



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:19 AM EDT

PDB ID : 4NZB / pdb\_00004nzb  
Title : NS9283 bound to Ls-AChBP  
Authors : Olsen, J.A.; Kastrup, J.S.; Gajhede, M.  
Deposited on : 2013-12-11  
Resolution : 2.68 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

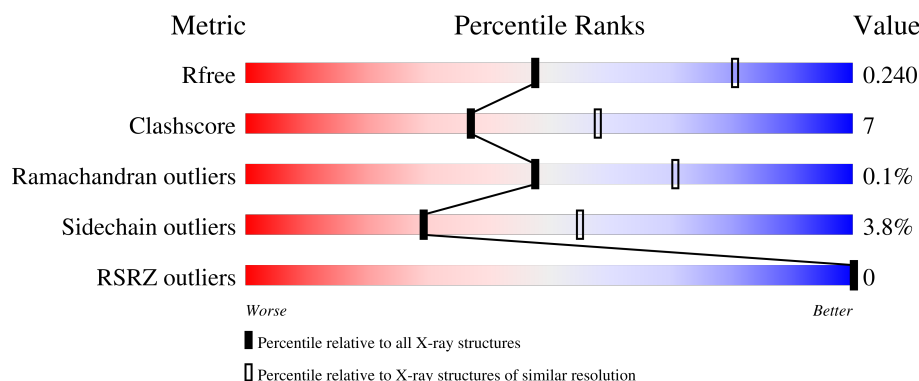
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.68 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                      | 5070 (2.70-2.66)                                      |
| Clashscore            | 190562                      | 5409 (2.70-2.66)                                      |
| Ramachandran outliers | 187476                      | 5324 (2.70-2.66)                                      |
| Sidechain outliers    | 187428                      | 5324 (2.70-2.66)                                      |
| RSRZ outliers         | 180081                      | 5070 (2.70-2.66)                                      |

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     | 210    | <div> <div>76%</div> <div>15%</div> <div>6%</div> </div> |
| 1   | B     | 210    | <div> <div>76%</div> <div>15%</div> <div>6%</div> </div> |
| 1   | C     | 210    | <div> <div>77%</div> <div>13%</div> <div>6%</div> </div> |
| 1   | D     | 210    | <div> <div>78%</div> <div>13%</div> <div>6%</div> </div> |
| 1   | E     | 210    | <div> <div>77%</div> <div>14%</div> <div>6%</div> </div> |

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| Mol | Chain | Length | Quality of chain                                                                                 |
|-----|-------|--------|--------------------------------------------------------------------------------------------------|
| 1   | F     | 210    |  77% 16% •• 5% |
| 1   | G     | 210    |  75% 15% •• 6% |
| 1   | H     | 210    |  79% 12% •• 6% |
| 1   | I     | 210    |  76% 15% • 7%  |
| 1   | J     | 210    |  75% 17% • 6%  |
| 1   | K     | 210    |  78% 13% • 6%  |
| 1   | L     | 210    |  78% 14% • 6%  |
| 1   | M     | 210    |  78% 11% •• 8% |
| 1   | N     | 210    |  77% 13% •• 6% |
| 1   | O     | 210    |  78% 12% • 6%  |

## 2 Entry composition

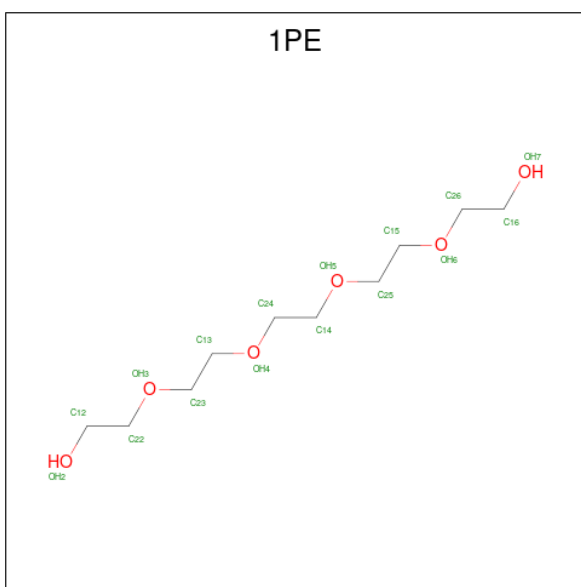
There are 9 unique types of molecules in this entry. The entry contains 24523 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Acetylcholine-binding protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | G     | 198      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1591  | 1002 | 272 | 312 | 5 |         |         |       |
| 1   | D     | 197      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1578  | 991  | 271 | 311 | 5 |         |         |       |
| 1   | E     | 198      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1586  | 997  | 272 | 312 | 5 |         |         |       |
| 1   | A     | 198      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1586  | 997  | 272 | 312 | 5 |         |         |       |
| 1   | B     | 198      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1586  | 997  | 272 | 312 | 5 |         |         |       |
| 1   | C     | 198      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1586  | 997  | 272 | 312 | 5 |         |         |       |
| 1   | F     | 200      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1607  | 1010 | 274 | 318 | 5 |         |         |       |
| 1   | H     | 198      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1586  | 997  | 272 | 312 | 5 |         |         |       |
| 1   | I     | 195      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1568  | 988  | 269 | 308 | 3 |         |         |       |
| 1   | J     | 198      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1586  | 997  | 272 | 312 | 5 |         |         |       |
| 1   | K     | 197      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1571  | 989  | 268 | 309 | 5 |         |         |       |
| 1   | L     | 198      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1591  | 1000 | 272 | 314 | 5 |         |         |       |
| 1   | M     | 194      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1566  | 988  | 268 | 307 | 3 |         |         |       |
| 1   | N     | 198      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1586  | 997  | 272 | 312 | 5 |         |         |       |
| 1   | O     | 198      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1586  | 997  | 272 | 312 | 5 |         |         |       |

- Molecule 2 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 2   | G     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 16    | 10 | 6 |         |         |
| 2   | D     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 16    | 10 | 6 |         |         |
| 2   | E     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 16    | 10 | 6 |         |         |
| 2   | A     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 16    | 10 | 6 |         |         |
| 2   | B     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 16    | 10 | 6 |         |         |
| 2   | C     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 16    | 10 | 6 |         |         |
| 2   | H     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 16    | 10 | 6 |         |         |
| 2   | I     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 16    | 10 | 6 |         |         |

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 3   | G     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |

- Molecule 4 is SULFATE ION (CCD ID: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4   | G     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | G     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

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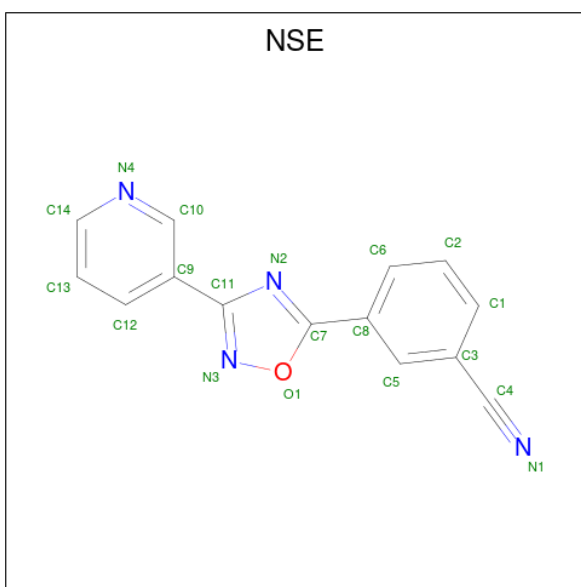
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4   | G     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | D     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | D     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | E     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | E     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | E     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | E     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | E     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | F     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | F     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | I     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | J     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | M     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 5   | G     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 5   | G     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 5   | G     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 5   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 5   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 5   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 5   | F     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 5   | F     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 5   | F     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 5   | F     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 5   | J     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 5   | O     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |

- Molecule 6 is 3-[3-(pyridin-3-yl)-1,2,4-oxadiazol-5-yl]benzonitrile (CCD ID: NSE) (formula: C<sub>14</sub>H<sub>8</sub>N<sub>4</sub>O).



| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 6   | E     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 19    | 14 | 4 | 1 |         |         |
| 6   | A     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 19    | 14 | 4 | 1 |         |         |
| 6   | B     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 19    | 14 | 4 | 1 |         |         |
| 6   | I     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 19    | 14 | 4 | 1 |         |         |
| 6   | K     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 19    | 14 | 4 | 1 |         |         |
| 6   | M     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 19    | 14 | 4 | 1 |         |         |

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

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 7   | A     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 7   | K     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 7   | L     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 7   | N     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 8   | J     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |

- Molecule 9 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 9   | G     | 28       | Total | O  | 0       | 0       |
|     |       |          | 28    | 28 |         |         |
| 9   | D     | 27       | Total | O  | 0       | 0       |
|     |       |          | 27    | 27 |         |         |
| 9   | E     | 23       | Total | O  | 0       | 0       |
|     |       |          | 23    | 23 |         |         |
| 9   | A     | 28       | Total | O  | 0       | 0       |
|     |       |          | 28    | 28 |         |         |
| 9   | B     | 19       | Total | O  | 0       | 0       |
|     |       |          | 19    | 19 |         |         |
| 9   | C     | 22       | Total | O  | 0       | 0       |
|     |       |          | 22    | 22 |         |         |
| 9   | F     | 31       | Total | O  | 0       | 0       |
|     |       |          | 31    | 31 |         |         |
| 9   | H     | 26       | Total | O  | 0       | 0       |
|     |       |          | 26    | 26 |         |         |
| 9   | I     | 21       | Total | O  | 0       | 0       |
|     |       |          | 21    | 21 |         |         |
| 9   | J     | 21       | Total | O  | 0       | 0       |
|     |       |          | 21    | 21 |         |         |
| 9   | K     | 26       | Total | O  | 0       | 0       |
|     |       |          | 26    | 26 |         |         |

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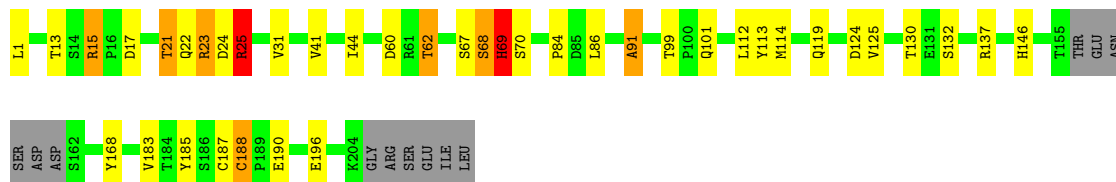
| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 9   | L     | 24       | Total<br>24 | O<br>24 | 0       | 0       |
| 9   | M     | 21       | Total<br>21 | O<br>21 | 0       | 0       |
| 9   | N     | 5        | Total<br>5  | O<br>5  | 0       | 0       |
| 9   | O     | 13       | Total<br>13 | O<br>13 | 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.

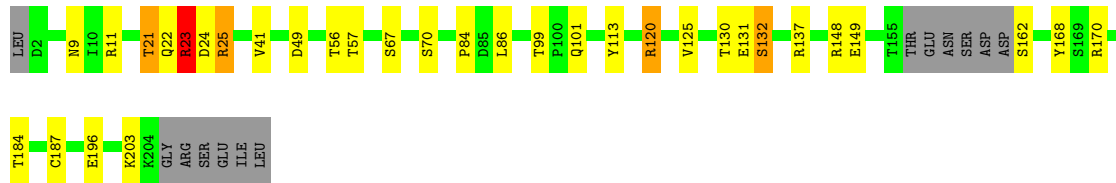
#### • Molecule 1: Acetylcholine-binding protein

Chain G: 



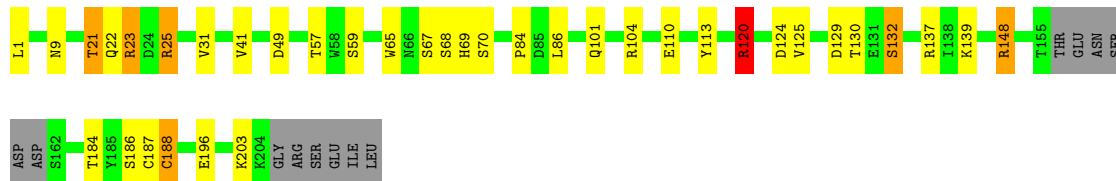
#### • Molecule 1: Acetylcholine-binding protein

Chain D: 



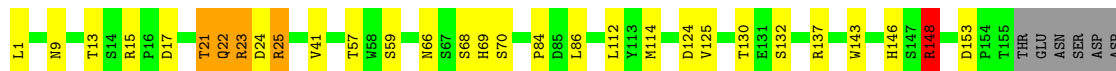
#### • Molecule 1: Acetylcholine-binding protein

Chain E: 



#### • Molecule 1: Acetylcholine-binding protein

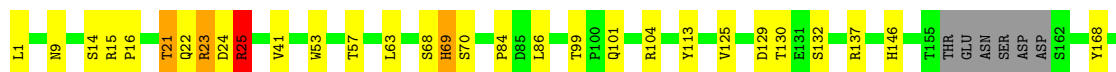
Chain A: 





- Molecule 1: Acetylcholine-binding protein

Chain B: 76% 15% 6%



- Molecule 1: Acetylcholine-binding protein

Chain C: 77% 13% 6%



- Molecule 1: Acetylcholine-binding protein

Chain F: 77% 16% 5%



- Molecule 1: Acetylcholine-binding protein

Chain H: 79% 12% 6%



- Molecule 1: Acetylcholine-binding protein

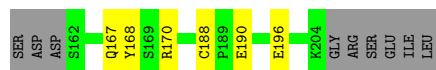
Chain I: 76% 15% 7%





- Molecule 1: Acetylcholine-binding protein

Chain J: 75% 17% 6%



- Molecule 1: Acetylcholine-binding protein

Chain K: 78% 13% 6%



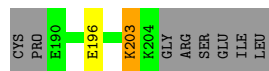
- Molecule 1: Acetylcholine-binding protein

Chain L: 78% 14% 6%



- Molecule 1: Acetylcholine-binding protein

Chain M: 78% 11% 8%



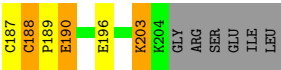
- Molecule 1: Acetylcholine-binding protein

Chain N: 77% 13% 6%





● Molecule 1: Acetylcholine-binding protein



## 4 Data and refinement statistics

| Property                                                                | Value                                                                                                                                                                                 | Source           |
|-------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------|
| Space group                                                             | C 1 2 1                                                                                                                                                                               | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 231.73Å 140.38Å 119.55Å<br>90.00° 89.98° 90.00°                                                                                                                                       | Depositor        |
| Resolution (Å)                                                          | 28.24 – 2.68<br>28.24 – 2.68                                                                                                                                                          | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.2 (28.24-2.68)<br>98.1 (28.24-2.68)                                                                                                                                                | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                                                                                                                                                       | Depositor        |
| $R_{sym}$                                                               | 0.07                                                                                                                                                                                  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.69 (at 2.68Å)                                                                                                                                                                       | Xtriage          |
| Refinement program                                                      | PHENIX 1.8.4_1496                                                                                                                                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.207 , 0.240<br>0.208 , 0.240                                                                                                                                                        | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 5278 reflections (4.92%)                                                                                                                                                              | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 52.7                                                                                                                                                                                  | Xtriage          |
| Anisotropy                                                              | 0.296                                                                                                                                                                                 | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.35 , 35.2                                                                                                                                                                           | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$                                                                                                                           | Xtriage          |
| Estimated twinning fraction                                             | 0.069 for -1/2*h+3/2*k,1/2*h+1/2*k,-l<br>0.064 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l<br>0.075 for 1/2*h+3/2*k,1/2*h-1/2*k,-l<br>0.064 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l<br>0.104 for -h,-k,l | Xtriage          |
| $F_o$ , $F_c$ correlation                                               | 0.96                                                                                                                                                                                  | EDS              |
| Total number of atoms                                                   | 24523                                                                                                                                                                                 | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 53.0                                                                                                                                                                                  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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: SO4, NSE, GOL, CL, NAG, ACT, 1PE

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     | 0.70         | 1/1621 (0.1%)   | 1.04        | 10/2211 (0.5%)   |
| 1   | B     | 0.69         | 4/1621 (0.2%)   | 0.97        | 8/2211 (0.4%)    |
| 1   | C     | 0.63         | 2/1621 (0.1%)   | 0.96        | 8/2211 (0.4%)    |
| 1   | D     | 0.82         | 8/1613 (0.5%)   | 1.24        | 18/2200 (0.8%)   |
| 1   | E     | 0.74         | 4/1621 (0.2%)   | 0.98        | 7/2211 (0.3%)    |
| 1   | F     | 0.79         | 4/1645 (0.2%)   | 1.05        | 11/2244 (0.5%)   |
| 1   | G     | 0.79         | 4/1629 (0.2%)   | 1.03        | 6/2222 (0.3%)    |
| 1   | H     | 0.78         | 8/1621 (0.5%)   | 1.08        | 18/2211 (0.8%)   |
| 1   | I     | 0.71         | 6/1602 (0.4%)   | 0.94        | 10/2183 (0.5%)   |
| 1   | J     | 0.72         | 5/1621 (0.3%)   | 0.98        | 8/2211 (0.4%)    |
| 1   | K     | 0.62         | 1/1605 (0.1%)   | 0.97        | 7/2188 (0.3%)    |
| 1   | L     | 0.71         | 2/1629 (0.1%)   | 0.96        | 8/2222 (0.4%)    |
| 1   | M     | 0.87         | 9/1602 (0.6%)   | 1.03        | 11/2183 (0.5%)   |
| 1   | N     | 0.77         | 5/1621 (0.3%)   | 1.15        | 17/2211 (0.8%)   |
| 1   | O     | 0.64         | 2/1621 (0.1%)   | 0.94        | 10/2211 (0.5%)   |
| All | All   | 0.74         | 65/24293 (0.3%) | 1.02        | 157/33130 (0.5%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |
| 1   | D     | 0                   | 1                   |
| 1   | F     | 0                   | 4                   |
| 1   | G     | 0                   | 2                   |
| 1   | M     | 0                   | 1                   |
| 1   | N     | 0                   | 2                   |
| 1   | O     | 0                   | 1                   |
| All | All   | 0                   | 12                  |

All (65) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | N     | 25  | ARG  | CZ-NH1 | -14.96 | 1.11        | 1.32     |
| 1   | M     | 25  | ARG  | CZ-NH2 | -12.83 | 1.16        | 1.33     |
| 1   | G     | 23  | ARG  | CZ-NH1 | -12.79 | 1.14        | 1.32     |
| 1   | D     | 11  | ARG  | CZ-NH1 | -11.13 | 1.17        | 1.32     |
| 1   | L     | 131 | GLU  | CD-OE1 | -10.61 | 1.05        | 1.25     |
| 1   | D     | 23  | ARG  | CZ-NH1 | -10.43 | 1.18        | 1.32     |
| 1   | H     | 131 | GLU  | CD-OE1 | -9.59  | 1.07        | 1.25     |
| 1   | M     | 25  | ARG  | CB-CG  | -9.46  | 1.24        | 1.52     |
| 1   | E     | 23  | ARG  | CG-CD  | -9.36  | 1.24        | 1.52     |
| 1   | N     | 25  | ARG  | CG-CD  | -9.28  | 1.24        | 1.52     |
| 1   | F     | 23  | ARG  | CZ-NH1 | -9.19  | 1.19        | 1.32     |
| 1   | M     | 25  | ARG  | CD-NE  | -9.08  | 1.33        | 1.46     |
| 1   | D     | 25  | ARG  | CG-CD  | -9.04  | 1.25        | 1.52     |
| 1   | D     | 23  | ARG  | CD-NE  | -8.76  | 1.33        | 1.46     |
| 1   | J     | 23  | ARG  | CG-CD  | -8.66  | 1.26        | 1.52     |
| 1   | I     | 23  | ARG  | CB-CG  | -8.40  | 1.27        | 1.52     |
| 1   | L     | 23  | ARG  | CG-CD  | -8.12  | 1.28        | 1.52     |
| 1   | O     | 23  | ARG  | CG-CD  | -7.87  | 1.28        | 1.52     |
| 1   | D     | 131 | GLU  | CD-OE1 | -7.63  | 1.10        | 1.25     |
| 1   | B     | 23  | ARG  | CG-CD  | -7.56  | 1.29        | 1.52     |
| 1   | F     | 23  | ARG  | CG-CD  | -7.42  | 1.30        | 1.52     |
| 1   | A     | 23  | ARG  | CG-CD  | -7.37  | 1.30        | 1.52     |
| 1   | F     | 25  | ARG  | CB-CG  | -7.23  | 1.30        | 1.52     |
| 1   | M     | 25  | ARG  | NE-CZ  | -7.23  | 1.25        | 1.33     |
| 1   | G     | 23  | ARG  | CB-CG  | -7.00  | 1.31        | 1.52     |
| 1   | B     | 25  | ARG  | CB-CG  | -6.84  | 1.31        | 1.52     |
| 1   | J     | 167 | GLN  | CB-CG  | -6.78  | 1.32        | 1.52     |
| 1   | I     | 23  | ARG  | CZ-NH1 | -6.76  | 1.23        | 1.32     |
| 1   | N     | 23  | ARG  | CB-CG  | -6.72  | 1.32        | 1.52     |
| 1   | D     | 25  | ARG  | CB-CG  | -6.70  | 1.32        | 1.52     |
| 1   | H     | 23  | ARG  | CB-CG  | -6.58  | 1.32        | 1.52     |
| 1   | M     | 131 | GLU  | CB-CG  | -6.51  | 1.32        | 1.52     |
| 1   | B     | 25  | ARG  | CG-CD  | -6.48  | 1.33        | 1.52     |
| 1   | J     | 23  | ARG  | CB-CG  | -6.43  | 1.33        | 1.52     |
| 1   | H     | 23  | ARG  | CZ-NH1 | -6.43  | 1.23        | 1.32     |
| 1   | G     | 25  | ARG  | CB-CG  | -6.37  | 1.33        | 1.52     |
| 1   | J     | 22  | GLN  | CD-OE1 | -6.27  | 1.11        | 1.23     |
| 1   | K     | 25  | ARG  | CZ-NH1 | -6.21  | 1.24        | 1.32     |
| 1   | H     | 131 | GLU  | CB-CG  | -6.17  | 1.33        | 1.52     |
| 1   | H     | 23  | ARG  | CG-CD  | -6.11  | 1.34        | 1.52     |
| 1   | M     | 25  | ARG  | CG-CD  | -6.00  | 1.34        | 1.52     |
| 1   | E     | 23  | ARG  | CB-CG  | -6.00  | 1.34        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | C     | 23  | ARG  | CB-CG   | -6.00 | 1.34        | 1.52     |
| 1   | I     | 131 | GLU  | CB-CG   | -5.84 | 1.34        | 1.52     |
| 1   | I     | 23  | ARG  | CG-CD   | -5.76 | 1.35        | 1.52     |
| 1   | D     | 23  | ARG  | CB-CG   | -5.62 | 1.35        | 1.52     |
| 1   | H     | 25  | ARG  | CB-CG   | -5.57 | 1.35        | 1.52     |
| 1   | H     | 25  | ARG  | CG-CD   | -5.53 | 1.35        | 1.52     |
| 1   | E     | 25  | ARG  | CB-CG   | -5.52 | 1.35        | 1.52     |
| 1   | G     | 91  | ALA  | CA-CB   | -5.50 | 1.44        | 1.53     |
| 1   | M     | 25  | ARG  | CA-CB   | -5.46 | 1.46        | 1.53     |
| 1   | M     | 22  | GLN  | CA-C    | -5.44 | 1.46        | 1.52     |
| 1   | H     | 22  | GLN  | CA-C    | -5.39 | 1.46        | 1.52     |
| 1   | M     | 23  | ARG  | CG-CD   | -5.38 | 1.36        | 1.52     |
| 1   | N     | 25  | ARG  | CB-CG   | -5.35 | 1.36        | 1.52     |
| 1   | F     | 23  | ARG  | CB-CG   | -5.34 | 1.36        | 1.52     |
| 1   | E     | 25  | ARG  | CG-CD   | -5.30 | 1.36        | 1.52     |
| 1   | D     | 25  | ARG  | CA-C    | -5.28 | 1.46        | 1.52     |
| 1   | O     | 25  | ARG  | CB-CG   | -5.22 | 1.36        | 1.52     |
| 1   | I     | 69  | HIS  | ND1-CE1 | -5.21 | 1.27        | 1.32     |
| 1   | B     | 25  | ARG  | CA-C    | -5.13 | 1.46        | 1.52     |
| 1   | J     | 25  | ARG  | CG-CD   | -5.12 | 1.37        | 1.52     |
| 1   | C     | 25  | ARG  | CB-CG   | -5.05 | 1.37        | 1.52     |
| 1   | N     | 23  | ARG  | CG-CD   | -5.01 | 1.37        | 1.52     |
| 1   | I     | 25  | ARG  | CG-CD   | -5.00 | 1.37        | 1.52     |

All (157) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | D     | 23  | ARG  | NE-CZ-NH2 | 19.09  | 136.38      | 119.20   |
| 1   | N     | 25  | ARG  | NE-CZ-NH2 | 17.20  | 134.68      | 119.20   |
| 1   | H     | 131 | GLU  | CA-CB-CG  | 17.12  | 148.34      | 114.10   |
| 1   | D     | 11  | ARG  | NE-CZ-NH2 | 16.18  | 133.76      | 119.20   |
| 1   | D     | 25  | ARG  | CG-CD-NE  | 15.37  | 145.81      | 112.00   |
| 1   | G     | 23  | ARG  | NE-CZ-NH2 | 14.98  | 132.69      | 119.20   |
| 1   | D     | 11  | ARG  | NE-CZ-NH1 | -13.10 | 108.40      | 121.50   |
| 1   | M     | 203 | LYS  | CG-CD-CE  | 13.03  | 141.27      | 111.30   |
| 1   | A     | 148 | ARG  | CB-CG-CD  | -12.90 | 81.63       | 111.30   |
| 1   | G     | 23  | ARG  | NE-CZ-NH1 | -12.89 | 108.61      | 121.50   |
| 1   | N     | 139 | LYS  | CG-CD-CE  | 12.74  | 140.61      | 111.30   |
| 1   | F     | 23  | ARG  | NE-CZ-NH2 | 12.66  | 130.59      | 119.20   |
| 1   | N     | 25  | ARG  | NE-CZ-NH1 | -12.59 | 108.91      | 121.50   |
| 1   | D     | 23  | ARG  | NE-CZ-NH1 | -12.57 | 108.93      | 121.50   |
| 1   | A     | 148 | ARG  | CG-CD-NE  | 12.11  | 138.63      | 112.00   |

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| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | E     | 148 | ARG  | CB-CG-CD  | -11.22 | 85.49       | 111.30   |
| 1   | K     | 203 | LYS  | CG-CD-CE  | 10.80  | 136.15      | 111.30   |
| 1   | F     | 186 | SER  | CA-CB-OG  | 10.55  | 132.19      | 111.10   |
| 1   | L     | 131 | GLU  | CG-CD-OE2 | 10.00  | 141.41      | 118.40   |
| 1   | H     | 131 | GLU  | CB-CA-C   | -9.92  | 92.28       | 110.63   |
| 1   | D     | 25  | ARG  | CD-NE-CZ  | -9.80  | 110.67      | 124.40   |
| 1   | K     | 15  | ARG  | CA-C-N    | 9.41   | 129.16      | 119.56   |
| 1   | K     | 15  | ARG  | C-N-CA    | 9.41   | 129.16      | 119.56   |
| 1   | J     | 120 | ARG  | CG-CD-NE  | 9.18   | 132.20      | 112.00   |
| 1   | M     | 203 | LYS  | CB-CG-CD  | -9.18  | 90.19       | 111.30   |
| 1   | A     | 148 | ARG  | CD-NE-CZ  | 9.00   | 137.00      | 124.40   |
| 1   | J     | 22  | GLN  | CA-CB-CG  | 8.89   | 131.89      | 114.10   |
| 1   | D     | 120 | ARG  | CG-CD-NE  | 8.86   | 131.48      | 112.00   |
| 1   | M     | 15  | ARG  | CA-C-N    | 8.84   | 128.57      | 119.56   |
| 1   | M     | 15  | ARG  | C-N-CA    | 8.84   | 128.57      | 119.56   |
| 1   | K     | 25  | ARG  | NE-CZ-NH2 | 8.81   | 127.13      | 119.20   |
| 1   | M     | 120 | ARG  | CB-CG-CD  | 8.37   | 130.56      | 111.30   |
| 1   | F     | 25  | ARG  | CG-CD-NE  | 8.34   | 130.34      | 112.00   |
| 1   | I     | 203 | LYS  | CG-CD-CE  | 8.31   | 130.41      | 111.30   |
| 1   | N     | 23  | ARG  | CG-CD-NE  | 8.19   | 130.02      | 112.00   |
| 1   | F     | 23  | ARG  | NE-CZ-NH1 | -8.15  | 113.35      | 121.50   |
| 1   | B     | 25  | ARG  | CG-CD-NE  | 8.15   | 129.93      | 112.00   |
| 1   | K     | 25  | ARG  | NE-CZ-NH1 | -8.07  | 113.43      | 121.50   |
| 1   | I     | 23  | ARG  | NE-CZ-NH2 | 8.03   | 126.43      | 119.20   |
| 1   | B     | 23  | ARG  | NE-CZ-NH2 | 8.03   | 126.42      | 119.20   |
| 1   | H     | 120 | ARG  | CG-CD-NE  | 8.02   | 129.64      | 112.00   |
| 1   | E     | 120 | ARG  | CG-CD-NE  | 7.99   | 129.57      | 112.00   |
| 1   | F     | 162 | SER  | CA-C-N    | -7.88  | 109.11      | 120.29   |
| 1   | F     | 162 | SER  | C-N-CA    | -7.88  | 109.11      | 120.29   |
| 1   | K     | 203 | LYS  | CB-CG-CD  | -7.81  | 93.33       | 111.30   |
| 1   | D     | 120 | ARG  | CB-CG-CD  | 7.79   | 129.22      | 111.30   |
| 1   | N     | 139 | LYS  | CB-CG-CD  | 7.75   | 129.12      | 111.30   |
| 1   | H     | 132 | SER  | N-CA-C    | -7.69  | 103.36      | 112.89   |
| 1   | N     | 23  | ARG  | CB-CG-CD  | 7.64   | 128.88      | 111.30   |
| 1   | D     | 132 | SER  | N-CA-C    | -7.59  | 103.47      | 112.89   |
| 1   | J     | 25  | ARG  | CG-CD-NE  | 7.51   | 128.52      | 112.00   |
| 1   | L     | 24  | ASP  | N-CA-C    | -7.49  | 102.39      | 113.40   |
| 1   | L     | 23  | ARG  | CD-NE-CZ  | -7.47  | 113.95      | 124.40   |
| 1   | E     | 23  | ARG  | NE-CZ-NH2 | 7.45   | 125.91      | 119.20   |
| 1   | B     | 25  | ARG  | CD-NE-CZ  | -7.43  | 114.00      | 124.40   |
| 1   | G     | 25  | ARG  | CG-CD-NE  | 7.35   | 128.18      | 112.00   |
| 1   | D     | 23  | ARG  | CD-NE-CZ  | 7.31   | 134.63      | 124.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | H     | 23  | ARG  | NE-CZ-NH2  | 7.24  | 125.72      | 119.20   |
| 1   | A     | 23  | ARG  | NE-CZ-NH1  | -7.24 | 114.26      | 121.50   |
| 1   | M     | 22  | GLN  | CA-C-O     | -7.21 | 112.74      | 120.46   |
| 1   | O     | 23  | ARG  | NE-CZ-NH2  | 7.21  | 125.69      | 119.20   |
| 1   | J     | 120 | ARG  | CB-CG-CD   | 7.20  | 127.86      | 111.30   |
| 1   | J     | 23  | ARG  | NE-CZ-NH2  | 7.17  | 125.65      | 119.20   |
| 1   | A     | 25  | ARG  | CB-CG-CD   | -7.14 | 94.87       | 111.30   |
| 1   | B     | 190 | GLU  | CA-CB-CG   | -7.10 | 99.89       | 114.10   |
| 1   | H     | 120 | ARG  | CB-CG-CD   | 7.09  | 127.60      | 111.30   |
| 1   | D     | 131 | GLU  | CG-CD-OE2  | 7.03  | 134.57      | 118.40   |
| 1   | H     | 131 | GLU  | N-CA-CB    | 6.97  | 120.95      | 110.22   |
| 1   | A     | 22  | GLN  | N-CA-C     | -6.91 | 95.92       | 108.02   |
| 1   | B     | 25  | ARG  | NE-CZ-NH1  | -6.89 | 114.61      | 121.50   |
| 1   | N     | 120 | ARG  | CG-CD-NE   | 6.85  | 127.08      | 112.00   |
| 1   | B     | 23  | ARG  | NE-CZ-NH1  | -6.79 | 114.70      | 121.50   |
| 1   | L     | 25  | ARG  | CB-CG-CD   | -6.78 | 95.71       | 111.30   |
| 1   | D     | 25  | ARG  | NE-CZ-NH1  | -6.77 | 114.73      | 121.50   |
| 1   | I     | 25  | ARG  | CB-CG-CD   | -6.77 | 95.72       | 111.30   |
| 1   | I     | 131 | GLU  | CG-CD-OE2  | 6.67  | 133.74      | 118.40   |
| 1   | D     | 25  | ARG  | CB-CG-CD   | 6.62  | 126.54      | 111.30   |
| 1   | N     | 25  | ARG  | N-CA-CB    | 6.62  | 119.28      | 109.88   |
| 1   | N     | 25  | ARG  | CB-CA-C    | -6.58 | 99.15       | 109.09   |
| 1   | L     | 23  | ARG  | NE-CZ-NH2  | 6.57  | 125.12      | 119.20   |
| 1   | M     | 23  | ARG  | CA-CB-CG   | 6.54  | 127.17      | 114.10   |
| 1   | C     | 129 | ASP  | N-CA-C     | -6.54 | 105.44      | 113.41   |
| 1   | A     | 23  | ARG  | NE-CZ-NH2  | 6.50  | 125.05      | 119.20   |
| 1   | O     | 23  | ARG  | NE-CZ-NH1  | -6.47 | 115.03      | 121.50   |
| 1   | O     | 25  | ARG  | CB-CG-CD   | -6.46 | 96.43       | 111.30   |
| 1   | N     | 120 | ARG  | NE-CZ-NH1  | -6.41 | 115.09      | 121.50   |
| 1   | D     | 25  | ARG  | NE-CZ-NH2  | 6.40  | 124.96      | 119.20   |
| 1   | C     | 23  | ARG  | NE-CZ-NH2  | 6.38  | 124.94      | 119.20   |
| 1   | N     | 25  | ARG  | CA-CB-CG   | 6.36  | 126.82      | 114.10   |
| 1   | K     | 120 | ARG  | CG-CD-NE   | 6.32  | 125.90      | 112.00   |
| 1   | E     | 23  | ARG  | NE-CZ-NH1  | -6.26 | 115.24      | 121.50   |
| 1   | C     | 23  | ARG  | CA-CB-CG   | 6.26  | 126.61      | 114.10   |
| 1   | A     | 23  | ARG  | CD-NE-CZ   | -6.16 | 115.78      | 124.40   |
| 1   | L     | 131 | GLU  | CA-CB-CG   | 6.13  | 126.37      | 114.10   |
| 1   | I     | 23  | ARG  | CB-CA-C    | -6.12 | 97.41       | 110.76   |
| 1   | O     | 25  | ARG  | NE-CZ-NH1  | -6.12 | 115.38      | 121.50   |
| 1   | D     | 23  | ARG  | NH1-CZ-NH2 | -6.12 | 111.34      | 119.30   |
| 1   | M     | 25  | ARG  | NE-CZ-NH2  | -6.09 | 113.71      | 119.20   |
| 1   | I     | 23  | ARG  | NE-CZ-NH1  | -6.07 | 115.43      | 121.50   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | M     | 131 | GLU  | CA-CB-CG   | 6.01  | 126.13      | 114.10   |
| 1   | H     | 120 | ARG  | CA-CB-CG   | 5.98  | 126.06      | 114.10   |
| 1   | H     | 131 | GLU  | CB-CG-CD   | 5.95  | 122.71      | 112.60   |
| 1   | H     | 179 | LYS  | CD-CE-NZ   | 5.93  | 130.89      | 111.90   |
| 1   | G     | 23  | ARG  | CB-CA-C    | -5.78 | 99.30       | 110.35   |
| 1   | O     | 23  | ARG  | CD-NE-CZ   | -5.77 | 116.32      | 124.40   |
| 1   | H     | 22  | GLN  | N-CA-C     | -5.77 | 97.93       | 108.02   |
| 1   | E     | 120 | ARG  | CB-CG-CD   | 5.72  | 124.45      | 111.30   |
| 1   | H     | 131 | GLU  | CG-CD-OE2  | 5.71  | 131.54      | 118.40   |
| 1   | H     | 25  | ARG  | NE-CZ-NH1  | -5.70 | 115.81      | 121.50   |
| 1   | F     | 23  | ARG  | NH1-CZ-NH2 | -5.68 | 111.91      | 119.30   |
| 1   | O     | 183 | VAL  | N-CA-C     | 5.68  | 116.06      | 108.11   |
| 1   | G     | 68  | SER  | CA-C-N     | -5.67 | 115.38      | 123.20   |
| 1   | G     | 68  | SER  | C-N-CA     | -5.67 | 115.38      | 123.20   |
| 1   | D     | 203 | LYS  | CG-CD-CE   | 5.64  | 124.27      | 111.30   |
| 1   | B     | 23  | ARG  | CD-NE-CZ   | -5.62 | 116.53      | 124.40   |
| 1   | C     | 23  | ARG  | CB-CA-C    | -5.62 | 99.62       | 110.35   |
| 1   | O     | 203 | LYS  | CG-CD-CE   | 5.59  | 124.17      | 111.30   |
| 1   | C     | 15  | ARG  | CA-C-N     | 5.57  | 126.80      | 119.84   |
| 1   | C     | 15  | ARG  | C-N-CA     | 5.57  | 126.80      | 119.84   |
| 1   | N     | 23  | ARG  | CA-CB-CG   | 5.56  | 125.23      | 114.10   |
| 1   | N     | 120 | ARG  | CA-CB-CG   | -5.55 | 103.01      | 114.10   |
| 1   | E     | 25  | ARG  | CD-NE-CZ   | -5.54 | 116.64      | 124.40   |
| 1   | N     | 23  | ARG  | N-CA-CB    | -5.49 | 103.29      | 113.89   |
| 1   | L     | 131 | GLU  | OE1-CD-OE2 | -5.49 | 109.72      | 122.90   |
| 1   | D     | 25  | ARG  | CA-CB-CG   | -5.49 | 103.12      | 114.10   |
| 1   | E     | 25  | ARG  | NE-CZ-NH1  | -5.49 | 116.01      | 121.50   |
| 1   | F     | 15  | ARG  | CA-C-N     | 5.46  | 125.13      | 119.56   |
| 1   | F     | 15  | ARG  | C-N-CA     | 5.46  | 125.13      | 119.56   |
| 1   | H     | 192 | TYR  | CA-C-N     | -5.42 | 115.07      | 122.93   |
| 1   | H     | 192 | TYR  | C-N-CA     | -5.42 | 115.07      | 122.93   |
| 1   | D     | 120 | ARG  | CA-CB-CG   | 5.42  | 124.94      | 114.10   |
| 1   | H     | 25  | ARG  | CB-CG-CD   | -5.41 | 98.86       | 111.30   |
| 1   | C     | 11  | ARG  | NE-CZ-NH1  | -5.39 | 116.11      | 121.50   |
| 1   | F     | 23  | ARG  | CG-CD-NE   | 5.38  | 123.83      | 112.00   |
| 1   | B     | 25  | ARG  | NE-CZ-NH2  | 5.34  | 124.00      | 119.20   |
| 1   | C     | 13  | THR  | N-CA-C     | -5.28 | 106.16      | 112.59   |
| 1   | J     | 25  | ARG  | CB-CG-CD   | -5.27 | 99.18       | 111.30   |
| 1   | I     | 15  | ARG  | CA-C-N     | 5.25  | 126.41      | 119.84   |
| 1   | I     | 15  | ARG  | C-N-CA     | 5.25  | 126.41      | 119.84   |
| 1   | M     | 23  | ARG  | CB-CG-CD   | -5.23 | 99.26       | 111.30   |
| 1   | H     | 25  | ARG  | CG-CD-NE   | 5.22  | 123.48      | 112.00   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | O     | 25  | ARG  | CD-NE-CZ  | -5.19 | 117.14      | 124.40   |
| 1   | A     | 148 | ARG  | NE-CZ-NH2 | -5.19 | 114.53      | 119.20   |
| 1   | J     | 149 | GLU  | N-CA-C    | -5.18 | 107.03      | 113.55   |
| 1   | M     | 23  | ARG  | NE-CZ-NH1 | -5.17 | 116.33      | 121.50   |
| 1   | I     | 203 | LYS  | CB-CG-CD  | -5.17 | 99.42       | 111.30   |
| 1   | L     | 21  | THR  | N-CA-C    | -5.14 | 102.25      | 109.96   |
| 1   | I     | 203 | LYS  | CD-CE-NZ  | 5.12  | 128.27      | 111.90   |
| 1   | A     | 203 | LYS  | CG-CD-CE  | 5.11  | 123.05      | 111.30   |
| 1   | J     | 23  | ARG  | NE-CZ-NH1 | -5.09 | 116.41      | 121.50   |
| 1   | O     | 22  | GLN  | N-CA-C    | -5.09 | 100.22      | 108.52   |
| 1   | H     | 131 | GLU  | CG-CD-OE1 | -5.08 | 106.72      | 118.40   |
| 1   | O     | 120 | ARG  | CB-CG-CD  | 5.08  | 122.98      | 111.30   |
| 1   | N     | 23  | ARG  | CD-NE-CZ  | 5.07  | 131.50      | 124.40   |
| 1   | N     | 24  | ASP  | N-CA-C    | -5.02 | 107.11      | 113.23   |
| 1   | F     | 23  | ARG  | CA-CB-CG  | 5.01  | 124.12      | 114.10   |
| 1   | N     | 187 | CYS  | N-CA-C    | 5.00  | 121.46      | 110.80   |

There are no chirality outliers.

All (12) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 148 | ARG  | Sidechain |
| 1   | D     | 23  | ARG  | Sidechain |
| 1   | F     | 185 | TYR  | Sidechain |
| 1   | F     | 23  | ARG  | Sidechain |
| 1   | F     | 25  | ARG  | Sidechain |
| 1   | F     | 40  | GLU  | Sidechain |
| 1   | G     | 25  | ARG  | Sidechain |
| 1   | G     | 69  | HIS  | Sidechain |
| 1   | M     | 25  | ARG  | Sidechain |
| 1   | N     | 120 | ARG  | Sidechain |
| 1   | N     | 23  | ARG  | Sidechain |
| 1   | O     | 170 | ARG  | Sidechain |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1586  | 0        | 1545     | 28      | 0            |
| 1   | B     | 1586  | 0        | 1545     | 28      | 0            |
| 1   | C     | 1586  | 0        | 1545     | 22      | 0            |
| 1   | D     | 1578  | 0        | 1530     | 18      | 0            |
| 1   | E     | 1586  | 0        | 1545     | 35      | 0            |
| 1   | F     | 1607  | 0        | 1564     | 35      | 0            |
| 1   | G     | 1591  | 0        | 1557     | 29      | 0            |
| 1   | H     | 1586  | 0        | 1545     | 21      | 0            |
| 1   | I     | 1568  | 0        | 1532     | 28      | 0            |
| 1   | J     | 1586  | 0        | 1545     | 25      | 0            |
| 1   | K     | 1571  | 0        | 1530     | 19      | 0            |
| 1   | L     | 1591  | 0        | 1549     | 21      | 0            |
| 1   | M     | 1566  | 0        | 1535     | 31      | 0            |
| 1   | N     | 1586  | 0        | 1545     | 22      | 0            |
| 1   | O     | 1586  | 0        | 1545     | 18      | 0            |
| 2   | A     | 16    | 0        | 22       | 0       | 0            |
| 2   | B     | 16    | 0        | 22       | 2       | 0            |
| 2   | C     | 16    | 0        | 22       | 1       | 0            |
| 2   | D     | 16    | 0        | 22       | 3       | 0            |
| 2   | E     | 16    | 0        | 22       | 2       | 0            |
| 2   | G     | 16    | 0        | 22       | 1       | 0            |
| 2   | H     | 16    | 0        | 22       | 3       | 0            |
| 2   | I     | 16    | 0        | 22       | 5       | 0            |
| 3   | D     | 14    | 0        | 13       | 0       | 0            |
| 3   | G     | 14    | 0        | 12       | 0       | 0            |
| 4   | A     | 10    | 0        | 0        | 1       | 0            |
| 4   | B     | 10    | 0        | 0        | 1       | 0            |
| 4   | C     | 5     | 0        | 0        | 0       | 0            |
| 4   | D     | 10    | 0        | 0        | 0       | 0            |
| 4   | E     | 25    | 0        | 0        | 1       | 0            |
| 4   | F     | 10    | 0        | 0        | 0       | 0            |
| 4   | G     | 15    | 0        | 0        | 0       | 0            |
| 4   | I     | 5     | 0        | 0        | 0       | 0            |
| 4   | J     | 5     | 0        | 0        | 1       | 0            |
| 4   | M     | 5     | 0        | 0        | 0       | 0            |
| 5   | A     | 8     | 0        | 6        | 0       | 0            |
| 5   | D     | 4     | 0        | 3        | 0       | 0            |
| 5   | F     | 16    | 0        | 12       | 1       | 0            |
| 5   | G     | 12    | 0        | 9        | 0       | 0            |
| 5   | J     | 4     | 0        | 3        | 0       | 0            |
| 5   | O     | 4     | 0        | 3        | 0       | 0            |
| 6   | A     | 19    | 0        | 8        | 2       | 0            |
| 6   | B     | 19    | 0        | 8        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6   | E     | 19    | 0        | 8        | 1       | 0            |
| 6   | I     | 19    | 0        | 8        | 1       | 0            |
| 6   | K     | 19    | 0        | 8        | 2       | 0            |
| 6   | M     | 19    | 0        | 8        | 2       | 0            |
| 7   | A     | 1     | 0        | 0        | 0       | 0            |
| 7   | K     | 1     | 0        | 0        | 0       | 0            |
| 7   | L     | 1     | 0        | 0        | 0       | 0            |
| 7   | N     | 1     | 0        | 0        | 0       | 0            |
| 8   | J     | 6     | 0        | 8        | 0       | 0            |
| 9   | A     | 28    | 0        | 0        | 1       | 0            |
| 9   | B     | 19    | 0        | 0        | 0       | 0            |
| 9   | C     | 22    | 0        | 0        | 1       | 0            |
| 9   | D     | 27    | 0        | 0        | 2       | 0            |
| 9   | E     | 23    | 0        | 0        | 1       | 0            |
| 9   | F     | 31    | 0        | 0        | 0       | 0            |
| 9   | G     | 28    | 0        | 0        | 0       | 0            |
| 9   | H     | 26    | 0        | 0        | 1       | 0            |
| 9   | I     | 21    | 0        | 0        | 0       | 0            |
| 9   | J     | 21    | 0        | 0        | 1       | 0            |
| 9   | K     | 26    | 0        | 0        | 2       | 0            |
| 9   | L     | 24    | 0        | 0        | 0       | 0            |
| 9   | M     | 21    | 0        | 0        | 1       | 0            |
| 9   | N     | 5     | 0        | 0        | 0       | 0            |
| 9   | O     | 13    | 0        | 0        | 0       | 0            |
| All | All   | 24523 | 0        | 23450    | 335     | 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 7.

All (335) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:E:148:ARG:CZ  | 1:M:25:ARG:HH22  | 1.57                     | 1.18              |
| 1:E:148:ARG:CZ  | 1:M:25:ARG:NH2   | 2.21                     | 1.02              |
| 1:A:153:ASP:OD1 | 1:F:179:LYS:NZ   | 1.93                     | 1.01              |
| 1:E:65:TRP:HB3  | 2:E:302:1PE:H261 | 1.43                     | 0.98              |
| 1:D:23:ARG:O    | 1:D:23:ARG:HG3   | 1.67                     | 0.93              |
| 1:E:148:ARG:HD3 | 1:M:25:ARG:CZ    | 2.04                     | 0.88              |
| 1:E:148:ARG:HD3 | 1:M:25:ARG:NH2   | 1.93                     | 0.84              |
| 1:J:30:SER:HB2  | 1:J:57:THR:HG22  | 1.61                     | 0.82              |
| 1:I:65:TRP:HB3  | 2:I:302:1PE:H151 | 1.62                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:9:ASN:HD22   | 2:E:302:1PE:H162 | 1.44                     | 0.82              |
| 1:H:15:ARG:NH2   | 1:I:4:ALA:O      | 2.13                     | 0.81              |
| 1:H:22:GLN:O     | 1:H:23:ARG:HB3   | 1.81                     | 0.80              |
| 1:E:148:ARG:NE   | 1:M:25:ARG:HH22  | 1.78                     | 0.80              |
| 1:F:23:ARG:HG3   | 1:F:25:ARG:HD2   | 1.63                     | 0.80              |
| 1:E:148:ARG:NE   | 1:M:25:ARG:NH2   | 2.31                     | 0.77              |
| 1:K:170:ARG:HH21 | 1:K:203:LYS:HE2  | 1.50                     | 0.77              |
| 1:F:160:ASP:HB3  | 1:F:163:GLU:HB2  | 1.67                     | 0.77              |
| 1:C:22:GLN:O     | 1:C:23:ARG:HB2   | 1.82                     | 0.77              |
| 1:L:23:ARG:HB3   | 1:L:25:ARG:HG3   | 1.66                     | 0.77              |
| 1:M:170:ARG:HH21 | 1:M:203:LYS:HE2  | 1.50                     | 0.76              |
| 1:G:91:ALA:HB1   | 1:G:119:GLN:HE21 | 1.51                     | 0.75              |
| 1:N:22:GLN:O     | 1:N:23:ARG:HB3   | 1.86                     | 0.74              |
| 1:E:148:ARG:CD   | 1:M:25:ARG:NH2   | 2.50                     | 0.74              |
| 1:F:23:ARG:HG2   | 1:F:23:ARG:HH11  | 1.52                     | 0.74              |
| 1:G:23:ARG:HB2   | 1:G:25:ARG:HD2   | 1.69                     | 0.73              |
| 1:H:130:THR:HG22 | 1:H:132:SER:H    | 1.53                     | 0.73              |
| 1:M:130:THR:HG22 | 1:M:132:SER:H    | 1.55                     | 0.72              |
| 1:D:130:THR:HG22 | 1:D:132:SER:H    | 1.55                     | 0.71              |
| 1:E:148:ARG:NH1  | 1:M:25:ARG:NH2   | 2.38                     | 0.71              |
| 1:L:61:ARG:NH1   | 1:L:108:ASP:O    | 2.24                     | 0.71              |
| 1:G:15:ARG:NH2   | 1:G:17:ASP:OD2   | 2.23                     | 0.70              |
| 1:M:22:GLN:O     | 1:M:23:ARG:HB3   | 1.89                     | 0.70              |
| 1:D:148:ARG:NH1  | 9:D:407:HOH:O    | 2.25                     | 0.69              |
| 1:I:1:LEU:HD11   | 2:I:302:1PE:H161 | 1.75                     | 0.69              |
| 1:A:23:ARG:HB3   | 1:A:25:ARG:HG3   | 1.75                     | 0.68              |
| 1:B:130:THR:HG22 | 1:B:132:SER:H    | 1.58                     | 0.67              |
| 1:C:202:ARG:NH2  | 9:C:412:HOH:O    | 2.17                     | 0.67              |
| 1:G:22:GLN:O     | 1:G:23:ARG:HB2   | 1.94                     | 0.67              |
| 1:I:130:THR:HG22 | 1:I:132:SER:H    | 1.58                     | 0.67              |
| 1:E:148:ARG:CD   | 1:M:25:ARG:CZ    | 2.72                     | 0.67              |
| 1:O:130:THR:HG22 | 1:O:132:SER:H    | 1.58                     | 0.67              |
| 1:F:130:THR:HG22 | 1:F:132:SER:H    | 1.60                     | 0.67              |
| 1:A:181:ASN:HA   | 1:F:182:SER:O    | 1.94                     | 0.67              |
| 1:F:22:GLN:O     | 1:F:23:ARG:HB3   | 1.94                     | 0.67              |
| 1:K:15:ARG:NH2   | 1:L:4:ALA:O      | 2.28                     | 0.66              |
| 1:K:130:THR:HG22 | 1:K:132:SER:H    | 1.61                     | 0.66              |
| 6:M:301:NSE:H5   | 1:N:53:TRP:CH2   | 2.30                     | 0.66              |
| 1:F:183:VAL:CG1  | 1:F:185:TYR:HE1  | 2.08                     | 0.66              |
| 1:G:124:ASP:HB2  | 1:H:168:TYR:CE1  | 2.31                     | 0.65              |
| 1:O:187:CYS:SG   | 1:O:188:CYS:N    | 2.69                     | 0.65              |

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| Atom-1              | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|------------------|--------------------------|-------------------|
| 1:G:130:THR:HG22    | 1:G:132:SER:H    | 1.61                     | 0.65              |
| 1:J:130:THR:HG22    | 1:J:132:SER:H    | 1.62                     | 0.65              |
| 1:C:130:THR:HG22    | 1:C:132:SER:H    | 1.61                     | 0.65              |
| 1:M:170:ARG:NH2     | 1:M:203:LYS:HE2  | 2.11                     | 0.65              |
| 1:C:65:TRP:HB3      | 2:C:301:1PE:H261 | 1.78                     | 0.65              |
| 1:F:187:CYS:SG      | 1:F:188:CYS:N    | 2.70                     | 0.64              |
| 1:N:130:THR:HG22    | 1:N:132:SER:H    | 1.61                     | 0.64              |
| 1:H:61:ARG:NH2      | 9:H:403:HOH:O    | 2.29                     | 0.64              |
| 1:L:130:THR:HG22    | 1:L:132:SER:H    | 1.62                     | 0.64              |
| 1:F:23:ARG:CG       | 1:F:25:ARG:HD2   | 2.28                     | 0.64              |
| 1:B:129:ASP:OD1     | 1:B:203:LYS:HE3  | 1.98                     | 0.64              |
| 1:A:130:THR:HG22    | 1:A:132:SER:H    | 1.63                     | 0.63              |
| 1:O:23:ARG:HB3      | 1:O:25:ARG:HG3   | 1.80                     | 0.63              |
| 1:J:25:ARG:HH11     | 1:J:25:ARG:HG2   | 1.62                     | 0.63              |
| 1:A:22:GLN:O        | 1:A:23:ARG:HB3   | 1.99                     | 0.62              |
| 1:O:22:GLN:O        | 1:O:23:ARG:HB3   | 2.00                     | 0.62              |
| 1:K:22:GLN:O        | 1:K:25:ARG:HG3   | 2.00                     | 0.62              |
| 1:O:129:ASP:OD1     | 1:O:203:LYS:HE3  | 1.98                     | 0.62              |
| 1:D:168:TYR:CE1     | 1:C:124:ASP:HB2  | 2.35                     | 0.62              |
| 1:I:14:SER:O        | 1:I:16:PRO:HD3   | 2.00                     | 0.62              |
| 1:L:23:ARG:O        | 1:L:24:ASP:HB2   | 2.00                     | 0.62              |
| 1:K:4:ALA:O         | 1:O:15:ARG:NH1   | 2.32                     | 0.62              |
| 6:M:301:NSE:H5      | 1:N:53:TRP:CZ3   | 2.35                     | 0.62              |
| 1:B:22:GLN:O        | 1:B:23:ARG:HB3   | 2.00                     | 0.61              |
| 6:K:301:NSE:H8      | 1:L:104:ARG:HB2  | 1.81                     | 0.61              |
| 1:A:181:ASN:OD1     | 1:F:182:SER:HB3  | 2.01                     | 0.60              |
| 1:L:22:GLN:O        | 1:L:23:ARG:HB3   | 2.01                     | 0.60              |
| 1:N:23:ARG:O        | 1:N:24:ASP:HB2   | 2.01                     | 0.60              |
| 1:D:162:SER:O       | 9:D:413:HOH:O    | 2.17                     | 0.60              |
| 1:C:187:CYS:SG      | 1:C:188:CYS:N    | 2.74                     | 0.59              |
| 1:A:15:ARG:NH2      | 1:A:17:ASP:OD2   | 2.35                     | 0.59              |
| 1:L:94:LYS:HE3      | 1:M:97:VAL:O     | 2.01                     | 0.59              |
| 1:G:44:ILE:HG22     | 1:H:170:ARG:HD2  | 1.84                     | 0.59              |
| 1:G:23:ARG:O        | 1:G:24:ASP:HB2   | 2.03                     | 0.59              |
| 1:D:170:ARG:HD2     | 1:C:44:ILE:HG22  | 1.84                     | 0.59              |
| 1:F:160:ASP:OD1     | 1:L:189:PRO:HB3  | 2.03                     | 0.58              |
| 1:E:21:THR:HG22     | 1:E:25:ARG:O     | 2.04                     | 0.58              |
| 1:B:137:ARG:NH1     | 4:B:303:SO4:O2   | 2.33                     | 0.58              |
| 1:C:14:SER:C        | 1:C:16:PRO:HD3   | 2.28                     | 0.58              |
| 1:L:21:THR:HG22     | 1:L:25:ARG:O     | 2.03                     | 0.58              |
| 1:G:112[A]:LEU:HD11 | 1:G:114:MET:HE2  | 1.86                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:10:ILE:O     | 1:L:14:SER:HB3   | 2.03                     | 0.58              |
| 1:N:21:THR:HG22  | 1:N:25:ARG:O     | 2.04                     | 0.57              |
| 1:G:187:CYS:C    | 1:G:188:CYS:SG   | 2.87                     | 0.57              |
| 1:G:23:ARG:CB    | 1:G:25:ARG:HD2   | 2.35                     | 0.57              |
| 1:E:148:ARG:CD   | 1:M:25:ARG:NH1   | 2.67                     | 0.57              |
| 1:M:124:ASP:HB2  | 1:N:168:TYR:CE1  | 2.40                     | 0.56              |
| 1:L:187:CYS:SG   | 1:L:188:CYS:N    | 2.78                     | 0.56              |
| 1:B:23:ARG:O     | 1:B:24:ASP:HB2   | 2.05                     | 0.56              |
| 1:B:187:CYS:SG   | 1:B:188:CYS:N    | 2.79                     | 0.56              |
| 1:G:91:ALA:HB1   | 1:G:119:GLN:NE2  | 2.19                     | 0.56              |
| 1:A:21:THR:HG22  | 1:A:25:ARG:O     | 2.05                     | 0.56              |
| 1:B:23:ARG:HB3   | 1:B:25:ARG:HG3   | 1.87                     | 0.56              |
| 1:G:60:ASP:OD1   | 1:G:62:THR:HB    | 2.06                     | 0.56              |
| 1:F:183:VAL:CG1  | 1:F:185:TYR:CE1  | 2.89                     | 0.55              |
| 1:K:139:LYS:NZ   | 9:K:426:HOH:O    | 2.39                     | 0.55              |
| 1:A:23:ARG:O     | 1:A:24:ASP:HB2   | 2.08                     | 0.54              |
| 1:H:15:ARG:HH21  | 1:I:4:ALA:HA     | 1.72                     | 0.54              |
| 1:K:21:THR:HG22  | 1:K:25:ARG:O     | 2.08                     | 0.54              |
| 1:E:148:ARG:CG   | 1:M:25:ARG:NH1   | 2.70                     | 0.54              |
| 1:C:23:ARG:O     | 1:C:24:ASP:HB2   | 2.08                     | 0.54              |
| 1:O:23:ARG:O     | 1:O:24:ASP:HB2   | 2.07                     | 0.54              |
| 1:I:6:ILE:HG23   | 2:I:302:1PE:H152 | 1.88                     | 0.54              |
| 1:K:170:ARG:NH2  | 1:K:203:LYS:HE2  | 2.19                     | 0.54              |
| 1:F:14:SER:OG    | 1:F:80:SER:O     | 2.17                     | 0.54              |
| 1:I:21:THR:HG22  | 1:I:25:ARG:O     | 2.08                     | 0.54              |
| 1:G:21:THR:HG22  | 1:G:25:ARG:O     | 2.08                     | 0.54              |
| 1:F:183:VAL:HG12 | 1:F:185:TYR:CE1  | 2.42                     | 0.54              |
| 1:O:21:THR:HG22  | 1:O:25:ARG:O     | 2.07                     | 0.54              |
| 1:D:23:ARG:O     | 1:D:24:ASP:HB2   | 2.06                     | 0.54              |
| 1:E:148:ARG:HG3  | 1:M:25:ARG:NH1   | 2.22                     | 0.54              |
| 1:C:11:ARG:O     | 1:C:14:SER:HB3   | 2.08                     | 0.53              |
| 1:L:22:GLN:O     | 1:L:23:ARG:CB    | 2.55                     | 0.53              |
| 6:A:301:NSE:H5   | 1:B:53:TRP:CZ3   | 2.43                     | 0.53              |
| 1:D:21:THR:HG22  | 1:D:25:ARG:O     | 2.07                     | 0.53              |
| 1:K:124:ASP:HB2  | 1:L:168:TYR:CE1  | 2.43                     | 0.53              |
| 1:I:9:ASN:ND2    | 2:I:302:1PE:H162 | 2.24                     | 0.53              |
| 1:E:148:ARG:NH1  | 1:M:25:ARG:HH21  | 2.05                     | 0.53              |
| 1:H:22:GLN:O     | 1:H:25:ARG:HG3   | 2.09                     | 0.53              |
| 1:I:23:ARG:HG2   | 1:I:23:ARG:HH11  | 1.72                     | 0.53              |
| 1:B:9:ASN:HB3    | 2:B:302:1PE:H151 | 1.90                     | 0.52              |
| 1:M:14:SER:HB3   | 9:M:401:HOH:O    | 2.08                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:23:ARG:HG2   | 1:M:25:ARG:HE    | 1.73                     | 0.52              |
| 1:I:22:GLN:O     | 1:I:23:ARG:HB2   | 2.07                     | 0.52              |
| 1:A:184:THR:O    | 1:F:186:SER:HB3  | 2.09                     | 0.52              |
| 6:K:301:NSE:H5   | 1:L:53:TRP:CH2   | 2.44                     | 0.52              |
| 1:N:94:LYS:HE3   | 1:O:97:VAL:O     | 2.07                     | 0.52              |
| 1:A:22:GLN:O     | 1:A:23:ARG:CB    | 2.57                     | 0.52              |
| 1:I:22:GLN:O     | 1:I:25:ARG:HG3   | 2.09                     | 0.52              |
| 1:M:143:TRP:CZ2  | 1:N:99:THR:HG21  | 2.45                     | 0.52              |
| 1:E:124:ASP:HB2  | 1:A:168:TYR:CE1  | 2.44                     | 0.52              |
| 1:J:21:THR:HG22  | 1:J:25:ARG:O     | 2.10                     | 0.52              |
| 1:C:21:THR:HG22  | 1:C:25:ARG:O     | 2.10                     | 0.52              |
| 1:F:129:ASP:OD1  | 1:F:203:LYS:HE3  | 2.10                     | 0.52              |
| 1:H:21:THR:HG22  | 1:H:25:ARG:O     | 2.09                     | 0.51              |
| 1:I:23:ARG:HB2   | 1:I:25:ARG:HG3   | 1.92                     | 0.51              |
| 1:M:22:GLN:O     | 1:M:25:ARG:HG3   | 2.11                     | 0.51              |
| 1:B:21:THR:HG22  | 1:B:25:ARG:O     | 2.10                     | 0.51              |
| 1:F:167:GLN:NE2  | 5:F:306:ACT:OXT  | 2.44                     | 0.51              |
| 1:C:15:ARG:NH2   | 1:C:17:ASP:OD2   | 2.43                     | 0.51              |
| 1:H:137:ARG:HD2  | 1:H:196:GLU:OE1  | 2.10                     | 0.51              |
| 1:D:9:ASN:HB2    | 2:D:301:1PE:H162 | 1.94                     | 0.50              |
| 1:I:124:ASP:HB2  | 1:J:168:TYR:CE1  | 2.46                     | 0.50              |
| 1:E:139:LYS:NZ   | 9:E:414:HOH:O    | 2.33                     | 0.50              |
| 1:I:137:ARG:HD2  | 1:I:196:GLU:OE1  | 2.10                     | 0.50              |
| 1:A:84:PRO:HB2   | 1:A:86:LEU:HG    | 1.94                     | 0.50              |
| 1:G:13:THR:HG21  | 2:G:301:1PE:H142 | 1.93                     | 0.50              |
| 1:A:137:ARG:HD2  | 1:A:196:GLU:OE1  | 2.11                     | 0.50              |
| 1:F:21:THR:HG22  | 1:F:25:ARG:O     | 2.12                     | 0.50              |
| 1:E:22:GLN:O     | 1:E:25:ARG:HG3   | 2.12                     | 0.49              |
| 1:H:9:ASN:HB2    | 2:H:301:1PE:H161 | 1.92                     | 0.49              |
| 1:F:183:VAL:HG12 | 1:F:185:TYR:HE1  | 1.77                     | 0.49              |
| 1:J:190:GLU:HG3  | 9:J:412:HOH:O    | 2.12                     | 0.49              |
| 1:I:44:ILE:HG22  | 1:J:170:ARG:HD2  | 1.95                     | 0.49              |
| 1:L:137:ARG:HD2  | 1:L:196:GLU:OE1  | 2.13                     | 0.49              |
| 1:G:137:ARG:HD2  | 1:G:196:GLU:OE1  | 2.13                     | 0.49              |
| 1:A:180:LYS:O    | 1:F:182:SER:N    | 2.37                     | 0.49              |
| 1:J:137:ARG:HD2  | 1:J:196:GLU:OE1  | 2.13                     | 0.48              |
| 1:F:101:GLN:OE1  | 1:F:113:TYR:OH   | 2.28                     | 0.48              |
| 1:J:49:ASP:OD2   | 1:J:120:ARG:HD2  | 2.11                     | 0.48              |
| 1:F:137:ARG:HD2  | 1:F:196:GLU:OE1  | 2.13                     | 0.48              |
| 1:D:49:ASP:OD2   | 1:D:120:ARG:HD2  | 2.12                     | 0.48              |
| 1:E:137:ARG:HD2  | 1:E:196:GLU:OE1  | 2.14                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:23:ARG:O     | 1:F:24:ASP:HB2   | 2.13                     | 0.48              |
| 1:E:23:ARG:HB3   | 1:E:25:ARG:HG3   | 1.94                     | 0.48              |
| 1:E:139:LYS:HE3  | 4:E:307:SO4:O4   | 2.14                     | 0.48              |
| 1:G:68:SER:OG    | 1:G:69:HIS:N     | 2.44                     | 0.47              |
| 1:F:99:THR:HG21  | 1:J:143:TRP:CZ2  | 2.49                     | 0.47              |
| 1:N:22:GLN:O     | 1:N:25:ARG:HG2   | 2.14                     | 0.47              |
| 1:O:137:ARG:HD2  | 1:O:196:GLU:OE1  | 2.14                     | 0.47              |
| 6:A:301:NSE:H8   | 1:B:104:ARG:HB2  | 1.96                     | 0.47              |
| 1:B:41:VAL:HG13  | 1:B:125:VAL:HG11 | 1.97                     | 0.47              |
| 1:I:185:TYR:CD1  | 1:I:185:TYR:N    | 2.82                     | 0.47              |
| 1:K:99:THR:HG21  | 1:O:143:TRP:CZ2  | 2.49                     | 0.47              |
| 1:A:66:ASN:ND2   | 9:A:416:HOH:O    | 2.46                     | 0.47              |
| 1:H:23:ARG:O     | 1:H:23:ARG:HG3   | 2.14                     | 0.47              |
| 1:J:146:HIS:CD2  | 1:J:190:GLU:HG2  | 2.50                     | 0.47              |
| 1:O:10:ILE:O     | 1:O:14:SER:HB2   | 2.14                     | 0.47              |
| 1:B:15:ARG:N     | 1:B:16:PRO:HD3   | 2.29                     | 0.47              |
| 1:B:146:HIS:CE1  | 1:B:190:GLU:OE1  | 2.68                     | 0.47              |
| 1:J:84:PRO:HB2   | 1:J:86:LEU:HG    | 1.96                     | 0.47              |
| 1:K:137:ARG:HD2  | 1:K:196:GLU:OE1  | 2.14                     | 0.47              |
| 1:O:101:GLN:OE1  | 1:O:113:TYR:OH   | 2.29                     | 0.47              |
| 1:D:101:GLN:OE1  | 1:D:113:TYR:OH   | 2.31                     | 0.47              |
| 1:B:137:ARG:HD2  | 1:B:196:GLU:OE1  | 2.14                     | 0.47              |
| 1:N:137:ARG:HD2  | 1:N:196:GLU:OE1  | 2.14                     | 0.47              |
| 1:J:72:ASP:N     | 4:J:301:SO4:O1   | 2.26                     | 0.47              |
| 1:K:84:PRO:HB2   | 1:K:86:LEU:HG    | 1.96                     | 0.47              |
| 1:D:149:GLU:CD   | 1:E:104:ARG:HH22 | 2.23                     | 0.46              |
| 1:K:168:TYR:CE1  | 1:O:124:ASP:HB2  | 2.50                     | 0.46              |
| 1:A:137:ARG:NH2  | 4:A:303:SO4:O1   | 2.36                     | 0.46              |
| 1:L:41:VAL:HG13  | 1:L:125:VAL:HG11 | 1.97                     | 0.46              |
| 1:E:129:ASP:OD1  | 1:E:203:LYS:HE3  | 2.14                     | 0.46              |
| 1:F:41:VAL:HG13  | 1:F:125:VAL:HG11 | 1.97                     | 0.46              |
| 1:H:49:ASP:OD2   | 1:H:120:ARG:HD2  | 2.16                     | 0.46              |
| 1:J:146:HIS:CG   | 1:J:190:GLU:HG2  | 2.50                     | 0.46              |
| 1:N:84:PRO:HB2   | 1:N:86:LEU:HG    | 1.96                     | 0.46              |
| 2:D:301:1PE:OH2  | 2:D:301:1PE:H232 | 2.16                     | 0.46              |
| 1:A:112:LEU:HD11 | 1:A:114:MET:HE2  | 1.96                     | 0.46              |
| 1:A:185:TYR:HA   | 1:F:186:SER:HB3  | 1.97                     | 0.46              |
| 1:C:137:ARG:HD2  | 1:C:196:GLU:OE1  | 2.14                     | 0.46              |
| 1:H:41:VAL:HG13  | 1:H:125:VAL:HG11 | 1.97                     | 0.46              |
| 1:J:10:ILE:O     | 1:J:14:SER:HB2   | 2.16                     | 0.46              |
| 1:I:185:TYR:N    | 1:I:185:TYR:HD1  | 2.13                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:91:ALA:CB    | 1:G:119:GLN:NE2  | 2.79                     | 0.46              |
| 1:L:185:TYR:N    | 1:L:185:TYR:CD1  | 2.84                     | 0.46              |
| 1:J:23:ARG:O     | 1:J:24:ASP:HB2   | 2.14                     | 0.46              |
| 1:E:59:SER:OG    | 1:E:110:GLU:OE2  | 2.32                     | 0.45              |
| 1:A:143:TRP:CZ2  | 1:B:99:THR:HG21  | 2.50                     | 0.45              |
| 1:M:41:VAL:HG13  | 1:M:125:VAL:HG11 | 1.98                     | 0.45              |
| 1:M:137:ARG:HD2  | 1:M:196:GLU:OE1  | 2.17                     | 0.45              |
| 1:D:137:ARG:HD2  | 1:D:196:GLU:OE1  | 2.17                     | 0.45              |
| 1:D:41:VAL:HG13  | 1:D:125:VAL:HG11 | 1.98                     | 0.45              |
| 1:G:101:GLN:OE1  | 1:G:113:TYR:OH   | 2.32                     | 0.45              |
| 1:B:22:GLN:O     | 1:B:25:ARG:HG3   | 2.17                     | 0.45              |
| 1:B:23:ARG:HB3   | 1:B:25:ARG:CG    | 2.47                     | 0.45              |
| 1:F:67:SER:HA    | 1:F:70:SER:HB2   | 1.98                     | 0.45              |
| 1:N:25:ARG:HH11  | 1:N:25:ARG:HD3   | 1.33                     | 0.45              |
| 1:N:41:VAL:HG13  | 1:N:125:VAL:HG11 | 1.97                     | 0.45              |
| 1:A:41:VAL:HG13  | 1:A:125:VAL:HG11 | 1.98                     | 0.45              |
| 1:C:84:PRO:HB2   | 1:C:86:LEU:HG    | 1.99                     | 0.45              |
| 1:C:185:TYR:N    | 1:C:185:TYR:CD1  | 2.85                     | 0.45              |
| 1:K:41:VAL:HG13  | 1:K:125:VAL:HG11 | 1.97                     | 0.45              |
| 1:O:41:VAL:HG13  | 1:O:125:VAL:HG11 | 1.99                     | 0.45              |
| 1:E:101:GLN:OE1  | 1:E:113:TYR:OH   | 2.31                     | 0.45              |
| 1:G:99:THR:HG21  | 1:F:143:TRP:CZ2  | 2.52                     | 0.45              |
| 1:C:101:GLN:OE1  | 1:C:113:TYR:OH   | 2.30                     | 0.45              |
| 1:L:183:VAL:HG12 | 1:L:185:TYR:CE1  | 2.52                     | 0.45              |
| 1:E:22:GLN:O     | 1:E:23:ARG:CB    | 2.64                     | 0.44              |
| 1:I:84:PRO:HB2   | 1:I:86:LEU:HG    | 1.99                     | 0.44              |
| 1:J:25:ARG:HB3   | 1:J:26:PRO:HD2   | 1.99                     | 0.44              |
| 1:D:84:PRO:HB2   | 1:D:86:LEU:HG    | 1.99                     | 0.44              |
| 1:B:183:VAL:HG12 | 1:B:185:TYR:CE1  | 2.52                     | 0.44              |
| 1:B:185:TYR:CD1  | 1:B:185:TYR:N    | 2.85                     | 0.44              |
| 1:D:22:GLN:O     | 1:D:23:ARG:HB3   | 2.14                     | 0.44              |
| 1:E:49:ASP:OD2   | 1:E:120:ARG:HD2  | 2.17                     | 0.44              |
| 1:E:187:CYS:SG   | 1:E:188:CYS:N    | 2.90                     | 0.44              |
| 1:A:9:ASN:O      | 1:A:13:THR:OG1   | 2.31                     | 0.44              |
| 1:I:189:PRO:C    | 1:I:190:GLU:HG2  | 2.43                     | 0.44              |
| 1:O:25:ARG:HH11  | 1:O:25:ARG:HD3   | 1.40                     | 0.44              |
| 2:D:301:1PE:H131 | 2:D:301:1PE:H141 | 1.79                     | 0.44              |
| 1:K:193:GLU:O    | 9:K:408:HOH:O    | 2.21                     | 0.44              |
| 1:B:68:SER:OG    | 1:B:69:HIS:N     | 2.51                     | 0.44              |
| 1:G:185:TYR:CD1  | 1:G:185:TYR:N    | 2.86                     | 0.44              |
| 1:D:67:SER:HA    | 1:D:70:SER:HB2   | 2.00                     | 0.44              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:1:LEU:HB2   | 1:A:70:SER:OG    | 2.18                     | 0.44              |
| 1:J:68:SER:OG   | 1:J:69:HIS:N     | 2.51                     | 0.44              |
| 1:M:84:PRO:HB2  | 1:M:86:LEU:HG    | 1.99                     | 0.44              |
| 1:N:187:CYS:SG  | 1:N:188:CYS:N    | 2.91                     | 0.44              |
| 1:A:124:ASP:HB2 | 1:B:168:TYR:CE1  | 2.52                     | 0.43              |
| 1:H:84:PRO:HB2  | 1:H:86:LEU:HG    | 1.99                     | 0.43              |
| 1:D:99:THR:HG21 | 1:C:143:TRP:CZ2  | 2.54                     | 0.43              |
| 1:B:84:PRO:HB2  | 1:B:86:LEU:HG    | 1.99                     | 0.43              |
| 1:E:67:SER:HA   | 1:E:70:SER:HB2   | 2.00                     | 0.43              |
| 1:C:41:VAL:HG13 | 1:C:125:VAL:HG11 | 2.00                     | 0.43              |
| 1:J:41:VAL:HG13 | 1:J:125:VAL:HG11 | 1.99                     | 0.43              |
| 1:K:68:SER:OG   | 1:K:69:HIS:N     | 2.51                     | 0.43              |
| 1:E:41:VAL:HG13 | 1:E:125:VAL:HG11 | 1.99                     | 0.43              |
| 1:B:22:GLN:O    | 1:B:23:ARG:CB    | 2.59                     | 0.43              |
| 1:B:101:GLN:OE1 | 1:B:113:TYR:OH   | 2.30                     | 0.43              |
| 1:C:67:SER:HA   | 1:C:70:SER:HB2   | 2.00                     | 0.43              |
| 6:I:301:NSE:H8  | 1:J:104:ARG:HB2  | 2.00                     | 0.43              |
| 1:J:1:LEU:HB2   | 1:J:70:SER:OG    | 2.18                     | 0.43              |
| 1:O:67:SER:HA   | 1:O:70:SER:HB2   | 2.00                     | 0.43              |
| 1:I:41:VAL:HG13 | 1:I:125:VAL:HG11 | 2.00                     | 0.43              |
| 1:K:1:LEU:HB2   | 1:K:70:SER:OG    | 2.18                     | 0.43              |
| 1:M:1:LEU:HB2   | 1:M:70:SER:OG    | 2.18                     | 0.43              |
| 1:F:1:LEU:HB2   | 1:F:70:SER:OG    | 2.19                     | 0.43              |
| 1:H:25:ARG:HH11 | 1:H:25:ARG:HD3   | 1.39                     | 0.43              |
| 1:J:15:ARG:HE   | 1:J:15:ARG:HB3   | 1.77                     | 0.43              |
| 1:G:41:VAL:HG13 | 1:G:125:VAL:HG11 | 2.00                     | 0.42              |
| 1:E:1:LEU:HB2   | 1:E:70:SER:OG    | 2.19                     | 0.42              |
| 1:A:146:HIS:CE1 | 1:A:190:GLU:HG2  | 2.54                     | 0.42              |
| 1:F:99:THR:HG21 | 1:J:143:TRP:CE2  | 2.54                     | 0.42              |
| 1:H:101:GLN:OE1 | 1:H:113:TYR:OH   | 2.33                     | 0.42              |
| 1:L:84:PRO:HB2  | 1:L:86:LEU:HG    | 2.00                     | 0.42              |
| 1:H:67:SER:HA   | 1:H:70:SER:HB2   | 2.00                     | 0.42              |
| 1:E:68:SER:OG   | 1:E:69:HIS:N     | 2.52                     | 0.42              |
| 1:I:23:ARG:O    | 1:I:24:ASP:HB2   | 2.20                     | 0.42              |
| 1:L:67:SER:HA   | 1:L:70:SER:HB2   | 2.00                     | 0.42              |
| 1:F:84:PRO:HB2  | 1:F:86:LEU:HG    | 2.01                     | 0.42              |
| 1:I:67:SER:HA   | 1:I:70:SER:HB2   | 2.01                     | 0.42              |
| 1:J:67:SER:HA   | 1:J:70:SER:HB2   | 2.02                     | 0.42              |
| 1:N:129:ASP:OD1 | 1:N:203:LYS:HE3  | 2.19                     | 0.42              |
| 1:N:185:TYR:N   | 1:N:185:TYR:CD1  | 2.87                     | 0.42              |
| 1:B:1:LEU:HB2   | 1:B:70:SER:OG    | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:E:301:NSE:C2   | 1:A:114:MET:HB3  | 2.49                     | 0.42              |
| 1:K:187:CYS:SG   | 1:K:188:CYS:N    | 2.93                     | 0.42              |
| 1:B:23:ARG:HH11  | 1:B:23:ARG:HD3   | 1.40                     | 0.42              |
| 2:H:301:1PE:H142 | 2:H:301:1PE:H151 | 1.81                     | 0.42              |
| 1:M:183:VAL:HG12 | 1:M:185:TYR:CE1  | 2.55                     | 0.42              |
| 1:O:84:PRO:HB2   | 1:O:86:LEU:HG    | 2.01                     | 0.42              |
| 1:G:67:SER:HA    | 1:G:70:SER:HB2   | 2.01                     | 0.41              |
| 1:A:153:ASP:CG   | 1:F:179:LYS:NZ   | 2.74                     | 0.41              |
| 1:M:101:GLN:OE1  | 1:M:113:TYR:OH   | 2.36                     | 0.41              |
| 1:G:1:LEU:HB2    | 1:G:70:SER:OG    | 2.20                     | 0.41              |
| 1:J:17:ASP:OD1   | 1:J:17:ASP:N     | 2.50                     | 0.41              |
| 1:B:63:LEU:O     | 2:B:302:1PE:H262 | 2.20                     | 0.41              |
| 1:C:1:LEU:HB2    | 1:C:70:SER:OG    | 2.21                     | 0.41              |
| 1:G:168:TYR:CE1  | 1:F:124:ASP:HB2  | 2.55                     | 0.41              |
| 1:H:143:TRP:CZ2  | 1:I:99:THR:HG21  | 2.55                     | 0.41              |
| 1:N:189:PRO:C    | 1:N:190:GLU:HG2  | 2.46                     | 0.41              |
| 1:H:1:LEU:HB2    | 1:H:70:SER:OG    | 2.20                     | 0.41              |
| 1:I:101:GLN:OE1  | 1:I:113:TYR:OH   | 2.35                     | 0.41              |
| 1:M:185:TYR:CD1  | 1:M:185:TYR:N    | 2.88                     | 0.41              |
| 1:N:183:VAL:HG12 | 1:N:185:TYR:CE1  | 2.55                     | 0.41              |
| 1:G:84:PRO:HB2   | 1:G:86:LEU:HG    | 2.03                     | 0.41              |
| 1:E:84:PRO:HB2   | 1:E:86:LEU:HG    | 2.02                     | 0.41              |
| 1:G:1:LEU:HD23   | 1:G:1:LEU:HA     | 1.90                     | 0.41              |
| 1:G:183:VAL:HG12 | 1:G:185:TYR:CE1  | 2.56                     | 0.41              |
| 1:E:130:THR:HG22 | 1:E:132:SER:H    | 1.85                     | 0.41              |
| 1:C:112:LEU:HD11 | 1:C:114:MET:HE2  | 2.02                     | 0.41              |
| 1:C:183:VAL:HG12 | 1:C:185:TYR:CE1  | 2.56                     | 0.41              |
| 1:G:146:HIS:CE1  | 1:G:190:GLU:OE1  | 2.74                     | 0.41              |
| 1:N:67:SER:HA    | 1:N:70:SER:HB2   | 2.03                     | 0.41              |
| 1:A:68:SER:OG    | 1:A:69:HIS:N     | 2.54                     | 0.40              |
| 1:I:183:VAL:HG12 | 1:I:185:TYR:CE1  | 2.56                     | 0.40              |
| 1:N:1:LEU:HB2    | 1:N:70:SER:OG    | 2.21                     | 0.40              |
| 1:I:9:ASN:HD22   | 2:I:302:1PE:H162 | 1.84                     | 0.40              |
| 1:K:67:SER:HA    | 1:K:70:SER:HB2   | 2.03                     | 0.40              |
| 1:N:61:ARG:NH1   | 1:N:108:ASP:O    | 2.50                     | 0.40              |
| 1:F:23:ARG:HH11  | 1:F:23:ARG:CG    | 2.23                     | 0.40              |
| 1:H:143:TRP:CE2  | 1:I:99:THR:HG21  | 2.56                     | 0.40              |
| 2:H:301:1PE:H151 | 2:H:301:1PE:H162 | 1.66                     | 0.40              |
| 1:M:67:SER:HA    | 1:M:70:SER:HB2   | 2.02                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 1   | A     | 194/210 (92%)   | 187 (96%)  | 7 (4%)  | 0        | 100         | 100 |
| 1   | B     | 194/210 (92%)   | 189 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 1   | C     | 194/210 (92%)   | 185 (95%)  | 9 (5%)  | 0        | 100         | 100 |
| 1   | D     | 193/210 (92%)   | 186 (96%)  | 6 (3%)  | 1 (0%)   | 24          | 45  |
| 1   | E     | 194/210 (92%)   | 189 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 1   | F     | 197/210 (94%)   | 186 (94%)  | 11 (6%) | 0        | 100         | 100 |
| 1   | G     | 195/210 (93%)   | 189 (97%)  | 6 (3%)  | 0        | 100         | 100 |
| 1   | H     | 194/210 (92%)   | 187 (96%)  | 7 (4%)  | 0        | 100         | 100 |
| 1   | I     | 189/210 (90%)   | 185 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 1   | J     | 194/210 (92%)   | 186 (96%)  | 8 (4%)  | 0        | 100         | 100 |
| 1   | K     | 191/210 (91%)   | 186 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 1   | L     | 195/210 (93%)   | 189 (97%)  | 6 (3%)  | 0        | 100         | 100 |
| 1   | M     | 189/210 (90%)   | 184 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 1   | N     | 194/210 (92%)   | 186 (96%)  | 7 (4%)  | 1 (0%)   | 24          | 45  |
| 1   | O     | 194/210 (92%)   | 185 (95%)  | 7 (4%)  | 2 (1%)   | 12          | 28  |
| All | All   | 2901/3150 (92%) | 2799 (96%) | 98 (3%) | 4 (0%)   | 48          | 71  |

All (4) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 187 | CYS  |
| 1   | O     | 189 | PRO  |
| 1   | N     | 187 | CYS  |
| 1   | O     | 190 | GLU  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 185/196 (94%)   | 178 (96%)  | 7 (4%)   | 29          | 55 |
| 1   | B     | 185/196 (94%)   | 178 (96%)  | 7 (4%)   | 29          | 55 |
| 1   | C     | 185/196 (94%)   | 178 (96%)  | 7 (4%)   | 29          | 55 |
| 1   | D     | 184/196 (94%)   | 179 (97%)  | 5 (3%)   | 39          | 67 |
| 1   | E     | 185/196 (94%)   | 177 (96%)  | 8 (4%)   | 26          | 51 |
| 1   | F     | 188/196 (96%)   | 183 (97%)  | 5 (3%)   | 39          | 67 |
| 1   | G     | 186/196 (95%)   | 179 (96%)  | 7 (4%)   | 29          | 55 |
| 1   | H     | 185/196 (94%)   | 175 (95%)  | 10 (5%)  | 20          | 42 |
| 1   | I     | 182/196 (93%)   | 178 (98%)  | 4 (2%)   | 45          | 72 |
| 1   | J     | 185/196 (94%)   | 178 (96%)  | 7 (4%)   | 29          | 55 |
| 1   | K     | 183/196 (93%)   | 174 (95%)  | 9 (5%)   | 22          | 46 |
| 1   | L     | 186/196 (95%)   | 180 (97%)  | 6 (3%)   | 34          | 61 |
| 1   | M     | 182/196 (93%)   | 175 (96%)  | 7 (4%)   | 29          | 55 |
| 1   | N     | 185/196 (94%)   | 175 (95%)  | 10 (5%)  | 20          | 42 |
| 1   | O     | 185/196 (94%)   | 179 (97%)  | 6 (3%)   | 34          | 61 |
| All | All   | 2771/2940 (94%) | 2666 (96%) | 105 (4%) | 29          | 55 |

All (105) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 15  | ARG  |
| 1   | G     | 21  | THR  |
| 1   | G     | 25  | ARG  |
| 1   | G     | 31  | VAL  |
| 1   | G     | 62  | THR  |
| 1   | G     | 69  | HIS  |
| 1   | G     | 188 | CYS  |
| 1   | D     | 21  | THR  |
| 1   | D     | 23  | ARG  |
| 1   | D     | 56  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 57  | THR  |
| 1   | D     | 184 | THR  |
| 1   | E     | 21  | THR  |
| 1   | E     | 31  | VAL  |
| 1   | E     | 57  | THR  |
| 1   | E     | 120 | ARG  |
| 1   | E     | 132 | SER  |
| 1   | E     | 184 | THR  |
| 1   | E     | 186 | SER  |
| 1   | E     | 188 | CYS  |
| 1   | A     | 21  | THR  |
| 1   | A     | 57  | THR  |
| 1   | A     | 59  | SER  |
| 1   | A     | 148 | ARG  |
| 1   | A     | 184 | THR  |
| 1   | A     | 188 | CYS  |
| 1   | A     | 203 | LYS  |
| 1   | B     | 14  | SER  |
| 1   | B     | 21  | THR  |
| 1   | B     | 25  | ARG  |
| 1   | B     | 57  | THR  |
| 1   | B     | 69  | HIS  |
| 1   | B     | 186 | SER  |
| 1   | B     | 188 | CYS  |
| 1   | C     | 21  | THR  |
| 1   | C     | 25  | ARG  |
| 1   | C     | 129 | ASP  |
| 1   | C     | 185 | TYR  |
| 1   | C     | 186 | SER  |
| 1   | C     | 187 | CYS  |
| 1   | C     | 188 | CYS  |
| 1   | F     | 21  | THR  |
| 1   | F     | 25  | ARG  |
| 1   | F     | 57  | THR  |
| 1   | F     | 185 | TYR  |
| 1   | F     | 188 | CYS  |
| 1   | H     | 21  | THR  |
| 1   | H     | 23  | ARG  |
| 1   | H     | 31  | VAL  |
| 1   | H     | 57  | THR  |
| 1   | H     | 61  | ARG  |
| 1   | H     | 120 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 179 | LYS  |
| 1   | H     | 182 | SER  |
| 1   | H     | 184 | THR  |
| 1   | H     | 188 | CYS  |
| 1   | I     | 21  | THR  |
| 1   | I     | 25  | ARG  |
| 1   | I     | 57  | THR  |
| 1   | I     | 185 | TYR  |
| 1   | J     | 21  | THR  |
| 1   | J     | 25  | ARG  |
| 1   | J     | 31  | VAL  |
| 1   | J     | 57  | THR  |
| 1   | J     | 61  | ARG  |
| 1   | J     | 131 | GLU  |
| 1   | J     | 188 | CYS  |
| 1   | K     | 11  | ARG  |
| 1   | K     | 21  | THR  |
| 1   | K     | 25  | ARG  |
| 1   | K     | 57  | THR  |
| 1   | K     | 69  | HIS  |
| 1   | K     | 179 | LYS  |
| 1   | K     | 184 | THR  |
| 1   | K     | 186 | SER  |
| 1   | K     | 188 | CYS  |
| 1   | L     | 15  | ARG  |
| 1   | L     | 21  | THR  |
| 1   | L     | 31  | VAL  |
| 1   | L     | 57  | THR  |
| 1   | L     | 186 | SER  |
| 1   | L     | 188 | CYS  |
| 1   | M     | 15  | ARG  |
| 1   | M     | 23  | ARG  |
| 1   | M     | 41  | VAL  |
| 1   | M     | 57  | THR  |
| 1   | M     | 62  | THR  |
| 1   | M     | 69  | HIS  |
| 1   | M     | 120 | ARG  |
| 1   | N     | 21  | THR  |
| 1   | N     | 25  | ARG  |
| 1   | N     | 31  | VAL  |
| 1   | N     | 44  | ILE  |
| 1   | N     | 139 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | N     | 185 | TYR  |
| 1   | N     | 186 | SER  |
| 1   | N     | 187 | CYS  |
| 1   | N     | 188 | CYS  |
| 1   | N     | 202 | ARG  |
| 1   | O     | 21  | THR  |
| 1   | O     | 57  | THR  |
| 1   | O     | 61  | ARG  |
| 1   | O     | 120 | ARG  |
| 1   | O     | 188 | CYS  |
| 1   | O     | 190 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 119 | GLN  |
| 1   | D     | 167 | GLN  |
| 1   | E     | 9   | ASN  |
| 1   | A     | 54  | GLN  |
| 1   | C     | 9   | ASN  |
| 1   | I     | 9   | ASN  |
| 1   | J     | 54  | GLN  |

### 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 53 ligands modelled in this entry, 4 are monoatomic - leaving 49 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 |
| 4   | SO4  | M     | 302 | -    | 4,4,4        | 0.25 | 0        | 6,6,6       | 0.14 | 0        |
| 2   | 1PE  | I     | 302 | -    | 15,15,15     | 0.88 | 0        | 14,14,14    | 1.10 | 2 (14%)  |
| 3   | NAG  | D     | 302 | 1    | 14,14,15     | 2.18 | 2 (14%)  | 17,19,21    | 2.06 | 5 (29%)  |
| 4   | SO4  | D     | 305 | -    | 4,4,4        | 0.24 | 0        | 6,6,6       | 0.15 | 0        |
| 5   | ACT  | G     | 308 | -    | 3,3,3        | 0.76 | 0        | 3,3,3       | 1.08 | 0        |
| 2   | 1PE  | G     | 301 | -    | 15,15,15     | 0.60 | 0        | 14,14,14    | 1.35 | 2 (14%)  |
| 5   | ACT  | A     | 305 | -    | 3,3,3        | 0.82 | 0        | 3,3,3       | 1.01 | 0        |
| 4   | SO4  | E     | 303 | -    | 4,4,4        | 0.25 | 0        | 6,6,6       | 0.27 | 0        |
| 4   | SO4  | F     | 301 | -    | 4,4,4        | 0.23 | 0        | 6,6,6       | 0.27 | 0        |
| 4   | SO4  | G     | 304 | -    | 4,4,4        | 0.24 | 0        | 6,6,6       | 0.16 | 0        |
| 4   | SO4  | E     | 305 | -    | 4,4,4        | 0.29 | 0        | 6,6,6       | 0.09 | 0        |
| 4   | SO4  | E     | 306 | -    | 4,4,4        | 0.30 | 0        | 6,6,6       | 0.15 | 0        |
| 4   | SO4  | B     | 303 | -    | 4,4,4        | 0.26 | 0        | 6,6,6       | 0.21 | 0        |
| 4   | SO4  | A     | 304 | -    | 4,4,4        | 0.30 | 0        | 6,6,6       | 0.08 | 0        |
| 4   | SO4  | A     | 303 | -    | 4,4,4        | 0.24 | 0        | 6,6,6       | 0.25 | 0        |
| 5   | ACT  | F     | 306 | -    | 3,3,3        | 0.78 | 0        | 3,3,3       | 0.85 | 0        |
| 5   | ACT  | A     | 307 | -    | 3,3,3        | 0.82 | 0        | 3,3,3       | 0.83 | 0        |
| 4   | SO4  | I     | 303 | -    | 4,4,4        | 0.27 | 0        | 6,6,6       | 0.05 | 0        |
| 2   | 1PE  | D     | 301 | -    | 15,15,15     | 0.84 | 0        | 14,14,14    | 1.14 | 1 (7%)   |
| 5   | ACT  | F     | 305 | -    | 3,3,3        | 0.74 | 0        | 3,3,3       | 0.98 | 0        |
| 4   | SO4  | E     | 307 | -    | 4,4,4        | 0.29 | 0        | 6,6,6       | 0.22 | 0        |
| 4   | SO4  | E     | 304 | -    | 4,4,4        | 0.30 | 0        | 6,6,6       | 0.31 | 0        |
| 2   | 1PE  | A     | 302 | -    | 15,15,15     | 0.77 | 0        | 14,14,14    | 1.15 | 2 (14%)  |
| 6   | NSE  | I     | 301 | -    | 21,21,21     | 0.87 | 0        | 28,28,28    | 1.41 | 4 (14%)  |
| 5   | ACT  | D     | 304 | -    | 3,3,3        | 0.79 | 0        | 3,3,3       | 0.78 | 0        |
| 2   | 1PE  | E     | 302 | -    | 15,15,15     | 0.73 | 0        | 14,14,14    | 1.98 | 3 (21%)  |
| 5   | ACT  | O     | 301 | -    | 3,3,3        | 0.84 | 0        | 3,3,3       | 0.70 | 0        |
| 6   | NSE  | K     | 301 | -    | 21,21,21     | 0.71 | 0        | 28,28,28    | 1.69 | 7 (25%)  |
| 6   | NSE  | M     | 301 | -    | 21,21,21     | 0.71 | 0        | 28,28,28    | 0.72 | 0        |
| 2   | 1PE  | H     | 301 | -    | 15,15,15     | 0.82 | 0        | 14,14,14    | 1.29 | 2 (14%)  |
| 8   | GOL  | J     | 303 | -    | 5,5,5        | 0.35 | 0        | 5,5,5       | 0.47 | 0        |
| 4   | SO4  | J     | 301 | -    | 4,4,4        | 0.24 | 0        | 6,6,6       | 0.21 | 0        |
| 5   | ACT  | G     | 307 | -    | 3,3,3        | 0.79 | 0        | 3,3,3       | 1.04 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 5   | ACT  | F     | 303 | -    | 3,3,3        | 0.73 | 0        | 3,3,3       | 0.96 | 0        |
| 5   | ACT  | G     | 306 | -    | 3,3,3        | 0.89 | 0        | 3,3,3       | 0.65 | 0        |
| 2   | 1PE  | B     | 302 | -    | 15,15,15     | 0.76 | 0        | 14,14,14    | 1.92 | 4 (28%)  |
| 6   | NSE  | B     | 301 | -    | 21,21,21     | 0.93 | 1 (4%)   | 28,28,28    | 0.95 | 1 (3%)   |
| 4   | SO4  | C     | 302 | -    | 4,4,4        | 0.26 | 0        | 6,6,6       | 0.11 | 0        |
| 6   | NSE  | A     | 301 | -    | 21,21,21     | 0.70 | 0        | 28,28,28    | 1.67 | 5 (17%)  |
| 2   | 1PE  | C     | 301 | -    | 15,15,15     | 1.03 | 0        | 14,14,14    | 1.36 | 3 (21%)  |
| 5   | ACT  | J     | 302 | -    | 3,3,3        | 1.08 | 0        | 3,3,3       | 0.72 | 0        |
| 4   | SO4  | D     | 303 | -    | 4,4,4        | 0.38 | 0        | 6,6,6       | 0.26 | 0        |
| 6   | NSE  | E     | 301 | -    | 21,21,21     | 0.83 | 0        | 28,28,28    | 0.97 | 1 (3%)   |
| 4   | SO4  | F     | 302 | -    | 4,4,4        | 0.26 | 0        | 6,6,6       | 0.32 | 0        |
| 4   | SO4  | B     | 304 | -    | 4,4,4        | 0.31 | 0        | 6,6,6       | 0.24 | 0        |
| 3   | NAG  | G     | 302 | 1    | 14,14,15     | 4.33 | 7 (50%)  | 17,19,21    | 3.93 | 12 (70%) |
| 4   | SO4  | G     | 303 | -    | 4,4,4        | 0.30 | 0        | 6,6,6       | 0.16 | 0        |
| 5   | ACT  | F     | 304 | -    | 3,3,3        | 0.83 | 0        | 3,3,3       | 0.78 | 0        |
| 4   | SO4  | G     | 305 | -    | 4,4,4        | 0.32 | 0        | 6,6,6       | 0.26 | 0        |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 2   | 1PE  | D     | 301 | -    | -       | 1/13/13/13 | -       |
| 6   | NSE  | E     | 301 | -    | -       | 3/10/10/10 | 0/3/3/3 |
| 2   | 1PE  | I     | 302 | -    | -       | 3/13/13/13 | -       |
| 3   | NAG  | D     | 302 | 1    | -       | 2/6/23/26  | 0/1/1/1 |
| 8   | GOL  | J     | 303 | -    | -       | 3/4/4/4    | -       |
| 2   | 1PE  | G     | 301 | -    | -       | 1/13/13/13 | -       |
| 2   | 1PE  | A     | 302 | -    | -       | 3/13/13/13 | -       |
| 3   | NAG  | G     | 302 | 1    | -       | 2/6/23/26  | 0/1/1/1 |
| 6   | NSE  | I     | 301 | -    | -       | 4/10/10/10 | 0/3/3/3 |
| 2   | 1PE  | E     | 302 | -    | -       | 4/13/13/13 | -       |
| 2   | 1PE  | B     | 302 | -    | -       | 5/13/13/13 | -       |
| 6   | NSE  | B     | 301 | -    | -       | 3/10/10/10 | 0/3/3/3 |
| 6   | NSE  | K     | 301 | -    | -       | 4/10/10/10 | 0/3/3/3 |
| 6   | NSE  | A     | 301 | -    | -       | 4/10/10/10 | 0/3/3/3 |
| 6   | NSE  | M     | 301 | -    | -       | 0/10/10/10 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings |
|-----|------|-------|-----|------|---------|------------|-------|
| 2   | 1PE  | C     | 301 | -    | -       | 5/13/13/13 | -     |
| 2   | 1PE  | H     | 301 | -    | -       | 3/13/13/13 | -     |

All (10) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 3   | G     | 302 | NAG  | C1-C2 | -10.96 | 1.37        | 1.52     |
| 3   | G     | 302 | NAG  | C8-C7 | 8.20   | 1.67        | 1.50     |
| 3   | G     | 302 | NAG  | O7-C7 | -5.96  | 1.09        | 1.23     |
| 3   | D     | 302 | NAG  | C1-C2 | 5.76   | 1.60        | 1.52     |
| 3   | D     | 302 | NAG  | C2-N2 | 5.02   | 1.54        | 1.46     |
| 3   | G     | 302 | NAG  | C2-N2 | -3.85  | 1.39        | 1.46     |
| 3   | G     | 302 | NAG  | C7-N2 | 2.92   | 1.43        | 1.34     |
| 3   | G     | 302 | NAG  | C3-C2 | -2.36  | 1.47        | 1.52     |
| 3   | G     | 302 | NAG  | C4-C3 | -2.21  | 1.46        | 1.52     |
| 6   | B     | 301 | NSE  | O1-C7 | 2.10   | 1.36        | 1.34     |

All (54) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | G     | 302 | NAG  | C1-O5-C5    | 7.38  | 122.08      | 112.19   |
| 3   | G     | 302 | NAG  | C2-N2-C7    | 7.08  | 132.39      | 122.90   |
| 3   | G     | 302 | NAG  | O7-C7-N2    | -6.43 | 110.61      | 121.98   |
| 6   | A     | 301 | NSE  | C9-C11-N3   | 5.89  | 127.25      | 122.22   |
| 3   | D     | 302 | NAG  | O5-C1-C2    | -5.60 | 102.63      | 111.29   |
| 3   | G     | 302 | NAG  | O5-C1-C2    | -5.04 | 103.49      | 111.29   |
| 6   | K     | 301 | NSE  | C9-C11-N3   | 4.59  | 126.13      | 122.22   |
| 3   | D     | 302 | NAG  | C1-O5-C5    | 4.29  | 117.93      | 112.19   |
| 3   | G     | 302 | NAG  | O5-C5-C4    | 3.94  | 120.42      | 110.83   |
| 2   | E     | 302 | 1PE  | C26-OH6-C15 | 3.90  | 130.33      | 113.26   |
| 2   | E     | 302 | 1PE  | OH6-C26-C16 | 3.85  | 127.08      | 110.11   |
| 3   | G     | 302 | NAG  | O3-C3-C4    | -3.78 | 101.47      | 110.38   |
| 2   | B     | 302 | 1PE  | OH3-C23-C13 | 3.77  | 127.53      | 110.35   |
| 2   | E     | 302 | 1PE  | C25-OH5-C14 | -3.54 | 97.76       | 113.26   |
| 3   | G     | 302 | NAG  | C6-C5-C4    | 3.42  | 121.43      | 113.02   |
| 3   | G     | 302 | NAG  | C1-C2-N2    | -3.25 | 105.31      | 110.43   |
| 6   | K     | 301 | NSE  | C5-C8-C7    | -3.22 | 114.66      | 120.04   |
| 2   | B     | 302 | 1PE  | OH6-C26-C16 | 3.20  | 124.23      | 110.11   |
| 3   | G     | 302 | NAG  | O5-C5-C6    | 3.17  | 113.84      | 107.66   |
| 6   | I     | 301 | NSE  | C9-C11-N3   | 3.16  | 124.91      | 122.22   |
| 2   | G     | 301 | 1PE  | OH3-C23-C13 | -2.98 | 96.78       | 110.35   |
| 2   | A     | 302 | 1PE  | OH3-C23-C13 | -2.90 | 97.15       | 110.35   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | G     | 302 | NAG  | O6-C6-C5    | 2.80  | 120.88      | 111.33   |
| 2   | D     | 301 | 1PE  | OH6-C15-C25 | -2.77 | 97.73       | 110.35   |
| 6   | I     | 301 | NSE  | C10-C9-C11  | -2.76 | 117.47      | 121.00   |
| 2   | B     | 302 | 1PE  | C23-OH3-C22 | 2.69  | 125.05      | 113.26   |
| 6   | K     | 301 | NSE  | O1-C7-C8    | 2.67  | 123.52      | 117.89   |
| 2   | C     | 301 | 1PE  | OH6-C15-C25 | -2.66 | 98.24       | 110.35   |
| 6   | K     | 301 | NSE  | C6-C8-C7    | 2.64  | 124.56      | 120.56   |
| 2   | I     | 302 | 1PE  | OH4-C24-C14 | -2.61 | 98.47       | 110.35   |
| 6   | A     | 301 | NSE  | C5-C8-C7    | -2.60 | 115.69      | 120.04   |
| 2   | C     | 301 | 1PE  | OH3-C23-C13 | 2.55  | 121.98      | 110.35   |
| 2   | B     | 302 | 1PE  | OH3-C22-C12 | 2.54  | 121.31      | 110.11   |
| 2   | I     | 302 | 1PE  | OH6-C15-C25 | 2.50  | 121.77      | 110.35   |
| 3   | G     | 302 | NAG  | C3-C4-C5    | -2.43 | 105.82      | 110.23   |
| 2   | H     | 301 | 1PE  | OH3-C22-C12 | 2.39  | 120.63      | 110.11   |
| 3   | D     | 302 | NAG  | C1-C2-N2    | -2.38 | 106.69      | 110.43   |
| 2   | H     | 301 | 1PE  | OH4-C13-C23 | 2.37  | 121.17      | 110.35   |
| 3   | D     | 302 | NAG  | C4-C3-C2    | -2.33 | 107.61      | 111.02   |
| 6   | K     | 301 | NSE  | C5-C3-C4    | -2.32 | 116.42      | 119.55   |
| 6   | A     | 301 | NSE  | C9-C11-N2   | -2.29 | 118.92      | 122.92   |
| 3   | D     | 302 | NAG  | O5-C5-C4    | -2.24 | 105.39      | 110.83   |
| 6   | A     | 301 | NSE  | O1-C7-C8    | 2.20  | 122.53      | 117.89   |
| 2   | C     | 301 | 1PE  | OH6-C26-C16 | -2.20 | 100.44      | 110.11   |
| 6   | K     | 301 | NSE  | C8-C7-N2    | -2.19 | 123.04      | 127.80   |
| 6   | A     | 301 | NSE  | C2-C6-C8    | -2.18 | 118.22      | 120.36   |
| 2   | G     | 301 | 1PE  | OH6-C15-C25 | 2.17  | 120.23      | 110.35   |
| 2   | A     | 302 | 1PE  | OH6-C26-C16 | 2.16  | 119.62      | 110.11   |
| 6   | B     | 301 | NSE  | C13-C12-C9  | -2.14 | 118.26      | 120.36   |
| 3   | G     | 302 | NAG  | O4-C4-C3    | -2.12 | 105.38      | 110.38   |
| 6   | I     | 301 | NSE  | C13-C12-C9  | -2.12 | 118.28      | 120.36   |
| 6   | E     | 301 | NSE  | O1-N3-C11   | 2.08  | 104.50      | 103.28   |
| 6   | I     | 301 | NSE  | C6-C8-C5    | 2.04  | 121.60      | 119.25   |
| 6   | K     | 301 | NSE  | C1-C3-C4    | 2.00  | 123.24      | 119.97   |

There are no chirality outliers.

All (50) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 6   | A     | 301 | NSE  | N3-C11-C9-C12 |
| 6   | I     | 301 | NSE  | O1-C7-C8-C5   |
| 6   | I     | 301 | NSE  | O1-C7-C8-C6   |
| 3   | G     | 302 | NAG  | O7-C7-N2-C2   |
| 3   | G     | 302 | NAG  | O5-C5-C6-O6   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | D     | 302 | NAG  | O5-C5-C6-O6     |
| 2   | E     | 302 | 1PE  | C14-C24-OH4-C13 |
| 3   | D     | 302 | NAG  | C4-C5-C6-O6     |
| 6   | A     | 301 | NSE  | N2-C11-C9-C12   |
| 6   | I     | 301 | NSE  | N2-C7-C8-C6     |
| 2   | B     | 302 | 1PE  | C15-C25-OH5-C14 |
| 6   | I     | 301 | NSE  | N2-C7-C8-C5     |
| 8   | J     | 303 | GOL  | O1-C1-C2-C3     |
| 8   | J     | 303 | GOL  | C1-C2-C3-O3     |
| 6   | A     | 301 | NSE  | N3-C11-C9-C10   |
| 2   | E     | 302 | 1PE  | C25-C15-OH6-C26 |
| 2   | A     | 302 | 1PE  | C15-C25-OH5-C14 |
| 6   | K     | 301 | NSE  | O1-C7-C8-C6     |
| 6   | A     | 301 | NSE  | N2-C11-C9-C10   |
| 2   | B     | 302 | 1PE  | C16-C26-OH6-C15 |
| 2   | I     | 302 | 1PE  | C13-C23-OH3-C22 |
| 6   | K     | 301 | NSE  | N2-C7-C8-C6     |
| 2   | H     | 301 | 1PE  | C16-C26-OH6-C15 |
| 8   | J     | 303 | GOL  | O2-C2-C3-O3     |
| 2   | I     | 302 | 1PE  | C25-C15-OH6-C26 |
| 6   | K     | 301 | NSE  | N2-C7-C8-C5     |
| 2   | C     | 301 | 1PE  | C13-C23-OH3-C22 |
| 6   | E     | 301 | NSE  | N2-C7-C8-C6     |
| 6   | B     | 301 | NSE  | N2-C7-C8-C6     |
| 2   | G     | 301 | 1PE  | C25-C15-OH6-C26 |
| 2   | A     | 302 | 1PE  | C16-C26-OH6-C15 |
| 2   | B     | 302 | 1PE  | C12-C22-OH3-C23 |
| 2   | C     | 301 | 1PE  | C12-C22-OH3-C23 |
| 2   | C     | 301 | 1PE  | C23-C13-OH4-C24 |
| 2   | E     | 302 | 1PE  | C24-C14-OH5-C25 |
| 6   | K     | 301 | NSE  | O1-C7-C8-C5     |
| 6   | E     | 301 | NSE  | N2-C7-C8-C5     |
| 6   | B     | 301 | NSE  | N2-C7-C8-C5     |
| 2   | B     | 302 | 1PE  | C13-C23-OH3-C22 |
| 2   | B     | 302 | 1PE  | OH6-C15-C25-OH5 |
| 2   | H     | 301 | 1PE  | OH6-C15-C25-OH5 |
| 2   | D     | 301 | 1PE  | OH4-C13-C23-OH3 |
| 2   | A     | 302 | 1PE  | OH6-C15-C25-OH5 |
| 2   | C     | 301 | 1PE  | OH4-C13-C23-OH3 |
| 6   | E     | 301 | NSE  | O1-C7-C8-C6     |
| 6   | B     | 301 | NSE  | O1-C7-C8-C6     |
| 2   | I     | 302 | 1PE  | OH4-C13-C23-OH3 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | H     | 301 | 1PE  | C15-C25-OH5-C14 |
| 2   | E     | 302 | 1PE  | OH5-C14-C24-OH4 |
| 2   | C     | 301 | 1PE  | C14-C24-OH4-C13 |

There are no ring outliers.

17 monomers are involved in 30 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | I     | 302 | 1PE  | 5       | 0            |
| 2   | G     | 301 | 1PE  | 1       | 0            |
| 4   | B     | 303 | SO4  | 1       | 0            |
| 4   | A     | 303 | SO4  | 1       | 0            |
| 5   | F     | 306 | ACT  | 1       | 0            |
| 2   | D     | 301 | 1PE  | 3       | 0            |
| 4   | E     | 307 | SO4  | 1       | 0            |
| 6   | I     | 301 | NSE  | 1       | 0            |
| 2   | E     | 302 | 1PE  | 2       | 0            |
| 6   | K     | 301 | NSE  | 2       | 0            |
| 6   | M     | 301 | NSE  | 2       | 0            |
| 2   | H     | 301 | 1PE  | 3       | 0            |
| 4   | J     | 301 | SO4  | 1       | 0            |
| 2   | B     | 302 | 1PE  | 2       | 0            |
| 6   | A     | 301 | NSE  | 2       | 0            |
| 2   | C     | 301 | 1PE  | 1       | 0            |
| 6   | E     | 301 | NSE  | 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     | 198/210 (94%)   | -1.61  | 0 100 100 | 28, 45, 79, 97        | 0      |
| 1   | B     | 198/210 (94%)   | -1.58  | 0 100 100 | 33, 51, 87, 102       | 0      |
| 1   | C     | 198/210 (94%)   | -1.56  | 0 100 100 | 34, 51, 82, 101       | 0      |
| 1   | D     | 197/210 (93%)   | -1.62  | 0 100 100 | 30, 47, 76, 99        | 0      |
| 1   | E     | 198/210 (94%)   | -1.61  | 0 100 100 | 29, 47, 81, 99        | 0      |
| 1   | F     | 200/210 (95%)   | -1.64  | 0 100 100 | 25, 42, 78, 95        | 1 (0%) |
| 1   | G     | 198/210 (94%)   | -1.63  | 0 100 100 | 27, 46, 79, 102       | 1 (0%) |
| 1   | H     | 198/210 (94%)   | -1.58  | 0 100 100 | 29, 50, 82, 103       | 0      |
| 1   | I     | 195/210 (92%)   | -1.53  | 0 100 100 | 37, 56, 84, 106       | 0      |
| 1   | J     | 198/210 (94%)   | -1.59  | 0 100 100 | 32, 50, 74, 96        | 0      |
| 1   | K     | 197/210 (93%)   | -1.55  | 0 100 100 | 31, 54, 78, 88        | 0      |
| 1   | L     | 198/210 (94%)   | -1.59  | 0 100 100 | 26, 48, 77, 99        | 1 (0%) |
| 1   | M     | 194/210 (92%)   | -1.53  | 0 100 100 | 33, 56, 80, 107       | 1 (0%) |
| 1   | N     | 198/210 (94%)   | -1.49  | 0 100 100 | 38, 64, 89, 112       | 0      |
| 1   | O     | 198/210 (94%)   | -1.52  | 0 100 100 | 41, 58, 83, 98        | 0      |
| All | All   | 2963/3150 (94%) | -1.58  | 0 100 100 | 25, 51, 83, 112       | 4 (0%) |

There are no RSRZ outliers to report.

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

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

### 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 3   | NAG  | G     | 302 | 14/15 | 0.96 | 0.07 | 93,103,106,109             | 0     |
| 4   | SO4  | J     | 301 | 5/5   | 0.96 | 0.06 | 88,90,97,112               | 0     |
| 4   | SO4  | M     | 302 | 5/5   | 0.96 | 0.09 | 80,82,96,100               | 0     |
| 5   | ACT  | G     | 307 | 4/4   | 0.96 | 0.07 | 58,61,70,73                | 0     |
| 5   | ACT  | A     | 305 | 4/4   | 0.96 | 0.06 | 47,60,61,61                | 0     |
| 5   | ACT  | F     | 304 | 4/4   | 0.96 | 0.05 | 36,51,56,68                | 0     |
| 5   | ACT  | F     | 306 | 4/4   | 0.96 | 0.06 | 45,52,57,58                | 0     |
| 8   | GOL  | J     | 303 | 6/6   | 0.96 | 0.09 | 64,75,83,86                | 0     |
| 4   | SO4  | D     | 305 | 5/5   | 0.97 | 0.07 | 75,85,105,110              | 0     |
| 5   | ACT  | D     | 304 | 4/4   | 0.97 | 0.07 | 62,63,63,72                | 0     |
| 4   | SO4  | E     | 306 | 5/5   | 0.97 | 0.05 | 82,85,104,121              | 0     |
| 4   | SO4  | F     | 301 | 5/5   | 0.98 | 0.04 | 67,71,76,78                | 0     |
| 4   | SO4  | I     | 303 | 5/5   | 0.98 | 0.03 | 95,97,105,111              | 0     |
| 4   | SO4  | G     | 305 | 5/5   | 0.98 | 0.07 | 64,81,87,93                | 0     |
| 3   | NAG  | D     | 302 | 14/15 | 0.98 | 0.04 | 80,85,91,92                | 0     |
| 5   | ACT  | G     | 306 | 4/4   | 0.98 | 0.05 | 48,52,60,62                | 0     |
| 4   | SO4  | E     | 305 | 5/5   | 0.98 | 0.05 | 79,79,90,94                | 0     |
| 4   | SO4  | G     | 304 | 5/5   | 0.98 | 0.04 | 87,91,106,110              | 0     |
| 4   | SO4  | E     | 307 | 5/5   | 0.98 | 0.03 | 76,82,96,96                | 0     |
| 5   | ACT  | A     | 307 | 4/4   | 0.98 | 0.04 | 43,66,70,71                | 0     |
| 5   | ACT  | F     | 303 | 4/4   | 0.98 | 0.06 | 59,62,64,69                | 0     |
| 4   | SO4  | A     | 304 | 5/5   | 0.98 | 0.05 | 78,80,93,104               | 0     |
| 5   | ACT  | F     | 305 | 4/4   | 0.98 | 0.06 | 51,60,67,69                | 0     |
| 4   | SO4  | B     | 303 | 5/5   | 0.98 | 0.03 | 86,87,91,101               | 0     |
| 6   | NSE  | M     | 301 | 19/19 | 0.98 | 0.05 | 61,74,79,80                | 0     |
| 7   | CL   | A     | 306 | 1/1   | 0.98 | 0.08 | 86,86,86,86                | 0     |
| 7   | CL   | K     | 302 | 1/1   | 0.98 | 0.04 | 69,69,69,69                | 0     |
| 7   | CL   | L     | 301 | 1/1   | 0.98 | 0.04 | 60,60,60,60                | 0     |
| 4   | SO4  | C     | 302 | 5/5   | 0.98 | 0.04 | 84,85,107,110              | 0     |
| 2   | 1PE  | B     | 302 | 16/16 | 0.99 | 0.05 | 47,57,64,69                | 0     |
| 4   | SO4  | E     | 303 | 5/5   | 0.99 | 0.03 | 58,60,66,74                | 0     |
| 4   | SO4  | E     | 304 | 5/5   | 0.99 | 0.04 | 64,67,85,94                | 0     |
| 5   | ACT  | G     | 308 | 4/4   | 0.99 | 0.04 | 44,44,58,59                | 0     |
| 2   | 1PE  | C     | 301 | 16/16 | 0.99 | 0.04 | 49,57,61,63                | 0     |
| 2   | 1PE  | H     | 301 | 16/16 | 0.99 | 0.04 | 38,46,58,62                | 0     |
| 2   | 1PE  | I     | 302 | 16/16 | 0.99 | 0.04 | 46,59,67,69                | 0     |
| 4   | SO4  | A     | 303 | 5/5   | 0.99 | 0.03 | 71,75,77,79                | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | 1PE  | G     | 301 | 16/16 | 0.99 | 0.04 | 33,34,35,35                 | 16    |
| 2   | 1PE  | D     | 301 | 16/16 | 0.99 | 0.04 | 47,55,67,70                 | 0     |
| 4   | SO4  | B     | 304 | 5/5   | 0.99 | 0.04 | 54,61,89,90                 | 0     |
| 5   | ACT  | J     | 302 | 4/4   | 0.99 | 0.05 | 34,35,41,55                 | 0     |
| 5   | ACT  | O     | 301 | 4/4   | 0.99 | 0.04 | 37,43,45,49                 | 0     |
| 6   | NSE  | E     | 301 | 19/19 | 0.99 | 0.04 | 45,57,74,75                 | 0     |
| 6   | NSE  | A     | 301 | 19/19 | 0.99 | 0.04 | 50,58,68,69                 | 0     |
| 6   | NSE  | B     | 301 | 19/19 | 0.99 | 0.04 | 54,67,78,78                 | 0     |
| 6   | NSE  | I     | 301 | 19/19 | 0.99 | 0.05 | 60,70,78,80                 | 0     |
| 6   | NSE  | K     | 301 | 19/19 | 0.99 | 0.04 | 51,58,68,68                 | 0     |
| 4   | SO4  | G     | 303 | 5/5   | 0.99 | 0.03 | 63,64,79,83                 | 0     |
| 2   | 1PE  | E     | 302 | 16/16 | 0.99 | 0.05 | 46,55,63,64                 | 0     |
| 4   | SO4  | F     | 302 | 5/5   | 0.99 | 0.10 | 64,69,75,106                | 0     |
| 2   | 1PE  | A     | 302 | 16/16 | 0.99 | 0.04 | 36,48,56,62                 | 0     |
| 7   | CL   | N     | 301 | 1/1   | 0.99 | 0.02 | 54,54,54,54                 | 0     |
| 4   | SO4  | D     | 303 | 5/5   | 0.99 | 0.08 | 56,61,72,92                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.