



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:59 AM GMT

PDB ID : 2VAT  
Title : CRYSTAL STRUCTURE OF DEACETYLCEPHALOSPORIN C ACETYL-TRANSFERASE IN COMPLEX WITH COENZYME A  
Authors : Lejon, S.; Ellis, J.; Valegard, K.  
Deposited on : 2007-09-04  
Resolution : 2.20 Å(reported)

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

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

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

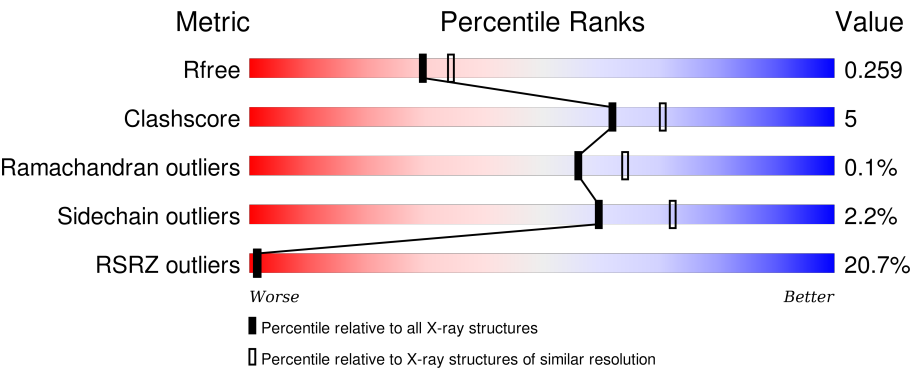
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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 <sub>free</sub>     | 91344                       | 3774 (2.20-2.20)                                      |
| Clashscore            | 102246                      | 4477 (2.20-2.20)                                      |
| Ramachandran outliers | 100387                      | 4404 (2.20-2.20)                                      |
| Sidechain outliers    | 100360                      | 4405 (2.20-2.20)                                      |
| RSRZ outliers         | 91569                       | 3781 (2.20-2.20)                                      |

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

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | A     | 444    | <div><div>3%</div><div></div><div>68%</div><div>10%</div><div>22%</div></div> |
| 1   | B     | 444    | <div><div>8%</div><div></div><div>71%</div><div>7%</div><div>22%</div></div>  |
| 1   | C     | 444    | <div><div>11%</div><div></div><div>69%</div><div>7%</div><div>22%</div></div> |
| 1   | D     | 444    | <div><div>8%</div><div></div><div>70%</div><div>6%</div><div>22%</div></div>  |
| 1   | E     | 444    | <div><div>3%</div><div></div><div>70%</div><div>7%</div><div>22%</div></div>  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | F     | 444    |                  |
| 1   | G     | 444    |                  |
| 1   | H     | 444    |                  |
| 1   | I     | 444    |                  |
| 1   | J     | 444    |                  |
| 1   | K     | 444    |                  |
| 1   | L     | 444    |                  |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 2   | COA  | B     | 1383 | -         | -        | -       | X                |
| 2   | COA  | C     | 1383 | -         | -        | -       | X                |
| 2   | COA  | D     | 1383 | -         | -        | -       | X                |
| 2   | COA  | F     | 1383 | -         | -        | -       | X                |
| 2   | COA  | G     | 1383 | -         | -        | -       | X                |
| 2   | COA  | L     | 1383 | -         | -        | -       | X                |
| 3   | ACT  | A     | 1384 | -         | -        | -       | X                |
| 3   | ACT  | C     | 1384 | -         | -        | -       | X                |
| 3   | ACT  | D     | 1384 | -         | -        | -       | X                |
| 3   | ACT  | F     | 1384 | -         | -        | -       | X                |
| 3   | ACT  | H     | 1384 | -         | -        | X       | -                |
| 3   | ACT  | I     | 1385 | -         | -        | -       | X                |
| 3   | ACT  | K     | 1386 | -         | -        | X       | -                |
| 4   | GOL  | B     | 1384 | -         | -        | -       | X                |
| 4   | GOL  | I     | 1384 | -         | -        | -       | X                |

## 2 Entry composition

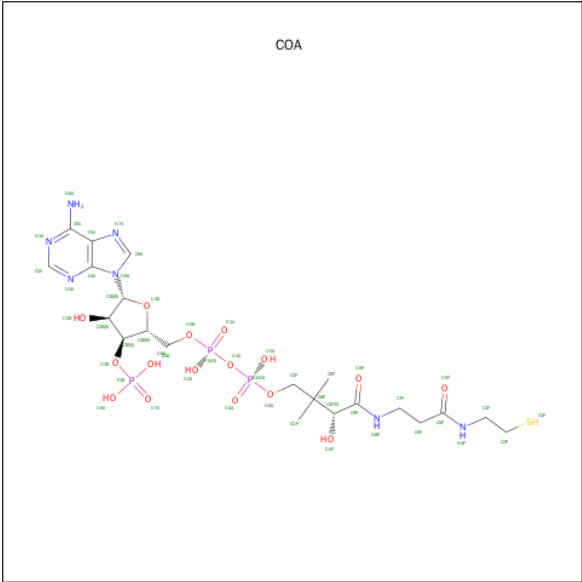
There are 5 unique types of molecules in this entry. The entry contains 35013 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 347      | Total | C    | N   | O   | S  | 0       | 4       | 0     |
|     |       |          | 2744  | 1731 | 485 | 509 | 19 |         |         |       |
| 1   | B     | 347      | Total | C    | N   | O   | S  | 0       | 3       | 0     |
|     |       |          | 2744  | 1731 | 488 | 506 | 19 |         |         |       |
| 1   | C     | 345      | Total | C    | N   | O   | S  | 0       | 4       | 0     |
|     |       |          | 2745  | 1730 | 488 | 508 | 19 |         |         |       |
| 1   | D     | 345      | Total | C    | N   | O   | S  | 0       | 4       | 0     |
|     |       |          | 2748  | 1732 | 488 | 509 | 19 |         |         |       |
| 1   | E     | 346      | Total | C    | N   | O   | S  | 0       | 5       | 0     |
|     |       |          | 2744  | 1732 | 487 | 506 | 19 |         |         |       |
| 1   | F     | 342      | Total | C    | N   | O   | S  | 0       | 2       | 0     |
|     |       |          | 2694  | 1700 | 474 | 501 | 19 |         |         |       |
| 1   | G     | 342      | Total | C    | N   | O   | S  | 0       | 6       | 0     |
|     |       |          | 2733  | 1724 | 484 | 506 | 19 |         |         |       |
| 1   | H     | 345      | Total | C    | N   | O   | S  | 0       | 8       | 0     |
|     |       |          | 2760  | 1741 | 492 | 508 | 19 |         |         |       |
| 1   | I     | 347      | Total | C    | N   | O   | S  | 0       | 3       | 0     |
|     |       |          | 2739  | 1728 | 485 | 507 | 19 |         |         |       |
| 1   | J     | 344      | Total | C    | N   | O   | S  | 0       | 4       | 0     |
|     |       |          | 2724  | 1719 | 482 | 504 | 19 |         |         |       |
| 1   | K     | 344      | Total | C    | N   | O   | S  | 0       | 5       | 0     |
|     |       |          | 2732  | 1724 | 485 | 504 | 19 |         |         |       |
| 1   | L     | 341      | Total | C    | N   | O   | S  | 0       | 3       | 0     |
|     |       |          | 2697  | 1702 | 476 | 500 | 19 |         |         |       |

- Molecule 2 is COENZYME A (three-letter code: COA) (formula:  $C_{21}H_{36}N_7O_{16}P_3S$ ).



| Mol | Chain | Residues | Atoms |    |   |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---|---------|---------|
| 2   | A     | 1        | Total | C  | N | O  | P | S | 0       | 0       |
|     |       |          | 48    | 21 | 7 | 16 | 3 | 1 |         |         |
| 2   | B     | 1        | Total | C  | N | O  | P | S | 0       | 0       |
|     |       |          | 48    | 21 | 7 | 16 | 3 | 1 |         |         |
| 2   | C     | 1        | Total | C  | N | O  | P | S | 0       | 0       |
|     |       |          | 48    | 21 | 7 | 16 | 3 | 1 |         |         |
| 2   | D     | 1        | Total | C  | N | O  | P | S | 0       | 0       |
|     |       |          | 48    | 21 | 7 | 16 | 3 | 1 |         |         |
| 2   | E     | 1        | Total | C  | N | O  | P | S | 0       | 0       |
|     |       |          | 48    | 21 | 7 | 16 | 3 | 1 |         |         |
| 2   | F     | 1        | Total | C  | N | O  | P | S | 0       | 0       |
|     |       |          | 48    | 21 | 7 | 16 | 3 | 1 |         |         |
| 2   | G     | 1        | Total | C  | N | O  | P | S | 0       | 0       |
|     |       |          | 48    | 21 | 7 | 16 | 3 | 1 |         |         |
| 2   | H     | 1        | Total | C  | N | O  | P | S | 0       | 0       |
|     |       |          | 48    | 21 | 7 | 16 | 3 | 1 |         |         |
| 2   | I     | 1        | Total | C  | N | O  | P | S | 0       | 0       |
|     |       |          | 48    | 21 | 7 | 16 | 3 | 1 |         |         |
| 2   | J     | 1        | Total | C  | N | O  | P | S | 0       | 0       |
|     |       |          | 48    | 21 | 7 | 16 | 3 | 1 |         |         |
| 2   | K     | 1        | Total | C  | N | O  | P | S | 0       | 0       |
|     |       |          | 48    | 21 | 7 | 16 | 3 | 1 |         |         |
| 2   | L     | 1        | Total | C  | N | O  | P | S | 0       | 0       |
|     |       |          | 48    | 21 | 7 | 16 | 3 | 1 |         |         |

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | F     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | G     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | H     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | I     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | J     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | K     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | L     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 4   | I     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 5   | A     | 165      | Total | O   | 0       | 0       |
|     |       |          | 165   | 165 |         |         |
| 5   | B     | 171      | Total | O   | 0       | 0       |
|     |       |          | 171   | 171 |         |         |
| 5   | C     | 137      | Total | O   | 0       | 0       |
|     |       |          | 137   | 137 |         |         |
| 5   | D     | 123      | Total | O   | 0       | 0       |
|     |       |          | 123   | 123 |         |         |
| 5   | E     | 165      | Total | O   | 0       | 0       |
|     |       |          | 165   | 165 |         |         |
| 5   | F     | 102      | Total | O   | 0       | 0       |
|     |       |          | 102   | 102 |         |         |
| 5   | G     | 140      | Total | O   | 0       | 0       |
|     |       |          | 140   | 140 |         |         |
| 5   | H     | 144      | Total | O   | 0       | 0       |
|     |       |          | 144   | 144 |         |         |
| 5   | I     | 164      | Total | O   | 0       | 0       |
|     |       |          | 164   | 164 |         |         |
| 5   | J     | 80       | Total | O   | 0       | 0       |
|     |       |          | 80    | 80  |         |         |

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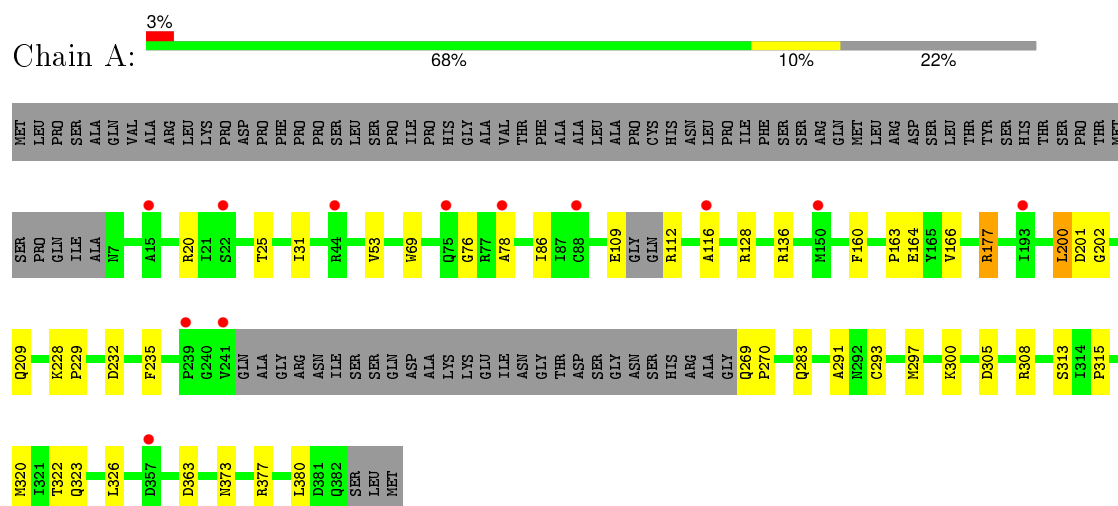
| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 5   | K     | 78       | Total<br>78  | O<br>78  | 0       | 0       |
| 5   | L     | 104      | Total<br>104 | O<br>104 | 0       | 0       |



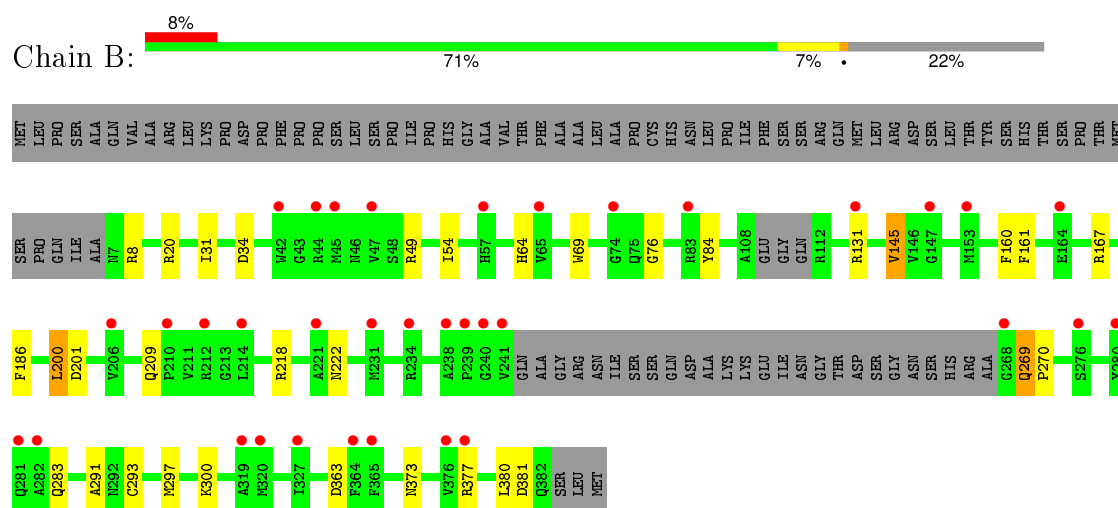
### 3 Residue-property plots [i](#)

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

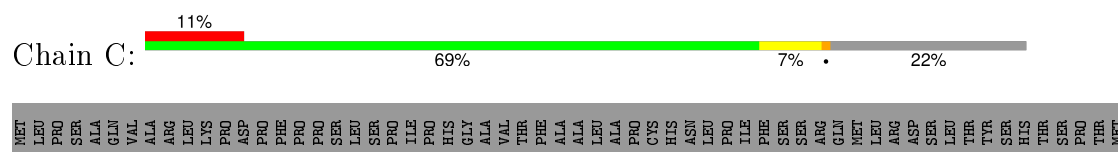
#### • Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

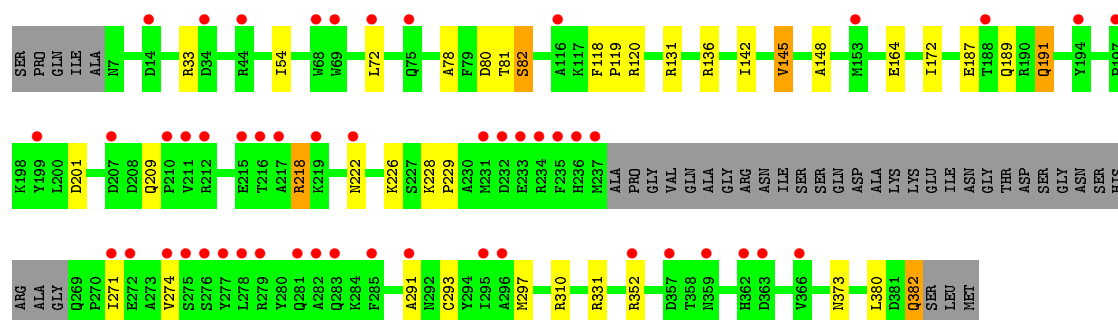


#### • Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

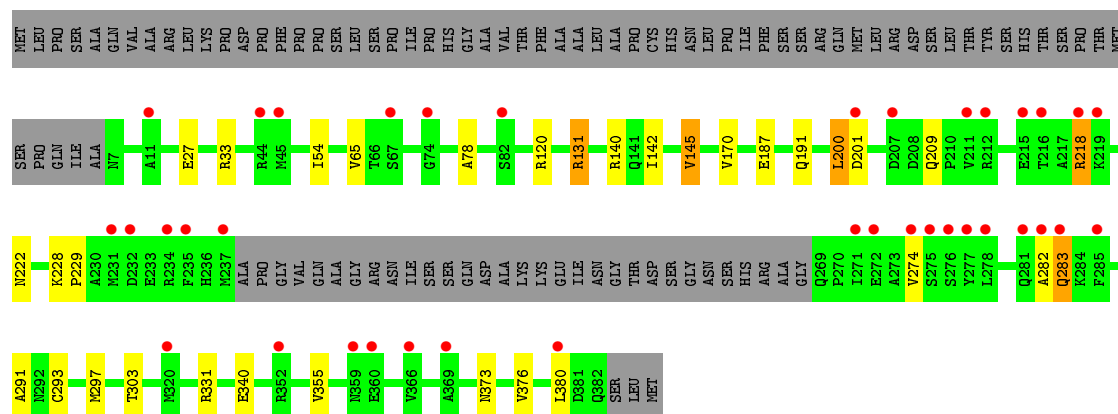


#### • Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

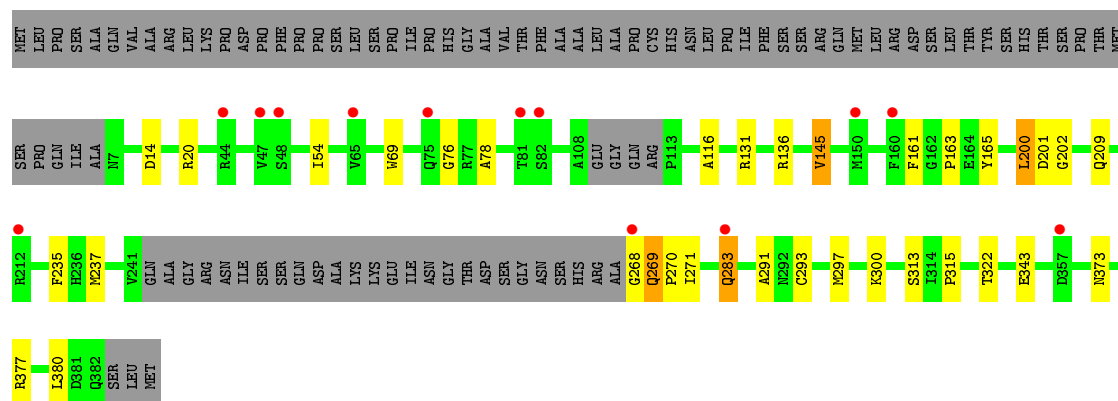




• Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE



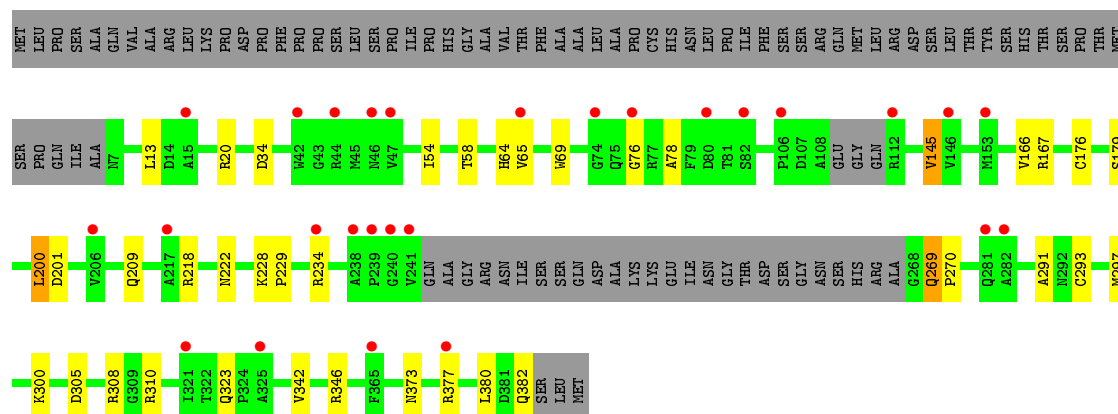
• Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE



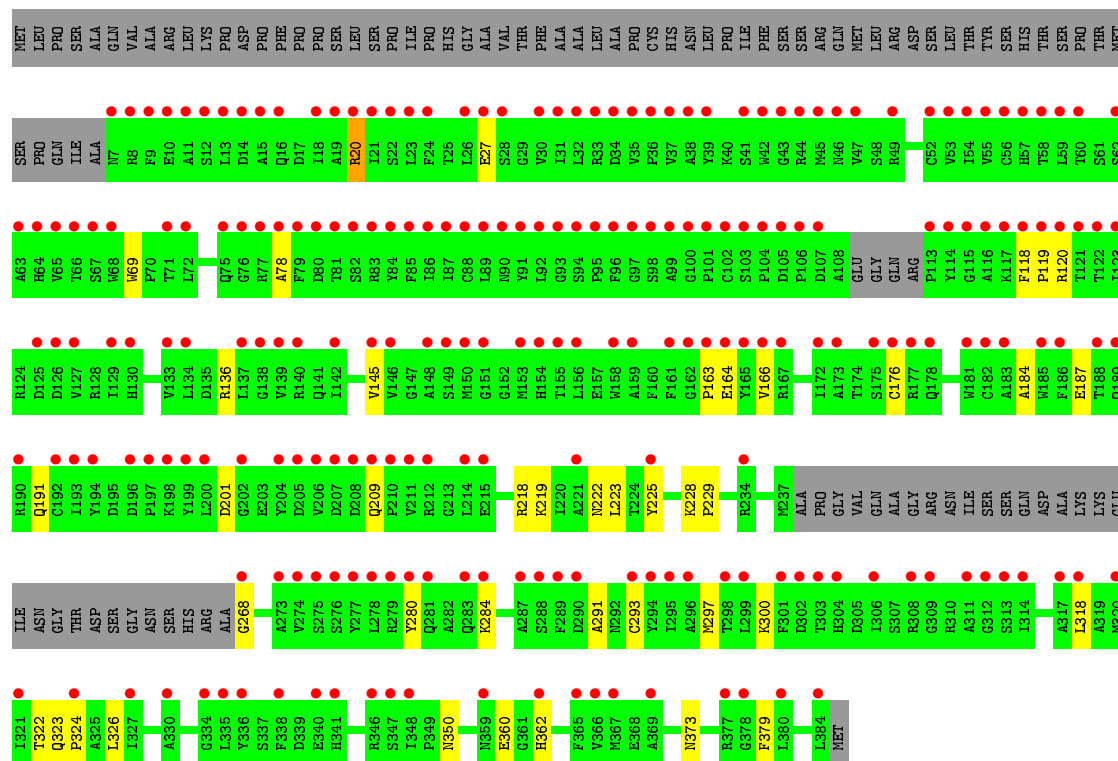
• Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE



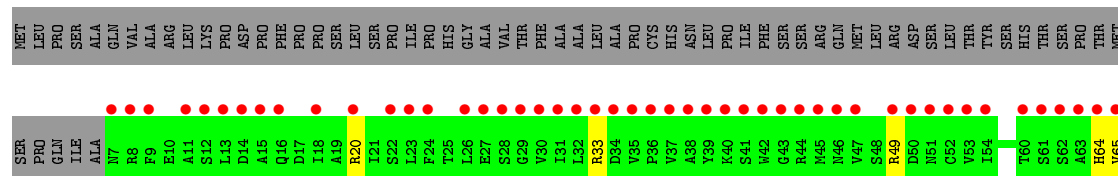


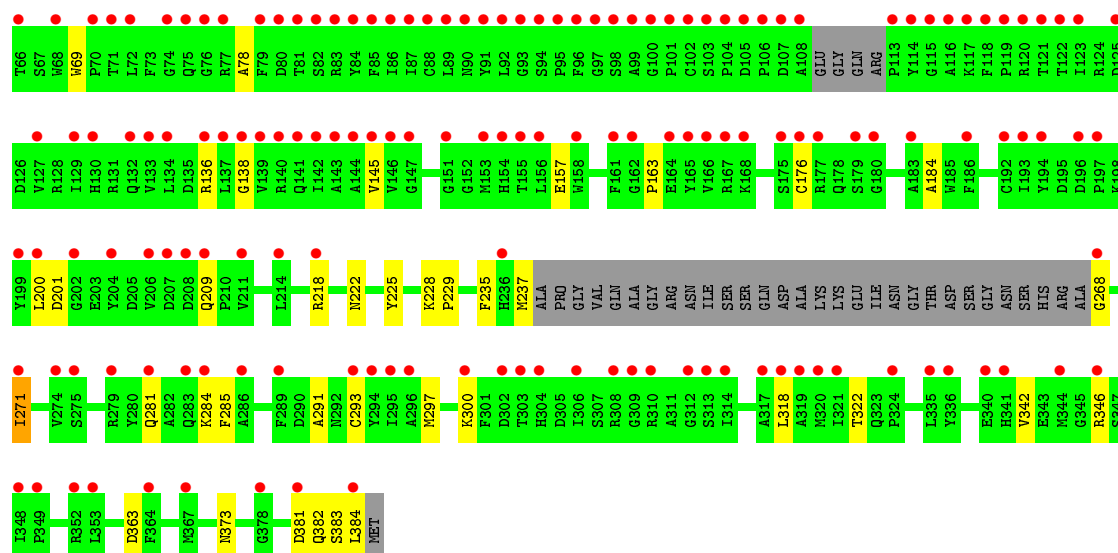


● Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

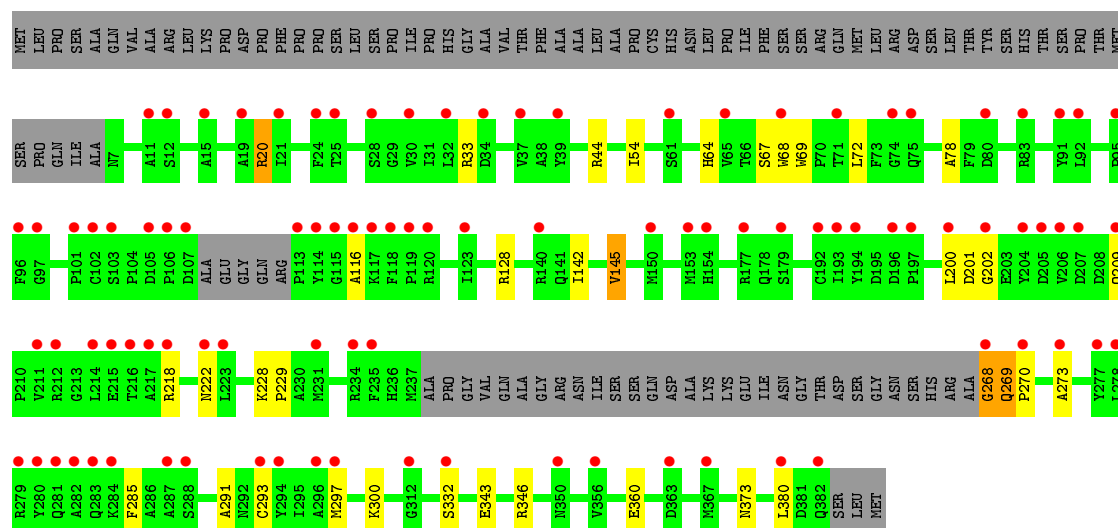


● Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE





● Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1 21 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 121.96Å 109.28Å 197.00Å<br>90.00° 90.23° 90.00°             | Depositor        |
| Resolution (Å)  | 122.17 – 2.20<br>27.45 – 2.40                               | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.5 (122.17-2.20)<br>98.9 (27.45-2.40)                     | Depositor<br>EDS |
| $R_{merge}$   | 0.09  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.37 (at 2.39Å)   | Xtriage          |
| Refinement program  | REFMAC 5.2.0019   | Depositor        |
| R, $R_{free}$   | 0.200 , 0.230<br>0.263 , 0.259                              | Depositor<br>DCC |
| $R_{free}$ test set   | 10106 reflections (5.30%)                                   | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 30.2  | Xtriage          |
| Anisotropy  | 0.195   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.38 , 16.2   | EDS              |
| Estimated twinning fraction   | 0.479 for h,-k,-l   | Xtriage          |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Outliers  | 0 of 200784 reflections                                     | Xtriage          |
| $F_o, F_c$ correlation  | 0.89  | EDS              |
| Total number of atoms   | 35013   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 24.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.77% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: COA, GOL, ACT

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     | 0.89         | 3/2816 (0.1%)   | 0.75        | 4/3817 (0.1%)   |
| 1   | B     | 0.99         | 10/2816 (0.4%)  | 0.76        | 3/3816 (0.1%)   |
| 1   | C     | 0.89         | 6/2820 (0.2%)   | 0.71        | 1/3821 (0.0%)   |
| 1   | D     | 0.94         | 5/2826 (0.2%)   | 0.74        | 2/3829 (0.1%)   |
| 1   | E     | 0.85         | 1/2822 (0.0%)   | 0.70        | 0/3823          |
| 1   | F     | 0.89         | 5/2759 (0.2%)   | 0.75        | 6/3739 (0.2%)   |
| 1   | G     | 0.87         | 3/2813 (0.1%)   | 0.73        | 3/3811 (0.1%)   |
| 1   | H     | 0.84         | 0/2844          | 0.73        | 4/3852 (0.1%)   |
| 1   | I     | 0.87         | 2/2811 (0.1%)   | 0.73        | 3/3810 (0.1%)   |
| 1   | J     | 0.89         | 2/2795 (0.1%)   | 0.72        | 1/3786 (0.0%)   |
| 1   | K     | 0.86         | 1/2806 (0.0%)   | 0.69        | 0/3800          |
| 1   | L     | 0.86         | 1/2765 (0.0%)   | 0.71        | 0/3746          |
| All | All   | 0.89         | 39/33693 (0.1%) | 0.73        | 27/45650 (0.1%) |

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   | L     | 0                   | 1                   |

All (39) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | B     | 186 | PHE  | CE1-CZ | -11.74 | 1.15        | 1.37     |
| 1   | B     | 186 | PHE  | CG-CD2 | -11.20 | 1.22        | 1.38     |
| 1   | D     | 340 | GLU  | CD-OE1 | -10.64 | 1.14        | 1.25     |
| 1   | D     | 340 | GLU  | CD-OE2 | -10.50 | 1.14        | 1.25     |
| 1   | B     | 186 | PHE  | CE2-CZ | -9.88  | 1.18        | 1.37     |
| 1   | D     | 27  | GLU  | CD-OE1 | -9.79  | 1.14        | 1.25     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 8   | ARG  | CZ-NH1 | -9.34 | 1.21        | 1.33     |
| 1   | B     | 186 | PHE  | CG-CD1 | -9.34 | 1.24        | 1.38     |
| 1   | F     | 190 | ARG  | CZ-NH1 | -9.25 | 1.21        | 1.33     |
| 1   | J     | 27  | GLU  | CD-OE1 | -8.68 | 1.16        | 1.25     |
| 1   | B     | 8   | ARG  | CZ-NH2 | -8.47 | 1.22        | 1.33     |
| 1   | A     | 326 | LEU  | CG-CD1 | -8.46 | 1.20        | 1.51     |
| 1   | D     | 27  | GLU  | CD-OE2 | -7.39 | 1.17        | 1.25     |
| 1   | J     | 27  | GLU  | CD-OE2 | -7.33 | 1.17        | 1.25     |
| 1   | F     | 190 | ARG  | CZ-NH2 | -7.07 | 1.23        | 1.33     |
| 1   | F     | 176 | CYS  | CB-SG  | -6.41 | 1.71        | 1.82     |
| 1   | D     | 200 | LEU  | CG-CD1 | -6.34 | 1.28        | 1.51     |
| 1   | C     | 189 | GLN  | CD-NE2 | -6.34 | 1.17        | 1.32     |
| 1   | C     | 191 | GLN  | CD-NE2 | -6.16 | 1.17        | 1.32     |
| 1   | G     | 102 | CYS  | CB-SG  | -6.13 | 1.71        | 1.82     |
| 1   | B     | 373 | ASN  | CG-OD1 | -6.06 | 1.10        | 1.24     |
| 1   | G     | 332 | SER  | CB-OG  | 5.87  | 1.49        | 1.42     |
| 1   | C     | 382 | GLN  | CD-OE1 | -5.79 | 1.11        | 1.24     |
| 1   | A     | 326 | LEU  | CG-CD2 | -5.71 | 1.30        | 1.51     |
| 1   | E     | 200 | LEU  | CG-CD1 | -5.67 | 1.30        | 1.51     |
| 1   | C     | 189 | GLN  | CD-OE1 | -5.64 | 1.11        | 1.24     |
| 1   | I     | 200 | LEU  | CG-CD1 | -5.64 | 1.30        | 1.51     |
| 1   | B     | 373 | ASN  | CG-ND2 | -5.62 | 1.18        | 1.32     |
| 1   | A     | 200 | LEU  | CG-CD1 | -5.54 | 1.31        | 1.51     |
| 1   | G     | 200 | LEU  | CG-CD1 | -5.53 | 1.31        | 1.51     |
| 1   | I     | 176 | CYS  | CB-SG  | -5.46 | 1.73        | 1.81     |
| 1   | C     | 191 | GLN  | CD-OE1 | -5.17 | 1.12        | 1.24     |
| 1   | B     | 200 | LEU  | CG-CD2 | -5.16 | 1.32        | 1.51     |
| 1   | L     | 200 | LEU  | CG-CD2 | -5.12 | 1.32        | 1.51     |
| 1   | K     | 200 | LEU  | CG-CD1 | -5.08 | 1.33        | 1.51     |
| 1   | C     | 82  | SER  | CB-OG  | -5.05 | 1.35        | 1.42     |
| 1   | F     | 200 | LEU  | CG-CD1 | -5.05 | 1.33        | 1.51     |
| 1   | B     | 200 | LEU  | CG-CD1 | -5.04 | 1.33        | 1.51     |
| 1   | F     | 191 | GLN  | CD-OE1 | -5.00 | 1.12        | 1.24     |

All (27) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | A     | 177 | ARG  | NE-CZ-NH1  | 11.47  | 126.04      | 120.30   |
| 1   | B     | 8   | ARG  | NE-CZ-NH2  | 10.40  | 125.50      | 120.30   |
| 1   | D     | 340 | GLU  | OE1-CD-OE2 | -10.00 | 111.30      | 123.30   |
| 1   | D     | 27  | GLU  | OE1-CD-OE2 | -9.88  | 111.44      | 123.30   |
| 1   | J     | 27  | GLU  | OE1-CD-OE2 | -9.78  | 111.56      | 123.30   |

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| Mol | Chain | Res    | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 1   | F     | 190    | ARG  | NE-CZ-NH1  | 9.21  | 124.90      | 120.30   |
| 1   | A     | 177    | ARG  | NE-CZ-NH2  | -8.32 | 116.14      | 120.30   |
| 1   | B     | 8      | ARG  | NH1-CZ-NH2 | -8.10 | 110.49      | 119.40   |
| 1   | A     | 326    | LEU  | CD1-CG-CD2 | -7.87 | 86.89       | 110.50   |
| 1   | F     | 190    | ARG  | NH1-CZ-NH2 | -7.46 | 111.20      | 119.40   |
| 1   | B     | 8      | ARG  | NE-CZ-NH1  | 7.41  | 124.01      | 120.30   |
| 1   | F     | 190    | ARG  | NE-CZ-NH2  | 7.20  | 123.90      | 120.30   |
| 1   | C     | 310    | ARG  | NE-CZ-NH2  | -6.89 | 116.85      | 120.30   |
| 1   | G     | 297    | MET  | CG-SD-CE   | 6.54  | 110.66      | 100.20   |
| 1   | H     | 297    | MET  | CG-SD-CE   | 6.49  | 110.58      | 100.20   |
| 1   | H     | 310    | ARG  | NE-CZ-NH2  | -6.47 | 117.06      | 120.30   |
| 1   | H     | 310    | ARG  | NE-CZ-NH1  | 6.01  | 123.31      | 120.30   |
| 1   | I     | 310    | ARG  | NE-CZ-NH1  | 5.72  | 123.16      | 120.30   |
| 1   | I     | 167    | ARG  | NE-CZ-NH1  | 5.63  | 123.12      | 120.30   |
| 1   | A     | 128[A] | ARG  | NE-CZ-NH1  | -5.61 | 117.50      | 120.30   |
| 1   | G     | 310    | ARG  | NE-CZ-NH2  | -5.54 | 117.53      | 120.30   |
| 1   | H     | 30     | VAL  | CG1-CB-CG2 | 5.47  | 119.66      | 110.90   |
| 1   | F     | 310    | ARG  | NE-CZ-NH1  | 5.37  | 122.99      | 120.30   |
| 1   | G     | 134    | LEU  | CB-CG-CD1  | 5.35  | 120.09      | 111.00   |
| 1   | I     | 310    | ARG  | NE-CZ-NH2  | -5.29 | 117.66      | 120.30   |
| 1   | F     | 310    | ARG  | NE-CZ-NH2  | -5.18 | 117.71      | 120.30   |
| 1   | F     | 167    | ARG  | NE-CZ-NH2  | -5.03 | 117.78      | 120.30   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | L     | 268 | GLY  | Peptide |

## 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     | 2744  | 0        | 2656     | 25      | 0            |
| 1   | B     | 2744  | 0        | 2663     | 18      | 0            |
| 1   | C     | 2745  | 0        | 2662     | 30      | 0            |
| 1   | D     | 2748  | 0        | 2669     | 29      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | E     | 2744  | 0        | 2669     | 26      | 0            |
| 1   | F     | 2694  | 0        | 2599     | 30      | 0            |
| 1   | G     | 2733  | 0        | 2652     | 27      | 0            |
| 1   | H     | 2760  | 0        | 2685     | 44      | 0            |
| 1   | I     | 2739  | 0        | 2655     | 33      | 0            |
| 1   | J     | 2724  | 0        | 2641     | 33      | 0            |
| 1   | K     | 2732  | 0        | 2653     | 44      | 0            |
| 1   | L     | 2697  | 0        | 2607     | 33      | 0            |
| 2   | A     | 48    | 0        | 32       | 2       | 0            |
| 2   | B     | 48    | 0        | 32       | 2       | 0            |
| 2   | C     | 48    | 0        | 32       | 0       | 0            |
| 2   | D     | 48    | 0        | 32       | 0       | 0            |
| 2   | E     | 48    | 0        | 31       | 1       | 0            |
| 2   | F     | 48    | 0        | 32       | 3       | 0            |
| 2   | G     | 48    | 0        | 32       | 5       | 0            |
| 2   | H     | 48    | 0        | 32       | 6       | 0            |
| 2   | I     | 48    | 0        | 32       | 1       | 0            |
| 2   | J     | 48    | 0        | 32       | 3       | 0            |
| 2   | K     | 48    | 0        | 32       | 4       | 0            |
| 2   | L     | 48    | 0        | 32       | 1       | 0            |
| 3   | A     | 4     | 0        | 3        | 0       | 0            |
| 3   | B     | 4     | 0        | 3        | 1       | 0            |
| 3   | C     | 4     | 0        | 3        | 0       | 0            |
| 3   | D     | 4     | 0        | 3        | 0       | 0            |
| 3   | E     | 4     | 0        | 3        | 0       | 0            |
| 3   | F     | 4     | 0        | 3        | 0       | 0            |
| 3   | G     | 4     | 0        | 3        | 1       | 0            |
| 3   | H     | 4     | 0        | 3        | 3       | 0            |
| 3   | I     | 4     | 0        | 3        | 0       | 0            |
| 3   | J     | 4     | 0        | 3        | 0       | 0            |
| 3   | K     | 4     | 0        | 3        | 2       | 0            |
| 3   | L     | 4     | 0        | 3        | 1       | 0            |
| 4   | B     | 6     | 0        | 8        | 0       | 0            |
| 4   | I     | 6     | 0        | 8        | 0       | 0            |
| 5   | A     | 165   | 0        | 0        | 0       | 0            |
| 5   | B     | 171   | 0        | 0        | 6       | 0            |
| 5   | C     | 137   | 0        | 0        | 8       | 0            |
| 5   | D     | 123   | 0        | 0        | 5       | 0            |
| 5   | E     | 165   | 0        | 0        | 3       | 0            |
| 5   | F     | 102   | 0        | 0        | 7       | 0            |
| 5   | G     | 140   | 0        | 0        | 3       | 0            |
| 5   | H     | 144   | 0        | 0        | 5       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5   | I     | 164   | 0        | 0        | 3       | 0            |
| 5   | J     | 80    | 0        | 0        | 3       | 0            |
| 5   | K     | 78    | 0        | 0        | 5       | 0            |
| 5   | L     | 104   | 0        | 0        | 7       | 0            |
| All | All   | 35013 | 0        | 32246    | 357     | 0            |

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

All (357) 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:K:218[A]:ARG:NE   | 1:K:222[A]:ASN:HD21 | 1.04                     | 1.42              |
| 1:K:218[A]:ARG:NE   | 1:K:222[A]:ASN:ND2  | 1.78                     | 1.29              |
| 1:J:218:ARG:CZ      | 1:J:222[A]:ASN:OD1  | 1.98                     | 1.11              |
| 1:H:363[A]:ASP:OD1  | 2:H:1383:COA:C6P    | 1.99                     | 1.11              |
| 1:E:14:ASP:OD1      | 5:E:2005:HOH:O      | 1.72                     | 1.08              |
| 1:K:218[A]:ARG:CZ   | 1:K:222[A]:ASN:ND2  | 2.20                     | 1.04              |
| 1:H:363[A]:ASP:OD1  | 2:H:1383:COA:H61    | 1.60                     | 1.01              |
| 1:D:120[B]:ARG:HH11 | 1:D:120[B]:ARG:HG3  | 1.29                     | 0.98              |
| 1:H:363[A]:ASP:OD1  | 2:H:1383:COA:H62    | 1.62                     | 0.98              |
| 1:J:218:ARG:NH2     | 1:J:222[A]:ASN:OD1  | 1.98                     | 0.95              |
| 1:E:269:GLN:H       | 1:E:270:PRO:HD2     | 1.31                     | 0.94              |
| 1:K:218[A]:ARG:HE   | 1:K:222[A]:ASN:HD21 | 1.08                     | 0.94              |
| 1:C:120[B]:ARG:HD3  | 5:C:2107:HOH:O      | 1.66                     | 0.93              |
| 1:H:131[A]:ARG:HH11 | 1:H:131[A]:ARG:HG3  | 1.35                     | 0.90              |
| 1:D:331:ARG:NH1     | 1:I:382:GLN:HE21    | 1.69                     | 0.89              |
| 1:J:360:GLU:O       | 5:J:2076:HOH:O      | 1.89                     | 0.88              |
| 1:C:120[B]:ARG:HG3  | 1:C:120[B]:ARG:HH21 | 1.37                     | 0.87              |
| 1:K:218[A]:ARG:CD   | 1:K:222[A]:ASN:HD21 | 1.89                     | 0.85              |
| 1:L:20:ARG:HG3      | 1:L:20:ARG:HH11     | 1.39                     | 0.85              |
| 1:K:218[A]:ARG:CD   | 1:K:222[A]:ASN:ND2  | 2.40                     | 0.84              |
| 1:L:269:GLN:H       | 1:L:270:PRO:HD2     | 1.39                     | 0.84              |
| 1:K:78:ALA:H        | 1:K:373:ASN:HD21    | 1.26                     | 0.84              |
| 1:D:120[B]:ARG:HD3  | 5:D:2098:HOH:O      | 1.79                     | 0.82              |
| 1:J:218:ARG:NE      | 1:J:222[A]:ASN:HD21 | 1.78                     | 0.80              |
| 1:D:65:VAL:HG22     | 5:D:2030:HOH:O      | 1.80                     | 0.79              |
| 1:D:120[B]:ARG:HH11 | 1:D:120[B]:ARG:CG   | 1.95                     | 0.79              |
| 1:H:131[A]:ARG:CG   | 1:H:131[A]:ARG:HH11 | 1.95                     | 0.79              |
| 1:J:78:ALA:H        | 1:J:373:ASN:HD21    | 1.31                     | 0.79              |
| 2:B:1383:COA:O9A    | 5:B:2170:HOH:O      | 2.01                     | 0.78              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:H:332:SER:OG     | 1:H:360:GLU:O       | 2.01                     | 0.78              |
| 1:G:331:ARG:HH11   | 1:G:331:ARG:HG3     | 1.49                     | 0.78              |
| 1:E:269:GLN:H      | 1:E:270:PRO:CD      | 1.98                     | 0.77              |
| 1:D:331:ARG:NH1    | 1:I:382:GLN:NE2     | 2.33                     | 0.76              |
| 1:H:308[B]:ARG:HG3 | 1:H:308[B]:ARG:HH21 | 1.51                     | 0.76              |
| 1:H:303:THR:OG1    | 5:H:2117:HOH:O      | 1.67                     | 0.75              |
| 1:K:218[A]:ARG:CZ  | 1:K:222[A]:ASN:HD21 | 1.86                     | 0.74              |
| 1:C:164:GLU:HB3    | 5:C:2066:HOH:O      | 1.87                     | 0.74              |
| 1:I:78:ALA:H       | 1:I:373:ASN:HD21    | 1.35                     | 0.73              |
| 1:F:332:SER:OG     | 1:F:360:GLU:O       | 2.05                     | 0.73              |
| 2:H:1383:COA:H131  | 2:H:1383:COA:O9P    | 1.87                     | 0.72              |
| 1:A:78:ALA:H       | 1:A:373:ASN:ND2     | 1.87                     | 0.72              |
| 1:F:64:HIS:HD2     | 5:F:2003:HOH:O      | 1.73                     | 0.72              |
| 1:A:209:GLN:HE22   | 1:A:291:ALA:H       | 1.37                     | 0.72              |
| 1:D:209:GLN:HE22   | 1:D:291:ALA:H       | 1.39                     | 0.71              |
| 1:I:209:GLN:HE22   | 1:I:291:ALA:H       | 1.38                     | 0.71              |
| 1:E:209:GLN:HE22   | 1:E:291:ALA:H       | 1.38                     | 0.71              |
| 1:E:78:ALA:H       | 1:E:373:ASN:HD21    | 1.38                     | 0.71              |
| 1:G:281:GLN:HE22   | 2:G:1383:COA:H52A   | 1.54                     | 0.71              |
| 1:A:78:ALA:H       | 1:A:373:ASN:HD21    | 1.36                     | 0.71              |
| 1:F:68:TRP:CZ2     | 5:F:2018:HOH:O      | 2.42                     | 0.71              |
| 1:C:120[B]:ARG:CG  | 1:C:120[B]:ARG:HH21 | 2.04                     | 0.70              |
| 1:K:218[B]:ARG:NH2 | 1:K:281:GLN:O       | 2.25                     | 0.70              |
| 1:L:343:GLU:HG3    | 5:L:2092:HOH:O      | 1.91                     | 0.70              |
| 1:H:64:HIS:HD2     | 5:H:2003:HOH:O      | 1.75                     | 0.69              |
| 1:K:297:MET:O      | 1:K:300:LYS:HB2     | 1.92                     | 0.69              |
| 1:L:332:SER:OG     | 1:L:360:GLU:O       | 2.06                     | 0.69              |
| 1:K:363:ASP:OD1    | 2:K:1385:COA:H62    | 1.93                     | 0.69              |
| 1:K:78:ALA:H       | 1:K:373:ASN:ND2     | 1.90                     | 0.68              |
| 1:I:78:ALA:H       | 1:I:373:ASN:ND2     | 1.90                     | 0.68              |
| 1:C:209:GLN:HE22   | 1:C:291:ALA:H       | 1.41                     | 0.68              |
| 1:H:128[A]:ARG:HE  | 3:H:1384:ACT:H1     | 1.59                     | 0.67              |
| 1:E:78:ALA:H       | 1:E:373:ASN:ND2     | 1.91                     | 0.67              |
| 1:B:209:GLN:HE22   | 1:B:291:ALA:H       | 1.42                     | 0.67              |
| 1:D:331:ARG:HH12   | 1:I:382:GLN:HE21    | 1.42                     | 0.67              |
| 1:G:209:GLN:HE22   | 1:G:291:ALA:H       | 1.42                     | 0.67              |
| 1:J:78:ALA:H       | 1:J:373:ASN:ND2     | 1.92                     | 0.66              |
| 1:L:68:TRP:CZ2     | 5:L:2021:HOH:O      | 2.47                     | 0.66              |
| 1:D:33:ARG:HD2     | 5:D:2037:HOH:O      | 1.96                     | 0.66              |
| 1:F:50:ASP:HB3     | 1:F:140[A]:ARG:NH1  | 2.10                     | 0.66              |
| 1:G:64:HIS:HD2     | 5:G:2005:HOH:O      | 1.79                     | 0.66              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:J:164:GLU:HB3    | 5:J:2029:HOH:O      | 1.95                     | 0.66              |
| 1:I:293:CYS:O      | 1:I:297:MET:HG3     | 1.96                     | 0.66              |
| 1:D:293:CYS:O      | 1:D:297:MET:HG3     | 1.96                     | 0.66              |
| 1:H:209:GLN:HE22   | 1:H:291:ALA:H       | 1.44                     | 0.65              |
| 1:D:218:ARG:CZ     | 1:D:222:ASN:HB2     | 2.26                     | 0.65              |
| 1:K:268:GLY:N      | 2:K:1385:COA:H62A   | 1.94                     | 0.65              |
| 1:F:343:GLU:HG3    | 5:F:2090:HOH:O      | 1.97                     | 0.65              |
| 1:J:209:GLN:HE22   | 1:J:291:ALA:H       | 1.45                     | 0.65              |
| 1:K:64:HIS:HD2     | 5:K:2003:HOH:O      | 1.80                     | 0.65              |
| 1:D:228:LYS:HB3    | 1:D:229:PRO:HD3     | 1.79                     | 0.65              |
| 1:A:109:GLU:HA     | 1:A:109:GLU:OE1     | 1.97                     | 0.64              |
| 1:J:218:ARG:NE     | 1:J:222[A]:ASN:ND2  | 2.44                     | 0.64              |
| 1:F:209:GLN:HE22   | 1:F:291:ALA:H       | 1.46                     | 0.64              |
| 1:K:381:ASP:HB3    | 5:K:2076:HOH:O      | 1.97                     | 0.64              |
| 1:K:209:GLN:HE22   | 1:K:291:ALA:H       | 1.44                     | 0.64              |
| 1:L:209:GLN:HE22   | 1:L:291:ALA:H       | 1.46                     | 0.63              |
| 1:B:293:CYS:O      | 1:B:297:MET:HG3     | 1.98                     | 0.63              |
| 1:J:293:CYS:O      | 1:J:297:MET:HG3     | 1.98                     | 0.63              |
| 1:B:269:GLN:H      | 1:B:270:PRO:HD2     | 1.64                     | 0.63              |
| 1:D:120[B]:ARG:NH1 | 1:D:120[B]:ARG:CG   | 2.58                     | 0.63              |
| 1:C:120[B]:ARG:CD  | 5:C:2107:HOH:O      | 2.37                     | 0.63              |
| 1:D:78:ALA:H       | 1:D:373:ASN:HD21    | 1.46                     | 0.63              |
| 1:F:78:ALA:H       | 1:F:373:ASN:HD21    | 1.45                     | 0.63              |
| 1:E:237:MET:HG3    | 1:E:271:ILE:HD12    | 1.81                     | 0.63              |
| 1:L:78:ALA:H       | 1:L:373:ASN:HD21    | 1.46                     | 0.63              |
| 1:K:218[A]:ARG:HD2 | 1:K:222[A]:ASN:OD1  | 1.99                     | 0.62              |
| 1:C:293:CYS:O      | 1:C:297:MET:HG3     | 1.98                     | 0.62              |
| 1:J:218:ARG:CZ     | 1:J:222[A]:ASN:CG   | 2.68                     | 0.62              |
| 1:F:293:CYS:O      | 1:F:297:MET:HG3     | 1.99                     | 0.62              |
| 1:J:297:MET:O      | 1:J:300:LYS:HB2     | 1.99                     | 0.62              |
| 1:G:331:ARG:NH1    | 1:G:331:ARG:HG3     | 2.15                     | 0.61              |
| 1:H:33[A]:ARG:NH2  | 1:H:107:ASP:OD2     | 2.24                     | 0.61              |
| 1:C:81:THR:OG1     | 1:F:138:GLY:HA2     | 2.00                     | 0.61              |
| 1:L:20:ARG:HH11    | 1:L:20:ARG:CG       | 2.12                     | 0.61              |
| 1:L:20:ARG:NH1     | 1:L:20:ARG:HG3      | 2.14                     | 0.61              |
| 1:L:269:GLN:H      | 1:L:270:PRO:CD      | 2.12                     | 0.61              |
| 1:L:68:TRP:NE1     | 5:L:2021:HOH:O      | 2.33                     | 0.61              |
| 1:I:64:HIS:HD2     | 5:I:2004:HOH:O      | 1.82                     | 0.61              |
| 1:J:218:ARG:HE     | 1:J:222[A]:ASN:HD21 | 1.47                     | 0.61              |
| 1:J:218:ARG:NE     | 1:J:222[A]:ASN:OD1  | 2.34                     | 0.61              |
| 1:H:281:GLN:HE22   | 2:H:1383:COA:H52A   | 1.66                     | 0.61              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:K:218[B]:ARG:HG3 | 1:K:285:PHE:CG      | 2.37                     | 0.60              |
| 1:L:293:CYS:O      | 1:L:297:MET:HG3     | 2.01                     | 0.60              |
| 1:K:218[A]:ARG:HD2 | 1:K:222[A]:ASN:CG   | 2.22                     | 0.59              |
| 1:B:84:TYR:HE1     | 1:B:377[B]:ARG:HH22 | 1.50                     | 0.59              |
| 1:B:76:GLY:O       | 1:B:377[A]:ARG:HD3  | 2.03                     | 0.59              |
| 1:D:78:ALA:H       | 1:D:373:ASN:ND2     | 1.99                     | 0.59              |
| 1:G:78:ALA:H       | 1:G:373:ASN:HD21    | 1.48                     | 0.59              |
| 1:H:131[A]:ARG:NH1 | 1:H:131[A]:ARG:HG3  | 2.10                     | 0.59              |
| 1:K:218[A]:ARG:CD  | 1:K:222[A]:ASN:CG   | 2.71                     | 0.59              |
| 1:E:237:MET:CG     | 1:E:271:ILE:HD12    | 2.33                     | 0.59              |
| 1:F:50:ASP:HB3     | 1:F:140[A]:ARG:HH12 | 1.68                     | 0.58              |
| 1:E:237:MET:HG3    | 1:E:271:ILE:CD1     | 2.34                     | 0.57              |
| 1:F:78:ALA:H       | 1:F:373:ASN:ND2     | 2.02                     | 0.57              |
| 1:C:331:ARG:NH2    | 5:C:2114:HOH:O      | 2.38                     | 0.57              |
| 1:G:226:LYS:NZ     | 1:G:363[B]:ASP:OD1  | 2.24                     | 0.56              |
| 1:K:293:CYS:O      | 1:K:297:MET:HG3     | 2.04                     | 0.56              |
| 1:H:27:GLU:OE1     | 1:H:308[A]:ARG:NH2  | 2.35                     | 0.56              |
| 1:G:78:ALA:H       | 1:G:373:ASN:ND2     | 2.03                     | 0.56              |
| 1:A:25:THR:HG21    | 3:B:1385:ACT:H3     | 1.86                     | 0.56              |
| 1:F:268:GLY:O      | 1:F:273:ALA:HB3     | 2.05                     | 0.56              |
| 1:L:64:HIS:HD2     | 5:L:2003:HOH:O      | 1.89                     | 0.56              |
| 1:H:75:GLN:HG3     | 1:H:82:SER:OG       | 2.05                     | 0.56              |
| 1:G:363[A]:ASP:OD1 | 2:G:1383:COA:H61    | 2.05                     | 0.56              |
| 1:G:332:SER:OG     | 1:G:360:GLU:O       | 2.13                     | 0.56              |
| 1:H:308[B]:ARG:CG  | 1:H:308[B]:ARG:HH21 | 2.17                     | 0.56              |
| 1:L:78:ALA:H       | 1:L:373:ASN:ND2     | 2.03                     | 0.56              |
| 1:C:228:LYS:HB3    | 1:C:229:PRO:HD3     | 1.87                     | 0.56              |
| 1:J:280:TYR:OH     | 2:J:1385:COA:O7A    | 2.17                     | 0.56              |
| 1:C:78:ALA:H       | 1:C:373:ASN:HD21    | 1.53                     | 0.56              |
| 1:K:235:PHE:CE2    | 1:K:268:GLY:O       | 2.60                     | 0.55              |
| 1:H:226:LYS:NZ     | 1:H:363[B]:ASP:OD1  | 2.27                     | 0.55              |
| 1:K:281:GLN:HB2    | 5:K:2043:HOH:O      | 2.06                     | 0.55              |
| 1:G:116:ALA:HB2    | 1:G:202:GLY:HA3     | 1.88                     | 0.55              |
| 1:L:297:MET:O      | 1:L:300:LYS:HB2     | 2.06                     | 0.55              |
| 1:I:346:ARG:CZ     | 1:K:346[B]:ARG:HG3  | 2.37                     | 0.55              |
| 1:C:120[A]:ARG:NH1 | 5:C:2054:HOH:O      | 2.40                     | 0.54              |
| 1:G:76:GLY:O       | 1:G:377:ARG:NH1     | 2.40                     | 0.54              |
| 1:L:68:TRP:CE2     | 5:L:2021:HOH:O      | 2.61                     | 0.54              |
| 1:C:33:ARG:HD2     | 5:C:2047:HOH:O      | 2.07                     | 0.54              |
| 1:G:164[B]:GLU:HB2 | 5:G:2071:HOH:O      | 2.06                     | 0.54              |
| 1:I:218:ARG:CZ     | 1:I:222:ASN:HB2     | 2.37                     | 0.54              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:G:297:MET:O      | 1:G:300:LYS:HB2     | 2.07                     | 0.54              |
| 1:E:131[A]:ARG:HD3 | 1:E:161:PHE:CE1     | 2.43                     | 0.54              |
| 1:F:297:MET:O      | 1:F:300:LYS:HB2     | 2.07                     | 0.53              |
| 1:H:116:ALA:HB2    | 1:H:202:GLY:HA3     | 1.89                     | 0.53              |
| 1:H:27:GLU:CD      | 1:H:308[A]:ARG:HH12 | 2.11                     | 0.53              |
| 1:K:20:ARG:O       | 1:K:136[A]:ARG:NH2  | 2.41                     | 0.53              |
| 1:B:20:ARG:HD3     | 1:B:34:ASP:OD1      | 2.09                     | 0.53              |
| 1:K:163:PRO:HG3    | 1:K:322:THR:CG2     | 2.39                     | 0.53              |
| 1:B:377[B]:ARG:NH1 | 1:B:381:ASP:OD1     | 2.40                     | 0.53              |
| 1:K:218[B]:ARG:CZ  | 1:K:285:PHE:HB2     | 2.38                     | 0.53              |
| 1:A:293:CYS:O      | 1:A:297:MET:HG3     | 2.09                     | 0.53              |
| 1:D:283:GLN:HB3    | 5:D:2088:HOH:O      | 2.09                     | 0.53              |
| 1:E:343:GLU:HG3    | 5:E:2150:HOH:O      | 2.08                     | 0.52              |
| 1:F:68:TRP:HZ2     | 5:F:2018:HOH:O      | 1.88                     | 0.52              |
| 1:E:283:GLN:HB3    | 5:E:2117:HOH:O      | 2.08                     | 0.52              |
| 1:C:78:ALA:H       | 1:C:373:ASN:ND2     | 2.07                     | 0.52              |
| 1:H:28:SER:OG      | 1:H:30:VAL:HG13     | 2.08                     | 0.52              |
| 1:G:48:SER:O       | 1:G:140[A]:ARG:NE   | 2.43                     | 0.52              |
| 1:G:281:GLN:NE2    | 2:G:1383:COA:H52A   | 2.23                     | 0.52              |
| 1:G:128[A]:ARG:HE  | 3:G:1384:ACT:H1     | 1.75                     | 0.52              |
| 1:I:20:ARG:HD3     | 1:I:34:ASP:OD1      | 2.09                     | 0.52              |
| 1:F:218:ARG:HD2    | 1:F:218:ARG:O       | 2.10                     | 0.52              |
| 1:H:61:SER:CB      | 5:H:2035:HOH:O      | 2.59                     | 0.51              |
| 1:F:218:ARG:CZ     | 1:F:222:ASN:HB2     | 2.41                     | 0.51              |
| 1:C:120[B]:ARG:CG  | 1:C:120[B]:ARG:NH2  | 2.67                     | 0.51              |
| 1:H:128[A]:ARG:HE  | 3:H:1384:ACT:CH3    | 2.23                     | 0.51              |
| 1:K:163:PRO:HG3    | 1:K:322:THR:HG22    | 1.92                     | 0.51              |
| 1:L:20:ARG:NH1     | 1:L:20:ARG:CG       | 2.69                     | 0.51              |
| 1:J:268:GLY:N      | 2:J:1385:COA:H62A   | 2.09                     | 0.51              |
| 1:J:163:PRO:HG3    | 1:J:322:THR:CG2     | 2.41                     | 0.51              |
| 1:H:61:SER:HB2     | 5:H:2035:HOH:O      | 2.10                     | 0.51              |
| 1:B:269:GLN:H      | 1:B:270:PRO:CD      | 2.23                     | 0.50              |
| 1:B:297:MET:O      | 1:B:300:LYS:HB2     | 2.10                     | 0.50              |
| 1:C:72:LEU:HA      | 1:C:373:ASN:HD22    | 1.77                     | 0.50              |
| 1:C:191:GLN:HE21   | 1:J:219:LYS:NZ      | 2.10                     | 0.50              |
| 1:H:128[A]:ARG:NE  | 3:H:1384:ACT:H1     | 2.27                     | 0.50              |
| 1:F:23:LEU:HD23    | 1:F:33:ARG:HG2      | 1.94                     | 0.50              |
| 1:E:131[A]:ARG:HD2 | 1:E:165:TYR:CE2     | 2.46                     | 0.50              |
| 1:J:120:ARG:HD3    | 5:J:2019:HOH:O      | 2.11                     | 0.50              |
| 1:C:218:ARG:CZ     | 1:C:222:ASN:HB2     | 2.42                     | 0.50              |
| 1:L:116:ALA:HB2    | 1:L:202:GLY:HA3     | 1.94                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:H:78:ALA:H       | 1:H:373:ASN:HD21   | 1.58                     | 0.49              |
| 1:F:54:ILE:HB      | 1:F:145:VAL:HB     | 1.94                     | 0.49              |
| 1:I:65:VAL:HA      | 5:I:2036:HOH:O     | 2.11                     | 0.49              |
| 1:E:76:GLY:O       | 1:E:377:ARG:HD3    | 2.12                     | 0.49              |
| 1:L:54:ILE:HB      | 1:L:145:VAL:HB     | 1.94                     | 0.49              |
| 1:K:157:GLU:O      | 3:K:1386:ACT:OXT   | 2.30                     | 0.49              |
| 1:K:65:VAL:HG22    | 5:K:2012:HOH:O     | 2.12                     | 0.49              |
| 1:H:164[B]:GLU:HB2 | 5:H:2075:HOH:O     | 2.11                     | 0.49              |
| 1:H:78:ALA:H       | 1:H:373:ASN:ND2    | 2.11                     | 0.48              |
| 1:F:228:LYS:HB3    | 1:F:229:PRO:HD3    | 1.95                     | 0.48              |
| 1:G:366:VAL:HG21   | 2:G:1383:COA:H71   | 1.95                     | 0.48              |
| 1:G:228:LYS:HB3    | 1:G:229:PRO:HD3    | 1.96                     | 0.48              |
| 1:L:218[A]:ARG:CZ  | 1:L:222[A]:ASN:HB2 | 2.43                     | 0.48              |
| 1:J:163:PRO:HG3    | 1:J:322:THR:HG22   | 1.94                     | 0.48              |
| 1:D:331:ARG:HH11   | 1:I:382:GLN:NE2    | 2.07                     | 0.48              |
| 1:I:228:LYS:HB3    | 1:I:229:PRO:HD3    | 1.95                     | 0.48              |
| 1:I:346:ARG:NH2    | 1:K:346[A]:ARG:CD  | 2.76                     | 0.48              |
| 1:G:331:ARG:CG     | 1:G:331:ARG:HH11   | 2.22                     | 0.48              |
| 1:I:297:MET:O      | 1:I:300:LYS:HB2    | 2.13                     | 0.48              |
| 1:H:23:LEU:HD23    | 1:H:33[B]:ARG:HB3  | 1.95                     | 0.48              |
| 1:L:128[A]:ARG:HE  | 3:L:1384:ACT:H2    | 1.79                     | 0.48              |
| 1:I:76:GLY:O       | 1:I:377:ARG:HD3    | 2.14                     | 0.48              |
| 1:I:342:VAL:O      | 1:I:346:ARG:HG3    | 2.14                     | 0.47              |
| 1:L:228:LYS:HB3    | 1:L:229:PRO:HD3    | 1.96                     | 0.47              |
| 1:F:191:GLN:HE21   | 1:H:219:LYS:NZ     | 2.11                     | 0.47              |
| 1:L:218[A]:ARG:NH2 | 1:L:222[A]:ASN:HB2 | 2.30                     | 0.47              |
| 1:D:218:ARG:HG2    | 1:D:282:ALA:HA     | 1.95                     | 0.47              |
| 1:A:235:PHE:HA     | 1:A:269:GLN:O      | 2.15                     | 0.47              |
| 1:B:218:ARG:CZ     | 1:B:222:ASN:HB2    | 2.45                     | 0.47              |
| 1:H:228:LYS:HB3    | 1:H:229:PRO:HD3    | 1.97                     | 0.47              |
| 1:A:160:PHE:HB3    | 1:B:31:ILE:HD12    | 1.96                     | 0.47              |
| 1:F:54:ILE:CD1     | 1:F:142:ILE:HD13   | 2.45                     | 0.47              |
| 1:I:13:LEU:HB2     | 1:L:44:ARG:NH2     | 2.30                     | 0.47              |
| 1:H:297:MET:O      | 1:H:300:LYS:HB2    | 2.15                     | 0.47              |
| 1:I:305:ASP:O      | 1:I:308:ARG:HG2    | 2.15                     | 0.47              |
| 1:E:20:ARG:O       | 1:E:136:ARG:NH1    | 2.48                     | 0.47              |
| 1:F:54:ILE:HD11    | 1:F:142:ILE:HD13   | 1.97                     | 0.46              |
| 1:D:120[B]:ARG:HG3 | 1:D:120[B]:ARG:NH1 | 2.09                     | 0.46              |
| 1:A:76:GLY:O       | 1:A:377:ARG:HD3    | 2.16                     | 0.46              |
| 1:B:131[A]:ARG:HD3 | 1:B:161:PHE:CZ     | 2.51                     | 0.46              |
| 1:C:54:ILE:HB      | 1:C:145:VAL:HB     | 1.98                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:A:166:VAL:O     | 1:A:323:GLN:HG2    | 2.15                     | 0.46              |
| 1:I:65:VAL:HG22   | 5:I:2036:HOH:O     | 2.14                     | 0.46              |
| 3:K:1386:ACT:H3   | 5:K:2055:HOH:O     | 2.15                     | 0.46              |
| 1:I:269:GLN:H     | 1:I:270:PRO:CD     | 2.28                     | 0.46              |
| 1:B:64:HIS:HD2    | 5:B:2004:HOH:O     | 1.99                     | 0.46              |
| 2:F:1383:COA:H131 | 2:F:1383:COA:H72   | 1.98                     | 0.46              |
| 1:F:363:ASP:OD1   | 2:F:1383:COA:C7P   | 2.63                     | 0.45              |
| 1:A:363:ASP:OD1   | 2:A:1383:COA:H62   | 2.15                     | 0.45              |
| 1:E:54:ILE:HB     | 1:E:145:VAL:HB     | 1.98                     | 0.45              |
| 1:L:33:ARG:HD3    | 5:L:2028:HOH:O     | 2.16                     | 0.45              |
| 1:B:167:ARG:HD2   | 5:B:2079:HOH:O     | 2.17                     | 0.45              |
| 1:H:49:ARG:HG3    | 1:H:49:ARG:HH21    | 1.81                     | 0.45              |
| 1:L:72:LEU:HA     | 1:L:373:ASN:HD22   | 1.82                     | 0.45              |
| 1:B:54:ILE:HB     | 1:B:145:VAL:HB     | 1.99                     | 0.45              |
| 1:G:57:HIS:HB2    | 1:G:61:SER:OG      | 2.16                     | 0.45              |
| 1:F:218:ARG:NH2   | 1:F:222:ASN:HB2    | 2.32                     | 0.45              |
| 1:A:297:MET:O     | 1:A:300:LYS:HB2    | 2.17                     | 0.45              |
| 1:G:234:ARG:O     | 1:G:269:GLN:HA     | 2.16                     | 0.45              |
| 1:F:68:TRP:CE2    | 5:F:2018:HOH:O     | 2.65                     | 0.45              |
| 1:A:20:ARG:O      | 1:A:136:ARG:NH1    | 2.50                     | 0.45              |
| 1:H:234:ARG:O     | 1:H:269:GLN:HA     | 2.16                     | 0.45              |
| 1:I:346:ARG:HH22  | 1:K:346[A]:ARG:HG2 | 1.82                     | 0.44              |
| 1:C:226:LYS:HD3   | 5:C:2132:HOH:O     | 2.18                     | 0.44              |
| 1:H:365:PHE:HZ    | 2:H:1383:COA:H32   | 1.83                     | 0.44              |
| 1:D:303:THR:CG2   | 5:D:2098:HOH:O     | 2.66                     | 0.44              |
| 1:J:326:LEU:HD22  | 1:J:379:PHE:HB2    | 1.98                     | 0.44              |
| 1:L:68:TRP:HZ2    | 5:L:2021:HOH:O     | 1.93                     | 0.44              |
| 1:H:36:PRO:HD2    | 1:H:99:ALA:HB2     | 1.99                     | 0.44              |
| 1:I:346:ARG:NH2   | 1:K:346[A]:ARG:HG2 | 2.33                     | 0.44              |
| 1:K:342:VAL:O     | 1:K:346[A]:ARG:HG3 | 2.18                     | 0.44              |
| 1:D:331:ARG:HH11  | 1:I:382:GLN:HE21   | 1.58                     | 0.44              |
| 1:E:297:MET:O     | 1:E:300:LYS:HB2    | 2.17                     | 0.44              |
| 1:C:80:ASP:OD1    | 1:C:82:SER:HB2     | 2.18                     | 0.44              |
| 1:F:68:TRP:NE1    | 5:F:2018:HOH:O     | 2.51                     | 0.44              |
| 1:K:225:TYR:CD2   | 2:K:1385:COA:H61   | 2.52                     | 0.44              |
| 1:H:235:PHE:HA    | 1:H:269:GLN:O      | 2.18                     | 0.44              |
| 1:D:187:GLU:O     | 1:D:191:GLN:HG3    | 2.18                     | 0.44              |
| 1:L:268:GLY:HA2   | 1:L:273:ALA:CB     | 2.48                     | 0.44              |
| 1:D:274:VAL:HG11  | 1:K:184:ALA:HA     | 1.98                     | 0.43              |
| 1:J:187:GLU:O     | 1:J:191:GLN:HG3    | 2.17                     | 0.43              |
| 1:A:228:LYS:HB3   | 1:A:229:PRO:HD3    | 2.00                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:L:1383:COA:H71   | 2:L:1383:COA:H131  | 1.99                     | 0.43              |
| 1:A:320:MET:HE3    | 5:B:2012:HOH:O     | 2.18                     | 0.43              |
| 1:C:54:ILE:CD1     | 1:C:142:ILE:HD13   | 2.49                     | 0.43              |
| 1:F:363:ASP:OD1    | 2:F:1383:COA:H71   | 2.19                     | 0.43              |
| 1:D:355:VAL:HB     | 1:I:382:GLN:HG2    | 2.00                     | 0.43              |
| 1:I:346:ARG:HD2    | 1:K:346[B]:ARG:NH1 | 2.34                     | 0.43              |
| 1:J:166:VAL:O      | 1:J:323:GLN:HG2    | 2.18                     | 0.43              |
| 1:D:54:ILE:CD1     | 1:D:142:ILE:HD13   | 2.49                     | 0.43              |
| 1:A:320:MET:CE     | 5:B:2012:HOH:O     | 2.67                     | 0.43              |
| 1:K:218[A]:ARG:CD  | 1:K:222[A]:ASN:OD1 | 2.53                     | 0.43              |
| 1:D:170:VAL:HG11   | 1:D:376:VAL:HG22   | 1.99                     | 0.43              |
| 1:A:163:PRO:HG3    | 1:A:322:THR:CG2    | 2.49                     | 0.43              |
| 1:A:305:ASP:O      | 1:A:308:ARG:HG2    | 2.18                     | 0.43              |
| 1:I:234:ARG:O      | 1:I:269:GLN:HB3    | 2.18                     | 0.42              |
| 1:G:367:MET:SD     | 2:G:1383:COA:H132  | 2.59                     | 0.42              |
| 1:E:268:GLY:N      | 2:E:1383:COA:H62A  | 2.17                     | 0.42              |
| 1:G:225:TYR:HA     | 1:G:362:HIS:HB3    | 2.00                     | 0.42              |
| 1:E:163:PRO:HG3    | 1:E:322:THR:CG2    | 2.48                     | 0.42              |
| 1:F:318:LEU:HD13   | 1:F:344:MET:HA     | 2.01                     | 0.42              |
| 1:C:218:ARG:HG3    | 1:C:218:ARG:O      | 2.10                     | 0.42              |
| 1:J:228:LYS:HB3    | 1:J:229:PRO:HD3    | 2.02                     | 0.42              |
| 1:I:166:VAL:O      | 1:I:323:GLN:HG2    | 2.20                     | 0.42              |
| 1:C:118:PHE:HA     | 1:C:119:PRO:HD3    | 1.91                     | 0.42              |
| 1:A:269:GLN:N      | 1:A:270:PRO:HD2    | 2.35                     | 0.42              |
| 1:K:228:LYS:HB3    | 1:K:229:PRO:HD3    | 2.02                     | 0.42              |
| 1:I:54:ILE:HB      | 1:I:145:VAL:HB     | 2.02                     | 0.42              |
| 1:A:313:SER:HB2    | 1:A:315:PRO:HD2    | 2.02                     | 0.42              |
| 1:E:209:GLN:HB3    | 1:E:209:GLN:HE21   | 1.66                     | 0.42              |
| 2:A:1383:COA:H10   | 2:A:1383:COA:H71   | 1.90                     | 0.42              |
| 1:E:116:ALA:HB2    | 1:E:202:GLY:HA3    | 2.01                     | 0.42              |
| 1:C:148:ALA:HA     | 1:C:172:ILE:O      | 2.20                     | 0.42              |
| 1:A:232:ASP:OD1    | 1:I:179:SER:HB2    | 2.20                     | 0.41              |
| 1:A:53:VAL:HB      | 1:A:86:ILE:HD13    | 2.02                     | 0.41              |
| 1:L:218[B]:ARG:HB2 | 1:L:285:PHE:CD1    | 2.55                     | 0.41              |
| 1:J:225:TYR:HA     | 1:J:362:HIS:HB3    | 2.02                     | 0.41              |
| 1:J:218:ARG:NE     | 1:J:222[A]:ASN:CG  | 2.72                     | 0.41              |
| 1:F:54:ILE:HD11    | 1:F:142:ILE:CD1    | 2.50                     | 0.41              |
| 1:D:54:ILE:HB      | 1:D:145:VAL:HB     | 2.02                     | 0.41              |
| 1:K:382:GLN:HB3    | 1:K:384:LEU:CD2    | 2.51                     | 0.41              |
| 1:E:235:PHE:HA     | 1:E:269:GLN:O      | 2.20                     | 0.41              |
| 1:C:187:GLU:O      | 1:C:191:GLN:HG3    | 2.20                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:I:58:THR:HB      | 2:I:1383:COA:H31   | 2.02                     | 0.41              |
| 1:K:176:CYS:SG     | 1:K:318:LEU:HD21   | 2.60                     | 0.41              |
| 1:H:27:GLU:OE1     | 1:H:308[A]:ARG:NH1 | 2.53                     | 0.41              |
| 1:E:237:MET:HG2    | 1:E:271:ILE:HD12   | 2.03                     | 0.41              |
| 1:C:54:ILE:HD11    | 1:C:142:ILE:HD13   | 2.03                     | 0.41              |
| 1:A:31:ILE:HD12    | 1:B:160:PHE:HB3    | 2.03                     | 0.41              |
| 1:J:324:PRO:HA     | 1:J:350:ASN:O      | 2.21                     | 0.41              |
| 1:E:293:CYS:O      | 1:E:297:MET:HG3    | 2.21                     | 0.41              |
| 1:J:20:ARG:O       | 1:J:136[A]:ARG:NH1 | 2.53                     | 0.41              |
| 1:K:284:LYS:NZ     | 2:K:1385:COA:O9A   | 2.48                     | 0.41              |
| 1:G:164[A]:GLU:HB3 | 5:G:2071:HOH:O     | 2.19                     | 0.41              |
| 1:C:274:VAL:HG11   | 1:J:184:ALA:HA     | 2.01                     | 0.41              |
| 1:D:131:ARG:HG3    | 1:D:131:ARG:O      | 2.19                     | 0.41              |
| 1:A:109:GLU:CD     | 1:A:112:ARG:N      | 2.74                     | 0.41              |
| 1:J:284:LYS:NZ     | 2:J:1385:COA:O9A   | 2.46                     | 0.41              |
| 1:I:13:LEU:HB2     | 1:L:44:ARG:HH21    | 1.86                     | 0.41              |
| 1:E:163:PRO:HG3    | 1:E:322:THR:HG22   | 2.02                     | 0.41              |
| 1:J:176:CYS:SG     | 1:J:318:LEU:HD21   | 2.60                     | 0.41              |
| 1:J:223:LEU:HA     | 1:J:223:LEU:HD23   | 1.93                     | 0.41              |
| 1:J:118:PHE:HA     | 1:J:119:PRO:HD3    | 1.90                     | 0.41              |
| 1:G:32:LEU:HD21    | 1:G:119:PRO:HG2    | 2.02                     | 0.41              |
| 1:H:118:PHE:HA     | 1:H:119:PRO:HD3    | 1.91                     | 0.41              |
| 1:D:54:ILE:HD11    | 1:D:142:ILE:HD13   | 2.02                     | 0.41              |
| 1:C:352:ARG:NH1    | 5:C:2126:HOH:O     | 2.48                     | 0.41              |
| 1:E:313:SER:HB2    | 1:E:315:PRO:HD2    | 2.04                     | 0.40              |
| 1:K:237:MET:HG3    | 1:K:271:ILE:HD12   | 2.03                     | 0.40              |
| 1:B:363:ASP:OD1    | 2:B:1383:COA:H72   | 2.21                     | 0.40              |
| 1:H:225:TYR:HA     | 1:H:362:HIS:HB3    | 2.03                     | 0.40              |
| 1:B:49:ARG:NH2     | 5:B:2033:HOH:O     | 2.52                     | 0.40              |
| 1:F:65:VAL:HG22    | 5:F:2018:HOH:O     | 2.21                     | 0.40              |
| 1:L:54:ILE:HD11    | 1:L:142:ILE:HD13   | 2.03                     | 0.40              |
| 1:G:118:PHE:HA     | 1:G:119:PRO:HD3    | 1.94                     | 0.40              |
| 1:H:187:GLU:O      | 1:H:191:GLN:HG3    | 2.22                     | 0.40              |
| 1:A:116:ALA:HB2    | 1:A:202:GLY:HA3    | 2.03                     | 0.40              |
| 1:K:49:ARG:HD2     | 1:K:138:GLY:O      | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 343/444 (77%)   | 332 (97%)  | 11 (3%)  | 0        | 100         | 100 |
| 1   | B     | 343/444 (77%)   | 332 (97%)  | 10 (3%)  | 1 (0%)   | 46          | 50  |
| 1   | C     | 344/444 (78%)   | 334 (97%)  | 10 (3%)  | 0        | 100         | 100 |
| 1   | D     | 345/444 (78%)   | 335 (97%)  | 10 (3%)  | 0        | 100         | 100 |
| 1   | E     | 344/444 (78%)   | 333 (97%)  | 10 (3%)  | 1 (0%)   | 46          | 50  |
| 1   | F     | 336/444 (76%)   | 325 (97%)  | 11 (3%)  | 0        | 100         | 100 |
| 1   | G     | 341/444 (77%)   | 332 (97%)  | 9 (3%)   | 0        | 100         | 100 |
| 1   | H     | 345/444 (78%)   | 334 (97%)  | 11 (3%)  | 0        | 100         | 100 |
| 1   | I     | 343/444 (77%)   | 333 (97%)  | 9 (3%)   | 1 (0%)   | 46          | 50  |
| 1   | J     | 340/444 (77%)   | 327 (96%)  | 13 (4%)  | 0        | 100         | 100 |
| 1   | K     | 341/444 (77%)   | 328 (96%)  | 13 (4%)  | 0        | 100         | 100 |
| 1   | L     | 336/444 (76%)   | 327 (97%)  | 8 (2%)   | 1 (0%)   | 46          | 50  |
| All | All   | 4101/5328 (77%) | 3972 (97%) | 125 (3%) | 4 (0%)   | 56          | 64  |

All (4) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 269 | GLN  |
| 1   | E     | 269 | GLN  |
| 1   | I     | 269 | GLN  |
| 1   | L     | 269 | GLN  |

### 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     | 293/372 (79%)   | 286 (98%)  | 7 (2%)   | 57          | 69 |
| 1   | B     | 292/372 (78%)   | 286 (98%)  | 6 (2%)   | 61          | 74 |
| 1   | C     | 293/372 (79%)   | 286 (98%)  | 7 (2%)   | 57          | 69 |
| 1   | D     | 294/372 (79%)   | 286 (97%)  | 8 (3%)   | 52          | 64 |
| 1   | E     | 293/372 (79%)   | 287 (98%)  | 6 (2%)   | 63          | 76 |
| 1   | F     | 287/372 (77%)   | 280 (98%)  | 7 (2%)   | 57          | 69 |
| 1   | G     | 293/372 (79%)   | 283 (97%)  | 10 (3%)  | 44          | 54 |
| 1   | H     | 295/372 (79%)   | 286 (97%)  | 9 (3%)   | 47          | 59 |
| 1   | I     | 292/372 (78%)   | 287 (98%)  | 5 (2%)   | 68          | 81 |
| 1   | J     | 291/372 (78%)   | 287 (99%)  | 4 (1%)   | 74          | 85 |
| 1   | K     | 292/372 (78%)   | 286 (98%)  | 6 (2%)   | 61          | 74 |
| 1   | L     | 288/372 (77%)   | 281 (98%)  | 7 (2%)   | 57          | 69 |
| All | All   | 3503/4464 (78%) | 3421 (98%) | 82 (2%)  | 60          | 71 |

All (82) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 69  | TRP  |
| 1   | A     | 164 | GLU  |
| 1   | A     | 177 | ARG  |
| 1   | A     | 200 | LEU  |
| 1   | A     | 201 | ASP  |
| 1   | A     | 283 | GLN  |
| 1   | A     | 380 | LEU  |
| 1   | B     | 69  | TRP  |
| 1   | B     | 145 | VAL  |
| 1   | B     | 200 | LEU  |
| 1   | B     | 201 | ASP  |
| 1   | B     | 283 | GLN  |
| 1   | B     | 380 | LEU  |
| 1   | C     | 131 | ARG  |
| 1   | C     | 145 | VAL  |
| 1   | C     | 201 | ASP  |
| 1   | C     | 218 | ARG  |
| 1   | C     | 271 | ILE  |
| 1   | C     | 380 | LEU  |
| 1   | C     | 382 | GLN  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | D     | 131    | ARG  |
| 1   | D     | 140    | ARG  |
| 1   | D     | 145    | VAL  |
| 1   | D     | 200    | LEU  |
| 1   | D     | 201    | ASP  |
| 1   | D     | 218    | ARG  |
| 1   | D     | 283    | GLN  |
| 1   | D     | 380    | LEU  |
| 1   | E     | 69     | TRP  |
| 1   | E     | 145    | VAL  |
| 1   | E     | 200    | LEU  |
| 1   | E     | 201    | ASP  |
| 1   | E     | 283    | GLN  |
| 1   | E     | 380    | LEU  |
| 1   | F     | 69     | TRP  |
| 1   | F     | 82     | SER  |
| 1   | F     | 145    | VAL  |
| 1   | F     | 201    | ASP  |
| 1   | F     | 269    | GLN  |
| 1   | F     | 271    | ILE  |
| 1   | F     | 380    | LEU  |
| 1   | G     | 69     | TRP  |
| 1   | G     | 134    | LEU  |
| 1   | G     | 140[A] | ARG  |
| 1   | G     | 140[B] | ARG  |
| 1   | G     | 145    | VAL  |
| 1   | G     | 164[A] | GLU  |
| 1   | G     | 164[B] | GLU  |
| 1   | G     | 331    | ARG  |
| 1   | G     | 377    | ARG  |
| 1   | G     | 380    | LEU  |
| 1   | H     | 33[A]  | ARG  |
| 1   | H     | 33[B]  | ARG  |
| 1   | H     | 69     | TRP  |
| 1   | H     | 131[A] | ARG  |
| 1   | H     | 131[B] | ARG  |
| 1   | H     | 140[A] | ARG  |
| 1   | H     | 140[B] | ARG  |
| 1   | H     | 145    | VAL  |
| 1   | H     | 380    | LEU  |
| 1   | I     | 69     | TRP  |
| 1   | I     | 145    | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 200 | LEU  |
| 1   | I     | 201 | ASP  |
| 1   | I     | 380 | LEU  |
| 1   | J     | 20  | ARG  |
| 1   | J     | 69  | TRP  |
| 1   | J     | 145 | VAL  |
| 1   | J     | 201 | ASP  |
| 1   | K     | 33  | ARG  |
| 1   | K     | 69  | TRP  |
| 1   | K     | 145 | VAL  |
| 1   | K     | 201 | ASP  |
| 1   | K     | 271 | ILE  |
| 1   | K     | 383 | SER  |
| 1   | L     | 20  | ARG  |
| 1   | L     | 67  | SER  |
| 1   | L     | 69  | TRP  |
| 1   | L     | 145 | VAL  |
| 1   | L     | 201 | ASP  |
| 1   | L     | 346 | ARG  |
| 1   | L     | 380 | LEU  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 209 | GLN  |
| 1   | A     | 373 | ASN  |
| 1   | B     | 64  | HIS  |
| 1   | B     | 75  | GLN  |
| 1   | B     | 209 | GLN  |
| 1   | B     | 269 | GLN  |
| 1   | C     | 189 | GLN  |
| 1   | C     | 191 | GLN  |
| 1   | C     | 209 | GLN  |
| 1   | C     | 373 | ASN  |
| 1   | D     | 209 | GLN  |
| 1   | D     | 269 | GLN  |
| 1   | D     | 373 | ASN  |
| 1   | E     | 209 | GLN  |
| 1   | E     | 373 | ASN  |
| 1   | F     | 64  | HIS  |
| 1   | F     | 191 | GLN  |
| 1   | F     | 209 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 269 | GLN  |
| 1   | F     | 373 | ASN  |
| 1   | G     | 64  | HIS  |
| 1   | G     | 209 | GLN  |
| 1   | G     | 269 | GLN  |
| 1   | G     | 281 | GLN  |
| 1   | G     | 373 | ASN  |
| 1   | H     | 64  | HIS  |
| 1   | H     | 209 | GLN  |
| 1   | H     | 281 | GLN  |
| 1   | H     | 373 | ASN  |
| 1   | I     | 209 | GLN  |
| 1   | I     | 373 | ASN  |
| 1   | I     | 382 | GLN  |
| 1   | J     | 64  | HIS  |
| 1   | J     | 209 | GLN  |
| 1   | J     | 373 | ASN  |
| 1   | K     | 64  | HIS  |
| 1   | K     | 209 | GLN  |
| 1   | K     | 373 | ASN  |
| 1   | L     | 64  | HIS  |
| 1   | L     | 209 | GLN  |
| 1   | L     | 373 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

26 ligands are modelled in this entry.



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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 2   | COA  | A     | 1383 | -    | 40,50,50     | 2.19 | 14 (35%)    | 50,75,75    | 2.17 | 9 (18%)     |
| 3   | ACT  | A     | 1384 | -    | 1,3,3        | 1.27 | 0           | 0,3,3       | 0.00 | -           |
| 2   | COA  | B     | 1383 | -    | 40,50,50     | 1.69 | 3 (7%)      | 50,75,75    | 2.13 | 6 (12%)     |
| 4   | GOL  | B     | 1384 | -    | 5,5,5        | 0.30 | 0           | 5,5,5       | 0.36 | 0           |
| 3   | ACT  | B     | 1385 | -    | 1,3,3        | 0.68 | 0           | 0,3,3       | 0.00 | -           |
| 2   | COA  | C     | 1383 | -    | 40,50,50     | 1.85 | 4 (10%)     | 50,75,75    | 2.07 | 4 (8%)      |
| 3   | ACT  | C     | 1384 | -    | 1,3,3        | 0.91 | 0           | 0,3,3       | 0.00 | -           |
| 2   | COA  | D     | 1383 | -    | 40,50,50     | 1.85 | 4 (10%)     | 50,75,75    | 2.03 | 5 (10%)     |
| 3   | ACT  | D     | 1384 | -    | 1,3,3        | 0.28 | 0           | 0,3,3       | 0.00 | -           |
| 2   | COA  | E     | 1383 | -    | 40,50,50     | 2.13 | 12 (30%)    | 50,75,75    | 2.03 | 9 (18%)     |
| 3   | ACT  | E     | 1384 | -    | 1,3,3        | 1.31 | 0           | 0,3,3       | 0.00 | -           |
| 2   | COA  | F     | 1383 | -    | 40,50,50     | 1.86 | 3 (7%)      | 50,75,75    | 2.03 | 3 (6%)      |
| 3   | ACT  | F     | 1384 | -    | 1,3,3        | 1.74 | 0           | 0,3,3       | 0.00 | -           |
| 2   | COA  | G     | 1383 | -    | 40,50,50     | 1.79 | 3 (7%)      | 50,75,75    | 1.92 | 5 (10%)     |
| 3   | ACT  | G     | 1384 | -    | 1,3,3        | 1.11 | 0           | 0,3,3       | 0.00 | -           |
| 2   | COA  | H     | 1383 | -    | 40,50,50     | 2.03 | 9 (22%)     | 50,75,75    | 2.33 | 11 (22%)    |
| 3   | ACT  | H     | 1384 | -    | 1,3,3        | 1.87 | 0           | 0,3,3       | 0.00 | -           |
| 2   | COA  | I     | 1383 | -    | 40,50,50     | 1.70 | 3 (7%)      | 50,75,75    | 2.15 | 7 (14%)     |
| 4   | GOL  | I     | 1384 | -    | 5,5,5        | 0.35 | 0           | 5,5,5       | 0.21 | 0           |
| 3   | ACT  | I     | 1385 | -    | 1,3,3        | 1.44 | 0           | 0,3,3       | 0.00 | -           |
| 2   | COA  | J     | 1385 | -    | 40,50,50     | 1.80 | 4 (10%)     | 50,75,75    | 1.95 | 3 (6%)      |
| 3   | ACT  | J     | 1386 | -    | 1,3,3        | 1.71 | 0           | 0,3,3       | 0.00 | -           |
| 2   | COA  | K     | 1385 | -    | 40,50,50     | 1.81 | 4 (10%)     | 50,75,75    | 2.12 | 5 (10%)     |
| 3   | ACT  | K     | 1386 | -    | 1,3,3        | 1.75 | 0           | 0,3,3       | 0.00 | -           |
| 2   | COA  | L     | 1383 | -    | 40,50,50     | 1.80 | 3 (7%)      | 50,75,75    | 2.15 | 3 (6%)      |
| 3   | ACT  | L     | 1384 | -    | 1,3,3        | 1.77 | 0           | 0,3,3       | 0.00 | -           |

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   | COA  | A     | 1383 | -    | -       | 2/44/64/64 | 0/3/3/3 |
| 3   | ACT  | A     | 1384 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 2   | COA  | B     | 1383 | -    | -       | 1/44/64/64 | 0/3/3/3 |
| 4   | GOL  | B     | 1384 | -    | -       | 0/4/4/4    | 0/0/0/0 |
| 3   | ACT  | B     | 1385 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 2   | COA  | C     | 1383 | -    | -       | 0/44/64/64 | 0/3/3/3 |
| 3   | ACT  | C     | 1384 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 2   | COA  | D     | 1383 | -    | -       | 0/44/64/64 | 0/3/3/3 |
| 3   | ACT  | D     | 1384 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 2   | COA  | E     | 1383 | -    | -       | 1/44/64/64 | 0/3/3/3 |
| 3   | ACT  | E     | 1384 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 2   | COA  | F     | 1383 | -    | -       | 1/44/64/64 | 0/3/3/3 |
| 3   | ACT  | F     | 1384 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 2   | COA  | G     | 1383 | -    | -       | 0/44/64/64 | 0/3/3/3 |
| 3   | ACT  | G     | 1384 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 2   | COA  | H     | 1383 | -    | -       | 0/44/64/64 | 0/3/3/3 |
| 3   | ACT  | H     | 1384 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 2   | COA  | I     | 1383 | -    | -       | 1/44/64/64 | 0/3/3/3 |
| 4   | GOL  | I     | 1384 | -    | -       | 0/4/4/4    | 0/0/0/0 |
| 3   | ACT  | I     | 1385 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 2   | COA  | J     | 1385 | -    | -       | 0/44/64/64 | 0/3/3/3 |
| 3   | ACT  | J     | 1386 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 2   | COA  | K     | 1385 | -    | -       | 0/44/64/64 | 0/3/3/3 |
| 3   | ACT  | K     | 1386 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 2   | COA  | L     | 1383 | -    | -       | 0/44/64/64 | 0/3/3/3 |
| 3   | ACT  | L     | 1384 | -    | -       | 0/0/0/0    | 0/0/0/0 |

All (66) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | E     | 1383 | COA  | P3B-O8A | -3.78 | 1.41        | 1.54     |
| 2   | A     | 1383 | COA  | P1A-O2A | -3.48 | 1.40        | 1.54     |
| 2   | E     | 1383 | COA  | P1A-O2A | -3.47 | 1.40        | 1.54     |
| 2   | A     | 1383 | COA  | O4B-C1B | -3.40 | 1.36        | 1.41     |
| 2   | A     | 1383 | COA  | P3B-O8A | -3.26 | 1.43        | 1.54     |
| 2   | A     | 1383 | COA  | P3B-O9A | -3.06 | 1.43        | 1.54     |
| 2   | H     | 1383 | COA  | P3B-O9A | -2.81 | 1.44        | 1.54     |
| 2   | E     | 1383 | COA  | P3B-O9A | -2.77 | 1.44        | 1.54     |
| 2   | H     | 1383 | COA  | P3B-O8A | -2.77 | 1.44        | 1.54     |
| 2   | A     | 1383 | COA  | C6A-N6A | -2.71 | 1.26        | 1.34     |
| 2   | E     | 1383 | COA  | C6A-N6A | -2.68 | 1.26        | 1.34     |
| 2   | H     | 1383 | COA  | C5A-C4A | -2.63 | 1.34        | 1.40     |
| 2   | A     | 1383 | COA  | P2A-O4A | -2.61 | 1.41        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | E     | 1383 | COA  | O2B-C2B | -2.59 | 1.36        | 1.43     |
| 2   | E     | 1383 | COA  | P1A-O1A | -2.58 | 1.41        | 1.51     |
| 2   | A     | 1383 | COA  | C5A-C4A | -2.56 | 1.34        | 1.40     |
| 2   | H     | 1383 | COA  | C8A-N7A | -2.52 | 1.29        | 1.34     |
| 2   | A     | 1383 | COA  | C5A-N7A | -2.44 | 1.31        | 1.39     |
| 2   | E     | 1383 | COA  | P2A-O4A | -2.44 | 1.42        | 1.51     |
| 2   | E     | 1383 | COA  | C5A-N7A | -2.39 | 1.31        | 1.39     |
| 2   | H     | 1383 | COA  | O2B-C2B | -2.34 | 1.37        | 1.43     |
| 2   | A     | 1383 | COA  | P1A-O1A | -2.30 | 1.42        | 1.51     |
| 2   | E     | 1383 | COA  | P2A-O5A | -2.28 | 1.45        | 1.54     |
| 2   | H     | 1383 | COA  | P1A-O2A | -2.28 | 1.45        | 1.54     |
| 2   | A     | 1383 | COA  | P2A-O5A | -2.27 | 1.45        | 1.54     |
| 2   | H     | 1383 | COA  | C5A-N7A | -2.26 | 1.31        | 1.39     |
| 2   | A     | 1383 | COA  | C9P-N8P | -2.26 | 1.28        | 1.33     |
| 2   | E     | 1383 | COA  | C5A-C4A | -2.17 | 1.35        | 1.40     |
| 2   | A     | 1383 | COA  | C4A-N3A | -2.12 | 1.32        | 1.35     |
| 2   | E     | 1383 | COA  | O4B-C4B | -2.07 | 1.40        | 1.45     |
| 2   | A     | 1383 | COA  | O2B-C2B | -2.00 | 1.38        | 1.43     |
| 2   | H     | 1383 | COA  | C2A-N3A | 2.14  | 1.36        | 1.32     |
| 2   | I     | 1383 | COA  | C2A-N1A | 2.18  | 1.38        | 1.33     |
| 2   | J     | 1385 | COA  | O4B-C1B | 2.21  | 1.44        | 1.41     |
| 2   | K     | 1385 | COA  | C2A-N1A | 2.22  | 1.38        | 1.33     |
| 2   | C     | 1383 | COA  | O4B-C1B | 2.43  | 1.44        | 1.41     |
| 2   | B     | 1383 | COA  | C2A-N1A | 2.43  | 1.38        | 1.33     |
| 2   | D     | 1383 | COA  | C2A-N1A | 2.60  | 1.38        | 1.33     |
| 2   | L     | 1383 | COA  | C2A-N1A | 2.68  | 1.39        | 1.33     |
| 2   | C     | 1383 | COA  | C2A-N1A | 2.69  | 1.39        | 1.33     |
| 2   | D     | 1383 | COA  | O4B-C1B | 2.79  | 1.44        | 1.41     |
| 2   | J     | 1385 | COA  | C2A-N1A | 2.79  | 1.39        | 1.33     |
| 2   | F     | 1383 | COA  | C2A-N1A | 2.82  | 1.39        | 1.33     |
| 2   | G     | 1383 | COA  | C2A-N1A | 2.85  | 1.39        | 1.33     |
| 2   | K     | 1385 | COA  | O4B-C1B | 2.87  | 1.44        | 1.41     |
| 2   | B     | 1383 | COA  | C2A-N3A | 3.38  | 1.38        | 1.32     |
| 2   | I     | 1383 | COA  | C2A-N3A | 3.50  | 1.38        | 1.32     |
| 2   | K     | 1385 | COA  | C2A-N3A | 3.73  | 1.38        | 1.32     |
| 2   | G     | 1383 | COA  | C2A-N3A | 3.84  | 1.39        | 1.32     |
| 2   | J     | 1385 | COA  | C2A-N3A | 3.84  | 1.39        | 1.32     |
| 2   | L     | 1383 | COA  | C2A-N3A | 3.85  | 1.39        | 1.32     |
| 2   | F     | 1383 | COA  | C2A-N3A | 4.00  | 1.39        | 1.32     |
| 2   | C     | 1383 | COA  | C2A-N3A | 4.12  | 1.39        | 1.32     |
| 2   | D     | 1383 | COA  | C2A-N3A | 4.32  | 1.39        | 1.32     |
| 2   | E     | 1383 | COA  | O9P-C9P | 8.09  | 1.39        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 2   | A     | 1383 | COA  | O9P-C9P | 8.14 | 1.39        | 1.23     |
| 2   | H     | 1383 | COA  | O9P-C9P | 8.82 | 1.40        | 1.23     |
| 2   | B     | 1383 | COA  | O9P-C9P | 8.91 | 1.40        | 1.23     |
| 2   | I     | 1383 | COA  | O9P-C9P | 9.16 | 1.41        | 1.23     |
| 2   | J     | 1385 | COA  | O9P-C9P | 9.27 | 1.41        | 1.23     |
| 2   | D     | 1383 | COA  | O9P-C9P | 9.57 | 1.42        | 1.23     |
| 2   | K     | 1385 | COA  | O9P-C9P | 9.58 | 1.42        | 1.23     |
| 2   | G     | 1383 | COA  | O9P-C9P | 9.61 | 1.42        | 1.23     |
| 2   | L     | 1383 | COA  | O9P-C9P | 9.68 | 1.42        | 1.23     |
| 2   | C     | 1383 | COA  | O9P-C9P | 9.76 | 1.42        | 1.23     |
| 2   | F     | 1383 | COA  | O9P-C9P | 9.97 | 1.42        | 1.23     |

All (70) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 2   | L     | 1383 | COA  | N3A-C2A-N1A | -13.37 | 118.66      | 128.89   |
| 2   | K     | 1385 | COA  | N3A-C2A-N1A | -12.92 | 119.00      | 128.89   |
| 2   | I     | 1383 | COA  | N3A-C2A-N1A | -12.61 | 119.24      | 128.89   |
| 2   | F     | 1383 | COA  | N3A-C2A-N1A | -12.35 | 119.44      | 128.89   |
| 2   | B     | 1383 | COA  | N3A-C2A-N1A | -12.27 | 119.50      | 128.89   |
| 2   | C     | 1383 | COA  | N3A-C2A-N1A | -12.20 | 119.56      | 128.89   |
| 2   | D     | 1383 | COA  | N3A-C2A-N1A | -12.04 | 119.67      | 128.89   |
| 2   | J     | 1385 | COA  | N3A-C2A-N1A | -11.98 | 119.72      | 128.89   |
| 2   | G     | 1383 | COA  | N3A-C2A-N1A | -11.69 | 119.94      | 128.89   |
| 2   | A     | 1383 | COA  | N3A-C2A-N1A | -11.67 | 119.96      | 128.89   |
| 2   | H     | 1383 | COA  | N3A-C2A-N1A | -10.34 | 120.98      | 128.89   |
| 2   | E     | 1383 | COA  | N3A-C2A-N1A | -9.98  | 121.25      | 128.89   |
| 2   | B     | 1383 | COA  | P2A-O3A-P1A | -3.88  | 121.84      | 132.73   |
| 2   | I     | 1383 | COA  | P2A-O3A-P1A | -3.83  | 121.98      | 132.73   |
| 2   | E     | 1383 | COA  | C4A-C5A-N7A | -3.61  | 106.16      | 109.48   |
| 2   | B     | 1383 | COA  | C2B-C1B-N9A | -3.35  | 109.17      | 114.29   |
| 2   | K     | 1385 | COA  | P2A-O3A-P1A | -3.34  | 123.34      | 132.73   |
| 2   | I     | 1383 | COA  | C2B-C1B-N9A | -3.19  | 109.42      | 114.29   |
| 2   | C     | 1383 | COA  | C7P-C6P-C5P | -2.99  | 107.39      | 112.31   |
| 2   | F     | 1383 | COA  | P2A-O3A-P1A | -2.99  | 124.34      | 132.73   |
| 2   | L     | 1383 | COA  | P2A-O3A-P1A | -2.96  | 124.42      | 132.73   |
| 2   | E     | 1383 | COA  | C1B-N9A-C4A | -2.96  | 122.48      | 126.94   |
| 2   | C     | 1383 | COA  | P2A-O3A-P1A | -2.96  | 124.43      | 132.73   |
| 2   | E     | 1383 | COA  | C3P-N4P-C5P | -2.92  | 117.05      | 122.79   |
| 2   | H     | 1383 | COA  | CDP-CBP-CAP | -2.92  | 104.02      | 109.34   |
| 2   | G     | 1383 | COA  | P2A-O3A-P1A | -2.85  | 124.72      | 132.73   |
| 2   | D     | 1383 | COA  | P2A-O3A-P1A | -2.83  | 124.80      | 132.73   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | A     | 1383 | COA  | OAP-CAP-C9P | -2.82 | 103.91      | 110.38   |
| 2   | H     | 1383 | COA  | C4A-C5A-N7A | -2.68 | 107.01      | 109.48   |
| 2   | H     | 1383 | COA  | C2B-C1B-N9A | -2.67 | 110.20      | 114.29   |
| 2   | J     | 1385 | COA  | P2A-O3A-P1A | -2.66 | 125.25      | 132.73   |
| 2   | E     | 1383 | COA  | C7P-C6P-C5P | -2.60 | 108.03      | 112.31   |
| 2   | K     | 1385 | COA  | C2B-C1B-N9A | -2.58 | 110.35      | 114.29   |
| 2   | B     | 1383 | COA  | C7P-C6P-C5P | -2.52 | 108.15      | 112.31   |
| 2   | I     | 1383 | COA  | C3P-N4P-C5P | -2.49 | 117.89      | 122.79   |
| 2   | A     | 1383 | COA  | C4A-C5A-N7A | -2.49 | 107.19      | 109.48   |
| 2   | G     | 1383 | COA  | C4A-C5A-N7A | -2.39 | 107.28      | 109.48   |
| 2   | A     | 1383 | COA  | C5B-C4B-C3B | -2.36 | 105.83      | 114.31   |
| 2   | D     | 1383 | COA  | C7P-C6P-C5P | -2.33 | 108.48      | 112.31   |
| 2   | G     | 1383 | COA  | C1B-N9A-C4A | -2.31 | 123.45      | 126.94   |
| 2   | I     | 1383 | COA  | C4A-C5A-N7A | -2.22 | 107.44      | 109.48   |
| 2   | I     | 1383 | COA  | C7P-C6P-C5P | -2.14 | 108.78      | 112.31   |
| 2   | K     | 1385 | COA  | C1B-N9A-C4A | -2.10 | 123.77      | 126.94   |
| 2   | F     | 1383 | COA  | O5P-C5P-C6P | -2.07 | 118.41      | 121.98   |
| 2   | H     | 1383 | COA  | O8A-P3B-O7A | -2.07 | 103.92      | 110.58   |
| 2   | E     | 1383 | COA  | OAP-CAP-C9P | -2.03 | 105.72      | 110.38   |
| 2   | A     | 1383 | COA  | C1B-N9A-C4A | -2.02 | 123.89      | 126.94   |
| 2   | B     | 1383 | COA  | O3A-P1A-O5B | -2.00 | 97.62       | 102.94   |
| 2   | H     | 1383 | COA  | O9A-P3B-O7A | 2.02  | 117.08      | 110.58   |
| 2   | G     | 1383 | COA  | CDP-CBP-CCP | 2.06  | 111.17      | 108.50   |
| 2   | D     | 1383 | COA  | P3B-O3B-C3B | 2.11  | 126.63      | 121.56   |
| 2   | B     | 1383 | COA  | O4B-C1B-N9A | 2.17  | 112.64      | 108.10   |
| 2   | H     | 1383 | COA  | O3A-P2A-O6A | 2.18  | 108.71      | 102.94   |
| 2   | H     | 1383 | COA  | O2A-P1A-O3A | 2.22  | 115.15      | 105.09   |
| 2   | E     | 1383 | COA  | CAP-C9P-N8P | 2.23  | 121.42      | 116.47   |
| 2   | A     | 1383 | COA  | CDP-CBP-CAP | 2.30  | 113.55      | 109.34   |
| 2   | L     | 1383 | COA  | P3B-O3B-C3B | 2.39  | 127.29      | 121.56   |
| 2   | I     | 1383 | COA  | O4B-C1B-N9A | 2.50  | 113.33      | 108.10   |
| 2   | A     | 1383 | COA  | O6A-CCP-CBP | 2.57  | 114.67      | 110.55   |
| 2   | J     | 1385 | COA  | O4B-C1B-N9A | 2.58  | 113.50      | 108.10   |
| 2   | A     | 1383 | COA  | CDP-CBP-CCP | 2.67  | 111.97      | 108.50   |
| 2   | H     | 1383 | COA  | C7P-N8P-C9P | 2.77  | 128.01      | 122.53   |
| 2   | K     | 1385 | COA  | O4B-C1B-N9A | 2.98  | 114.35      | 108.10   |
| 2   | E     | 1383 | COA  | O4B-C1B-N9A | 3.04  | 114.47      | 108.10   |
| 2   | C     | 1383 | COA  | O4B-C1B-N9A | 3.20  | 114.80      | 108.10   |
| 2   | D     | 1383 | COA  | O4B-C1B-N9A | 3.29  | 114.99      | 108.10   |
| 2   | A     | 1383 | COA  | O4B-C1B-N9A | 3.34  | 115.09      | 108.10   |
| 2   | E     | 1383 | COA  | O6A-CCP-CBP | 3.36  | 115.94      | 110.55   |
| 2   | H     | 1383 | COA  | O6A-CCP-CBP | 5.05  | 118.66      | 110.55   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|-------------|------|------------------------|---------------------|
| 2   | H     | 1383 | COA  | CDP-CBP-CCP | 7.12 | 117.73                 | 108.50              |

There are no chirality outliers.

All (6) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 2   | I     | 1383 | COA  | CAP-C9P-N8P-C7P |
| 2   | A     | 1383 | COA  | C6P-C5P-N4P-C3P |
| 2   | B     | 1383 | COA  | CAP-C9P-N8P-C7P |
| 2   | F     | 1383 | COA  | CAP-C9P-N8P-C7P |
| 2   | E     | 1383 | COA  | CAP-C9P-N8P-C7P |
| 2   | A     | 1383 | COA  | CAP-C9P-N8P-C7P |

There are no ring outliers.

15 monomers are involved in 36 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2   | A     | 1383 | COA  | 2       | 0            |
| 2   | B     | 1383 | COA  | 2       | 0            |
| 3   | B     | 1385 | ACT  | 1       | 0            |
| 2   | E     | 1383 | COA  | 1       | 0            |
| 2   | F     | 1383 | COA  | 3       | 0            |
| 2   | G     | 1383 | COA  | 5       | 0            |
| 3   | G     | 1384 | ACT  | 1       | 0            |
| 2   | H     | 1383 | COA  | 6       | 0            |
| 3   | H     | 1384 | ACT  | 3       | 0            |
| 2   | I     | 1383 | COA  | 1       | 0            |
| 2   | J     | 1385 | COA  | 3       | 0            |
| 2   | K     | 1385 | COA  | 4       | 0            |
| 3   | K     | 1386 | ACT  | 2       | 0            |
| 2   | L     | 1383 | COA  | 1       | 0            |
| 3   | L     | 1384 | ACT  | 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     | 347/444 (78%)   | 0.79   | 12 (3%)   | 48 | 46 | 11, 22, 38, 57        | 2 (0%)  |
| 1   | B     | 347/444 (78%)   | 1.10   | 35 (10%)  | 9  | 8  | 12, 22, 38, 51        | 1 (0%)  |
| 1   | C     | 345/444 (77%)   | 1.14   | 50 (14%)  | 3  | 3  | 12, 22, 39, 59        | 1 (0%)  |
| 1   | D     | 345/444 (77%)   | 1.04   | 37 (10%)  | 8  | 7  | 12, 22, 38, 55        | 0       |
| 1   | E     | 346/444 (77%)   | 0.79   | 13 (3%)   | 44 | 43 | 9, 22, 36, 51         | 1 (0%)  |
| 1   | F     | 342/444 (77%)   | 1.40   | 84 (24%)  | 1  | 1  | 12, 23, 37, 51        | 2 (0%)  |
| 1   | G     | 342/444 (77%)   | 1.10   | 38 (11%)  | 7  | 7  | 12, 22, 37, 51        | 1 (0%)  |
| 1   | H     | 345/444 (77%)   | 1.00   | 37 (10%)  | 8  | 7  | 12, 22, 38, 52        | 2 (0%)  |
| 1   | I     | 347/444 (78%)   | 1.04   | 27 (7%)   | 16 | 15 | 10, 22, 38, 51        | 1 (0%)  |
| 1   | J     | 344/444 (77%)   | 2.91   | 227 (65%) | 0  | 0  | 13, 23, 38, 54        | 2 (0%)  |
| 1   | K     | 344/444 (77%)   | 2.66   | 200 (58%) | 0  | 0  | 13, 23, 38, 53        | 2 (0%)  |
| 1   | L     | 341/444 (76%)   | 1.45   | 96 (28%)  | 1  | 1  | 12, 23, 37, 51        | 2 (0%)  |
| All | All   | 4135/5328 (77%) | 1.37   | 856 (20%) | 1  | 1  | 9, 22, 38, 59         | 17 (0%) |

All (856) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | J     | 193 | ILE  | 11.6 |
| 1   | K     | 106 | PRO  | 11.5 |
| 1   | J     | 104 | PRO  | 10.6 |
| 1   | K     | 104 | PRO  | 10.5 |
| 1   | K     | 193 | ILE  | 10.5 |
| 1   | J     | 106 | PRO  | 9.1  |
| 1   | J     | 47  | VAL  | 9.0  |
| 1   | J     | 200 | LEU  | 8.7  |
| 1   | J     | 97  | GLY  | 8.6  |
| 1   | K     | 317 | ALA  | 8.6  |
| 1   | J     | 113 | PRO  | 8.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | K     | 88  | CYS  | 8.0  |
| 1   | K     | 47  | VAL  | 7.9  |
| 1   | J     | 115 | GLY  | 7.8  |
| 1   | K     | 96  | PHE  | 7.7  |
| 1   | C     | 282 | ALA  | 7.6  |
| 1   | H     | 282 | ALA  | 7.5  |
| 1   | K     | 137 | LEU  | 7.1  |
| 1   | J     | 103 | SER  | 7.1  |
| 1   | J     | 96  | PHE  | 7.1  |
| 1   | D     | 271 | ILE  | 7.0  |
| 1   | K     | 42  | TRP  | 7.0  |
| 1   | K     | 115 | GLY  | 7.0  |
| 1   | K     | 97  | GLY  | 6.8  |
| 1   | J     | 32  | LEU  | 6.7  |
| 1   | J     | 102 | CYS  | 6.7  |
| 1   | J     | 161 | PHE  | 6.7  |
| 1   | J     | 95  | PRO  | 6.7  |
| 1   | C     | 278 | LEU  | 6.6  |
| 1   | J     | 206 | VAL  | 6.6  |
| 1   | J     | 15  | ALA  | 6.6  |
| 1   | K     | 75  | GLN  | 6.5  |
| 1   | J     | 137 | LEU  | 6.4  |
| 1   | J     | 134 | LEU  | 6.4  |
| 1   | J     | 91  | TYR  | 6.3  |
| 1   | J     | 18  | ILE  | 6.3  |
| 1   | K     | 38  | ALA  | 6.3  |
| 1   | K     | 113 | PRO  | 6.2  |
| 1   | H     | 275 | SER  | 6.2  |
| 1   | J     | 123 | ILE  | 6.1  |
| 1   | D     | 278 | LEU  | 6.1  |
| 1   | K     | 139 | VAL  | 6.1  |
| 1   | J     | 90  | ASN  | 6.1  |
| 1   | L     | 205 | ASP  | 6.1  |
| 1   | J     | 192 | CYS  | 6.1  |
| 1   | I     | 238 | ALA  | 6.0  |
| 1   | J     | 199 | TYR  | 6.0  |
| 1   | J     | 24  | PHE  | 6.0  |
| 1   | J     | 88  | CYS  | 6.0  |
| 1   | K     | 134 | LEU  | 5.9  |
| 1   | K     | 140 | ARG  | 5.9  |
| 1   | K     | 24  | PHE  | 5.7  |
| 1   | J     | 12  | SER  | 5.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 274 | VAL  | 5.7  |
| 1   | J     | 211 | VAL  | 5.7  |
| 1   | J     | 214 | LEU  | 5.7  |
| 1   | J     | 127 | VAL  | 5.7  |
| 1   | K     | 102 | CYS  | 5.6  |
| 1   | L     | 202 | GLY  | 5.5  |
| 1   | K     | 80  | ASP  | 5.5  |
| 1   | K     | 321 | ILE  | 5.5  |
| 1   | G     | 206 | VAL  | 5.5  |
| 1   | B     | 241 | VAL  | 5.5  |
| 1   | K     | 32  | LEU  | 5.4  |
| 1   | K     | 122 | THR  | 5.4  |
| 1   | K     | 107 | ASP  | 5.4  |
| 1   | I     | 239 | PRO  | 5.3  |
| 1   | L     | 197 | PRO  | 5.3  |
| 1   | K     | 105 | ASP  | 5.3  |
| 1   | K     | 12  | SER  | 5.3  |
| 1   | J     | 76  | GLY  | 5.3  |
| 1   | K     | 43  | GLY  | 5.3  |
| 1   | K     | 268 | GLY  | 5.3  |
| 1   | K     | 214 | LEU  | 5.3  |
| 1   | J     | 294 | TYR  | 5.2  |
| 1   | J     | 11  | ALA  | 5.2  |
| 1   | J     | 130 | HIS  | 5.2  |
| 1   | J     | 197 | PRO  | 5.2  |
| 1   | J     | 105 | ASP  | 5.2  |
| 1   | J     | 64  | HIS  | 5.1  |
| 1   | K     | 39  | TYR  | 5.1  |
| 1   | D     | 282 | ALA  | 5.1  |
| 1   | J     | 63  | ALA  | 5.1  |
| 1   | J     | 7   | ASN  | 5.1  |
| 1   | B     | 282 | ALA  | 5.0  |
| 1   | C     | 234 | ARG  | 5.0  |
| 1   | H     | 212 | ARG  | 5.0  |
| 1   | J     | 39  | TYR  | 5.0  |
| 1   | K     | 143 | ALA  | 5.0  |
| 1   | K     | 209 | GLN  | 4.9  |
| 1   | K     | 200 | LEU  | 4.9  |
| 1   | K     | 52  | CYS  | 4.9  |
| 1   | K     | 86  | ILE  | 4.9  |
| 1   | K     | 123 | ILE  | 4.9  |
| 1   | K     | 129 | ILE  | 4.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | L     | 193 | ILE  | 4.9  |
| 1   | K     | 206 | VAL  | 4.9  |
| 1   | K     | 87  | ILE  | 4.9  |
| 1   | J     | 42  | TRP  | 4.8  |
| 1   | F     | 268 | GLY  | 4.8  |
| 1   | J     | 207 | ASP  | 4.8  |
| 1   | K     | 293 | CYS  | 4.8  |
| 1   | K     | 92  | LEU  | 4.8  |
| 1   | L     | 211 | VAL  | 4.7  |
| 1   | J     | 158 | TRP  | 4.7  |
| 1   | K     | 114 | TYR  | 4.7  |
| 1   | D     | 274 | VAL  | 4.7  |
| 1   | J     | 38  | ALA  | 4.7  |
| 1   | J     | 92  | LEU  | 4.7  |
| 1   | J     | 122 | THR  | 4.7  |
| 1   | K     | 95  | PRO  | 4.7  |
| 1   | K     | 103 | SER  | 4.6  |
| 1   | F     | 15  | ALA  | 4.6  |
| 1   | K     | 74  | GLY  | 4.6  |
| 1   | K     | 133 | VAL  | 4.6  |
| 1   | L     | 204 | TYR  | 4.6  |
| 1   | K     | 44  | ARG  | 4.6  |
| 1   | H     | 44  | ARG  | 4.6  |
| 1   | J     | 84  | TYR  | 4.6  |
| 1   | J     | 186 | PHE  | 4.6  |
| 1   | J     | 293 | CYS  | 4.6  |
| 1   | F     | 282 | ALA  | 4.5  |
| 1   | K     | 161 | PHE  | 4.5  |
| 1   | K     | 166 | VAL  | 4.5  |
| 1   | K     | 36  | PRO  | 4.5  |
| 1   | K     | 82  | SER  | 4.5  |
| 1   | G     | 212 | ARG  | 4.5  |
| 1   | J     | 83  | ARG  | 4.5  |
| 1   | C     | 219 | LYS  | 4.5  |
| 1   | J     | 99  | ALA  | 4.5  |
| 1   | J     | 139 | VAL  | 4.5  |
| 1   | J     | 16  | GLN  | 4.5  |
| 1   | J     | 57  | HIS  | 4.5  |
| 1   | J     | 89  | LEU  | 4.5  |
| 1   | J     | 317 | ALA  | 4.5  |
| 1   | B     | 238 | ALA  | 4.5  |
| 1   | J     | 44  | ARG  | 4.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | K     | 50  | ASP  | 4.4  |
| 1   | K     | 61  | SER  | 4.4  |
| 1   | K     | 167 | ARG  | 4.4  |
| 1   | J     | 138 | GLY  | 4.4  |
| 1   | K     | 15  | ALA  | 4.4  |
| 1   | J     | 133 | VAL  | 4.4  |
| 1   | K     | 165 | TYR  | 4.4  |
| 1   | J     | 296 | ALA  | 4.4  |
| 1   | L     | 102 | CYS  | 4.4  |
| 1   | L     | 280 | TYR  | 4.3  |
| 1   | J     | 121 | THR  | 4.3  |
| 1   | J     | 202 | GLY  | 4.3  |
| 1   | C     | 210 | PRO  | 4.3  |
| 1   | J     | 321 | ILE  | 4.3  |
| 1   | J     | 22  | SER  | 4.3  |
| 1   | J     | 98  | SER  | 4.3  |
| 1   | K     | 211 | VAL  | 4.3  |
| 1   | J     | 71  | THR  | 4.3  |
| 1   | G     | 201 | ASP  | 4.2  |
| 1   | C     | 359 | ASN  | 4.2  |
| 1   | J     | 126 | ASP  | 4.2  |
| 1   | K     | 91  | TYR  | 4.2  |
| 1   | K     | 199 | TYR  | 4.2  |
| 1   | J     | 30  | VAL  | 4.2  |
| 1   | J     | 36  | PRO  | 4.2  |
| 1   | K     | 79  | PHE  | 4.2  |
| 1   | H     | 276 | SER  | 4.2  |
| 1   | J     | 87  | ILE  | 4.2  |
| 1   | J     | 107 | ASP  | 4.2  |
| 1   | K     | 296 | ALA  | 4.2  |
| 1   | J     | 314 | ILE  | 4.1  |
| 1   | K     | 121 | THR  | 4.1  |
| 1   | L     | 115 | GLY  | 4.1  |
| 1   | J     | 114 | TYR  | 4.1  |
| 1   | L     | 212 | ARG  | 4.1  |
| 1   | L     | 282 | ALA  | 4.1  |
| 1   | F     | 197 | PRO  | 4.1  |
| 1   | J     | 26  | LEU  | 4.1  |
| 1   | K     | 18  | ILE  | 4.0  |
| 1   | J     | 167 | ARG  | 4.0  |
| 1   | C     | 235 | PHE  | 4.0  |
| 1   | F     | 115 | GLY  | 4.0  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | L     | 113    | PRO  | 4.0  |
| 1   | E     | 75     | GLN  | 4.0  |
| 1   | J     | 176    | CYS  | 4.0  |
| 1   | F     | 202    | GLY  | 4.0  |
| 1   | F     | 11     | ALA  | 4.0  |
| 1   | G     | 277    | TYR  | 4.0  |
| 1   | K     | 45     | MET  | 4.0  |
| 1   | D     | 212    | ARG  | 4.0  |
| 1   | K     | 49     | ARG  | 4.0  |
| 1   | B     | 268    | GLY  | 4.0  |
| 1   | K     | 41     | SER  | 4.0  |
| 1   | J     | 194    | TYR  | 4.0  |
| 1   | J     | 384    | LEU  | 4.0  |
| 1   | L     | 117    | LYS  | 4.0  |
| 1   | J     | 154    | HIS  | 4.0  |
| 1   | F     | 18     | ILE  | 4.0  |
| 1   | B     | 239    | PRO  | 3.9  |
| 1   | K     | 197    | PRO  | 3.9  |
| 1   | J     | 378    | GLY  | 3.9  |
| 1   | F     | 280    | TYR  | 3.9  |
| 1   | K     | 37     | VAL  | 3.9  |
| 1   | J     | 173    | ALA  | 3.9  |
| 1   | H     | 235    | PHE  | 3.9  |
| 1   | K     | 118    | PHE  | 3.9  |
| 1   | H     | 280    | TYR  | 3.9  |
| 1   | K     | 318    | LEU  | 3.9  |
| 1   | F     | 207    | ASP  | 3.9  |
| 1   | K     | 46     | ASN  | 3.9  |
| 1   | K     | 89     | LEU  | 3.9  |
| 1   | K     | 127    | VAL  | 3.9  |
| 1   | K     | 207    | ASP  | 3.9  |
| 1   | J     | 119    | PRO  | 3.9  |
| 1   | J     | 125    | ASP  | 3.8  |
| 1   | J     | 280    | TYR  | 3.8  |
| 1   | J     | 101    | PRO  | 3.8  |
| 1   | K     | 320    | MET  | 3.8  |
| 1   | K     | 62     | SER  | 3.8  |
| 1   | F     | 205    | ASP  | 3.8  |
| 1   | J     | 303    | THR  | 3.8  |
| 1   | L     | 218[A] | ARG  | 3.8  |
| 1   | K     | 304    | HIS  | 3.8  |
| 1   | K     | 22     | SER  | 3.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | K     | 175 | SER  | 3.7  |
| 1   | G     | 44  | ARG  | 3.7  |
| 1   | J     | 283 | GLN  | 3.7  |
| 1   | K     | 158 | TRP  | 3.7  |
| 1   | L     | 123 | ILE  | 3.7  |
| 1   | J     | 55  | VAL  | 3.7  |
| 1   | F     | 100 | GLY  | 3.7  |
| 1   | J     | 299 | LEU  | 3.7  |
| 1   | J     | 35  | VAL  | 3.7  |
| 1   | J     | 82  | SER  | 3.7  |
| 1   | K     | 83  | ARG  | 3.7  |
| 1   | L     | 268 | GLY  | 3.7  |
| 1   | K     | 119 | PRO  | 3.7  |
| 1   | J     | 347 | SER  | 3.7  |
| 1   | K     | 90  | ASN  | 3.7  |
| 1   | J     | 311 | ALA  | 3.7  |
| 1   | A     | 75  | GLN  | 3.7  |
| 1   | K     | 81  | THR  | 3.7  |
| 1   | J     | 204 | TYR  | 3.7  |
| 1   | J     | 306 | ILE  | 3.6  |
| 1   | J     | 8   | ARG  | 3.6  |
| 1   | K     | 130 | HIS  | 3.6  |
| 1   | K     | 120 | ARG  | 3.6  |
| 1   | F     | 200 | LEU  | 3.6  |
| 1   | J     | 308 | ARG  | 3.6  |
| 1   | J     | 86  | ILE  | 3.6  |
| 1   | I     | 206 | VAL  | 3.6  |
| 1   | G     | 282 | ALA  | 3.6  |
| 1   | D     | 352 | ARG  | 3.6  |
| 1   | J     | 212 | ARG  | 3.6  |
| 1   | I     | 281 | GLN  | 3.6  |
| 1   | G     | 235 | PHE  | 3.6  |
| 1   | J     | 117 | LYS  | 3.6  |
| 1   | D     | 275 | SER  | 3.6  |
| 1   | C     | 237 | MET  | 3.6  |
| 1   | J     | 23  | LEU  | 3.6  |
| 1   | K     | 294 | TYR  | 3.6  |
| 1   | K     | 208 | ASP  | 3.5  |
| 1   | J     | 165 | TYR  | 3.5  |
| 1   | J     | 276 | SER  | 3.5  |
| 1   | K     | 26  | LEU  | 3.5  |
| 1   | K     | 85  | PHE  | 3.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | K     | 138 | GLY  | 3.5  |
| 1   | A     | 15  | ALA  | 3.5  |
| 1   | J     | 156 | LEU  | 3.5  |
| 1   | K     | 76  | GLY  | 3.5  |
| 1   | J     | 177 | ARG  | 3.5  |
| 1   | K     | 236 | HIS  | 3.5  |
| 1   | J     | 166 | VAL  | 3.4  |
| 1   | J     | 151 | GLY  | 3.4  |
| 1   | F     | 106 | PRO  | 3.4  |
| 1   | H     | 278 | LEU  | 3.4  |
| 1   | J     | 335 | LEU  | 3.4  |
| 1   | L     | 106 | PRO  | 3.4  |
| 1   | B     | 44  | ARG  | 3.4  |
| 1   | F     | 212 | ARG  | 3.4  |
| 1   | H     | 238 | ALA  | 3.4  |
| 1   | K     | 142 | ILE  | 3.4  |
| 1   | F     | 23  | LEU  | 3.4  |
| 1   | J     | 234 | ARG  | 3.4  |
| 1   | K     | 144 | ALA  | 3.4  |
| 1   | K     | 94  | SER  | 3.4  |
| 1   | J     | 37  | VAL  | 3.4  |
| 1   | L     | 380 | LEU  | 3.4  |
| 1   | J     | 338 | PHE  | 3.4  |
| 1   | K     | 9   | PHE  | 3.4  |
| 1   | G     | 276 | SER  | 3.4  |
| 1   | J     | 66  | THR  | 3.4  |
| 1   | J     | 140 | ARG  | 3.4  |
| 1   | L     | 103 | SER  | 3.4  |
| 1   | J     | 142 | ILE  | 3.4  |
| 1   | G     | 65  | VAL  | 3.3  |
| 1   | K     | 303 | THR  | 3.3  |
| 1   | F     | 218 | ARG  | 3.3  |
| 1   | J     | 46  | ASN  | 3.3  |
| 1   | K     | 192 | CYS  | 3.3  |
| 1   | K     | 8   | ARG  | 3.3  |
| 1   | K     | 306 | ILE  | 3.3  |
| 1   | K     | 204 | TYR  | 3.3  |
| 1   | J     | 93  | GLY  | 3.3  |
| 1   | K     | 367 | MET  | 3.3  |
| 1   | K     | 384 | LEU  | 3.3  |
| 1   | L     | 75  | GLN  | 3.3  |
| 1   | K     | 71  | THR  | 3.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 372 | VAL  | 3.3  |
| 1   | J     | 150 | MET  | 3.3  |
| 1   | I     | 282 | ALA  | 3.3  |
| 1   | J     | 120 | ARG  | 3.3  |
| 1   | J     | 129 | ILE  | 3.3  |
| 1   | L     | 200 | LEU  | 3.3  |
| 1   | J     | 348 | ILE  | 3.3  |
| 1   | K     | 84  | TYR  | 3.3  |
| 1   | K     | 13  | LEU  | 3.3  |
| 1   | J     | 287 | ALA  | 3.3  |
| 1   | J     | 181 | TRP  | 3.2  |
| 1   | L     | 68  | TRP  | 3.2  |
| 1   | K     | 194 | TYR  | 3.2  |
| 1   | D     | 369 | ALA  | 3.2  |
| 1   | J     | 116 | ALA  | 3.2  |
| 1   | L     | 11  | ALA  | 3.2  |
| 1   | L     | 234 | ARG  | 3.2  |
| 1   | J     | 9   | PHE  | 3.2  |
| 1   | F     | 204 | TYR  | 3.2  |
| 1   | J     | 182 | CYS  | 3.2  |
| 1   | K     | 309 | GLY  | 3.2  |
| 1   | K     | 310 | ARG  | 3.2  |
| 1   | F     | 192 | CYS  | 3.2  |
| 1   | F     | 105 | ASP  | 3.2  |
| 1   | L     | 207 | ASP  | 3.2  |
| 1   | J     | 289 | PHE  | 3.2  |
| 1   | E     | 44  | ARG  | 3.2  |
| 1   | F     | 281 | GLN  | 3.2  |
| 1   | G     | 194 | TYR  | 3.2  |
| 1   | J     | 367 | MET  | 3.2  |
| 1   | K     | 101 | PRO  | 3.2  |
| 1   | J     | 34  | ASP  | 3.2  |
| 1   | J     | 65  | VAL  | 3.2  |
| 1   | G     | 272 | GLU  | 3.2  |
| 1   | K     | 33  | ARG  | 3.2  |
| 1   | L     | 209 | GLN  | 3.2  |
| 1   | D     | 237 | MET  | 3.2  |
| 1   | L     | 214 | LEU  | 3.2  |
| 1   | J     | 336 | TYR  | 3.2  |
| 1   | F     | 139 | VAL  | 3.2  |
| 1   | J     | 53  | VAL  | 3.2  |
| 1   | K     | 16  | GLN  | 3.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 213 | GLY  | 3.1  |
| 1   | J     | 273 | ALA  | 3.1  |
| 1   | K     | 70  | PRO  | 3.1  |
| 1   | J     | 304 | HIS  | 3.1  |
| 1   | F     | 30  | VAL  | 3.1  |
| 1   | K     | 66  | THR  | 3.1  |
| 1   | H     | 234 | ARG  | 3.1  |
| 1   | J     | 45  | MET  | 3.1  |
| 1   | K     | 348 | ILE  | 3.1  |
| 1   | J     | 380 | LEU  | 3.1  |
| 1   | J     | 49  | ARG  | 3.1  |
| 1   | J     | 277 | TYR  | 3.1  |
| 1   | F     | 10  | GLU  | 3.1  |
| 1   | J     | 75  | GLN  | 3.1  |
| 1   | K     | 279 | ARG  | 3.1  |
| 1   | L     | 196 | ASP  | 3.1  |
| 1   | K     | 35  | VAL  | 3.1  |
| 1   | J     | 288 | SER  | 3.1  |
| 1   | J     | 21  | ILE  | 3.0  |
| 1   | F     | 214 | LEU  | 3.0  |
| 1   | L     | 283 | GLN  | 3.0  |
| 1   | I     | 47  | VAL  | 3.0  |
| 1   | K     | 53  | VAL  | 3.0  |
| 1   | K     | 116 | ALA  | 3.0  |
| 1   | L     | 15  | ALA  | 3.0  |
| 1   | D     | 281 | GLN  | 3.0  |
| 1   | K     | 29  | GLY  | 3.0  |
| 1   | H     | 116 | ALA  | 3.0  |
| 1   | K     | 99  | ALA  | 3.0  |
| 1   | H     | 381 | ASP  | 3.0  |
| 1   | J     | 209 | GLN  | 3.0  |
| 1   | G     | 117 | LYS  | 3.0  |
| 1   | C     | 275 | SER  | 3.0  |
| 1   | J     | 85  | PHE  | 3.0  |
| 1   | J     | 284 | LYS  | 3.0  |
| 1   | F     | 306 | ILE  | 3.0  |
| 1   | J     | 33  | ARG  | 3.0  |
| 1   | K     | 117 | LYS  | 3.0  |
| 1   | L     | 356 | VAL  | 3.0  |
| 1   | C     | 285 | PHE  | 3.0  |
| 1   | J     | 188 | THR  | 3.0  |
| 1   | K     | 100 | GLY  | 2.9  |

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| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 1   | C     | 212   | ARG  | 2.9  |
| 1   | G     | 234   | ARG  | 2.9  |
| 1   | F     | 92    | LEU  | 2.9  |
| 1   | I     | 240   | GLY  | 2.9  |
| 1   | J     | 301   | PHE  | 2.9  |
| 1   | J     | 295   | ILE  | 2.9  |
| 1   | C     | 231   | MET  | 2.9  |
| 1   | K     | 168   | LYS  | 2.9  |
| 1   | C     | 211   | VAL  | 2.9  |
| 1   | J     | 183   | ALA  | 2.9  |
| 1   | K     | 30    | VAL  | 2.9  |
| 1   | D     | 82[A] | SER  | 2.9  |
| 1   | L     | 179   | SER  | 2.9  |
| 1   | G     | 280   | TYR  | 2.9  |
| 1   | J     | 60    | THR  | 2.9  |
| 1   | K     | 141   | GLN  | 2.9  |
| 1   | B     | 74    | GLY  | 2.9  |
| 1   | B     | 319   | ALA  | 2.9  |
| 1   | F     | 12    | SER  | 2.9  |
| 1   | K     | 108   | ALA  | 2.9  |
| 1   | F     | 102   | CYS  | 2.9  |
| 1   | J     | 58    | THR  | 2.9  |
| 1   | C     | 271   | ILE  | 2.9  |
| 1   | J     | 118   | PHE  | 2.9  |
| 1   | K     | 151   | GLY  | 2.9  |
| 1   | K     | 153   | MET  | 2.9  |
| 1   | D     | 359   | ASN  | 2.9  |
| 1   | J     | 67    | SER  | 2.9  |
| 1   | J     | 94    | SER  | 2.9  |
| 1   | H     | 206   | VAL  | 2.9  |
| 1   | J     | 279   | ARG  | 2.9  |
| 1   | F     | 193   | ILE  | 2.9  |
| 1   | J     | 41    | SER  | 2.9  |
| 1   | K     | 98    | SER  | 2.9  |
| 1   | K     | 275   | SER  | 2.9  |
| 1   | K     | 77    | ARG  | 2.8  |
| 1   | J     | 146   | VAL  | 2.8  |
| 1   | G     | 283   | GLN  | 2.8  |
| 1   | B     | 212   | ARG  | 2.8  |
| 1   | K     | 378   | GLY  | 2.8  |
| 1   | F     | 287   | ALA  | 2.8  |
| 1   | K     | 202   | GLY  | 2.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | H     | 356 | VAL  | 2.8  |
| 1   | F     | 215 | GLU  | 2.8  |
| 1   | D     | 235 | PHE  | 2.8  |
| 1   | J     | 54  | ILE  | 2.8  |
| 1   | L     | 21  | ILE  | 2.8  |
| 1   | K     | 176 | CYS  | 2.8  |
| 1   | C     | 116 | ALA  | 2.8  |
| 1   | A     | 239 | PRO  | 2.8  |
| 1   | L     | 25  | THR  | 2.8  |
| 1   | J     | 28  | SER  | 2.8  |
| 1   | L     | 231 | MET  | 2.8  |
| 1   | K     | 283 | GLN  | 2.8  |
| 1   | J     | 185 | TRP  | 2.8  |
| 1   | J     | 208 | ASP  | 2.8  |
| 1   | J     | 340 | GLU  | 2.8  |
| 1   | D     | 234 | ARG  | 2.8  |
| 1   | L     | 287 | ALA  | 2.8  |
| 1   | K     | 349 | PRO  | 2.8  |
| 1   | H     | 195 | ASP  | 2.8  |
| 1   | L     | 96  | PHE  | 2.8  |
| 1   | C     | 277 | TYR  | 2.8  |
| 1   | J     | 281 | GLN  | 2.7  |
| 1   | F     | 29  | GLY  | 2.7  |
| 1   | L     | 97  | GLY  | 2.7  |
| 1   | F     | 31  | ILE  | 2.7  |
| 1   | F     | 116 | ALA  | 2.7  |
| 1   | K     | 302 | ASP  | 2.7  |
| 1   | F     | 37  | VAL  | 2.7  |
| 1   | G     | 215 | GLU  | 2.7  |
| 1   | H     | 216 | THR  | 2.7  |
| 1   | J     | 52  | CYS  | 2.7  |
| 1   | H     | 283 | GLN  | 2.7  |
| 1   | F     | 118 | PHE  | 2.7  |
| 1   | K     | 314 | ILE  | 2.7  |
| 1   | D     | 218 | ARG  | 2.7  |
| 1   | H     | 279 | ARG  | 2.7  |
| 1   | J     | 10  | GLU  | 2.7  |
| 1   | L     | 30  | VAL  | 2.7  |
| 1   | C     | 44  | ARG  | 2.7  |
| 1   | F     | 279 | ARG  | 2.7  |
| 1   | F     | 150 | MET  | 2.7  |
| 1   | H     | 231 | MET  | 2.7  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | K     | 335    | LEU  | 2.7  |
| 1   | K     | 186    | PHE  | 2.7  |
| 1   | C     | 215    | GLU  | 2.7  |
| 1   | F     | 222    | ASN  | 2.7  |
| 1   | K     | 156    | LEU  | 2.7  |
| 1   | G     | 275    | SER  | 2.7  |
| 1   | J     | 365    | PHE  | 2.7  |
| 1   | C     | 236    | HIS  | 2.7  |
| 1   | I     | 76     | GLY  | 2.7  |
| 1   | C     | 233    | GLU  | 2.7  |
| 1   | K     | 14     | ASP  | 2.7  |
| 1   | K     | 125    | ASP  | 2.7  |
| 1   | K     | 196    | ASP  | 2.7  |
| 1   | K     | 23     | LEU  | 2.6  |
| 1   | K     | 295    | ILE  | 2.6  |
| 1   | D     | 44     | ARG  | 2.6  |
| 1   | G     | 112    | ARG  | 2.6  |
| 1   | I     | 74     | GLY  | 2.6  |
| 1   | J     | 377    | ARG  | 2.6  |
| 1   | D     | 232    | ASP  | 2.6  |
| 1   | J     | 14     | ASP  | 2.6  |
| 1   | L     | 284    | LYS  | 2.6  |
| 1   | L     | 270    | PRO  | 2.6  |
| 1   | H     | 359    | ASN  | 2.6  |
| 1   | G     | 13     | LEU  | 2.6  |
| 1   | J     | 62     | SER  | 2.6  |
| 1   | J     | 366    | VAL  | 2.6  |
| 1   | K     | 218[A] | ARG  | 2.6  |
| 1   | L     | 154    | HIS  | 2.6  |
| 1   | L     | 312    | GLY  | 2.6  |
| 1   | J     | 298    | THR  | 2.6  |
| 1   | C     | 34     | ASP  | 2.6  |
| 1   | J     | 196    | ASP  | 2.6  |
| 1   | B     | 280    | TYR  | 2.6  |
| 1   | F     | 176    | CYS  | 2.6  |
| 1   | L     | 192    | CYS  | 2.6  |
| 1   | D     | 276    | SER  | 2.6  |
| 1   | K     | 308    | ARG  | 2.6  |
| 1   | L     | 12     | SER  | 2.6  |
| 1   | C     | 72     | LEU  | 2.6  |
| 1   | D     | 231    | MET  | 2.6  |
| 1   | C     | 68     | TRP  | 2.6  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | I     | 321    | ILE  | 2.6  |
| 1   | L     | 222[A] | ASN  | 2.6  |
| 1   | E     | 47     | VAL  | 2.6  |
| 1   | F     | 38     | ALA  | 2.6  |
| 1   | I     | 241    | VAL  | 2.6  |
| 1   | J     | 81     | THR  | 2.6  |
| 1   | J     | 77     | ARG  | 2.6  |
| 1   | F     | 284    | LYS  | 2.6  |
| 1   | F     | 113    | PRO  | 2.6  |
| 1   | F     | 64     | HIS  | 2.6  |
| 1   | J     | 80     | ASP  | 2.6  |
| 1   | K     | 312    | GLY  | 2.6  |
| 1   | J     | 178    | GLN  | 2.6  |
| 1   | F     | 234    | ARG  | 2.6  |
| 1   | I     | 112    | ARG  | 2.6  |
| 1   | K     | 7      | ASN  | 2.6  |
| 1   | J     | 205    | ASP  | 2.6  |
| 1   | L     | 91     | TYR  | 2.6  |
| 1   | E     | 283    | GLN  | 2.6  |
| 1   | K     | 281    | GLN  | 2.6  |
| 1   | A     | 44     | ARG  | 2.6  |
| 1   | I     | 44     | ARG  | 2.6  |
| 1   | D     | 366    | VAL  | 2.6  |
| 1   | J     | 320    | MET  | 2.6  |
| 1   | G     | 216    | THR  | 2.6  |
| 1   | J     | 175    | SER  | 2.5  |
| 1   | J     | 275    | SER  | 2.5  |
| 1   | J     | 290    | ASP  | 2.5  |
| 1   | G     | 202    | GLY  | 2.5  |
| 1   | J     | 225    | TYR  | 2.5  |
| 1   | I     | 15     | ALA  | 2.5  |
| 1   | K     | 63     | ALA  | 2.5  |
| 1   | B     | 147    | GLY  | 2.5  |
| 1   | J     | 79     | PHE  | 2.5  |
| 1   | C     | 199    | TYR  | 2.5  |
| 1   | A     | 357    | ASP  | 2.5  |
| 1   | L     | 150    | MET  | 2.5  |
| 1   | K     | 20     | ARG  | 2.5  |
| 1   | K     | 54     | ILE  | 2.5  |
| 1   | K     | 154    | HIS  | 2.5  |
| 1   | L     | 215    | GLU  | 2.5  |
| 1   | F     | 68     | TRP  | 2.5  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | D     | 11     | ALA  | 2.5  |
| 1   | F     | 114    | TYR  | 2.5  |
| 1   | G     | 22     | SER  | 2.5  |
| 1   | L     | 332    | SER  | 2.5  |
| 1   | L     | 118    | PHE  | 2.5  |
| 1   | D     | 207    | ASP  | 2.5  |
| 1   | E     | 357    | ASP  | 2.5  |
| 1   | L     | 293    | CYS  | 2.5  |
| 1   | C     | 283    | GLN  | 2.5  |
| 1   | E     | 212    | ARG  | 2.5  |
| 1   | J     | 189    | GLN  | 2.5  |
| 1   | K     | 136[A] | ARG  | 2.5  |
| 1   | I     | 42     | TRP  | 2.5  |
| 1   | J     | 148    | ALA  | 2.5  |
| 1   | L     | 116    | ALA  | 2.5  |
| 1   | C     | 276    | SER  | 2.5  |
| 1   | J     | 318    | LEU  | 2.5  |
| 1   | K     | 72     | LEU  | 2.5  |
| 1   | D     | 285    | PHE  | 2.5  |
| 1   | L     | 235    | PHE  | 2.5  |
| 1   | F     | 108    | ALA  | 2.5  |
| 1   | J     | 221    | ALA  | 2.5  |
| 1   | K     | 162    | GLY  | 2.5  |
| 1   | B     | 153    | MET  | 2.5  |
| 1   | I     | 106    | PRO  | 2.5  |
| 1   | L     | 37     | VAL  | 2.5  |
| 1   | I     | 80     | ASP  | 2.5  |
| 1   | G     | 203    | GLU  | 2.5  |
| 1   | J     | 100    | GLY  | 2.4  |
| 1   | D     | 360    | GLU  | 2.4  |
| 1   | G     | 279    | ARG  | 2.4  |
| 1   | H     | 272    | GLU  | 2.4  |
| 1   | L     | 32     | LEU  | 2.4  |
| 1   | L     | 119    | PRO  | 2.4  |
| 1   | K     | 68     | TRP  | 2.4  |
| 1   | B     | 206    | VAL  | 2.4  |
| 1   | F     | 211    | VAL  | 2.4  |
| 1   | D     | 219    | LYS  | 2.4  |
| 1   | K     | 28     | SER  | 2.4  |
| 1   | E     | 81     | THR  | 2.4  |
| 1   | C     | 207    | ASP  | 2.4  |
| 1   | F     | 32     | LEU  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | L     | 297 | MET  | 2.4  |
| 1   | H     | 277 | TYR  | 2.4  |
| 1   | L     | 114 | TYR  | 2.4  |
| 1   | K     | 40  | LYS  | 2.4  |
| 1   | F     | 123 | ILE  | 2.4  |
| 1   | J     | 31  | ILE  | 2.4  |
| 1   | K     | 274 | VAL  | 2.4  |
| 1   | L     | 206 | VAL  | 2.4  |
| 1   | F     | 9   | PHE  | 2.4  |
| 1   | K     | 93  | GLY  | 2.4  |
| 1   | K     | 364 | PHE  | 2.4  |
| 1   | C     | 222 | ASN  | 2.4  |
| 1   | J     | 159 | ALA  | 2.4  |
| 1   | H     | 113 | PRO  | 2.4  |
| 1   | K     | 336 | TYR  | 2.4  |
| 1   | F     | 88  | CYS  | 2.4  |
| 1   | J     | 20  | ARG  | 2.4  |
| 1   | D     | 201 | ASP  | 2.4  |
| 1   | J     | 302 | ASP  | 2.4  |
| 1   | K     | 313 | SER  | 2.4  |
| 1   | H     | 188 | THR  | 2.4  |
| 1   | H     | 358 | THR  | 2.4  |
| 1   | J     | 155 | THR  | 2.4  |
| 1   | J     | 153 | MET  | 2.4  |
| 1   | L     | 177 | ARG  | 2.4  |
| 1   | A     | 241 | VAL  | 2.4  |
| 1   | G     | 193 | ILE  | 2.4  |
| 1   | H     | 274 | VAL  | 2.4  |
| 1   | I     | 65  | VAL  | 2.4  |
| 1   | J     | 274 | VAL  | 2.4  |
| 1   | J     | 56  | CYS  | 2.4  |
| 1   | E     | 160 | PHE  | 2.4  |
| 1   | F     | 297 | MET  | 2.4  |
| 1   | H     | 302 | ASP  | 2.4  |
| 1   | K     | 147 | GLY  | 2.4  |
| 1   | A     | 22  | SER  | 2.4  |
| 1   | F     | 206 | VAL  | 2.4  |
| 1   | J     | 362 | HIS  | 2.4  |
| 1   | K     | 64  | HIS  | 2.4  |
| 1   | A     | 116 | ALA  | 2.4  |
| 1   | F     | 8   | ARG  | 2.4  |
| 1   | F     | 95  | PRO  | 2.4  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | L     | 296    | ALA  | 2.4  |
| 1   | K     | 346[A] | ARG  | 2.4  |
| 1   | F     | 350    | ASN  | 2.3  |
| 1   | J     | 59     | LEU  | 2.3  |
| 1   | A     | 193    | ILE  | 2.3  |
| 1   | B     | 47     | VAL  | 2.3  |
| 1   | K     | 65     | VAL  | 2.3  |
| 1   | J     | 346[A] | ARG  | 2.3  |
| 1   | C     | 216    | THR  | 2.3  |
| 1   | H     | 285    | PHE  | 2.3  |
| 1   | I     | 325    | ALA  | 2.3  |
| 1   | K     | 155    | THR  | 2.3  |
| 1   | K     | 324    | PRO  | 2.3  |
| 1   | G     | 153    | MET  | 2.3  |
| 1   | L     | 92     | LEU  | 2.3  |
| 1   | E     | 82[A]  | SER  | 2.3  |
| 1   | K     | 177    | ARG  | 2.3  |
| 1   | G     | 191    | GLN  | 2.3  |
| 1   | K     | 132    | GLN  | 2.3  |
| 1   | L     | 39     | TYR  | 2.3  |
| 1   | F     | 36     | PRO  | 2.3  |
| 1   | J     | 330    | ALA  | 2.3  |
| 1   | L     | 71     | THR  | 2.3  |
| 1   | F     | 309    | GLY  | 2.3  |
| 1   | J     | 190    | ARG  | 2.3  |
| 1   | L     | 278    | LEU  | 2.3  |
| 1   | C     | 295    | ILE  | 2.3  |
| 1   | K     | 145    | VAL  | 2.3  |
| 1   | G     | 270    | PRO  | 2.3  |
| 1   | L     | 194    | TYR  | 2.3  |
| 1   | F     | 19     | ALA  | 2.3  |
| 1   | J     | 162    | GLY  | 2.3  |
| 1   | J     | 312    | GLY  | 2.3  |
| 1   | D     | 272    | GLU  | 2.3  |
| 1   | J     | 313    | SER  | 2.3  |
| 1   | K     | 164    | GLU  | 2.3  |
| 1   | L     | 288    | SER  | 2.3  |
| 1   | J     | 278    | LEU  | 2.3  |
| 1   | K     | 353    | LEU  | 2.3  |
| 1   | C     | 194    | TYR  | 2.3  |
| 1   | D     | 211    | VAL  | 2.3  |
| 1   | I     | 217    | ALA  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | L     | 74  | GLY  | 2.3  |
| 1   | B     | 281 | GLN  | 2.3  |
| 1   | G     | 285 | PHE  | 2.3  |
| 1   | B     | 42  | TRP  | 2.3  |
| 1   | F     | 13  | LEU  | 2.3  |
| 1   | B     | 83  | ARG  | 2.3  |
| 1   | J     | 324 | PRO  | 2.3  |
| 1   | C     | 188 | THR  | 2.3  |
| 1   | D     | 216 | THR  | 2.3  |
| 1   | F     | 91  | TYR  | 2.3  |
| 1   | F     | 199 | TYR  | 2.3  |
| 1   | J     | 78  | ALA  | 2.3  |
| 1   | B     | 276 | SER  | 2.3  |
| 1   | B     | 320 | MET  | 2.3  |
| 1   | H     | 153 | MET  | 2.3  |
| 1   | J     | 72  | LEU  | 2.3  |
| 1   | L     | 350 | ASN  | 2.3  |
| 1   | H     | 146 | VAL  | 2.2  |
| 1   | K     | 183 | ALA  | 2.2  |
| 1   | K     | 284 | LYS  | 2.2  |
| 1   | B     | 365 | PHE  | 2.2  |
| 1   | F     | 338 | PHE  | 2.2  |
| 1   | B     | 234 | ARG  | 2.2  |
| 1   | C     | 281 | GLN  | 2.2  |
| 1   | H     | 281 | GLN  | 2.2  |
| 1   | L     | 382 | GLN  | 2.2  |
| 1   | K     | 180 | GLY  | 2.2  |
| 1   | C     | 69  | TRP  | 2.2  |
| 1   | F     | 296 | ALA  | 2.2  |
| 1   | L     | 19  | ALA  | 2.2  |
| 1   | L     | 105 | ASP  | 2.2  |
| 1   | L     | 107 | ASP  | 2.2  |
| 1   | K     | 300 | LYS  | 2.2  |
| 1   | L     | 223 | LEU  | 2.2  |
| 1   | L     | 95  | PRO  | 2.2  |
| 1   | L     | 101 | PRO  | 2.2  |
| 1   | C     | 14  | ASP  | 2.2  |
| 1   | C     | 272 | GLU  | 2.2  |
| 1   | C     | 363 | ASP  | 2.2  |
| 1   | H     | 108 | ALA  | 2.2  |
| 1   | J     | 68  | TRP  | 2.2  |
| 1   | G     | 220 | ILE  | 2.2  |

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| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 1   | K     | 271   | ILE  | 2.2  |
| 1   | B     | 214   | LEU  | 2.2  |
| 1   | C     | 153   | MET  | 2.2  |
| 1   | J     | 210   | PRO  | 2.2  |
| 1   | C     | 352   | ARG  | 2.2  |
| 1   | I     | 82[A] | SER  | 2.2  |
| 1   | L     | 216   | THR  | 2.2  |
| 1   | I     | 46    | ASN  | 2.2  |
| 1   | K     | 319   | ALA  | 2.2  |
| 1   | J     | 172   | ILE  | 2.2  |
| 1   | C     | 366   | VAL  | 2.2  |
| 1   | K     | 146   | VAL  | 2.2  |
| 1   | D     | 277   | TYR  | 2.2  |
| 1   | J     | 43    | GLY  | 2.2  |
| 1   | F     | 104   | PRO  | 2.2  |
| 1   | B     | 231   | MET  | 2.2  |
| 1   | F     | 153   | MET  | 2.2  |
| 1   | G     | 297   | MET  | 2.2  |
| 1   | F     | 198   | LYS  | 2.2  |
| 1   | G     | 48    | SER  | 2.2  |
| 1   | L     | 281   | GLN  | 2.2  |
| 1   | A     | 78    | ALA  | 2.2  |
| 1   | F     | 291   | ALA  | 2.2  |
| 1   | K     | 27    | GLU  | 2.2  |
| 1   | K     | 286   | ALA  | 2.2  |
| 1   | C     | 279   | ARG  | 2.2  |
| 1   | D     | 74    | GLY  | 2.2  |
| 1   | F     | 83    | ARG  | 2.2  |
| 1   | E     | 150   | MET  | 2.2  |
| 1   | J     | 13    | LEU  | 2.2  |
| 1   | F     | 103   | SER  | 2.2  |
| 1   | K     | 51    | ASN  | 2.2  |
| 1   | F     | 317   | ALA  | 2.2  |
| 1   | L     | 273   | ALA  | 2.2  |
| 1   | L     | 80    | ASP  | 2.1  |
| 1   | I     | 377   | ARG  | 2.1  |
| 1   | B     | 65    | VAL  | 2.1  |
| 1   | B     | 376   | VAL  | 2.1  |
| 1   | D     | 283   | GLN  | 2.1  |
| 1   | B     | 210   | PRO  | 2.1  |
| 1   | D     | 215   | GLU  | 2.1  |
| 1   | J     | 215   | GLU  | 2.1  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | D     | 67     | SER  | 2.1  |
| 1   | H     | 297    | MET  | 2.1  |
| 1   | J     | 341    | HIS  | 2.1  |
| 1   | K     | 344    | MET  | 2.1  |
| 1   | B     | 327    | ILE  | 2.1  |
| 1   | F     | 129    | ILE  | 2.1  |
| 1   | J     | 268    | GLY  | 2.1  |
| 1   | K     | 340    | GLU  | 2.1  |
| 1   | B     | 364    | PHE  | 2.1  |
| 1   | H     | 200    | LEU  | 2.1  |
| 1   | I     | 153    | MET  | 2.1  |
| 1   | L     | 367    | MET  | 2.1  |
| 1   | B     | 131[A] | ARG  | 2.1  |
| 1   | K     | 34     | ASP  | 2.1  |
| 1   | C     | 75[A]  | GLN  | 2.1  |
| 1   | C     | 217    | ALA  | 2.1  |
| 1   | J     | 369    | ALA  | 2.1  |
| 1   | J     | 327    | ILE  | 2.1  |
| 1   | J     | 359    | ASN  | 2.1  |
| 1   | E     | 65     | VAL  | 2.1  |
| 1   | F     | 119    | PRO  | 2.1  |
| 1   | J     | 145    | VAL  | 2.1  |
| 1   | B     | 57     | HIS  | 2.1  |
| 1   | F     | 24     | PHE  | 2.1  |
| 1   | F     | 107    | ASP  | 2.1  |
| 1   | I     | 365    | PHE  | 2.1  |
| 1   | L     | 24     | PHE  | 2.1  |
| 1   | L     | 83     | ARG  | 2.1  |
| 1   | L     | 279    | ARG  | 2.1  |
| 1   | C     | 296    | ALA  | 2.1  |
| 1   | J     | 19     | ALA  | 2.1  |
| 1   | B     | 377[A] | ARG  | 2.1  |
| 1   | J     | 164    | GLU  | 2.1  |
| 1   | C     | 357    | ASP  | 2.1  |
| 1   | L     | 28     | SER  | 2.1  |
| 1   | K     | 289    | PHE  | 2.1  |
| 1   | G     | 84     | TYR  | 2.1  |
| 1   | L     | 277    | TYR  | 2.1  |
| 1   | E     | 268    | GLY  | 2.1  |
| 1   | K     | 11     | ALA  | 2.1  |
| 1   | J     | 27     | GLU  | 2.1  |
| 1   | K     | 352    | ARG  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 48  | SER  | 2.1  |
| 1   | F     | 302 | ASP  | 2.1  |
| 1   | K     | 381 | ASP  | 2.1  |
| 1   | L     | 363 | ASP  | 2.1  |
| 1   | G     | 231 | MET  | 2.1  |
| 1   | L     | 294 | TYR  | 2.1  |
| 1   | I     | 234 | ARG  | 2.1  |
| 1   | C     | 232 | ASP  | 2.1  |
| 1   | H     | 370 | ASP  | 2.1  |
| 1   | F     | 28  | SER  | 2.1  |
| 1   | K     | 341 | HIS  | 2.1  |
| 1   | I     | 146 | VAL  | 2.1  |
| 1   | K     | 60  | THR  | 2.0  |
| 1   | A     | 150 | MET  | 2.0  |
| 1   | F     | 381 | ASP  | 2.0  |
| 1   | L     | 34  | ASP  | 2.0  |
| 1   | J     | 149 | SER  | 2.0  |
| 1   | L     | 61  | SER  | 2.0  |
| 1   | G     | 87  | ILE  | 2.0  |
| 1   | B     | 240 | GLY  | 2.0  |
| 1   | J     | 309 | GLY  | 2.0  |
| 1   | J     | 334 | GLY  | 2.0  |
| 1   | L     | 140 | ARG  | 2.0  |
| 1   | D     | 45  | MET  | 2.0  |
| 1   | D     | 320 | MET  | 2.0  |
| 1   | D     | 380 | LEU  | 2.0  |
| 1   | A     | 88  | CYS  | 2.0  |
| 1   | B     | 164 | GLU  | 2.0  |
| 1   | C     | 197 | PRO  | 2.0  |
| 1   | J     | 163 | PRO  | 2.0  |
| 1   | K     | 179 | SER  | 2.0  |
| 1   | F     | 33  | ARG  | 2.0  |
| 1   | F     | 359 | ASN  | 2.0  |
| 1   | K     | 31  | ILE  | 2.0  |
| 1   | J     | 198 | LYS  | 2.0  |
| 1   | G     | 370 | ASP  | 2.0  |
| 1   | L     | 65  | VAL  | 2.0  |
| 1   | B     | 45  | MET  | 2.0  |
| 1   | B     | 221 | ALA  | 2.0  |
| 1   | C     | 291 | ALA  | 2.0  |
| 1   | H     | 78  | ALA  | 2.0  |
| 1   | L     | 153 | MET  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | L     | 217 | ALA  | 2.0  |
| 1   | C     | 362 | HIS  | 2.0  |
| 1   | F     | 332 | SER  | 2.0  |
| 1   | H     | 194 | TYR  | 2.0  |
| 1   | L     | 120 | ARG  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 3   | ACT  | F     | 1384 | 4/4   | 0.70 | 0.39 | 15.37 | 39,40,42,42                | 0     |
| 4   | GOL  | B     | 1384 | 6/6   | 0.74 | 0.42 | 11.04 | 33,36,39,40                | 0     |
| 3   | ACT  | I     | 1385 | 4/4   | 0.80 | 0.29 | 5.40  | 20,20,22,23                | 0     |
| 2   | COA  | D     | 1383 | 48/48 | 0.47 | 0.57 | 4.89  | 35,47,70,72                | 0     |
| 3   | ACT  | A     | 1384 | 4/4   | 0.91 | 0.28 | 4.79  | 27,27,28,29                | 0     |
| 3   | ACT  | C     | 1384 | 4/4   | 0.94 | 0.28 | 4.51  | 30,31,31,31                | 0     |
| 2   | COA  | C     | 1383 | 48/48 | 0.59 | 0.58 | 4.22  | 36,46,73,80                | 0     |
| 3   | ACT  | D     | 1384 | 4/4   | 0.92 | 0.32 | 3.97  | 28,29,29,29                | 0     |
| 2   | COA  | F     | 1383 | 48/48 | 0.62 | 0.50 | 3.16  | 39,59,69,70                | 0     |
| 4   | GOL  | I     | 1384 | 6/6   | 0.79 | 0.24 | 3.03  | 35,37,39,44                | 0     |
| 2   | COA  | L     | 1383 | 48/48 | 0.67 | 0.49 | 2.89  | 37,57,65,65                | 0     |
| 2   | COA  | G     | 1383 | 48/48 | 0.74 | 0.37 | 2.38  | 21,53,83,86                | 0     |
| 2   | COA  | B     | 1383 | 48/48 | 0.74 | 0.35 | 2.21  | 28,42,54,57                | 0     |
| 2   | COA  | H     | 1383 | 48/48 | 0.78 | 0.37 | 1.67  | 21,53,75,76                | 0     |
| 3   | ACT  | E     | 1384 | 4/4   | 0.94 | 0.24 | 1.67  | 30,31,31,31                | 0     |
| 3   | ACT  | H     | 1384 | 4/4   | 0.85 | 0.21 | 1.62  | 31,32,32,33                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 2   | COA  | I     | 1383 | 48/48 | 0.81 | 0.30 | 1.43  | 29,41,57,59                 | 0     |
| 3   | ACT  | L     | 1384 | 4/4   | 0.82 | 0.21 | 0.56  | 46,48,48,48                 | 0     |
| 3   | ACT  | K     | 1386 | 4/4   | 0.84 | 0.32 | 0.51  | 45,45,45,46                 | 0     |
| 2   | COA  | A     | 1383 | 48/48 | 0.92 | 0.18 | 0.22  | 17,29,48,50                 | 0     |
| 2   | COA  | J     | 1385 | 48/48 | 0.76 | 0.29 | 0.10  | 23,55,68,70                 | 0     |
| 3   | ACT  | B     | 1385 | 4/4   | 0.84 | 0.20 | 0.02  | 20,22,23,24                 | 0     |
| 2   | COA  | K     | 1385 | 48/48 | 0.78 | 0.24 | -0.08 | 20,50,65,72                 | 0     |
| 3   | ACT  | G     | 1384 | 4/4   | 0.85 | 0.18 | -0.13 | 37,37,38,38                 | 0     |
| 3   | ACT  | J     | 1386 | 4/4   | 0.86 | 0.24 | -0.71 | 47,49,50,50                 | 0     |
| 2   | COA  | E     | 1383 | 48/48 | 0.93 | 0.15 | -1.31 | 14,27,49,52                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.