | 2.8  |
| 1   | I     | 444 | HIS  | 2.8  |
| 1   | C     | 316 | VAL  | 2.8  |
| 1   | W     | 117 | ALA  | 2.8  |
| 1   | W     | 364 | ALA  | 2.8  |
| 2   | P     | 58  | MET  | 2.8  |
| 1   | K     | 95  | VAL  | 2.8  |
| 1   | W     | 28  | VAL  | 2.8  |
| 1   | O     | 260 | THR  | 2.8  |
| 1   | W     | 166 | ALA  | 2.8  |
| 1   | K     | 127 | TYR  | 2.8  |
| 1   | M     | 201 | THR  | 2.8  |
| 1   | O     | 105 | MET  | 2.8  |
| 1   | A     | 261 | LYS  | 2.8  |
| 1   | M     | 307 | GLN  | 2.8  |
| 1   | O     | 109 | ARG  | 2.8  |
| 1   | U     | 275 | GLY  | 2.7  |
| 1   | W     | 378 | PHE  | 2.8  |
| 2   | D     | 8   | PHE  | 2.8  |
| 1   | W     | 293 | THR  | 2.7  |
| 2   | H     | 27  | ILE  | 2.7  |
| 1   | C     | 193 | TYR  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | I     | 316 | VAL  | 2.7  |
| 1   | U     | 196 | VAL  | 2.7  |
| 1   | O     | 291 | LYS  | 2.7  |
| 2   | V     | 58  | MET  | 2.7  |
| 2   | X     | 45  | ALA  | 2.7  |
| 1   | C     | 255 | GLN  | 2.7  |
| 2   | V     | 8   | PHE  | 2.7  |
| 1   | K     | 251 | MET  | 2.7  |
| 2   | H     | 94  | ARG  | 2.7  |
| 1   | E     | 235 | GLY  | 2.7  |
| 1   | K     | 414 | GLY  | 2.7  |
| 1   | U     | 291 | LYS  | 2.7  |
| 1   | W     | 109 | ARG  | 2.7  |
| 1   | W     | 190 | ALA  | 2.7  |
| 1   | U     | 261 | LYS  | 2.6  |
| 1   | W     | 258 | ILE  | 2.6  |
| 1   | W     | 278 | VAL  | 2.6  |
| 1   | C     | 314 | MET  | 2.6  |
| 1   | K     | 203 | ALA  | 2.6  |
| 1   | I     | 431 | TYR  | 2.6  |
| 1   | W     | 46  | TYR  | 2.6  |
| 1   | U     | 296 | TRP  | 2.6  |
| 1   | W     | 276 | TRP  | 2.6  |
| 2   | V     | 179 | LEU  | 2.6  |
| 2   | P     | 11  | THR  | 2.6  |
| 1   | W     | 248 | PRO  | 2.6  |
| 1   | I     | 285 | LEU  | 2.6  |
| 2   | X     | 21  | LEU  | 2.6  |
| 1   | U     | 274 | SER  | 2.6  |
| 2   | R     | 16  | SER  | 2.6  |
| 2   | V     | 94  | ARG  | 2.5  |
| 2   | L     | 165 | PHE  | 2.5  |
| 2   | X     | 8   | PHE  | 2.5  |
| 1   | C     | 309 | LEU  | 2.5  |
| 1   | I     | 432 | VAL  | 2.5  |
| 1   | W     | 92  | SER  | 2.5  |
| 2   | V     | 14  | TRP  | 2.5  |
| 1   | W     | 241 | SER  | 2.5  |
| 1   | W     | 105 | MET  | 2.5  |
| 2   | B     | 58  | MET  | 2.5  |
| 1   | W     | 315 | PRO  | 2.5  |
| 1   | S     | 416 | GLY  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 24  | ILE  | 2.5  |
| 2   | V     | 57  | PHE  | 2.5  |
| 1   | O     | 257 | GLN  | 2.5  |
| 1   | I     | 305 | ALA  | 2.5  |
| 1   | K     | 109 | ARG  | 2.5  |
| 1   | W     | 331 | SER  | 2.5  |
| 1   | U     | 448 | MET  | 2.5  |
| 1   | C     | 131 | GLY  | 2.5  |
| 1   | S     | 107 | ILE  | 2.5  |
| 1   | K     | 94  | LYS  | 2.5  |
| 1   | K     | 454 | TRP  | 2.5  |
| 2   | H     | 119 | VAL  | 2.5  |
| 1   | G     | 109 | ARG  | 2.5  |
| 1   | U     | 434 | ALA  | 2.5  |
| 1   | W     | 174 | ALA  | 2.5  |
| 1   | K     | 204 | GLY  | 2.4  |
| 1   | U     | 118 | PHE  | 2.4  |
| 1   | U     | 336 | PHE  | 2.4  |
| 2   | B     | 8   | PHE  | 2.4  |
| 1   | W     | 296 | TRP  | 2.4  |
| 1   | W     | 84  | VAL  | 2.4  |
| 1   | W     | 251 | MET  | 2.4  |
| 1   | W     | 354 | ALA  | 2.4  |
| 2   | V     | 181 | SER  | 2.4  |
| 1   | C     | 321 | GLY  | 2.4  |
| 1   | W     | 59  | LEU  | 2.4  |
| 2   | H     | 8   | PHE  | 2.4  |
| 2   | X     | 94  | ARG  | 2.4  |
| 1   | G     | 434 | ALA  | 2.4  |
| 1   | W     | 126 | ALA  | 2.4  |
| 1   | U     | 321 | GLY  | 2.4  |
| 1   | U     | 348 | ASN  | 2.4  |
| 1   | S     | 434 | ALA  | 2.4  |
| 1   | I     | 94  | LYS  | 2.4  |
| 2   | H     | 11  | THR  | 2.4  |
| 2   | X     | 169 | LYS  | 2.4  |
| 1   | W     | 398 | GLY  | 2.4  |
| 1   | W     | 304 | LEU  | 2.4  |
| 2   | T     | 73  | TYR  | 2.4  |
| 1   | C     | 301 | ALA  | 2.4  |
| 1   | S     | 438 | ALA  | 2.4  |
| 1   | U     | 362 | ALA  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | V     | 26  | GLU  | 2.4  |
| 1   | E     | 137 | PRO  | 2.3  |
| 2   | X     | 166 | SER  | 2.3  |
| 1   | W     | 97  | LEU  | 2.3  |
| 1   | W     | 198 | LEU  | 2.3  |
| 2   | D     | 160 | ASP  | 2.3  |
| 1   | W     | 193 | TYR  | 2.3  |
| 1   | S     | 19  | TRP  | 2.3  |
| 1   | I     | 414 | GLY  | 2.3  |
| 1   | M     | 289 | GLY  | 2.3  |
| 2   | V     | 101 | GLY  | 2.3  |
| 1   | I     | 187 | LEU  | 2.3  |
| 1   | W     | 366 | ILE  | 2.3  |
| 2   | N     | 55  | HIS  | 2.3  |
| 1   | W     | 448 | MET  | 2.3  |
| 2   | L     | 8   | PHE  | 2.3  |
| 2   | P     | 10  | LYS  | 2.3  |
| 1   | I     | 277 | TYR  | 2.3  |
| 1   | S     | 47  | GLU  | 2.3  |
| 1   | S     | 163 | ALA  | 2.3  |
| 2   | D     | 176 | ALA  | 2.3  |
| 1   | W     | 43  | GLN  | 2.3  |
| 1   | W     | 381 | GLY  | 2.3  |
| 1   | K     | 96  | PHE  | 2.3  |
| 2   | N     | 15  | PRO  | 2.3  |
| 1   | K     | 159 | GLY  | 2.3  |
| 1   | S     | 48  | LEU  | 2.3  |
| 1   | K     | 319 | MET  | 2.3  |
| 1   | I     | 153 | PHE  | 2.3  |
| 1   | S     | 265 | PHE  | 2.3  |
| 2   | P     | 8   | PHE  | 2.3  |
| 1   | U     | 432 | VAL  | 2.3  |
| 1   | I     | 263 | ASN  | 2.2  |
| 2   | H     | 168 | ALA  | 2.2  |
| 2   | T     | 176 | ALA  | 2.2  |
| 2   | X     | 48  | ALA  | 2.2  |
| 1   | W     | 189 | ASP  | 2.2  |
| 1   | W     | 332 | PHE  | 2.2  |
| 2   | R     | 9   | PHE  | 2.2  |
| 1   | C     | 417 | ARG  | 2.2  |
| 1   | M     | 109 | ARG  | 2.2  |
| 1   | M     | 422 | HIS  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 270 | GLY  | 2.2  |
| 1   | W     | 401 | GLY  | 2.2  |
| 2   | V     | 167 | ILE  | 2.2  |
| 1   | U     | 276 | TRP  | 2.2  |
| 1   | I     | 300 | PRO  | 2.2  |
| 1   | U     | 429 | VAL  | 2.2  |
| 2   | P     | 18  | ALA  | 2.2  |
| 1   | I     | 89  | LYS  | 2.2  |
| 1   | M     | 291 | LYS  | 2.2  |
| 1   | U     | 431 | TYR  | 2.2  |
| 1   | C     | 124 | GLY  | 2.2  |
| 1   | M     | 105 | MET  | 2.2  |
| 2   | X     | 58  | MET  | 2.2  |
| 1   | M     | 309 | LEU  | 2.2  |
| 1   | K     | 107 | ILE  | 2.2  |
| 1   | U     | 24  | ILE  | 2.2  |
| 1   | M     | 298 | GLU  | 2.2  |
| 1   | W     | 223 | ALA  | 2.2  |
| 1   | G     | 255 | GLN  | 2.2  |
| 1   | U     | 413 | MET  | 2.2  |
| 1   | W     | 319 | MET  | 2.2  |
| 1   | Q     | 389 | GLY  | 2.2  |
| 2   | X     | 20  | GLY  | 2.2  |
| 1   | I     | 258 | ILE  | 2.2  |
| 1   | W     | 95  | VAL  | 2.1  |
| 1   | S     | 166 | ALA  | 2.1  |
| 1   | U     | 197 | MET  | 2.1  |
| 1   | U     | 263 | ASN  | 2.1  |
| 1   | W     | 301 | ALA  | 2.1  |
| 1   | U     | 242 | GLY  | 2.1  |
| 1   | W     | 271 | GLY  | 2.1  |
| 1   | W     | 350 | ILE  | 2.1  |
| 2   | H     | 68  | GLU  | 2.1  |
| 1   | C     | 265 | PHE  | 2.1  |
| 1   | G     | 19  | TRP  | 2.1  |
| 1   | S     | 153 | PHE  | 2.1  |
| 1   | S     | 136 | VAL  | 2.1  |
| 1   | U     | 438 | ALA  | 2.1  |
| 2   | X     | 71  | LEU  | 2.1  |
| 1   | A     | 372 | ARG  | 2.1  |
| 2   | N     | 121 | GLU  | 2.1  |
| 1   | W     | 283 | SER  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | M     | 281 | PRO  | 2.1  |
| 1   | W     | 21  | PRO  | 2.1  |
| 1   | W     | 281 | PRO  | 2.1  |
| 1   | K     | 86  | VAL  | 2.1  |
| 1   | U     | 19  | TRP  | 2.1  |
| 2   | N     | 123 | ALA  | 2.1  |
| 1   | U     | 312 | THR  | 2.1  |
| 1   | W     | 26  | GLY  | 2.1  |
| 2   | L     | 11  | THR  | 2.1  |
| 1   | S     | 140 | LYS  | 2.1  |
| 1   | W     | 413 | MET  | 2.1  |
| 2   | T     | 58  | MET  | 2.1  |
| 1   | M     | 432 | VAL  | 2.1  |
| 1   | S     | 86  | VAL  | 2.1  |
| 1   | U     | 278 | VAL  | 2.1  |
| 2   | T     | 8   | PHE  | 2.1  |
| 1   | C     | 364 | ALA  | 2.1  |
| 1   | K     | 305 | ALA  | 2.1  |
| 2   | X     | 19  | ALA  | 2.1  |
| 1   | I     | 296 | TRP  | 2.1  |
| 1   | I     | 109 | ARG  | 2.1  |
| 1   | S     | 52  | ARG  | 2.1  |
| 1   | U     | 62  | GLY  | 2.1  |
| 1   | W     | 273 | GLY  | 2.1  |
| 1   | A     | 431 | TYR  | 2.1  |
| 1   | C     | 186 | TYR  | 2.1  |
| 2   | J     | 160 | ASP  | 2.1  |
| 1   | I     | 165 | VAL  | 2.0  |
| 1   | W     | 222 | PHE  | 2.0  |
| 2   | V     | 21  | LEU  | 2.0  |
| 1   | E     | 414 | GLY  | 2.0  |
| 1   | U     | 176 | TRP  | 2.0  |
| 1   | I     | 243 | ILE  | 2.0  |
| 2   | L     | 58  | MET  | 2.0  |
| 1   | S     | 118 | PHE  | 2.0  |
| 1   | K     | 23  | ALA  | 2.0  |
| 1   | M     | 305 | ALA  | 2.0  |
| 1   | U     | 309 | LEU  | 2.0  |
| 1   | W     | 321 | GLY  | 2.0  |
| 1   | W     | 93  | ILE  | 2.0  |
| 2   | D     | 11  | THR  | 2.0  |
| 2   | L     | 132 | SER  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | P     | 16  | SER  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 5   | BNL  | K     | 1462 | 12/12 | 0.82 | 0.22 | 86,86,87,87                | 0     |
| 5   | BNL  | G     | 1462 | 12/12 | 0.84 | 0.16 | 63,64,64,64                | 0     |
| 5   | BNL  | A     | 1462 | 12/12 | 0.86 | 0.19 | 76,76,76,76                | 0     |
| 5   | BNL  | W     | 1462 | 12/12 | 0.86 | 0.22 | 87,87,88,88                | 0     |
| 5   | BNL  | S     | 1462 | 12/12 | 0.87 | 0.23 | 82,82,82,82                | 0     |
| 5   | BNL  | U     | 1462 | 12/12 | 0.88 | 0.16 | 86,86,86,86                | 0     |
| 5   | BNL  | I     | 1462 | 12/12 | 0.89 | 0.15 | 63,63,64,64                | 0     |
| 5   | BNL  | O     | 1462 | 12/12 | 0.91 | 0.11 | 44,44,45,45                | 0     |
| 5   | BNL  | Q     | 1462 | 12/12 | 0.91 | 0.13 | 40,40,41,41                | 0     |
| 3   | FES  | S     | 1460 | 4/4   | 0.91 | 0.10 | 86,86,86,87                | 0     |
| 3   | FES  | E     | 1460 | 4/4   | 0.91 | 0.08 | 44,46,47,50                | 0     |
| 5   | BNL  | E     | 1462 | 12/12 | 0.91 | 0.13 | 49,49,49,49                | 0     |
| 5   | BNL  | M     | 1462 | 12/12 | 0.92 | 0.14 | 55,56,56,56                | 0     |
| 5   | BNL  | C     | 1462 | 12/12 | 0.92 | 0.14 | 55,56,56,56                | 0     |
| 3   | FES  | A     | 1460 | 4/4   | 0.93 | 0.09 | 43,44,46,48                | 0     |
| 3   | FES  | I     | 1460 | 4/4   | 0.94 | 0.08 | 45,46,48,50                | 0     |
| 3   | FES  | W     | 1460 | 4/4   | 0.94 | 0.11 | 74,75,76,77                | 0     |
| 3   | FES  | M     | 1460 | 4/4   | 0.95 | 0.06 | 38,38,39,42                | 0     |
| 3   | FES  | U     | 1460 | 4/4   | 0.95 | 0.08 | 48,48,49,49                | 0     |
| 3   | FES  | O     | 1460 | 4/4   | 0.95 | 0.07 | 44,45,46,48                | 0     |
| 4   | FE2  | W     | 1461 | 1/1   | 0.95 | 0.06 | 68,68,68,68                | 0     |
| 3   | FES  | G     | 1460 | 4/4   | 0.96 | 0.06 | 54,54,54,56                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 4   | FE2  | U     | 1461 | 1/1   | 0.96 | 0.04 | 57,57,57,57                 | 0     |
| 3   | FES  | Q     | 1460 | 4/4   | 0.96 | 0.08 | 39,39,41,44                 | 0     |
| 4   | FE2  | I     | 1461 | 1/1   | 0.97 | 0.07 | 58,58,58,58                 | 0     |
| 4   | FE2  | K     | 1461 | 1/1   | 0.97 | 0.07 | 59,59,59,59                 | 0     |
| 3   | FES  | C     | 1460 | 4/4   | 0.97 | 0.06 | 43,44,45,46                 | 0     |
| 3   | FES  | K     | 1460 | 4/4   | 0.97 | 0.06 | 74,75,75,76                 | 0     |
| 4   | FE2  | A     | 1461 | 1/1   | 0.98 | 0.09 | 53,53,53,53                 | 0     |
| 4   | FE2  | E     | 1461 | 1/1   | 0.98 | 0.06 | 41,41,41,41                 | 0     |
| 4   | FE2  | S     | 1461 | 1/1   | 0.99 | 0.04 | 51,51,51,51                 | 0     |
| 4   | FE2  | G     | 1461 | 1/1   | 0.99 | 0.04 | 52,52,52,52                 | 0     |
| 4   | FE2  | M     | 1461 | 1/1   | 0.99 | 0.05 | 43,43,43,43                 | 0     |
| 4   | FE2  | C     | 1461 | 1/1   | 1.00 | 0.05 | 44,44,44,44                 | 0     |
| 4   | FE2  | O     | 1461 | 1/1   | 1.00 | 0.06 | 34,34,34,34                 | 0     |
| 4   | FE2  | Q     | 1461 | 1/1   | 1.00 | 0.03 | 37,37,37,37                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.