



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 07:48 AM UTC

PDB ID : 4V4G / pdb\_00004v4g  
Title : Crystal structure of five 70s ribosomes from Escherichia Coli in complex with protein Y.  
Authors : Vila-Sanjurjo, A.; Schuwirth, B.S.; Hau, C.W.; Cate, J.H.  
Deposited on : 2004-10-06  
Resolution : 11.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                    |
|--------------------------------|---|--------------------------------------------------------------------|
| MolProbity                     | : | <b>FAILED</b>                                                      |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                       |
| Xtriage (Phenix)               | : | 2.0                                                                |
| EDS                            | : | 3.0                                                                |
| Percentile statistics          | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| CCP4                           | : | 9.0.010 (Gargrove)                                                 |
| Density-Fitness                | : | 1.0.12                                                             |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                                |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                            |
| Validation Pipeline (wwPDB-VP) | : | 2.48.1                                                             |

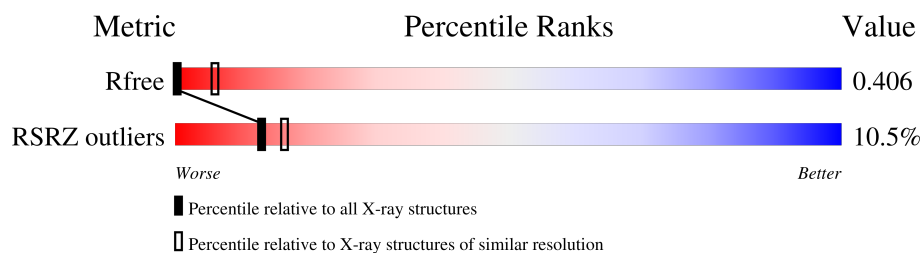
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 11.50 Å.

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



| Metric        | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|---------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$    | 164625                      | 1107 (10.00-4.00)                                     |
| RSRZ outliers | 164620                      | 1102 (10.00-4.00)                                     |

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 717805 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 RNA chain called 16S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1   | AA    | 1526     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32799 | 14601 | 6082 | 10590 | 1526 |         |         |       |
| 1   | CA    | 1526     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32799 | 14601 | 6082 | 10590 | 1526 |         |         |       |
| 1   | EA    | 1526     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32799 | 14601 | 6082 | 10590 | 1526 |         |         |       |
| 1   | GA    | 1526     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32799 | 14601 | 6082 | 10590 | 1526 |         |         |       |
| 1   | IA    | 1526     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32799 | 14601 | 6082 | 10590 | 1526 |         |         |       |

- Molecule 2 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | AB    | 234      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1901  | 1213 | 341 | 342 | 5 |         |         |       |
| 2   | CB    | 234      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1901  | 1213 | 341 | 342 | 5 |         |         |       |
| 2   | EB    | 234      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1901  | 1213 | 341 | 342 | 5 |         |         |       |
| 2   | GB    | 234      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1901  | 1213 | 341 | 342 | 5 |         |         |       |
| 2   | IB    | 234      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1901  | 1213 | 341 | 342 | 5 |         |         |       |

- Molecule 3 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | AC    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1613  | 1016 | 314 | 282 | 1 |         |         |       |
| 3   | CC    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1613  | 1016 | 314 | 282 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | EC    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1613  | 1016 | 314 | 282 | 1 |         |         |       |
| 3   | GC    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1613  | 1016 | 314 | 282 | 1 |         |         |       |
| 3   | IC    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1613  | 1016 | 314 | 282 | 1 |         |         |       |

- Molecule 4 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | AD    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1703  | 1066 | 339 | 291 | 7 |         |         |       |
| 4   | CD    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1703  | 1066 | 339 | 291 | 7 |         |         |       |
| 4   | ED    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1703  | 1066 | 339 | 291 | 7 |         |         |       |
| 4   | GD    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1703  | 1066 | 339 | 291 | 7 |         |         |       |
| 4   | ID    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1703  | 1066 | 339 | 291 | 7 |         |         |       |

- Molecule 5 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | AE    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1147  | 724 | 217 | 202 | 4 |         |         |       |
| 5   | CE    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1147  | 724 | 217 | 202 | 4 |         |         |       |
| 5   | EE    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1147  | 724 | 217 | 202 | 4 |         |         |       |
| 5   | GE    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1147  | 724 | 217 | 202 | 4 |         |         |       |
| 5   | IE    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1147  | 724 | 217 | 202 | 4 |         |         |       |

- Molecule 6 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | AF    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 843   | 531 | 155 | 154 | 3 |         |         |       |
| 6   | CF    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 843   | 531 | 155 | 154 | 3 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | EF    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 843   | 531 | 155 | 154 | 3 |         |         |       |
| 6   | GF    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 843   | 531 | 155 | 154 | 3 |         |         |       |
| 6   | IF    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 843   | 531 | 155 | 154 | 3 |         |         |       |

- Molecule 7 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | AG    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1257  | 781 | 252 | 218 | 6 |         |         |       |
| 7   | CG    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1257  | 781 | 252 | 218 | 6 |         |         |       |
| 7   | EG    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1257  | 781 | 252 | 218 | 6 |         |         |       |
| 7   | GG    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1257  | 781 | 252 | 218 | 6 |         |         |       |
| 7   | IG    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1257  | 781 | 252 | 218 | 6 |         |         |       |

- Molecule 8 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | AH    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1116  | 705 | 215 | 193 | 3 |         |         |       |
| 8   | CH    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1116  | 705 | 215 | 193 | 3 |         |         |       |
| 8   | EH    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1116  | 705 | 215 | 193 | 3 |         |         |       |
| 8   | GH    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1116  | 705 | 215 | 193 | 3 |         |         |       |
| 8   | IH    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1116  | 705 | 215 | 193 | 3 |         |         |       |

- Molecule 9 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 9   | AI    | 127      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1011  | 639 | 198 | 174 |         |         |       |
| 9   | CI    | 127      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1011  | 639 | 198 | 174 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 9   | EI    | 127      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1011  | 639 | 198 | 174 |         |         |       |
| 9   | GI    | 127      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1011  | 639 | 198 | 174 |         |         |       |
| 9   | II    | 127      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1011  | 639 | 198 | 174 |         |         |       |

- Molecule 10 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | AJ    | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 795   | 499 | 156 | 139 | 1 |         |         |       |
| 10  | CJ    | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 795   | 499 | 156 | 139 | 1 |         |         |       |
| 10  | EJ    | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 795   | 499 | 156 | 139 | 1 |         |         |       |
| 10  | GJ    | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 795   | 499 | 156 | 139 | 1 |         |         |       |
| 10  | IJ    | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 795   | 499 | 156 | 139 | 1 |         |         |       |

- Molecule 11 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | AK    | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 885   | 549 | 168 | 165 | 3 |         |         |       |
| 11  | CK    | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 885   | 549 | 168 | 165 | 3 |         |         |       |
| 11  | EK    | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 885   | 549 | 168 | 165 | 3 |         |         |       |
| 11  | GK    | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 885   | 549 | 168 | 165 | 3 |         |         |       |
| 11  | IK    | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 885   | 549 | 168 | 165 | 3 |         |         |       |

- Molecule 12 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | AL    | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 971   | 611 | 195 | 164 | 1 |         |         |       |
| 12  | CL    | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 971   | 611 | 195 | 164 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | EL    | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 971   | 611 | 195 | 164 | 1 |         |         |       |
| 12  | GL    | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 971   | 611 | 195 | 164 | 1 |         |         |       |
| 12  | IL    | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 971   | 611 | 195 | 164 | 1 |         |         |       |

- Molecule 13 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | AM    | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 997   | 617 | 207 | 171 | 2 |         |         |       |
| 13  | CM    | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 997   | 617 | 207 | 171 | 2 |         |         |       |
| 13  | EM    | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 997   | 617 | 207 | 171 | 2 |         |         |       |
| 13  | GM    | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 997   | 617 | 207 | 171 | 2 |         |         |       |
| 13  | IM    | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 997   | 617 | 207 | 171 | 2 |         |         |       |

- Molecule 14 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 14  | AN    | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 492   | 312 | 104 | 72 | 4 |         |         |       |
| 14  | CN    | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 492   | 312 | 104 | 72 | 4 |         |         |       |
| 14  | EN    | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 492   | 312 | 104 | 72 | 4 |         |         |       |
| 14  | GN    | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 492   | 312 | 104 | 72 | 4 |         |         |       |
| 14  | IN    | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 492   | 312 | 104 | 72 | 4 |         |         |       |

- Molecule 15 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | AO    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 734   | 459 | 147 | 126 | 2 |         |         |       |
| 15  | CO    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 734   | 459 | 147 | 126 | 2 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | EO    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 734   | 459 | 147 | 126 | 2 |         |         |       |
| 15  | GO    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 734   | 459 | 147 | 126 | 2 |         |         |       |
| 15  | IO    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 734   | 459 | 147 | 126 | 2 |         |         |       |

- Molecule 16 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | AP    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 701   | 443 | 139 | 118 | 1 |         |         |       |
| 16  | CP    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 701   | 443 | 139 | 118 | 1 |         |         |       |
| 16  | EP    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 701   | 443 | 139 | 118 | 1 |         |         |       |
| 16  | GP    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 701   | 443 | 139 | 118 | 1 |         |         |       |
| 16  | IP    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 701   | 443 | 139 | 118 | 1 |         |         |       |

- Molecule 17 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | AQ    | 104      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 857   | 547 | 161 | 147 | 2 |         |         |       |
| 17  | CQ    | 104      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 857   | 547 | 161 | 147 | 2 |         |         |       |
| 17  | EQ    | 104      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 857   | 547 | 161 | 147 | 2 |         |         |       |
| 17  | GQ    | 104      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 857   | 547 | 161 | 147 | 2 |         |         |       |
| 17  | IQ    | 104      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 857   | 547 | 161 | 147 | 2 |         |         |       |

- Molecule 18 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 18  | AR    | 73       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 597   | 380 | 118 | 99 |         |         |       |
| 18  | CR    | 73       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 597   | 380 | 118 | 99 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 18  | ER    | 73       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 597   | 380 | 118 | 99 |         |         |       |
| 18  | GR    | 73       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 597   | 380 | 118 | 99 |         |         |       |
| 18  | IR    | 73       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 597   | 380 | 118 | 99 |         |         |       |

- Molecule 19 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | AS    | 80       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 648   | 414 | 119 | 113 | 2 |         |         |       |
| 19  | CS    | 80       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 648   | 414 | 119 | 113 | 2 |         |         |       |
| 19  | ES    | 80       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 648   | 414 | 119 | 113 | 2 |         |         |       |
| 19  | GS    | 80       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 648   | 414 | 119 | 113 | 2 |         |         |       |
| 19  | IS    | 80       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 648   | 414 | 119 | 113 | 2 |         |         |       |

- Molecule 20 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | AT    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 762   | 469 | 162 | 129 | 2 |         |         |       |
| 20  | CT    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 762   | 469 | 162 | 129 | 2 |         |         |       |
| 20  | ET    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 762   | 469 | 162 | 129 | 2 |         |         |       |
| 20  | GT    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 762   | 469 | 162 | 129 | 2 |         |         |       |
| 20  | IT    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 762   | 469 | 162 | 129 | 2 |         |         |       |

- Molecule 21 is a protein called protein Y.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21  | Aa    | 90       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 719   | 452 | 131 | 133 | 3 |         |         |       |
| 21  | Ca    | 90       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 719   | 452 | 131 | 133 | 3 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21  | Ea    | 90       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 719   | 452 | 131 | 133 | 3 |         |         |       |
| 21  | Ga    | 90       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 719   | 452 | 131 | 133 | 3 |         |         |       |
| 21  | Ia    | 90       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 719   | 452 | 131 | 133 | 3 |         |         |       |

- Molecule 22 is a RNA chain called 23S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 22  | BB    | 2825     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 60635 | 27047 | 11190 | 19573 | 2825 |         |         |       |
| 22  | DB    | 2825     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 60635 | 27047 | 11190 | 19573 | 2825 |         |         |       |
| 22  | FB    | 2825     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 60635 | 27047 | 11190 | 19573 | 2825 |         |         |       |
| 22  | HB    | 2825     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 60635 | 27047 | 11190 | 19573 | 2825 |         |         |       |
| 22  | JB    | 2825     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 60635 | 27047 | 11190 | 19573 | 2825 |         |         |       |

- Molecule 23 is a RNA chain called 5S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 23  | BA    | 118      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2519  | 1124 | 464 | 813 | 118 |         |         |       |
| 23  | DA    | 118      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2519  | 1124 | 464 | 813 | 118 |         |         |       |
| 23  | FA    | 118      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2519  | 1124 | 464 | 813 | 118 |         |         |       |
| 23  | HA    | 118      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2519  | 1124 | 464 | 813 | 118 |         |         |       |
| 23  | JA    | 118      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2519  | 1124 | 464 | 813 | 118 |         |         |       |

- Molecule 24 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 24  | BD    | 270      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2079  | 1294 | 417 | 365 | 3 |         |         |       |
| 24  | DD    | 270      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2079  | 1294 | 417 | 365 | 3 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 24  | FD    | 270      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2079  | 1294 | 417 | 365 | 3 |         |         |       |
| 24  | HD    | 270      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2079  | 1294 | 417 | 365 | 3 |         |         |       |
| 24  | JD    | 270      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2079  | 1294 | 417 | 365 | 3 |         |         |       |

- Molecule 25 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 25  | BE    | 205      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1540  | 965 | 295 | 272 | 8 |         |         |       |
| 25  | DE    | 205      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1540  | 965 | 295 | 272 | 8 |         |         |       |
| 25  | FE    | 205      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1540  | 965 | 295 | 272 | 8 |         |         |       |
| 25  | HE    | 205      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1540  | 965 | 295 | 272 | 8 |         |         |       |
| 25  | JE    | 205      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1540  | 965 | 295 | 272 | 8 |         |         |       |

- Molecule 26 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26  | BF    | 197      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1507  | 935 | 287 | 283 | 2 |         |         |       |
| 26  | DF    | 197      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1507  | 935 | 287 | 283 | 2 |         |         |       |
| 26  | FF    | 197      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1507  | 935 | 287 | 283 | 2 |         |         |       |
| 26  | HF    | 197      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1507  | 935 | 287 | 283 | 2 |         |         |       |
| 26  | JF    | 197      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1507  | 935 | 287 | 283 | 2 |         |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 27  | BG    | 178      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1410  | 897 | 249 | 257 | 7 |         |         |       |
| 27  | DG    | 178      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1410  | 897 | 249 | 257 | 7 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 27  | FG    | 178      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1410  | 897 | 249 | 257 | 7 |         |         |       |
| 27  | HG    | 178      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1410  | 897 | 249 | 257 | 7 |         |         |       |
| 27  | JG    | 178      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1410  | 897 | 249 | 257 | 7 |         |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28  | BH    | 177      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1316  | 828 | 243 | 244 | 1 |         |         |       |
| 28  | DH    | 177      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1316  | 828 | 243 | 244 | 1 |         |         |       |
| 28  | FH    | 177      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1316  | 828 | 243 | 244 | 1 |         |         |       |
| 28  | HH    | 177      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1316  | 828 | 243 | 244 | 1 |         |         |       |
| 28  | JH    | 177      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1316  | 828 | 243 | 244 | 1 |         |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 29  | BI    | 52       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 401   | 251 | 73 | 75 | 2 |         |         |       |
| 29  | DI    | 52       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 401   | 251 | 73 | 75 | 2 |         |         |       |
| 29  | FI    | 52       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 401   | 251 | 73 | 75 | 2 |         |         |       |
| 29  | HI    | 52       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 401   | 251 | 73 | 75 | 2 |         |         |       |
| 29  | JI    | 52       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 401   | 251 | 73 | 75 | 2 |         |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30  | BJ    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1039  | 660 | 178 | 196 | 5 |         |         |       |
| 30  | DJ    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1039  | 660 | 178 | 196 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30  | FJ    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1039  | 660 | 178 | 196 | 5 |         |         |       |
| 30  | HJ    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1039  | 660 | 178 | 196 | 5 |         |         |       |
| 30  | JJ    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1039  | 660 | 178 | 196 | 5 |         |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31  | BK    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 709 | 210 | 200 | 3 |         |         |       |
| 31  | DK    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 709 | 210 | 200 | 3 |         |         |       |
| 31  | FK    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 709 | 210 | 200 | 3 |         |         |       |
| 31  | HK    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 709 | 210 | 200 | 3 |         |         |       |
| 31  | JK    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 709 | 210 | 200 | 3 |         |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32  | BL    | 132      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 981   | 603 | 196 | 178 | 4 |         |         |       |
| 32  | DL    | 132      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 981   | 603 | 196 | 178 | 4 |         |         |       |
| 32  | FL    | 132      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 981   | 603 | 196 | 178 | 4 |         |         |       |
| 32  | HL    | 132      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 981   | 603 | 196 | 178 | 4 |         |         |       |
| 32  | JL    | 132      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 981   | 603 | 196 | 178 | 4 |         |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 33  | BM    | 141      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1068  | 655 | 216 | 197 |         |         |       |
| 33  | DM    | 141      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1068  | 655 | 216 | 197 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 33  | FM    | 141      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1068  | 655 | 216 | 197 |         |         |       |
| 33  | HM    | 141      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1068  | 655 | 216 | 197 |         |         |       |
| 33  | JM    | 141      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1068  | 655 | 216 | 197 |         |         |       |

- Molecule 34 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34  | BN    | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 986   | 631 | 182 | 167 | 6 |         |         |       |
| 34  | DN    | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 986   | 631 | 182 | 167 | 6 |         |         |       |
| 34  | FN    | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 986   | 631 | 182 | 167 | 6 |         |         |       |
| 34  | HN    | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 986   | 631 | 182 | 167 | 6 |         |         |       |
| 34  | JN    | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 986   | 631 | 182 | 167 | 6 |         |         |       |

- Molecule 35 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35  | BO    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 886   | 546 | 179 | 159 | 2 |         |         |       |
| 35  | DO    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 886   | 546 | 179 | 159 | 2 |         |         |       |
| 35  | FO    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 886   | 546 | 179 | 159 | 2 |         |         |       |
| 35  | HO    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 886   | 546 | 179 | 159 | 2 |         |         |       |
| 35  | JO    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 886   | 546 | 179 | 159 | 2 |         |         |       |

- Molecule 36 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 36  | BP    | 111      | Total | C   | N   | O   | 8       | 0       | 0     |
|     |       |          | 834   | 512 | 168 | 154 |         |         |       |
| 36  | DP    | 111      | Total | C   | N   | O   | 8       | 0       | 0     |
|     |       |          | 834   | 512 | 168 | 154 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 36  | FP    | 111      | Total | C   | N   | O   | 8       | 0       | 0     |
|     |       |          | 834   | 512 | 168 | 154 |         |         |       |
| 36  | HP    | 111      | Total | C   | N   | O   | 8       | 0       | 0     |
|     |       |          | 834   | 512 | 168 | 154 |         |         |       |
| 36  | JP    | 111      | Total | C   | N   | O   | 8       | 0       | 0     |
|     |       |          | 834   | 512 | 168 | 154 |         |         |       |

- Molecule 37 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37  | BQ    | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1008  | 625 | 204 | 178 | 1 |         |         |       |
| 37  | DQ    | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1008  | 625 | 204 | 178 | 1 |         |         |       |
| 37  | FQ    | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1008  | 625 | 204 | 178 | 1 |         |         |       |
| 37  | HQ    | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1008  | 625 | 204 | 178 | 1 |         |         |       |
| 37  | JQ    | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1008  | 625 | 204 | 178 | 1 |         |         |       |

- Molecule 38 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38  | BR    | 117      | Total | C   | N   | O   | S | 16      | 0       | 0     |
|     |       |          | 978   | 608 | 210 | 159 | 1 |         |         |       |
| 38  | DR    | 117      | Total | C   | N   | O   | S | 16      | 0       | 0     |
|     |       |          | 978   | 608 | 210 | 159 | 1 |         |         |       |
| 38  | FR    | 117      | Total | C   | N   | O   | S | 16      | 0       | 0     |
|     |       |          | 978   | 608 | 210 | 159 | 1 |         |         |       |
| 38  | HR    | 117      | Total | C   | N   | O   | S | 16      | 0       | 0     |
|     |       |          | 978   | 608 | 210 | 159 | 1 |         |         |       |
| 38  | JR    | 117      | Total | C   | N   | O   | S | 16      | 0       | 0     |
|     |       |          | 978   | 608 | 210 | 159 | 1 |         |         |       |

- Molecule 39 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39  | BS    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 787   | 495 | 146 | 145 | 1 |         |         |       |
| 39  | DS    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 787   | 495 | 146 | 145 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39  | FS    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 787   | 495 | 146 | 145 | 1 |         |         |       |
| 39  | HS    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 787   | 495 | 146 | 145 | 1 |         |         |       |
| 39  | JS    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 787   | 495 | 146 | 145 | 1 |         |         |       |

- Molecule 40 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40  | BT    | 130      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1039  | 653 | 203 | 181 | 2 |         |         |       |
| 40  | DT    | 130      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1039  | 653 | 203 | 181 | 2 |         |         |       |
| 40  | FT    | 130      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1039  | 653 | 203 | 181 | 2 |         |         |       |
| 40  | HT    | 130      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1039  | 653 | 203 | 181 | 2 |         |         |       |
| 40  | JT    | 130      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1039  | 653 | 203 | 181 | 2 |         |         |       |

- Molecule 41 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41  | BU    | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 727   | 458 | 136 | 131 | 2 |         |         |       |
| 41  | DU    | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 727   | 458 | 136 | 131 | 2 |         |         |       |
| 41  | FU    | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 727   | 458 | 136 | 131 | 2 |         |         |       |
| 41  | HU    | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 727   | 458 | 136 | 131 | 2 |         |         |       |
| 41  | JU    | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 727   | 458 | 136 | 131 | 2 |         |         |       |

- Molecule 42 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | BV    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 852   | 530 | 166 | 155 | 1 |         |         |       |
| 42  | DV    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 852   | 530 | 166 | 155 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | FV    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 852   | 530 | 166 | 155 | 1 |         |         |       |
| 42  | HV    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 852   | 530 | 166 | 155 | 1 |         |         |       |
| 42  | JV    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 852   | 530 | 166 | 155 | 1 |         |         |       |

- Molecule 43 is a protein called general stress protein Ctc.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43  | BW    | 173      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1328  | 838 | 231 | 253 | 6 |         |         |       |
| 43  | DW    | 173      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1328  | 838 | 231 | 253 | 6 |         |         |       |
| 43  | FW    | 173      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1328  | 838 | 231 | 253 | 6 |         |         |       |
| 43  | HW    | 173      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1328  | 838 | 231 | 253 | 6 |         |         |       |
| 43  | JW    | 173      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1328  | 838 | 231 | 253 | 6 |         |         |       |

- Molecule 44 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44  | BX    | 86       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 642   | 402 | 124 | 115 | 1 |         |         |       |
| 44  | DX    | 86       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 642   | 402 | 124 | 115 | 1 |         |         |       |
| 44  | FX    | 86       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 642   | 402 | 124 | 115 | 1 |         |         |       |
| 44  | HX    | 86       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 642   | 402 | 124 | 115 | 1 |         |         |       |
| 44  | JX    | 86       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 642   | 402 | 124 | 115 | 1 |         |         |       |

- Molecule 45 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 45  | BY    | 65       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 526   | 322 | 106 | 96 | 2 |         |         |       |
| 45  | DY    | 65       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 526   | 322 | 106 | 96 | 2 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 45  | FY    | 65       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 526   | 322 | 106 | 96 | 2 |         |         |       |
| 45  | HY    | 65       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 526   | 322 | 106 | 96 | 2 |         |         |       |
| 45  | JY    | 65       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 526   | 322 | 106 | 96 | 2 |         |         |       |

- Molecule 46 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 46  | BZ    | 55       | Total | C   | N  | O  | S | 4       | 0       | 0     |
|     |       |          | 424   | 264 | 82 | 76 | 2 |         |         |       |
| 46  | DZ    | 55       | Total | C   | N  | O  | S | 4       | 0       | 0     |
|     |       |          | 424   | 264 | 82 | 76 | 2 |         |         |       |
| 46  | FZ    | 55       | Total | C   | N  | O  | S | 4       | 0       | 0     |
|     |       |          | 424   | 264 | 82 | 76 | 2 |         |         |       |
| 46  | HZ    | 55       | Total | C   | N  | O  | S | 4       | 0       | 0     |
|     |       |          | 424   | 264 | 82 | 76 | 2 |         |         |       |
| 46  | JZ    | 55       | Total | C   | N  | O  | S | 4       | 0       | 0     |
|     |       |          | 424   | 264 | 82 | 76 | 2 |         |         |       |

- Molecule 47 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47  | B1    | 73       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 604   | 382 | 110 | 108 | 4 |         |         |       |
| 47  | D1    | 73       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 604   | 382 | 110 | 108 | 4 |         |         |       |
| 47  | F1    | 73       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 604   | 382 | 110 | 108 | 4 |         |         |       |
| 47  | H1    | 73       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 604   | 382 | 110 | 108 | 4 |         |         |       |
| 47  | J1    | 73       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 604   | 382 | 110 | 108 | 4 |         |         |       |

- Molecule 48 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 48  | B2    | 58       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 458   | 281 | 94 | 78 | 5 |         |         |       |
| 48  | D2    | 58       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 458   | 281 | 94 | 78 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 48  | F2    | 58       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 458   | 281 | 94 | 78 | 5 |         |         |       |
| 48  | H2    | 58       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 458   | 281 | 94 | 78 | 5 |         |         |       |
| 48  | J2    | 58       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 458   | 281 | 94 | 78 | 5 |         |         |       |

- Molecule 49 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 49  | B3    | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 432   | 274 | 80 | 77 | 1 |         |         |       |
| 49  | D3    | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 432   | 274 | 80 | 77 | 1 |         |         |       |
| 49  | F3    | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 432   | 274 | 80 | 77 | 1 |         |         |       |
| 49  | H3    | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 432   | 274 | 80 | 77 | 1 |         |         |       |
| 49  | J3    | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 432   | 274 | 80 | 77 | 1 |         |         |       |

- Molecule 50 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 50  | B4    | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 384   | 230 | 91 | 61 | 2 |         |         |       |
| 50  | D4    | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 384   | 230 | 91 | 61 | 2 |         |         |       |
| 50  | F4    | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 384   | 230 | 91 | 61 | 2 |         |         |       |
| 50  | H4    | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 384   | 230 | 91 | 61 | 2 |         |         |       |
| 50  | J4    | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 384   | 230 | 91 | 61 | 2 |         |         |       |

- Molecule 51 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 51  | B5    | 63       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 496   | 312 | 101 | 78 | 5 |         |         |       |
| 51  | D5    | 63       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 496   | 312 | 101 | 78 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 51  | F5    | 63       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 496   | 312 | 101 | 78 | 5 |         |         |       |
| 51  | H5    | 63       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 496   | 312 | 101 | 78 | 5 |         |         |       |
| 51  | J5    | 63       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 496   | 312 | 101 | 78 | 5 |         |         |       |

- Molecule 52 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 52  | B6    | 35       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 285   | 172 | 64 | 45 | 4 |         |         |       |
| 52  | D6    | 35       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 285   | 172 | 64 | 45 | 4 |         |         |       |
| 52  | F6    | 35       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 285   | 172 | 64 | 45 | 4 |         |         |       |
| 52  | H6    | 35       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 285   | 172 | 64 | 45 | 4 |         |         |       |
| 52  | J6    | 35       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 285   | 172 | 64 | 45 | 4 |         |         |       |

- Molecule 53 is a protein called 50S ribosomal protein L1P.

| Mol | Chain | Residues | Atoms |      |     |     |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|----|---------|---------|-------|
| 53  | B7    | 217      | Total | C    | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 1720  | 1098 | 304 | 313 | 1 | 4  |         |         |       |
| 53  | D7    | 217      | Total | C    | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 1720  | 1098 | 304 | 313 | 1 | 4  |         |         |       |
| 53  | F7    | 217      | Total | C    | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 1720  | 1098 | 304 | 313 | 1 | 4  |         |         |       |
| 53  | H7    | 217      | Total | C    | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 1720  | 1098 | 304 | 313 | 1 | 4  |         |         |       |
| 53  | J7    | 217      | Total | C    | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 1720  | 1098 | 304 | 313 | 1 | 4  |         |         |       |

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### 3 Data and refinement statistics

| Property                                                                | Value                                                                            | Source           |
|-------------------------------------------------------------------------|----------------------------------------------------------------------------------|------------------|
| Space group                                                             | I 4 2 2                                                                          | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 687.90Å 687.90Å 1933.30Å<br>90.00° 90.00° 90.00°                                 | Depositor        |
| Resolution (Å)                                                          | 500.00 – 11.50<br>500.00 – 11.53                                                 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 93.9 (500.00-11.50)<br>76.2 (500.00-11.53)                                       | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                                                  | Depositor        |
| $R_{sym}$                                                               | 0.18                                                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$                                           | -                                                                                | Xtrriage         |
| Refinement program                                                      | CNS                                                                              | Depositor        |
| R, $R_{free}$                                                           | 0.395 , 0.401<br>0.405 , 0.406                                                   | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 7421 reflections (10.12%)                                                        | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | (Not available)                                                                  | Xtrriage         |
| Anisotropy                                                              | (Not available)                                                                  | Xtrriage         |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.22 , 999.0                                                                     | EDS              |
| L-test for twinning <sup>1</sup>                                        | $\langle  L  \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available) | Xtrriage         |
| Estimated twinning fraction                                             | No twinning to report.                                                           | Xtrriage         |
| $F_o, F_c$ correlation                                                  | 0.90                                                                             | EDS              |
| Total number of atoms                                                   | 717805                                                                           | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 803.0                                                                            | wwPDB-VP         |

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

<sup>1</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

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

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### 4.3 Torsion angles [i](#)

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

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

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

### 4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 4.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 4.7 Other polymers [i](#)

There are no such residues in this entry.

## 4.8 Polymer linkage issues

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 22  | FB    | 56               |
| 22  | HB    | 55               |
| 22  | JB    | 52               |
| 22  | DB    | 51               |
| 22  | BB    | 51               |
| 1   | EA    | 5                |
| 1   | AA    | 4                |
| 1   | CA    | 4                |
| 1   | GA    | 4                |
| 1   | IA    | 4                |
| 12  | AL    | 3                |
| 12  | GL    | 3                |
| 12  | CL    | 3                |
| 12  | IL    | 3                |
| 43  | DW    | 2                |
| 43  | JW    | 2                |
| 43  | FW    | 2                |
| 43  | BW    | 2                |
| 13  | IM    | 2                |
| 13  | EM    | 2                |
| 13  | CM    | 2                |
| 43  | HW    | 2                |
| 12  | EL    | 2                |
| 13  | GM    | 2                |
| 13  | AM    | 1                |

The worst 5 of 319 chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | JB    | 373:A     | O3'    | 387:A     | P      | 28.29        |
| 1     | HB    | 373:A     | O3'    | 387:A     | P      | 28.03        |
| 1     | FB    | 373:A     | O3'    | 387:A     | P      | 28.01        |
| 1     | DB    | 373:A     | O3'    | 387:A     | P      | 27.91        |
| 1     | FB    | 248:A     | O3'    | 292:A     | P      | 27.80        |

## 5 Fit of model and data ⓘ

### 5.1 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(Å²) | Q<0.9              |   |
|-----|-------|------------------|--------|----------|----|----------|--------------------|---|
| 1   | AA    | 1526/1526 (100%) | 0.05   | 105 (6%) | 24 | 24       | 521, 521, 521, 521 | 0 |
| 1   | CA    | 1526/1526 (100%) | -0.01  | 102 (6%) | 25 | 24       | 607, 607, 607, 607 | 0 |
| 1   | EA    | 1526/1526 (100%) | 0.05   | 111 (7%) | 22 | 23       | 628, 628, 628, 628 | 0 |
| 1   | GA    | 1526/1526 (100%) | 0.09   | 114 (7%) | 22 | 23       | 669, 669, 669, 669 | 0 |
| 1   | IA    | 1526/1526 (100%) | 0.07   | 108 (7%) | 23 | 24       | 743, 743, 743, 743 | 0 |
| 2   | AB    | 234/234 (100%)   | 1.69   | 69 (29%) | 1  | 5        | 521, 521, 521, 521 | 0 |
| 2   | CB    | 234/234 (100%)   | 1.57   | 57 (24%) | 2  | 7        | 607, 607, 607, 607 | 0 |
| 2   | EB    | 234/234 (100%)   | 2.06   | 54 (23%) | 2  | 7        | 628, 628, 628, 628 | 0 |
| 2   | GB    | 234/234 (100%)   | 2.14   | 62 (26%) | 2  | 6        | 669, 669, 669, 669 | 0 |
| 2   | IB    | 234/234 (100%)   | 2.50   | 53 (22%) | 3  | 7        | 743, 743, 743, 743 | 0 |
| 3   | AC    | 206/206 (100%)   | 0.92   | 41 (19%) | 3  | 8        | 521, 521, 521, 521 | 0 |
| 3   | CC    | 206/206 (100%)   | 0.81   | 33 (16%) | 6  | 11       | 607, 607, 607, 607 | 0 |
| 3   | EC    | 206/206 (100%)   | 1.27   | 48 (23%) | 2  | 7        | 628, 628, 628, 628 | 0 |
| 3   | GC    | 206/206 (100%)   | 1.24   | 52 (25%) | 2  | 6        | 669, 669, 669, 669 | 0 |
| 3   | IC    | 206/206 (100%)   | 1.47   | 50 (24%) | 2  | 7        | 743, 743, 743, 743 | 0 |
| 4   | AD    | 208/208 (100%)   | 0.59   | 34 (16%) | 5  | 10       | 521, 521, 521, 521 | 0 |
| 4   | CD    | 208/208 (100%)   | 0.26   | 22 (10%) | 13 | 16       | 607, 607, 607, 607 | 0 |
| 4   | ED    | 208/208 (100%)   | 0.50   | 33 (15%) | 6  | 11       | 628, 628, 628, 628 | 0 |
| 4   | GD    | 208/208 (100%)   | 1.00   | 50 (24%) | 2  | 7        | 669, 669, 669, 669 | 0 |
| 4   | ID    | 208/208 (100%)   | 1.11   | 40 (19%) | 4  | 9        | 743, 743, 743, 743 | 0 |
| 5   | AE    | 150/150 (100%)   | 0.22   | 15 (10%) | 14 | 17       | 521, 521, 521, 521 | 0 |
| 5   | CE    | 150/150 (100%)   | 0.09   | 8 (5%)   | 33 | 30       | 607, 607, 607, 607 | 0 |
| 5   | EE    | 150/150 (100%)   | 0.65   | 19 (12%) | 9  | 14       | 628, 628, 628, 628 | 0 |
| 5   | GE    | 150/150 (100%)   | 0.52   | 22 (14%) | 7  | 12       | 669, 669, 669, 669 | 0 |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2  |       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|----------|-------|-----------------------|-------|
| 5   | IE    | 150/150 (100%) | 0.90   | 27 (18%) | 4 9   | 743, 743, 743, 743    | 0     |
| 6   | AF    | 101/101 (100%) | 0.92   | 20 (19%) | 3 9   | 521, 521, 521, 521    | 0     |
| 6   | CF    | 101/101 (100%) | 0.74   | 16 (15%) | 6 11  | 607, 607, 607, 607    | 0     |
| 6   | EF    | 101/101 (100%) | 0.96   | 19 (18%) | 4 9   | 628, 628, 628, 628    | 0     |
| 6   | GF    | 101/101 (100%) | 1.14   | 21 (20%) | 3 8   | 669, 669, 669, 669    | 0     |
| 6   | IF    | 101/101 (100%) | 0.87   | 14 (13%) | 7 13  | 743, 743, 743, 743    | 0     |
| 7   | AG    | 155/155 (100%) | 0.76   | 20 (12%) | 9 13  | 521, 521, 521, 521    | 0     |
| 7   | CG    | 155/155 (100%) | 0.61   | 17 (10%) | 12 16 | 607, 607, 607, 607    | 0     |
| 7   | EG    | 155/155 (100%) | 0.91   | 27 (17%) | 5 10  | 628, 628, 628, 628    | 0     |
| 7   | GG    | 155/155 (100%) | 0.67   | 27 (17%) | 5 10  | 669, 669, 669, 669    | 0     |
| 7   | IG    | 155/155 (100%) | 0.90   | 29 (18%) | 4 9   | 743, 743, 743, 743    | 0     |
| 8   | AH    | 138/138 (100%) | 0.41   | 12 (8%)  | 17 19 | 521, 521, 521, 521    | 0     |
| 8   | CH    | 138/138 (100%) | -0.03  | 8 (5%)   | 30 28 | 607, 607, 607, 607    | 0     |
| 8   | EH    | 138/138 (100%) | 0.32   | 16 (11%) | 11 15 | 628, 628, 628, 628    | 0     |
| 8   | GH    | 138/138 (100%) | 0.27   | 8 (5%)   | 30 28 | 669, 669, 669, 669    | 0     |
| 8   | IH    | 138/138 (100%) | 0.03   | 10 (7%)  | 23 23 | 743, 743, 743, 743    | 0     |
| 9   | AI    | 127/127 (100%) | 0.31   | 14 (11%) | 12 16 | 521, 521, 521, 521    | 0     |
| 9   | CI    | 127/127 (100%) | 0.18   | 14 (11%) | 12 16 | 607, 607, 607, 607    | 0     |
| 9   | EI    | 127/127 (100%) | 0.37   | 15 (11%) | 10 15 | 628, 628, 628, 628    | 0     |
| 9   | GI    | 127/127 (100%) | 0.82   | 21 (16%) | 5 10  | 669, 669, 669, 669    | 0     |
| 9   | II    | 127/127 (100%) | 0.61   | 16 (12%) | 9 14  | 743, 743, 743, 743    | 0     |
| 10  | AJ    | 98/98 (100%)   | 0.08   | 4 (4%)   | 42 35 | 521, 521, 521, 521    | 0     |
| 10  | CJ    | 98/98 (100%)   | 0.13   | 6 (6%)   | 28 27 | 607, 607, 607, 607    | 0     |
| 10  | EJ    | 98/98 (100%)   | 0.44   | 13 (13%) | 8 13  | 628, 628, 628, 628    | 0     |
| 10  | GJ    | 98/98 (100%)   | 0.29   | 10 (10%) | 13 16 | 669, 669, 669, 669    | 0     |
| 10  | IJ    | 98/98 (100%)   | 0.41   | 10 (10%) | 13 16 | 743, 743, 743, 743    | 0     |
| 11  | AK    | 119/119 (100%) | 0.86   | 23 (19%) | 4 9   | 521, 521, 521, 521    | 0     |
| 11  | CK    | 119/119 (100%) | 0.59   | 15 (12%) | 9 14  | 607, 607, 607, 607    | 0     |
| 11  | EK    | 119/119 (100%) | 0.49   | 11 (9%)  | 16 18 | 628, 628, 628, 628    | 0     |
| 11  | GK    | 119/119 (100%) | 0.99   | 32 (26%) | 2 6   | 669, 669, 669, 669    | 0     |
| 11  | IK    | 119/119 (100%) | 1.09   | 25 (21%) | 3 8   | 743, 743, 743, 743    | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|----------------|-----------------------|-------|
| 12  | AL    | 124/124 (100%) | 1.23   | 21 (16%) 5 10  | 521, 521, 521, 521    | 0     |
| 12  | CL    | 124/124 (100%) | 0.56   | 13 (10%) 13 16 | 607, 607, 607, 607    | 0     |
| 12  | EL    | 124/124 (100%) | 0.74   | 14 (11%) 11 15 | 628, 628, 628, 628    | 0     |
| 12  | GL    | 124/124 (100%) | 1.07   | 29 (23%) 2 7   | 669, 669, 669, 669    | 0     |
| 12  | IL    | 124/124 (100%) | 0.98   | 24 (19%) 4 9   | 743, 743, 743, 743    | 0     |
| 13  | AM    | 125/125 (100%) | 0.84   | 26 (20%) 3 8   | 521, 521, 521, 521    | 0     |
| 13  | CM    | 125/125 (100%) | 0.94   | 19 (15%) 6 12  | 607, 607, 607, 607    | 0     |
| 13  | EM    | 125/125 (100%) | 1.29   | 27 (21%) 3 8   | 628, 628, 628, 628    | 0     |
| 13  | GM    | 125/125 (100%) | 0.84   | 23 (18%) 4 9   | 669, 669, 669, 669    | 0     |
| 13  | IM    | 125/125 (100%) | 1.06   | 24 (19%) 4 9   | 743, 743, 743, 743    | 0     |
| 14  | AN    | 60/60 (100%)   | 0.46   | 8 (13%) 8 13   | 521, 521, 521, 521    | 0     |
| 14  | CN    | 60/60 (100%)   | 0.61   | 9 (15%) 6 12   | 607, 607, 607, 607    | 0     |
| 14  | EN    | 60/60 (100%)   | 1.11   | 12 (20%) 3 8   | 628, 628, 628, 628    | 0     |
| 14  | GN    | 60/60 (100%)   | 0.73   | 8 (13%) 8 13   | 669, 669, 669, 669    | 0     |
| 14  | IN    | 60/60 (100%)   | 0.95   | 10 (16%) 5 10  | 743, 743, 743, 743    | 0     |
| 15  | AO    | 88/88 (100%)   | 0.76   | 17 (19%) 4 9   | 521, 521, 521, 521    | 0     |
| 15  | CO    | 88/88 (100%)   | 1.24   | 17 (19%) 4 9   | 607, 607, 607, 607    | 0     |
| 15  | EO    | 88/88 (100%)   | 1.86   | 16 (18%) 4 9   | 628, 628, 628, 628    | 0     |
| 15  | GO    | 88/88 (100%)   | 0.83   | 14 (15%) 6 11  | 669, 669, 669, 669    | 0     |
| 15  | IO    | 88/88 (100%)   | 1.39   | 13 (14%) 7 12  | 743, 743, 743, 743    | 0     |
| 16  | AP    | 83/83 (100%)   | 0.40   | 8 (9%) 15 17   | 521, 521, 521, 521    | 0     |
| 16  | CP    | 83/83 (100%)   | 0.98   | 12 (14%) 7 12  | 607, 607, 607, 607    | 0     |
| 16  | EP    | 83/83 (100%)   | 0.12   | 9 (10%) 12 16  | 628, 628, 628, 628    | 0     |
| 16  | GP    | 83/83 (100%)   | 0.35   | 9 (10%) 12 16  | 669, 669, 669, 669    | 0     |
| 16  | IP    | 83/83 (100%)   | 0.27   | 9 (10%) 12 16  | 743, 743, 743, 743    | 0     |
| 17  | AQ    | 104/104 (100%) | 0.46   | 13 (12%) 9 14  | 521, 521, 521, 521    | 0     |
| 17  | CQ    | 104/104 (100%) | -0.09  | 5 (4%) 36 33   | 607, 607, 607, 607    | 0     |
| 17  | EQ    | 104/104 (100%) | -0.10  | 5 (4%) 36 33   | 628, 628, 628, 628    | 0     |
| 17  | GQ    | 104/104 (100%) | 0.08   | 5 (4%) 36 33   | 669, 669, 669, 669    | 0     |
| 17  | IQ    | 104/104 (100%) | -0.12  | 6 (5%) 30 28   | 743, 743, 743, 743    | 0     |
| 18  | AR    | 73/73 (100%)   | 0.48   | 7 (9%) 15 17   | 521, 521, 521, 521    | 0     |

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| Mol | Chain | Analysed         | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9     |
|-----|-------|------------------|--------|----------------|-----------------------|-----------|
| 18  | CR    | 73/73 (100%)     | 0.19   | 6 (8%) 19 20   | 607, 607, 607, 607    | 0         |
| 18  | ER    | 73/73 (100%)     | 0.52   | 9 (12%) 9 14   | 628, 628, 628, 628    | 0         |
| 18  | GR    | 73/73 (100%)     | 0.77   | 15 (20%) 3 8   | 669, 669, 669, 669    | 0         |
| 18  | IR    | 73/73 (100%)     | 0.82   | 9 (12%) 9 14   | 743, 743, 743, 743    | 0         |
| 19  | AS    | 80/80 (100%)     | 0.10   | 6 (7%) 22 23   | 521, 521, 521, 521    | 0         |
| 19  | CS    | 80/80 (100%)     | 0.37   | 9 (11%) 11 15  | 607, 607, 607, 607    | 0         |
| 19  | ES    | 80/80 (100%)     | -0.14  | 3 (3%) 44 37   | 628, 628, 628, 628    | 0         |
| 19  | GS    | 80/80 (100%)     | 0.28   | 7 (8%) 17 19   | 669, 669, 669, 669    | 0         |
| 19  | IS    | 80/80 (100%)     | 0.07   | 8 (10%) 14 17  | 743, 743, 743, 743    | 0         |
| 20  | AT    | 99/99 (100%)     | 0.71   | 16 (16%) 5 11  | 521, 521, 521, 521    | 0         |
| 20  | CT    | 99/99 (100%)     | 0.66   | 14 (14%) 7 13  | 607, 607, 607, 607    | 0         |
| 20  | ET    | 99/99 (100%)     | 0.55   | 13 (13%) 8 13  | 628, 628, 628, 628    | 0         |
| 20  | GT    | 99/99 (100%)     | 1.07   | 23 (23%) 2 7   | 669, 669, 669, 669    | 0         |
| 20  | IT    | 99/99 (100%)     | 0.32   | 10 (10%) 14 16 | 743, 743, 743, 743    | 0         |
| 21  | Aa    | 90/90 (100%)     | 0.98   | 14 (15%) 6 11  | 0, 0, 0, 0            | 90 (100%) |
| 21  | Ca    | 90/90 (100%)     | 0.82   | 17 (18%) 4 9   | 0, 0, 0, 0            | 90 (100%) |
| 21  | Ea    | 90/90 (100%)     | 0.64   | 17 (18%) 4 9   | 0, 0, 0, 0            | 90 (100%) |
| 21  | Ga    | 90/90 (100%)     | 1.08   | 23 (25%) 2 6   | 0, 0, 0, 0            | 90 (100%) |
| 21  | Ia    | 90/90 (100%)     | 1.23   | 15 (16%) 5 10  | 0, 0, 0, 0            | 90 (100%) |
| 22  | BB    | 2825/2825 (100%) | 0.11   | 221 (7%) 20 21 | 849, 855, 857, 859    | 0         |
| 22  | DB    | 2825/2825 (100%) | 0.18   | 241 (8%) 18 20 | 895, 902, 903, 904    | 0         |
| 22  | FB    | 2825/2825 (100%) | 0.22   | 254 (8%) 17 19 | 896, 902, 905, 905    | 0         |
| 22  | HB    | 2825/2825 (100%) | 0.07   | 210 (7%) 22 23 | 894, 902, 903, 903    | 0         |
| 22  | JB    | 2825/2825 (100%) | 0.08   | 204 (7%) 23 23 | 897, 902, 906, 908    | 0         |
| 23  | BA    | 118/119 (99%)    | 0.10   | 8 (6%) 25 24   | 809, 846, 846, 846    | 0         |
| 23  | DA    | 118/119 (99%)    | -0.08  | 6 (5%) 34 30   | 854, 893, 893, 893    | 0         |
| 23  | FA    | 118/119 (99%)    | -0.38  | 5 (4%) 41 35   | 857, 896, 896, 896    | 0         |
| 23  | HA    | 118/119 (99%)    | 0.02   | 7 (5%) 29 28   | 855, 894, 894, 894    | 0         |
| 23  | JA    | 118/119 (99%)    | -0.14  | 8 (6%) 25 24   | 855, 894, 894, 894    | 0         |
| 24  | BD    | 270/270 (100%)   | 0.30   | 31 (11%) 11 15 | 904, 904, 904, 904    | 0         |
| 24  | DD    | 270/270 (100%)   | 0.50   | 38 (14%) 7 13  | 950, 950, 950, 950    | 0         |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|----------------|-----------------------|-------|
| 24  | FD    | 270/270 (100%) | 0.80   | 39 (14%) 7 12  | 950, 950, 950, 950    | 0     |
| 24  | HD    | 270/270 (100%) | 0.66   | 37 (13%) 8 13  | 950, 950, 950, 950    | 0     |
| 24  | JD    | 270/270 (100%) | 0.18   | 26 (9%) 15 17  | 950, 950, 950, 950    | 0     |
| 25  | BE    | 205/205 (100%) | 0.64   | 25 (12%) 10 15 | 904, 904, 904, 904    | 0     |
| 25  | DE    | 205/205 (100%) | 0.05   | 13 (6%) 27 27  | 950, 950, 950, 950    | 0     |
| 25  | FE    | 205/205 (100%) | 0.47   | 21 (10%) 13 16 | 950, 950, 950, 950    | 0     |
| 25  | HE    | 205/205 (100%) | 0.95   | 34 (16%) 5 10  | 950, 950, 950, 950    | 0     |
| 25  | JE    | 205/205 (100%) | 1.52   | 42 (20%) 3 8   | 950, 950, 950, 950    | 0     |
| 26  | BF    | 197/198 (99%)  | 0.06   | 11 (5%) 31 28  | 904, 904, 904, 904    | 0     |
| 26  | DF    | 197/198 (99%)  | 0.29   | 18 (9%) 16 18  | 950, 950, 950, 950    | 0     |
| 26  | FF    | 197/198 (99%)  | 0.43   | 20 (10%) 13 16 | 950, 950, 950, 950    | 0     |
| 26  | HF    | 197/198 (99%)  | 0.25   | 14 (7%) 23 24  | 950, 950, 950, 950    | 0     |
| 26  | JF    | 197/198 (99%)  | 0.44   | 19 (9%) 15 17  | 950, 950, 950, 950    | 0     |
| 27  | BG    | 178/178 (100%) | 0.97   | 22 (12%) 9 14  | 904, 904, 904, 904    | 0     |
| 27  | DG    | 178/178 (100%) | 0.21   | 11 (6%) 28 27  | 950, 950, 950, 950    | 0     |
| 27  | FG    | 178/178 (100%) | 0.46   | 9 (5%) 34 30   | 950, 950, 950, 950    | 0     |
| 27  | HG    | 178/178 (100%) | 2.00   | 31 (17%) 5 10  | 950, 950, 950, 950    | 0     |
| 27  | JG    | 178/178 (100%) | 1.02   | 26 (14%) 7 12  | 950, 950, 950, 950    | 0     |
| 28  | BH    | 177/177 (100%) | 2.13   | 70 (39%) 1 4   | 904, 904, 904, 904    | 0     |
| 28  | DH    | 177/177 (100%) | 1.42   | 38 (21%) 3 8   | 950, 950, 950, 950    | 0     |
| 28  | FH    | 177/177 (100%) | 0.89   | 23 (12%) 9 13  | 950, 950, 950, 950    | 0     |
| 28  | HH    | 177/177 (100%) | 2.53   | 66 (37%) 1 4   | 950, 950, 950, 950    | 0     |
| 28  | JH    | 177/177 (100%) | 1.70   | 41 (23%) 2 7   | 950, 950, 950, 950    | 0     |
| 29  | BI    | 52/52 (100%)   | 0.59   | 5 (9%) 15 17   | 904, 904, 904, 904    | 0     |
| 29  | DI    | 52/52 (100%)   | 0.81   | 8 (15%) 6 11   | 950, 950, 950, 950    | 0     |
| 29  | FI    | 52/52 (100%)   | 0.84   | 7 (13%) 8 13   | 950, 950, 950, 950    | 0     |
| 29  | HI    | 52/52 (100%)   | 0.47   | 2 (3%) 44 37   | 950, 950, 950, 950    | 0     |
| 29  | JI    | 52/52 (100%)   | 0.22   | 4 (7%) 21 22   | 950, 950, 950, 950    | 0     |
| 30  | BJ    | 143/143 (100%) | -0.10  | 9 (6%) 27 27   | 904, 904, 904, 904    | 0     |
| 30  | DJ    | 143/143 (100%) | 0.16   | 7 (4%) 36 32   | 950, 950, 950, 950    | 0     |
| 30  | FJ    | 143/143 (100%) | 0.31   | 9 (6%) 27 27   | 950, 950, 950, 950    | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2  |         | OWAB(Å <sup>2</sup> ) | Q<0.9  |
|-----|-------|----------------|--------|----------|---------|-----------------------|--------|
| 30  | HJ    | 143/143 (100%) | -0.04  | 15 (10%) | 13 16   | 950, 950, 950, 950    | 0      |
| 30  | JJ    | 143/143 (100%) | 0.02   | 7 (4%)   | 36 32   | 950, 950, 950, 950    | 0      |
| 31  | BK    | 143/143 (100%) | 0.52   | 15 (10%) | 13 16   | 904, 904, 904, 904    | 0      |
| 31  | DK    | 143/143 (100%) | 0.42   | 14 (9%)  | 14 17   | 950, 950, 950, 950    | 0      |
| 31  | FK    | 143/143 (100%) | 1.15   | 20 (13%) | 7 13    | 950, 950, 950, 950    | 0      |
| 31  | HK    | 143/143 (100%) | 0.93   | 18 (12%) | 9 14    | 950, 950, 950, 950    | 0      |
| 31  | JK    | 143/143 (100%) | 2.42   | 34 (23%) | 2 7     | 950, 950, 950, 950    | 0      |
| 32  | BL    | 132/132 (100%) | 0.65   | 20 (15%) | 6 12    | 904, 904, 904, 904    | 0      |
| 32  | DL    | 132/132 (100%) | 0.23   | 12 (9%)  | 16 18   | 950, 950, 950, 950    | 0      |
| 32  | FL    | 132/132 (100%) | 0.34   | 13 (9%)  | 14 17   | 950, 950, 950, 950    | 0      |
| 32  | HL    | 132/132 (100%) | 0.75   | 21 (15%) | 6 11    | 950, 950, 950, 950    | 0      |
| 32  | JL    | 132/132 (100%) | 0.37   | 16 (12%) | 10 15   | 950, 950, 950, 950    | 0      |
| 33  | BM    | 141/141 (100%) | 1.31   | 15 (10%) | 13 16   | 904, 904, 904, 904    | 0      |
| 33  | DM    | 141/141 (100%) | 1.39   | 11 (7%)  | 20 21   | 950, 950, 950, 950    | 0      |
| 33  | FM    | 141/141 (100%) | 1.70   | 13 (9%)  | 16 18   | 950, 950, 950, 950    | 0      |
| 33  | HM    | 141/141 (100%) | 0.90   | 14 (9%)  | 14 17   | 950, 950, 950, 950    | 0      |
| 33  | JM    | 141/141 (100%) | 1.17   | 16 (11%) | 11 15   | 950, 950, 950, 950    | 0      |
| 34  | BN    | 124/124 (100%) | -0.32  | 3 (2%)   | 59 49   | 904, 904, 904, 904    | 0      |
| 34  | DN    | 124/124 (100%) | -0.39  | 1 (0%)   | 82 71   | 950, 950, 950, 950    | 0      |
| 34  | FN    | 124/124 (100%) | 0.33   | 10 (8%)  | 19 21   | 950, 950, 950, 950    | 0      |
| 34  | HN    | 124/124 (100%) | -0.14  | 7 (5%)   | 31 28   | 950, 950, 950, 950    | 0      |
| 34  | JN    | 124/124 (100%) | 0.14   | 8 (6%)   | 26 26   | 950, 950, 950, 950    | 0      |
| 35  | BO    | 114/114 (100%) | -0.05  | 2 (1%)   | 67 56   | 904, 904, 904, 904    | 0      |
| 35  | DO    | 114/114 (100%) | -0.29  | 1 (0%)   | 81 69   | 950, 950, 950, 950    | 0      |
| 35  | FO    | 114/114 (100%) | -0.30  | 2 (1%)   | 67 56   | 950, 950, 950, 950    | 0      |
| 35  | HO    | 114/114 (100%) | -0.25  | 2 (1%)   | 67 56   | 950, 950, 950, 950    | 0      |
| 35  | JO    | 114/114 (100%) | -0.52  | 0        | 100 100 | 950, 950, 950, 950    | 0      |
| 36  | BP    | 111/111 (100%) | -0.28  | 0        | 100 100 | 678, 904, 904, 904    | 7 (6%) |
| 36  | DP    | 111/111 (100%) | -0.40  | 2 (1%)   | 67 56   | 712, 950, 950, 950    | 7 (6%) |
| 36  | FP    | 111/111 (100%) | -0.21  | 6 (5%)   | 32 29   | 712, 950, 950, 950    | 7 (6%) |
| 36  | HP    | 111/111 (100%) | -0.14  | 3 (2%)   | 56 45   | 712, 950, 950, 950    | 7 (6%) |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2  |    |    | OWAB(Å <sup>2</sup> ) | Q<0.9  |
|-----|-------|----------------|--------|----------|----|----|-----------------------|--------|
| 36  | JP    | 111/111 (100%) | -0.35  | 4 (3%)   | 46 | 38 | 712, 950, 950, 950    | 7 (6%) |
| 37  | BQ    | 125/125 (100%) | 0.83   | 15 (12%) | 10 | 15 | 904, 904, 904, 904    | 0      |
| 37  | DQ    | 125/125 (100%) | 0.90   | 20 (16%) | 6  | 11 | 950, 950, 950, 950    | 0      |
| 37  | FQ    | 125/125 (100%) | 0.78   | 18 (14%) | 7  | 12 | 950, 950, 950, 950    | 0      |
| 37  | HQ    | 125/125 (100%) | 0.55   | 12 (9%)  | 15 | 17 | 950, 950, 950, 950    | 0      |
| 37  | JQ    | 125/125 (100%) | -0.08  | 8 (6%)   | 27 | 26 | 950, 950, 950, 950    | 0      |
| 38  | BR    | 117/117 (100%) | 0.41   | 14 (11%) | 10 | 15 | 678, 904, 904, 904    | 9 (7%) |
| 38  | DR    | 117/117 (100%) | -0.15  | 6 (5%)   | 34 | 30 | 712, 950, 950, 950    | 9 (7%) |
| 38  | FR    | 117/117 (100%) | -0.34  | 7 (5%)   | 29 | 27 | 712, 950, 950, 950    | 9 (7%) |
| 38  | HR    | 117/117 (100%) | 0.40   | 11 (9%)  | 15 | 17 | 712, 950, 950, 950    | 9 (7%) |
| 38  | JR    | 117/117 (100%) | -0.07  | 8 (6%)   | 25 | 24 | 712, 950, 950, 950    | 9 (7%) |
| 39  | BS    | 100/100 (100%) | 0.94   | 20 (20%) | 3  | 8  | 904, 904, 904, 904    | 0      |
| 39  | DS    | 100/100 (100%) | 0.83   | 16 (16%) | 6  | 11 | 950, 950, 950, 950    | 0      |
| 39  | FS    | 100/100 (100%) | 0.47   | 13 (13%) | 9  | 13 | 950, 950, 950, 950    | 0      |
| 39  | HS    | 100/100 (100%) | 1.25   | 18 (18%) | 4  | 9  | 950, 950, 950, 950    | 0      |
| 39  | JS    | 100/100 (100%) | 0.89   | 20 (20%) | 3  | 8  | 950, 950, 950, 950    | 0      |
| 40  | BT    | 130/130 (100%) | -0.19  | 9 (6%)   | 24 | 24 | 904, 904, 904, 904    | 0      |
| 40  | DT    | 130/130 (100%) | 0.63   | 18 (13%) | 8  | 13 | 950, 950, 950, 950    | 0      |
| 40  | FT    | 130/130 (100%) | 1.37   | 20 (15%) | 6  | 11 | 950, 950, 950, 950    | 0      |
| 40  | HT    | 130/130 (100%) | -0.36  | 3 (2%)   | 61 | 50 | 950, 950, 950, 950    | 0      |
| 40  | JT    | 130/130 (100%) | 0.71   | 9 (6%)   | 24 | 24 | 950, 950, 950, 950    | 0      |
| 41  | BU    | 93/93 (100%)   | -0.18  | 2 (2%)   | 62 | 51 | 904, 904, 904, 904    | 0      |
| 41  | DU    | 93/93 (100%)   | -0.31  | 1 (1%)   | 77 | 65 | 950, 950, 950, 950    | 0      |
| 41  | FU    | 93/93 (100%)   | -0.35  | 1 (1%)   | 77 | 65 | 950, 950, 950, 950    | 0      |
| 41  | HU    | 93/93 (100%)   | -0.34  | 1 (1%)   | 77 | 65 | 950, 950, 950, 950    | 0      |
| 41  | JU    | 93/93 (100%)   | -0.10  | 2 (2%)   | 62 | 51 | 950, 950, 950, 950    | 0      |
| 42  | BV    | 113/113 (100%) | 0.87   | 21 (18%) | 4  | 9  | 904, 904, 904, 904    | 0      |
| 42  | DV    | 113/113 (100%) | 0.25   | 10 (8%)  | 17 | 19 | 950, 950, 950, 950    | 0      |
| 42  | FV    | 113/113 (100%) | -0.14  | 7 (6%)   | 28 | 27 | 950, 950, 950, 950    | 0      |
| 42  | HV    | 113/113 (100%) | 1.06   | 22 (19%) | 4  | 9  | 950, 950, 950, 950    | 0      |
| 42  | JV    | 113/113 (100%) | 0.19   | 11 (9%)  | 15 | 17 | 950, 950, 950, 950    | 0      |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9  |
|-----|-------|----------------|--------|---------------|-----------------------|--------|
| 43  | BW    | 173/173 (100%) | -0.09  | 5 (2%) 54 43  | 904, 904, 904, 904    | 0      |
| 43  | DW    | 173/173 (100%) | 0.17   | 15 (8%) 17 19 | 950, 950, 950, 950    | 0      |
| 43  | FW    | 173/173 (100%) | 0.02   | 0 100 100     | 950, 950, 950, 950    | 0      |
| 43  | HW    | 173/173 (100%) | 0.22   | 10 (5%) 30 28 | 950, 950, 950, 950    | 0      |
| 43  | JW    | 173/173 (100%) | 0.31   | 13 (7%) 22 23 | 950, 950, 950, 950    | 0      |
| 44  | BX    | 86/86 (100%)   | 0.39   | 7 (8%) 19 21  | 904, 904, 904, 904    | 0      |
| 44  | DX    | 86/86 (100%)   | 0.26   | 7 (8%) 19 21  | 950, 950, 950, 950    | 0      |
| 44  | FX    | 86/86 (100%)   | 0.57   | 7 (8%) 19 21  | 950, 950, 950, 950    | 0      |
| 44  | HX    | 86/86 (100%)   | 0.27   | 7 (8%) 19 21  | 950, 950, 950, 950    | 0      |
| 44  | JX    | 86/86 (100%)   | 1.27   | 12 (13%) 7 13 | 950, 950, 950, 950    | 0      |
| 45  | BY    | 65/65 (100%)   | 0.04   | 3 (4%) 38 34  | 904, 904, 904, 904    | 0      |
| 45  | DY    | 65/65 (100%)   | 0.39   | 7 (10%) 12 16 | 950, 950, 950, 950    | 0      |
| 45  | FY    | 65/65 (100%)   | 0.16   | 4 (6%) 28 27  | 950, 950, 950, 950    | 0      |
| 45  | HY    | 65/65 (100%)   | -0.35  | 5 (7%) 21 22  | 950, 950, 950, 950    | 0      |
| 45  | JY    | 65/65 (100%)   | -0.20  | 5 (7%) 21 22  | 950, 950, 950, 950    | 0      |
| 46  | BZ    | 55/55 (100%)   | -0.49  | 0 100 100     | 791, 904, 904, 904    | 3 (5%) |
| 46  | DZ    | 55/55 (100%)   | -0.47  | 0 100 100     | 831, 950, 950, 950    | 3 (5%) |
| 46  | FZ    | 55/55 (100%)   | -0.68  | 0 100 100     | 831, 950, 950, 950    | 3 (5%) |
| 46  | HZ    | 55/55 (100%)   | -0.19  | 2 (3%) 46 38  | 831, 950, 950, 950    | 3 (5%) |
| 46  | JZ    | 55/55 (100%)   | -0.40  | 0 100 100     | 831, 950, 950, 950    | 3 (5%) |
| 47  | B1    | 73/73 (100%)   | 0.30   | 4 (5%) 32 29  | 904, 904, 904, 904    | 0      |
| 47  | D1    | 73/73 (100%)   | 0.18   | 4 (5%) 32 29  | 950, 950, 950, 950    | 0      |
| 47  | F1    | 73/73 (100%)   | 0.41   | 6 (8%) 19 20  | 950, 950, 950, 950    | 0      |
| 47  | H1    | 73/73 (100%)   | -0.05  | 5 (6%) 25 24  | 950, 950, 950, 950    | 0      |
| 47  | J1    | 73/73 (100%)   | 0.15   | 7 (9%) 15 17  | 950, 950, 950, 950    | 0      |
| 48  | B2    | 58/58 (100%)   | 0.47   | 7 (12%) 10 15 | 904, 904, 904, 904    | 0      |
| 48  | D2    | 58/58 (100%)   | 0.73   | 8 (13%) 8 13  | 950, 950, 950, 950    | 0      |
| 48  | F2    | 58/58 (100%)   | 0.76   | 10 (17%) 5 10 | 950, 950, 950, 950    | 0      |
| 48  | H2    | 58/58 (100%)   | 0.16   | 2 (3%) 48 39  | 950, 950, 950, 950    | 0      |
| 48  | J2    | 58/58 (100%)   | -0.13  | 4 (6%) 24 24  | 950, 950, 950, 950    | 0      |
| 49  | B3    | 53/53 (100%)   | 1.63   | 14 (26%) 2 6  | 904, 904, 904, 904    | 0      |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2          | OWAB(Å <sup>2</sup> ) | Q<0.9    |
|-----|-------|-------------------|--------|------------------|-----------------------|----------|
| 49  | D3    | 53/53 (100%)      | 2.29   | 18 (33%) 1 5     | 950, 950, 950, 950    | 0        |
| 49  | F3    | 53/53 (100%)      | 1.07   | 10 (18%) 4 9     | 950, 950, 950, 950    | 0        |
| 49  | H3    | 53/53 (100%)      | 1.42   | 10 (18%) 4 9     | 950, 950, 950, 950    | 0        |
| 49  | J3    | 53/53 (100%)      | 0.25   | 3 (5%) 30 28     | 950, 950, 950, 950    | 0        |
| 50  | B4    | 46/46 (100%)      | -0.65  | 0 100 100        | 904, 904, 904, 904    | 0        |
| 50  | D4    | 46/46 (100%)      | -0.70  | 0 100 100        | 950, 950, 950, 950    | 0        |
| 50  | F4    | 46/46 (100%)      | -0.58  | 0 100 100        | 950, 950, 950, 950    | 0        |
| 50  | H4    | 46/46 (100%)      | -0.53  | 0 100 100        | 950, 950, 950, 950    | 0        |
| 50  | J4    | 46/46 (100%)      | -0.54  | 0 100 100        | 950, 950, 950, 950    | 0        |
| 51  | B5    | 63/63 (100%)      | -0.51  | 1 (1%) 70 58     | 904, 904, 904, 904    | 0        |
| 51  | D5    | 63/63 (100%)      | -0.60  | 1 (1%) 70 58     | 950, 950, 950, 950    | 0        |
| 51  | F5    | 63/63 (100%)      | -0.99  | 0 100 100        | 950, 950, 950, 950    | 0        |
| 51  | H5    | 63/63 (100%)      | -0.37  | 1 (1%) 70 58     | 950, 950, 950, 950    | 0        |
| 51  | J5    | 63/63 (100%)      | -0.73  | 0 100 100        | 950, 950, 950, 950    | 0        |
| 52  | B6    | 35/35 (100%)      | 0.23   | 3 (8%) 18 19     | 904, 904, 904, 904    | 0        |
| 52  | D6    | 35/35 (100%)      | -0.48  | 0 100 100        | 950, 950, 950, 950    | 0        |
| 52  | F6    | 35/35 (100%)      | -0.35  | 1 (2%) 54 43     | 950, 950, 950, 950    | 0        |
| 52  | H6    | 35/35 (100%)      | 0.07   | 0 100 100        | 950, 950, 950, 950    | 0        |
| 52  | J6    | 35/35 (100%)      | -0.12  | 2 (5%) 30 28     | 950, 950, 950, 950    | 0        |
| 53  | B7    | 213/217 (98%)     | 1.14   | 50 (23%) 2 7     | 904, 904, 904, 904    | 0        |
| 53  | D7    | 213/217 (98%)     | 1.10   | 31 (14%) 7 12    | 950, 950, 950, 950    | 0        |
| 53  | F7    | 213/217 (98%)     | 1.34   | 53 (24%) 2 7     | 950, 950, 950, 950    | 0        |
| 53  | H7    | 213/217 (98%)     | 0.87   | 37 (17%) 5 10    | 950, 950, 950, 950    | 0        |
| 53  | J7    | 213/217 (98%)     | 0.84   | 36 (16%) 5 10    | 950, 950, 950, 950    | 0        |
| All | All   | 52580/52610 (99%) | 0.39   | 5533 (10%) 13 16 | 0, 900, 950, 950      | 545 (1%) |

The worst 5 of 5533 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 31  | JK    | 156 | HIS  | 71.0 |
| 2   | IB    | 240 | GLN  | 56.3 |
| 33  | HM    | 7   | LYS  | 54.9 |
| 33  | BM    | 7   | LYS  | 54.7 |
| 33  | DM    | 4   | HIS  | 54.5 |

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

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

## 5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.4 Ligands [i](#)

There are no ligands in this entry.

## 5.5 Other polymers [i](#)

There are no such residues in this entry.