



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:04 PM UTC

PDB ID : 6Y0G / pdb\_00006y0g  
EMDB ID : EMD-10668  
Title : Structure of human ribosome in classical-PRE state  
Authors : Bhaskar, V.; Schenk, A.D.; Cavadini, S.; von Loeffelholz, O.; Natchiar, S.K.; Klaholz, B.P.; Chao, J.A.  
Deposited on : 2020-02-07  
Resolution : 3.20 Å(reported)  
Based on initial models : 5LKS, 6QZP, 5AJ0

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

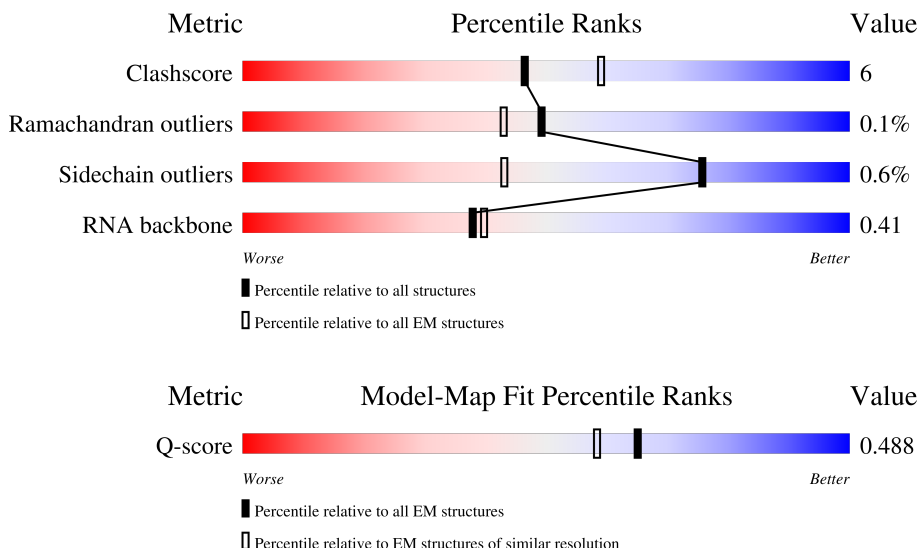
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 15020 ( 2.70 - 3.70 )                                    |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A4    | 28     |                  |
| 2   | B4    | 76     |                  |
| 2   | D4    | 76     |                  |

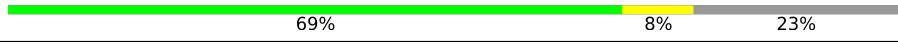
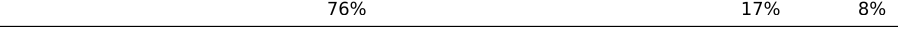
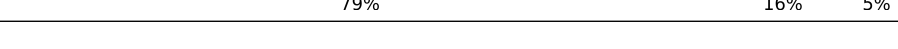
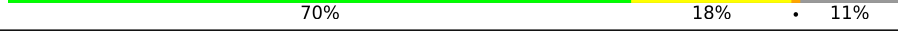
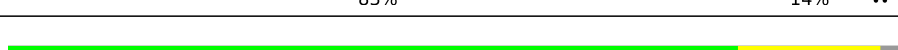
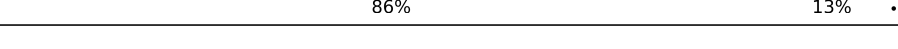
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | C4    | 2      | 100%             |
| 4   | L5    | 5070   | 47% 21% . 28%    |
| 5   | L7    | 120    | 72% 24% .        |
| 6   | L8    | 156    | 71% 25% .        |
| 7   | LA    | 257    | 81% 15% .        |
| 8   | LB    | 403    | 78% 21% .        |
| 9   | LC    | 427    | 73% 12% 15%      |
| 10  | LD    | 297    | 84% 14% .        |
| 11  | LE    | 288    | 61% 15% 23%      |
| 12  | LF    | 248    | 82% 9% 9%        |
| 13  | LG    | 266    | 70% 15% 15%      |
| 14  | LH    | 192    | 82% 17% ..       |
| 15  | LI    | 214    | 76% 22% .        |
| 16  | LJ    | 178    | . 75% 22% ..     |
| 17  | LL    | 211    | 77% 21% .        |
| 18  | LM    | 215    | 51% 12% 37%      |
| 19  | LN    | 204    | 86% 14%          |
| 20  | LO    | 203    | 85% 14% .        |
| 21  | LP    | 184    | 74% 9% 17%       |
| 22  | LQ    | 188    | 79% 20% ..       |
| 23  | LR    | 196    | . 78% 14% 8%     |
| 24  | LS    | 176    | 84% 15% .        |
| 25  | LT    | 160    | 81% 18% .        |
| 26  | LU    | 128    | 67% 12% 21%      |
| 27  | LV    | 140    | 76% 18% 6%       |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 28  | LW    | 157    |    |
| 29  | LX    | 156    |    |
| 30  | LY    | 145    |    |
| 31  | LZ    | 136    |    |
| 32  | La    | 148    |    |
| 33  | Lb    | 159    |    |
| 34  | Lc    | 115    |    |
| 35  | Ld    | 125    |    |
| 36  | Le    | 135    |    |
| 37  | Lf    | 110    |   |
| 38  | Lg    | 117    |  |
| 39  | Lh    | 123    |  |
| 40  | Li    | 105    |  |
| 41  | Lj    | 97     |  |
| 42  | Lk    | 70     |  |
| 43  | Ll    | 51     |  |
| 44  | Lm    | 128    |  |
| 45  | Ln    | 25     |  |
| 46  | Lo    | 106    |  |
| 47  | Lp    | 92     |  |
| 48  | Lr    | 137    |  |
| 49  | S2    | 1869   |  |
| 50  | SA    | 295    |  |
| 51  | SB    | 264    |  |
| 52  | SC    | 293    |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 53  | SD    | 243    |                  |
| 54  | SE    | 263    |                  |
| 55  | SF    | 204    |                  |
| 56  | SG    | 249    |                  |
| 57  | SH    | 194    |                  |
| 58  | SI    | 208    |                  |
| 59  | SJ    | 194    |                  |
| 60  | SK    | 165    |                  |
| 61  | SL    | 158    |                  |
| 62  | SM    | 132    |                  |
| 63  | SN    | 151    |                  |
| 64  | SO    | 151    |                  |
| 65  | SP    | 145    |                  |
| 66  | SQ    | 146    |                  |
| 67  | SR    | 135    |                  |
| 68  | SS    | 152    |                  |
| 69  | ST    | 145    |                  |
| 70  | SU    | 119    |                  |
| 71  | SV    | 83     |                  |
| 72  | SW    | 130    |                  |
| 73  | SX    | 143    |                  |
| 74  | SY    | 133    |                  |
| 75  | SZ    | 125    |                  |
| 76  | Sa    | 115    |                  |
| 77  | Sb    | 84     |                  |

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| Mol | Chain | Length | Quality of chain                                                                                  |
|-----|-------|--------|---------------------------------------------------------------------------------------------------|
| 78  | Sc    | 69     | <br>65% 26% 9%  |
| 79  | Sd    | 56     | <br>68% 25% 7%  |
| 80  | Se    | 59     | <br>86% 10% .   |
| 81  | Sf    | 156    | <br>28% 15% 57% |
| 82  | Sg    | 317    | <br>66% 33% .   |

## 2 Entry composition [i](#)

There are 86 unique types of molecules in this entry. The entry contains 215032 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 mRNA.

| Mol | Chain | Residues | Atoms |     |    |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 1   | A4    | 17       | Total | C   | N  | O   | P  | 0       | 0     |
|     |       |          | 340   | 153 | 34 | 136 | 17 |         |       |

- Molecule 2 is a RNA chain called tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 2   | B4    | 76       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1623  | 723 | 290 | 534 | 76 |         |       |
| 2   | D4    | 76       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1623  | 723 | 290 | 534 | 76 |         |       |

- Molecule 3 is a protein called Nascent peptide.

| Mol | Chain | Residues | Atoms |   |   |   | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---------|-------|
| 3   | C4    | 2        | Total | C | N | O | 0       | 0     |
|     |       |          | 10    | 6 | 2 | 2 |         |       |

- Molecule 4 is a RNA chain called 28S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 4   | L5    | 3644     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 78119 | 34786 | 14297 | 25393 | 3643 |         |       |

- Molecule 5 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 5   | L7    | 120      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2558  | 1141 | 456 | 842 | 119 |         |       |

- Molecule 6 is a RNA chain called 5.8S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 6   | L8    | 156      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3314  | 1480 | 585 | 1094 | 155 |         |       |

- Molecule 7 is a protein called 60S ribosomal protein L8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7   | LA    | 247      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1891  | 1185 | 388 | 312 | 6 |         |       |

- Molecule 8 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 8   | LB    | 398      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3211  | 2045 | 604 | 548 | 14 |         |       |

- Molecule 9 is a protein called 60S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9   | LC    | 365      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2897  | 1823 | 579 | 480 | 15 |         |       |

- Molecule 10 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 10  | LD    | 293      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2379  | 1506 | 434 | 425 | 14 |         |       |

- Molecule 11 is a protein called 60S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 11  | LE    | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1785  | 1148 | 338 | 295 | 4 |         |       |

- Molecule 12 is a protein called 60S ribosomal protein L7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 12  | LF    | 225      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1870  | 1202 | 358 | 301 | 9 |         |       |

- Molecule 13 is a protein called 60S ribosomal protein L7a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13  | LG    | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1832  | 1168 | 352 | 308 | 4 |         |       |

- Molecule 14 is a protein called 60S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | LH    | 190      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1518  | 956 | 284 | 272 | 6 |         |       |

- Molecule 15 is a protein called 60S ribosomal protein L10-like.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 15  | LI    | 209      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1681  | 1065 | 325 | 278 | 13 |         |       |

- Molecule 16 is a protein called 60S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | LJ    | 175      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1401  | 882 | 261 | 252 | 6 |         |       |

- Molecule 17 is a protein called 60S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 17  | LL    | 208      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1682  | 1052 | 348 | 278 | 4 |         |       |

- Molecule 18 is a protein called 60S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | LM    | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1120  | 719 | 215 | 179 | 7 |         |       |

- Molecule 19 is a protein called 60S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 19  | LN    | 203      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1701  | 1072 | 359 | 266 | 4 |         |       |

- Molecule 20 is a protein called 60S ribosomal protein L13a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 20  | LO    | 200      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1641  | 1058 | 320 | 258 | 5 |         |       |

- Molecule 21 is a protein called 60S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | LP    | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1242  | 776 | 241 | 216 | 9 |         |       |

- Molecule 22 is a protein called 60S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | LQ    | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1513  | 944 | 314 | 250 | 5 |         |       |

- Molecule 23 is a protein called 60S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | LR    | 180      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1508  | 933 | 328 | 238 | 9 |         |       |

- Molecule 24 is a protein called 60S ribosomal protein L18a.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 24  | LS    | 175      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1453  | 925 | 283 | 235 | 10 |         |       |

- Molecule 25 is a protein called 60S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | LT    | 159      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1298  | 823 | 252 | 217 | 6 |         |       |

- Molecule 26 is a protein called 60S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | LU    | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 821   | 526 | 143 | 150 | 2 |         |       |

- Molecule 27 is a protein called 60S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | LV    | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 979   | 618 | 184 | 172 | 5 |         |       |

- Molecule 28 is a protein called 60S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | LW    | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 914   | 571 | 186 | 153 | 4 |         |       |

- Molecule 29 is a protein called 60S ribosomal protein L23a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | LX    | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 981   | 628 | 185 | 167 | 1 |         |       |

- Molecule 30 is a protein called 60S ribosomal protein L26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | LY    | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1115  | 700 | 226 | 186 | 3 |         |       |

- Molecule 31 is a protein called 60S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | LZ    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1107  | 714 | 208 | 182 | 3 |         |       |

- Molecule 32 is a protein called 60S ribosomal protein L27a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | La    | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1162  | 736 | 237 | 186 | 3 |         |       |

- Molecule 33 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 33  | Lb    | 75       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 601   | 370 | 129 | 99 | 3 |         |       |

- Molecule 34 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | Lc    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 764   | 485 | 135 | 138 | 6 |         |       |

- Molecule 35 is a protein called 60S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | Ld    | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 888   | 560 | 171 | 155 | 2 |         |       |

- Molecule 36 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | Le    | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1053  | 667 | 216 | 165 | 5 |         |       |

- Molecule 37 is a protein called 60S ribosomal protein L35a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | Lf    | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 876   | 555 | 174 | 144 | 3 |         |       |

- Molecule 38 is a protein called 60S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | Lg    | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 906   | 566 | 187 | 147 | 6 |         |       |

- Molecule 39 is a protein called 60S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | Lh    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1015  | 641 | 205 | 168 | 1 |         |       |

- Molecule 40 is a protein called 60S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | Li    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 832   | 521 | 177 | 129 | 5 |         |       |

- Molecule 41 is a protein called 60S ribosomal protein L37.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | Lj    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 705   | 434 | 155 | 111 | 5 |         |       |

- Molecule 42 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 42  | Lk    | 69       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 569   | 366 | 103 | 99 | 1 |         |       |

- Molecule 43 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 43  | Ll    | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 444   | 281 | 98 | 64 | 1 |         |       |

- Molecule 44 is a protein called Ubiquitin-60S ribosomal protein L40.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 44  | Lm    | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 429   | 266 | 90 | 67 | 6 |         |       |

- Molecule 45 is a protein called 60S ribosomal protein L41.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 45  | Ln    | 24       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 230   | 139 | 62 | 26 | 3 |         |       |

- Molecule 46 is a protein called 60S ribosomal protein L36a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | Lo    | 105      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 862   | 542 | 175 | 139 | 6 |         |       |

- Molecule 47 is a protein called 60S ribosomal protein L37a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | Lp    | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 708   | 445 | 136 | 120 | 7 |         |       |

- Molecule 48 is a protein called 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48  | Lr    | 125      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1002  | 622 | 207 | 168 | 5 |         |       |

- Molecule 49 is a RNA chain called 18S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 49  | S2    | 1697     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 36223 | 16169 | 6504 | 11854 | 1696 |         |       |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference |
|-------|---------|----------|--------|----------|-----------|
| S2    | 582     | C        | U      | conflict | GB 36162  |
| S2    | 583     | C        | A      | conflict | GB 36162  |
| S2    | 584     | G        | A      | conflict | GB 36162  |
| S2    | 798     | A        | G      | conflict | GB 36162  |
| S2    | 1095    | U        | C      | conflict | GB 36162  |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 50  | SA    | 215      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1695  | 1077 | 297 | 313 | 8 |         |       |

- Molecule 51 is a protein called 40S ribosomal protein S3a.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 51  | SB    | 214      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1738  | 1103 | 310 | 311 | 14 |         |       |

- Molecule 52 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 52  | SC    | 219      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1692  | 1096 | 291 | 295 | 10 |         |       |

- Molecule 53 is a protein called 40S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 53  | SD    | 218      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1689  | 1075 | 307 | 300 | 7 |         |       |

- Molecule 54 is a protein called 40S ribosomal protein S4, X isoform.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 54  | SE    | 262      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2070  | 1321 | 383 | 358 | 8 |         |       |

- Molecule 55 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 55  | SF    | 186      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1447  | 907 | 269 | 264 | 7 |         |       |

- Molecule 56 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 56  | SG    | 237      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1917  | 1197 | 384 | 329 | 7 |         |       |

- Molecule 57 is a protein called 40S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57  | SH    | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1510  | 963 | 278 | 268 | 1 |         |       |

- Molecule 58 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 58  | SI    | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1674  | 1049 | 329 | 291 | 5 |         |       |

- Molecule 59 is a protein called 40S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 59  | SJ    | 182      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1506  | 959 | 300 | 245 | 2 |         |       |

- Molecule 60 is a protein called 40S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 60  | SK    | 96       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 810   | 530 | 143 | 131 | 6 |         |       |

- Molecule 61 is a protein called 40S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 61  | SL    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1203  | 766 | 226 | 205 | 6 |         |       |

- Molecule 62 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 62  | SM    | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 796   | 497 | 146 | 147 | 6 |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| SM    | 52      | GLN      | LEU    | conflict | UNP P25398 |
| SM    | 69      | LEU      | CYS    | conflict | UNP P25398 |
| SM    | 99      | ASN      | LYS    | conflict | UNP P25398 |

- Molecule 63 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 63  | SN    | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1208  | 773 | 229 | 205 | 1 |         |       |

- Molecule 64 is a protein called 40S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 64  | SO    | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1002  | 612 | 197 | 187 | 6 |         |       |

- Molecule 65 is a protein called 40S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 65  | SP    | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1103  | 703 | 208 | 185 | 7 |         |       |

- Molecule 66 is a protein called 40S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 66  | SQ    | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1128  | 717 | 213 | 195 | 3 |         |       |

- Molecule 67 is a protein called 40S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 67  | SR    | 130      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1051  | 661 | 196 | 189 | 5 |         |       |

- Molecule 68 is a protein called 40S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 68  | SS    | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1169  | 731 | 236 | 201 | 1 |         |       |

- Molecule 69 is a protein called 40S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 69  | ST    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1096  | 686 | 211 | 196 | 3 |         |       |

- Molecule 70 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 70  | SU    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 799   | 501 | 153 | 141 | 4 |         |       |

- Molecule 71 is a protein called 40S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 71  | SV    | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 636   | 393 | 117 | 121 | 5 |         |       |

- Molecule 72 is a protein called 40S ribosomal protein S15a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 72  | SW    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1034  | 659 | 193 | 176 | 6 |         |       |

- Molecule 73 is a protein called 40S ribosomal protein S23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 73  | SX    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1098  | 693 | 219 | 183 | 3 |         |       |

- Molecule 74 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 74  | SY    | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1002  | 634 | 196 | 167 | 5 |         |       |

- Molecule 75 is a protein called 40S ribosomal protein S25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 75  | SZ    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 680   | 436 | 127 | 116 | 1 |         |       |

- Molecule 76 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 76  | Sa    | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 792   | 492 | 165 | 130 | 5 |         |       |

- Molecule 77 is a protein called 40S ribosomal protein S27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 77  | Sb    | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 643   | 402 | 119 | 115 | 7 |         |       |

- Molecule 78 is a protein called 40S ribosomal protein S28.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 78  | Sc    | 63       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 480   | 293 | 92 | 93 | 2 |         |       |

- Molecule 79 is a protein called 40S ribosomal protein S29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 79  | Sd    | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 432   | 271 | 87 | 69 | 5 |         |       |

- Molecule 80 is a protein called 40S ribosomal protein S30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 80  | Se    | 57       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 452   | 279 | 99 | 73 | 1 |         |       |

- Molecule 81 is a protein called Ubiquitin-40S ribosomal protein S27a.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 81  | Sf    | 67       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 537   | 338 | 102 | 90 | 7 |         |       |

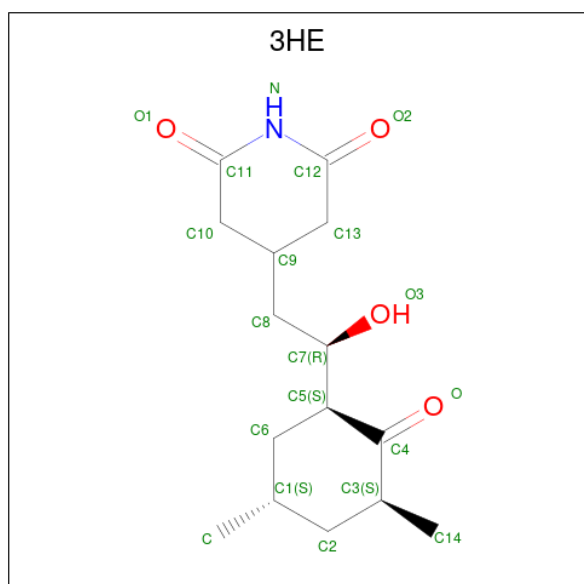
- Molecule 82 is a protein called Receptor of activated protein C kinase 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 82  | Sg    | 313      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2436  | 1535 | 424 | 465 | 12 |         |       |

- Molecule 83 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 83  | A4    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 83  | L5    | 36       | Total | Mg | 0       |
|     |       |          | 36    | 36 |         |
| 83  | L7    | 2        | Total | Mg | 0       |
|     |       |          | 2     | 2  |         |
| 83  | L8    | 4        | Total | Mg | 0       |
|     |       |          | 4     | 4  |         |
| 83  | LI    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 83  | S2    | 28       | Total | Mg | 0       |
|     |       |          | 28    | 28 |         |

- Molecule 84 is 4-{(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl}piperidine-2,6-dione (CCD ID: 3HE) (formula: C<sub>15</sub>H<sub>23</sub>NO<sub>4</sub>).



| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 84  | L5    | 1        | Total | C  | N | O | 0       |
|     |       |          | 20    | 15 | 1 | 4 |         |

- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 85  | Lg    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 85  | Lj    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 85  | Lm    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 85  | Lo    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 85  | Lp    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 85  | Sa    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 85  | Sd    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

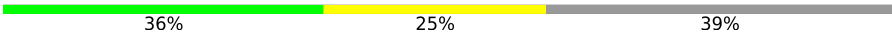
- Molecule 86 is water.

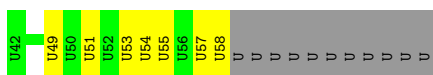
| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 86  | L5    | 2        | Total | O | 0       |
|     |       |          | 2     | 2 |         |
| 86  | L8    | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 86  | LC    | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 86  | LI    | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 86  | LP    | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 86  | LV    | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 86  | S2    | 4        | Total | O | 0       |
|     |       |          | 4     | 4 |         |
| 86  | SN    | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |

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

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: mRNA

Chain A4: 



- Molecule 2: tRNA

Chain B4: 

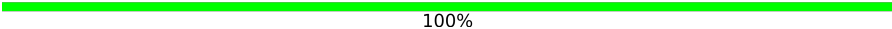


- Molecule 2: tRNA

Chain D4: 



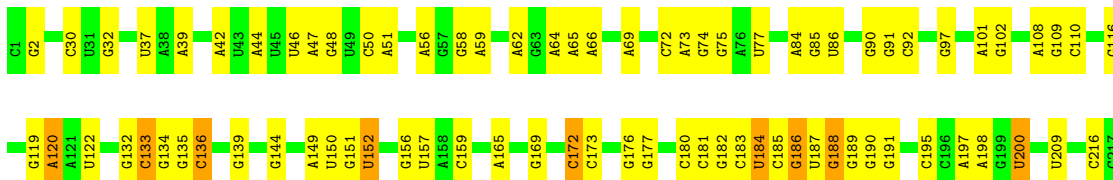
- Molecule 3: Nascent peptide

Chain C4: 

There are no outlier residues recorded for this chain.

- Molecule 4: 28S ribosomal RNA

Chain L5: 





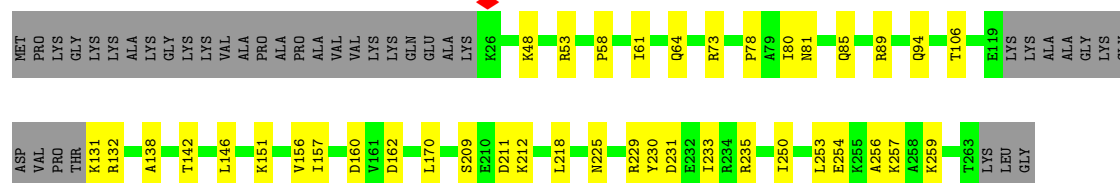


|       |       |       |       |       |   |   |       |       |       |       |   |
|-------|-------|-------|-------|-------|---|---|-------|-------|-------|-------|---|
| C4674 | M4553 | G4432 | A4279 | C4141 | U | C | G3938 | U3802 | G3689 | G3592 | G |
| U4677 | G4554 | G4433 | A4280 | C4142 | C | C | G3939 | U3802 | U3690 | C3593 | C |
| G4678 | U4558 | C4434 | A4281 | C4143 | G | G | U3940 | G3811 | G3691 | C3594 | G |
| G4679 | A4559 | G4440 | U4290 | C4144 | A | A | G3941 | C3812 | U3692 | U3595 | C |
| G4686 | C4560 | U4440 | G4291 | C4145 | U | U | A3942 | A3813 | C3693 | A3596 | C |
| A4691 | G4567 | U4444 | A4292 | C4146 | C | A | A3943 | U3814 | U3697 | G3597 | C |
| U4694 | A4568 | U4445 | U4293 | C4148 | G | G | G3944 | U3815 | G3698 | C3598 | C |
| G4694 | A4569 | U4446 | G4297 | C4149 | G | G | A3947 | A3817 | U3709 | A3604 | G |
| C4695 | G4570 | U4448 | U4297 | C4150 | C | C | C3948 | G3819 | G3710 | C3605 | C |
| U4699 | G4573 | U4452 | A4304 | C4160 | U | U | A3949 | G3823 | A3711 | U3606 | C |
| A4700 | U4574 | C4453 | G4305 | C4161 | G | G | U     | G3823 | A3712 | U3607 | C |
| A4707 | G4575 | U4464 | U4306 | C4162 | G | G | G     | U3838 | U3612 | G     | U |
| U4708 | A4586 | C4464 | C4314 | U4163 | G | G | A     | U3839 | U3613 | C     | G |
| U4709 | U4465 | U4465 | G4314 | C4164 | G | G | A     | U3840 | G3614 | C     | G |
| A4717 | A4589 | U4466 | G4330 | A4170 | C | A | G     | C3841 | G3615 | U     | A |
| G4718 | A4590 | G4472 | G4331 | C4171 | G | G | U     | C3842 | U3616 | C     | G |
| G4719 | U4591 | U4475 | C4332 | C4177 | G | G | U     | C3843 | G3617 | C     | G |
| C4720 | C4592 | U4479 | U4333 | C4177 | G | G | U     | G3859 | C3618 | C     | A |
| U4728 | G4600 | A4479 | G4338 | G4183 | U | U | A     | A3726 | A3621 | C     | G |
| A4729 | A4604 | C4485 | G4341 | C4184 | C | C | A     | U3727 | G     | C     | G |
| G4730 | A4605 | U4489 | C4349 | U4191 | G | G | A     | U3728 | G3626 | C     | C |
| G4731 | G4606 | U4489 | C4350 | C4195 | C | C | U     | U3729 | A3630 | C     | G |
| G4732 | U4492 | U4492 | U4351 | C4195 | C | A | A     | A3732 | A3635 | C     | G |
| C4733 | G4617 | U4492 | U4352 | A4203 | G | G | A     | G3733 | G     | C     | C |
| A4734 | C4618 | G4495 | U4353 | C4207 | C | C | U     | U3734 | U3641 | C     | C |
| G4740 | A4622 | U4500 | U4354 | C4207 | C | C | U     | A3735 | A     | G     | U |
| C4741 | G4623 | U4500 | G4373 | U4208 | C | G | U     | A3736 | U3644 | C     | U |
| G4742 | A4624 | A4507 | G4373 | U4208 | C | G | A     | A3747 | U3645 | C     | U |
| G4743 | C4625 | U4507 | G4373 | A4212 | U | U | A     | C3749 | A3646 | C     | C |
| A4744 | G4633 | U4512 | G4377 | G4222 | G | G | G     | G3750 | A3651 | C     | G |
| G4745 | U4634 | A4513 | A4378 | C4223 | G | C | C     | G3751 | A3652 | C     | U |
| U4748 | A4635 | A4517 | A4379 | A4224 | G | C | C     | G3752 | A3653 | C     | G |
| C4749 | U4636 | A4518 | A4380 | G4225 | C | C | C     | G3753 | G3654 | C     | G |
| G4750 | G4637 | A4519 | A4381 | C4225 | C | C | C     | G3754 | G     | C     | A |
| A4754 | A4647 | C4520 | C4387 | U4229 | C | C | C     | G3755 | C3658 | C     | U |
| G4755 | A4648 | U4521 | G4391 | A4233 | C | G | G     | A3756 | G3659 | C     | U |
| C4756 | G4652 | G4522 | A4394 | G4249 | C | G | C     | U3757 | C3660 | C     | C |
| U4758 | C4653 | G4524 | A4394 | A4251 | C | C | C     | A3759 | G3661 | C     | C |
| C4759 | A4654 | C4525 | G4410 | A4251 | U | U | G     | A3760 | A3662 | C     | C |
| G4760 | A4655 | U4541 | G4410 | G4254 | C | C | C     | A3766 | G3664 | C     | C |
| G4761 | U4657 | A4544 | A4415 | A4257 | A | C | C     | C3767 | C3667 | C     | A |
| A4764 | G4658 | G4545 | G4416 | C4258 | A | C | C     | U3768 | C3672 | C     | C |
| G4765 | G4663 | C4547 | U4419 | U4265 | C | G | C     | U3914 | C3673 | C     | U |
| C4771 | C4670 | U4548 | A4422 | U4265 | A | U | U     | U3915 | G3674 | C     | C |
| C4772 | C4671 | G4549 | C4429 | A4268 | C | G | G     | G3777 | G3678 | C     | C |
| C4773 | U4672 | G4550 | G4430 | A4273 | C | U | U     | A3784 | U3679 | C     | C |
| C4774 | U4673 | G4550 | U4431 | A4273 | A | C | C     | A3785 | U3680 | C     | A |
|       |       |       |       |       | C | C | C     | U3786 | U3688 | C     | G |



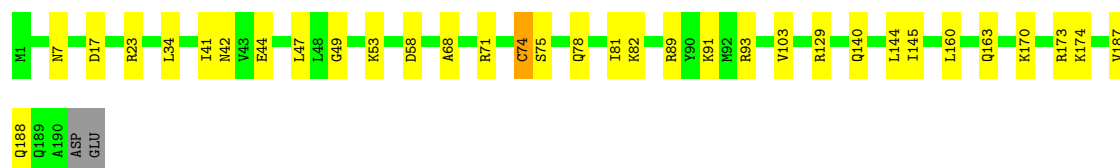


Chain LG:  70% 15% 15%



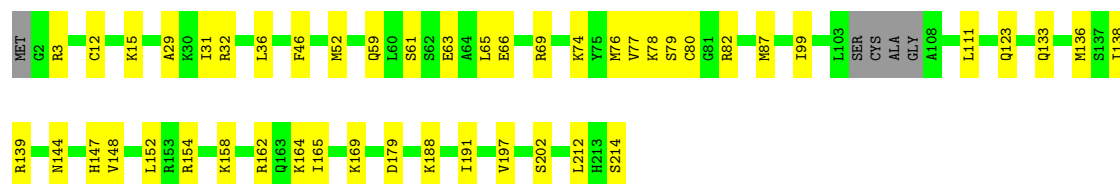
- Molecule 14: 60S ribosomal protein L9

Chain LH:  82% 17% ..



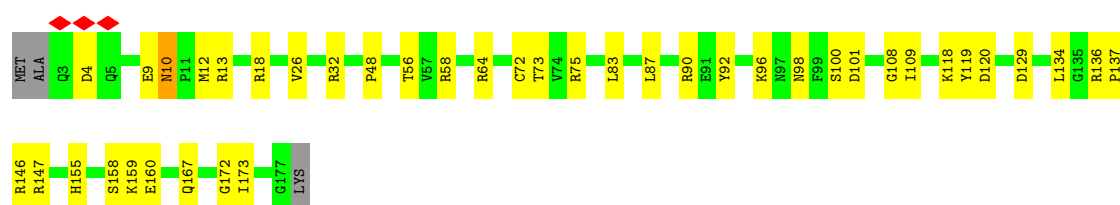
- Molecule 15: 60S ribosomal protein L10-like

Chain LI:  76% 22% .



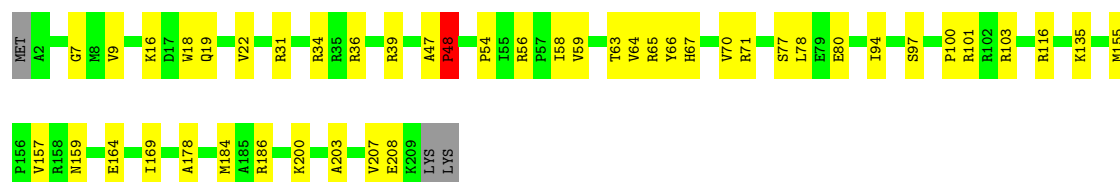
- Molecule 16: 60S ribosomal protein L11

Chain LJ:  75% 22% ..

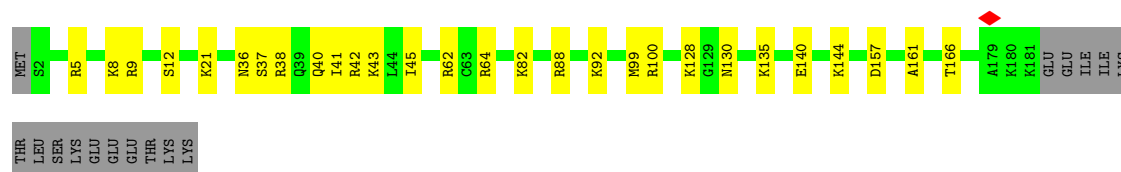


- Molecule 17: 60S ribosomal protein L13

Chain LL:  77% 21% .



- Chain LR:  78% 14% 8%



- Molecule 24: 60S ribosomal protein L18a

Chain LS: 84% 15% .



- Molecule 25: 60S ribosomal protein L21

Chain LT: 81% 18% .



- Molecule 26: 60S ribosomal protein L22

Chain LU: 67% 12% 21%



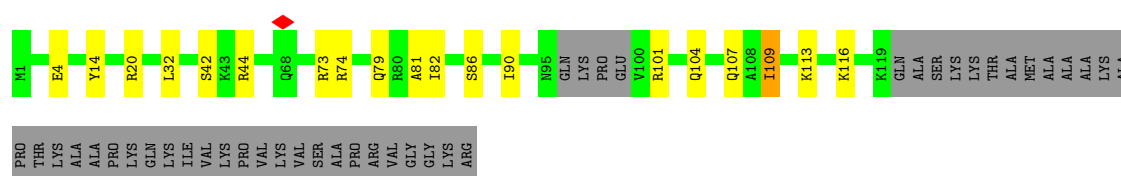
- Molecule 27: 60S ribosomal protein L23

Chain LV: 76% 18% 6%



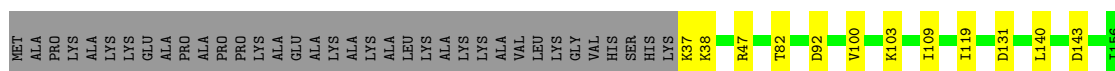
- Molecule 28: 60S ribosomal protein L24

Chain LW: 61% 11% 27%



- Molecule 29: 60S ribosomal protein L23a

Chain LX: 69% 8% 23%



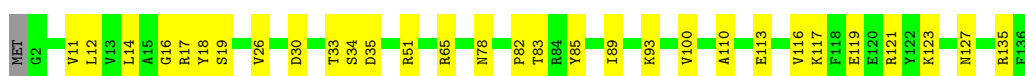
- Molecule 30: 60S ribosomal protein L26

Chain LY: 76% 17% 8%



- Molecule 31: 60S ribosomal protein L27

Chain LZ: 77% 22%



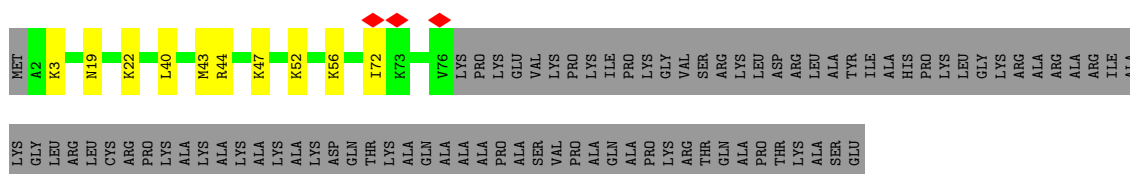
- Molecule 32: 60S ribosomal protein L27a

Chain La: 83% 16%



- Molecule 33: 60S ribosomal protein L29

Chain Lb: 41% 6% 53%



- Molecule 34: 60S ribosomal protein L30

Chain Lc: 63% 22% 15%



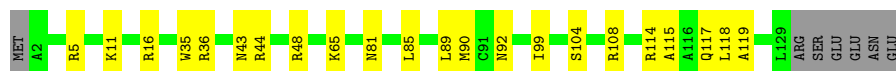
- Molecule 35: 60S ribosomal protein L31

Chain Ld: 73% 12% 14%



- Molecule 36: 60S ribosomal protein L32

Chain Le:  79% 16% 5%



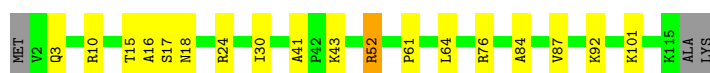
- Molecule 37: 60S ribosomal protein L35a

Chain Lf:  78% 20% ..



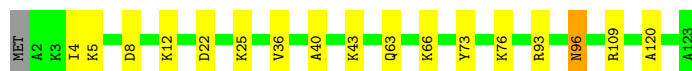
- Molecule 38: 60S ribosomal protein L34

Chain Lg:  82% 15% ..



- Molecule 39: 60S ribosomal protein L35

Chain Lh:  85% 13% ..



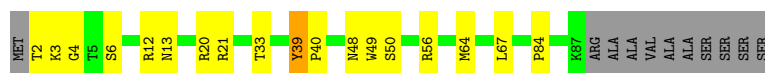
- Molecule 40: 60S ribosomal protein L36

Chain Li:  88% 9% ..



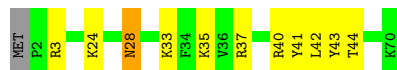
- Molecule 41: 60S ribosomal protein L37

Chain Lj:  70% 18% 11%



- Molecule 42: 60S ribosomal protein L38

Chain Lk:  83% 14% ..



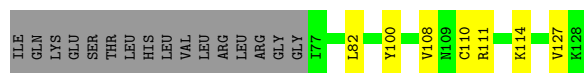
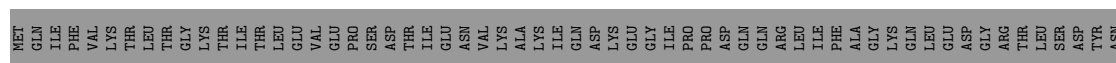
- Molecule 43: 60S ribosomal protein L39

Chain Ll:  82% 16%



- Molecule 44: Ubiquitin-60S ribosomal protein L40

Chain Lm:  35% 5% 59%



- Molecule 45: 60S ribosomal protein L41

Chain Ln:  76% 20%



- Molecule 46: 60S ribosomal protein L36a

Chain Lo:  84% 15%



- Molecule 47: 60S ribosomal protein L37a

Chain Lp:  86% 13%



- Molecule 48: 60S ribosomal protein L28

Chain Lr:  78% 13% 9%

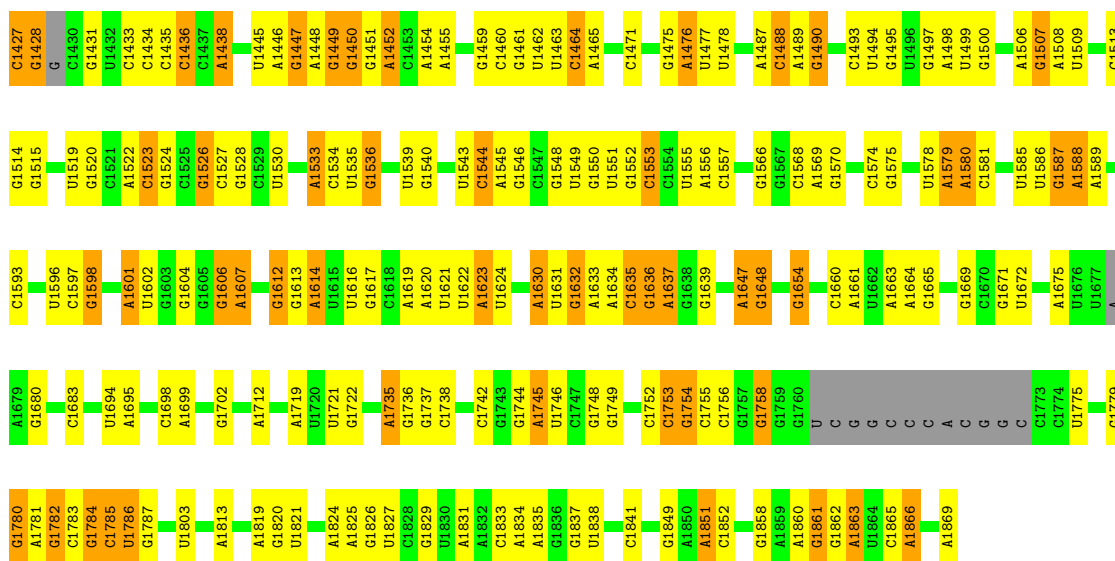


- Molecule 49: 18S ribosomal RNA

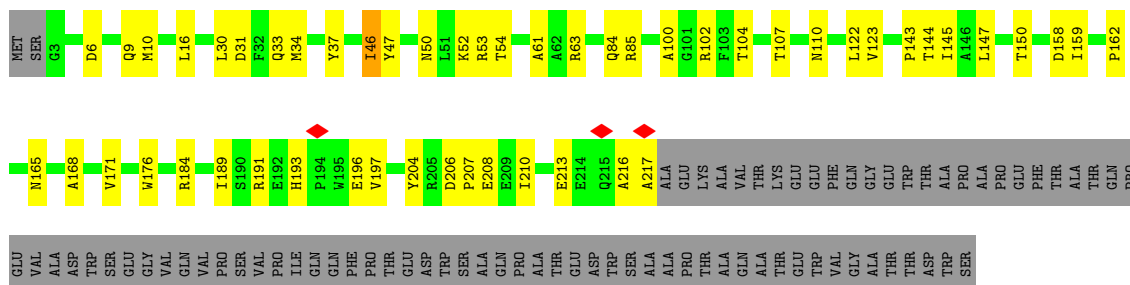
Chain S2:  51% 31% 9% 9%



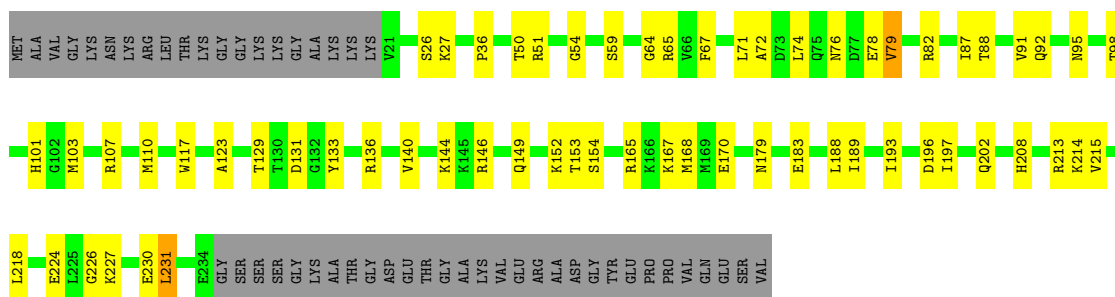




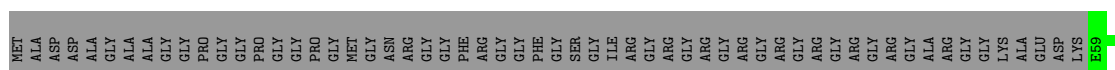
• Molecule 50: 40S ribosomal protein SA

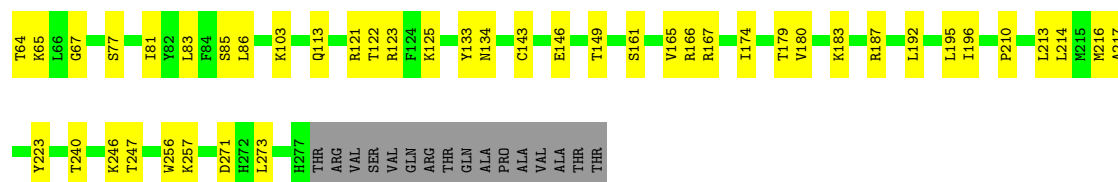


• Molecule 51: 40S ribosomal protein S3a



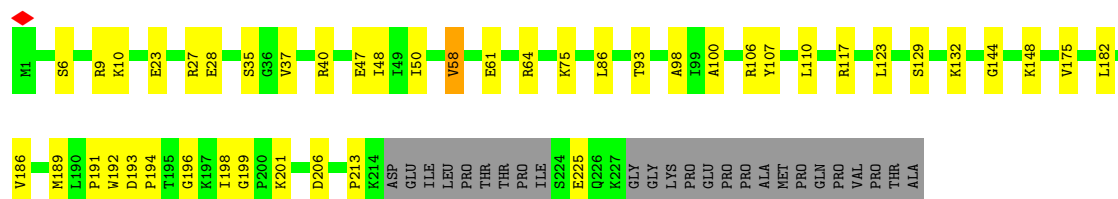
• Molecule 52: 40S ribosomal protein S2





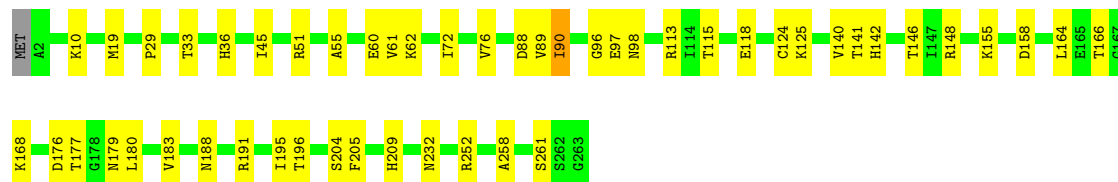
• Molecule 53: 40S ribosomal protein S3

Chain SD:



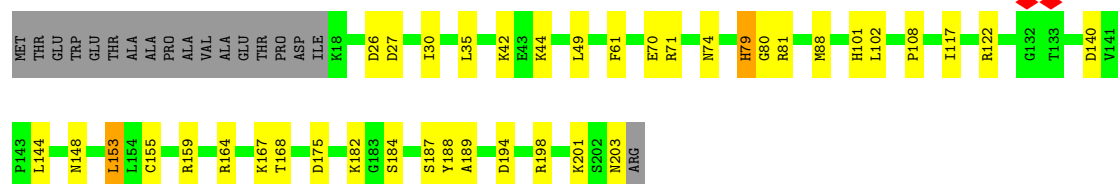
• Molecule 54: 40S ribosomal protein S4, X isoform

Chain SE:



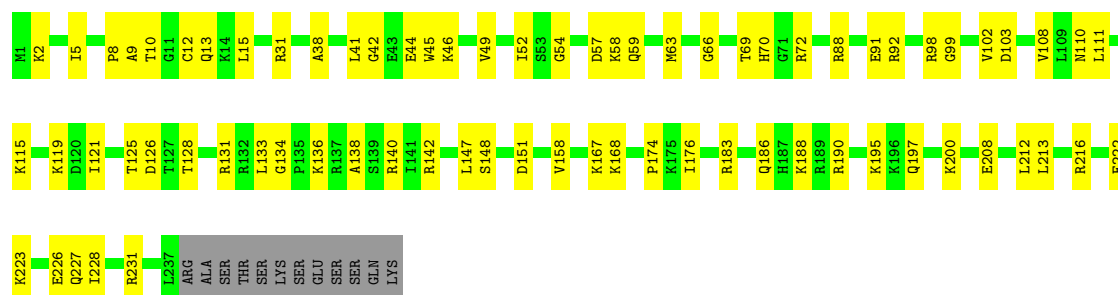
• Molecule 55: 40S ribosomal protein S5

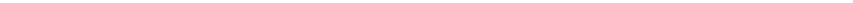
Chain SF:

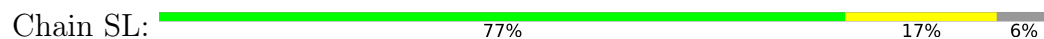


• Molecule 56: 40S ribosomal protein S6

Chain SG:

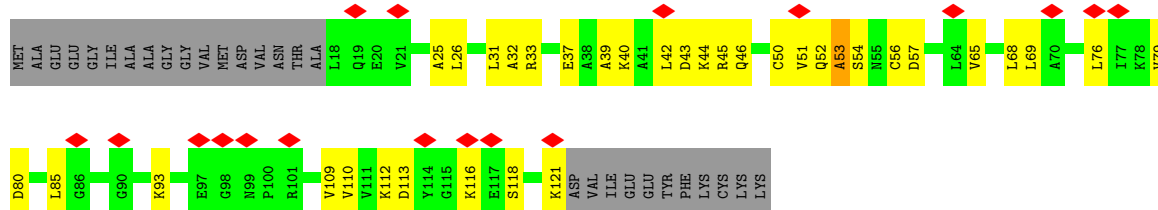


- Chain SH:  69% 27%

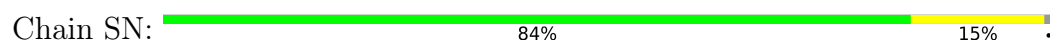




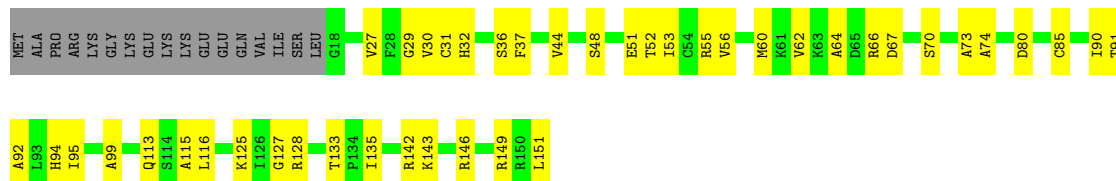
- Molecule 62: 40S ribosomal protein S12



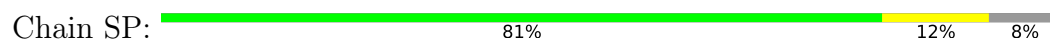
- Molecule 63: 40S ribosomal protein S13



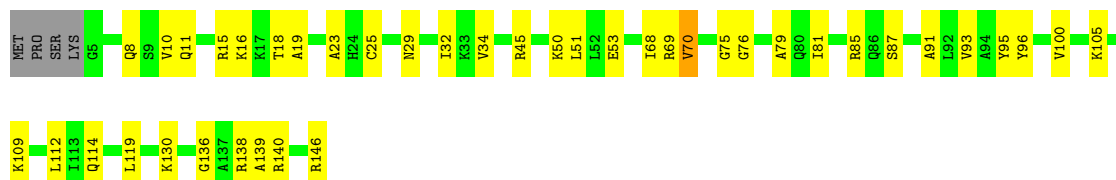
- Molecule 64: 40S ribosomal protein S14



- Molecule 65: 40S ribosomal protein S15



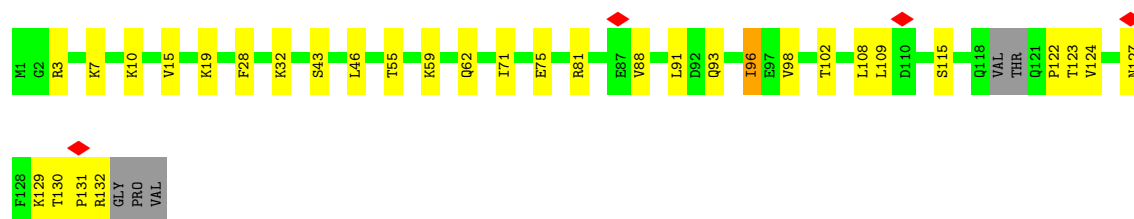
- Molecule 66: 40S ribosomal protein S16



- Molecule 67: 40S ribosomal protein S17

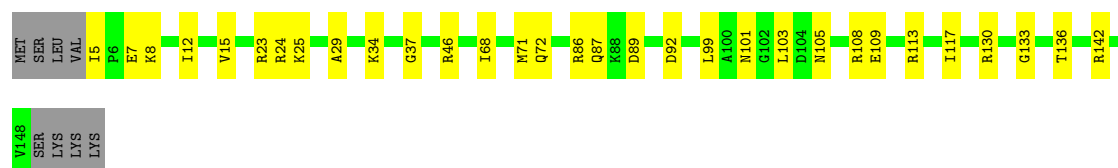


Chain SR:  73% 23%



- Molecule 68: 40S ribosomal protein S18

Chain SS:  74% 20% 5%



- Molecule 69: 40S ribosomal protein S19

Chain ST:  75% 22%



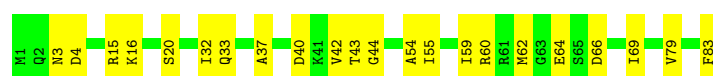
- Molecule 70: 40S ribosomal protein S20

Chain SU:  58% 28% 14%



- Molecule 71: 40S ribosomal protein S21

Chain SV:  73% 27%



- Molecule 72: 40S ribosomal protein S15a

Chain SW:  80% 19%



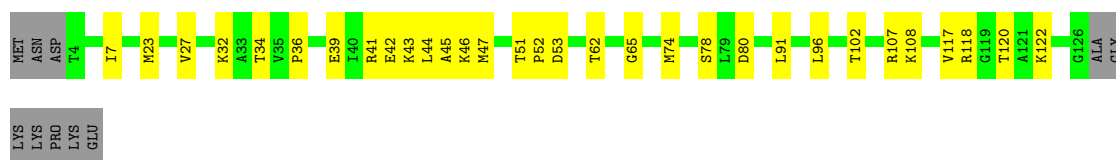
- Molecule 73: 40S ribosomal protein S23

Chain SX: 84% 15% .



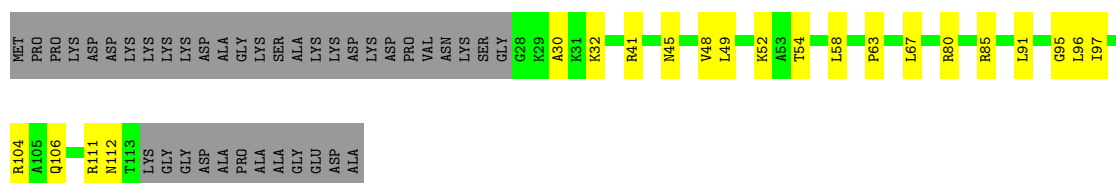
- Molecule 74: 40S ribosomal protein S24

Chain SY: 69% 23% 8%



- Molecule 75: 40S ribosomal protein S25

Chain SZ: 52% 17% 31%



- Molecule 76: 40S ribosomal protein S26

Chain Sa: 65% 21% 14%



- Molecule 77: 40S ribosomal protein S27

Chain Sb: 77% 21% .



- Molecule 78: 40S ribosomal protein S28

Chain Sc: 65% 26% 9%



- Molecule 79: 40S ribosomal protein S29

Chain Sd:  68% 25% 7%



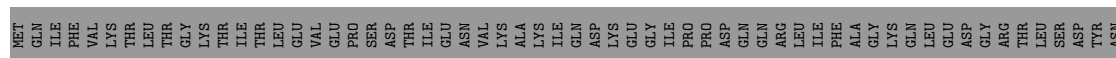
- Molecule 80: 40S ribosomal protein S30

Chain Se:  86% 10% .



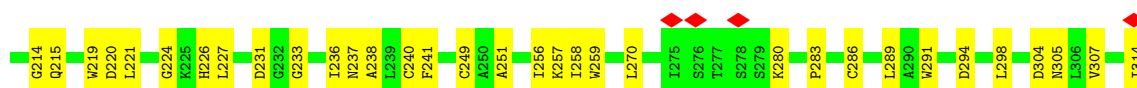
- Molecule 81: Ubiquitin-40S ribosomal protein S27a

Chain Sf:  28% 15% 57%



- Molecule 82: Receptor of activated protein C kinase 1

Chain Sg:  66% 33% .



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 21820                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 40                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 0.101                                   | Depositor |
| Minimum map value                    | -0.033                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.005                                   | Depositor |
| Recommended contour level            | 0.0092                                  | Depositor |
| Map size (Å)                         | 473.0, 473.0, 473.0                     | wwPDB     |
| Map dimensions                       | 550, 550, 550                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.86, 0.86, 0.86                        | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 3HE, ZN

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

| Mol | Chain | Bond lengths |             | Bond angles |                 |
|-----|-------|--------------|-------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$     |
| 1   | A4    | 0.27         | 0/373       | 0.50        | 0/574           |
| 2   | B4    | 0.25         | 0/1813      | 0.39        | 0/2823          |
| 2   | D4    | 0.24         | 0/1813      | 0.36        | 0/2823          |
| 4   | L5    | 0.36         | 0/87379     | 0.37        | 3/136294 (0.0%) |
| 5   | L7    | 0.33         | 0/2858      | 0.33        | 0/4455          |
| 6   | L8    | 0.38         | 0/3701      | 0.39        | 0/5766          |
| 7   | LA    | 0.40         | 0/1929      | 0.63        | 0/2586          |
| 8   | LB    | 0.37         | 0/3279      | 0.60        | 0/4388          |
| 9   | LC    | 0.39         | 0/2951      | 0.57        | 2/3963 (0.1%)   |
| 10  | LD    | 0.32         | 0/2425      | 0.58        | 1/3248 (0.0%)   |
| 11  | LE    | 0.33         | 0/1819      | 0.66        | 0/2439          |
| 12  | LF    | 0.37         | 0/1905      | 0.58        | 0/2539          |
| 13  | LG    | 0.32         | 0/1863      | 0.57        | 1/2510 (0.0%)   |
| 14  | LH    | 0.33         | 0/1537      | 0.56        | 0/2066          |
| 15  | LI    | 0.32         | 0/1720      | 0.55        | 0/2298          |
| 16  | LJ    | 0.27         | 0/1424      | 0.60        | 0/1904          |
| 17  | LL    | 0.37         | 0/1713      | 0.60        | 1/2293 (0.0%)   |
| 18  | LM    | 0.33         | 0/1142      | 0.57        | 0/1527          |
| 19  | LN    | 0.42         | 0/1746      | 0.49        | 0/2338          |
| 20  | LO    | 0.37         | 0/1673      | 0.51        | 0/2238          |
| 21  | LP    | 0.38         | 0/1268      | 0.50        | 0/1701          |
| 22  | LQ    | 0.39         | 0/1537      | 0.59        | 0/2052          |
| 23  | LR    | 0.33         | 0/1524      | 0.51        | 0/2013          |
| 24  | LS    | 0.36         | 0/1493      | 0.53        | 0/2003          |
| 25  | LT    | 0.34         | 0/1326      | 0.49        | 0/1770          |
| 26  | LU    | 0.30         | 0/835       | 0.58        | 0/1122          |
| 27  | LV    | 0.35         | 0/993       | 0.55        | 0/1332          |
| 28  | LW    | 0.29         | 0/927       | 0.51        | 0/1232          |
| 29  | LX    | 0.34         | 0/998       | 0.58        | 0/1340          |
| 30  | LY    | 0.37         | 0/1132      | 0.57        | 0/1504          |
| 31  | LZ    | 0.33         | 0/1130      | 0.51        | 0/1507          |
| 32  | La    | 0.40         | 0/1191      | 0.56        | 0/1591          |

| Mol | Chain | Bond lengths |         | Bond angles |                |
|-----|-------|--------------|---------|-------------|----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5        |
| 33  | Lb    | 0.32         | 0/611   | 0.52        | 0/808          |
| 34  | Lc    | 0.32         | 0/774   | 0.50        | 0/1038         |
| 35  | Ld    | 0.36         | 0/903   | 0.50        | 0/1216         |
| 36  | Le    | 0.39         | 0/1071  | 0.50        | 0/1429         |
| 37  | Lf    | 0.39         | 0/895   | 0.62        | 0/1198         |
| 38  | Lg    | 0.35         | 0/916   | 0.59        | 0/1220         |
| 39  | Lh    | 0.34         | 0/1023  | 0.47        | 0/1351         |
| 40  | Li    | 0.33         | 0/843   | 0.57        | 0/1115         |
| 41  | Lj    | 0.41         | 0/720   | 0.59        | 0/952          |
| 42  | Lk    | 0.29         | 0/575   | 0.51        | 0/761          |
| 43  | Ll    | 0.36         | 0/454   | 0.50        | 0/599          |
| 44  | Lm    | 0.33         | 0/435   | 0.55        | 0/575          |
| 45  | Ln    | 0.33         | 0/231   | 0.49        | 0/294          |
| 46  | Lo    | 0.36         | 0/876   | 0.61        | 2/1156 (0.2%)  |
| 47  | Lp    | 0.36         | 0/718   | 0.53        | 0/953          |
| 48  | Lr    | 0.39         | 0/1017  | 0.51        | 0/1364         |
| 49  | S2    | 0.32         | 0/40504 | 0.41        | 3/63126 (0.0%) |
| 50  | SA    | 0.28         | 0/1732  | 0.56        | 0/2355         |
| 51  | SB    | 0.26         | 0/1765  | 0.56        | 2/2362 (0.1%)  |
| 52  | SC    | 0.31         | 0/1729  | 0.58        | 0/2337         |
| 53  | SD    | 0.28         | 0/1714  | 0.63        | 2/2304 (0.1%)  |
| 54  | SE    | 0.28         | 0/2112  | 0.49        | 0/2842         |
| 55  | SF    | 0.28         | 0/1468  | 0.60        | 0/1977         |
| 56  | SG    | 0.25         | 0/1940  | 0.51        | 0/2583         |
| 57  | SH    | 0.27         | 0/1533  | 0.65        | 0/2053         |
| 58  | SI    | 0.28         | 0/1703  | 0.52        | 0/2275         |
| 59  | SJ    | 0.28         | 0/1531  | 0.58        | 0/2045         |
| 60  | SK    | 0.25         | 0/834   | 0.53        | 0/1125         |
| 61  | SL    | 0.32         | 0/1223  | 0.58        | 1/1637 (0.1%)  |
| 62  | SM    | 0.27         | 0/804   | 0.73        | 0/1081         |
| 63  | SN    | 0.28         | 0/1232  | 0.54        | 0/1656         |
| 64  | SO    | 0.31         | 0/1015  | 0.58        | 0/1361         |
| 65  | SP    | 0.27         | 0/1126  | 0.53        | 0/1505         |
| 66  | SQ    | 0.29         | 0/1146  | 0.69        | 0/1534         |
| 67  | SR    | 0.27         | 0/1064  | 0.65        | 2/1425 (0.1%)  |
| 68  | SS    | 0.29         | 0/1187  | 0.68        | 2/1593 (0.1%)  |
| 69  | ST    | 0.28         | 0/1114  | 0.60        | 0/1493         |
| 70  | SU    | 0.30         | 0/809   | 0.72        | 0/1087         |
| 71  | SV    | 0.31         | 0/643   | 0.56        | 0/860          |
| 72  | SW    | 0.32         | 0/1051  | 0.59        | 0/1406         |
| 73  | SX    | 0.33         | 0/1116  | 0.51        | 0/1490         |
| 74  | SY    | 0.26         | 0/1019  | 0.53        | 0/1355         |
| 75  | SZ    | 0.26         | 0/688   | 0.65        | 0/921          |

| Mol | Chain | Bond lengths |             | Bond angles |                  |
|-----|-------|--------------|-------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$      |
| 76  | Sa    | 0.31         | 0/805       | 0.54        | 0/1079           |
| 77  | Sb    | 0.27         | 0/657       | 0.60        | 0/883            |
| 78  | Sc    | 0.28         | 0/482       | 0.76        | 0/648            |
| 79  | Sd    | 0.29         | 0/442       | 0.55        | 0/586            |
| 80  | Se    | 0.24         | 0/458       | 0.47        | 0/602            |
| 81  | Sf    | 0.21         | 0/548       | 0.56        | 0/728            |
| 82  | Sg    | 0.28         | 0/2493      | 0.69        | 2/3394 (0.1%)    |
| All | All   | 0.34         | 0/231166    | 0.46        | 24/339976 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 7   | LA    | 0                   | 2                   |
| 8   | LB    | 0                   | 1                   |
| 9   | LC    | 0                   | 2                   |
| 10  | LD    | 0                   | 1                   |
| 11  | LE    | 0                   | 1                   |
| 12  | LF    | 0                   | 2                   |
| 13  | LG    | 0                   | 1                   |
| 17  | LL    | 0                   | 1                   |
| 18  | LM    | 0                   | 1                   |
| 21  | LP    | 0                   | 2                   |
| 22  | LQ    | 0                   | 1                   |
| 24  | LS    | 0                   | 1                   |
| 25  | LT    | 0                   | 1                   |
| 28  | LW    | 0                   | 1                   |
| 37  | Lf    | 0                   | 1                   |
| 38  | Lg    | 0                   | 1                   |
| 40  | Li    | 0                   | 1                   |
| 41  | Lj    | 0                   | 1                   |
| 51  | SB    | 0                   | 2                   |
| 52  | SC    | 0                   | 1                   |
| 55  | SF    | 0                   | 1                   |
| 62  | SM    | 0                   | 1                   |
| 70  | SU    | 0                   | 2                   |
| 82  | Sg    | 0                   | 2                   |
| All | All   | 0                   | 31                  |

There are no bond length outliers.

All (24) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 10  | LD    | 125  | VAL  | N-CA-C      | 7.02  | 117.53      | 110.23   |
| 13  | LG    | 80   | ILE  | N-CA-C      | -6.45 | 106.51      | 112.96   |
| 53  | SD    | 225  | GLU  | CA-C-N      | 6.18  | 129.90      | 120.82   |
| 53  | SD    | 225  | GLU  | C-N-CA      | 6.18  | 129.90      | 120.82   |
| 82  | Sg    | 49   | GLU  | CA-C-N      | 5.79  | 136.70      | 126.45   |
| 82  | Sg    | 49   | GLU  | C-N-CA      | 5.79  | 136.70      | 126.45   |
| 61  | SL    | 4    | ILE  | N-CA-C      | -5.77 | 107.66      | 113.20   |
| 46  | Lo    | 101  | GLY  | CA-C-N      | 5.67  | 131.90      | 121.70   |
| 46  | Lo    | 101  | GLY  | C-N-CA      | 5.67  | 131.90      | 121.70   |
| 4   | L5    | 2117 | G    | P-O3'-C3'   | 5.59  | 128.59      | 120.20   |
| 67  | SR    | 96   | ILE  | CA-C-N      | 5.52  | 132.08      | 121.54   |
| 67  | SR    | 96   | ILE  | C-N-CA      | 5.52  | 132.08      | 121.54   |
| 17  | LL    | 48   | PRO  | N-CA-C      | 5.47  | 123.73      | 112.47   |
| 51  | SB    | 78   | GLU  | CA-C-N      | 5.46  | 131.81      | 121.97   |
| 51  | SB    | 78   | GLU  | C-N-CA      | 5.46  | 131.81      | 121.97   |
| 49  | S2    | 32   | U    | C2'-C3'-O3' | 5.24  | 117.36      | 109.50   |
| 4   | L5    | 914  | U    | P-O3'-C3'   | 5.22  | 128.03      | 120.20   |
| 9   | LC    | 318  | PRO  | CA-C-N      | 5.18  | 131.43      | 121.54   |
| 9   | LC    | 318  | PRO  | C-N-CA      | 5.18  | 131.43      | 121.54   |
| 68  | SS    | 87   | GLN  | CA-C-N      | 5.07  | 131.21      | 121.54   |
| 68  | SS    | 87   | GLN  | C-N-CA      | 5.07  | 131.21      | 121.54   |
| 49  | S2    | 531  | A    | P-O3'-C3'   | -5.06 | 112.61      | 120.20   |
| 49  | S2    | 32   | U    | P-O3'-C3'   | 5.03  | 127.74      | 120.20   |
| 4   | L5    | 2760 | G    | P-O3'-C3'   | 5.02  | 127.73      | 120.20   |

There are no chirality outliers.

All (31) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 7   | LA    | 205 | ASN  | Peptide |
| 7   | LA    | 239 | ALA  | Peptide |
| 8   | LB    | 258 | HIS  | Peptide |
| 9   | LC    | 279 | LEU  | Peptide |
| 9   | LC    | 70  | GLY  | Peptide |
| 10  | LD    | 124 | GLU  | Peptide |
| 11  | LE    | 130 | LYS  | Peptide |
| 12  | LF    | 163 | ASN  | Peptide |
| 12  | LF    | 86  | GLU  | Peptide |
| 13  | LG    | 162 | ASP  | Peptide |
| 17  | LL    | 47  | ALA  | Peptide |
| 18  | LM    | 96  | GLU  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 21  | LP    | 131 | ARG  | Peptide |
| 21  | LP    | 20  | SER  | Peptide |
| 22  | LQ    | 159 | PRO  | Peptide |
| 24  | LS    | 155 | PRO  | Peptide |
| 25  | LT    | 80  | VAL  | Peptide |
| 28  | LW    | 14  | TYR  | Peptide |
| 37  | Lf    | 103 | VAL  | Peptide |
| 38  | Lg    | 52  | ARG  | Peptide |
| 40  | Li    | 87  | ARG  | Peptide |
| 41  | Lj    | 39  | TYR  | Peptide |
| 51  | SB    | 189 | ILE  | Peptide |
| 51  | SB    | 50  | THR  | Peptide |
| 52  | SC    | 77  | SER  | Peptide |
| 55  | SF    | 79  | HIS  | Peptide |
| 62  | SM    | 53  | ALA  | Peptide |
| 70  | SU    | 42  | GLY  | Peptide |
| 70  | SU    | 43  | ALA  | Peptide |
| 82  | Sg    | 149 | GLU  | Peptide |
| 82  | Sg    | 233 | GLY  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A4    | 340   | 0        | 171      | 1       | 0            |
| 2   | B4    | 1623  | 0        | 821      | 7       | 0            |
| 2   | D4    | 1623  | 0        | 821      | 7       | 0            |
| 3   | C4    | 10    | 0        | 4        | 0       | 0            |
| 4   | L5    | 78119 | 0        | 39488    | 462     | 0            |
| 5   | L7    | 2558  | 0        | 1296     | 14      | 0            |
| 6   | L8    | 3314  | 0        | 1683     | 16      | 0            |
| 7   | LA    | 1891  | 0        | 1986     | 29      | 0            |
| 8   | LB    | 3211  | 0        | 3356     | 60      | 0            |
| 9   | LC    | 2897  | 0        | 3077     | 39      | 0            |
| 10  | LD    | 2379  | 0        | 2408     | 28      | 0            |
| 11  | LE    | 1785  | 0        | 1939     | 38      | 0            |
| 12  | LF    | 1870  | 0        | 1996     | 14      | 0            |
| 13  | LG    | 1832  | 0        | 1962     | 24      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 14  | LH    | 1518  | 0        | 1601     | 26      | 0            |
| 15  | LI    | 1681  | 0        | 1712     | 34      | 0            |
| 16  | LJ    | 1401  | 0        | 1428     | 30      | 0            |
| 17  | LL    | 1682  | 0        | 1792     | 33      | 0            |
| 18  | LM    | 1120  | 0        | 1187     | 20      | 0            |
| 19  | LN    | 1701  | 0        | 1749     | 20      | 0            |
| 20  | LO    | 1641  | 0        | 1788     | 19      | 0            |
| 21  | LP    | 1242  | 0        | 1269     | 10      | 0            |
| 22  | LQ    | 1513  | 0        | 1628     | 29      | 0            |
| 23  | LR    | 1508  | 0        | 1664     | 23      | 0            |
| 24  | LS    | 1453  | 0        | 1490     | 22      | 0            |
| 25  | LT    | 1298  | 0        | 1366     | 21      | 0            |
| 26  | LU    | 821   | 0        | 839      | 10      | 0            |
| 27  | LV    | 979   | 0        | 1039     | 17      | 0            |
| 28  | LW    | 914   | 0        | 937      | 14      | 0            |
| 29  | LX    | 981   | 0        | 1062     | 9       | 0            |
| 30  | LY    | 1115  | 0        | 1205     | 20      | 0            |
| 31  | LZ    | 1107  | 0        | 1182     | 21      | 0            |
| 32  | La    | 1162  | 0        | 1213     | 18      | 0            |
| 33  | Lb    | 601   | 0        | 623      | 10      | 0            |
| 34  | Lc    | 764   | 0        | 804      | 14      | 0            |
| 35  | Ld    | 888   | 0        | 930      | 13      | 0            |
| 36  | Le    | 1053  | 0        | 1147     | 18      | 0            |
| 37  | Lf    | 876   | 0        | 912      | 16      | 0            |
| 38  | Lg    | 906   | 0        | 998      | 14      | 0            |
| 39  | Lh    | 1015  | 0        | 1148     | 14      | 0            |
| 40  | Li    | 832   | 0        | 917      | 8       | 0            |
| 41  | Lj    | 705   | 0        | 737      | 15      | 0            |
| 42  | Lk    | 569   | 0        | 637      | 8       | 0            |
| 43  | Ll    | 444   | 0        | 483      | 5       | 0            |
| 44  | Lm    | 429   | 0        | 466      | 5       | 0            |
| 45  | Ln    | 230   | 0        | 276      | 4       | 0            |
| 46  | Lo    | 862   | 0        | 931      | 11      | 0            |
| 47  | Lp    | 708   | 0        | 756      | 12      | 0            |
| 48  | Lr    | 1002  | 0        | 1068     | 15      | 0            |
| 49  | S2    | 36223 | 0        | 18298    | 299     | 0            |
| 50  | SA    | 1695  | 0        | 1690     | 39      | 0            |
| 51  | SB    | 1738  | 0        | 1809     | 42      | 0            |
| 52  | SC    | 1692  | 0        | 1774     | 28      | 0            |
| 53  | SD    | 1689  | 0        | 1775     | 31      | 0            |
| 54  | SE    | 2070  | 0        | 2166     | 29      | 0            |
| 55  | SF    | 1447  | 0        | 1481     | 30      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 56  | SG    | 1917  | 0        | 2078     | 53      | 0            |
| 57  | SH    | 1510  | 0        | 1606     | 37      | 0            |
| 58  | SI    | 1674  | 0        | 1739     | 44      | 0            |
| 59  | SJ    | 1506  | 0        | 1618     | 30      | 0            |
| 60  | SK    | 810   | 0        | 836      | 23      | 0            |
| 61  | SL    | 1203  | 0        | 1264     | 19      | 0            |
| 62  | SM    | 796   | 0        | 821      | 22      | 0            |
| 63  | SN    | 1208  | 0        | 1294     | 18      | 0            |
| 64  | SO    | 1002  | 0        | 1023     | 35      | 0            |
| 65  | SP    | 1103  | 0        | 1156     | 13      | 0            |
| 66  | SQ    | 1128  | 0        | 1195     | 29      | 0            |
| 67  | SR    | 1051  | 0        | 1105     | 27      | 0            |
| 68  | SS    | 1169  | 0        | 1198     | 23      | 0            |
| 69  | ST    | 1096  | 0        | 1125     | 25      | 0            |
| 70  | SU    | 799   | 0        | 850      | 22      | 0            |
| 71  | SV    | 636   | 0        | 637      | 18      | 0            |
| 72  | SW    | 1034  | 0        | 1080     | 16      | 0            |
| 73  | SX    | 1098  | 0        | 1167     | 14      | 0            |
| 74  | SY    | 1002  | 0        | 1067     | 21      | 0            |
| 75  | SZ    | 680   | 0        | 744      | 17      | 0            |
| 76  | Sa    | 792   | 0        | 843      | 19      | 0            |
| 77  | Sb    | 643   | 0        | 650      | 11      | 0            |
| 78  | Sc    | 480   | 0        | 492      | 14      | 0            |
| 79  | Sd    | 432   | 0        | 424      | 13      | 0            |
| 80  | Se    | 452   | 0        | 494      | 5       | 0            |
| 81  | Sf    | 537   | 0        | 538      | 24      | 0            |
| 82  | Sg    | 2436  | 0        | 2393     | 65      | 0            |
| 83  | A4    | 1     | 0        | 0        | 0       | 0            |
| 83  | L5    | 36    | 0        | 0        | 0       | 0            |
| 83  | L7    | 2     | 0        | 0        | 0       | 0            |
| 83  | L8    | 4     | 0        | 0        | 0       | 0            |
| 83  | LI    | 1     | 0        | 0        | 0       | 0            |
| 83  | S2    | 28    | 0        | 0        | 0       | 0            |
| 84  | L5    | 20    | 0        | 23       | 0       | 0            |
| 85  | Lg    | 1     | 0        | 0        | 0       | 0            |
| 85  | Lj    | 1     | 0        | 0        | 0       | 0            |
| 85  | Lm    | 1     | 0        | 0        | 0       | 0            |
| 85  | Lo    | 1     | 0        | 0        | 0       | 0            |
| 85  | Lp    | 1     | 0        | 0        | 0       | 0            |
| 85  | Sa    | 1     | 0        | 0        | 0       | 0            |
| 85  | Sd    | 1     | 0        | 0        | 0       | 0            |
| 86  | L5    | 2     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 86  | L8    | 1      | 0        | 0        | 0       | 0            |
| 86  | LC    | 1      | 0        | 0        | 0       | 0            |
| 86  | LI    | 1      | 0        | 0        | 0       | 0            |
| 86  | LP    | 1      | 0        | 0        | 0       | 0            |
| 86  | LV    | 1      | 0        | 0        | 0       | 0            |
| 86  | S2    | 4      | 0        | 0        | 0       | 0            |
| 86  | SN    | 1      | 0        | 0        | 0       | 0            |
| All | All   | 215032 | 0        | 158445   | 1954    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1954) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:Lj:2:THR:N      | 41:Lj:6:SER:HG     | 1.77                     | 0.83              |
| 62:SM:45:ARG:HG2   | 62:SM:46:GLN:HG2   | 1.72                     | 0.71              |
| 49:S2:1550:G:H3'   | 49:S2:1579:A:H61   | 1.55                     | 0.70              |
| 49:S2:291:G:H1'    | 49:S2:292:A:H2'    | 1.75                     | 0.68              |
| 60:SK:80:ARG:HD3   | 60:SK:87:PRO:HA    | 1.75                     | 0.68              |
| 4:L5:490:C:H1'     | 4:L5:666:G:H1      | 1.58                     | 0.68              |
| 4:L5:1524:A:H61    | 4:L5:1651:G:H22    | 1.39                     | 0.68              |
| 49:S2:928:G:H1     | 49:S2:1013:U:H3    | 1.41                     | 0.68              |
| 64:SO:113:GLN:HE22 | 76:Sa:47:ALA:HB3   | 1.59                     | 0.68              |
| 36:Le:114:ARG:HH11 | 36:Le:117:GLN:HE21 | 1.40                     | 0.68              |
| 4:L5:1387:A:H62    | 32:La:74:ASN:HD21  | 1.41                     | 0.67              |
| 1:A4:51:U:H3       | 2:D4:34:G:H1       | 1.40                     | 0.67              |
| 49:S2:1252:C:H41   | 66:SQ:146:ARG:HH11 | 1.42                     | 0.67              |
| 58:SI:129:LEU:HB3  | 58:SI:132:GLU:HB2  | 1.76                     | 0.67              |
| 4:L5:1570:G:N7     | 47:Lp:3:LYS:NZ     | 2.42                     | 0.67              |
| 8:LB:89:ILE:HG22   | 8:LB:162:VAL:HG23  | 1.77                     | 0.67              |
| 4:L5:1100:U:H3     | 4:L5:1195:G:H1     | 1.43                     | 0.67              |
| 14:LH:44:GLU:HB3   | 14:LH:58:ASP:HB2   | 1.76                     | 0.67              |
| 2:D4:51:U:H3       | 2:D4:63:G:H1       | 1.41                     | 0.66              |
| 4:L5:2481:G:H1     | 4:L5:2497:C:H42    | 1.43                     | 0.66              |
| 4:L5:1267:C:OP2    | 4:L5:2121:C:N4     | 2.28                     | 0.66              |
| 59:SJ:121:LYS:H    | 59:SJ:125:HIS:HD2  | 1.42                     | 0.66              |
| 8:LB:95:THR:HG23   | 8:LB:97:ARG:H      | 1.61                     | 0.65              |
| 57:SH:11:PRO:HG3   | 57:SH:44:ASN:HD22  | 1.62                     | 0.65              |
| 4:L5:1656:U:OP2    | 32:La:26:ARG:NH2   | 2.30                     | 0.65              |
| 62:SM:52:GLN:HG2   | 62:SM:76:LEU:HD11  | 1.78                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:S2:1416:C:H42   | 49:S2:1422:G:H1    | 1.43                     | 0.65              |
| 54:SE:19:MET:HB2   | 54:SE:51:ARG:HH22  | 1.62                     | 0.65              |
| 55:SF:122:ARG:HE   | 78:Sc:59:LEU:HD11  | 1.62                     | 0.65              |
| 82:Sg:158:PRO:HG2  | 82:Sg:202:PRO:HA   | 1.79                     | 0.64              |
| 4:L5:502:C:H3'     | 4:L5:503:C:H3'     | 1.79                     | 0.64              |
| 4:L5:700:G:O2'     | 4:L5:969:C:N4      | 2.31                     | 0.64              |
| 56:SG:10:THR:HG23  | 56:SG:128:THR:HA   | 1.79                     | 0.64              |
| 4:L5:4133:C:H5'    | 4:L5:4144:C:H42    | 1.63                     | 0.64              |
| 38:Lg:3:GLN:HE21   | 38:Lg:30:ILE:HG22  | 1.62                     | 0.64              |
| 50:SA:16:LEU:O     | 67:SR:93:GLN:NE2   | 2.30                     | 0.64              |
| 55:SF:144:LEU:HD21 | 78:Sc:49:PRO:HG2   | 1.80                     | 0.64              |
| 62:SM:46:GLN:HE21  | 62:SM:112:LYS:HE3  | 1.62                     | 0.64              |
| 4:L5:1961:G:H1     | 4:L5:2024:G:HO2'   | 1.43                     | 0.64              |
| 24:LS:85:ASP:HB3   | 24:LS:90:THR:HG22  | 1.79                     | 0.64              |
| 4:L5:1701:A:OP2    | 4:L5:2096:G:N2     | 2.31                     | 0.64              |
| 49:S2:973:C:N3     | 64:SO:55:ARG:NH1   | 2.46                     | 0.64              |
| 49:S2:455:A:O2'    | 49:S2:1735:A:N1    | 2.30                     | 0.64              |
| 49:S2:1415:C:N4    | 49:S2:1424:G:O6    | 2.31                     | 0.64              |
| 54:SE:55:ALA:HB1   | 54:SE:60:GLU:HG3   | 1.80                     | 0.64              |
| 54:SE:125:LYS:H    | 54:SE:142:HIS:HD2  | 1.44                     | 0.64              |
| 49:S2:1754:G:N7    | 49:S2:1779:G:N2    | 2.46                     | 0.63              |
| 49:S2:1256:G:N2    | 70:SU:64:THR:O     | 2.31                     | 0.63              |
| 81:Sf:118:ARG:HH11 | 81:Sf:134:SER:HB3  | 1.63                     | 0.63              |
| 4:L5:1755:C:N4     | 4:L5:1776:A:N1     | 2.47                     | 0.63              |
| 4:L5:2838:G:H5'    | 8:LB:247:GLY:HA2   | 1.79                     | 0.63              |
| 11:LE:96:VAL:HG11  | 11:LE:105:ARG:HD2  | 1.80                     | 0.63              |
| 49:S2:1471:C:H42   | 49:S2:1476:A:H62   | 1.47                     | 0.63              |
| 4:L5:489:C:H42     | 4:L5:664:G:H1      | 1.45                     | 0.63              |
| 4:L5:1440:U:O2'    | 4:L5:2109:G:N3     | 2.31                     | 0.63              |
| 57:SH:83:LEU:HD21  | 57:SH:92:VAL:HG21  | 1.81                     | 0.63              |
| 4:L5:2601:A:N6     | 4:L5:2744:A:OP2    | 2.32                     | 0.63              |
| 56:SG:98:ARG:NH2   | 56:SG:103:ASP:OD1  | 2.32                     | 0.63              |
| 7:LA:28:ARG:HB2    | 7:LA:123:ARG:HB3   | 1.79                     | 0.62              |
| 50:SA:54:THR:HG22  | 50:SA:162:PRO:HG2  | 1.81                     | 0.62              |
| 14:LH:89:ARG:HH11  | 14:LH:187:VAL:HA   | 1.65                     | 0.62              |
| 70:SU:19:ARG:HH11  | 70:SU:92:HIS:HB2   | 1.64                     | 0.62              |
| 49:S2:1248:U:O3'   | 66:SQ:146:ARG:NH2  | 2.32                     | 0.62              |
| 49:S2:335:G:N7     | 56:SG:190:ARG:NH2  | 2.46                     | 0.62              |
| 49:S2:624:C:N4     | 73:SX:63:ASN:OD1   | 2.32                     | 0.62              |
| 70:SU:26:SER:HB2   | 70:SU:110:VAL:HG23 | 1.81                     | 0.62              |
| 50:SA:52:LYS:HE3   | 67:SR:108:LEU:HD13 | 1.81                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:L5:4096:C:H42    | 4:L5:4113:U:H1'    | 1.65                     | 0.62              |
| 7:LA:30:ARG:O      | 7:LA:163:ARG:NH2   | 2.32                     | 0.62              |
| 29:LX:37:LYS:HG3   | 29:LX:38:LYS:HG2   | 1.82                     | 0.62              |
| 55:SF:49:LEU:HD12  | 66:SQ:50:LYS:HB2   | 1.81                     | 0.62              |
| 57:SH:143:ARG:HB2  | 57:SH:155:LYS:HB2  | 1.82                     | 0.62              |
| 17:LL:116:ARG:NH1  | 17:LL:155:MET:O    | 2.33                     | 0.62              |
| 57:SH:57:ARG:NH2   | 57:SH:58:LYS:O     | 2.33                     | 0.62              |
| 4:L5:3723:A:N7     | 40:Li:68:ARG:NH1   | 2.47                     | 0.62              |
| 50:SA:84:GLN:HG2   | 50:SA:100:ALA:HB1  | 1.81                     | 0.62              |
| 4:L5:2562:G:O2'    | 4:L5:2565:A:N6     | 2.32                     | 0.62              |
| 49:S2:65:C:N4      | 56:SG:134:GLY:O    | 2.33                     | 0.62              |
| 4:L5:3651:A:OP2    | 7:LA:200:ARG:NH1   | 2.33                     | 0.61              |
| 4:L5:4093:G:H2'    | 4:L5:4094:G:H8     | 1.65                     | 0.61              |
| 38:Lg:43:LYS:HZ3   | 38:Lg:52:ARG:HE    | 1.48                     | 0.61              |
| 76:Sa:38:LYS:HB3   | 76:Sa:71:LEU:HB2   | 1.80                     | 0.61              |
| 15:LI:87:MET:HB3   | 15:LI:138:ILE:HG12 | 1.81                     | 0.61              |
| 38:Lg:41:ALA:O     | 38:Lg:52:ARG:NH1   | 2.32                     | 0.61              |
| 4:L5:1970:A:O2'    | 4:L5:2017:A:N7     | 2.33                     | 0.61              |
| 4:L5:4985:U:O2     | 8:LB:174:ARG:NH2   | 2.33                     | 0.61              |
| 5:L7:99:G:N7       | 24:LS:55:LYS:NZ    | 2.48                     | 0.61              |
| 8:LB:378:ARG:HG2   | 28:LW:32:LEU:HD21  | 1.81                     | 0.61              |
| 59:SJ:137:VAL:HG22 | 59:SJ:157:ILE:HG22 | 1.81                     | 0.61              |
| 32:La:37:GLY:H     | 32:La:41:HIS:HB2   | 1.66                     | 0.61              |
| 49:S2:1630:A:H5'   | 68:SS:37:GLY:HA3   | 1.82                     | 0.61              |
| 77:Sb:36:LYS:HB2   | 77:Sb:78:SER:HB2   | 1.82                     | 0.61              |
| 4:L5:493:G:N1      | 4:L5:661:C:O2      | 2.34                     | 0.61              |
| 24:LS:83:ARG:NH2   | 25:LT:154:ILE:O    | 2.33                     | 0.61              |
| 8:LB:184:GLN:HE21  | 8:LB:186:ASN:HD21  | 1.46                     | 0.61              |
| 19:LN:73:ARG:HH21  | 19:LN:92:LEU:HD21  | 1.64                     | 0.61              |
| 31:LZ:83:THR:HG22  | 31:LZ:85:TYR:H     | 1.66                     | 0.61              |
| 4:L5:3641:U:OP2    | 4:L5:3646:A:N6     | 2.34                     | 0.60              |
| 12:LF:62:ARG:HD2   | 12:LF:66:ARG:HH21  | 1.66                     | 0.60              |
| 4:L5:2611:A:H5'    | 4:L5:2688:G:H4'    | 1.83                     | 0.60              |
| 4:L5:4686:G:N3     | 14:LH:163:GLN:NE2  | 2.48                     | 0.60              |
| 51:SB:36:PRO:HB3   | 51:SB:231:LEU:HD21 | 1.83                     | 0.60              |
| 54:SE:166:THR:HG23 | 54:SE:168:LYS:H    | 1.64                     | 0.60              |
| 4:L5:1761:G:H1     | 4:L5:1771:U:H3     | 1.50                     | 0.60              |
| 68:SS:15:VAL:HG13  | 68:SS:68:ILE:HD11  | 1.82                     | 0.60              |
| 4:L5:182:G:H1      | 4:L5:254:G:H22     | 1.48                     | 0.60              |
| 4:L5:2334:C:OP2    | 9:LC:195:LYS:NZ    | 2.34                     | 0.60              |
| 17:LL:56:ARG:O     | 17:LL:116:ARG:NH2  | 2.35                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:La:71:PRO:HG2   | 32:La:108:TYR:HA   | 1.83                     | 0.60              |
| 49:S2:49:C:N4      | 49:S2:472:C:O2'    | 2.33                     | 0.60              |
| 81:Sf:140:TYR:HA   | 81:Sf:147:THR:HA   | 1.83                     | 0.60              |
| 4:L5:4101:C:H1'    | 4:L5:4109:G:H1     | 1.66                     | 0.60              |
| 8:LB:254:ILE:HG23  | 8:LB:266:VAL:HG11  | 1.82                     | 0.60              |
| 16:LJ:72:CYS:SG    | 16:LJ:73:THR:N     | 2.74                     | 0.60              |
| 49:S2:526:A:O2'    | 59:SJ:125:HIS:ND1  | 2.34                     | 0.60              |
| 4:L5:1070:G:N7     | 11:LE:46:ARG:NH2   | 2.48                     | 0.60              |
| 4:L5:1313:C:H5''   | 36:Le:44:ARG:HH12  | 1.66                     | 0.60              |
| 4:L5:4740:G:H1'    | 4:L5:4742:G:H5''   | 1.82                     | 0.60              |
| 49:S2:1606:G:OP1   | 69:ST:84:ARG:NH1   | 2.34                     | 0.60              |
| 51:SB:107:ARG:NH2  | 64:SO:133:THR:O    | 2.35                     | 0.60              |
| 69:ST:125:PRO:HA   | 69:ST:128:GLN:HB3  | 1.83                     | 0.60              |
| 70:SU:23:THR:HB    | 70:SU:113:GLU:HB2  | 1.82                     | 0.60              |
| 4:L5:90:G:OP2      | 46:Lo:40:ARG:NH2   | 2.35                     | 0.60              |
| 4:L5:1493:G:OP2    | 33:Lb:44:ARG:NH1   | 2.35                     | 0.60              |
| 52:SC:65:LYS:HG3   | 52:SC:273:LEU:HD21 | 1.84                     | 0.60              |
| 4:L5:1974:U:O2'    | 4:L5:1994:C:N4     | 2.34                     | 0.60              |
| 49:S2:745:C:H5'    | 49:S2:746:C:H4'    | 1.83                     | 0.60              |
| 53:SD:28:GLU:HB2   | 60:SK:61:GLN:HG2   | 1.83                     | 0.60              |
| 75:SZ:95:GLY:O     | 75:SZ:112:ASN:ND2  | 2.35                     | 0.60              |
| 31:LZ:121:ARG:NH2  | 31:LZ:127:ASN:OD1  | 2.35                     | 0.60              |
| 49:S2:962:A:H5''   | 64:SO:66:ARG:HB2   | 1.83                     | 0.60              |
| 58:SI:158:ILE:HD12 | 58:SI:162:LEU:HB3  | 1.84                     | 0.59              |
| 64:SO:62:VAL:HG22  | 64:SO:64:ALA:H     | 1.67                     | 0.59              |
| 67:SR:59:LYS:HA    | 67:SR:62:GLN:HE21  | 1.65                     | 0.59              |
| 6:L8:96:C:H5''     | 39:Lh:66:LYS:HD2   | 1.84                     | 0.59              |
| 4:L5:2598:A:OP1    | 38:Lg:52:ARG:NH2   | 2.35                     | 0.59              |
| 63:SN:23:PRO:HG2   | 63:SN:26:LEU:HD23  | 1.83                     | 0.59              |
| 8:LB:10:ARG:NH1    | 8:LB:265:SER:O     | 2.36                     | 0.59              |
| 49:S2:1230:C:OP1   | 68:SS:130:ARG:NH2  | 2.36                     | 0.59              |
| 82:Sg:164:ILE:HD12 | 82:Sg:221:LEU:HB2  | 1.82                     | 0.59              |
| 4:L5:1508:A:OP1    | 9:LC:110:ARG:NH1   | 2.35                     | 0.59              |
| 4:L5:2487:G:N1     | 4:L5:2492:C:O2     | 2.33                     | 0.59              |
| 4:L5:4586:G:OP2    | 20:LO:74:ARG:NH1   | 2.36                     | 0.59              |
| 49:S2:1488:C:O2'   | 49:S2:1490:G:OP2   | 2.20                     | 0.59              |
| 56:SG:49:VAL:HG12  | 56:SG:115:LYS:HB3  | 1.83                     | 0.59              |
| 4:L5:4884:G:N7     | 11:LE:272:ARG:NH2  | 2.51                     | 0.59              |
| 2:D4:19:G:OP2      | 2:D4:57:G:N2       | 2.35                     | 0.59              |
| 51:SB:71:LEU:HD22  | 51:SB:82:ARG:HB3   | 1.84                     | 0.59              |
| 62:SM:50:CYS:SG    | 62:SM:51:VAL:N     | 2.76                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 64:SO:85:CYS:HB2   | 64:SO:90:ILE:HB    | 1.85                     | 0.59              |
| 4:L5:200:U:O2'     | 30:LY:59:ARG:NH1   | 2.36                     | 0.59              |
| 49:S2:193:C:OP2    | 58:SI:141:ARG:NH2  | 2.36                     | 0.59              |
| 49:S2:533:A:N3     | 49:S2:552:G:N2     | 2.50                     | 0.59              |
| 49:S2:1617:G:N1    | 49:S2:1620:A:OP2   | 2.36                     | 0.59              |
| 49:S2:1834:A:H2    | 49:S2:1837:G:H1    | 1.50                     | 0.59              |
| 61:SL:57:ASP:OD2   | 61:SL:84:ARG:NH1   | 2.36                     | 0.59              |
| 4:L5:3842:C:OP1    | 8:LB:238:LYS:NZ    | 2.31                     | 0.59              |
| 14:LH:44:GLU:OE2   | 18:LM:2:VAL:N      | 2.36                     | 0.59              |
| 28:LW:73:ARG:HH22  | 49:S2:1784:G:H8    | 1.51                     | 0.59              |
| 49:S2:527:C:O2     | 49:S2:559:G:N2     | 2.33                     | 0.59              |
| 60:SK:11:ILE:HA    | 60:SK:14:LEU:HD12  | 1.85                     | 0.59              |
| 68:SS:71:MET:HB3   | 68:SS:99:LEU:HD21  | 1.84                     | 0.59              |
| 69:ST:104:LEU:HD22 | 69:ST:121:ARG:HG3  | 1.85                     | 0.59              |
| 82:Sg:14:HIS:HB3   | 82:Sg:305:ASN:HB2  | 1.85                     | 0.59              |
| 4:L5:1269:G:N2     | 4:L5:2109:G:N7     | 2.49                     | 0.58              |
| 49:S2:1533:A:OP2   | 55:SF:164:ARG:NH1  | 2.35                     | 0.58              |
| 64:SO:125:LYS:HA   | 76:Sa:56:ALA:HB1   | 1.85                     | 0.58              |
| 4:L5:280:G:OP1     | 19:LN:47:LYS:NZ    | 2.36                     | 0.58              |
| 4:L5:4429:C:N3     | 15:LI:158:LYS:NZ   | 2.51                     | 0.58              |
| 4:L5:4472:G:O2'    | 44:Lm:100:TYR:O    | 2.20                     | 0.58              |
| 4:L5:4691:A:OP1    | 14:LH:71:ARG:NH1   | 2.37                     | 0.58              |
| 9:LC:109:ARG:O     | 19:LN:204:ARG:NH2  | 2.36                     | 0.58              |
| 4:L5:1797:G:OP1    | 12:LF:104:LYS:NZ   | 2.37                     | 0.58              |
| 4:L5:4935:C:H2'    | 4:L5:4936:G:H8     | 1.69                     | 0.58              |
| 19:LN:137:PRO:O    | 19:LN:143:ARG:NH1  | 2.36                     | 0.58              |
| 61:SL:59:LYS:HD3   | 61:SL:134:LEU:HD13 | 1.86                     | 0.58              |
| 6:L8:99:U:O2'      | 29:LX:103:LYS:NZ   | 2.36                     | 0.58              |
| 51:SB:36:PRO:HD3   | 51:SB:98:THR:HG23  | 1.85                     | 0.58              |
| 52:SC:64:THR:HG23  | 52:SC:67:GLY:H     | 1.69                     | 0.58              |
| 61:SL:103:GLU:OE2  | 73:SX:14:ARG:NH2   | 2.37                     | 0.58              |
| 4:L5:4250:G:OP1    | 16:LJ:98:ASN:ND2   | 2.37                     | 0.58              |
| 49:S2:1858:G:OP2   | 64:SO:146:ARG:NH2  | 2.32                     | 0.58              |
| 70:SU:62:ARG:HE    | 70:SU:81:GLN:HE22  | 1.50                     | 0.58              |
| 4:L5:4517:A:OP2    | 8:LB:2:SER:N       | 2.37                     | 0.58              |
| 16:LJ:90:ARG:NH2   | 16:LJ:108:GLY:O    | 2.37                     | 0.58              |
| 49:S2:153:G:N3     | 56:SG:13:GLN:NE2   | 2.52                     | 0.58              |
| 49:S2:302:A:OP1    | 58:SI:74:ARG:NH1   | 2.37                     | 0.58              |
| 49:S2:1477:U:OP2   | 67:SR:3:ARG:NH1    | 2.37                     | 0.58              |
| 50:SA:61:ALA:HB2   | 50:SA:159:ILE:HG21 | 1.85                     | 0.58              |
| 78:Sc:13:ARG:HB3   | 78:Sc:33:GLU:HB2   | 1.84                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 82:Sg:118:ARG:HD2  | 82:Sg:119:GLN:HG2  | 1.85                     | 0.58              |
| 4:L5:1253:G:O2'    | 4:L5:1257:A:N6     | 2.37                     | 0.58              |
| 4:L5:4755:G:N7     | 11:LE:279:ASN:ND2  | 2.51                     | 0.58              |
| 60:SK:65:ARG:HE    | 79:Sd:25:SER:HB2   | 1.69                     | 0.58              |
| 5:L7:7:G:OP1       | 10:LD:33:ARG:NE    | 2.33                     | 0.58              |
| 4:L5:500:G:N2      | 4:L5:655:C:O2      | 2.36                     | 0.58              |
| 49:S2:1551:U:OP1   | 53:SD:9:ARG:NH1    | 2.37                     | 0.58              |
| 52:SC:83:LEU:O     | 71:SV:15:ARG:NE    | 2.35                     | 0.58              |
| 60:SK:3:MET:HE3    | 60:SK:44:HIS:HB3   | 1.84                     | 0.58              |
| 18:LM:41:PRO:HG3   | 18:LM:73:VAL:HG23  | 1.84                     | 0.57              |
| 49:S2:919:A:N1     | 63:SN:70:LYS:NZ    | 2.51                     | 0.57              |
| 49:S2:1616:U:H3    | 49:S2:1620:A:H2    | 1.50                     | 0.57              |
| 54:SE:36:HIS:NE2   | 54:SE:88:ASP:OD2   | 2.36                     | 0.57              |
| 69:ST:18:LEU:HD11  | 69:ST:131:LEU:HD22 | 1.85                     | 0.57              |
| 82:Sg:40:ILE:HB    | 82:Sg:59:LEU:HB2   | 1.86                     | 0.57              |
| 4:L5:75:G:O2'      | 17:LL:101:ARG:NH1  | 2.37                     | 0.57              |
| 4:L5:2621:A:OP1    | 26:LU:80:LYS:NZ    | 2.37                     | 0.57              |
| 14:LH:7:ASN:ND2    | 14:LH:58:ASP:OD1   | 2.37                     | 0.57              |
| 39:Lh:40:ALA:HB3   | 39:Lh:43:LYS:HG3   | 1.85                     | 0.57              |
| 49:S2:111:A:O2'    | 61:SL:69:ARG:NH1   | 2.38                     | 0.57              |
| 49:S2:317:C:OP2    | 56:SG:183:ARG:NH2  | 2.36                     | 0.57              |
| 4:L5:703:G:O2'     | 36:Le:5:ARG:NH2    | 2.38                     | 0.57              |
| 28:LW:101:ARG:HA   | 28:LW:104:GLN:HG2  | 1.85                     | 0.57              |
| 67:SR:15:VAL:O     | 67:SR:19:LYS:NZ    | 2.37                     | 0.57              |
| 82:Sg:220:ASP:H    | 82:Sg:224:GLY:HA2  | 1.69                     | 0.57              |
| 4:L5:711:A:HO2'    | 11:LE:136:HIS:HD1  | 1.52                     | 0.57              |
| 20:LO:8:VAL:HG22   | 20:LO:117:ARG:HG3  | 1.87                     | 0.57              |
| 46:Lo:33:LEU:HA    | 46:Lo:38:LYS:HG2   | 1.86                     | 0.57              |
| 49:S2:333:G:O6     | 56:SG:186:GLN:NE2  | 2.38                     | 0.57              |
| 55:SF:153:LEU:HD22 | 55:SF:189:ALA:HA   | 1.85                     | 0.57              |
| 57:SH:60:ILE:HG22  | 57:SH:90:LYS:HB3   | 1.85                     | 0.57              |
| 58:SI:57:ALA:HB2   | 58:SI:183:GLY:HA2  | 1.85                     | 0.57              |
| 4:L5:4146:G:H2'    | 4:L5:4147:G:H8     | 1.69                     | 0.57              |
| 4:L5:4618:G:H5''   | 27:LV:15:ARG:HB2   | 1.85                     | 0.57              |
| 7:LA:104:VAL:HA    | 7:LA:107:MET:HG3   | 1.86                     | 0.57              |
| 49:S2:943:U:OP1    | 51:SB:214:LYS:NZ   | 2.38                     | 0.57              |
| 64:SO:149:ARG:HH21 | 64:SO:151:LEU:HD13 | 1.69                     | 0.57              |
| 82:Sg:66:VAL:HA    | 82:Sg:82:SER:HA    | 1.87                     | 0.57              |
| 8:LB:58:ARG:HE     | 8:LB:60:VAL:HG12   | 1.68                     | 0.57              |
| 8:LB:214:ASP:OD1   | 8:LB:214:ASP:N     | 2.37                     | 0.57              |
| 51:SB:71:LEU:HD21  | 51:SB:79:VAL:HG13  | 1.86                     | 0.57              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 62:SM:50:CYS:SG   | 62:SM:52:GLN:NE2   | 2.78                     | 0.57              |
| 4:L5:1390:G:N2    | 4:L5:1393:G:OP2    | 2.38                     | 0.57              |
| 8:LB:83:PRO:O     | 8:LB:167:GLN:NE2   | 2.37                     | 0.57              |
| 63:SN:55:ARG:HH21 | 63:SN:56:ASP:HB3   | 1.69                     | 0.57              |
| 4:L5:374:G:OP2    | 41:Lj:56:ARG:NH1   | 2.37                     | 0.57              |
| 4:L5:2130:G:N2    | 4:L5:2249:C:O2     | 2.37                     | 0.57              |
| 4:L5:4717:A:OP2   | 8:LB:30:LYS:NZ     | 2.36                     | 0.57              |
| 49:S2:1349:G:O6   | 49:S2:1379:A:N6    | 2.38                     | 0.57              |
| 50:SA:85:ARG:NH1  | 67:SR:81:ARG:O     | 2.38                     | 0.57              |
| 82:Sg:132:TRP:HA  | 82:Sg:138:CYS:HA   | 1.85                     | 0.57              |
| 4:L5:2404:A:H1'   | 41:Lj:12:ARG:HH21  | 1.68                     | 0.57              |
| 64:SO:56:VAL:HG11 | 64:SO:80:ASP:HB3   | 1.86                     | 0.57              |
| 67:SR:124:VAL:O   | 67:SR:127:ASN:ND2  | 2.37                     | 0.57              |
| 82:Sg:72:SER:OG   | 82:Sg:74:ASP:O     | 2.22                     | 0.57              |
| 82:Sg:237:ASN:ND2 | 82:Sg:286:CYS:O    | 2.38                     | 0.57              |
| 4:L5:1755:C:N3    | 10:LD:2:GLY:N      | 2.52                     | 0.57              |
| 31:LZ:89:ILE:HD11 | 31:LZ:117:LYS:HB3  | 1.87                     | 0.57              |
| 49:S2:383:G:H4'   | 61:SL:132:ARG:HD2  | 1.86                     | 0.57              |
| 49:S2:1293:A:H1'  | 81:Sf:138:ARG:HH11 | 1.69                     | 0.57              |
| 49:S2:1623:A:H5'' | 68:SS:133:GLY:HA3  | 1.86                     | 0.56              |
| 63:SN:99:ARG:NH1  | 63:SN:143:SER:O    | 2.38                     | 0.56              |
| 12:LF:127:LYS:HB2 | 25:LT:133:ALA:HB3  | 1.87                     | 0.56              |
| 30:LY:112:ASP:H   | 30:LY:115:ARG:HB3  | 1.70                     | 0.56              |
| 49:S2:444:G:N7    | 58:SI:47:ARG:NH1   | 2.53                     | 0.56              |
| 49:S2:466:G:O2'   | 56:SG:72:ARG:NH1   | 2.38                     | 0.56              |
| 49:S2:1544:C:N4   | 49:S2:1588:A:O2'   | 2.38                     | 0.56              |
| 59:SJ:136:ARG:HA  | 59:SJ:141:VAL:HA   | 1.87                     | 0.56              |
| 67:SR:98:VAL:HB   | 67:SR:115:SER:HB2  | 1.86                     | 0.56              |
| 82:Sg:65:PHE:O    | 82:Sg:83:TRP:N     | 2.36                     | 0.56              |
| 4:L5:347:A:O2'    | 9:LC:50:GLN:NE2    | 2.39                     | 0.56              |
| 4:L5:394:G:N2     | 4:L5:397:G:OP2     | 2.36                     | 0.56              |
| 4:L5:1351:G:OP1   | 9:LC:33:ARG:NH1    | 2.39                     | 0.56              |
| 4:L5:4479:A:OP1   | 14:LH:170:LYS:NZ   | 2.39                     | 0.56              |
| 9:LC:208:CYS:HB2  | 9:LC:248:ARG:HE    | 1.69                     | 0.56              |
| 16:LJ:48:PRO:HB3  | 16:LJ:72:CYS:HB2   | 1.86                     | 0.56              |
| 25:LT:41:ASP:N    | 25:LT:41:ASP:OD1   | 2.38                     | 0.56              |
| 34:Lc:14:ILE:O    | 34:Lc:18:LEU:N     | 2.36                     | 0.56              |
| 45:Ln:9:ARG:NH2   | 49:S2:1851:A:OP1   | 2.39                     | 0.56              |
| 49:S2:434:G:H21   | 49:S2:473:A:H8     | 1.53                     | 0.56              |
| 49:S2:1060:A:O2'  | 49:S2:1062:A:N7    | 2.34                     | 0.56              |
| 52:SC:210:PRO:HB3 | 52:SC:240:THR:HG21 | 1.88                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 78:Sc:20:ARG:HD2  | 78:Sc:28:THR:HG22  | 1.87                     | 0.56              |
| 81:Sf:141:CYS:SG  | 81:Sf:142:GLY:N    | 2.79                     | 0.56              |
| 2:B4:19:G:OP2     | 2:B4:57:G:N2       | 2.39                     | 0.56              |
| 4:L5:3688:U:OP2   | 7:LA:198:ARG:NH1   | 2.37                     | 0.56              |
| 16:LJ:9:GLU:HG3   | 16:LJ:13:ARG:HD2   | 1.86                     | 0.56              |
| 16:LJ:18:ARG:H    | 16:LJ:134:LEU:HA   | 1.69                     | 0.56              |
| 29:LX:92:ASP:OD1  | 29:LX:92:ASP:N     | 2.39                     | 0.56              |
| 46:Lo:45:GLN:NE2  | 46:Lo:51:GLN:OE1   | 2.39                     | 0.56              |
| 47:Lp:19:GLY:O    | 47:Lp:23:ARG:NH1   | 2.39                     | 0.56              |
| 49:S2:528:A:OP1   | 59:SJ:121:LYS:NZ   | 2.37                     | 0.56              |
| 53:SD:75:LYS:NZ   | 60:SK:20:VAL:O     | 2.38                     | 0.56              |
| 82:Sg:89:LEU:HD13 | 82:Sg:99:ARG:HB3   | 1.87                     | 0.56              |
| 4:L5:2578:G:N7    | 31:LZ:17:ARG:NH1   | 2.54                     | 0.56              |
| 4:L5:2693:G:OP1   | 42:Lk:35:LYS:NZ    | 2.38                     | 0.56              |
| 4:L5:4139:G:O2'   | 4:L5:4146:G:N2     | 2.38                     | 0.56              |
| 15:LI:31:ILE:O    | 15:LI:32:ARG:NH1   | 2.35                     | 0.56              |
| 15:LI:179:ASP:OD1 | 15:LI:179:ASP:N    | 2.38                     | 0.56              |
| 4:L5:169:G:O2'    | 17:LL:135:LYS:NZ   | 2.36                     | 0.56              |
| 6:L8:22:U:OP1     | 30:LY:11:ARG:NH1   | 2.38                     | 0.56              |
| 7:LA:120:PRO:HA   | 7:LA:162:ASN:HB3   | 1.87                     | 0.56              |
| 24:LS:80:ILE:HG12 | 24:LS:129:VAL:HG23 | 1.87                     | 0.56              |
| 49:S2:493:A:H1'   | 49:S2:574:A:H5'    | 1.86                     | 0.56              |
| 49:S2:957:A:O2'   | 49:S2:958:G:N3     | 2.34                     | 0.56              |
| 49:S2:1139:C:O2   | 49:S2:1148:A:N6    | 2.38                     | 0.56              |
| 49:S2:1199:A:H5'' | 76:Sa:2:THR:HB     | 1.88                     | 0.56              |
| 82:Sg:35:SER:OG   | 82:Sg:36:ARG:N     | 2.38                     | 0.56              |
| 4:L5:518:G:H1     | 4:L5:643:C:H3'     | 1.71                     | 0.56              |
| 4:L5:1697:G:N2    | 4:L5:2084:C:OP2    | 2.38                     | 0.56              |
| 8:LB:234:ARG:NH1  | 8:LB:268:ARG:O     | 2.39                     | 0.56              |
| 13:LG:61:ILE:HA   | 13:LG:64:GLN:HG2   | 1.88                     | 0.56              |
| 27:LV:83:ARG:NH2  | 27:LV:120:PRO:O    | 2.37                     | 0.56              |
| 49:S2:1109:C:N4   | 67:SR:123:THR:OG1  | 2.39                     | 0.56              |
| 49:S2:1255:G:HO2' | 70:SU:70:CYS:HG    | 1.53                     | 0.56              |
| 82:Sg:289:LEU:HB3 | 82:Sg:298:LEU:HD21 | 1.86                     | 0.56              |
| 4:L5:1098:G:N2    | 4:L5:1197:C:O2     | 2.39                     | 0.56              |
| 12:LF:108:VAL:HA  | 12:LF:111:LEU:HD12 | 1.88                     | 0.56              |
| 49:S2:190:G:O2'   | 49:S2:191:A:N7     | 2.38                     | 0.56              |
| 51:SB:179:ASN:HB3 | 51:SB:183:GLU:HB3  | 1.88                     | 0.56              |
| 72:SW:27:ILE:HB   | 72:SW:61:ILE:HG23  | 1.87                     | 0.56              |
| 4:L5:2544:G:N2    | 6:L8:126:C:OP1     | 2.39                     | 0.56              |
| 9:LC:140:LYS:O    | 9:LC:204:ARG:NH1   | 2.39                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:SH:122:LEU:HA   | 57:SH:125:VAL:HG22 | 1.88                     | 0.56              |
| 4:L5:937:U:OP1     | 18:LM:46:ARG:NH1   | 2.38                     | 0.56              |
| 4:L5:1398:A:OP1    | 32:La:136:LYS:NZ   | 2.35                     | 0.56              |
| 4:L5:4088:C:O2     | 13:LG:53:ARG:NH2   | 2.39                     | 0.56              |
| 4:L5:4485:C:O2'    | 44:Lm:114:LYS:NZ   | 2.38                     | 0.56              |
| 39:Lh:8:ASP:O      | 39:Lh:12:LYS:NZ    | 2.39                     | 0.56              |
| 49:S2:466:G:O2'    | 56:SG:59:GLN:NE2   | 2.38                     | 0.56              |
| 49:S2:1115:U:O2'   | 49:S2:1117:C:OP2   | 2.23                     | 0.56              |
| 49:S2:1278:A:N6    | 49:S2:1318:G:O6    | 2.39                     | 0.56              |
| 49:S2:1426:U:OP1   | 66:SQ:69:ARG:NH1   | 2.38                     | 0.56              |
| 53:SD:93:THR:HG21  | 53:SD:198:ILE:HD12 | 1.88                     | 0.56              |
| 56:SG:197:GLN:HA   | 56:SG:200:LYS:HB3  | 1.88                     | 0.56              |
| 58:SI:158:ILE:HD11 | 58:SI:163:GLU:HB3  | 1.87                     | 0.56              |
| 82:Sg:107:ASP:HB2  | 82:Sg:125:ARG:HD3  | 1.88                     | 0.55              |
| 8:LB:389:MET:HE2   | 8:LB:392:LEU:HD21  | 1.89                     | 0.55              |
| 19:LN:68:ARG:NH1   | 19:LN:124:ASP:O    | 2.40                     | 0.55              |
| 26:LU:111:GLU:OE2  | 26:LU:113:ARG:NH2  | 2.39                     | 0.55              |
| 49:S2:751:G:N2     | 49:S2:753:C:OP1    | 2.40                     | 0.55              |
| 49:S2:1507:G:N1    | 81:Sf:87:THR:O     | 2.37                     | 0.55              |
| 49:S2:1746:U:OP1   | 56:SG:31:ARG:NH2   | 2.39                     | 0.55              |
| 51:SB:92:GLN:HE21  | 51:SB:95:ASN:HB3   | 1.71                     | 0.55              |
| 60:SK:35:LEU:HD11  | 60:SK:40:VAL:HG12  | 1.88                     | 0.55              |
| 73:SX:63:ASN:ND2   | 73:SX:114:ASP:OD2  | 2.39                     | 0.55              |
| 4:L5:3929:G:OP1    | 19:LN:72:LYS:NZ    | 2.39                     | 0.55              |
| 11:LE:50:LEU:HD12  | 11:LE:51:VAL:HG22  | 1.87                     | 0.55              |
| 46:Lo:11:PHE:O     | 46:Lo:81:ARG:NH1   | 2.39                     | 0.55              |
| 49:S2:1199:A:OP1   | 76:Sa:2:THR:N      | 2.39                     | 0.55              |
| 52:SC:121:ARG:HH22 | 52:SC:123:ARG:HH11 | 1.55                     | 0.55              |
| 68:SS:68:ILE:O     | 68:SS:72:GLN:NE2   | 2.39                     | 0.55              |
| 4:L5:701:G:H5'     | 4:L5:969:C:H42     | 1.71                     | 0.55              |
| 4:L5:1506:G:O2'    | 9:LC:116:ASN:ND2   | 2.39                     | 0.55              |
| 4:L5:1972:G:O2'    | 4:L5:1995:G:N2     | 2.39                     | 0.55              |
| 4:L5:2696:A:N1     | 42:Lk:24:LYS:NZ    | 2.49                     | 0.55              |
| 4:L5:3709:U:O2'    | 4:L5:3711:A:N1     | 2.39                     | 0.55              |
| 49:S2:851:C:H5''   | 49:S2:852:G:H5'    | 1.89                     | 0.55              |
| 57:SH:69:LEU:O     | 57:SH:73:GLN:NE2   | 2.40                     | 0.55              |
| 59:SJ:110:LEU:HB2  | 59:SJ:147:PHE:HB3  | 1.88                     | 0.55              |
| 4:L5:1707:C:O2'    | 4:L5:2118:G:N2     | 2.40                     | 0.55              |
| 4:L5:1962:A:H5''   | 4:L5:2024:G:H22    | 1.71                     | 0.55              |
| 4:L5:2279:A:O2'    | 36:Le:48:ARG:NH2   | 2.40                     | 0.55              |
| 4:L5:3888:G:O6     | 20:LO:96:GLN:NE2   | 2.40                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:LH:17:ASP:N     | 14:LH:17:ASP:OD1   | 2.40                     | 0.55              |
| 17:LL:186:ARG:HG3  | 40:Li:9:VAL:HG11   | 1.87                     | 0.55              |
| 49:S2:1142:G:N2    | 49:S2:1145:A:OP2   | 2.38                     | 0.55              |
| 53:SD:23:GLU:OE2   | 53:SD:27:ARG:NH2   | 2.39                     | 0.55              |
| 58:SI:101:ILE:HD12 | 58:SI:190:LEU:HD11 | 1.87                     | 0.55              |
| 75:SZ:96:LEU:HD23  | 75:SZ:97:ILE:HG23  | 1.88                     | 0.55              |
| 4:L5:2266:C:O2'    | 48:Lr:39:ARG:NH1   | 2.40                     | 0.55              |
| 49:S2:1309:C:OP1   | 81:Sf:118:ARG:NH1  | 2.40                     | 0.55              |
| 49:S2:1669:G:OP1   | 70:SU:79:ARG:NH2   | 2.40                     | 0.55              |
| 65:SP:81:ARG:NH1   | 65:SP:120:SER:OG   | 2.39                     | 0.55              |
| 43:Ll:2:SER:O      | 43:Ll:5:LYS:NZ     | 2.40                     | 0.55              |
| 53:SD:106:ARG:HG3  | 53:SD:175:VAL:HG12 | 1.88                     | 0.55              |
| 4:L5:4625:C:HO2'   | 8:LB:336:CYS:HG    | 1.55                     | 0.55              |
| 36:Le:35:TRP:O     | 36:Le:36:ARG:NH2   | 2.36                     | 0.55              |
| 50:SA:191:ARG:NH2  | 71:SV:44:GLY:O     | 2.34                     | 0.55              |
| 56:SG:54:GLY:O     | 56:SG:110:ASN:ND2  | 2.40                     | 0.55              |
| 82:Sg:108:VAL:HA   | 82:Sg:124:SER:HA   | 1.89                     | 0.55              |
| 4:L5:1763:C:H42    | 4:L5:1769:G:H1     | 1.53                     | 0.55              |
| 4:L5:5032:C:N4     | 4:L5:5033:G:O6     | 2.40                     | 0.55              |
| 5:L7:34:C:N3       | 5:L7:46:C:O2'      | 2.40                     | 0.55              |
| 22:LQ:41:SER:OG    | 22:LQ:44:ASN:ND2   | 2.40                     | 0.55              |
| 4:L5:1316:G:OP1    | 36:Le:43:ASN:ND2   | 2.40                     | 0.54              |
| 16:LJ:4:ASP:N      | 16:LJ:4:ASP:OD1    | 2.39                     | 0.54              |
| 41:Lj:2:THR:N      | 41:Lj:6:SER:OG     | 2.40                     | 0.54              |
| 49:S2:830:A:OP2    | 49:S2:846:G:N2     | 2.40                     | 0.54              |
| 51:SB:123:ALA:HB2  | 51:SB:165:ARG:HB2  | 1.89                     | 0.54              |
| 60:SK:25:LYS:HB3   | 60:SK:67:PHE:HE1   | 1.71                     | 0.54              |
| 4:L5:280:G:H5''    | 19:LN:14:LYS:HE2   | 1.89                     | 0.54              |
| 4:L5:2263:A:OP1    | 48:Lr:107:ARG:NH2  | 2.41                     | 0.54              |
| 4:L5:4415:A:OP1    | 15:LI:154:ARG:NH1  | 2.41                     | 0.54              |
| 16:LJ:101:ASP:HA   | 16:LJ:159:LYS:HB2  | 1.89                     | 0.54              |
| 24:LS:95:ARG:NH2   | 24:LS:112:ASP:OD1  | 2.41                     | 0.54              |
| 28:LW:81:ALA:HB2   | 56:SG:131:ARG:HH21 | 1.72                     | 0.54              |
| 50:SA:53:ARG:NH2   | 71:SV:83:PHE:O     | 2.39                     | 0.54              |
| 70:SU:60:THR:HG22  | 70:SU:83:ARG:HD3   | 1.89                     | 0.54              |
| 6:L8:155:C:OP2     | 13:LG:89:ARG:NH2   | 2.40                     | 0.54              |
| 9:LC:204:ARG:NH2   | 9:LC:205:ARG:O     | 2.40                     | 0.54              |
| 12:LF:153:LEU:HD11 | 12:LF:244:ILE:HD11 | 1.88                     | 0.54              |
| 22:LQ:69:LYS:O     | 22:LQ:75:ARG:NH1   | 2.40                     | 0.54              |
| 49:S2:1255:G:O2'   | 70:SU:70:CYS:SG    | 2.64                     | 0.54              |
| 49:S2:1416:C:O2    | 69:ST:3:GLY:N      | 2.40                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:SB:67:PHE:HB3   | 64:SO:48:SER:HA    | 1.90                     | 0.54              |
| 4:L5:1594:C:HO2'   | 4:L5:1597:G:HO2'   | 1.52                     | 0.54              |
| 20:LO:9:LEU:HD23   | 20:LO:118:MET:HB2  | 1.90                     | 0.54              |
| 31:LZ:26:VAL:O     | 31:LZ:93:LYS:NZ    | 2.37                     | 0.54              |
| 49:S2:65:C:N4      | 56:SG:133:LEU:O    | 2.39                     | 0.54              |
| 49:S2:1536:G:O6    | 49:S2:1597:C:N4    | 2.41                     | 0.54              |
| 49:S2:1607:A:N1    | 49:S2:1632:G:O2'   | 2.38                     | 0.54              |
| 72:SW:49:GLU:O     | 72:SW:64:ASN:ND2   | 2.40                     | 0.54              |
| 4:L5:3697:U:H5''   | 4:L5:3698:G:H5'    | 1.89                     | 0.54              |
| 49:S2:223:C:H2'    | 49:S2:224:A:H8     | 1.71                     | 0.54              |
| 54:SE:204:SER:OG   | 54:SE:205:PHE:N    | 2.40                     | 0.54              |
| 60:SK:13:GLU:O     | 60:SK:17:LYS:N     | 2.38                     | 0.54              |
| 4:L5:188:G:N2      | 4:L5:191:G:O6      | 2.38                     | 0.54              |
| 4:L5:496:G:O6      | 4:L5:497:G:N2      | 2.40                     | 0.54              |
| 4:L5:517:C:N4      | 4:L5:646:G:O2'     | 2.41                     | 0.54              |
| 4:L5:1479:G:H21    | 17:LL:184:MET:HE2  | 1.73                     | 0.54              |
| 4:L5:1555:G:N7     | 47:Lp:4:ARG:NH2    | 2.48                     | 0.54              |
| 4:L5:3756:A:N6     | 4:L5:3757:G:O6     | 2.41                     | 0.54              |
| 57:SH:36:LEU:HD21  | 57:SH:40:LEU:H     | 1.72                     | 0.54              |
| 4:L5:667:A:N3      | 48:Lr:46:ARG:NH1   | 2.55                     | 0.54              |
| 14:LH:23:ARG:NH2   | 14:LH:41:ILE:O     | 2.40                     | 0.54              |
| 50:SA:158:ASP:OD1  | 71:SV:60:ARG:NH1   | 2.40                     | 0.54              |
| 52:SC:81:ILE:HA    | 52:SC:86:LEU:HD12  | 1.90                     | 0.54              |
| 4:L5:1355:G:OP1    | 22:LQ:108:ARG:NH2  | 2.41                     | 0.54              |
| 4:L5:2083:C:OP2    | 22:LQ:14:ARG:NH1   | 2.41                     | 0.54              |
| 4:L5:4093:G:OP2    | 4:L5:4093:G:N2     | 2.36                     | 0.54              |
| 4:L5:5001:U:H4'    | 8:LB:317:LEU:HB3   | 1.89                     | 0.54              |
| 19:LN:115:VAL:HG11 | 19:LN:160:GLU:HB3  | 1.90                     | 0.54              |
| 23:LR:166:THR:HG21 | 49:S2:873:G:H5'    | 1.90                     | 0.54              |
| 48:Lr:26:SER:OG    | 48:Lr:31:ASN:ND2   | 2.41                     | 0.54              |
| 49:S2:588:G:OP2    | 49:S2:588:G:N2     | 2.34                     | 0.54              |
| 55:SF:187:SER:OG   | 55:SF:188:TYR:N    | 2.38                     | 0.54              |
| 58:SI:139:LYS:HD2  | 58:SI:146:GLN:HB2  | 1.90                     | 0.54              |
| 8:LB:10:ARG:NH2    | 8:LB:12:GLY:O      | 2.40                     | 0.54              |
| 22:LQ:157:GLY:O    | 22:LQ:188:ASN:ND2  | 2.40                     | 0.54              |
| 46:Lo:78:ARG:O     | 46:Lo:80:LYS:NZ    | 2.39                     | 0.54              |
| 49:S2:570:C:H4'    | 74:SY:36:PRO:HG3   | 1.90                     | 0.54              |
| 49:S2:640:A:OP2    | 80:Se:110:GLN:NE2  | 2.41                     | 0.54              |
| 49:S2:1749:G:H1    | 49:S2:1785:C:H42   | 1.56                     | 0.54              |
| 52:SC:213:LEU:HD23 | 52:SC:240:THR:HG23 | 1.90                     | 0.54              |
| 60:SK:83:LEU:HB3   | 60:SK:85:LEU:HD13  | 1.90                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 68:SS:101:ASN:O   | 68:SS:105:ASN:ND2  | 2.40                     | 0.54              |
| 4:L5:1637:A:OP1   | 4:L5:1640:C:N4     | 2.35                     | 0.54              |
| 4:L5:5062:G:H2'   | 4:L5:5063:G:H8     | 1.73                     | 0.54              |
| 30:LY:85:VAL:HG11 | 30:LY:99:ILE:HD11  | 1.89                     | 0.54              |
| 42:Lk:28:ASN:N    | 42:Lk:28:ASN:OD1   | 2.40                     | 0.54              |
| 49:S2:1121:G:N2   | 51:SB:202:GLN:O    | 2.39                     | 0.54              |
| 51:SB:226:GLY:O   | 51:SB:230:GLU:N    | 2.41                     | 0.54              |
| 55:SF:44:LYS:NZ   | 66:SQ:114:GLN:O    | 2.41                     | 0.54              |
| 68:SS:24:ARG:HB2  | 68:SS:29:ALA:HB2   | 1.90                     | 0.54              |
| 10:LD:155:THR:OG1 | 10:LD:179:ARG:NH2  | 2.41                     | 0.53              |
| 67:SR:7:LYS:HA    | 67:SR:10:LYS:HB2   | 1.90                     | 0.53              |
| 4:L5:3660:C:OP1   | 7:LA:241:ARG:NH2   | 2.41                     | 0.53              |
| 5:L7:27:G:OP1     | 16:LJ:146:ARG:NH1  | 2.41                     | 0.53              |
| 8:LB:350:SER:OG   | 8:LB:352:LEU:O     | 2.26                     | 0.53              |
| 19:LN:17:ASP:N    | 19:LN:17:ASP:OD1   | 2.40                     | 0.53              |
| 19:LN:120:TRP:HE1 | 19:LN:123:GLU:HG3  | 1.71                     | 0.53              |
| 44:Lm:110:CYS:SG  | 44:Lm:111:ARG:N    | 2.81                     | 0.53              |
| 49:S2:4:C:O2      | 59:SJ:18:ARG:NH1   | 2.41                     | 0.53              |
| 50:SA:207:PRO:HA  | 50:SA:210:ILE:HG12 | 1.89                     | 0.53              |
| 74:SY:91:LEU:HD22 | 74:SY:96:LEU:HD11  | 1.90                     | 0.53              |
| 4:L5:736:C:OP1    | 18:LM:74:ARG:NH1   | 2.41                     | 0.53              |
| 4:L5:1687:U:OP2   | 33:Lb:19:ASN:ND2   | 2.40                     | 0.53              |
| 11:LE:287:VAL:H   | 18:LM:109:ARG:HH12 | 1.55                     | 0.53              |
| 42:Lk:35:LYS:HG2  | 42:Lk:44:THR:HG22  | 1.90                     | 0.53              |
| 49:S2:1264:C:H4'  | 49:S2:1265:A:H5'   | 1.89                     | 0.53              |
| 56:SG:42:GLY:O    | 56:SG:46:LYS:NZ    | 2.42                     | 0.53              |
| 58:SI:177:SER:OG  | 58:SI:182:CYS:SG   | 2.66                     | 0.53              |
| 63:SN:99:ARG:NH1  | 63:SN:143:SER:OG   | 2.41                     | 0.53              |
| 82:Sg:114:SER:O   | 82:Sg:117:ASN:ND2  | 2.41                     | 0.53              |
| 4:L5:2582:A:HO2'  | 4:L5:2653:C:HO2'   | 1.56                     | 0.53              |
| 4:L5:3598:C:H2'   | 4:L5:3599:A:H8     | 1.74                     | 0.53              |
| 4:L5:4293:U:O2'   | 46:Lo:81:ARG:NH2   | 2.41                     | 0.53              |
| 9:LC:293:LEU:O    | 9:LC:299:GLN:NE2   | 2.41                     | 0.53              |
| 79:Sd:21:CYS:SG   | 79:Sd:22:ARG:N     | 2.81                     | 0.53              |
| 82:Sg:124:SER:OG  | 82:Sg:128:THR:OG1  | 2.25                     | 0.53              |
| 4:L5:382:G:N1     | 4:L5:385:A:OP2     | 2.39                     | 0.53              |
| 4:L5:4748:U:OP1   | 37:Lf:54:LYS:NZ    | 2.41                     | 0.53              |
| 49:S2:919:A:OP2   | 63:SN:64:ARG:NH2   | 2.42                     | 0.53              |
| 49:S2:1378:A:OP2  | 50:SA:102:ARG:NH2  | 2.41                     | 0.53              |
| 49:S2:1752:C:OP2  | 49:S2:1753:C:N4    | 2.41                     | 0.53              |
| 4:L5:5024:C:OP1   | 58:SI:124:LYS:NZ   | 2.39                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 30:LY:54:GLU:HB3  | 30:LY:108:ARG:HB2  | 1.89                     | 0.53              |
| 69:ST:110:LEU:HB2 | 69:ST:112:MET:HG2  | 1.90                     | 0.53              |
| 81:Sf:118:ARG:HD3 | 81:Sf:134:SER:HB3  | 1.91                     | 0.53              |
| 4:L5:706:C:HO2'   | 4:L5:1298:C:HO2'   | 1.56                     | 0.53              |
| 4:L5:1683:U:OP1   | 32:La:44:ASN:ND2   | 2.42                     | 0.53              |
| 4:L5:1785:C:OP1   | 15:LI:133:GLN:NE2  | 2.41                     | 0.53              |
| 4:L5:2479:G:H2'   | 4:L5:2480:G:H8     | 1.73                     | 0.53              |
| 10:LD:75:VAL:O    | 10:LD:112:ARG:NH1  | 2.41                     | 0.53              |
| 11:LE:101:ASN:OD1 | 11:LE:105:ARG:NH2  | 2.42                     | 0.53              |
| 15:LI:79:SER:OG   | 15:LI:147:HIS:ND1  | 2.41                     | 0.53              |
| 36:Le:99:ILE:HG21 | 36:Le:108:ARG:HG3  | 1.91                     | 0.53              |
| 41:Lj:20:ARG:NH1  | 41:Lj:39:TYR:OH    | 2.42                     | 0.53              |
| 49:S2:753:C:OP2   | 49:S2:791:C:O2'    | 2.26                     | 0.53              |
| 64:SO:99:ALA:H    | 64:SO:133:THR:HG22 | 1.73                     | 0.53              |
| 68:SS:7:GLU:HG3   | 68:SS:8:LYS:HD3    | 1.91                     | 0.53              |
| 49:S2:678:U:OP2   | 49:S2:1026:C:N4    | 2.40                     | 0.53              |
| 49:S2:943:U:O2'   | 64:SO:135:ILE:O    | 2.26                     | 0.53              |
| 82:Sg:122:SER:OG  | 82:Sg:132:TRP:NE1  | 2.42                     | 0.53              |
| 4:L5:970:G:H2'    | 11:LE:126:LEU:HD11 | 1.91                     | 0.53              |
| 4:L5:1364:U:OP2   | 17:LL:36:ARG:NH2   | 2.42                     | 0.53              |
| 4:L5:1375:C:OP1   | 9:LC:274:LYS:NZ    | 2.41                     | 0.53              |
| 4:L5:4507:A:HO2'  | 27:LV:41:SER:HG    | 1.55                     | 0.53              |
| 11:LE:216:TYR:O   | 11:LE:246:ARG:NH2  | 2.42                     | 0.53              |
| 16:LJ:10:ASN:OD1  | 16:LJ:10:ASN:N     | 2.41                     | 0.53              |
| 49:S2:922:A:OP1   | 72:SW:28:ARG:NH2   | 2.42                     | 0.53              |
| 4:L5:2382:A:N1    | 4:L5:2829:U:O2'    | 2.39                     | 0.53              |
| 4:L5:2743:A:O2'   | 7:LA:21:LYS:NZ     | 2.41                     | 0.53              |
| 16:LJ:119:TYR:HB3 | 68:SS:12:ILE:HG12  | 1.90                     | 0.53              |
| 21:LP:69:ARG:HA   | 21:LP:80:GLN:HA    | 1.90                     | 0.53              |
| 37:Lf:109:ARG:HG3 | 37:Lf:110:ILE:HD12 | 1.91                     | 0.53              |
| 43:LI:20:ASN:O    | 43:LI:41:ARG:NH1   | 2.42                     | 0.53              |
| 49:S2:748:C:H1'   | 49:S2:794:A:H61    | 1.74                     | 0.53              |
| 50:SA:63:ARG:HB3  | 71:SV:37:ALA:H     | 1.74                     | 0.53              |
| 82:Sg:219:TRP:HE1 | 82:Sg:226:HIS:CD2  | 2.27                     | 0.53              |
| 4:L5:305:A:OP2    | 19:LN:15:GLN:NE2   | 2.43                     | 0.52              |
| 4:L5:2633:U:OP1   | 23:LR:64:ARG:NH2   | 2.42                     | 0.52              |
| 37:Lf:33:VAL:HG23 | 37:Lf:38:GLU:HG3   | 1.91                     | 0.52              |
| 49:S2:1738:C:OP1  | 56:SG:92:ARG:NH1   | 2.39                     | 0.52              |
| 49:S2:1753:C:O2'  | 49:S2:1779:G:N2    | 2.42                     | 0.52              |
| 62:SM:33:ARG:N    | 62:SM:37:GLU:OE2   | 2.41                     | 0.52              |
| 65:SP:53:GLN:HG3  | 65:SP:80:LEU:HD21  | 1.92                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 81:Sf:118:ARG:NH2  | 81:Sf:132:MET:O    | 2.43                     | 0.52              |
| 32:La:75:LEU:HD13  | 32:La:113:GLY:HA2  | 1.91                     | 0.52              |
| 24:LS:86:SER:OG    | 24:LS:87:ARG:N     | 2.42                     | 0.52              |
| 28:LW:113:LYS:HA   | 28:LW:116:LYS:HG2  | 1.91                     | 0.52              |
| 49:S2:387:C:OP2    | 58:SI:10:LYS:NZ    | 2.42                     | 0.52              |
| 55:SF:70:GLU:O     | 55:SF:74:ASN:ND2   | 2.41                     | 0.52              |
| 20:LO:130:LYS:HB2  | 20:LO:133:ARG:HG2  | 1.90                     | 0.52              |
| 29:LX:119:ILE:HG21 | 29:LX:140:LEU:HD22 | 1.91                     | 0.52              |
| 49:S2:554:A:N7     | 49:S2:555:A:N6     | 2.57                     | 0.52              |
| 49:S2:744:G:N2     | 57:SH:105:THR:O    | 2.41                     | 0.52              |
| 56:SG:8:PRO:O      | 56:SG:131:ARG:NH1  | 2.42                     | 0.52              |
| 57:SH:21:SER:O     | 57:SH:24:SER:OG    | 2.25                     | 0.52              |
| 59:SJ:28:GLU:HB2   | 59:SJ:43:VAL:HG21  | 1.91                     | 0.52              |
| 59:SJ:53:ILE:HG23  | 59:SJ:77:LEU:HD11  | 1.91                     | 0.52              |
| 64:SO:44:VAL:HG22  | 64:SO:53:ILE:HD12  | 1.91                     | 0.52              |
| 82:Sg:2:THR:HA     | 82:Sg:314:ILE:HB   | 1.91                     | 0.52              |
| 4:L5:1378:C:N4     | 17:LL:159:ASN:O    | 2.43                     | 0.52              |
| 4:L5:5006:U:H4'    | 4:L5:5007:A:H5'    | 1.91                     | 0.52              |
| 9:LC:94:ASN:HD22   | 9:LC:102:PHE:HB2   | 1.75                     | 0.52              |
| 49:S2:142:C:OP2    | 56:SG:188:LYS:NZ   | 2.43                     | 0.52              |
| 49:S2:446:G:OP2    | 58:SI:47:ARG:NH2   | 2.38                     | 0.52              |
| 49:S2:1452:A:O2'   | 49:S2:1475:G:N2    | 2.42                     | 0.52              |
| 51:SB:65:ARG:HH12  | 64:SO:51:GLU:HG2   | 1.74                     | 0.52              |
| 82:Sg:120:ILE:HB   | 82:Sg:132:TRP:HB2  | 1.90                     | 0.52              |
| 4:L5:310:G:H5''    | 40:Li:85:ARG:HH12  | 1.75                     | 0.52              |
| 4:L5:4985:U:O5'    | 8:LB:175:GLN:NE2   | 2.43                     | 0.52              |
| 6:L8:55:U:H3       | 6:L8:62:A:H2       | 1.57                     | 0.52              |
| 9:LC:292:ILE:HG23  | 22:LQ:128:LEU:HD13 | 1.91                     | 0.52              |
| 11:LE:101:ASN:O    | 11:LE:105:ARG:NH1  | 2.42                     | 0.52              |
| 19:LN:143:ARG:NH2  | 39:Lh:93:ARG:O     | 2.43                     | 0.52              |
| 23:LR:38:ARG:HA    | 23:LR:41:ILE:HG22  | 1.91                     | 0.52              |
| 49:S2:827:A:OP1    | 59:SJ:10:ARG:NH1   | 2.42                     | 0.52              |
| 49:S2:838:G:N2     | 49:S2:840:C:O2'    | 2.42                     | 0.52              |
| 74:SY:41:ARG:NH2   | 74:SY:52:PRO:O     | 2.42                     | 0.52              |
| 8:LB:36:ASP:N      | 8:LB:36:ASP:OD1    | 2.42                     | 0.52              |
| 41:Lj:33:THR:HA    | 41:Lj:40:PRO:HD3   | 1.92                     | 0.52              |
| 46:Lo:74:GLU:O     | 46:Lo:78:ARG:NH2   | 2.43                     | 0.52              |
| 4:L5:2378:G:N2     | 4:L5:2381:A:OP2    | 2.42                     | 0.52              |
| 4:L5:3654:G:O2'    | 4:L5:3693:U:OP1    | 2.25                     | 0.52              |
| 4:L5:3717:A:OP2    | 4:L5:3735:G:N2     | 2.43                     | 0.52              |
| 10:LD:286:SER:HA   | 10:LD:289:ARG:HD2  | 1.92                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:LO:22:ILE:HG21  | 20:LO:120:VAL:HG11 | 1.92                     | 0.52              |
| 48:Lr:39:ARG:O     | 48:Lr:103:ARG:NH2  | 2.42                     | 0.52              |
| 49:S2:207:G:H3'    | 49:S2:208:G:H8     | 1.74                     | 0.52              |
| 49:S2:1201:U:HO2'  | 49:S2:1358:U:HO2'  | 1.52                     | 0.52              |
| 49:S2:1660:C:H3'   | 79:Sd:32:ARG:HH22  | 1.73                     | 0.52              |
| 81:Sf:133:ALA:N    | 81:Sf:140:TYR:O    | 2.37                     | 0.52              |
| 82:Sg:304:ASP:OD1  | 82:Sg:304:ASP:N    | 2.43                     | 0.52              |
| 4:L5:224:U:OP1     | 9:LC:163:LYS:NZ    | 2.43                     | 0.52              |
| 4:L5:2005:G:N3     | 4:L5:2016:C:N4     | 2.57                     | 0.52              |
| 4:L5:2461:G:O3'    | 19:LN:108:ARG:NH1  | 2.43                     | 0.52              |
| 4:L5:2847:G:OP1    | 27:LV:85:ARG:NH1   | 2.42                     | 0.52              |
| 9:LC:296:PRO:O     | 9:LC:300:ARG:NH1   | 2.43                     | 0.52              |
| 18:LM:41:PRO:HB3   | 18:LM:70:GLN:HG2   | 1.90                     | 0.52              |
| 30:LY:50:ARG:NH1   | 30:LY:52:ASP:OD1   | 2.43                     | 0.52              |
| 31:LZ:119:GLU:O    | 31:LZ:123:LYS:NZ   | 2.41                     | 0.52              |
| 40:Li:62:LYS:HB3   | 40:Li:94:LEU:HD21  | 1.91                     | 0.52              |
| 51:SB:146:ARG:HB2  | 51:SB:149:GLN:HB2  | 1.91                     | 0.52              |
| 4:L5:86:U:OP1      | 22:LQ:168:ARG:NH1  | 2.42                     | 0.52              |
| 4:L5:1655:C:HO2'   | 4:L5:4391:G:HO2'   | 1.58                     | 0.52              |
| 4:L5:3938:G:N2     | 4:L5:4171:C:OP2    | 2.43                     | 0.52              |
| 4:L5:4674:C:O2'    | 8:LB:282:LYS:NZ    | 2.43                     | 0.52              |
| 6:L8:23:C:OP2      | 30:LY:15:ARG:NE    | 2.38                     | 0.52              |
| 28:LW:74:ARG:NH2   | 49:S2:1749:G:N7    | 2.52                     | 0.52              |
| 31:LZ:100:VAL:HG21 | 31:LZ:110:ALA:HB2  | 1.91                     | 0.52              |
| 49:S2:538:U:H1'    | 49:S2:544:G:H1     | 1.75                     | 0.52              |
| 49:S2:816:A:OP2    | 59:SJ:10:ARG:NH2   | 2.33                     | 0.52              |
| 49:S2:1110:G:H1'   | 67:SR:122:PRO:HB3  | 1.92                     | 0.52              |
| 64:SO:95:ILE:HD12  | 64:SO:116:LEU:HD11 | 1.92                     | 0.52              |
| 4:L5:308:G:OP2     | 4:L5:308:G:N2      | 2.37                     | 0.51              |
| 4:L5:2891:U:HO2'   | 4:L5:5017:G:HO2'   | 1.56                     | 0.51              |
| 11:LE:273:SER:OG   | 11:LE:274:VAL:N    | 2.43                     | 0.51              |
| 22:LQ:86:ILE:HG13  | 22:LQ:105:VAL:HG13 | 1.92                     | 0.51              |
| 29:LX:100:VAL:HG21 | 29:LX:109:ILE:HD11 | 1.92                     | 0.51              |
| 49:S2:377:G:H5'    | 58:SI:98:LYS:HB3   | 1.92                     | 0.51              |
| 49:S2:570:C:O2     | 74:SY:34:THR:OG1   | 2.28                     | 0.51              |
| 57:SH:79:LEU:HD23  | 57:SH:83:LEU:HD22  | 1.92                     | 0.51              |
| 82:Sg:116:ASP:OD1  | 82:Sg:116:ASP:N    | 2.43                     | 0.51              |
| 4:L5:1968:G:OP2    | 4:L5:1970:A:N6     | 2.43                     | 0.51              |
| 4:L5:4604:G:OP1    | 14:LH:174:LYS:NZ   | 2.43                     | 0.51              |
| 4:L5:4870:G:OP2    | 18:LM:5:ARG:NH2    | 2.42                     | 0.51              |
| 24:LS:85:ASP:HA    | 24:LS:90:THR:HA    | 1.92                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:LZ:17:ARG:NH2  | 31:LZ:18:TYR:OH    | 2.43                     | 0.51              |
| 34:Lc:48:LEU:HD21 | 34:Lc:60:ILE:HG21  | 1.92                     | 0.51              |
| 49:S2:380:G:N1    | 49:S2:383:G:OP2    | 2.39                     | 0.51              |
| 51:SB:136:ARG:HB2 | 51:SB:218:LEU:HD11 | 1.91                     | 0.51              |
| 75:SZ:48:VAL:HG23 | 75:SZ:80:ARG:HD2   | 1.92                     | 0.51              |
| 79:Sd:49:ASP:N    | 79:Sd:49:ASP:OD1   | 2.43                     | 0.51              |
| 2:B4:51:U:H3      | 2:B4:63:G:H22      | 1.57                     | 0.51              |
| 4:L5:969:C:H1'    | 11:LE:123:ARG:HD3  | 1.91                     | 0.51              |
| 4:L5:1269:G:H1'   | 4:L5:2109:G:H2'    | 1.91                     | 0.51              |
| 19:LN:63:ARG:HG2  | 19:LN:131:GLU:HG2  | 1.91                     | 0.51              |
| 28:LW:42:SER:OG   | 28:LW:44:ARG:NH1   | 2.43                     | 0.51              |
| 49:S2:1169:G:N2   | 49:S2:1189:A:N7    | 2.59                     | 0.51              |
| 49:S2:1396:A:O2'  | 49:S2:1398:G:N7    | 2.43                     | 0.51              |
| 55:SF:168:THR:OG1 | 75:SZ:106:GLN:NE2  | 2.43                     | 0.51              |
| 61:SL:77:VAL:HG13 | 61:SL:123:GLY:H    | 1.75                     | 0.51              |
| 62:SM:56:CYS:SG   | 62:SM:57:ASP:N     | 2.80                     | 0.51              |
| 4:L5:230:G:OP1    | 30:LY:15:ARG:NH1   | 2.43                     | 0.51              |
| 4:L5:264:C:N3     | 4:L5:265:C:N4      | 2.59                     | 0.51              |
| 12:LF:83:VAL:HG12 | 24:LS:62:VAL:HA    | 1.92                     | 0.51              |
| 15:LI:99:ILE:HB   | 15:LI:123:GLN:HE21 | 1.75                     | 0.51              |
| 16:LJ:120:ASP:N   | 16:LJ:120:ASP:OD1  | 2.42                     | 0.51              |
| 27:LV:35:LYS:NZ   | 49:S2:1803:U:OP1   | 2.44                     | 0.51              |
| 52:SC:134:ASN:O   | 52:SC:167:ARG:NH2  | 2.44                     | 0.51              |
| 52:SC:271:ASP:OD1 | 52:SC:271:ASP:N    | 2.43                     | 0.51              |
| 68:SS:5:ILE:HG22  | 75:SZ:49:LEU:HD21  | 1.93                     | 0.51              |
| 2:D4:18:G:H3'     | 2:D4:57:G:H22      | 1.75                     | 0.51              |
| 4:L5:953:C:OP1    | 37:Lf:73:LYS:NZ    | 2.42                     | 0.51              |
| 4:L5:2583:C:OP2   | 38:Lg:76:ARG:NH2   | 2.41                     | 0.51              |
| 35:Ld:114:PHE:HA  | 35:Ld:117:LEU:HD12 | 1.93                     | 0.51              |
| 49:S2:122:G:H21   | 54:SE:146:THR:HG21 | 1.75                     | 0.51              |
| 49:S2:375:U:OP2   | 61:SL:59:LYS:NZ    | 2.44                     | 0.51              |
| 49:S2:1781:A:O2'  | 49:S2:1782:G:N7    | 2.44                     | 0.51              |
| 50:SA:206:ASP:HB3 | 50:SA:208:GLU:HG2  | 1.92                     | 0.51              |
| 64:SO:94:HIS:ND1  | 64:SO:127:GLY:O    | 2.43                     | 0.51              |
| 4:L5:97:G:OP1     | 17:LL:16:LYS:NZ    | 2.44                     | 0.51              |
| 4:L5:2088:A:OP2   | 22:LQ:37:ARG:NH1   | 2.44                     | 0.51              |
| 4:L5:2503:G:O2'   | 4:L5:2505:C:O2     | 2.28                     | 0.51              |
| 15:LI:52:MET:HE2  | 15:LI:136:MET:HG2  | 1.93                     | 0.51              |
| 28:LW:104:GLN:O   | 28:LW:107:GLN:NE2  | 2.40                     | 0.51              |
| 41:Lj:2:THR:OG1   | 41:Lj:3:LYS:N      | 2.41                     | 0.51              |
| 41:Lj:2:THR:HG23  | 41:Lj:4:GLY:H      | 1.75                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:S2:355:G:OP1    | 61:SL:105:ARG:NH2  | 2.40                     | 0.51              |
| 49:S2:441:C:OP2    | 58:SI:2:GLY:N      | 2.43                     | 0.51              |
| 62:SM:26:LEU:HD21  | 62:SM:33:ARG:HH22  | 1.76                     | 0.51              |
| 67:SR:124:VAL:HG22 | 67:SR:127:ASN:HD21 | 1.76                     | 0.51              |
| 4:L5:690:C:OP2     | 11:LE:111:LYS:NZ   | 2.43                     | 0.51              |
| 4:L5:2006:U:O2'    | 4:L5:2012:A:N6     | 2.44                     | 0.51              |
| 4:L5:4691:A:O2'    | 14:LH:68:ALA:O     | 2.29                     | 0.51              |
| 20:LO:190:ASP:OD1  | 20:LO:190:ASP:N    | 2.43                     | 0.51              |
| 49:S2:126:G:OP2    | 56:SG:195:LYS:NZ   | 2.43                     | 0.51              |
| 49:S2:1455:A:N1    | 49:S2:1476:A:N6    | 2.58                     | 0.51              |
| 49:S2:1619:A:OP2   | 65:SP:47:ARG:NH2   | 2.44                     | 0.51              |
| 56:SG:45:TRP:O     | 56:SG:46:LYS:NZ    | 2.40                     | 0.51              |
| 82:Sg:119:GLN:NE2  | 82:Sg:132:TRP:O    | 2.44                     | 0.51              |
| 4:L5:4095:G:H22    | 4:L5:4114:C:H1'    | 1.75                     | 0.51              |
| 23:LR:37:SER:OG    | 23:LR:38:ARG:O     | 2.29                     | 0.51              |
| 39:Lh:4:ILE:HD11   | 39:Lh:8:ASP:HB2    | 1.92                     | 0.51              |
| 56:SG:44:GLU:OE2   | 56:SG:119:LYS:NZ   | 2.32                     | 0.51              |
| 66:SQ:53:GLU:HB2   | 66:SQ:85:ARG:HD3   | 1.93                     | 0.51              |
| 69:ST:40:ALA:HB3   | 69:ST:43:LYS:HG2   | 1.91                     | 0.51              |
| 4:L5:989:U:O2'     | 4:L5:990:C:O4'     | 2.28                     | 0.51              |
| 4:L5:2613:C:OP1    | 38:Lg:24:ARG:NH2   | 2.44                     | 0.51              |
| 4:L5:2622:G:O6     | 26:LU:81:ARG:NH2   | 2.38                     | 0.51              |
| 4:L5:4419:U:OP1    | 4:L5:4475:G:N2     | 2.44                     | 0.51              |
| 18:LM:96:GLU:HA    | 18:LM:99:GLU:HB3   | 1.93                     | 0.51              |
| 49:S2:603:C:N4     | 49:S2:620:G:O6     | 2.44                     | 0.51              |
| 49:S2:962:A:N1     | 49:S2:1055:A:O2'   | 2.43                     | 0.51              |
| 56:SG:228:ILE:HA   | 56:SG:231:ARG:HB2  | 1.93                     | 0.51              |
| 67:SR:28:PHE:HA    | 67:SR:55:THR:HG21  | 1.92                     | 0.51              |
| 82:Sg:152:SER:H    | 82:Sg:169:GLY:HA2  | 1.74                     | 0.51              |
| 4:L5:1971:C:OP2    | 4:L5:2005:G:N2     | 2.44                     | 0.51              |
| 4:L5:2527:A:OP2    | 23:LR:38:ARG:NH2   | 2.43                     | 0.51              |
| 50:SA:33:GLN:NE2   | 71:SV:64:GLU:OE1   | 2.43                     | 0.51              |
| 62:SM:33:ARG:HA    | 62:SM:109:VAL:HG12 | 1.92                     | 0.51              |
| 82:Sg:238:ALA:HB3  | 82:Sg:251:ALA:HB3  | 1.92                     | 0.51              |
| 2:D4:18:G:N2       | 2:D4:58:A:O4'      | 2.44                     | 0.50              |
| 4:L5:1172:C:O2'    | 4:L5:1189:G:N2     | 2.43                     | 0.50              |
| 4:L5:1500:A:H5''   | 4:L5:1501:C:H5''   | 1.92                     | 0.50              |
| 10:LD:19:LYS:O     | 10:LD:24:ARG:NH2   | 2.44                     | 0.50              |
| 23:LR:157:ASP:O    | 23:LR:161:ALA:N    | 2.43                     | 0.50              |
| 49:S2:67:C:N4      | 56:SG:168:LYS:O    | 2.36                     | 0.50              |
| 49:S2:1758:G:O2'   | 49:S2:1775:U:N3    | 2.44                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:SH:8:ILE:HD12   | 57:SH:28:LEU:HD13  | 1.92                     | 0.50              |
| 62:SM:40:LYS:O     | 62:SM:44:LYS:NZ    | 2.36                     | 0.50              |
| 4:L5:151:G:OP2     | 19:LN:4:TYR:OH     | 2.25                     | 0.50              |
| 4:L5:1969:G:O2'    | 4:L5:1999:A:N6     | 2.45                     | 0.50              |
| 4:L5:3908:A:N7     | 4:L5:4449:A:N6     | 2.60                     | 0.50              |
| 31:LZ:33:THR:OG1   | 31:LZ:34:SER:N     | 2.44                     | 0.50              |
| 49:S2:1540:G:OP1   | 69:ST:43:LYS:NZ    | 2.38                     | 0.50              |
| 51:SB:129:THR:HG22 | 51:SB:133:TYR:H    | 1.76                     | 0.50              |
| 57:SH:144:ILE:HG12 | 57:SH:154:ILE:HG23 | 1.93                     | 0.50              |
| 59:SJ:142:VAL:HG12 | 59:SJ:144:ILE:H    | 1.75                     | 0.50              |
| 4:L5:2322:G:OP1    | 36:Le:36:ARG:NH1   | 2.41                     | 0.50              |
| 49:S2:1033:G:N1    | 49:S2:1080:A:O2'   | 2.38                     | 0.50              |
| 51:SB:103:MET:HG3  | 51:SB:215:VAL:HG22 | 1.93                     | 0.50              |
| 75:SZ:63:PRO:HG3   | 75:SZ:96:LEU:HD21  | 1.94                     | 0.50              |
| 82:Sg:206:LEU:HD11 | 82:Sg:227:LEU:HD22 | 1.93                     | 0.50              |
| 4:L5:1669:A:N3     | 4:L5:1852:U:O2'    | 2.44                     | 0.50              |
| 4:L5:1706:A:N6     | 4:L5:2118:G:O4'    | 2.44                     | 0.50              |
| 4:L5:2754:G:OP1    | 31:LZ:135:ARG:NH1  | 2.44                     | 0.50              |
| 4:L5:3653:A:N6     | 4:L5:3691:G:O2'    | 2.38                     | 0.50              |
| 4:L5:3689:G:O2'    | 4:L5:3818:U:OP2    | 2.29                     | 0.50              |
| 47:Lp:3:LYS:HG3    | 47:Lp:4:ARG:HG3    | 1.93                     | 0.50              |
| 49:S2:289:G:OP1    | 54:SE:155:LYS:NZ   | 2.44                     | 0.50              |
| 49:S2:1304:U:H5'   | 81:Sf:93:HIS:HB2   | 1.94                     | 0.50              |
| 49:S2:1593:C:OP2   | 75:SZ:104:ARG:NH2  | 2.44                     | 0.50              |
| 63:SN:40:LEU:HD23  | 63:SN:43:LYS:HD2   | 1.92                     | 0.50              |
| 66:SQ:96:TYR:HA    | 66:SQ:100:VAL:HG12 | 1.93                     | 0.50              |
| 82:Sg:203:ASP:OD1  | 82:Sg:203:ASP:N    | 2.44                     | 0.50              |
| 4:L5:74:G:H5'      | 17:LL:59:VAL:HG13  | 1.92                     | 0.50              |
| 4:L5:513:U:O2'     | 4:L5:647:G:N2      | 2.44                     | 0.50              |
| 4:L5:2705:G:H22    | 4:L5:2710:C:H5     | 1.57                     | 0.50              |
| 18:LM:11:ARG:NH2   | 18:LM:58:THR:O     | 2.41                     | 0.50              |
| 66:SQ:32:ILE:HD12  | 66:SQ:68:ILE:HB    | 1.93                     | 0.50              |
| 82:Sg:162:ASN:OD1  | 82:Sg:162:ASN:N    | 2.43                     | 0.50              |
| 4:L5:518:G:N1      | 4:L5:644:G:OP2     | 2.45                     | 0.50              |
| 4:L5:2362:U:OP1    | 21:LP:82:ARG:NH2   | 2.44                     | 0.50              |
| 4:L5:5040:U:OP2    | 8:LB:396:ARG:NH2   | 2.43                     | 0.50              |
| 11:LE:278:THR:OG1  | 11:LE:279:ASN:N    | 2.44                     | 0.50              |
| 12:LF:115:ARG:NH1  | 22:LQ:4:ASP:O      | 2.45                     | 0.50              |
| 49:S2:954:U:O2'    | 64:SO:55:ARG:NH2   | 2.44                     | 0.50              |
| 4:L5:517:C:O2'     | 4:L5:644:G:O6      | 2.24                     | 0.50              |
| 4:L5:1676:C:O2'    | 4:L5:3914:U:N3     | 2.43                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:L5:2416:G:N2    | 4:L5:2426:U:O4     | 2.45                     | 0.50              |
| 4:L5:4084:G:O6    | 7:LA:72:ARG:NH2    | 2.45                     | 0.50              |
| 4:L5:5063:G:O6    | 8:LB:124:LYS:NZ    | 2.43                     | 0.50              |
| 4:L5:5063:G:H2'   | 4:L5:5064:G:H8     | 1.74                     | 0.50              |
| 11:LE:95:PRO:HA   | 11:LE:104:THR:HG23 | 1.93                     | 0.50              |
| 15:LI:31:ILE:HD12 | 15:LI:65:LEU:HB3   | 1.93                     | 0.50              |
| 35:Ld:24:GLU:HG2  | 35:Ld:85:ARG:HD2   | 1.93                     | 0.50              |
| 49:S2:1236:G:O2'  | 65:SP:131:PRO:O    | 2.24                     | 0.50              |
| 49:S2:1416:C:N3   | 49:S2:1417:C:N4    | 2.60                     | 0.50              |
| 51:SB:26:SER:O    | 51:SB:51:ARG:NH1   | 2.44                     | 0.50              |
| 51:SB:152:LYS:HE3 | 67:SR:131:PRO:HG2  | 1.94                     | 0.50              |
| 63:SN:56:ASP:OD2  | 63:SN:57:SER:N     | 2.44                     | 0.50              |
| 69:ST:85:ASN:HB3  | 69:ST:88:MET:HB2   | 1.94                     | 0.50              |
| 4:L5:1629:G:N1    | 7:LA:208:GLU:OE1   | 2.36                     | 0.50              |
| 4:L5:5000:G:OP1   | 8:LB:394:LYS:NZ    | 2.43                     | 0.50              |
| 13:LG:160:ASP:OD1 | 13:LG:160:ASP:N    | 2.44                     | 0.50              |
| 49:S2:1065:G:OP1  | 64:SO:149:ARG:NH1  | 2.45                     | 0.50              |
| 49:S2:1614:A:OP2  | 65:SP:42:ARG:NH1   | 2.34                     | 0.50              |
| 64:SO:36:SER:OG   | 64:SO:37:PHE:N     | 2.45                     | 0.50              |
| 4:L5:1516:G:O2'   | 17:LL:18:TRP:NE1   | 2.37                     | 0.50              |
| 4:L5:4728:U:OP1   | 8:LB:132:LYS:NZ    | 2.44                     | 0.50              |
| 10:LD:33:ARG:NH1  | 10:LD:72:ASP:OD1   | 2.45                     | 0.50              |
| 36:Le:89:LEU:HD13 | 36:Le:118:LEU:HD22 | 1.93                     | 0.50              |
| 55:SF:142:SER:OG  | 78:Sc:49:PRO:O     | 2.30                     | 0.50              |
| 77:Sb:36:LYS:HG2  | 77:Sb:43:ILE:HD13  | 1.93                     | 0.50              |
| 79:Sd:22:ARG:NE   | 79:Sd:36:LEU:O     | 2.40                     | 0.50              |
| 4:L5:2326:G:OP1   | 36:Le:108:ARG:NH1  | 2.45                     | 0.49              |
| 4:L5:2708:U:O3'   | 23:LR:43:LYS:NZ    | 2.43                     | 0.49              |
| 4:L5:3720:G:OP1   | 40:Li:75:LYS:NZ    | 2.45                     | 0.49              |
| 49:S2:345:U:O2    | 54:SE:33:THR:OG1   | 2.28                     | 0.49              |
| 49:S2:1712:A:N6   | 49:S2:1820:G:O6    | 2.45                     | 0.49              |
| 49:S2:1752:C:H2'  | 49:S2:1780:G:H22   | 1.77                     | 0.49              |
| 51:SB:129:THR:OG1 | 51:SB:179:ASN:O    | 2.29                     | 0.49              |
| 71:SV:42:VAL:HG23 | 71:SV:43:THR:HG23  | 1.93                     | 0.49              |
| 4:L5:499:G:N3     | 4:L5:504:G:N2      | 2.61                     | 0.49              |
| 4:L5:1571:G:H4'   | 23:LR:130:ASN:HD22 | 1.77                     | 0.49              |
| 4:L5:4489:G:N2    | 4:L5:4592:C:OP1    | 2.44                     | 0.49              |
| 6:L8:14:U:H5''    | 21:LP:123:PRO:HD3  | 1.95                     | 0.49              |
| 9:LC:205:ARG:HB3  | 9:LC:248:ARG:HH12  | 1.76                     | 0.49              |
| 13:LG:131:LYS:NZ  | 13:LG:132:ARG:O    | 2.45                     | 0.49              |
| 15:LI:61:SER:OG   | 15:LI:63:GLU:OE1   | 2.30                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 20:LO:186:GLU:HA  | 20:LO:189:ILE:HG22 | 1.93                     | 0.49              |
| 56:SG:126:ASP:OD1 | 56:SG:126:ASP:N    | 2.41                     | 0.49              |
| 72:SW:65:LEU:HD12 | 72:SW:67:GLY:H     | 1.76                     | 0.49              |
| 82:Sg:237:ASN:N   | 82:Sg:237:ASN:OD1  | 2.42                     | 0.49              |
| 24:LS:147:ASP:HB3 | 24:LS:150:ILE:HB   | 1.92                     | 0.49              |
| 31:LZ:78:ASN:OD1  | 34:Lc:39:ARG:NH1   | 2.45                     | 0.49              |
| 35:Ld:24:GLU:HG2  | 35:Ld:85:ARG:HH11  | 1.77                     | 0.49              |
| 55:SF:26:ASP:N    | 55:SF:26:ASP:OD1   | 2.44                     | 0.49              |
| 62:SM:53:ALA:HA   | 62:SM:79:VAL:HG12  | 1.94                     | 0.49              |
| 77:Sb:14:GLU:HA   | 77:Sb:17:ARG:HB3   | 1.94                     | 0.49              |
| 4:L5:1704:C:O5'   | 12:LF:43:ARG:NH1   | 2.45                     | 0.49              |
| 4:L5:2845:A:H61   | 4:L5:3843:C:H42    | 1.61                     | 0.49              |
| 17:LL:58:ILE:HG12 | 17:LL:157:VAL:HG12 | 1.94                     | 0.49              |
| 42:Lk:40:ARG:NH1  | 42:Lk:41:TYR:OH    | 2.45                     | 0.49              |
| 49:S2:191:A:H5''  | 58:SI:140:LYS:HG3  | 1.95                     | 0.49              |
| 55:SF:35:LEU:HD12 | 55:SF:117:ILE:HD13 | 1.94                     | 0.49              |
| 55:SF:194:ASP:O   | 55:SF:198:ARG:N    | 2.42                     | 0.49              |
| 56:SG:136:LYS:HG3 | 56:SG:174:PRO:HB2  | 1.95                     | 0.49              |
| 69:ST:64:LEU:HD11 | 69:ST:121:ARG:HB2  | 1.93                     | 0.49              |
| 4:L5:46:U:H5''    | 17:LL:16:LYS:HG3   | 1.93                     | 0.49              |
| 4:L5:184:U:O2'    | 4:L5:189:G:O4'     | 2.29                     | 0.49              |
| 4:L5:3746:A:H5''  | 7:LA:244:GLY:HA3   | 1.94                     | 0.49              |
| 8:LB:92:TYR:HB2   | 8:LB:159:VAL:HB    | 1.93                     | 0.49              |
| 39:Lh:96:ASN:OD1  | 39:Lh:96:ASN:N     | 2.33                     | 0.49              |
| 67:SR:28:PHE:O    | 67:SR:32:LYS:N     | 2.46                     | 0.49              |
| 4:L5:290:U:O2'    | 19:LN:188:ARG:NH2  | 2.45                     | 0.49              |
| 4:L5:715:G:OP1    | 9:LC:321:ASN:ND2   | 2.45                     | 0.49              |
| 4:L5:2658:G:O6    | 34:Lc:32:LYS:NZ    | 2.42                     | 0.49              |
| 6:L8:2:G:H3'      | 6:L8:3:A:H8        | 1.77                     | 0.49              |
| 20:LO:115:LYS:O   | 20:LO:117:ARG:NH1  | 2.46                     | 0.49              |
| 49:S2:382:C:OP2   | 58:SI:54:LYS:NZ    | 2.45                     | 0.49              |
| 54:SE:176:ASP:O   | 54:SE:179:ASN:ND2  | 2.44                     | 0.49              |
| 2:B4:20:U:OP1     | 16:LJ:58:ARG:NH1   | 2.45                     | 0.49              |
| 4:L5:238:C:OP2    | 30:LY:45:ARG:NH2   | 2.44                     | 0.49              |
| 6:L8:95:A:N3      | 39:Lh:63:GLN:NE2   | 2.61                     | 0.49              |
| 16:LJ:96:LYS:O    | 16:LJ:159:LYS:NZ   | 2.45                     | 0.49              |
| 36:Le:92:ASN:ND2  | 36:Le:119:ALA:O    | 2.42                     | 0.49              |
| 78:Sc:8:PRO:O     | 78:Sc:10:LYS:NZ    | 2.37                     | 0.49              |
| 81:Sf:132:MET:HG2 | 81:Sf:141:CYS:HA   | 1.94                     | 0.49              |
| 8:LB:329:ASP:OD1  | 8:LB:329:ASP:N     | 2.39                     | 0.49              |
| 17:LL:65:ARG:HD2  | 17:LL:66:TYR:CZ    | 2.48                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:LR:99:MET:HE1   | 23:LR:128:LYS:HA   | 1.94                     | 0.49              |
| 46:Lo:71:GLU:HB3   | 46:Lo:80:LYS:HG2   | 1.94                     | 0.49              |
| 49:S2:556:U:N3     | 49:S2:559:G:N7     | 2.61                     | 0.49              |
| 49:S2:1402:A:H5'   | 70:SU:51:LYS:HD2   | 1.94                     | 0.49              |
| 68:SS:23:ARG:HB3   | 75:SZ:48:VAL:HG11  | 1.95                     | 0.49              |
| 82:Sg:256:ILE:HB   | 82:Sg:270:LEU:HB3  | 1.95                     | 0.49              |
| 2:B4:11:C:O2'      | 4:L5:3756:A:O2'    | 2.29                     | 0.49              |
| 4:L5:508:G:N3      | 32:La:85:GLN:NE2   | 2.53                     | 0.49              |
| 16:LJ:167:GLN:HE21 | 16:LJ:173:ILE:HA   | 1.78                     | 0.49              |
| 26:LU:98:ASP:OD1   | 26:LU:98:ASP:N     | 2.44                     | 0.49              |
| 37:Lf:50:VAL:HG12  | 37:Lf:69:VAL:HG12  | 1.93                     | 0.49              |
| 59:SJ:136:ARG:HD2  | 59:SJ:139:LYS:HA   | 1.95                     | 0.49              |
| 65:SP:51:ARG:O     | 65:SP:55:SER:N     | 2.46                     | 0.49              |
| 75:SZ:91:LEU:HD23  | 75:SZ:96:LEU:HD22  | 1.94                     | 0.49              |
| 76:Sa:3:LYS:NZ     | 76:Sa:5:ARG:O      | 2.46                     | 0.49              |
| 76:Sa:94:ASP:OD1   | 76:Sa:94:ASP:N     | 2.42                     | 0.49              |
| 82:Sg:21:ILE:HD11  | 82:Sg:31:ILE:HG13  | 1.95                     | 0.49              |
| 4:L5:1480:C:O2'    | 4:L5:1482:G:OP2    | 2.31                     | 0.49              |
| 4:L5:2693:G:OP2    | 42:Lk:33:LYS:NZ    | 2.46                     | 0.49              |
| 4:L5:4162:C:O2     | 13:LG:73:ARG:NH2   | 2.39                     | 0.49              |
| 4:L5:4541:G:N2     | 4:L5:4544:A:OP2    | 2.42                     | 0.49              |
| 22:LQ:16:LYS:O     | 22:LQ:33:ARG:NH2   | 2.46                     | 0.49              |
| 34:Lc:69:THR:OG1   | 34:Lc:70:GLY:N     | 2.46                     | 0.49              |
| 49:S2:380:G:OP1    | 58:SI:56:ARG:NH2   | 2.44                     | 0.49              |
| 49:S2:1535:U:O2'   | 55:SF:88:MET:SD    | 2.70                     | 0.49              |
| 49:S2:1647:A:OP1   | 66:SQ:138:ARG:NH1  | 2.43                     | 0.49              |
| 49:S2:1654:G:H5'   | 69:ST:91:HIS:HA    | 1.95                     | 0.49              |
| 53:SD:40:ARG:HB3   | 53:SD:47:GLU:HB2   | 1.94                     | 0.49              |
| 56:SG:98:ARG:NH1   | 56:SG:99:GLY:O     | 2.46                     | 0.49              |
| 77:Sb:23:ARG:NH1   | 77:Sb:27:SER:OG    | 2.46                     | 0.49              |
| 4:L5:1553:A:O2'    | 47:Lp:9:GLY:O      | 2.26                     | 0.48              |
| 4:L5:2128:G:H21    | 4:L5:2252:G:H5''   | 1.77                     | 0.48              |
| 4:L5:2898:G:OP2    | 23:LR:135:LYS:NZ   | 2.40                     | 0.48              |
| 4:L5:2905:C:O2'    | 4:L5:3590:G:O6     | 2.27                     | 0.48              |
| 4:L5:5002:U:OP2    | 8:LB:385:LYS:NZ    | 2.41                     | 0.48              |
| 14:LH:93:ARG:HH22  | 14:LH:140:GLN:HG2  | 1.77                     | 0.48              |
| 54:SE:96:GLY:O     | 54:SE:98:ASN:ND2   | 2.46                     | 0.48              |
| 56:SG:213:LEU:HA   | 56:SG:216:ARG:HB2  | 1.94                     | 0.48              |
| 62:SM:32:ALA:HB3   | 62:SM:110:VAL:HG13 | 1.95                     | 0.48              |
| 82:Sg:249:CYS:HA   | 82:Sg:258:ILE:HA   | 1.95                     | 0.48              |
| 4:L5:62:A:N3       | 4:L5:77:U:O2'      | 2.43                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:L5:945:U:OP1    | 9:LC:342:ARG:NH2   | 2.38                     | 0.48              |
| 4:L5:3786:U:OP1   | 4:L5:4550:G:O2'    | 2.28                     | 0.48              |
| 4:L5:4898:G:N2    | 4:L5:4923:C:O2     | 2.47                     | 0.48              |
| 21:LP:24:VAL:HG12 | 21:LP:86:LYS:HG2   | 1.95                     | 0.48              |
| 49:S2:1426:U:H1'  | 69:ST:5:THR:HG21   | 1.95                     | 0.48              |
| 57:SH:40:LEU:HA   | 57:SH:43:LEU:HB2   | 1.95                     | 0.48              |
| 64:SO:67:ASP:OD1  | 64:SO:67:ASP:N     | 2.44                     | 0.48              |
| 70:SU:66:ARG:HG3  | 70:SU:68:THR:HG22  | 1.95                     | 0.48              |
| 4:L5:37:U:H4'     | 32:La:32:ARG:HD2   | 1.94                     | 0.48              |
| 4:L5:4635:A:H2    | 4:L5:4663:G:H21    | 1.61                     | 0.48              |
| 4:L5:4758:U:H5''  | 20:LO:116:LYS:HG3  | 1.94                     | 0.48              |
| 37:Lf:11:PHE:HB2  | 37:Lf:101:ILE:HD12 | 1.95                     | 0.48              |
| 49:S2:964:A:N3    | 49:S2:1054:G:O2'   | 2.38                     | 0.48              |
| 49:S2:1248:U:H4'  | 66:SQ:146:ARG:HE   | 1.79                     | 0.48              |
| 49:S2:1523:C:OP1  | 68:SS:142:ARG:N    | 2.46                     | 0.48              |
| 59:SJ:24:ARG:NH1  | 59:SJ:28:GLU:OE2   | 2.46                     | 0.48              |
| 82:Sg:14:HIS:NE2  | 82:Sg:33:SER:OG    | 2.35                     | 0.48              |
| 82:Sg:87:LEU:H    | 82:Sg:101:PHE:HB2  | 1.78                     | 0.48              |
| 2:D4:54:U:OP1     | 15:LI:74:LYS:NZ    | 2.41                     | 0.48              |
| 4:L5:748:G:O3'    | 24:LS:148:SER:OG   | 2.32                     | 0.48              |
| 9:LC:94:ASN:OD1   | 9:LC:94:ASN:N      | 2.44                     | 0.48              |
| 35:Ld:64:ILE:HG23 | 35:Ld:68:LEU:HD23  | 1.96                     | 0.48              |
| 40:Li:34:THR:HB   | 40:Li:37:THR:HG22  | 1.95                     | 0.48              |
| 49:S2:96:C:O2     | 49:S2:473:A:O2'    | 2.29                     | 0.48              |
| 49:S2:629:A:O2'   | 49:S2:631:U:OP2    | 2.30                     | 0.48              |
| 49:S2:1083:A:N7   | 49:S2:1841:C:O2'   | 2.44                     | 0.48              |
| 63:SN:47:PRO:HD2  | 63:SN:86:GLU:HG3   | 1.96                     | 0.48              |
| 69:ST:97:LYS:O    | 69:ST:101:ARG:N    | 2.45                     | 0.48              |
| 4:L5:369:G:N2     | 4:L5:372:A:OP2     | 2.45                     | 0.48              |
| 4:L5:513:U:H5'    | 4:L5:514:U:H4'     | 1.95                     | 0.48              |
| 53:SD:48:ILE:HG13 | 53:SD:86:LEU:HG    | 1.95                     | 0.48              |
| 54:SE:258:ALA:HA  | 54:SE:261:SER:HB2  | 1.94                     | 0.48              |
| 57:SH:171:GLU:O   | 57:SH:174:SER:OG   | 2.31                     | 0.48              |
| 66:SQ:10:VAL:HG22 | 66:SQ:25:CYS:HB3   | 1.95                     | 0.48              |
| 4:L5:419:A:N3     | 4:L5:1332:C:O2'    | 2.41                     | 0.48              |
| 13:LG:209:SER:HA  | 13:LG:212:LYS:HE3  | 1.94                     | 0.48              |
| 16:LJ:136:ARG:NH1 | 16:LJ:155:HIS:O    | 2.44                     | 0.48              |
| 17:LL:64:VAL:HA   | 17:LL:67:HIS:CD2   | 2.49                     | 0.48              |
| 49:S2:1259:A:N6   | 49:S2:1519:U:O5'   | 2.46                     | 0.48              |
| 54:SE:124:CYS:HB3 | 54:SE:141:THR:HB   | 1.95                     | 0.48              |
| 56:SG:5:ILE:HG12  | 56:SG:111:LEU:HB2  | 1.95                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 56:SG:57:ASP:OD1  | 56:SG:58:LYS:N     | 2.45                     | 0.48              |
| 57:SH:167:GLU:HA  | 57:SH:170:VAL:HG13 | 1.94                     | 0.48              |
| 68:SS:113:ARG:HD3 | 68:SS:117:ILE:HD13 | 1.95                     | 0.48              |
| 75:SZ:54:THR:O    | 75:SZ:58:LEU:N     | 2.46                     | 0.48              |
| 2:B4:30:G:OP1     | 49:S2:1524:G:O2'   | 2.28                     | 0.48              |
| 13:LG:253:LEU:O   | 13:LG:257:LYS:N    | 2.45                     | 0.48              |
| 49:S2:155:G:H4'   | 56:SG:15:LEU:HD11  | 1.95                     | 0.48              |
| 56:SG:142:ARG:HA  | 56:SG:147:LEU:HD12 | 1.96                     | 0.48              |
| 66:SQ:130:LYS:HG3 | 66:SQ:136:GLY:H    | 1.79                     | 0.48              |
| 67:SR:129:LYS:O   | 67:SR:132:ARG:N    | 2.47                     | 0.48              |
| 72:SW:32:LYS:HA   | 72:SW:35:VAL:HG22  | 1.94                     | 0.48              |
| 4:L5:1543:G:OP1   | 4:L5:2514:G:O2'    | 2.32                     | 0.48              |
| 4:L5:1818:G:OP2   | 4:L5:1818:G:N2     | 2.40                     | 0.48              |
| 4:L5:4492:U:O2'   | 4:L5:4512:U:O2     | 2.26                     | 0.48              |
| 9:LC:60:HIS:HE1   | 9:LC:100:ARG:HH11  | 1.61                     | 0.48              |
| 17:LL:54:PRO:HB2  | 17:LL:97:SER:HB3   | 1.95                     | 0.48              |
| 58:SI:163:GLU:HA  | 58:SI:166:PHE:HB2  | 1.96                     | 0.48              |
| 60:SK:53:LYS:HZ3  | 60:SK:60:GLU:H     | 1.61                     | 0.48              |
| 71:SV:62:MET:HB3  | 71:SV:64:GLU:HG2   | 1.95                     | 0.48              |
| 4:L5:2740:U:O2'   | 4:L5:2742:G:N2     | 2.46                     | 0.48              |
| 5:L7:23:A:N3      | 5:L7:118:C:O2'     | 2.43                     | 0.48              |
| 6:L8:142:U:OP1    | 19:LN:38:ARG:NH2   | 2.43                     | 0.48              |
| 7:LA:28:ARG:HD2   | 7:LA:123:ARG:HD3   | 1.95                     | 0.48              |
| 13:LG:138:ALA:O   | 13:LG:142:THR:OG1  | 2.31                     | 0.48              |
| 28:LW:109:ILE:O   | 28:LW:113:LYS:N    | 2.44                     | 0.48              |
| 49:S2:360:A:N6    | 49:S2:400:C:O2'    | 2.47                     | 0.48              |
| 49:S2:1436:C:O2'  | 49:S2:1438:A:O5'   | 2.28                     | 0.48              |
| 49:S2:1863:A:N6   | 76:Sa:76:SER:OG    | 2.47                     | 0.48              |
| 59:SJ:129:LEU:HB2 | 59:SJ:134:HIS:HD2  | 1.79                     | 0.48              |
| 69:ST:23:LYS:O    | 69:ST:23:LYS:NZ    | 2.46                     | 0.48              |
| 4:L5:75:G:O6      | 17:LL:103:ARG:NH1  | 2.47                     | 0.48              |
| 4:L5:186:G:N2     | 4:L5:1365:C:O2'    | 2.47                     | 0.48              |
| 4:L5:438:G:OP1    | 36:Le:16:ARG:NH2   | 2.38                     | 0.48              |
| 4:L5:1812:C:H5''  | 33:Lb:56:LYS:HE2   | 1.96                     | 0.48              |
| 4:L5:3893:C:O2'   | 4:L5:4979:A:N1     | 2.46                     | 0.48              |
| 4:L5:4105:A:N3    | 4:L5:4106:G:N2     | 2.61                     | 0.48              |
| 5:L7:61:G:O3'     | 10:LD:279:ARG:NH1  | 2.46                     | 0.48              |
| 47:Lp:38:THR:HA   | 47:Lp:45:THR:HA    | 1.96                     | 0.48              |
| 49:S2:441:C:OP1   | 49:S2:1737:G:N2    | 2.44                     | 0.48              |
| 53:SD:194:PRO:HA  | 53:SD:201:LYS:HG3  | 1.96                     | 0.48              |
| 7:LA:90:CYS:HA    | 7:LA:101:VAL:HB    | 1.96                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 13:LG:85:GLN:HE22 | 13:LG:229:ARG:HH22 | 1.62                     | 0.47              |
| 13:LG:231:ASP:O   | 13:LG:235:ARG:NE   | 2.46                     | 0.47              |
| 37:Lf:24:HIS:O    | 37:Lf:87:LYS:NZ    | 2.46                     | 0.47              |
| 49:S2:30:C:O2'    | 49:S2:596:U:OP1    | 2.30                     | 0.47              |
| 66:SQ:93:VAL:O    | 66:SQ:105:LYS:NZ   | 2.43                     | 0.47              |
| 69:ST:42:HIS:HB2  | 69:ST:83:GLN:HA    | 1.95                     | 0.47              |
| 4:L5:2049:G:HO2'  | 4:L5:3884:U:HO2'   | 1.59                     | 0.47              |
| 4:L5:4927:G:H5''  | 4:L5:4928:C:H5     | 1.78                     | 0.47              |
| 11:LE:214:ASP:N   | 11:LE:214:ASP:OD1  | 2.46                     | 0.47              |
| 17:LL:48:PRO:HB2  | 39:Lh:120:ALA:HB2  | 1.95                     | 0.47              |
| 30:LY:31:SER:HA   | 30:LY:48:PRO:HA    | 1.96                     | 0.47              |
| 49:S2:688:U:OP1   | 57:SH:121:THR:OG1  | 2.32                     | 0.47              |
| 49:S2:1147:C:OP1  | 76:Sa:6:ARG:NH1    | 2.48                     | 0.47              |
| 49:S2:1404:U:OP2  | 70:SU:21:ARG:NH1   | 2.42                     | 0.47              |
| 49:S2:1459:G:OP2  | 82:Sg:280:LYS:NZ   | 2.40                     | 0.47              |
| 50:SA:213:GLU:O   | 50:SA:217:ALA:N    | 2.47                     | 0.47              |
| 55:SF:71:ARG:NH1  | 55:SF:148:ASN:OD1  | 2.47                     | 0.47              |
| 4:L5:969:C:O2'    | 11:LE:123:ARG:NH1  | 2.47                     | 0.47              |
| 4:L5:1274:A:H1'   | 4:L5:1275:G:H5'    | 1.96                     | 0.47              |
| 4:L5:3925:U:OP1   | 46:Lo:57:ARG:NH2   | 2.47                     | 0.47              |
| 4:L5:4094:G:H3'   | 4:L5:4095:G:H8     | 1.80                     | 0.47              |
| 4:L5:4558:U:OP2   | 8:LB:246:ARG:NH2   | 2.43                     | 0.47              |
| 7:LA:102:LEU:HG   | 7:LA:107:MET:HE2   | 1.96                     | 0.47              |
| 15:LI:191:ILE:N   | 15:LI:197:VAL:O    | 2.48                     | 0.47              |
| 17:LL:77:SER:HB3  | 17:LL:80:GLU:HG3   | 1.97                     | 0.47              |
| 50:SA:37:TYR:OH   | 71:SV:66:ASP:OD2   | 2.28                     | 0.47              |
| 69:ST:96:SER:HB2  | 69:ST:99:VAL:HG12  | 1.96                     | 0.47              |
| 78:Sc:12:ALA:HB1  | 78:Sc:32:VAL:HB    | 1.95                     | 0.47              |
| 4:L5:1444:G:N2    | 4:L5:2103:G:H22    | 2.13                     | 0.47              |
| 4:L5:2121:C:O2'   | 4:L5:2122:G:O4'    | 2.27                     | 0.47              |
| 16:LJ:12:MET:HA   | 16:LJ:137:PRO:HG2  | 1.96                     | 0.47              |
| 16:LJ:26:VAL:HB   | 16:LJ:32:ARG:HH12  | 1.80                     | 0.47              |
| 20:LO:43:ILE:HG13 | 20:LO:136:ALA:HB3  | 1.96                     | 0.47              |
| 22:LQ:53:MET:O    | 22:LQ:58:ARG:NH1   | 2.47                     | 0.47              |
| 36:Le:81:ASN:N    | 36:Le:81:ASN:OD1   | 2.47                     | 0.47              |
| 40:Li:70:LEU:HD12 | 40:Li:87:ARG:HE    | 1.79                     | 0.47              |
| 49:S2:1601:A:N1   | 49:S2:1636:G:N2    | 2.61                     | 0.47              |
| 63:SN:23:PRO:HB3  | 77:Sb:84:HIS:HB2   | 1.95                     | 0.47              |
| 66:SQ:29:ASN:OD1  | 66:SQ:29:ASN:N     | 2.45                     | 0.47              |
| 4:L5:1396:G:N7    | 32:La:110:LYS:NZ   | 2.48                     | 0.47              |
| 29:LX:143:ASP:N   | 29:LX:143:ASP:OD1  | 2.47                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:S2:1249:C:H5'   | 66:SQ:146:ARG:HH22 | 1.79                     | 0.47              |
| 49:S2:1253:A:OP2   | 49:S2:1526:G:N2    | 2.44                     | 0.47              |
| 49:S2:1637:A:N1    | 55:SF:81:ARG:NH1   | 2.62                     | 0.47              |
| 64:SO:53:ILE:HD13  | 64:SO:90:ILE:HG13  | 1.96                     | 0.47              |
| 82:Sg:198:VAL:HG12 | 82:Sg:209:SER:HA   | 1.95                     | 0.47              |
| 4:L5:267:G:OP1     | 39:Lh:109:ARG:NH2  | 2.45                     | 0.47              |
| 4:L5:679:C:H2'     | 4:L5:680:G:H8      | 1.78                     | 0.47              |
| 4:L5:2121:C:H4'    | 12:LF:41:MET:HE2   | 1.96                     | 0.47              |
| 9:LC:33:ARG:HE     | 9:LC:33:ARG:HB3    | 1.57                     | 0.47              |
| 9:LC:353:LYS:O     | 9:LC:357:ALA:N     | 2.48                     | 0.47              |
| 16:LJ:56:THR:OG1   | 16:LJ:64:ARG:N     | 2.48                     | 0.47              |
| 49:S2:1403:C:OP1   | 70:SU:51:LYS:NZ    | 2.45                     | 0.47              |
| 49:S2:1445:U:O4    | 49:S2:1446:A:N6    | 2.47                     | 0.47              |
| 49:S2:1520:G:OP1   | 68:SS:136:THR:N    | 2.46                     | 0.47              |
| 51:SB:154:SER:O    | 51:SB:154:SER:OG   | 2.32                     | 0.47              |
| 52:SC:195:LEU:HD22 | 52:SC:214:LEU:HD21 | 1.96                     | 0.47              |
| 53:SD:193:ASP:HB3  | 53:SD:199:GLY:HA3  | 1.96                     | 0.47              |
| 55:SF:203:ASN:N    | 55:SF:203:ASN:OD1  | 2.47                     | 0.47              |
| 66:SQ:18:THR:HB    | 66:SQ:75:GLY:HA2   | 1.97                     | 0.47              |
| 70:SU:68:THR:O     | 79:Sd:40:ARG:NH1   | 2.48                     | 0.47              |
| 76:Sa:11:ALA:H     | 76:Sa:33:ASP:HB2   | 1.80                     | 0.47              |
| 4:L5:51:A:N3       | 4:L5:1528:U:O2'    | 2.47                     | 0.47              |
| 4:L5:420:A:HO2'    | 4:L5:1331:C:HO2'   | 1.62                     | 0.47              |
| 4:L5:4207:C:OP2    | 25:LT:4:THR:OG1    | 2.33                     | 0.47              |
| 7:LA:29:LEU:O      | 7:LA:123:ARG:NH1   | 2.47                     | 0.47              |
| 15:LI:12:CYS:HB3   | 15:LI:59:GLN:HB3   | 1.96                     | 0.47              |
| 15:LI:36:LEU:HD11  | 15:LI:69:ARG:HD2   | 1.97                     | 0.47              |
| 22:LQ:72:LEU:HB3   | 22:LQ:75:ARG:HG3   | 1.96                     | 0.47              |
| 23:LR:8:LYS:O      | 23:LR:12:SER:OG    | 2.28                     | 0.47              |
| 24:LS:83:ARG:NH1   | 24:LS:125:GLN:OE1  | 2.48                     | 0.47              |
| 24:LS:85:ASP:OD1   | 24:LS:85:ASP:N     | 2.45                     | 0.47              |
| 25:LT:48:VAL:HG21  | 25:LT:94:GLU:HG2   | 1.95                     | 0.47              |
| 27:LV:83:ARG:HB2   | 27:LV:102:ALA:HB3  | 1.96                     | 0.47              |
| 53:SD:98:ALA:HB1   | 53:SD:186:VAL:HG23 | 1.95                     | 0.47              |
| 55:SF:30:ILE:HG22  | 55:SF:42:LYS:HZ3   | 1.80                     | 0.47              |
| 57:SH:57:ARG:HH22  | 57:SH:91:HIS:H     | 1.62                     | 0.47              |
| 58:SI:92:ARG:O     | 58:SI:94:LYS:NZ    | 2.41                     | 0.47              |
| 58:SI:163:GLU:O    | 58:SI:167:GLN:N    | 2.47                     | 0.47              |
| 4:L5:1269:G:N2     | 4:L5:2108:G:OP2    | 2.47                     | 0.47              |
| 5:L7:9:C:OP2       | 5:L7:10:C:N4       | 2.47                     | 0.47              |
| 6:L8:75:G:OP2      | 30:LY:74:TYR:OH    | 2.29                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:LB:315:ASN:OD1   | 8:LB:326:VAL:N     | 2.42                     | 0.47              |
| 13:LG:58:PRO:HD2   | 13:LG:61:ILE:HD11  | 1.95                     | 0.47              |
| 18:LM:90:ARG:O     | 18:LM:94:LYS:N     | 2.46                     | 0.47              |
| 33:Lb:40:LEU:HA    | 33:Lb:43:MET:HG2   | 1.96                     | 0.47              |
| 34:Lc:19:GLN:HE22  | 63:SN:151:ALA:HB1  | 1.78                     | 0.47              |
| 34:Lc:44:LYS:NZ    | 34:Lc:97:ILE:O     | 2.39                     | 0.47              |
| 38:Lg:15:THR:HG23  | 38:Lg:17:SER:H     | 1.80                     | 0.47              |
| 49:S2:1866:A:H5'   | 76:Sa:95:ARG:HG2   | 1.97                     | 0.47              |
| 82:Sg:133:ASN:ND2  | 82:Sg:137:VAL:O    | 2.37                     | 0.47              |
| 4:L5:1826:G:O2'    | 33:Lb:47:LYS:NZ    | 2.47                     | 0.47              |
| 4:L5:3680:U:OP1    | 7:LA:54:ARG:NH2    | 2.48                     | 0.47              |
| 4:L5:4525:C:OP1    | 8:LB:246:ARG:NH1   | 2.41                     | 0.47              |
| 10:LD:65:ALA:HB2   | 10:LD:74:ILE:HD13  | 1.97                     | 0.47              |
| 15:LI:66:GLU:HA    | 15:LI:69:ARG:HG2   | 1.96                     | 0.47              |
| 49:S2:496:C:H5'    | 54:SE:29:PRO:HG3   | 1.96                     | 0.47              |
| 57:SH:48:ALA:HA    | 57:SH:62:ILE:HA    | 1.96                     | 0.47              |
| 2:D4:26:A:H61      | 2:D4:44:G:H1       | 1.63                     | 0.47              |
| 10:LD:59:ASP:OD1   | 10:LD:81:HIS:N     | 2.47                     | 0.47              |
| 10:LD:191:ASN:HD22 | 10:LD:194:VAL:HG23 | 1.80                     | 0.47              |
| 11:LE:46:ARG:HG3   | 11:LE:62:MET:HE1   | 1.97                     | 0.47              |
| 31:LZ:14:LEU:HD21  | 38:Lg:92:LYS:HE3   | 1.96                     | 0.47              |
| 45:Ln:13:LEU:HD21  | 49:S2:1819:A:H4'   | 1.97                     | 0.47              |
| 53:SD:61:GLU:H     | 53:SD:64:ARG:HG2   | 1.79                     | 0.47              |
| 4:L5:667:A:OP1     | 48:Lr:67:ARG:NH2   | 2.47                     | 0.46              |
| 4:L5:1972:G:N2     | 4:L5:1973:G:N7     | 2.63                     | 0.46              |
| 4:L5:2262:G:OP1    | 48:Lr:94:ARG:NH1   | 2.45                     | 0.46              |
| 4:L5:5054:C:H4'    | 4:L5:5055:G:H5'    | 1.97                     | 0.46              |
| 8:LB:220:ILE:HD11  | 8:LB:348:ARG:HE    | 1.80                     | 0.46              |
| 14:LH:103:VAL:HG11 | 14:LH:144:LEU:HD21 | 1.97                     | 0.46              |
| 15:LI:36:LEU:HD13  | 15:LI:87:MET:HE3   | 1.96                     | 0.46              |
| 17:LL:207:VAL:HG23 | 17:LL:208:GLU:HG3  | 1.97                     | 0.46              |
| 25:LT:43:LYS:O     | 25:LT:58:HIS:ND1   | 2.41                     | 0.46              |
| 49:S2:96:C:H1'     | 49:S2:474:G:H5''   | 1.97                     | 0.46              |
| 49:S2:1017:U:H5'   | 63:SN:55:ARG:HD3   | 1.97                     | 0.46              |
| 49:S2:1298:G:H1'   | 65:SP:79:HIS:H     | 1.79                     | 0.46              |
| 49:S2:1427:C:H2'   | 49:S2:1428:G:C4    | 2.49                     | 0.46              |
| 49:S2:1648:G:N2    | 49:S2:1675:A:OP2   | 2.44                     | 0.46              |
| 50:SA:31:ASP:N     | 50:SA:150:THR:O    | 2.46                     | 0.46              |
| 52:SC:179:THR:OG1  | 52:SC:180:VAL:N    | 2.48                     | 0.46              |
| 59:SJ:158:ASP:OD1  | 59:SJ:158:ASP:N    | 2.46                     | 0.46              |
| 76:Sa:43:ASN:HB2   | 76:Sa:46:GLU:HB2   | 1.98                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:L5:512:U:H2'    | 4:L5:513:U:H4'     | 1.97                     | 0.46              |
| 4:L5:2501:C:N4    | 4:L5:2502:G:O6     | 2.47                     | 0.46              |
| 17:LL:19:GLN:HA   | 17:LL:22:VAL:HG13  | 1.97                     | 0.46              |
| 22:LQ:63:LEU:HB2  | 22:LQ:88:ASP:HA    | 1.96                     | 0.46              |
| 35:Ld:85:ARG:HH21 | 35:Ld:117:LEU:HB3  | 1.79                     | 0.46              |
| 38:Lg:61:PRO:HA   | 38:Lg:64:LEU:HD13  | 1.96                     | 0.46              |
| 49:S2:507:G:OP1   | 74:SY:108:LYS:NZ   | 2.49                     | 0.46              |
| 49:S2:1597:C:O2'  | 49:S2:1598:G:O4'   | 2.33                     | 0.46              |
| 49:S2:1694:U:O2'  | 49:S2:1833:C:O2'   | 2.33                     | 0.46              |
| 51:SB:103:MET:H   | 51:SB:215:VAL:HG22 | 1.80                     | 0.46              |
| 52:SC:85:SER:OG   | 52:SC:85:SER:O     | 2.33                     | 0.46              |
| 52:SC:146:GLU:HB2 | 52:SC:149:THR:HG22 | 1.97                     | 0.46              |
| 52:SC:256:TRP:CD2 | 72:SW:68:ARG:HD3   | 2.50                     | 0.46              |
| 68:SS:25:LYS:O    | 68:SS:29:ALA:N     | 2.46                     | 0.46              |
| 70:SU:55:ARG:HH11 | 70:SU:87:ARG:HE    | 1.63                     | 0.46              |
| 74:SY:44:LEU:HD12 | 74:SY:47:MET:HB2   | 1.97                     | 0.46              |
| 78:Sc:12:ALA:HB3  | 78:Sc:56:LEU:HB3   | 1.96                     | 0.46              |
| 82:Sg:214:GLY:HA2 | 82:Sg:236:ILE:HG23 | 1.98                     | 0.46              |
| 4:L5:2667:C:O2    | 23:LR:92:LYS:NZ    | 2.44                     | 0.46              |
| 4:L5:3612:C:H1'   | 4:L5:5016:A:H8     | 1.79                     | 0.46              |
| 4:L5:4098:A:H3'   | 4:L5:4099:G:H4'    | 1.96                     | 0.46              |
| 4:L5:4868:G:O3'   | 18:LM:90:ARG:NH1   | 2.48                     | 0.46              |
| 15:LI:77:VAL:HG23 | 15:LI:82:ARG:HA    | 1.96                     | 0.46              |
| 18:LM:26:ALA:HB2  | 18:LM:77:TRP:HZ3   | 1.81                     | 0.46              |
| 49:S2:525:A:OP2   | 80:Se:99:LYS:NZ    | 2.47                     | 0.46              |
| 58:SI:110:ARG:NH2 | 58:SI:121:LEU:O    | 2.48                     | 0.46              |
| 70:SU:48:LEU:HA   | 70:SU:49:LYS:HA    | 1.52                     | 0.46              |
| 82:Sg:257:LYS:HE3 | 82:Sg:259:TRP:HZ2  | 1.80                     | 0.46              |
| 4:L5:1362:G:OP1   | 17:LL:39:ARG:NH2   | 2.48                     | 0.46              |
| 4:L5:2418:A:H5'   | 21:LP:23:ARG:HH22  | 1.79                     | 0.46              |
| 4:L5:2590:G:O2'   | 4:L5:2755:A:N6     | 2.49                     | 0.46              |
| 13:LG:211:ASP:N   | 13:LG:211:ASP:OD1  | 2.49                     | 0.46              |
| 13:LG:250:ILE:O   | 13:LG:254:GLU:N    | 2.48                     | 0.46              |
| 49:S2:86:C:OP1    | 74:SY:118:ARG:NH2  | 2.49                     | 0.46              |
| 50:SA:213:GLU:HA  | 50:SA:216:ALA:HB3  | 1.98                     | 0.46              |
| 56:SG:222:GLU:O   | 56:SG:226:GLU:N    | 2.48                     | 0.46              |
| 64:SO:29:GLY:O    | 64:SO:94:HIS:N     | 2.45                     | 0.46              |
| 82:Sg:215:GLN:HA  | 82:Sg:231:ASP:HA   | 1.96                     | 0.46              |
| 4:L5:1270:A:O4'   | 4:L5:2109:G:N2     | 2.43                     | 0.46              |
| 4:L5:2282:A:OP1   | 32:La:21:ARG:NH1   | 2.48                     | 0.46              |
| 4:L5:2812:A:H5'   | 23:LR:88:ARG:HG2   | 1.97                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:LH:129:ARG:HH21 | 14:LH:160:LEU:HD11 | 1.81                     | 0.46              |
| 49:S2:1373:C:OP1   | 67:SR:7:LYS:N      | 2.45                     | 0.46              |
| 53:SD:206:ASP:OD1  | 53:SD:206:ASP:N    | 2.48                     | 0.46              |
| 55:SF:101:HIS:HB2  | 55:SF:108:PRO:HG3  | 1.96                     | 0.46              |
| 58:SI:57:ALA:HB1   | 58:SI:60:LEU:HD11  | 1.96                     | 0.46              |
| 60:SK:49:MET:HB3   | 60:SK:49:MET:HE2   | 1.80                     | 0.46              |
| 60:SK:57:TYR:O     | 60:SK:72:THR:OG1   | 2.34                     | 0.46              |
| 75:SZ:30:ALA:HB1   | 75:SZ:32:LYS:HE3   | 1.97                     | 0.46              |
| 4:L5:684:G:H4'     | 11:LE:100:LYS:HB2  | 1.98                     | 0.46              |
| 4:L5:1176:C:H2'    | 4:L5:1177:U:H6     | 1.80                     | 0.46              |
| 4:L5:1778:C:H5''   | 10:LD:5:LYS:HB2    | 1.98                     | 0.46              |
| 14:LH:173:ARG:HB3  | 44:Lm:127:VAL:HG12 | 1.97                     | 0.46              |
| 28:LW:86:SER:HB2   | 56:SG:158:VAL:HG13 | 1.97                     | 0.46              |
| 42:Lk:37:ARG:HH11  | 42:Lk:42:LEU:HB2   | 1.79                     | 0.46              |
| 49:S2:750:C:N4     | 49:S2:793:G:O2'    | 2.49                     | 0.46              |
| 49:S2:1354:G:N2    | 49:S2:1357:A:OP2   | 2.42                     | 0.46              |
| 49:S2:1786:U:H2'   | 49:S2:1787:G:H8    | 1.80                     | 0.46              |
| 53:SD:35:SER:HB2   | 53:SD:100:ALA:HB2  | 1.97                     | 0.46              |
| 56:SG:69:THR:OG1   | 56:SG:70:HIS:N     | 2.47                     | 0.46              |
| 81:Sf:132:MET:HE1  | 81:Sf:148:TYR:HB2  | 1.98                     | 0.46              |
| 4:L5:4093:G:O6     | 4:L5:4114:C:O2'    | 2.26                     | 0.46              |
| 12:LF:67:THR:OG1   | 12:LF:70:ARG:NH1   | 2.48                     | 0.46              |
| 13:LG:256:ALA:HA   | 13:LG:259:LYS:HD3  | 1.98                     | 0.46              |
| 17:LL:31:ARG:HA    | 17:LL:34:ARG:HG2   | 1.97                     | 0.46              |
| 20:LO:81:TRP:HB2   | 20:LO:104:VAL:HG11 | 1.98                     | 0.46              |
| 25:LT:79:GLN:HG2   | 25:LT:84:ILE:HG12  | 1.98                     | 0.46              |
| 35:Ld:19:GLU:OE1   | 35:Ld:92:ARG:NH1   | 2.49                     | 0.46              |
| 43:Ll:16:LYS:HA    | 43:Ll:19:GLN:HG2   | 1.98                     | 0.46              |
| 49:S2:165:G:OP2    | 49:S2:165:G:N2     | 2.41                     | 0.46              |
| 50:SA:46:ILE:H     | 50:SA:46:ILE:HG13  | 1.62                     | 0.46              |
| 63:SN:25:TRP:HE1   | 77:Sb:84:HIS:HA    | 1.80                     | 0.46              |
| 65:SP:81:ARG:NH1   | 65:SP:97:TYR:O     | 2.46                     | 0.46              |
| 2:B4:73:A:H1'      | 15:LI:111:LEU:HD13 | 1.97                     | 0.46              |
| 4:L5:4942:C:OP1    | 11:LE:187:ARG:NH2  | 2.49                     | 0.46              |
| 42:Lk:3:ARG:HB2    | 42:Lk:43:TYR:HD1   | 1.80                     | 0.46              |
| 49:S2:441:C:H5     | 49:S2:452:G:H1     | 1.62                     | 0.46              |
| 49:S2:1292:C:O2    | 81:Sf:138:ARG:NH1  | 2.49                     | 0.46              |
| 50:SA:104:THR:O    | 50:SA:107:THR:OG1  | 2.32                     | 0.46              |
| 53:SD:175:VAL:HG22 | 53:SD:182:LEU:HB2  | 1.98                     | 0.46              |
| 56:SG:136:LYS:HG2  | 56:SG:176:ILE:HA   | 1.98                     | 0.46              |
| 59:SJ:112:THR:HG22 | 59:SJ:123:ILE:HD11 | 1.97                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 82:Sg:62:HIS:O     | 82:Sg:88:ARG:NH2   | 2.49                     | 0.46              |
| 15:LI:46:PHE:HB2   | 15:LI:139:ARG:HD2  | 1.97                     | 0.46              |
| 17:LL:78:LEU:HD13  | 17:LL:100:PRO:HA   | 1.97                     | 0.46              |
| 17:LL:169:ILE:HG12 | 32:La:123:ILE:HD11 | 1.98                     | 0.46              |
| 24:LS:127:MET:HB3  | 25:LT:153:PRO:HG2  | 1.98                     | 0.46              |
| 39:Lh:73:TYR:HA    | 39:Lh:76:LYS:HD3   | 1.98                     | 0.46              |
| 47:Lp:57:CYS:SG    | 47:Lp:59:SER:OG    | 2.71                     | 0.46              |
| 49:S2:1745:A:H1'   | 56:SG:66:GLY:HA2   | 1.97                     | 0.46              |
| 53:SD:107:TYR:HA   | 53:SD:110:LEU:HB2  | 1.98                     | 0.46              |
| 56:SG:88:ARG:HB3   | 56:SG:91:GLU:HB2   | 1.98                     | 0.46              |
| 58:SI:84:ASN:HD22  | 58:SI:90:LEU:HB2   | 1.81                     | 0.46              |
| 72:SW:90:GLN:HB2   | 72:SW:94:LEU:HD12  | 1.97                     | 0.46              |
| 73:SX:124:LYS:HG2  | 73:SX:129:SER:HA   | 1.98                     | 0.46              |
| 81:Sf:118:ARG:HH21 | 81:Sf:131:PHE:HB3  | 1.80                     | 0.46              |
| 4:L5:960:A:N6      | 11:LE:125:LEU:O    | 2.48                     | 0.46              |
| 4:L5:3756:A:H61    | 4:L5:3768:U:H3     | 1.64                     | 0.46              |
| 10:LD:176:SER:OG   | 10:LD:177:THR:N    | 2.49                     | 0.46              |
| 24:LS:29:ARG:HB2   | 25:LT:148:PRO:HB2  | 1.96                     | 0.46              |
| 63:SN:37:ILE:HG23  | 63:SN:50:ILE:HD12  | 1.98                     | 0.46              |
| 65:SP:27:ASP:OD1   | 65:SP:27:ASP:N     | 2.44                     | 0.46              |
| 72:SW:115:GLU:O    | 72:SW:119:LYS:N    | 2.37                     | 0.46              |
| 82:Sg:173:LEU:HB3  | 82:Sg:175:LYS:HE3  | 1.98                     | 0.46              |
| 4:L5:2658:G:H2'    | 34:Lc:33:GLN:HE22  | 1.81                     | 0.45              |
| 5:L7:48:G:O2'      | 10:LD:222:GLN:O    | 2.27                     | 0.45              |
| 11:LE:270:TYR:OH   | 18:LM:106:ASP:OD2  | 2.33                     | 0.45              |
| 26:LU:28:PRO:HB2   | 26:LU:34:MET:HG2   | 1.98                     | 0.45              |
| 49:S2:683:G:N1     | 49:S2:1022:U:OP2   | 2.42                     | 0.45              |
| 49:S2:1206:G:O2'   | 49:S2:1208:A:OP1   | 2.32                     | 0.45              |
| 62:SM:68:LEU:HD12  | 81:Sf:114:ILE:HG13 | 1.98                     | 0.45              |
| 72:SW:8:ALA:HA     | 72:SW:74:VAL:HG11  | 1.98                     | 0.45              |
| 73:SX:98:ASP:OD2   | 73:SX:140:ARG:NH2  | 2.45                     | 0.45              |
| 74:SY:102:THR:O    | 74:SY:107:ARG:NH1  | 2.43                     | 0.45              |
| 4:L5:2519:U:O2'    | 4:L5:2530:U:O2     | 2.32                     | 0.45              |
| 9:LC:143:ARG:NH1   | 9:LC:145:GLU:OE2   | 2.50                     | 0.45              |
| 14:LH:49:GLY:HA3   | 14:LH:53:LYS:HA    | 1.99                     | 0.45              |
| 30:LY:112:ASP:O    | 30:LY:116:LYS:N    | 2.47                     | 0.45              |
| 34:Lc:38:ILE:HG21  | 34:Lc:63:TYR:HB3   | 1.98                     | 0.45              |
| 49:S2:628:A:H62    | 49:S2:1500:G:H21   | 1.62                     | 0.45              |
| 65:SP:81:ARG:HB3   | 65:SP:117:GLY:HA3  | 1.97                     | 0.45              |
| 82:Sg:291:TRP:HA   | 82:Sg:298:LEU:HA   | 1.98                     | 0.45              |
| 4:L5:1198:G:H2'    | 4:L5:1199:G:C8     | 2.52                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:L5:4633:G:O2'    | 4:L5:4635:A:OP2    | 2.29                     | 0.45              |
| 8:LB:302:ASN:HB3   | 8:LB:314:ILE:HB    | 1.99                     | 0.45              |
| 14:LH:78:GLN:HA    | 14:LH:81:ILE:HB    | 1.98                     | 0.45              |
| 21:LP:122:ALA:HB3  | 21:LP:143:PRO:HG2  | 1.98                     | 0.45              |
| 24:LS:46:TYR:OH    | 24:LS:125:GLN:NE2  | 2.49                     | 0.45              |
| 27:LV:90:ARG:NH1   | 27:LV:140:ALA:O    | 2.44                     | 0.45              |
| 32:La:102:ASP:OD2  | 32:La:105:ARG:N    | 2.49                     | 0.45              |
| 49:S2:1549:U:OP1   | 79:Sd:34:TYR:OH    | 2.32                     | 0.45              |
| 60:SK:43:LEU:HA    | 60:SK:46:MET:HE3   | 1.98                     | 0.45              |
| 62:SM:65:VAL:HG22  | 62:SM:69:LEU:HD23  | 1.98                     | 0.45              |
| 69:ST:39:LEU:HA    | 69:ST:39:LEU:HD23  | 1.82                     | 0.45              |
| 82:Sg:126:ASP:OD1  | 82:Sg:128:THR:OG1  | 2.33                     | 0.45              |
| 4:L5:152:U:H5'     | 19:LN:54:LYS:HB3   | 1.98                     | 0.45              |
| 9:LC:348:LYS:HA    | 9:LC:351:VAL:HG12  | 1.98                     | 0.45              |
| 10:LD:236:MET:HA   | 10:LD:239:MET:HB3  | 1.99                     | 0.45              |
| 11:LE:152:ILE:HG13 | 11:LE:162:VAL:HG11 | 1.98                     | 0.45              |
| 11:LE:176:THR:OG1  | 11:LE:177:GLY:O    | 2.33                     | 0.45              |
| 13:LG:146:LEU:HD22 | 13:LG:151:LYS:HB2  | 1.97                     | 0.45              |
| 16:LJ:158:SER:OG   | 16:LJ:159:LYS:N    | 2.50                     | 0.45              |
| 17:LL:70:VAL:HG12  | 17:LL:159:ASN:HD22 | 1.81                     | 0.45              |
| 34:Lc:30:GLY:O     | 34:Lc:93:THR:OG1   | 2.34                     | 0.45              |
| 53:SD:132:LYS:HD2  | 53:SD:189:MET:HE2  | 1.97                     | 0.45              |
| 58:SI:6:ASP:OD1    | 58:SI:6:ASP:N      | 2.44                     | 0.45              |
| 62:SM:39:ALA:HA    | 62:SM:42:LEU:HB2   | 1.97                     | 0.45              |
| 64:SO:142:ARG:NH1  | 76:Sa:23:CYS:O     | 2.49                     | 0.45              |
| 82:Sg:69:VAL:HG23  | 82:Sg:80:SER:HB3   | 1.99                     | 0.45              |
| 4:L5:188:G:O2'     | 4:L5:190:G:OP2     | 2.34                     | 0.45              |
| 4:L5:4882:U:OP1    | 18:LM:117:LYS:NZ   | 2.50                     | 0.45              |
| 49:S2:207:G:O6     | 58:SI:144:LYS:NZ   | 2.50                     | 0.45              |
| 49:S2:377:G:H5'    | 58:SI:98:LYS:HD3   | 1.99                     | 0.45              |
| 49:S2:1391:C:O2'   | 79:Sd:56:ASP:OD1   | 2.28                     | 0.45              |
| 49:S2:1447:G:OP1   | 70:SU:85:HIS:ND1   | 2.41                     | 0.45              |
| 49:S2:1553:C:N4    | 49:S2:1557:C:O2'   | 2.50                     | 0.45              |
| 57:SH:129:ILE:HD11 | 57:SH:180:LEU:HD13 | 1.99                     | 0.45              |
| 74:SY:7:ILE:HG22   | 74:SY:27:VAL:HG22  | 1.98                     | 0.45              |
| 77:Sb:67:THR:OG1   | 77:Sb:68:GLY:N     | 2.49                     | 0.45              |
| 79:Sd:31:ILE:HD11  | 79:Sd:40:ARG:HA    | 1.98                     | 0.45              |
| 4:L5:229:G:H5''    | 30:LY:11:ARG:HG3   | 1.98                     | 0.45              |
| 4:L5:467:U:O4      | 4:L5:686:A:N6      | 2.50                     | 0.45              |
| 4:L5:3667:C:H4'    | 7:LA:8:GLN:HA      | 1.99                     | 0.45              |
| 7:LA:101:VAL:HG22  | 7:LA:165:VAL:HG22  | 1.98                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:LB:90:VAL:HG12   | 8:LB:104:THR:HG23  | 1.98                     | 0.45              |
| 21:LP:119:VAL:HG12 | 21:LP:146:ILE:HG12 | 1.99                     | 0.45              |
| 24:LS:76:LYS:HD2   | 24:LS:131:GLU:HG3  | 1.99                     | 0.45              |
| 31:LZ:113:GLU:HA   | 31:LZ:116:VAL:HG22 | 1.98                     | 0.45              |
| 36:Le:11:LYS:HD2   | 36:Le:11:LYS:HA    | 1.86                     | 0.45              |
| 49:S2:113:G:C2     | 49:S2:292:A:H1'    | 2.51                     | 0.45              |
| 50:SA:184:ARG:HE   | 50:SA:189:ILE:HD11 | 1.81                     | 0.45              |
| 51:SB:72:ALA:HB3   | 64:SO:128:ARG:HH21 | 1.82                     | 0.45              |
| 51:SB:129:THR:HG23 | 51:SB:131:ASP:H    | 1.82                     | 0.45              |
| 56:SG:134:GLY:HA2  | 56:SG:158:VAL:HB   | 1.98                     | 0.45              |
| 57:SH:149:ASP:OD1  | 57:SH:149:ASP:N    | 2.50                     | 0.45              |
| 59:SJ:179:LYS:O    | 59:SJ:182:GLN:NE2  | 2.49                     | 0.45              |
| 64:SO:31:CYS:HB3   | 64:SO:95:ILE:HG22  | 1.98                     | 0.45              |
| 70:SU:95:SER:O     | 70:SU:99:LYS:NZ    | 2.39                     | 0.45              |
| 82:Sg:64:HIS:CG    | 82:Sg:84:ASP:HB2   | 2.51                     | 0.45              |
| 4:L5:318:A:H2'     | 4:L5:319:A:H8      | 1.82                     | 0.45              |
| 4:L5:495:C:H2'     | 4:L5:496:G:C8      | 2.51                     | 0.45              |
| 4:L5:513:U:H3'     | 4:L5:514:U:H4'     | 1.99                     | 0.45              |
| 4:L5:1758:G:H2'    | 4:L5:1759:G:H8     | 1.81                     | 0.45              |
| 4:L5:4279:A:H5'    | 4:L5:4281:A:H1'    | 1.98                     | 0.45              |
| 4:L5:4742:G:H2'    | 4:L5:4743:G:H8     | 1.82                     | 0.45              |
| 8:LB:11:HIS:HE2    | 8:LB:237:THR:HG22  | 1.82                     | 0.45              |
| 14:LH:42:ASN:HD21  | 20:LO:131:PRO:HB2  | 1.82                     | 0.45              |
| 52:SC:183:LYS:HG2  | 72:SW:95:PRO:HA    | 1.99                     | 0.45              |
| 53:SD:196:GLY:O    | 53:SD:201:LYS:NZ   | 2.42                     | 0.45              |
| 57:SH:136:PRO:HB2  | 57:SH:162:GLN:HG2  | 1.98                     | 0.45              |
| 59:SJ:160:SER:OG   | 59:SJ:161:LEU:N    | 2.50                     | 0.45              |
| 64:SO:31:CYS:HA    | 64:SO:44:VAL:HA    | 1.98                     | 0.45              |
| 66:SQ:15:ARG:HA    | 66:SQ:19:ALA:HB3   | 1.98                     | 0.45              |
| 73:SX:140:ARG:HD2  | 73:SX:141:PRO:HD2  | 1.99                     | 0.45              |
| 4:L5:1391:A:H5'    | 22:LQ:181:ARG:HH12 | 1.81                     | 0.45              |
| 22:LQ:53:MET:HB3   | 22:LQ:57:ASN:HB2   | 1.98                     | 0.45              |
| 23:LR:36:ASN:OD1   | 23:LR:40:GLN:NE2   | 2.47                     | 0.45              |
| 27:LV:38:TYR:N     | 27:LV:64:THR:O     | 2.45                     | 0.45              |
| 32:La:76:ASP:N     | 32:La:76:ASP:OD1   | 2.49                     | 0.45              |
| 35:Ld:33:ILE:HD11  | 35:Ld:44:ARG:HB3   | 1.98                     | 0.45              |
| 49:S2:25:A:O2'     | 49:S2:26:U:O5'     | 2.35                     | 0.45              |
| 54:SE:97:GLU:OE2   | 54:SE:113:ARG:NE   | 2.44                     | 0.45              |
| 4:L5:1238:A:OP2    | 11:LE:60:SER:OG    | 2.34                     | 0.45              |
| 4:L5:2408:U:OP1    | 43:Ll:42:ARG:NH1   | 2.38                     | 0.45              |
| 4:L5:3868:G:H22    | 4:L5:3900:G:H1'    | 1.81                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:L5:4089:G:H1     | 4:L5:4160:C:H42    | 1.65                     | 0.45              |
| 10:LD:164:LYS:HG2  | 10:LD:195:HIS:HE1  | 1.81                     | 0.45              |
| 17:LL:178:ALA:HB1  | 32:La:146:LEU:HD23 | 1.98                     | 0.45              |
| 18:LM:5:ARG:NE     | 18:LM:59:ASP:OD1   | 2.50                     | 0.45              |
| 19:LN:192:TRP:O    | 19:LN:196:ASN:ND2  | 2.41                     | 0.45              |
| 49:S2:94:G:HO2'    | 49:S2:508:A:HO2'   | 1.63                     | 0.45              |
| 49:S2:835:C:H2'    | 49:S2:837:A:C8     | 2.51                     | 0.45              |
| 49:S2:1379:A:H2    | 50:SA:110:ASN:HD21 | 1.65                     | 0.45              |
| 49:S2:1407:U:O4    | 49:S2:1438:A:N6    | 2.50                     | 0.45              |
| 55:SF:61:PHE:CE2   | 78:Sc:49:PRO:HB2   | 2.52                     | 0.45              |
| 58:SI:65:PHE:O     | 58:SI:109:TYR:OH   | 2.29                     | 0.45              |
| 61:SL:35:ARG:NH2   | 61:SL:55:TYR:O     | 2.32                     | 0.45              |
| 4:L5:2755:A:OP1    | 31:LZ:65:ARG:NH1   | 2.40                     | 0.45              |
| 10:LD:107:ARG:HH12 | 10:LD:120:GLU:HA   | 1.81                     | 0.45              |
| 15:LI:202:SER:O    | 15:LI:202:SER:OG   | 2.32                     | 0.45              |
| 23:LR:42:ARG:HA    | 23:LR:45:ILE:HD12  | 1.99                     | 0.45              |
| 31:LZ:16:GLY:O     | 31:LZ:19:SER:OG    | 2.34                     | 0.45              |
| 49:S2:1633:A:H2'   | 49:S2:1634:A:C8    | 2.52                     | 0.45              |
| 82:Sg:240:CYS:SG   | 82:Sg:241:PHE:N    | 2.90                     | 0.45              |
| 4:L5:102:G:OP1     | 17:LL:71:ARG:NH2   | 2.38                     | 0.44              |
| 4:L5:4887:C:N4     | 4:L5:4931:G:O6     | 2.50                     | 0.44              |
| 10:LD:67:ALA:HA    | 10:LD:72:ASP:HA    | 1.98                     | 0.44              |
| 37:Lf:45:LYS:HA    | 37:Lf:107:PRO:HD2  | 1.97                     | 0.44              |
| 39:Lh:22:ASP:HA    | 39:Lh:25:LYS:HB2   | 1.97                     | 0.44              |
| 49:S2:292:A:H5'    | 61:SL:41:GLY:H     | 1.83                     | 0.44              |
| 49:S2:523:A:OP1    | 59:SJ:127:ARG:NE   | 2.50                     | 0.44              |
| 51:SB:71:LEU:HA    | 51:SB:74:LEU:HG    | 1.98                     | 0.44              |
| 54:SE:180:LEU:HG   | 54:SE:232:ASN:HA   | 1.99                     | 0.44              |
| 56:SG:2:LYS:HB2    | 56:SG:108:VAL:HG22 | 1.99                     | 0.44              |
| 57:SH:66:VAL:HA    | 57:SH:69:LEU:HB2   | 1.99                     | 0.44              |
| 77:Sb:74:THR:OG1   | 77:Sb:75:GLU:N     | 2.50                     | 0.44              |
| 4:L5:92:C:OP2      | 4:L5:4341:C:O2'    | 2.31                     | 0.44              |
| 4:L5:2667:C:OP1    | 23:LR:100:ARG:NE   | 2.37                     | 0.44              |
| 4:L5:2705:G:H1     | 4:L5:2710:C:H41    | 1.63                     | 0.44              |
| 4:L5:3607:U:OP1    | 23:LR:88:ARG:NH1   | 2.51                     | 0.44              |
| 8:LB:240:LEU:HB3   | 8:LB:244:THR:HG21  | 1.99                     | 0.44              |
| 35:Ld:36:VAL:HG11  | 35:Ld:44:ARG:HD3   | 1.99                     | 0.44              |
| 41:Lj:13:ASN:N     | 41:Lj:13:ASN:OD1   | 2.46                     | 0.44              |
| 49:S2:146:G:O5'    | 56:SG:140:ARG:NH2  | 2.47                     | 0.44              |
| 49:S2:1161:U:O4    | 73:SX:3:LYS:NZ     | 2.40                     | 0.44              |
| 49:S2:1604:G:N2    | 49:S2:1635:C:O2    | 2.50                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:SA:37:TYR:HA    | 50:SA:53:ARG:HD2   | 1.98                     | 0.44              |
| 50:SA:122:LEU:HB3  | 50:SA:144:THR:HG22 | 1.99                     | 0.44              |
| 60:SK:2:LEU:HD12   | 60:SK:2:LEU:HA     | 1.87                     | 0.44              |
| 66:SQ:51:LEU:HA    | 66:SQ:85:ARG:HE    | 1.80                     | 0.44              |
| 74:SY:74:MET:HE2   | 74:SY:74:MET:HB3   | 1.87                     | 0.44              |
| 79:Sd:20:SER:OG    | 79:Sd:21:CYS:N     | 2.50                     | 0.44              |
| 82:Sg:205:SER:HB3  | 82:Sg:221:LEU:HG   | 1.99                     | 0.44              |
| 4:L5:706:C:O2'     | 4:L5:1298:C:O2'    | 2.31                     | 0.44              |
| 4:L5:1562:G:O6     | 63:SN:140:LYS:NZ   | 2.50                     | 0.44              |
| 4:L5:1646:A:OP1    | 9:LC:63:SER:OG     | 2.33                     | 0.44              |
| 4:L5:2422:C:OP1    | 21:LP:127:ARG:NH2  | 2.47                     | 0.44              |
| 4:L5:4648:A:OP1    | 23:LR:62:ARG:NH2   | 2.51                     | 0.44              |
| 17:LL:164:GLU:H    | 17:LL:164:GLU:HG3  | 1.55                     | 0.44              |
| 50:SA:123:VAL:HG12 | 50:SA:145:ILE:HG12 | 2.00                     | 0.44              |
| 52:SC:125:LYS:HG2  | 52:SC:143:CYS:HB3  | 1.98                     | 0.44              |
| 58:SI:76:THR:OG1   | 58:SI:77:ARG:N     | 2.51                     | 0.44              |
| 66:SQ:34:VAL:HB    | 66:SQ:70:VAL:HG22  | 2.00                     | 0.44              |
| 82:Sg:126:ASP:OD1  | 82:Sg:126:ASP:N    | 2.39                     | 0.44              |
| 4:L5:5041:G:H22    | 8:LB:391:PRO:HD2   | 1.82                     | 0.44              |
| 20:LO:10:ASP:HB2   | 20:LO:117:ARG:HB3  | 1.99                     | 0.44              |
| 25:LT:112:ASN:HD21 | 25:LT:128:LEU:HB3  | 1.82                     | 0.44              |
| 28:LW:4:GLU:OE2    | 28:LW:20:ARG:NH2   | 2.45                     | 0.44              |
| 28:LW:82:ILE:HG21  | 28:LW:90:ILE:HD13  | 1.99                     | 0.44              |
| 30:LY:103:LYS:HA   | 30:LY:103:LYS:HD3  | 1.84                     | 0.44              |
| 47:Lp:25:MET:HE3   | 47:Lp:25:MET:HB2   | 1.89                     | 0.44              |
| 49:S2:84:A:H5'     | 74:SY:122:LYS:HD2  | 1.98                     | 0.44              |
| 49:S2:591:U:H5''   | 49:S2:592:C:H3'    | 1.97                     | 0.44              |
| 49:S2:1310:U:OP2   | 81:Sf:105:TYR:OH   | 2.26                     | 0.44              |
| 49:S2:1530:U:O2'   | 49:S2:1606:G:OP1   | 2.31                     | 0.44              |
| 49:S2:1648:G:O6    | 66:SQ:16:LYS:NZ    | 2.46                     | 0.44              |
| 52:SC:174:ILE:HD13 | 71:SV:4:ASP:HB3    | 1.99                     | 0.44              |
| 53:SD:6:SER:O      | 53:SD:10:LYS:N     | 2.45                     | 0.44              |
| 54:SE:252:ARG:HH21 | 59:SJ:79:ARG:HH22  | 1.64                     | 0.44              |
| 57:SH:10:LYS:HZ3   | 57:SH:10:LYS:HG2   | 1.61                     | 0.44              |
| 58:SI:62:VAL:HA    | 58:SI:77:ARG:HA    | 1.99                     | 0.44              |
| 62:SM:80:ASP:OD1   | 62:SM:80:ASP:N     | 2.46                     | 0.44              |
| 62:SM:118:SER:HB3  | 62:SM:121:LYS:HG3  | 1.99                     | 0.44              |
| 73:SX:107:ARG:HD3  | 73:SX:112:VAL:HG22 | 2.00                     | 0.44              |
| 77:Sb:83:GLN:OE1   | 77:Sb:84:HIS:ND1   | 2.39                     | 0.44              |
| 4:L5:197:A:N1      | 4:L5:225:G:O2'     | 2.42                     | 0.44              |
| 4:L5:318:A:H2'     | 4:L5:319:A:C8      | 2.52                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:L5:1943:A:N6     | 4:L5:2039:G:O2'    | 2.47                     | 0.44              |
| 7:LA:92:LYS:HA     | 7:LA:103:PRO:HD2   | 2.00                     | 0.44              |
| 15:LI:188:LYS:HB3  | 15:LI:212:LEU:HD11 | 1.99                     | 0.44              |
| 18:LM:31:ILE:HD11  | 18:LM:37:LEU:HB2   | 1.99                     | 0.44              |
| 51:SB:76:ASN:OD1   | 51:SB:76:ASN:N     | 2.46                     | 0.44              |
| 55:SF:182:LYS:HZ2  | 55:SF:184:SER:HB2  | 1.83                     | 0.44              |
| 57:SH:25:GLN:HA    | 57:SH:28:LEU:HG    | 2.00                     | 0.44              |
| 59:SJ:108:ARG:HH21 | 59:SJ:149:VAL:HG23 | 1.81                     | 0.44              |
| 69:ST:7:LYS:HD2    | 69:ST:66:LEU:HD11  | 1.98                     | 0.44              |
| 70:SU:21:ARG:HA    | 70:SU:90:ASP:HA    | 2.00                     | 0.44              |
| 71:SV:3:ASN:ND2    | 71:SV:4:ASP:OD1    | 2.51                     | 0.44              |
| 71:SV:55:ILE:HD13  | 71:SV:69:ILE:HG21  | 1.98                     | 0.44              |
| 4:L5:4195:G:OP2    | 33:Lb:3:LYS:NZ     | 2.48                     | 0.44              |
| 49:S2:198:U:O2'    | 49:S2:200:G:OP2    | 2.36                     | 0.44              |
| 49:S2:563:G:H2'    | 49:S2:564:A:C8     | 2.52                     | 0.44              |
| 49:S2:1580:A:H5''  | 70:SU:56:MET:HE3   | 1.99                     | 0.44              |
| 50:SA:176:TRP:HE1  | 50:SA:197:VAL:HG23 | 1.82                     | 0.44              |
| 55:SF:27:ASP:OD1   | 55:SF:27:ASP:N     | 2.51                     | 0.44              |
| 56:SG:38:ALA:HB1   | 56:SG:41:LEU:HD22  | 2.00                     | 0.44              |
| 62:SM:93:LYS:HD3   | 62:SM:93:LYS:HA    | 1.67                     | 0.44              |
| 71:SV:32:ILE:HD12  | 71:SV:60:ARG:HD2   | 2.00                     | 0.44              |
| 74:SY:42:GLU:O     | 74:SY:46:LYS:NZ    | 2.48                     | 0.44              |
| 82:Sg:149:GLU:N    | 82:Sg:171:ASP:OD2  | 2.51                     | 0.44              |
| 4:L5:3621:A:O2'    | 4:L5:4658:G:O2'    | 2.33                     | 0.44              |
| 4:L5:4115:G:N7     | 7:LA:93:LYS:NZ     | 2.63                     | 0.44              |
| 4:L5:4895:C:O2'    | 18:LM:132:LYS:NZ   | 2.50                     | 0.44              |
| 12:LF:36:LYS:HD3   | 12:LF:36:LYS:HA    | 1.85                     | 0.44              |
| 45:Ln:21:ARG:NH2   | 49:S2:1175:G:OP1   | 2.51                     | 0.44              |
| 49:S2:1449:G:H1'   | 49:S2:1450:G:H5'   | 1.99                     | 0.44              |
| 50:SA:147:LEU:O    | 50:SA:165:ASN:ND2  | 2.39                     | 0.44              |
| 53:SD:50:ILE:HD11  | 53:SD:58:VAL:HG11  | 1.99                     | 0.44              |
| 54:SE:155:LYS:N    | 54:SE:158:ASP:OD2  | 2.46                     | 0.44              |
| 57:SH:142:LYS:HB2  | 72:SW:54:ASP:HB3   | 2.00                     | 0.44              |
| 61:SL:136:LYS:O    | 61:SL:139:ARG:NH2  | 2.49                     | 0.44              |
| 4:L5:733:A:N6      | 4:L5:933:G:O6      | 2.47                     | 0.44              |
| 4:L5:1802:A:H5''   | 4:L5:1803:G:H5'    | 1.99                     | 0.44              |
| 4:L5:2835:A:O2'    | 8:LB:228:TYR:O     | 2.34                     | 0.44              |
| 6:L8:102:G:OP2     | 6:L8:104:A:O2'     | 2.32                     | 0.44              |
| 8:LB:44:THR:O      | 8:LB:44:THR:OG1    | 2.33                     | 0.44              |
| 11:LE:114:ARG:HG2  | 48:Lr:87:ARG:HG3   | 1.99                     | 0.44              |
| 26:LU:63:ILE:HD12  | 26:LU:63:ILE:HA    | 1.92                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 49:S2:373:G:H21   | 61:SL:83:GLN:NE2   | 2.15                     | 0.44              |
| 49:S2:1507:G:N2   | 81:Sf:88:PRO:O     | 2.48                     | 0.44              |
| 51:SB:59:SER:HA   | 51:SB:91:VAL:HG11  | 1.99                     | 0.44              |
| 75:SZ:41:ARG:HA   | 75:SZ:41:ARG:HD2   | 1.80                     | 0.44              |
| 4:L5:132:G:H2'    | 4:L5:133:C:H4'     | 2.00                     | 0.44              |
| 4:L5:1367:C:O2'   | 4:L5:1369:C:OP2    | 2.34                     | 0.44              |
| 4:L5:1628:C:H5''  | 7:LA:15:VAL:HG21   | 2.00                     | 0.44              |
| 4:L5:2876:G:P     | 47:Lp:5:THR:HG1    | 2.40                     | 0.44              |
| 4:L5:4520:G:N2    | 8:LB:255:GLY:O     | 2.30                     | 0.44              |
| 13:LG:253:LEU:HA  | 13:LG:256:ALA:HB3  | 2.00                     | 0.44              |
| 16:LJ:108:GLY:HA2 | 16:LJ:129:ASP:HA   | 2.00                     | 0.44              |
| 18:LM:25:VAL:HG12 | 18:LM:38:VAL:HG22  | 1.99                     | 0.44              |
| 18:LM:25:VAL:HG22 | 18:LM:45:VAL:HG21  | 1.99                     | 0.44              |
| 20:LO:113:ASP:OD1 | 20:LO:113:ASP:N    | 2.50                     | 0.44              |
| 25:LT:157:GLU:HB3 | 25:LT:159:MET:HE2  | 1.99                     | 0.44              |
| 27:LV:28:CYS:HB2  | 27:LV:37:LEU:HG    | 2.00                     | 0.44              |
| 49:S2:1308:U:O4   | 81:Sf:96:LYS:NZ    | 2.49                     | 0.44              |
| 51:SB:193:ILE:HA  | 51:SB:196:ASP:HB2  | 2.00                     | 0.44              |
| 52:SC:257:LYS:O   | 71:SV:16:LYS:NZ    | 2.37                     | 0.44              |
| 56:SG:121:ILE:O   | 56:SG:125:THR:OG1  | 2.36                     | 0.44              |
| 56:SG:208:GLU:O   | 56:SG:212:LEU:N    | 2.51                     | 0.44              |
| 57:SH:49:LYS:HD3  | 57:SH:49:LYS:HA    | 1.77                     | 0.44              |
| 68:SS:89:ASP:O    | 68:SS:92:ASP:N     | 2.41                     | 0.44              |
| 71:SV:33:GLN:HA   | 71:SV:54:ALA:HA    | 1.99                     | 0.44              |
| 23:LR:21:LYS:HA   | 23:LR:21:LYS:HD3   | 1.88                     | 0.43              |
| 48:Lr:105:ASP:OD1 | 48:Lr:105:ASP:N    | 2.51                     | 0.43              |
| 49:S2:433:A:OP1   | 58:SI:25:ARG:NH1   | 2.46                     | 0.43              |
| 49:S2:557:U:H2'   | 49:S2:558:G:C8     | 2.52                     | 0.43              |
| 52:SC:166:ARG:HB3 | 52:SC:247:THR:HG22 | 1.99                     | 0.43              |
| 57:SH:50:GLU:HA   | 57:SH:60:ILE:HA    | 2.00                     | 0.43              |
| 57:SH:70:LYS:HA   | 57:SH:73:GLN:HB2   | 2.00                     | 0.43              |
| 4:L5:85:G:O2'     | 4:L5:97:G:O6       | 2.29                     | 0.43              |
| 4:L5:1174:G:H1    | 4:L5:1186:U:H3     | 1.67                     | 0.43              |
| 4:L5:2876:G:OP1   | 47:Lp:5:THR:OG1    | 2.36                     | 0.43              |
| 4:L5:4249:G:HO2'  | 16:LJ:100:SER:HG   | 1.61                     | 0.43              |
| 4:L5:4771:C:N4    | 4:L5:4862:G:O6     | 2.52                     | 0.43              |
| 7:LA:117:GLU:HB2  | 7:LA:162:ASN:HB2   | 2.00                     | 0.43              |
| 9:LC:316:LYS:HB2  | 9:LC:324:ILE:HG13  | 2.00                     | 0.43              |
| 16:LJ:83:LEU:O    | 16:LJ:87:LEU:N     | 2.51                     | 0.43              |
| 22:LQ:144:LYS:HE2 | 22:LQ:144:LYS:HB3  | 1.83                     | 0.43              |
| 49:S2:71:G:O2'    | 49:S2:73:C:N4      | 2.51                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 54:SE:62:LYS:HE3   | 54:SE:62:LYS:HB3   | 1.88                     | 0.43              |
| 54:SE:72:ILE:HG12  | 54:SE:90:ILE:HG13  | 2.00                     | 0.43              |
| 60:SK:5:LYS:HD3    | 60:SK:5:LYS:HA     | 1.80                     | 0.43              |
| 62:SM:43:ASP:HB3   | 81:Sf:116:ARG:HH22 | 1.83                     | 0.43              |
| 68:SS:108:ARG:NH1  | 68:SS:109:GLU:OE1  | 2.51                     | 0.43              |
| 79:Sd:14:PHE:O     | 79:Sd:18:SER:OG    | 2.30                     | 0.43              |
| 82:Sg:167:SER:N    | 82:Sg:175:LYS:O    | 2.47                     | 0.43              |
| 4:L5:440:U:O2'     | 37:Lf:91:ASN:O     | 2.36                     | 0.43              |
| 4:L5:3732:A:H2'    | 4:L5:3733:A:C8     | 2.53                     | 0.43              |
| 4:L5:4761:G:P      | 20:LO:37:ARG:HH12  | 2.41                     | 0.43              |
| 10:LD:280:VAL:O    | 10:LD:284:LYS:N    | 2.48                     | 0.43              |
| 30:LY:128:VAL:HA   | 30:LY:131:GLU:HB3  | 1.99                     | 0.43              |
| 53:SD:129:SER:O    | 53:SD:129:SER:OG   | 2.35                     | 0.43              |
| 54:SE:177:THR:HA   | 54:SE:195:ILE:HB   | 1.99                     | 0.43              |
| 59:SJ:117:LEU:HD22 | 59:SJ:157:ILE:HD11 | 1.99                     | 0.43              |
| 68:SS:23:ARG:NH2   | 75:SZ:45:ASN:OD1   | 2.51                     | 0.43              |
| 70:SU:46:LYS:HZ3   | 70:SU:97:ILE:C     | 2.26                     | 0.43              |
| 78:Sc:29:GLN:HA    | 78:Sc:45:ASN:HA    | 2.01                     | 0.43              |
| 4:L5:3617:G:OP1    | 28:LW:44:ARG:NH1   | 2.50                     | 0.43              |
| 4:L5:3766:A:N1     | 49:S2:1827:U:O2'   | 2.45                     | 0.43              |
| 4:L5:4212:A:OP2    | 15:LI:15:LYS:NZ    | 2.51                     | 0.43              |
| 9:LC:84:THR:OG1    | 9:LC:85:HIS:N      | 2.51                     | 0.43              |
| 9:LC:205:ARG:HA    | 9:LC:205:ARG:HD3   | 1.79                     | 0.43              |
| 22:LQ:20:SER:O     | 22:LQ:26:ARG:NH1   | 2.50                     | 0.43              |
| 25:LT:45:MET:HE2   | 25:LT:45:MET:HB3   | 1.83                     | 0.43              |
| 33:Lb:22:LYS:HA    | 33:Lb:22:LYS:HD2   | 1.87                     | 0.43              |
| 49:S2:445:A:H5''   | 58:SI:47:ARG:HH21  | 1.84                     | 0.43              |
| 49:S2:498:C:N4     | 49:S2:504:G:O6     | 2.50                     | 0.43              |
| 49:S2:1130:G:H4'   | 63:SN:10:GLY:HA2   | 2.00                     | 0.43              |
| 49:S2:1861:G:H5''  | 76:Sa:3:LYS:HA     | 2.01                     | 0.43              |
| 56:SG:52:ILE:HD11  | 56:SG:102:VAL:HG21 | 2.00                     | 0.43              |
| 57:SH:57:ARG:HH22  | 57:SH:90:LYS:HA    | 1.84                     | 0.43              |
| 57:SH:186:ASN:OD1  | 57:SH:186:ASN:N    | 2.50                     | 0.43              |
| 58:SI:81:VAL:HA    | 58:SI:102:VAL:HA   | 2.00                     | 0.43              |
| 59:SJ:151:LEU:HD23 | 59:SJ:151:LEU:HA   | 1.84                     | 0.43              |
| 66:SQ:112:LEU:HD22 | 66:SQ:119:LEU:HD21 | 2.00                     | 0.43              |
| 72:SW:42:MET:HB3   | 72:SW:42:MET:HE2   | 1.84                     | 0.43              |
| 4:L5:691:C:H2'     | 4:L5:692:A:C8      | 2.53                     | 0.43              |
| 4:L5:1970:A:O2'    | 4:L5:2018:C:N3     | 2.51                     | 0.43              |
| 9:LC:333:LYS:HD2   | 11:LE:54:ILE:HG12  | 2.01                     | 0.43              |
| 10:LD:223:PHE:HB3  | 10:LD:226:TYR:HB2  | 2.00                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:LG:212:LYS:HE3  | 13:LG:212:LYS:HB2  | 1.84                     | 0.43              |
| 20:LO:26:GLN:OE1   | 20:LO:31:ARG:NH1   | 2.51                     | 0.43              |
| 37:Lf:9:ALA:O      | 37:Lf:100:ARG:NH1  | 2.49                     | 0.43              |
| 37:Lf:45:LYS:HD2   | 37:Lf:105:LEU:HA   | 2.00                     | 0.43              |
| 76:Sa:59:PHE:HB2   | 76:Sa:62:TYR:HB2   | 1.99                     | 0.43              |
| 4:L5:957:G:OP1     | 36:Le:65:LYS:NZ    | 2.45                     | 0.43              |
| 4:L5:1895:G:O2'    | 4:L5:1907:A:N3     | 2.46                     | 0.43              |
| 4:L5:2906:G:H2'    | 4:L5:2908:U:H1'    | 2.00                     | 0.43              |
| 4:L5:3811:G:O2'    | 4:L5:3814:U:OP2    | 2.37                     | 0.43              |
| 4:L5:4122:G:O6     | 38:Lg:101:LYS:NZ   | 2.45                     | 0.43              |
| 8:LB:144:LYS:HE3   | 8:LB:144:LYS:HB3   | 1.77                     | 0.43              |
| 8:LB:189:THR:O     | 8:LB:193:LYS:N     | 2.52                     | 0.43              |
| 13:LG:94:GLN:HG3   | 13:LG:218:LEU:HD21 | 2.00                     | 0.43              |
| 49:S2:467:G:H4'    | 56:SG:72:ARG:HH22  | 1.83                     | 0.43              |
| 49:S2:1096:G:OP1   | 72:SW:22:LYS:NZ    | 2.52                     | 0.43              |
| 51:SB:103:MET:HG2  | 51:SB:188:LEU:HD13 | 2.01                     | 0.43              |
| 54:SE:45:ILE:HG13  | 54:SE:61:VAL:HG11  | 2.00                     | 0.43              |
| 58:SI:177:SER:OG   | 58:SI:178:ARG:N    | 2.52                     | 0.43              |
| 59:SJ:114:VAL:HG13 | 59:SJ:126:ALA:HB1  | 2.01                     | 0.43              |
| 81:Sf:134:SER:O    | 81:Sf:134:SER:OG   | 2.35                     | 0.43              |
| 4:L5:439:G:O3'     | 37:Lf:91:ASN:ND2   | 2.52                     | 0.43              |
| 4:L5:2370:A:N7     | 35:Ld:39:LYS:NZ    | 2.57                     | 0.43              |
| 4:L5:4546:A:N7     | 7:LA:215:ASN:ND2   | 2.66                     | 0.43              |
| 10:LD:27:LYS:HE2   | 16:LJ:147:ARG:HD3  | 2.01                     | 0.43              |
| 36:Le:90:MET:HG3   | 48:Lr:33:LYS:HA    | 2.00                     | 0.43              |
| 49:S2:560:A:H5'    | 59:SJ:174:LYS:HB3  | 2.00                     | 0.43              |
| 49:S2:1596:U:O4    | 49:S2:1597:C:N4    | 2.52                     | 0.43              |
| 52:SC:246:LYS:HE2  | 52:SC:246:LYS:HB3  | 1.77                     | 0.43              |
| 58:SI:86:SER:OG    | 58:SI:87:ASN:N     | 2.50                     | 0.43              |
| 60:SK:26:ASP:N     | 60:SK:26:ASP:OD1   | 2.49                     | 0.43              |
| 64:SO:70:SER:HB2   | 64:SO:73:ALA:H     | 1.84                     | 0.43              |
| 64:SO:92:ALA:HB2   | 64:SO:125:LYS:HB2  | 2.01                     | 0.43              |
| 81:Sf:135:HIS:CD2  | 81:Sf:138:ARG:HH22 | 2.37                     | 0.43              |
| 4:L5:700:G:H2'     | 4:L5:701:G:C8      | 2.53                     | 0.43              |
| 4:L5:1961:G:N1     | 4:L5:2024:G:O2'    | 2.42                     | 0.43              |
| 4:L5:2402:G:O2'    | 38:Lg:10:ARG:O     | 2.36                     | 0.43              |
| 8:LB:39:LYS:HB2    | 8:LB:187:GLY:HA2   | 2.01                     | 0.43              |
| 9:LC:231:ASN:HD22  | 9:LC:234:LYS:HD2   | 1.83                     | 0.43              |
| 22:LQ:66:MET:HE3   | 22:LQ:66:MET:HB2   | 1.95                     | 0.43              |
| 27:LV:82:ILE:HD12  | 27:LV:121:VAL:HG22 | 2.00                     | 0.43              |
| 49:S2:373:G:H1     | 49:S2:391:C:H42    | 1.67                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:S2:607:U:O4     | 53:SD:144:GLY:N    | 2.52                     | 0.43              |
| 49:S2:969:U:O2     | 49:S2:971:G:N1     | 2.51                     | 0.43              |
| 49:S2:975:G:O3'    | 64:SO:32:HIS:NE2   | 2.51                     | 0.43              |
| 50:SA:176:TRP:NE1  | 50:SA:197:VAL:O    | 2.49                     | 0.43              |
| 54:SE:196:THR:OG1  | 54:SE:209:HIS:O    | 2.31                     | 0.43              |
| 57:SH:109:ARG:HA   | 57:SH:109:ARG:HD3  | 1.79                     | 0.43              |
| 59:SJ:176:LYS:HA   | 59:SJ:179:LYS:HG2  | 2.01                     | 0.43              |
| 77:Sb:34:ASP:OD1   | 77:Sb:82:LYS:NZ    | 2.41                     | 0.43              |
| 4:L5:2341:A:OP2    | 32:La:4:ARG:NH2    | 2.44                     | 0.43              |
| 4:L5:4208:U:OP1    | 4:L5:4334:U:O2'    | 2.27                     | 0.43              |
| 8:LB:28:LYS:HE3    | 8:LB:28:LYS:HB2    | 1.74                     | 0.43              |
| 16:LJ:109:ILE:HD13 | 16:LJ:109:ILE:HA   | 1.88                     | 0.43              |
| 20:LO:47:PHE:HZ    | 20:LO:144:GLU:HG3  | 1.84                     | 0.43              |
| 24:LS:43:ARG:HA    | 24:LS:43:ARG:HD2   | 1.83                     | 0.43              |
| 49:S2:53:C:O2'     | 49:S2:507:G:N7     | 2.45                     | 0.43              |
| 56:SG:138:ALA:HA   | 56:SG:176:ILE:HD11 | 2.01                     | 0.43              |
| 57:SH:158:LEU:HD21 | 57:SH:187:PHE:HD2  | 1.82                     | 0.43              |
| 61:SL:12:LYS:HE3   | 61:SL:12:LYS:HB2   | 1.83                     | 0.43              |
| 80:Se:102:THR:HA   | 80:Se:106:LYS:HB2  | 1.99                     | 0.43              |
| 4:L5:713:C:O2      | 11:LE:130:LYS:NZ   | 2.41                     | 0.43              |
| 4:L5:2385:U:OP1    | 23:LR:5:ARG:NH2    | 2.45                     | 0.43              |
| 4:L5:4100:C:N4     | 4:L5:4110:C:H42    | 2.17                     | 0.43              |
| 4:L5:4635:A:O2'    | 4:L5:4637:G:OP1    | 2.37                     | 0.43              |
| 7:LA:33:ASP:OD2    | 7:LA:67:TYR:OH     | 2.32                     | 0.43              |
| 30:LY:52:ASP:OD1   | 30:LY:52:ASP:N     | 2.49                     | 0.43              |
| 41:Lj:64:MET:HG2   | 41:Lj:67:LEU:HB2   | 2.01                     | 0.43              |
| 49:S2:493:A:H61    | 49:S2:510:G:H1'    | 1.84                     | 0.43              |
| 56:SG:167:LYS:HE3  | 56:SG:167:LYS:HB3  | 1.82                     | 0.43              |
| 60:SK:41:PRO:HB2   | 60:SK:44:HIS:HD2   | 1.83                     | 0.43              |
| 61:SL:144:LYS:HE2  | 61:SL:144:LYS:HB3  | 1.84                     | 0.43              |
| 63:SN:5:HIS:HB2    | 63:SN:121:ARG:HH11 | 1.84                     | 0.43              |
| 71:SV:20:SER:HB3   | 71:SV:59:ILE:HD11  | 2.00                     | 0.43              |
| 76:Sa:22:ARG:HD2   | 76:Sa:27:ALA:HB1   | 2.01                     | 0.43              |
| 78:Sc:14:VAL:HB    | 78:Sc:54:ASP:H     | 1.84                     | 0.43              |
| 4:L5:486:C:N4      | 4:L5:487:G:O6      | 2.52                     | 0.42              |
| 4:L5:725:G:H5'     | 9:LC:346:ASN:HD22  | 1.83                     | 0.42              |
| 4:L5:2474:G:C5     | 29:LX:47:ARG:HG2   | 2.53                     | 0.42              |
| 4:L5:2874:U:H5''   | 4:L5:2875:C:H5     | 1.83                     | 0.42              |
| 4:L5:3658:C:H2'    | 4:L5:3659:G:C8     | 2.53                     | 0.42              |
| 8:LB:8:ALA:HB2     | 27:LV:49:LEU:HD22  | 2.00                     | 0.42              |
| 26:LU:64:GLU:OE1   | 26:LU:71:THR:OG1   | 2.37                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 49:S2:925:G:H1    | 49:S2:1017:U:H3    | 1.67                     | 0.42              |
| 50:SA:168:ALA:HB1 | 50:SA:204:TYR:HB3  | 2.00                     | 0.42              |
| 52:SC:113:GLN:HB3 | 52:SC:122:THR:HG22 | 2.00                     | 0.42              |
| 54:SE:10:LYS:HA   | 54:SE:10:LYS:HD3   | 1.87                     | 0.42              |
| 68:SS:46:ARG:HH12 | 69:ST:50:GLU:HA    | 1.84                     | 0.42              |
| 73:SX:142:ARG:HE  | 73:SX:142:ARG:HB2  | 1.69                     | 0.42              |
| 76:Sa:20:PRO:HA   | 76:Sa:31:PRO:HA    | 2.00                     | 0.42              |
| 4:L5:707:C:O2'    | 4:L5:4943:A:N1     | 2.49                     | 0.42              |
| 4:L5:1565:A:C5    | 4:L5:1566:C:H1'    | 2.55                     | 0.42              |
| 4:L5:2392:C:OP1   | 4:L5:4654:C:O2'    | 2.37                     | 0.42              |
| 4:L5:2652:G:H22   | 47:Lp:59:SER:HA    | 1.83                     | 0.42              |
| 5:L7:7:G:H4'      | 10:LD:33:ARG:HH11  | 1.84                     | 0.42              |
| 26:LU:20:LYS:HB3  | 26:LU:73:THR:HG23  | 2.00                     | 0.42              |
| 27:LV:43:LYS:HE3  | 27:LV:43:LYS:HB3   | 1.84                     | 0.42              |
| 29:LX:131:ASP:HA  | 43:Ll:14:ALA:HB1   | 2.01                     | 0.42              |
| 40:Li:75:LYS:HD2  | 40:Li:75:LYS:HA    | 1.79                     | 0.42              |
| 49:S2:114:G:O2'   | 49:S2:382:C:O2'    | 2.25                     | 0.42              |
| 49:S2:124:U:OP1   | 54:SE:148:ARG:NH2  | 2.48                     | 0.42              |
| 49:S2:1566:G:N7   | 69:ST:101:ARG:NH2  | 2.53                     | 0.42              |
| 49:S2:1612:G:OP1  | 65:SP:18:ARG:NH1   | 2.38                     | 0.42              |
| 50:SA:34:MET:HE1  | 50:SA:162:PRO:HB3  | 2.00                     | 0.42              |
| 51:SB:168:MET:HG3 | 51:SB:197:ILE:HG21 | 2.01                     | 0.42              |
| 55:SF:167:LYS:NZ  | 55:SF:175:ASP:OD1  | 2.49                     | 0.42              |
| 65:SP:21:ASP:OD1  | 65:SP:22:LEU:N     | 2.52                     | 0.42              |
| 69:ST:83:GLN:HB2  | 69:ST:93:SER:HB3   | 2.01                     | 0.42              |
| 74:SY:23:MET:SD   | 74:SY:23:MET:N     | 2.93                     | 0.42              |
| 74:SY:41:ARG:O    | 74:SY:45:ALA:N     | 2.47                     | 0.42              |
| 79:Sd:36:LEU:HD23 | 79:Sd:36:LEU:HA    | 1.90                     | 0.42              |
| 82:Sg:30:MET:HE1  | 82:Sg:44:LYS:HG3   | 2.00                     | 0.42              |
| 4:L5:136:C:OP1    | 39:Lh:96:ASN:ND2   | 2.52                     | 0.42              |
| 4:L5:1397:A:C8    | 32:La:114:LYS:HD2  | 2.54                     | 0.42              |
| 4:L5:1650:A:H61   | 9:LC:104:PRO:HD3   | 1.85                     | 0.42              |
| 4:L5:3879:G:O2'   | 4:L5:3881:G:OP2    | 2.35                     | 0.42              |
| 6:L8:87:G:OP2     | 39:Lh:5:LYS:NZ     | 2.41                     | 0.42              |
| 10:LD:220:LYS:O   | 10:LD:224:SER:OG   | 2.30                     | 0.42              |
| 11:LE:192:LYS:HG2 | 37:Lf:107:PRO:HA   | 2.01                     | 0.42              |
| 27:LV:26:ILE:HG23 | 27:LV:102:ALA:HA   | 2.01                     | 0.42              |
| 49:S2:950:C:H42   | 49:S2:976:G:H1     | 1.67                     | 0.42              |
| 49:S2:1348:G:H1   | 49:S2:1381:G:H22   | 1.67                     | 0.42              |
| 50:SA:143:PRO:HB3 | 71:SV:32:ILE:HG21  | 2.01                     | 0.42              |
| 51:SB:165:ARG:HA  | 51:SB:168:MET:HB3  | 2.01                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 64:SO:143:LYS:HE3  | 64:SO:143:LYS:HB2  | 1.83                     | 0.42              |
| 67:SR:88:VAL:HG23  | 67:SR:91:LEU:HB2   | 2.00                     | 0.42              |
| 68:SS:34:LYS:HB3   | 68:SS:103:LEU:HD23 | 2.02                     | 0.42              |
| 73:SX:51:VAL:HA    | 73:SX:72:VAL:HA    | 2.02                     | 0.42              |
| 76:Sa:86:ASN:OD1   | 76:Sa:86:ASN:N     | 2.50                     | 0.42              |
| 4:L5:338:A:OP1     | 17:LL:31:ARG:NH1   | 2.48                     | 0.42              |
| 4:L5:3711:A:H8     | 4:L5:3712:A:C8     | 2.37                     | 0.42              |
| 4:L5:4133:C:OP1    | 4:L5:4144:C:N4     | 2.52                     | 0.42              |
| 12:LF:247:MET:HE2  | 12:LF:247:MET:HB3  | 1.81                     | 0.42              |
| 36:Le:85:LEU:HD21  | 36:Le:115:ALA:HB2  | 2.01                     | 0.42              |
| 49:S2:492:C:H2'    | 49:S2:506:G:H22    | 1.85                     | 0.42              |
| 53:SD:37:VAL:HG12  | 53:SD:50:ILE:HA    | 2.01                     | 0.42              |
| 59:SJ:11:LYS:HD3   | 59:SJ:11:LYS:HA    | 1.57                     | 0.42              |
| 61:SL:111:VAL:HG11 | 61:SL:128:VAL:HG21 | 2.02                     | 0.42              |
| 74:SY:39:GLU:O     | 74:SY:43:LYS:N     | 2.46                     | 0.42              |
| 81:Sf:137:ASP:OD1  | 81:Sf:137:ASP:N    | 2.52                     | 0.42              |
| 4:L5:1501:C:H2'    | 22:LQ:68:ARG:HH22  | 1.83                     | 0.42              |
| 4:L5:2102:G:N3     | 4:L5:2103:G:N1     | 2.68                     | 0.42              |
| 5:L7:5:A:O2'       | 10:LD:63:GLN:NE2   | 2.52                     | 0.42              |
| 8:LB:14:LEU:HA     | 8:LB:17:LEU:HD13   | 2.01                     | 0.42              |
| 9:LC:24:LEU:HD12   | 9:LC:25:PRO:HD2    | 2.02                     | 0.42              |
| 11:LE:136:HIS:O    | 11:LE:138:ARG:NH1  | 2.52                     | 0.42              |
| 13:LG:230:TYR:HA   | 13:LG:233:ILE:HG12 | 2.02                     | 0.42              |
| 33:Lb:72:ILE:HD12  | 33:Lb:72:ILE:HA    | 1.94                     | 0.42              |
| 38:Lg:84:ALA:HA    | 38:Lg:87:VAL:HG12  | 2.01                     | 0.42              |
| 49:S2:1451:G:H4'   | 82:Sg:65:PHE:HZ    | 1.84                     | 0.42              |
| 4:L5:32:G:H21      | 4:L5:50:C:H5       | 1.67                     | 0.42              |
| 4:L5:156:G:N2      | 4:L5:157:U:O4      | 2.53                     | 0.42              |
| 7:LA:20:VAL:HG12   | 7:LA:23:ARG:HD2    | 2.01                     | 0.42              |
| 34:Lc:9:LYS:N      | 34:Lc:12:GLU:OE2   | 2.53                     | 0.42              |
| 35:Ld:92:ARG:HA    | 35:Ld:102:LEU:HD12 | 2.01                     | 0.42              |
| 48:Lr:56:ASP:OD1   | 48:Lr:56:ASP:N     | 2.52                     | 0.42              |
| 53:SD:148:LYS:HE2  | 53:SD:148:LYS:HB2  | 1.84                     | 0.42              |
| 56:SG:12:CYS:SG    | 56:SG:13:GLN:N     | 2.92                     | 0.42              |
| 66:SQ:87:SER:O     | 66:SQ:91:ALA:N     | 2.52                     | 0.42              |
| 66:SQ:105:LYS:HB2  | 66:SQ:105:LYS:HE2  | 1.77                     | 0.42              |
| 67:SR:98:VAL:HG13  | 67:SR:102:THR:HB   | 2.01                     | 0.42              |
| 4:L5:990:C:N4      | 4:L5:992:C:O2      | 2.52                     | 0.42              |
| 8:LB:63:PRO:HD2    | 8:LB:357:ARG:HH22  | 1.84                     | 0.42              |
| 17:LL:7:GLY:O      | 32:La:49:HIS:NE2   | 2.48                     | 0.42              |
| 46:Lo:75:PRO:HA    | 46:Lo:78:ARG:HH22  | 1.84                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:S2:192:C:H3'    | 58:SI:141:ARG:HH21 | 1.84                     | 0.42              |
| 49:S2:1566:G:H1    | 69:ST:97:LYS:HE3   | 1.85                     | 0.42              |
| 54:SE:183:VAL:HG11 | 54:SE:188:ASN:HB2  | 2.02                     | 0.42              |
| 58:SI:10:LYS:HB2   | 58:SI:10:LYS:HE3   | 1.81                     | 0.42              |
| 62:SM:113:ASP:HB2  | 62:SM:116:LYS:HG2  | 2.01                     | 0.42              |
| 82:Sg:74:ASP:OD1   | 82:Sg:74:ASP:N     | 2.41                     | 0.42              |
| 4:L5:688:U:OP1     | 11:LE:94:LYS:NZ    | 2.41                     | 0.42              |
| 4:L5:965:G:N2      | 4:L5:2092:G:H1'    | 2.34                     | 0.42              |
| 4:L5:1391:A:OP1    | 22:LQ:181:ARG:NH2  | 2.44                     | 0.42              |
| 4:L5:1646:A:O2'    | 41:Lj:49:TRP:O     | 2.29                     | 0.42              |
| 14:LH:129:ARG:HA   | 14:LH:129:ARG:HD3  | 1.86                     | 0.42              |
| 15:LI:169:LYS:HE2  | 15:LI:169:LYS:HB3  | 1.83                     | 0.42              |
| 27:LV:85:ARG:HE    | 27:LV:100:ASP:HA   | 1.85                     | 0.42              |
| 49:S2:463:C:O2'    | 49:S2:466:G:O6     | 2.27                     | 0.42              |
| 49:S2:527:C:OP2    | 80:Se:108:ARG:NH1  | 2.42                     | 0.42              |
| 49:S2:960:U:O2'    | 49:S2:962:A:N7     | 2.43                     | 0.42              |
| 49:S2:993:G:OP1    | 49:S2:1131:G:N2    | 2.45                     | 0.42              |
| 49:S2:1290:G:O6    | 81:Sf:95:ARG:NH2   | 2.30                     | 0.42              |
| 49:S2:1414:A:H4'   | 69:ST:125:PRO:HB3  | 2.02                     | 0.42              |
| 50:SA:168:ALA:HA   | 50:SA:171:VAL:HG12 | 2.02                     | 0.42              |
| 52:SC:103:LYS:HG3  | 52:SC:216:MET:HE1  | 2.01                     | 0.42              |
| 55:SF:140:ASP:HB2  | 78:Sc:46:VAL:HG23  | 2.02                     | 0.42              |
| 58:SI:134:GLU:HA   | 58:SI:137:LEU:HB2  | 2.02                     | 0.42              |
| 4:L5:223:G:N3      | 9:LC:223:ASN:ND2   | 2.51                     | 0.42              |
| 4:L5:1273:G:O6     | 4:L5:1274:A:N6     | 2.52                     | 0.42              |
| 4:L5:1503:A:H4'    | 4:L5:1504:G:H5'    | 2.01                     | 0.42              |
| 4:L5:1814:C:OP1    | 33:Lb:52:LYS:NZ    | 2.42                     | 0.42              |
| 9:LC:33:ARG:NH2    | 9:LC:35:ASP:OD2    | 2.44                     | 0.42              |
| 11:LE:149:ILE:O    | 11:LE:197:THR:OG1  | 2.38                     | 0.42              |
| 14:LH:82:LYS:HB2   | 14:LH:82:LYS:HE3   | 1.87                     | 0.42              |
| 31:LZ:51:ARG:HB3   | 31:LZ:65:ARG:HG2   | 2.02                     | 0.42              |
| 49:S2:1448:A:O2'   | 49:S2:1449:G:O4'   | 2.38                     | 0.42              |
| 50:SA:30:LEU:HD22  | 50:SA:47:TYR:CZ    | 2.55                     | 0.42              |
| 55:SF:102:LEU:HD11 | 75:SZ:67:LEU:HD13  | 2.01                     | 0.42              |
| 62:SM:42:LEU:HB3   | 62:SM:68:LEU:HD22  | 2.01                     | 0.42              |
| 69:ST:116:ASP:OD2  | 69:ST:122:LYS:N    | 2.53                     | 0.42              |
| 72:SW:36:ARG:HD3   | 72:SW:36:ARG:HA    | 1.89                     | 0.42              |
| 82:Sg:65:PHE:HB2   | 82:Sg:83:TRP:HD1   | 1.84                     | 0.42              |
| 4:L5:959:G:O2'     | 4:L5:2263:A:N6     | 2.53                     | 0.42              |
| 4:L5:2034:G:O2'    | 24:LS:118:ARG:NH2  | 2.51                     | 0.42              |
| 8:LB:268:ARG:HA    | 8:LB:268:ARG:HD3   | 1.72                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:LB:282:LYS:HA    | 8:LB:282:LYS:HD3   | 1.87                     | 0.42              |
| 9:LC:297:GLU:H     | 9:LC:297:GLU:HG3   | 1.72                     | 0.42              |
| 49:S2:573:U:O2'    | 49:S2:575:A:N7     | 2.47                     | 0.42              |
| 49:S2:604:A:N3     | 49:S2:639:C:O2'    | 2.48                     | 0.42              |
| 49:S2:1461:G:O2'   | 49:S2:1464:C:N4    | 2.41                     | 0.42              |
| 51:SB:87:ILE:H     | 51:SB:101:HIS:HB2  | 1.83                     | 0.42              |
| 58:SI:205:ARG:H    | 58:SI:205:ARG:HG3  | 1.66                     | 0.42              |
| 62:SM:25:ALA:HB1   | 62:SM:31:LEU:HB2   | 2.01                     | 0.42              |
| 67:SR:43:SER:HB3   | 67:SR:46:LEU:HB3   | 2.02                     | 0.42              |
| 82:Sg:185:LYS:HB3  | 82:Sg:186:THR:H    | 1.74                     | 0.42              |
| 4:L5:120:A:H2'     | 4:L5:149:A:H61     | 1.85                     | 0.41              |
| 4:L5:2527:A:OP1    | 23:LR:9:ARG:NH1    | 2.47                     | 0.41              |
| 4:L5:4941:G:OP2    | 11:LE:188:ARG:NH1  | 2.44                     | 0.41              |
| 15:LI:164:LYS:HE2  | 15:LI:164:LYS:HB3  | 1.87                     | 0.41              |
| 23:LR:140:GLU:O    | 23:LR:144:LYS:NZ   | 2.39                     | 0.41              |
| 24:LS:71:SER:O     | 24:LS:76:LYS:NZ    | 2.53                     | 0.41              |
| 27:LV:30:ASP:HB3   | 27:LV:104:VAL:HG12 | 2.01                     | 0.41              |
| 31:LZ:117:LYS:HD2  | 31:LZ:117:LYS:HA   | 1.90                     | 0.41              |
| 49:S2:595:U:O2'    | 49:S2:596:U:O4'    | 2.38                     | 0.41              |
| 49:S2:1493:C:O2'   | 49:S2:1499:U:O4    | 2.28                     | 0.41              |
| 51:SB:88:THR:HG22  | 51:SB:98:THR:HB    | 2.01                     | 0.41              |
| 52:SC:187:ARG:HD3  | 52:SC:192:LEU:HD12 | 2.02                     | 0.41              |
| 55:SF:201:LYS:HE3  | 55:SF:201:LYS:HB3  | 1.91                     | 0.41              |
| 60:SK:47:LYS:HA    | 60:SK:47:LYS:HD2   | 1.81                     | 0.41              |
| 67:SR:71:ILE:HD12  | 67:SR:71:ILE:HA    | 1.93                     | 0.41              |
| 74:SY:117:VAL:HG23 | 74:SY:122:LYS:HG2  | 2.02                     | 0.41              |
| 4:L5:172:C:H4'     | 4:L5:173:C:H5'     | 2.01                     | 0.41              |
| 4:L5:1502:G:OP1    | 22:LQ:65:ARG:NH1   | 2.53                     | 0.41              |
| 4:L5:2029:A:H2'    | 4:L5:2030:A:C8     | 2.55                     | 0.41              |
| 22:LQ:151:HIS:CE1  | 22:LQ:164:LYS:HD2  | 2.55                     | 0.41              |
| 25:LT:71:ALA:HA    | 25:LT:92:ARG:HA    | 2.02                     | 0.41              |
| 26:LU:65:ARG:HE    | 26:LU:65:ARG:HB2   | 1.68                     | 0.41              |
| 31:LZ:12:LEU:HD23  | 31:LZ:12:LEU:HA    | 1.87                     | 0.41              |
| 31:LZ:35:ASP:N     | 31:LZ:35:ASP:OD1   | 2.53                     | 0.41              |
| 35:Ld:95:ASP:N     | 35:Ld:95:ASP:OD1   | 2.50                     | 0.41              |
| 37:Lf:40:GLU:HA    | 37:Lf:43:LEU:HD23  | 2.02                     | 0.41              |
| 49:S2:1404:U:N3    | 49:S2:1580:A:OP1   | 2.53                     | 0.41              |
| 50:SA:184:ARG:HB3  | 50:SA:191:ARG:HE   | 1.85                     | 0.41              |
| 55:SF:155:CYS:SG   | 55:SF:159:ARG:NH1  | 2.81                     | 0.41              |
| 81:Sf:99:LYS:HB3   | 81:Sf:100:LEU:HD12 | 2.03                     | 0.41              |
| 4:L5:1590:C:H4'    | 4:L5:2857:A:H5'    | 2.02                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:L5:1741:G:O6     | 5:L7:103:A:O2'     | 2.27                     | 0.41              |
| 4:L5:1800:U:H2'    | 4:L5:1801:A:H8     | 1.85                     | 0.41              |
| 8:LB:85:VAL:HG22   | 8:LB:204:GLN:HG2   | 2.02                     | 0.41              |
| 15:LI:32:ARG:HA    | 15:LI:32:ARG:HD3   | 1.73                     | 0.41              |
| 18:LM:118:MET:HE3  | 18:LM:122:ILE:HD11 | 2.01                     | 0.41              |
| 49:S2:1387:G:N2    | 53:SD:206:ASP:OD2  | 2.51                     | 0.41              |
| 52:SC:161:SER:O    | 52:SC:161:SER:OG   | 2.34                     | 0.41              |
| 59:SJ:52:LYS:HB2   | 59:SJ:52:LYS:HE3   | 1.84                     | 0.41              |
| 66:SQ:109:LYS:HE3  | 66:SQ:109:LYS:HB3  | 1.90                     | 0.41              |
| 74:SY:51:THR:OG1   | 74:SY:53:ASP:OD1   | 2.37                     | 0.41              |
| 82:Sg:96:THR:OG1   | 82:Sg:97:THR:N     | 2.53                     | 0.41              |
| 82:Sg:124:SER:OG   | 82:Sg:126:ASP:OD1  | 2.33                     | 0.41              |
| 4:L5:1283:G:N1     | 4:L5:2076:G:OP1    | 2.42                     | 0.41              |
| 4:L5:3711:A:H2'    | 4:L5:3712:A:H8     | 1.86                     | 0.41              |
| 4:L5:4088:C:OP1    | 7:LA:37:ARG:NH2    | 2.41                     | 0.41              |
| 4:L5:4718:G:OP1    | 8:LB:20:LYS:NZ     | 2.46                     | 0.41              |
| 4:L5:4729:A:OP1    | 4:L5:4964:C:O2'    | 2.36                     | 0.41              |
| 5:L7:49:A:H5''     | 10:LD:224:SER:HB2  | 2.02                     | 0.41              |
| 10:LD:164:LYS:HD2  | 10:LD:164:LYS:HA   | 1.84                     | 0.41              |
| 11:LE:248:ILE:HD13 | 11:LE:248:ILE:HA   | 1.93                     | 0.41              |
| 13:LG:48:LYS:HA    | 13:LG:48:LYS:HD3   | 1.77                     | 0.41              |
| 15:LI:152:LEU:HB3  | 15:LI:165:ILE:HD12 | 2.01                     | 0.41              |
| 30:LY:32:SER:OG    | 30:LY:101:PRO:O    | 2.32                     | 0.41              |
| 31:LZ:11:VAL:HG23  | 31:LZ:82:PRO:HA    | 2.03                     | 0.41              |
| 49:S2:355:G:OP2    | 61:SL:107:LYS:NZ   | 2.40                     | 0.41              |
| 49:S2:683:G:H4'    | 72:SW:4:MET:HG3    | 2.02                     | 0.41              |
| 49:S2:1205:C:O2'   | 49:S2:1834:A:N6    | 2.53                     | 0.41              |
| 49:S2:1523:C:H2'   | 49:S2:1524:G:H8    | 1.85                     | 0.41              |
| 50:SA:9:GLN:HG3    | 50:SA:10:MET:H     | 1.84                     | 0.41              |
| 52:SC:103:LYS:HD2  | 52:SC:133:TYR:CZ   | 2.55                     | 0.41              |
| 71:SV:40:ASP:OD2   | 71:SV:40:ASP:N     | 2.53                     | 0.41              |
| 74:SY:32:LYS:HB3   | 74:SY:32:LYS:HE2   | 1.87                     | 0.41              |
| 82:Sg:35:SER:OG    | 82:Sg:37:ASP:OD1   | 2.22                     | 0.41              |
| 4:L5:499:G:H2'     | 4:L5:504:G:N2      | 2.36                     | 0.41              |
| 4:L5:711:A:O2'     | 11:LE:136:HIS:ND1  | 2.45                     | 0.41              |
| 4:L5:2318:G:N2     | 4:L5:2321:G:OP2    | 2.40                     | 0.41              |
| 9:LC:283:LYS:HE3   | 22:LQ:103:LEU:HD12 | 2.03                     | 0.41              |
| 10:LD:157:ASN:N    | 10:LD:157:ASN:OD1  | 2.51                     | 0.41              |
| 13:LG:78:PRO:HA    | 13:LG:81:ASN:HB3   | 2.03                     | 0.41              |
| 14:LH:160:LEU:HD23 | 14:LH:160:LEU:HA   | 1.93                     | 0.41              |
| 16:LJ:75:ARG:HA    | 16:LJ:75:ARG:HD3   | 1.81                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:LJ:92:TYR:HB3   | 16:LJ:172:GLY:HA2  | 2.02                     | 0.41              |
| 21:LP:94:MET:HE3   | 21:LP:94:MET:HB2   | 1.76                     | 0.41              |
| 22:LQ:19:LYS:HD2   | 22:LQ:19:LYS:HA    | 1.91                     | 0.41              |
| 25:LT:17:ARG:HA    | 25:LT:17:ARG:HD2   | 1.87                     | 0.41              |
| 27:LV:13:LYS:HA    | 27:LV:13:LYS:HD2   | 1.78                     | 0.41              |
| 35:Ld:33:ILE:HD12  | 35:Ld:33:ILE:HA    | 1.84                     | 0.41              |
| 49:S2:975:G:H2'    | 49:S2:976:G:C8     | 2.56                     | 0.41              |
| 52:SC:64:THR:OG1   | 52:SC:65:LYS:N     | 2.51                     | 0.41              |
| 53:SD:64:ARG:HH11  | 60:SK:94:LEU:HG    | 1.85                     | 0.41              |
| 58:SI:36:THR:HG21  | 58:SI:179:PRO:HB2  | 2.02                     | 0.41              |
| 61:SL:50:ALA:HA    | 61:SL:55:TYR:HE1   | 1.85                     | 0.41              |
| 4:L5:518:G:H1'     | 4:L5:644:G:C2      | 2.55                     | 0.41              |
| 5:L7:22:A:H2       | 5:L7:119:U:H4'     | 1.85                     | 0.41              |
| 14:LH:74:CYS:SG    | 14:LH:75:SER:N     | 2.93                     | 0.41              |
| 17:LL:200:LYS:HA   | 17:LL:203:ALA:HB3  | 2.02                     | 0.41              |
| 22:LQ:39:THR:HG22  | 22:LQ:41:SER:H     | 1.86                     | 0.41              |
| 34:Lc:21:VAL:HG11  | 34:Lc:96:ILE:HD12  | 2.01                     | 0.41              |
| 34:Lc:31:TYR:O     | 34:Lc:34:THR:OG1   | 2.37                     | 0.41              |
| 49:S2:1179:G:N2    | 49:S2:1182:A:OP2   | 2.53                     | 0.41              |
| 49:S2:1276:A:O2'   | 60:SK:50:GLN:NE2   | 2.54                     | 0.41              |
| 49:S2:1613:G:P     | 65:SP:42:ARG:HH12  | 2.44                     | 0.41              |
| 51:SB:224:GLU:HB3  | 51:SB:227:LYS:HG2  | 2.01                     | 0.41              |
| 58:SI:110:ARG:HG3  | 58:SI:121:LEU:HD23 | 2.02                     | 0.41              |
| 58:SI:150:ASP:OD1  | 58:SI:151:GLU:N    | 2.54                     | 0.41              |
| 63:SN:135:LEU:HD23 | 63:SN:135:LEU:HA   | 1.92                     | 0.41              |
| 74:SY:39:GLU:HA    | 74:SY:42:GLU:HB2   | 2.02                     | 0.41              |
| 2:B4:9:A:O2'       | 2:B4:10:G:N7       | 2.53                     | 0.41              |
| 4:L5:467:U:H2'     | 4:L5:468:U:O4'     | 2.21                     | 0.41              |
| 4:L5:1389:U:OP2    | 22:LQ:170:LYS:NZ   | 2.45                     | 0.41              |
| 4:L5:1405:C:H2'    | 4:L5:1406:G:H8     | 1.86                     | 0.41              |
| 4:L5:3612:C:H1'    | 4:L5:5016:A:C8     | 2.56                     | 0.41              |
| 4:L5:3717:A:H2'    | 4:L5:3718:A:C8     | 2.56                     | 0.41              |
| 4:L5:4250:G:H5''   | 16:LJ:98:ASN:HD22  | 1.86                     | 0.41              |
| 4:L5:4522:G:O2'    | 4:L5:4525:C:OP2    | 2.31                     | 0.41              |
| 4:L5:4940:C:OP2    | 11:LE:219:LYS:NZ   | 2.36                     | 0.41              |
| 24:LS:15:ARG:HH21  | 25:LT:141:VAL:HG23 | 1.86                     | 0.41              |
| 46:Lo:104:ILE:HA   | 46:Lo:105:GLN:HA   | 1.73                     | 0.41              |
| 48:Lr:21:ASN:OD1   | 48:Lr:21:ASN:N     | 2.52                     | 0.41              |
| 49:S2:581:U:OP1    | 74:SY:65:GLY:N     | 2.50                     | 0.41              |
| 49:S2:1275:G:O4'   | 49:S2:1506:A:N6    | 2.53                     | 0.41              |
| 51:SB:117:TRP:HB3  | 51:SB:153:THR:HA   | 2.02                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:SC:165:VAL:HG21 | 52:SC:217:ALA:HB1  | 2.02                     | 0.41              |
| 64:SO:91:THR:HB    | 64:SO:92:ALA:H     | 1.67                     | 0.41              |
| 4:L5:2263:A:O3'    | 48:Lr:112:ARG:NH1  | 2.52                     | 0.41              |
| 4:L5:2474:G:N2     | 4:L5:2502:G:O2'    | 2.53                     | 0.41              |
| 4:L5:3710:G:H4'    | 4:L5:3711:A:H5'    | 2.01                     | 0.41              |
| 4:L5:4305:G:N7     | 25:LT:87:LYS:NZ    | 2.58                     | 0.41              |
| 6:L8:94:G:C5       | 41:Lj:84:PRO:HG3   | 2.56                     | 0.41              |
| 8:LB:295:ASP:HA    | 8:LB:296:GLY:HA2   | 1.86                     | 0.41              |
| 14:LH:187:VAL:HG12 | 14:LH:188:GLN:H    | 1.86                     | 0.41              |
| 16:LJ:158:SER:OG   | 16:LJ:160:GLU:OE1  | 2.33                     | 0.41              |
| 38:Lg:15:THR:OG1   | 38:Lg:16:ALA:N     | 2.54                     | 0.41              |
| 44:Lm:82:LEU:HD12  | 44:Lm:82:LEU:HA    | 1.84                     | 0.41              |
| 48:Lr:101:LYS:HD2  | 48:Lr:101:LYS:HA   | 1.90                     | 0.41              |
| 49:S2:1297:U:O2'   | 49:S2:1299:A:N7    | 2.46                     | 0.41              |
| 49:S2:1391:C:H4'   | 79:Sd:55:LEU:HD21  | 2.03                     | 0.41              |
| 50:SA:50:ASN:HB3   | 50:SA:53:ARG:HG2   | 2.02                     | 0.41              |
| 50:SA:193:HIS:NE2  | 50:SA:196:GLU:OE1  | 2.47                     | 0.41              |
| 51:SB:27:LYS:HE2   | 51:SB:27:LYS:HB3   | 1.95                     | 0.41              |
| 51:SB:107:ARG:HA   | 51:SB:110:MET:HE2  | 2.03                     | 0.41              |
| 54:SE:164:LEU:HD23 | 54:SE:164:LEU:HA   | 1.88                     | 0.41              |
| 56:SG:223:LYS:O    | 56:SG:227:GLN:N    | 2.47                     | 0.41              |
| 67:SR:93:GLN:HB3   | 67:SR:96:ILE:HD13  | 2.02                     | 0.41              |
| 70:SU:28:ASN:O     | 70:SU:31:SER:OG    | 2.37                     | 0.41              |
| 74:SY:78:SER:OG    | 74:SY:80:ASP:OD1   | 2.33                     | 0.41              |
| 78:Sc:10:LYS:HE2   | 78:Sc:10:LYS:HB2   | 1.90                     | 0.41              |
| 4:L5:101:A:HO2'    | 17:LL:63:THR:HG1   | 1.67                     | 0.41              |
| 4:L5:1326:A:OP2    | 4:L5:4445:U:O2'    | 2.36                     | 0.41              |
| 4:L5:1971:C:N4     | 4:L5:2001:G:O5'    | 2.49                     | 0.41              |
| 4:L5:2041:A:N7     | 4:L5:4434:C:O2'    | 2.52                     | 0.41              |
| 4:L5:2863:G:O2'    | 23:LR:82:LYS:O     | 2.37                     | 0.41              |
| 4:L5:4431:U:OP2    | 15:LI:3:ARG:NH2    | 2.54                     | 0.41              |
| 4:L5:4622:A:H4'    | 8:LB:13:SER:HB2    | 2.02                     | 0.41              |
| 8:LB:231:VAL:HG11  | 8:LB:251:VAL:HG23  | 2.02                     | 0.41              |
| 8:LB:276:HIS:O     | 8:LB:277:ARG:NH1   | 2.45                     | 0.41              |
| 8:LB:277:ARG:HD3   | 8:LB:277:ARG:HA    | 1.87                     | 0.41              |
| 10:LD:166:ALA:HB1  | 10:LD:171:LEU:HD12 | 2.02                     | 0.41              |
| 12:LF:169:LEU:HD22 | 12:LF:175:ILE:HG12 | 2.03                     | 0.41              |
| 14:LH:47:LEU:HD23  | 14:LH:47:LEU:HA    | 1.91                     | 0.41              |
| 14:LH:91:LYS:HG2   | 14:LH:145:ILE:HG12 | 2.03                     | 0.41              |
| 22:LQ:69:LYS:HB2   | 22:LQ:139:LEU:HD21 | 2.02                     | 0.41              |
| 25:LT:18:PRO:HG2   | 25:LT:21:LYS:HB2   | 2.02                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:Lf:46:ARG:HA    | 37:Lf:73:LYS:HA    | 2.03                     | 0.41              |
| 37:Lf:49:TYR:HB2   | 37:Lf:101:ILE:HG12 | 2.03                     | 0.41              |
| 41:Lj:50:SER:O     | 41:Lj:50:SER:OG    | 2.39                     | 0.41              |
| 45:Ln:2:ARG:HB3    | 45:Ln:5:TRP:CD1    | 2.54                     | 0.41              |
| 48:Lr:46:ARG:O     | 48:Lr:70:GLN:NE2   | 2.54                     | 0.41              |
| 49:S2:616:A:H1'    | 80:Se:85:VAL:HG23  | 2.03                     | 0.41              |
| 49:S2:861:A:O4'    | 72:SW:107:SER:OG   | 2.38                     | 0.41              |
| 49:S2:1174:U:H2'   | 49:S2:1175:G:C8    | 2.56                     | 0.41              |
| 49:S2:1593:C:H4'   | 66:SQ:45:ARG:HH11  | 1.86                     | 0.41              |
| 50:SA:6:ASP:HA     | 50:SA:9:GLN:HB2    | 2.03                     | 0.41              |
| 50:SA:85:ARG:HD2   | 67:SR:81:ARG:HD3   | 2.03                     | 0.41              |
| 51:SB:140:VAL:HG13 | 51:SB:213:ARG:HB2  | 2.03                     | 0.41              |
| 57:SH:14:GLU:H     | 57:SH:14:GLU:HG3   | 1.79                     | 0.41              |
| 57:SH:18:GLU:OE2   | 57:SH:18:GLU:N     | 2.51                     | 0.41              |
| 57:SH:77:VAL:HG22  | 57:SH:81:ARG:HH11  | 1.86                     | 0.41              |
| 57:SH:103:LYS:HA   | 57:SH:103:LYS:HD3  | 1.80                     | 0.41              |
| 58:SI:165:GLN:O    | 58:SI:169:GLY:N    | 2.54                     | 0.41              |
| 59:SJ:35:TYR:HA    | 59:SJ:123:ILE:HD13 | 2.03                     | 0.41              |
| 60:SK:3:MET:HE2    | 60:SK:8:ARG:HA     | 2.01                     | 0.41              |
| 61:SL:45:LYS:HA    | 61:SL:45:LYS:HD3   | 1.81                     | 0.41              |
| 66:SQ:139:ALA:O    | 66:SQ:140:ARG:NH2  | 2.54                     | 0.41              |
| 68:SS:86:ARG:HD2   | 68:SS:86:ARG:HA    | 1.94                     | 0.41              |
| 82:Sg:20:GLN:HG2   | 82:Sg:69:VAL:H     | 1.86                     | 0.41              |
| 82:Sg:165:ILE:HD11 | 82:Sg:177:TRP:HB2  | 2.03                     | 0.41              |
| 4:L5:301:G:H5''    | 19:LN:98:LEU:HD13  | 2.03                     | 0.41              |
| 4:L5:1444:G:H1     | 4:L5:2102:G:N2     | 2.19                     | 0.41              |
| 4:L5:1613:A:H5''   | 7:LA:183:GLY:HA2   | 2.03                     | 0.41              |
| 7:LA:223:SER:O     | 7:LA:223:SER:OG    | 2.33                     | 0.41              |
| 13:LG:157:ILE:HG12 | 13:LG:170:LEU:HD23 | 2.02                     | 0.41              |
| 15:LI:76:MET:HE1   | 15:LI:148:VAL:HA   | 2.03                     | 0.41              |
| 15:LI:162:ARG:HE   | 15:LI:162:ARG:HB2  | 1.57                     | 0.41              |
| 25:LT:3:ASN:OD1    | 25:LT:3:ASN:N      | 2.51                     | 0.41              |
| 34:Lc:78:ASN:OD1   | 34:Lc:78:ASN:N     | 2.50                     | 0.41              |
| 49:S2:1597:C:OP2   | 75:SZ:85:ARG:NH2   | 2.54                     | 0.41              |
| 55:SF:88:MET:HE3   | 55:SF:88:MET:HB2   | 1.90                     | 0.41              |
| 56:SG:148:SER:N    | 56:SG:151:ASP:OD2  | 2.43                     | 0.41              |
| 66:SQ:8:GLN:NE2    | 66:SQ:95:TYR:OH    | 2.54                     | 0.41              |
| 67:SR:130:THR:HA   | 67:SR:131:PRO:HA   | 1.83                     | 0.41              |
| 76:Sa:41:ILE:HD12  | 76:Sa:41:ILE:HA    | 1.82                     | 0.41              |
| 4:L5:226:G:OP2     | 30:LY:1:MET:N      | 2.51                     | 0.40              |
| 4:L5:2303:C:H5''   | 36:Le:104:SER:HB3  | 2.01                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:L7:51:G:H21      | 16:LJ:12:MET:HE3   | 1.86                     | 0.40              |
| 9:LC:173:LYS:HD3   | 9:LC:173:LYS:HA    | 1.81                     | 0.40              |
| 13:LG:225:ASN:HA   | 13:LG:229:ARG:HD3  | 2.02                     | 0.40              |
| 15:LI:80:CYS:SG    | 15:LI:144:ASN:ND2  | 2.94                     | 0.40              |
| 20:LO:189:ILE:O    | 20:LO:193:THR:N    | 2.50                     | 0.40              |
| 49:S2:5:U:H2'      | 49:S2:6:G:H8       | 1.85                     | 0.40              |
| 51:SB:149:GLN:NE2  | 51:SB:153:THR:O    | 2.53                     | 0.40              |
| 54:SE:188:ASN:HB3  | 54:SE:191:ARG:HG3  | 2.02                     | 0.40              |
| 64:SO:30:VAL:HG12  | 64:SO:94:HIS:HB2   | 2.02                     | 0.40              |
| 67:SR:109:LEU:HD12 | 67:SR:109:LEU:HA   | 1.92                     | 0.40              |
| 68:SS:99:LEU:HD13  | 68:SS:99:LEU:HA    | 1.94                     | 0.40              |
| 4:L5:2361:G:O2'    | 4:L5:3859:G:O6     | 2.35                     | 0.40              |
| 4:L5:4625:C:O2'    | 8:LB:336:CYS:SG    | 2.69                     | 0.40              |
| 4:L5:4870:G:O6     | 24:LS:157:ARG:NH1  | 2.54                     | 0.40              |
| 15:LI:29:ALA:O     | 15:LI:32:ARG:NH1   | 2.39                     | 0.40              |
| 25:LT:69:GLN:H     | 25:LT:69:GLN:HG2   | 1.75                     | 0.40              |
| 30:LY:47:MET:HE3   | 30:LY:47:MET:HB3   | 1.92                     | 0.40              |
| 31:LZ:30:ASP:OD1   | 31:LZ:30:ASP:N     | 2.54                     | 0.40              |
| 41:Lj:48:ASN:OD1   | 41:Lj:48:ASN:N     | 2.42                     | 0.40              |
| 47:Lp:28:LYS:HE3   | 47:Lp:28:LYS:HB3   | 1.87                     | 0.40              |
| 49:S2:448:A:H5''   | 58:SI:25:ARG:HA    | 2.03                     | 0.40              |
| 49:S2:1010:G:H2'   | 49:S2:1011:A:C8    | 2.57                     | 0.40              |
| 53:SD:132:LYS:HE2  | 53:SD:191:PRO:HA   | 2.03                     | 0.40              |
| 53:SD:213:PRO:HB3  | 67:SR:19:LYS:HB3   | 2.04                     | 0.40              |
| 53:SD:213:PRO:HD3  | 67:SR:19:LYS:HD2   | 2.03                     | 0.40              |
| 55:SF:79:HIS:O     | 55:SF:81:ARG:N     | 2.53                     | 0.40              |
| 73:SX:135:LYS:HB2  | 73:SX:137:LYS:HG3  | 2.03                     | 0.40              |
| 77:Sb:64:CYS:O     | 77:Sb:65:GLN:NE2   | 2.52                     | 0.40              |
| 82:Sg:87:LEU:HD11  | 82:Sg:111:VAL:HG11 | 2.03                     | 0.40              |
| 82:Sg:294:ASP:OD1  | 82:Sg:294:ASP:N    | 2.52                     | 0.40              |
| 4:L5:425:U:OP1     | 21:LP:37:LYS:NZ    | 2.54                     | 0.40              |
| 4:L5:699:C:N4      | 4:L5:700:G:O6      | 2.53                     | 0.40              |
| 4:L5:1974:U:O2     | 4:L5:1994:C:N4     | 2.54                     | 0.40              |
| 9:LC:221:PHE:HB2   | 9:LC:229:LEU:HD11  | 2.02                     | 0.40              |
| 22:LQ:8:ASN:OD1    | 22:LQ:8:ASN:N      | 2.55                     | 0.40              |
| 24:LS:76:LYS:HE2   | 24:LS:76:LYS:HB2   | 1.93                     | 0.40              |
| 49:S2:17:C:O2'     | 49:S2:1194:A:N1    | 2.47                     | 0.40              |
| 49:S2:483:C:H5''   | 73:SX:48:LYS:HD3   | 2.03                     | 0.40              |
| 49:S2:1460:C:N4    | 49:S2:1461:G:O6    | 2.55                     | 0.40              |
| 51:SB:167:LYS:HA   | 51:SB:170:GLU:HG2  | 2.04                     | 0.40              |
| 52:SC:196:ILE:HB   | 52:SC:223:TYR:HB2  | 2.04                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:SD:192:TRP:CD2  | 53:SD:194:PRO:HD3  | 2.56                     | 0.40              |
| 56:SG:63:MET:HG2   | 56:SG:98:ARG:HD2   | 2.03                     | 0.40              |
| 61:SL:125:ILE:O    | 61:SL:146:THR:OG1  | 2.31                     | 0.40              |
| 75:SZ:52:LYS:HD3   | 75:SZ:52:LYS:HA    | 1.85                     | 0.40              |
| 4:L5:198:A:OP1     | 30:LY:126:ARG:NH2  | 2.54                     | 0.40              |
| 4:L5:1802:A:N3     | 25:LT:130:ARG:NH1  | 2.64                     | 0.40              |
| 6:L8:103:A:OP1     | 41:Lj:21:ARG:NH1   | 2.55                     | 0.40              |
| 7:LA:15:VAL:HG12   | 7:LA:194:ASN:HD22  | 1.86                     | 0.40              |
| 8:LB:219:VAL:HG11  | 8:LB:337:VAL:HG23  | 2.03                     | 0.40              |
| 25:LT:122:LYS:HE2  | 25:LT:122:LYS:HB2  | 1.92                     | 0.40              |
| 28:LW:79:GLN:HB2   | 56:SG:9:ALA:HA     | 2.02                     | 0.40              |
| 35:Ld:113:THR:OG1  | 35:Ld:114:PHE:N    | 2.55                     | 0.40              |
| 38:Lg:15:THR:HG22  | 38:Lg:18:ASN:HB2   | 2.02                     | 0.40              |
| 49:S2:616:A:OP1    | 73:SX:68:LYS:NZ    | 2.53                     | 0.40              |
| 49:S2:1587:G:H22   | 69:ST:63:HIS:HB3   | 1.87                     | 0.40              |
| 60:SK:7:ASN:OD1    | 60:SK:7:ASN:N      | 2.43                     | 0.40              |
| 64:SO:60:MET:HE3   | 64:SO:60:MET:HB2   | 1.80                     | 0.40              |
| 64:SO:74:ALA:HB1   | 64:SO:115:ALA:HB2  | 2.03                     | 0.40              |
| 73:SX:63:ASN:HD21  | 73:SX:67:ARG:HH11  | 1.69                     | 0.40              |
| 75:SZ:63:PRO:O     | 75:SZ:111:ARG:HB3  | 2.22                     | 0.40              |
| 4:L5:1099:C:O2     | 4:L5:1196:G:N1     | 2.55                     | 0.40              |
| 4:L5:1804:A:H5''   | 4:L5:1805:A:H2'    | 2.02                     | 0.40              |
| 4:L5:1975:G:O4'    | 4:L5:1983:A:O2'    | 2.39                     | 0.40              |
| 4:L5:3645:U:O2'    | 4:L5:4553:A:O2'    | 2.31                     | 0.40              |
| 4:L5:4139:G:N1     | 4:L5:4141:G:N3     | 2.69                     | 0.40              |
| 11:LE:205:ASN:OD1  | 11:LE:260:LYS:NZ   | 2.39                     | 0.40              |
| 12:LF:125:LEU:HD22 | 12:LF:130:ILE:HG22 | 2.03                     | 0.40              |
| 14:LH:34:LEU:HD23  | 14:LH:34:LEU:HA    | 1.89                     | 0.40              |
| 15:LI:78:LYS:HE3   | 15:LI:78:LYS:HB2   | 1.75                     | 0.40              |
| 15:LI:214:SER:OXT  | 15:LI:214:SER:OG   | 2.38                     | 0.40              |
| 26:LU:74:SER:OG    | 26:LU:75:GLU:N     | 2.54                     | 0.40              |
| 27:LV:68:GLY:H     | 27:LV:73:ARG:HD3   | 1.86                     | 0.40              |
| 29:LX:82:THR:HG22  | 39:Lh:36:VAL:HG12  | 2.04                     | 0.40              |
| 33:Lb:47:LYS:HZ2   | 33:Lb:47:LYS:HG2   | 1.75                     | 0.40              |
| 51:SB:64:GLY:HA2   | 51:SB:87:ILE:HD11  | 2.03                     | 0.40              |
| 51:SB:144:LYS:HA   | 51:SB:208:HIS:HD2  | 1.86                     | 0.40              |
| 53:SD:117:ARG:HD2  | 53:SD:117:ARG:HA   | 1.77                     | 0.40              |
| 54:SE:115:THR:OG1  | 54:SE:118:GLU:N    | 2.54                     | 0.40              |
| 55:SF:49:LEU:HD23  | 55:SF:49:LEU:HA    | 1.89                     | 0.40              |
| 66:SQ:11:GLN:NE2   | 66:SQ:23:ALA:O     | 2.54                     | 0.40              |
| 66:SQ:76:GLY:H     | 66:SQ:79:ALA:HB3   | 1.85                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 78:Sc:13:ARG:HB2 | 78:Sc:35:MET:SD | 2.62                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 7   | LA    | 245/257 (95%) | 223 (91%) | 22 (9%)  | 0        | 100         | 100 |
| 8   | LB    | 396/403 (98%) | 360 (91%) | 35 (9%)  | 1 (0%)   | 36          | 68  |
| 9   | LC    | 363/427 (85%) | 338 (93%) | 25 (7%)  | 0        | 100         | 100 |
| 10  | LD    | 291/297 (98%) | 267 (92%) | 24 (8%)  | 0        | 100         | 100 |
| 11  | LE    | 216/288 (75%) | 182 (84%) | 34 (16%) | 0        | 100         | 100 |
| 12  | LF    | 223/248 (90%) | 208 (93%) | 15 (7%)  | 0        | 100         | 100 |
| 13  | LG    | 223/266 (84%) | 208 (93%) | 14 (6%)  | 1 (0%)   | 30          | 62  |
| 14  | LH    | 188/192 (98%) | 167 (89%) | 21 (11%) | 0        | 100         | 100 |
| 15  | LI    | 205/214 (96%) | 185 (90%) | 20 (10%) | 0        | 100         | 100 |
| 16  | LJ    | 173/178 (97%) | 158 (91%) | 14 (8%)  | 1 (1%)   | 21          | 56  |
| 17  | LL    | 206/211 (98%) | 187 (91%) | 18 (9%)  | 1 (0%)   | 24          | 59  |
| 18  | LM    | 134/215 (62%) | 119 (89%) | 15 (11%) | 0        | 100         | 100 |
| 19  | LN    | 201/204 (98%) | 195 (97%) | 6 (3%)   | 0        | 100         | 100 |
| 20  | LO    | 198/203 (98%) | 190 (96%) | 8 (4%)   | 0        | 100         | 100 |
| 21  | LP    | 151/184 (82%) | 137 (91%) | 14 (9%)  | 0        | 100         | 100 |
| 22  | LQ    | 185/188 (98%) | 173 (94%) | 12 (6%)  | 0        | 100         | 100 |
| 23  | LR    | 178/196 (91%) | 175 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 24  | LS    | 173/176 (98%) | 159 (92%) | 14 (8%)  | 0        | 100         | 100 |
| 25  | LT    | 157/160 (98%) | 146 (93%) | 11 (7%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 26  | LU    | 99/128 (77%)  | 92 (93%)  | 7 (7%)   | 0        | 100         | 100 |
| 27  | LV    | 129/140 (92%) | 118 (92%) | 11 (8%)  | 0        | 100         | 100 |
| 28  | LW    | 111/157 (71%) | 103 (93%) | 8 (7%)   | 0        | 100         | 100 |
| 29  | LX    | 118/156 (76%) | 106 (90%) | 12 (10%) | 0        | 100         | 100 |
| 30  | LY    | 132/145 (91%) | 124 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 31  | LZ    | 133/136 (98%) | 123 (92%) | 10 (8%)  | 0        | 100         | 100 |
| 32  | La    | 145/148 (98%) | 129 (89%) | 16 (11%) | 0        | 100         | 100 |
| 33  | Lb    | 73/159 (46%)  | 66 (90%)  | 7 (10%)  | 0        | 100         | 100 |
| 34  | Lc    | 96/115 (84%)  | 90 (94%)  | 6 (6%)   | 0        | 100         | 100 |
| 35  | Ld    | 105/125 (84%) | 95 (90%)  | 10 (10%) | 0        | 100         | 100 |
| 36  | Le    | 126/135 (93%) | 123 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 37  | Lf    | 107/110 (97%) | 100 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 38  | Lg    | 112/117 (96%) | 102 (91%) | 10 (9%)  | 0        | 100         | 100 |
| 39  | Lh    | 120/123 (98%) | 118 (98%) | 2 (2%)   | 0        | 100         | 100 |
| 40  | Li    | 100/105 (95%) | 93 (93%)  | 7 (7%)   | 0        | 100         | 100 |
| 41  | Lj    | 84/97 (87%)   | 76 (90%)  | 8 (10%)  | 0        | 100         | 100 |
| 42  | Lk    | 67/70 (96%)   | 62 (92%)  | 5 (8%)   | 0        | 100         | 100 |
| 43  | Ll    | 48/51 (94%)   | 45 (94%)  | 3 (6%)   | 0        | 100         | 100 |
| 44  | Lm    | 50/128 (39%)  | 48 (96%)  | 2 (4%)   | 0        | 100         | 100 |
| 45  | Ln    | 22/25 (88%)   | 22 (100%) | 0        | 0        | 100         | 100 |
| 46  | Lo    | 103/106 (97%) | 95 (92%)  | 8 (8%)   | 0        | 100         | 100 |
| 47  | Lp    | 89/92 (97%)   | 83 (93%)  | 6 (7%)   | 0        | 100         | 100 |
| 48  | Lr    | 123/137 (90%) | 113 (92%) | 10 (8%)  | 0        | 100         | 100 |
| 50  | SA    | 213/295 (72%) | 201 (94%) | 12 (6%)  | 0        | 100         | 100 |
| 51  | SB    | 212/264 (80%) | 192 (91%) | 19 (9%)  | 1 (0%)   | 24          | 59  |
| 52  | SC    | 217/293 (74%) | 204 (94%) | 13 (6%)  | 0        | 100         | 100 |
| 53  | SD    | 214/243 (88%) | 189 (88%) | 25 (12%) | 0        | 100         | 100 |
| 54  | SE    | 260/263 (99%) | 247 (95%) | 13 (5%)  | 0        | 100         | 100 |
| 55  | SF    | 184/204 (90%) | 153 (83%) | 30 (16%) | 1 (0%)   | 24          | 59  |
| 56  | SG    | 235/249 (94%) | 219 (93%) | 16 (7%)  | 0        | 100         | 100 |
| 57  | SH    | 185/194 (95%) | 161 (87%) | 24 (13%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 58  | SI    | 204/208 (98%)     | 186 (91%)   | 18 (9%)  | 0        | 100         | 100 |
| 59  | SJ    | 180/194 (93%)     | 168 (93%)   | 12 (7%)  | 0        | 100         | 100 |
| 60  | SK    | 94/165 (57%)      | 89 (95%)    | 5 (5%)   | 0        | 100         | 100 |
| 61  | SL    | 144/158 (91%)     | 127 (88%)   | 17 (12%) | 0        | 100         | 100 |
| 62  | SM    | 102/132 (77%)     | 76 (74%)    | 25 (24%) | 1 (1%)   | 12          | 45  |
| 63  | SN    | 148/151 (98%)     | 140 (95%)   | 8 (5%)   | 0        | 100         | 100 |
| 64  | SO    | 132/151 (87%)     | 117 (89%)   | 15 (11%) | 0        | 100         | 100 |
| 65  | SP    | 132/145 (91%)     | 122 (92%)   | 10 (8%)  | 0        | 100         | 100 |
| 66  | SQ    | 140/146 (96%)     | 119 (85%)   | 21 (15%) | 0        | 100         | 100 |
| 67  | SR    | 126/135 (93%)     | 110 (87%)   | 16 (13%) | 0        | 100         | 100 |
| 68  | SS    | 142/152 (93%)     | 123 (87%)   | 19 (13%) | 0        | 100         | 100 |
| 69  | ST    | 139/145 (96%)     | 123 (88%)   | 16 (12%) | 0        | 100         | 100 |
| 70  | SU    | 100/119 (84%)     | 86 (86%)    | 14 (14%) | 0        | 100         | 100 |
| 71  | SV    | 81/83 (98%)       | 72 (89%)    | 9 (11%)  | 0        | 100         | 100 |
| 72  | SW    | 127/130 (98%)     | 118 (93%)   | 9 (7%)   | 0        | 100         | 100 |
| 73  | SX    | 139/143 (97%)     | 136 (98%)   | 2 (1%)   | 1 (1%)   | 18          | 52  |
| 74  | SY    | 121/133 (91%)     | 118 (98%)   | 3 (2%)   | 0        | 100         | 100 |
| 75  | SZ    | 84/125 (67%)      | 75 (89%)    | 9 (11%)  | 0        | 100         | 100 |
| 76  | Sa    | 97/115 (84%)      | 86 (89%)    | 11 (11%) | 0        | 100         | 100 |
| 77  | Sb    | 81/84 (96%)       | 67 (83%)    | 13 (16%) | 1 (1%)   | 10          | 42  |
| 78  | Sc    | 61/69 (88%)       | 47 (77%)    | 14 (23%) | 0        | 100         | 100 |
| 79  | Sd    | 50/56 (89%)       | 49 (98%)    | 1 (2%)   | 0        | 100         | 100 |
| 80  | Se    | 55/59 (93%)       | 50 (91%)    | 5 (9%)   | 0        | 100         | 100 |
| 81  | Sf    | 65/156 (42%)      | 60 (92%)    | 5 (8%)   | 0        | 100         | 100 |
| 82  | Sg    | 311/317 (98%)     | 254 (82%)   | 56 (18%) | 1 (0%)   | 36          | 68  |
| All | All   | 11173/12688 (88%) | 10187 (91%) | 976 (9%) | 10 (0%)  | 49          | 79  |

All (10) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | LL    | 48  | PRO  |
| 55  | SF    | 80  | GLY  |
| 77  | Sb    | 39  | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | LB    | 393 | LYS  |
| 82  | Sg    | 283 | PRO  |
| 62  | SM    | 54  | SER  |
| 13  | LG    | 106 | THR  |
| 16  | LJ    | 118 | LYS  |
| 51  | SB    | 54  | GLY  |
| 73  | SX    | 86  | PRO  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 7   | LA    | 189/199 (95%) | 188 (100%) | 1 (0%)   | 81          | 85  |
| 8   | LB    | 346/349 (99%) | 344 (99%)  | 2 (1%)   | 78          | 84  |
| 9   | LC    | 302/348 (87%) | 302 (100%) | 0        | 100         | 100 |
| 10  | LD    | 245/250 (98%) | 244 (100%) | 1 (0%)   | 84          | 86  |
| 11  | LE    | 196/252 (78%) | 195 (100%) | 1 (0%)   | 81          | 85  |
| 12  | LF    | 194/215 (90%) | 194 (100%) | 0        | 100         | 100 |
| 13  | LG    | 195/223 (87%) | 194 (100%) | 1 (0%)   | 81          | 85  |
| 14  | LH    | 169/171 (99%) | 168 (99%)  | 1 (1%)   | 78          | 84  |
| 15  | LI    | 175/181 (97%) | 175 (100%) | 0        | 100         | 100 |
| 16  | LJ    | 147/149 (99%) | 146 (99%)  | 1 (1%)   | 76          | 83  |
| 17  | LL    | 174/177 (98%) | 172 (99%)  | 2 (1%)   | 65          | 79  |
| 18  | LM    | 116/161 (72%) | 116 (100%) | 0        | 100         | 100 |
| 19  | LN    | 171/172 (99%) | 169 (99%)  | 2 (1%)   | 63          | 79  |
| 20  | LO    | 172/174 (99%) | 172 (100%) | 0        | 100         | 100 |
| 21  | LP    | 134/163 (82%) | 133 (99%)  | 1 (1%)   | 76          | 83  |
| 22  | LQ    | 164/165 (99%) | 162 (99%)  | 2 (1%)   | 63          | 79  |
| 23  | LR    | 159/175 (91%) | 159 (100%) | 0        | 100         | 100 |
| 24  | LS    | 156/157 (99%) | 155 (99%)  | 1 (1%)   | 78          | 84  |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 25  | LT    | 139/140 (99%) | 139 (100%) | 0        | 100         | 100 |
| 26  | LU    | 90/115 (78%)  | 90 (100%)  | 0        | 100         | 100 |
| 27  | LV    | 101/107 (94%) | 100 (99%)  | 1 (1%)   | 68          | 80  |
| 28  | LW    | 88/126 (70%)  | 87 (99%)   | 1 (1%)   | 65          | 79  |
| 29  | LX    | 107/133 (80%) | 107 (100%) | 0        | 100         | 100 |
| 30  | LY    | 124/135 (92%) | 124 (100%) | 0        | 100         | 100 |
| 31  | LZ    | 117/118 (99%) | 117 (100%) | 0        | 100         | 100 |
| 32  | La    | 120/121 (99%) | 118 (98%)  | 2 (2%)   | 53          | 75  |
| 33  | Lb    | 60/126 (48%)  | 60 (100%)  | 0        | 100         | 100 |
| 34  | Lc    | 83/97 (86%)   | 81 (98%)   | 2 (2%)   | 43          | 70  |
| 35  | Ld    | 98/110 (89%)  | 96 (98%)   | 2 (2%)   | 48          | 72  |
| 36  | Le    | 114/121 (94%) | 114 (100%) | 0        | 100         | 100 |
| 37  | Lf    | 88/89 (99%)   | 87 (99%)   | 1 (1%)   | 65          | 79  |
| 38  | Lg    | 98/100 (98%)  | 98 (100%)  | 0        | 100         | 100 |
| 39  | Lh    | 109/110 (99%) | 108 (99%)  | 1 (1%)   | 70          | 81  |
| 40  | Li    | 86/89 (97%)   | 86 (100%)  | 0        | 100         | 100 |
| 41  | Lj    | 73/80 (91%)   | 73 (100%)  | 0        | 100         | 100 |
| 42  | Lk    | 64/65 (98%)   | 63 (98%)   | 1 (2%)   | 55          | 75  |
| 43  | Ll    | 47/48 (98%)   | 47 (100%)  | 0        | 100         | 100 |
| 44  | Lm    | 48/116 (41%)  | 47 (98%)   | 1 (2%)   | 47          | 71  |
| 45  | Ln    | 23/24 (96%)   | 23 (100%)  | 0        | 100         | 100 |
| 46  | Lo    | 93/94 (99%)   | 93 (100%)  | 0        | 100         | 100 |
| 47  | Lp    | 74/75 (99%)   | 74 (100%)  | 0        | 100         | 100 |
| 48  | Lr    | 109/121 (90%) | 107 (98%)  | 2 (2%)   | 51          | 74  |
| 50  | SA    | 178/243 (73%) | 177 (99%)  | 1 (1%)   | 78          | 84  |
| 51  | SB    | 195/231 (84%) | 193 (99%)  | 2 (1%)   | 68          | 80  |
| 52  | SC    | 183/225 (81%) | 183 (100%) | 0        | 100         | 100 |
| 53  | SD    | 179/202 (89%) | 177 (99%)  | 2 (1%)   | 65          | 79  |
| 54  | SE    | 223/225 (99%) | 219 (98%)  | 4 (2%)   | 51          | 74  |
| 55  | SF    | 152/170 (89%) | 151 (99%)  | 1 (1%)   | 76          | 83  |
| 56  | SG    | 206/218 (94%) | 206 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|-------------|-----|
| 57  | SH    | 168/174 (97%)    | 166 (99%)  | 2 (1%)   | 63          | 79  |
| 58  | SI    | 175/180 (97%)    | 175 (100%) | 0        | 100         | 100 |
| 59  | SJ    | 160/168 (95%)    | 160 (100%) | 0        | 100         | 100 |
| 60  | SK    | 87/136 (64%)     | 87 (100%)  | 0        | 100         | 100 |
| 61  | SL    | 131/142 (92%)    | 130 (99%)  | 1 (1%)   | 73          | 82  |
| 62  | SM    | 85/108 (79%)     | 84 (99%)   | 1 (1%)   | 63          | 79  |
| 63  | SN    | 130/131 (99%)    | 129 (99%)  | 1 (1%)   | 73          | 82  |
| 64  | SO    | 104/119 (87%)    | 102 (98%)  | 2 (2%)   | 50          | 73  |
| 65  | SP    | 120/130 (92%)    | 119 (99%)  | 1 (1%)   | 73          | 82  |
| 66  | SQ    | 117/121 (97%)    | 115 (98%)  | 2 (2%)   | 53          | 75  |
| 67  | SR    | 116/122 (95%)    | 115 (99%)  | 1 (1%)   | 70          | 81  |
| 68  | SS    | 119/132 (90%)    | 119 (100%) | 0        | 100         | 100 |
| 69  | ST    | 111/115 (96%)    | 111 (100%) | 0        | 100         | 100 |
| 70  | SU    | 89/107 (83%)     | 88 (99%)   | 1 (1%)   | 65          | 79  |
| 71  | SV    | 67/67 (100%)     | 66 (98%)   | 1 (2%)   | 57          | 76  |
| 72  | SW    | 112/113 (99%)    | 110 (98%)  | 2 (2%)   | 51          | 74  |
| 73  | SX    | 113/115 (98%)    | 112 (99%)  | 1 (1%)   | 70          | 81  |
| 74  | SY    | 106/115 (92%)    | 104 (98%)  | 2 (2%)   | 50          | 73  |
| 75  | SZ    | 73/103 (71%)     | 73 (100%)  | 0        | 100         | 100 |
| 76  | Sa    | 86/98 (88%)      | 86 (100%)  | 0        | 100         | 100 |
| 77  | Sb    | 73/76 (96%)      | 73 (100%)  | 0        | 100         | 100 |
| 78  | Sc    | 53/62 (86%)      | 52 (98%)   | 1 (2%)   | 50          | 73  |
| 79  | Sd    | 45/49 (92%)      | 45 (100%)  | 0        | 100         | 100 |
| 80  | Se    | 46/48 (96%)      | 46 (100%)  | 0        | 100         | 100 |
| 81  | Sf    | 57/140 (41%)     | 57 (100%)  | 0        | 100         | 100 |
| 82  | Sg    | 272/275 (99%)    | 269 (99%)  | 3 (1%)   | 65          | 79  |
| All | All   | 9688/10801 (90%) | 9626 (99%) | 62 (1%)  | 76          | 84  |

All (62) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | LA    | 4   | VAL  |
| 8   | LB    | 57  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | LB    | 210 | VAL  |
| 10  | LD    | 153 | THR  |
| 11  | LE    | 106 | VAL  |
| 13  | LG    | 156 | VAL  |
| 14  | LH    | 74  | CYS  |
| 16  | LJ    | 10  | ASN  |
| 17  | LL    | 9   | VAL  |
| 17  | LL    | 94  | ILE  |
| 19  | LN    | 64  | ILE  |
| 19  | LN    | 80  | THR  |
| 21  | LP    | 58  | VAL  |
| 22  | LQ    | 13  | VAL  |
| 22  | LQ    | 86  | ILE  |
| 24  | LS    | 75  | VAL  |
| 27  | LV    | 65  | VAL  |
| 28  | LW    | 109 | ILE  |
| 32  | La    | 15  | VAL  |
| 32  | La    | 17  | HIS  |
| 34  | Lc    | 28  | VAL  |
| 34  | Lc    | 55  | LEU  |
| 35  | Ld    | 20  | VAL  |
| 35  | Ld    | 95  | ASP  |
| 37  | Lf    | 43  | LEU  |
| 39  | Lh    | 96  | ASN  |
| 42  | Lk    | 28  | ASN  |
| 44  | Lm    | 108 | VAL  |
| 48  | Lr    | 78  | VAL  |
| 48  | Lr    | 124 | VAL  |
| 50  | SA    | 46  | ILE  |
| 51  | SB    | 79  | VAL  |
| 51  | SB    | 231 | LEU  |
| 53  | SD    | 58  | VAL  |
| 53  | SD    | 123 | LEU  |
| 54  | SE    | 76  | VAL  |
| 54  | SE    | 89  | VAL  |
| 54  | SE    | 90  | ILE  |
| 54  | SE    | 140 | VAL  |
| 55  | SF    | 153 | LEU  |
| 57  | SH    | 170 | VAL  |
| 57  | SH    | 186 | ASN  |
| 61  | SL    | 87  | VAL  |
| 62  | SM    | 85  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 63  | SN    | 62  | GLN  |
| 64  | SO    | 27  | VAL  |
| 64  | SO    | 52  | THR  |
| 65  | SP    | 126 | VAL  |
| 66  | SQ    | 70  | VAL  |
| 66  | SQ    | 81  | ILE  |
| 67  | SR    | 75  | GLU  |
| 70  | SU    | 22  | ILE  |
| 71  | SV    | 79  | VAL  |
| 72  | SW    | 2   | VAL  |
| 72  | SW    | 33  | VAL  |
| 73  | SX    | 105 | PHE  |
| 74  | SY    | 62  | THR  |
| 74  | SY    | 120 | THR  |
| 78  | Sc    | 55  | VAL  |
| 82  | Sg    | 91  | ASP  |
| 82  | Sg    | 151 | VAL  |
| 82  | Sg    | 307 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (159) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | LA    | 95  | GLN  |
| 7   | LA    | 194 | ASN  |
| 7   | LA    | 218 | HIS  |
| 8   | LB    | 186 | ASN  |
| 8   | LB    | 328 | ASN  |
| 9   | LC    | 21  | ASN  |
| 9   | LC    | 50  | GLN  |
| 9   | LC    | 116 | ASN  |
| 9   | LC    | 215 | ASN  |
| 9   | LC    | 231 | ASN  |
| 9   | LC    | 276 | ASN  |
| 9   | LC    | 329 | ASN  |
| 9   | LC    | 346 | ASN  |
| 10  | LD    | 57  | ASN  |
| 10  | LD    | 63  | GLN  |
| 10  | LD    | 175 | HIS  |
| 10  | LD    | 191 | ASN  |
| 10  | LD    | 195 | HIS  |
| 10  | LD    | 267 | ASN  |
| 10  | LD    | 275 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | LD    | 282 | GLN  |
| 11  | LE    | 191 | GLN  |
| 11  | LE    | 256 | GLN  |
| 12  | LF    | 163 | ASN  |
| 13  | LG    | 94  | GLN  |
| 13  | LG    | 159 | HIS  |
| 13  | LG    | 227 | ASN  |
| 14  | LH    | 7   | ASN  |
| 14  | LH    | 63  | ASN  |
| 14  | LH    | 140 | GLN  |
| 15  | LI    | 123 | GLN  |
| 15  | LI    | 144 | ASN  |
| 15  | LI    | 203 | HIS  |
| 16  | LJ    | 3   | GLN  |
| 16  | LJ    | 46  | GLN  |
| 16  | LJ    | 98  | ASN  |
| 17  | LL    | 27  | ASN  |
| 17  | LL    | 104 | ASN  |
| 17  | LL    | 111 | GLN  |
| 17  | LL    | 115 | GLN  |
| 17  | LL    | 149 | GLN  |
| 17  | LL    | 159 | ASN  |
| 18  | LM    | 34  | ASN  |
| 18  | LM    | 44  | GLN  |
| 18  | LM    | 48  | GLN  |
| 18  | LM    | 56  | GLN  |
| 18  | LM    | 131 | GLN  |
| 19  | LN    | 15  | GLN  |
| 19  | LN    | 199 | GLN  |
| 20  | LO    | 42  | ASN  |
| 21  | LP    | 10  | ASN  |
| 21  | LP    | 28  | ASN  |
| 21  | LP    | 34  | GLN  |
| 21  | LP    | 80  | GLN  |
| 22  | LQ    | 7   | HIS  |
| 22  | LQ    | 44  | ASN  |
| 22  | LQ    | 77  | ASN  |
| 23  | LR    | 141 | HIS  |
| 24  | LS    | 156 | HIS  |
| 24  | LS    | 163 | HIS  |
| 25  | LT    | 66  | ASN  |
| 25  | LT    | 131 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | LU    | 44  | GLN  |
| 26  | LU    | 50  | ASN  |
| 27  | LV    | 107 | ASN  |
| 27  | LV    | 135 | ASN  |
| 28  | LW    | 45  | ASN  |
| 28  | LW    | 50  | ASN  |
| 28  | LW    | 95  | ASN  |
| 29  | LX    | 69  | ASN  |
| 30  | LY    | 14  | ASN  |
| 30  | LY    | 127 | GLN  |
| 31  | LZ    | 40  | HIS  |
| 32  | La    | 67  | GLN  |
| 32  | La    | 74  | ASN  |
| 32  | La    | 93  | ASN  |
| 33  | Lb    | 50  | ASN  |
| 34  | Lc    | 15  | ASN  |
| 34  | Lc    | 19  | GLN  |
| 34  | Lc    | 72  | HIS  |
| 36  | Le    | 43  | ASN  |
| 36  | Le    | 63  | ASN  |
| 36  | Le    | 68  | HIS  |
| 36  | Le    | 117 | GLN  |
| 37  | Lf    | 21  | GLN  |
| 38  | Lg    | 3   | GLN  |
| 38  | Lg    | 100 | GLN  |
| 39  | Lh    | 20  | GLN  |
| 41  | Lj    | 66  | HIS  |
| 44  | Lm    | 104 | HIS  |
| 44  | Lm    | 109 | ASN  |
| 46  | Lo    | 76  | ASN  |
| 46  | Lo    | 105 | GLN  |
| 48  | Lr    | 30  | ASN  |
| 48  | Lr    | 31  | ASN  |
| 48  | Lr    | 83  | ASN  |
| 50  | SA    | 29  | ASN  |
| 50  | SA    | 110 | ASN  |
| 51  | SB    | 53  | GLN  |
| 51  | SB    | 92  | GLN  |
| 51  | SB    | 147 | ASN  |
| 51  | SB    | 202 | GLN  |
| 52  | SC    | 115 | GLN  |
| 53  | SD    | 22  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | SD    | 101 | GLN  |
| 53  | SD    | 179 | GLN  |
| 54  | SE    | 142 | HIS  |
| 54  | SE    | 179 | ASN  |
| 55  | SF    | 101 | HIS  |
| 56  | SG    | 146 | ASN  |
| 56  | SG    | 177 | GLN  |
| 56  | SG    | 187 | HIS  |
| 56  | SG    | 197 | GLN  |
| 56  | SG    | 202 | ASN  |
| 56  | SG    | 227 | GLN  |
| 57  | SH    | 44  | ASN  |
| 57  | SH    | 162 | GLN  |
| 57  | SH    | 193 | GLN  |
| 58  | SI    | 84  | ASN  |
| 58  | SI    | 167 | GLN  |
| 59  | SJ    | 132 | GLN  |
| 59  | SJ    | 156 | HIS  |
| 60  | SK    | 50  | GLN  |
| 60  | SK    | 73  | ASN  |
| 61  | SL    | 83  | GLN  |
| 62  | SM    | 46  | GLN  |
| 62  | SM    | 52  | GLN  |
| 62  | SM    | 55  | ASN  |
| 63  | SN    | 36  | GLN  |
| 64  | SO    | 113 | GLN  |
| 65  | SP    | 35  | GLN  |
| 65  | SP    | 98  | ASN  |
| 65  | SP    | 103 | ASN  |
| 66  | SQ    | 8   | GLN  |
| 67  | SR    | 62  | GLN  |
| 67  | SR    | 127 | ASN  |
| 68  | SS    | 72  | GLN  |
| 70  | SU    | 47  | ASN  |
| 70  | SU    | 81  | GLN  |
| 71  | SV    | 33  | GLN  |
| 71  | SV    | 35  | ASN  |
| 71  | SV    | 49  | GLN  |
| 71  | SV    | 82  | ASN  |
| 72  | SW    | 24  | GLN  |
| 72  | SW    | 64  | ASN  |
| 73  | SX    | 16  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 74  | SY    | 94  | HIS  |
| 75  | SZ    | 106 | GLN  |
| 76  | Sa    | 43  | ASN  |
| 76  | Sa    | 72  | HIS  |
| 77  | Sb    | 51  | GLN  |
| 79  | Sd    | 16  | GLN  |
| 80  | Se    | 76  | HIS  |
| 80  | Se    | 88  | GLN  |
| 82  | Sg    | 64  | HIS  |
| 82  | Sg    | 119 | GLN  |
| 82  | Sg    | 215 | GLN  |
| 82  | Sg    | 222 | ASN  |
| 82  | Sg    | 285 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | A4    | 16/28 (57%)     | 6 (37%)           | 0               |
| 2   | B4    | 75/76 (98%)     | 20 (26%)          | 0               |
| 2   | D4    | 75/76 (98%)     | 19 (25%)          | 0               |
| 4   | L5    | 3626/5070 (71%) | 885 (24%)         | 14 (0%)         |
| 49  | S2    | 1688/1869 (90%) | 532 (31%)         | 17 (1%)         |
| 5   | L7    | 119/120 (99%)   | 20 (16%)          | 0               |
| 6   | L8    | 155/156 (99%)   | 34 (21%)          | 1 (0%)          |
| All | All   | 5754/7395 (77%) | 1516 (26%)        | 32 (0%)         |

All (1516) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A4    | 49  | U    |
| 1   | A4    | 53  | U    |
| 1   | A4    | 54  | U    |
| 1   | A4    | 55  | U    |
| 1   | A4    | 57  | U    |
| 1   | A4    | 58  | U    |
| 2   | B4    | 2   | C    |
| 2   | B4    | 4   | C    |
| 2   | B4    | 6   | G    |
| 2   | B4    | 7   | A    |
| 2   | B4    | 10  | G    |
| 2   | B4    | 17  | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B4    | 18  | G    |
| 2   | B4    | 19  | G    |
| 2   | B4    | 21  | A    |
| 2   | B4    | 37  | A    |
| 2   | B4    | 42  | C    |
| 2   | B4    | 47  | U    |
| 2   | B4    | 52  | G    |
| 2   | B4    | 59  | U    |
| 2   | B4    | 60  | U    |
| 2   | B4    | 62  | C    |
| 2   | B4    | 63  | G    |
| 2   | B4    | 66  | U    |
| 2   | B4    | 68  | C    |
| 2   | B4    | 76  | A    |
| 2   | D4    | 2   | C    |
| 2   | D4    | 4   | C    |
| 2   | D4    | 8   | U    |
| 2   | D4    | 9   | A    |
| 2   | D4    | 12  | U    |
| 2   | D4    | 13  | C    |
| 2   | D4    | 14  | A    |
| 2   | D4    | 17  | C    |
| 2   | D4    | 18  | G    |
| 2   | D4    | 19  | G    |
| 2   | D4    | 20  | U    |
| 2   | D4    | 21  | A    |
| 2   | D4    | 47  | U    |
| 2   | D4    | 48  | C    |
| 2   | D4    | 58  | A    |
| 2   | D4    | 59  | U    |
| 2   | D4    | 65  | G    |
| 2   | D4    | 74  | C    |
| 2   | D4    | 76  | A    |
| 4   | L5    | 2   | G    |
| 4   | L5    | 30  | C    |
| 4   | L5    | 39  | A    |
| 4   | L5    | 42  | A    |
| 4   | L5    | 44  | A    |
| 4   | L5    | 47  | A    |
| 4   | L5    | 48  | G    |
| 4   | L5    | 56  | A    |
| 4   | L5    | 58  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | L5    | 59  | A    |
| 4   | L5    | 64  | A    |
| 4   | L5    | 65  | A    |
| 4   | L5    | 66  | A    |
| 4   | L5    | 69  | A    |
| 4   | L5    | 72  | C    |
| 4   | L5    | 73  | A    |
| 4   | L5    | 84  | A    |
| 4   | L5    | 91  | G    |
| 4   | L5    | 108 | A    |
| 4   | L5    | 109 | G    |
| 4   | L5    | 110 | C    |
| 4   | L5    | 116 | G    |
| 4   | L5    | 119 | G    |
| 4   | L5    | 120 | A    |
| 4   | L5    | 122 | U    |
| 4   | L5    | 133 | C    |
| 4   | L5    | 134 | G    |
| 4   | L5    | 135 | G    |
| 4   | L5    | 136 | C    |
| 4   | L5    | 139 | G    |
| 4   | L5    | 144 | G    |
| 4   | L5    | 150 | U    |
| 4   | L5    | 152 | U    |
| 4   | L5    | 159 | C    |
| 4   | L5    | 165 | A    |
| 4   | L5    | 172 | C    |
| 4   | L5    | 176 | G    |
| 4   | L5    | 177 | G    |
| 4   | L5    | 180 | C    |
| 4   | L5    | 181 | C    |
| 4   | L5    | 183 | C    |
| 4   | L5    | 184 | U    |
| 4   | L5    | 185 | C    |
| 4   | L5    | 186 | G    |
| 4   | L5    | 187 | U    |
| 4   | L5    | 188 | G    |
| 4   | L5    | 195 | C    |
| 4   | L5    | 200 | U    |
| 4   | L5    | 209 | U    |
| 4   | L5    | 216 | C    |
| 4   | L5    | 218 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | L5    | 219 | G    |
| 4   | L5    | 233 | U    |
| 4   | L5    | 234 | G    |
| 4   | L5    | 256 | G    |
| 4   | L5    | 259 | C    |
| 4   | L5    | 261 | G    |
| 4   | L5    | 265 | C    |
| 4   | L5    | 266 | C    |
| 4   | L5    | 267 | G    |
| 4   | L5    | 272 | U    |
| 4   | L5    | 274 | C    |
| 4   | L5    | 276 | C    |
| 4   | L5    | 278 | G    |
| 4   | L5    | 280 | G    |
| 4   | L5    | 297 | U    |
| 4   | L5    | 306 | A    |
| 4   | L5    | 315 | G    |
| 4   | L5    | 316 | U    |
| 4   | L5    | 326 | C    |
| 4   | L5    | 340 | C    |
| 4   | L5    | 341 | G    |
| 4   | L5    | 344 | A    |
| 4   | L5    | 349 | A    |
| 4   | L5    | 379 | G    |
| 4   | L5    | 386 | A    |
| 4   | L5    | 387 | G    |
| 4   | L5    | 398 | A    |
| 4   | L5    | 401 | G    |
| 4   | L5    | 407 | A    |
| 4   | L5    | 408 | A    |
| 4   | L5    | 409 | G    |
| 4   | L5    | 410 | A    |
| 4   | L5    | 411 | G    |
| 4   | L5    | 412 | G    |
| 4   | L5    | 432 | U    |
| 4   | L5    | 437 | G    |
| 4   | L5    | 438 | G    |
| 4   | L5    | 440 | U    |
| 4   | L5    | 446 | C    |
| 4   | L5    | 449 | C    |
| 4   | L5    | 450 | G    |
| 4   | L5    | 452 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | L5    | 453 | G    |
| 4   | L5    | 454 | U    |
| 4   | L5    | 456 | C    |
| 4   | L5    | 457 | G    |
| 4   | L5    | 465 | G    |
| 4   | L5    | 467 | U    |
| 4   | L5    | 472 | C    |
| 4   | L5    | 483 | G    |
| 4   | L5    | 484 | U    |
| 4   | L5    | 485 | C    |
| 4   | L5    | 486 | C    |
| 4   | L5    | 487 | G    |
| 4   | L5    | 489 | C    |
| 4   | L5    | 492 | U    |
| 4   | L5    | 493 | G    |
| 4   | L5    | 494 | U    |
| 4   | L5    | 497 | G    |
| 4   | L5    | 498 | C    |
| 4   | L5    | 500 | G    |
| 4   | L5    | 501 | C    |
| 4   | L5    | 502 | C    |
| 4   | L5    | 503 | C    |
| 4   | L5    | 504 | G    |
| 4   | L5    | 505 | G    |
| 4   | L5    | 507 | G    |
| 4   | L5    | 509 | A    |
| 4   | L5    | 510 | U    |
| 4   | L5    | 511 | C    |
| 4   | L5    | 512 | U    |
| 4   | L5    | 513 | U    |
| 4   | L5    | 514 | U    |
| 4   | L5    | 515 | C    |
| 4   | L5    | 518 | G    |
| 4   | L5    | 519 | C    |
| 4   | L5    | 643 | C    |
| 4   | L5    | 644 | G    |
| 4   | L5    | 646 | G    |
| 4   | L5    | 654 | C    |
| 4   | L5    | 656 | C    |
| 4   | L5    | 657 | C    |
| 4   | L5    | 659 | G    |
| 4   | L5    | 665 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | L5    | 667 | A    |
| 4   | L5    | 668 | C    |
| 4   | L5    | 673 | C    |
| 4   | L5    | 674 | G    |
| 4   | L5    | 685 | C    |
| 4   | L5    | 686 | A    |
| 4   | L5    | 687 | U    |
| 4   | L5    | 688 | U    |
| 4   | L5    | 700 | G    |
| 4   | L5    | 703 | G    |
| 4   | L5    | 704 | C    |
| 4   | L5    | 719 | C    |
| 4   | L5    | 731 | G    |
| 4   | L5    | 738 | C    |
| 4   | L5    | 739 | G    |
| 4   | L5    | 740 | G    |
| 4   | L5    | 742 | G    |
| 4   | L5    | 753 | C    |
| 4   | L5    | 754 | U    |
| 4   | L5    | 757 | G    |
| 4   | L5    | 758 | G    |
| 4   | L5    | 759 | G    |
| 4   | L5    | 904 | C    |
| 4   | L5    | 906 | C    |
| 4   | L5    | 912 | G    |
| 4   | L5    | 913 | U    |
| 4   | L5    | 914 | U    |
| 4   | L5    | 915 | A    |
| 4   | L5    | 916 | C    |
| 4   | L5    | 917 | A    |
| 4   | L5    | 918 | G    |
| 4   | L5    | 923 | C    |
| 4   | L5    | 924 | C    |
| 4   | L5    | 926 | G    |
| 4   | L5    | 932 | A    |
| 4   | L5    | 933 | G    |
| 4   | L5    | 936 | C    |
| 4   | L5    | 937 | U    |
| 4   | L5    | 943 | A    |
| 4   | L5    | 944 | A    |
| 4   | L5    | 945 | U    |
| 4   | L5    | 959 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | L5    | 960  | A    |
| 4   | L5    | 961  | G    |
| 4   | L5    | 962  | C    |
| 4   | L5    | 963  | G    |
| 4   | L5    | 965  | G    |
| 4   | L5    | 966  | A    |
| 4   | L5    | 967  | C    |
| 4   | L5    | 968  | C    |
| 4   | L5    | 970  | G    |
| 4   | L5    | 972  | C    |
| 4   | L5    | 982  | U    |
| 4   | L5    | 988  | C    |
| 4   | L5    | 989  | U    |
| 4   | L5    | 990  | C    |
| 4   | L5    | 991  | C    |
| 4   | L5    | 992  | C    |
| 4   | L5    | 993  | G    |
| 4   | L5    | 995  | C    |
| 4   | L5    | 1066 | G    |
| 4   | L5    | 1068 | G    |
| 4   | L5    | 1070 | G    |
| 4   | L5    | 1072 | C    |
| 4   | L5    | 1075 | G    |
| 4   | L5    | 1083 | U    |
| 4   | L5    | 1092 | G    |
| 4   | L5    | 1168 | G    |
| 4   | L5    | 1170 | G    |
| 4   | L5    | 1172 | C    |
| 4   | L5    | 1173 | G    |
| 4   | L5    | 1174 | G    |
| 4   | L5    | 1178 | G    |
| 4   | L5    | 1179 | U    |
| 4   | L5    | 1180 | C    |
| 4   | L5    | 1181 | C    |
| 4   | L5    | 1182 | C    |
| 4   | L5    | 1183 | C    |
| 4   | L5    | 1184 | A    |
| 4   | L5    | 1187 | G    |
| 4   | L5    | 1193 | C    |
| 4   | L5    | 1196 | G    |
| 4   | L5    | 1202 | C    |
| 4   | L5    | 1203 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | L5    | 1205 | G    |
| 4   | L5    | 1209 | U    |
| 4   | L5    | 1211 | G    |
| 4   | L5    | 1214 | C    |
| 4   | L5    | 1215 | C    |
| 4   | L5    | 1216 | C    |
| 4   | L5    | 1217 | G    |
| 4   | L5    | 1218 | G    |
| 4   | L5    | 1221 | G    |
| 4   | L5    | 1222 | A    |
| 4   | L5    | 1241 | C    |
| 4   | L5    | 1245 | C    |
| 4   | L5    | 1253 | G    |
| 4   | L5    | 1258 | G    |
| 4   | L5    | 1259 | G    |
| 4   | L5    | 1260 | G    |
| 4   | L5    | 1261 | G    |
| 4   | L5    | 1262 | G    |
| 4   | L5    | 1266 | G    |
| 4   | L5    | 1269 | G    |
| 4   | L5    | 1271 | G    |
| 4   | L5    | 1272 | C    |
| 4   | L5    | 1273 | G    |
| 4   | L5    | 1274 | A    |
| 4   | L5    | 1275 | G    |
| 4   | L5    | 1277 | G    |
| 4   | L5    | 1280 | C    |
| 4   | L5    | 1284 | G    |
| 4   | L5    | 1287 | G    |
| 4   | L5    | 1294 | A    |
| 4   | L5    | 1295 | C    |
| 4   | L5    | 1301 | C    |
| 4   | L5    | 1302 | U    |
| 4   | L5    | 1313 | C    |
| 4   | L5    | 1314 | C    |
| 4   | L5    | 1326 | A    |
| 4   | L5    | 1354 | A    |
| 4   | L5    | 1358 | G    |
| 4   | L5    | 1359 | G    |
| 4   | L5    | 1365 | C    |
| 4   | L5    | 1366 | G    |
| 4   | L5    | 1370 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | L5    | 1377 | G    |
| 4   | L5    | 1378 | C    |
| 4   | L5    | 1379 | C    |
| 4   | L5    | 1381 | U    |
| 4   | L5    | 1387 | A    |
| 4   | L5    | 1394 | G    |
| 4   | L5    | 1398 | A    |
| 4   | L5    | 1399 | G    |
| 4   | L5    | 1402 | C    |
| 4   | L5    | 1404 | G    |
| 4   | L5    | 1405 | C    |
| 4   | L5    | 1407 | C    |
| 4   | L5    | 1409 | C    |
| 4   | L5    | 1410 | U    |
| 4   | L5    | 1411 | C    |
| 4   | L5    | 1417 | C    |
| 4   | L5    | 1418 | C    |
| 4   | L5    | 1420 | A    |
| 4   | L5    | 1425 | G    |
| 4   | L5    | 1435 | G    |
| 4   | L5    | 1439 | C    |
| 4   | L5    | 1441 | C    |
| 4   | L5    | 1442 | C    |
| 4   | L5    | 1443 | A    |
| 4   | L5    | 1444 | G    |
| 4   | L5    | 1445 | U    |
| 4   | L5    | 1447 | C    |
| 4   | L5    | 1482 | G    |
| 4   | L5    | 1483 | C    |
| 4   | L5    | 1494 | U    |
| 4   | L5    | 1497 | A    |
| 4   | L5    | 1498 | G    |
| 4   | L5    | 1516 | G    |
| 4   | L5    | 1518 | A    |
| 4   | L5    | 1525 | A    |
| 4   | L5    | 1534 | A    |
| 4   | L5    | 1543 | G    |
| 4   | L5    | 1547 | A    |
| 4   | L5    | 1549 | G    |
| 4   | L5    | 1563 | A    |
| 4   | L5    | 1566 | C    |
| 4   | L5    | 1578 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | L5    | 1591 | U    |
| 4   | L5    | 1596 | U    |
| 4   | L5    | 1605 | G    |
| 4   | L5    | 1624 | G    |
| 4   | L5    | 1625 | G    |
| 4   | L5    | 1631 | A    |
| 4   | L5    | 1633 | G    |
| 4   | L5    | 1634 | A    |
| 4   | L5    | 1641 | G    |
| 4   | L5    | 1642 | A    |
| 4   | L5    | 1649 | U    |
| 4   | L5    | 1650 | A    |
| 4   | L5    | 1654 | G    |
| 4   | L5    | 1661 | C    |
| 4   | L5    | 1663 | C    |
| 4   | L5    | 1676 | C    |
| 4   | L5    | 1681 | G    |
| 4   | L5    | 1685 | G    |
| 4   | L5    | 1691 | G    |
| 4   | L5    | 1694 | C    |
| 4   | L5    | 1697 | G    |
| 4   | L5    | 1699 | A    |
| 4   | L5    | 1700 | G    |
| 4   | L5    | 1701 | A    |
| 4   | L5    | 1703 | C    |
| 4   | L5    | 1704 | C    |
| 4   | L5    | 1705 | G    |
| 4   | L5    | 1707 | C    |
| 4   | L5    | 1715 | C    |
| 4   | L5    | 1718 | C    |
| 4   | L5    | 1731 | C    |
| 4   | L5    | 1734 | G    |
| 4   | L5    | 1741 | G    |
| 4   | L5    | 1742 | A    |
| 4   | L5    | 1750 | G    |
| 4   | L5    | 1755 | C    |
| 4   | L5    | 1757 | U    |
| 4   | L5    | 1758 | G    |
| 4   | L5    | 1760 | G    |
| 4   | L5    | 1763 | C    |
| 4   | L5    | 1765 | A    |
| 4   | L5    | 1767 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | L5    | 1785 | C    |
| 4   | L5    | 1787 | A    |
| 4   | L5    | 1804 | A    |
| 4   | L5    | 1806 | G    |
| 4   | L5    | 1810 | G    |
| 4   | L5    | 1815 | G    |
| 4   | L5    | 1820 | C    |
| 4   | L5    | 1821 | G    |
| 4   | L5    | 1822 | U    |
| 4   | L5    | 1823 | G    |
| 4   | L5    | 1824 | G    |
| 4   | L5    | 1833 | G    |
| 4   | L5    | 1834 | U    |
| 4   | L5    | 1836 | G    |
| 4   | L5    | 1837 | A    |
| 4   | L5    | 1842 | G    |
| 4   | L5    | 1855 | G    |
| 4   | L5    | 1869 | G    |
| 4   | L5    | 1882 | U    |
| 4   | L5    | 1893 | C    |
| 4   | L5    | 1897 | A    |
| 4   | L5    | 1915 | C    |
| 4   | L5    | 1917 | A    |
| 4   | L5    | 1918 | U    |
| 4   | L5    | 1919 | G    |
| 4   | L5    | 1920 | C    |
| 4   | L5    | 1921 | C    |
| 4   | L5    | 1922 | G    |
| 4   | L5    | 1925 | G    |
| 4   | L5    | 1930 | U    |
| 4   | L5    | 1931 | C    |
| 4   | L5    | 1932 | A    |
| 4   | L5    | 1935 | C    |
| 4   | L5    | 1940 | G    |
| 4   | L5    | 1948 | G    |
| 4   | L5    | 1953 | U    |
| 4   | L5    | 1959 | U    |
| 4   | L5    | 1960 | A    |
| 4   | L5    | 1961 | G    |
| 4   | L5    | 1962 | A    |
| 4   | L5    | 1966 | C    |
| 4   | L5    | 1967 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | L5    | 1971 | C    |
| 4   | L5    | 1972 | G    |
| 4   | L5    | 1973 | G    |
| 4   | L5    | 1974 | U    |
| 4   | L5    | 1975 | G    |
| 4   | L5    | 1976 | G    |
| 4   | L5    | 1977 | C    |
| 4   | L5    | 1984 | A    |
| 4   | L5    | 1985 | G    |
| 4   | L5    | 1995 | G    |
| 4   | L5    | 1996 | C    |
| 4   | L5    | 1997 | U    |
| 4   | L5    | 1998 | A    |
| 4   | L5    | 1999 | A    |
| 4   | L5    | 2001 | G    |
| 4   | L5    | 2002 | A    |
| 4   | L5    | 2003 | G    |
| 4   | L5    | 2006 | U    |
| 4   | L5    | 2007 | G    |
| 4   | L5    | 2009 | A    |
| 4   | L5    | 2010 | A    |
| 4   | L5    | 2011 | C    |
| 4   | L5    | 2012 | A    |
| 4   | L5    | 2013 | A    |
| 4   | L5    | 2015 | U    |
| 4   | L5    | 2017 | A    |
| 4   | L5    | 2018 | C    |
| 4   | L5    | 2020 | U    |
| 4   | L5    | 2025 | A    |
| 4   | L5    | 2026 | A    |
| 4   | L5    | 2031 | C    |
| 4   | L5    | 2038 | U    |
| 4   | L5    | 2046 | G    |
| 4   | L5    | 2048 | U    |
| 4   | L5    | 2055 | G    |
| 4   | L5    | 2056 | G    |
| 4   | L5    | 2062 | C    |
| 4   | L5    | 2069 | A    |
| 4   | L5    | 2084 | C    |
| 4   | L5    | 2085 | G    |
| 4   | L5    | 2089 | G    |
| 4   | L5    | 2092 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | L5    | 2093 | A    |
| 4   | L5    | 2094 | G    |
| 4   | L5    | 2095 | A    |
| 4   | L5    | 2096 | G    |
| 4   | L5    | 2097 | U    |
| 4   | L5    | 2098 | G    |
| 4   | L5    | 2101 | C    |
| 4   | L5    | 2102 | G    |
| 4   | L5    | 2103 | G    |
| 4   | L5    | 2106 | G    |
| 4   | L5    | 2107 | C    |
| 4   | L5    | 2108 | G    |
| 4   | L5    | 2109 | G    |
| 4   | L5    | 2116 | C    |
| 4   | L5    | 2117 | G    |
| 4   | L5    | 2118 | G    |
| 4   | L5    | 2119 | C    |
| 4   | L5    | 2120 | G    |
| 4   | L5    | 2121 | C    |
| 4   | L5    | 2123 | C    |
| 4   | L5    | 2128 | G    |
| 4   | L5    | 2129 | C    |
| 4   | L5    | 2130 | G    |
| 4   | L5    | 2250 | C    |
| 4   | L5    | 2252 | G    |
| 4   | L5    | 2253 | A    |
| 4   | L5    | 2255 | C    |
| 4   | L5    | 2256 | C    |
| 4   | L5    | 2257 | C    |
| 4   | L5    | 2258 | C    |
| 4   | L5    | 2259 | G    |
| 4   | L5    | 2270 | G    |
| 4   | L5    | 2289 | C    |
| 4   | L5    | 2294 | G    |
| 4   | L5    | 2300 | A    |
| 4   | L5    | 2301 | G    |
| 4   | L5    | 2313 | A    |
| 4   | L5    | 2316 | G    |
| 4   | L5    | 2322 | G    |
| 4   | L5    | 2333 | G    |
| 4   | L5    | 2346 | C    |
| 4   | L5    | 2348 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | L5    | 2350 | U    |
| 4   | L5    | 2351 | C    |
| 4   | L5    | 2357 | G    |
| 4   | L5    | 2389 | A    |
| 4   | L5    | 2395 | A    |
| 4   | L5    | 2396 | A    |
| 4   | L5    | 2397 | G    |
| 4   | L5    | 2398 | U    |
| 4   | L5    | 2402 | G    |
| 4   | L5    | 2404 | A    |
| 4   | L5    | 2416 | G    |
| 4   | L5    | 2417 | A    |
| 4   | L5    | 2421 | G    |
| 4   | L5    | 2422 | C    |
| 4   | L5    | 2424 | G    |
| 4   | L5    | 2425 | U    |
| 4   | L5    | 2437 | C    |
| 4   | L5    | 2441 | C    |
| 4   | L5    | 2447 | U    |
| 4   | L5    | 2450 | G    |
| 4   | L5    | 2453 | A    |
| 4   | L5    | 2464 | C    |
| 4   | L5    | 2465 | C    |
| 4   | L5    | 2474 | G    |
| 4   | L5    | 2475 | G    |
| 4   | L5    | 2478 | C    |
| 4   | L5    | 2483 | G    |
| 4   | L5    | 2484 | A    |
| 4   | L5    | 2487 | G    |
| 4   | L5    | 2489 | C    |
| 4   | L5    | 2490 | U    |
| 4   | L5    | 2491 | C    |
| 4   | L5    | 2493 | G    |
| 4   | L5    | 2503 | G    |
| 4   | L5    | 2504 | C    |
| 4   | L5    | 2505 | C    |
| 4   | L5    | 2506 | G    |
| 4   | L5    | 2511 | A    |
| 4   | L5    | 2513 | A    |
| 4   | L5    | 2519 | U    |
| 4   | L5    | 2537 | A    |
| 4   | L5    | 2544 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | L5    | 2546 | G    |
| 4   | L5    | 2547 | G    |
| 4   | L5    | 2554 | U    |
| 4   | L5    | 2555 | G    |
| 4   | L5    | 2556 | G    |
| 4   | L5    | 2566 | G    |
| 4   | L5    | 2567 | G    |
| 4   | L5    | 2573 | A    |
| 4   | L5    | 2583 | C    |
| 4   | L5    | 2587 | A    |
| 4   | L5    | 2588 | C    |
| 4   | L5    | 2600 | A    |
| 4   | L5    | 2601 | A    |
| 4   | L5    | 2618 | G    |
| 4   | L5    | 2627 | C    |
| 4   | L5    | 2653 | C    |
| 4   | L5    | 2662 | G    |
| 4   | L5    | 2663 | G    |
| 4   | L5    | 2669 | C    |
| 4   | L5    | 2670 | C    |
| 4   | L5    | 2673 | G    |
| 4   | L5    | 2675 | G    |
| 4   | L5    | 2676 | A    |
| 4   | L5    | 2687 | U    |
| 4   | L5    | 2694 | G    |
| 4   | L5    | 2695 | A    |
| 4   | L5    | 2696 | A    |
| 4   | L5    | 2707 | U    |
| 4   | L5    | 2708 | U    |
| 4   | L5    | 2710 | C    |
| 4   | L5    | 2711 | G    |
| 4   | L5    | 2719 | C    |
| 4   | L5    | 2721 | G    |
| 4   | L5    | 2724 | G    |
| 4   | L5    | 2726 | G    |
| 4   | L5    | 2739 | C    |
| 4   | L5    | 2742 | G    |
| 4   | L5    | 2743 | A    |
| 4   | L5    | 2746 | A    |
| 4   | L5    | 2754 | G    |
| 4   | L5    | 2756 | G    |
| 4   | L5    | 2761 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | L5    | 2763 | U    |
| 4   | L5    | 2764 | A    |
| 4   | L5    | 2770 | C    |
| 4   | L5    | 2788 | U    |
| 4   | L5    | 2790 | U    |
| 4   | L5    | 2794 | C    |
| 4   | L5    | 2814 | C    |
| 4   | L5    | 2815 | A    |
| 4   | L5    | 2819 | U    |
| 4   | L5    | 2827 | G    |
| 4   | L5    | 2829 | U    |
| 4   | L5    | 2830 | G    |
| 4   | L5    | 2835 | A    |
| 4   | L5    | 2838 | G    |
| 4   | L5    | 2842 | G    |
| 4   | L5    | 2855 | G    |
| 4   | L5    | 2856 | C    |
| 4   | L5    | 2874 | U    |
| 4   | L5    | 2877 | G    |
| 4   | L5    | 2900 | U    |
| 4   | L5    | 2902 | G    |
| 4   | L5    | 2903 | G    |
| 4   | L5    | 2904 | U    |
| 4   | L5    | 2905 | C    |
| 4   | L5    | 2906 | G    |
| 4   | L5    | 2907 | G    |
| 4   | L5    | 2908 | U    |
| 4   | L5    | 2910 | G    |
| 4   | L5    | 3585 | G    |
| 4   | L5    | 3588 | C    |
| 4   | L5    | 3590 | G    |
| 4   | L5    | 3591 | C    |
| 4   | L5    | 3592 | G    |
| 4   | L5    | 3593 | C    |
| 4   | L5    | 3594 | C    |
| 4   | L5    | 3595 | U    |
| 4   | L5    | 3596 | A    |
| 4   | L5    | 3597 | G    |
| 4   | L5    | 3599 | A    |
| 4   | L5    | 3604 | A    |
| 4   | L5    | 3605 | C    |
| 4   | L5    | 3606 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | L5    | 3615 | G    |
| 4   | L5    | 3616 | U    |
| 4   | L5    | 3618 | C    |
| 4   | L5    | 3626 | G    |
| 4   | L5    | 3630 | A    |
| 4   | L5    | 3635 | A    |
| 4   | L5    | 3644 | U    |
| 4   | L5    | 3662 | A    |
| 4   | L5    | 3664 | G    |
| 4   | L5    | 3672 | G    |
| 4   | L5    | 3673 | C    |
| 4   | L5    | 3674 | G    |
| 4   | L5    | 3678 | G    |
| 4   | L5    | 3680 | U    |
| 4   | L5    | 3691 | G    |
| 4   | L5    | 3692 | A    |
| 4   | L5    | 3711 | A    |
| 4   | L5    | 3726 | A    |
| 4   | L5    | 3727 | A    |
| 4   | L5    | 3729 | U    |
| 4   | L5    | 3735 | G    |
| 4   | L5    | 3736 | A    |
| 4   | L5    | 3748 | A    |
| 4   | L5    | 3750 | G    |
| 4   | L5    | 3753 | G    |
| 4   | L5    | 3754 | G    |
| 4   | L5    | 3757 | G    |
| 4   | L5    | 3758 | U    |
| 4   | L5    | 3760 | A    |
| 4   | L5    | 3771 | C    |
| 4   | L5    | 3775 | A    |
| 4   | L5    | 3776 | G    |
| 4   | L5    | 3777 | G    |
| 4   | L5    | 3784 | A    |
| 4   | L5    | 3786 | U    |
| 4   | L5    | 3802 | U    |
| 4   | L5    | 3811 | G    |
| 4   | L5    | 3812 | C    |
| 4   | L5    | 3814 | U    |
| 4   | L5    | 3817 | A    |
| 4   | L5    | 3818 | U    |
| 4   | L5    | 3819 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | L5    | 3823 | G    |
| 4   | L5    | 3838 | U    |
| 4   | L5    | 3839 | G    |
| 4   | L5    | 3840 | U    |
| 4   | L5    | 3867 | A    |
| 4   | L5    | 3877 | A    |
| 4   | L5    | 3878 | C    |
| 4   | L5    | 3879 | G    |
| 4   | L5    | 3880 | G    |
| 4   | L5    | 3885 | G    |
| 4   | L5    | 3890 | A    |
| 4   | L5    | 3892 | U    |
| 4   | L5    | 3897 | G    |
| 4   | L5    | 3898 | G    |
| 4   | L5    | 3901 | A    |
| 4   | L5    | 3905 | A    |
| 4   | L5    | 3906 | A    |
| 4   | L5    | 3907 | G    |
| 4   | L5    | 3908 | A    |
| 4   | L5    | 3915 | U    |
| 4   | L5    | 3926 | C    |
| 4   | L5    | 3938 | G    |
| 4   | L5    | 3939 | G    |
| 4   | L5    | 3941 | G    |
| 4   | L5    | 3942 | A    |
| 4   | L5    | 3943 | A    |
| 4   | L5    | 3944 | G    |
| 4   | L5    | 3947 | A    |
| 4   | L5    | 3948 | C    |
| 4   | L5    | 3949 | A    |
| 4   | L5    | 4066 | U    |
| 4   | L5    | 4067 | U    |
| 4   | L5    | 4069 | U    |
| 4   | L5    | 4076 | G    |
| 4   | L5    | 4086 | G    |
| 4   | L5    | 4099 | G    |
| 4   | L5    | 4102 | C    |
| 4   | L5    | 4104 | G    |
| 4   | L5    | 4105 | A    |
| 4   | L5    | 4107 | G    |
| 4   | L5    | 4108 | G    |
| 4   | L5    | 4111 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | L5    | 4113 | U    |
| 4   | L5    | 4114 | C    |
| 4   | L5    | 4115 | G    |
| 4   | L5    | 4116 | C    |
| 4   | L5    | 4119 | C    |
| 4   | L5    | 4121 | G    |
| 4   | L5    | 4122 | G    |
| 4   | L5    | 4127 | A    |
| 4   | L5    | 4132 | C    |
| 4   | L5    | 4133 | C    |
| 4   | L5    | 4138 | C    |
| 4   | L5    | 4139 | G    |
| 4   | L5    | 4140 | C    |
| 4   | L5    | 4141 | G    |
| 4   | L5    | 4142 | C    |
| 4   | L5    | 4143 | G    |
| 4   | L5    | 4145 | C    |
| 4   | L5    | 4148 | C    |
| 4   | L5    | 4149 | C    |
| 4   | L5    | 4150 | G    |
| 4   | L5    | 4162 | C    |
| 4   | L5    | 4163 | U    |
| 4   | L5    | 4164 | C    |
| 4   | L5    | 4170 | A    |
| 4   | L5    | 4177 | C    |
| 4   | L5    | 4183 | G    |
| 4   | L5    | 4184 | G    |
| 4   | L5    | 4191 | G    |
| 4   | L5    | 4203 | A    |
| 4   | L5    | 4212 | A    |
| 4   | L5    | 4222 | G    |
| 4   | L5    | 4224 | A    |
| 4   | L5    | 4225 | G    |
| 4   | L5    | 4229 | U    |
| 4   | L5    | 4233 | A    |
| 4   | L5    | 4249 | G    |
| 4   | L5    | 4251 | A    |
| 4   | L5    | 4254 | G    |
| 4   | L5    | 4257 | A    |
| 4   | L5    | 4258 | C    |
| 4   | L5    | 4265 | U    |
| 4   | L5    | 4268 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | L5    | 4273 | A    |
| 4   | L5    | 4281 | A    |
| 4   | L5    | 4290 | U    |
| 4   | L5    | 4291 | G    |
| 4   | L5    | 4297 | G    |
| 4   | L5    | 4304 | A    |
| 4   | L5    | 4305 | G    |
| 4   | L5    | 4306 | U    |
| 4   | L5    | 4314 | C    |
| 4   | L5    | 4330 | G    |
| 4   | L5    | 4332 | C    |
| 4   | L5    | 4338 | G    |
| 4   | L5    | 4349 | C    |
| 4   | L5    | 4350 | C    |
| 4   | L5    | 4352 | U    |
| 4   | L5    | 4354 | U    |
| 4   | L5    | 4373 | G    |
| 4   | L5    | 4377 | G    |
| 4   | L5    | 4378 | A    |
| 4   | L5    | 4379 | A    |
| 4   | L5    | 4380 | A    |
| 4   | L5    | 4381 | A    |
| 4   | L5    | 4387 | C    |
| 4   | L5    | 4391 | G    |
| 4   | L5    | 4394 | A    |
| 4   | L5    | 4410 | G    |
| 4   | L5    | 4416 | G    |
| 4   | L5    | 4422 | A    |
| 4   | L5    | 4433 | G    |
| 4   | L5    | 4440 | G    |
| 4   | L5    | 4444 | C    |
| 4   | L5    | 4448 | G    |
| 4   | L5    | 4449 | A    |
| 4   | L5    | 4452 | U    |
| 4   | L5    | 4453 | C    |
| 4   | L5    | 4464 | A    |
| 4   | L5    | 4466 | C    |
| 4   | L5    | 4495 | G    |
| 4   | L5    | 4500 | U    |
| 4   | L5    | 4512 | U    |
| 4   | L5    | 4513 | A    |
| 4   | L5    | 4519 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | L5    | 4524 | G    |
| 4   | L5    | 4545 | G    |
| 4   | L5    | 4548 | A    |
| 4   | L5    | 4549 | G    |
| 4   | L5    | 4554 | G    |
| 4   | L5    | 4560 | C    |
| 4   | L5    | 4567 | G    |
| 4   | L5    | 4569 | U    |
| 4   | L5    | 4570 | G    |
| 4   | L5    | 4573 | G    |
| 4   | L5    | 4575 | G    |
| 4   | L5    | 4589 | A    |
| 4   | L5    | 4590 | A    |
| 4   | L5    | 4600 | G    |
| 4   | L5    | 4606 | G    |
| 4   | L5    | 4617 | G    |
| 4   | L5    | 4624 | A    |
| 4   | L5    | 4635 | A    |
| 4   | L5    | 4636 | U    |
| 4   | L5    | 4637 | G    |
| 4   | L5    | 4647 | G    |
| 4   | L5    | 4652 | G    |
| 4   | L5    | 4656 | A    |
| 4   | L5    | 4658 | G    |
| 4   | L5    | 4670 | C    |
| 4   | L5    | 4672 | A    |
| 4   | L5    | 4677 | U    |
| 4   | L5    | 4679 | G    |
| 4   | L5    | 4694 | G    |
| 4   | L5    | 4695 | C    |
| 4   | L5    | 4700 | A    |
| 4   | L5    | 4707 | A    |
| 4   | L5    | 4708 | A    |
| 4   | L5    | 4709 | U    |
| 4   | L5    | 4719 | G    |
| 4   | L5    | 4720 | C    |
| 4   | L5    | 4728 | U    |
| 4   | L5    | 4731 | G    |
| 4   | L5    | 4732 | G    |
| 4   | L5    | 4733 | C    |
| 4   | L5    | 4734 | A    |
| 4   | L5    | 4740 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | L5    | 4741 | C    |
| 4   | L5    | 4742 | G    |
| 4   | L5    | 4745 | G    |
| 4   | L5    | 4750 | G    |
| 4   | L5    | 4754 | G    |
| 4   | L5    | 4757 | C    |
| 4   | L5    | 4759 | C    |
| 4   | L5    | 4761 | G    |
| 4   | L5    | 4764 | A    |
| 4   | L5    | 4765 | G    |
| 4   | L5    | 4771 | C    |
| 4   | L5    | 4772 | C    |
| 4   | L5    | 4774 | C    |
| 4   | L5    | 4775 | C    |
| 4   | L5    | 4776 | G    |
| 4   | L5    | 4860 | G    |
| 4   | L5    | 4870 | G    |
| 4   | L5    | 4871 | C    |
| 4   | L5    | 4875 | G    |
| 4   | L5    | 4877 | G    |
| 4   | L5    | 4881 | U    |
| 4   | L5    | 4882 | U    |
| 4   | L5    | 4883 | C    |
| 4   | L5    | 4887 | C    |
| 4   | L5    | 4888 | U    |
| 4   | L5    | 4894 | A    |
| 4   | L5    | 4895 | C    |
| 4   | L5    | 4896 | G    |
| 4   | L5    | 4898 | G    |
| 4   | L5    | 4900 | C    |
| 4   | L5    | 4901 | G    |
| 4   | L5    | 4902 | C    |
| 4   | L5    | 4910 | G    |
| 4   | L5    | 4911 | A    |
| 4   | L5    | 4912 | G    |
| 4   | L5    | 4913 | G    |
| 4   | L5    | 4914 | C    |
| 4   | L5    | 4923 | C    |
| 4   | L5    | 4926 | C    |
| 4   | L5    | 4928 | C    |
| 4   | L5    | 4931 | G    |
| 4   | L5    | 4937 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | L5    | 4938 | A    |
| 4   | L5    | 4940 | C    |
| 4   | L5    | 4941 | G    |
| 4   | L5    | 4942 | C    |
| 4   | L5    | 4943 | A    |
| 4   | L5    | 4949 | G    |
| 4   | L5    | 4950 | U    |
| 4   | L5    | 4955 | A    |
| 4   | L5    | 4960 | G    |
| 4   | L5    | 4961 | G    |
| 4   | L5    | 4967 | A    |
| 4   | L5    | 4976 | U    |
| 4   | L5    | 4985 | U    |
| 4   | L5    | 4988 | U    |
| 4   | L5    | 4989 | U    |
| 4   | L5    | 4991 | U    |
| 4   | L5    | 4993 | G    |
| 4   | L5    | 5006 | U    |
| 4   | L5    | 5014 | A    |
| 4   | L5    | 5017 | G    |
| 4   | L5    | 5022 | U    |
| 4   | L5    | 5023 | C    |
| 4   | L5    | 5024 | C    |
| 4   | L5    | 5026 | U    |
| 4   | L5    | 5028 | G    |
| 4   | L5    | 5030 | U    |
| 4   | L5    | 5034 | A    |
| 4   | L5    | 5035 | U    |
| 4   | L5    | 5040 | U    |
| 4   | L5    | 5041 | G    |
| 4   | L5    | 5050 | C    |
| 4   | L5    | 5054 | C    |
| 4   | L5    | 5055 | G    |
| 4   | L5    | 5060 | A    |
| 4   | L5    | 5061 | A    |
| 4   | L5    | 5069 | U    |
| 5   | L7    | 2    | U    |
| 5   | L7    | 7    | G    |
| 5   | L7    | 10   | C    |
| 5   | L7    | 13   | A    |
| 5   | L7    | 22   | A    |
| 5   | L7    | 23   | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | L7    | 25  | G    |
| 5   | L7    | 30  | C    |
| 5   | L7    | 33  | U    |
| 5   | L7    | 40  | U    |
| 5   | L7    | 41  | G    |
| 5   | L7    | 53  | U    |
| 5   | L7    | 54  | A    |
| 5   | L7    | 63  | C    |
| 5   | L7    | 64  | G    |
| 5   | L7    | 89  | G    |
| 5   | L7    | 97  | G    |
| 5   | L7    | 100 | A    |
| 5   | L7    | 115 | A    |
| 5   | L7    | 120 | U    |
| 6   | L8    | 2   | G    |
| 6   | L8    | 16  | G    |
| 6   | L8    | 23  | C    |
| 6   | L8    | 34  | U    |
| 6   | L8    | 35  | C    |
| 6   | L8    | 39  | G    |
| 6   | L8    | 48  | A    |
| 6   | L8    | 49  | G    |
| 6   | L8    | 59  | A    |
| 6   | L8    | 61  | A    |
| 6   | L8    | 63  | U    |
| 6   | L8    | 80  | A    |
| 6   | L8    | 81  | C    |
| 6   | L8    | 82  | A    |
| 6   | L8    | 84  | A    |
| 6   | L8    | 85  | U    |
| 6   | L8    | 86  | U    |
| 6   | L8    | 87  | G    |
| 6   | L8    | 88  | A    |
| 6   | L8    | 103 | A    |
| 6   | L8    | 104 | A    |
| 6   | L8    | 105 | C    |
| 6   | L8    | 110 | U    |
| 6   | L8    | 111 | U    |
| 6   | L8    | 114 | G    |
| 6   | L8    | 123 | U    |
| 6   | L8    | 124 | U    |
| 6   | L8    | 125 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | L8    | 126 | C    |
| 6   | L8    | 127 | U    |
| 6   | L8    | 147 | G    |
| 6   | L8    | 150 | C    |
| 6   | L8    | 151 | G    |
| 6   | L8    | 155 | C    |
| 49  | S2    | 2   | A    |
| 49  | S2    | 3   | C    |
| 49  | S2    | 9   | U    |
| 49  | S2    | 10  | G    |
| 49  | S2    | 11  | A    |
| 49  | S2    | 17  | C    |
| 49  | S2    | 21  | U    |
| 49  | S2    | 22  | A    |
| 49  | S2    | 24  | C    |
| 49  | S2    | 26  | U    |
| 49  | S2    | 32  | U    |
| 49  | S2    | 33  | G    |
| 49  | S2    | 35  | C    |
| 49  | S2    | 37  | C    |
| 49  | S2    | 41  | G    |
| 49  | S2    | 42  | A    |
| 49  | S2    | 43  | U    |
| 49  | S2    | 44  | U    |
| 49  | S2    | 45  | A    |
| 49  | S2    | 46  | A    |
| 49  | S2    | 47  | G    |
| 49  | S2    | 49  | C    |
| 49  | S2    | 53  | C    |
| 49  | S2    | 58  | C    |
| 49  | S2    | 59  | U    |
| 49  | S2    | 60  | A    |
| 49  | S2    | 64  | A    |
| 49  | S2    | 65  | C    |
| 49  | S2    | 66  | G    |
| 49  | S2    | 67  | C    |
| 49  | S2    | 68  | A    |
| 49  | S2    | 71  | G    |
| 49  | S2    | 72  | C    |
| 49  | S2    | 73  | C    |
| 49  | S2    | 74  | G    |
| 49  | S2    | 76  | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49  | S2    | 77  | A    |
| 49  | S2    | 78  | C    |
| 49  | S2    | 79  | A    |
| 49  | S2    | 80  | G    |
| 49  | S2    | 81  | U    |
| 49  | S2    | 82  | G    |
| 49  | S2    | 83  | A    |
| 49  | S2    | 84  | A    |
| 49  | S2    | 87  | U    |
| 49  | S2    | 97  | U    |
| 49  | S2    | 103 | A    |
| 49  | S2    | 111 | A    |
| 49  | S2    | 113 | G    |
| 49  | S2    | 114 | G    |
| 49  | S2    | 122 | G    |
| 49  | S2    | 126 | G    |
| 49  | S2    | 128 | U    |
| 49  | S2    | 129 | C    |
| 49  | S2    | 130 | G    |
| 49  | S2    | 143 | U    |
| 49  | S2    | 146 | G    |
| 49  | S2    | 149 | A    |
| 49  | S2    | 150 | A    |
| 49  | S2    | 155 | G    |
| 49  | S2    | 160 | U    |
| 49  | S2    | 161 | U    |
| 49  | S2    | 162 | C    |
| 49  | S2    | 163 | U    |
| 49  | S2    | 188 | C    |
| 49  | S2    | 190 | G    |
| 49  | S2    | 194 | C    |
| 49  | S2    | 196 | C    |
| 49  | S2    | 197 | U    |
| 49  | S2    | 198 | U    |
| 49  | S2    | 199 | C    |
| 49  | S2    | 202 | G    |
| 49  | S2    | 203 | G    |
| 49  | S2    | 214 | U    |
| 49  | S2    | 215 | G    |
| 49  | S2    | 290 | U    |
| 49  | S2    | 291 | G    |
| 49  | S2    | 292 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49  | S2    | 294 | U    |
| 49  | S2    | 295 | C    |
| 49  | S2    | 306 | C    |
| 49  | S2    | 307 | G    |
| 49  | S2    | 308 | G    |
| 49  | S2    | 309 | G    |
| 49  | S2    | 310 | C    |
| 49  | S2    | 311 | C    |
| 49  | S2    | 318 | A    |
| 49  | S2    | 319 | C    |
| 49  | S2    | 321 | C    |
| 49  | S2    | 322 | C    |
| 49  | S2    | 323 | C    |
| 49  | S2    | 328 | U    |
| 49  | S2    | 329 | G    |
| 49  | S2    | 331 | C    |
| 49  | S2    | 335 | G    |
| 49  | S2    | 339 | A    |
| 49  | S2    | 345 | U    |
| 49  | S2    | 346 | C    |
| 49  | S2    | 347 | G    |
| 49  | S2    | 351 | G    |
| 49  | S2    | 362 | C    |
| 49  | S2    | 364 | A    |
| 49  | S2    | 370 | G    |
| 49  | S2    | 380 | G    |
| 49  | S2    | 381 | C    |
| 49  | S2    | 382 | C    |
| 49  | S2    | 385 | G    |
| 49  | S2    | 386 | C    |
| 49  | S2    | 398 | A    |
| 49  | S2    | 400 | C    |
| 49  | S2    | 407 | G    |
| 49  | S2    | 408 | A    |
| 49  | S2    | 409 | C    |
| 49  | S2    | 413 | G    |
| 49  | S2    | 415 | A    |
| 49  | S2    | 416 | U    |
| 49  | S2    | 421 | G    |
| 49  | S2    | 426 | A    |
| 49  | S2    | 438 | G    |
| 49  | S2    | 441 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49  | S2    | 442 | C    |
| 49  | S2    | 445 | A    |
| 49  | S2    | 448 | A    |
| 49  | S2    | 449 | A    |
| 49  | S2    | 450 | C    |
| 49  | S2    | 451 | G    |
| 49  | S2    | 452 | G    |
| 49  | S2    | 464 | A    |
| 49  | S2    | 466 | G    |
| 49  | S2    | 467 | G    |
| 49  | S2    | 471 | G    |
| 49  | S2    | 472 | C    |
| 49  | S2    | 473 | A    |
| 49  | S2    | 474 | G    |
| 49  | S2    | 482 | G    |
| 49  | S2    | 485 | A    |
| 49  | S2    | 487 | U    |
| 49  | S2    | 488 | U    |
| 49  | S2    | 489 | A    |
| 49  | S2    | 492 | C    |
| 49  | S2    | 493 | A    |
| 49  | S2    | 496 | C    |
| 49  | S2    | 498 | C    |
| 49  | S2    | 506 | G    |
| 49  | S2    | 507 | G    |
| 49  | S2    | 517 | C    |
| 49  | S2    | 519 | A    |
| 49  | S2    | 520 | A    |
| 49  | S2    | 522 | A    |
| 49  | S2    | 523 | A    |
| 49  | S2    | 525 | A    |
| 49  | S2    | 527 | C    |
| 49  | S2    | 528 | A    |
| 49  | S2    | 529 | A    |
| 49  | S2    | 530 | U    |
| 49  | S2    | 532 | C    |
| 49  | S2    | 533 | A    |
| 49  | S2    | 534 | G    |
| 49  | S2    | 537 | C    |
| 49  | S2    | 538 | U    |
| 49  | S2    | 539 | C    |
| 49  | S2    | 540 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49  | S2    | 541 | U    |
| 49  | S2    | 544 | G    |
| 49  | S2    | 545 | A    |
| 49  | S2    | 548 | C    |
| 49  | S2    | 549 | C    |
| 49  | S2    | 551 | U    |
| 49  | S2    | 552 | G    |
| 49  | S2    | 554 | A    |
| 49  | S2    | 556 | U    |
| 49  | S2    | 557 | U    |
| 49  | S2    | 558 | G    |
| 49  | S2    | 560 | A    |
| 49  | S2    | 562 | U    |
| 49  | S2    | 563 | G    |
| 49  | S2    | 566 | U    |
| 49  | S2    | 568 | C    |
| 49  | S2    | 573 | U    |
| 49  | S2    | 575 | A    |
| 49  | S2    | 576 | A    |
| 49  | S2    | 582 | C    |
| 49  | S2    | 583 | C    |
| 49  | S2    | 584 | G    |
| 49  | S2    | 585 | C    |
| 49  | S2    | 587 | A    |
| 49  | S2    | 589 | G    |
| 49  | S2    | 590 | A    |
| 49  | S2    | 591 | U    |
| 49  | S2    | 592 | C    |
| 49  | S2    | 595 | U    |
| 49  | S2    | 596 | U    |
| 49  | S2    | 597 | G    |
| 49  | S2    | 598 | G    |
| 49  | S2    | 604 | A    |
| 49  | S2    | 605 | A    |
| 49  | S2    | 606 | G    |
| 49  | S2    | 608 | C    |
| 49  | S2    | 612 | U    |
| 49  | S2    | 614 | C    |
| 49  | S2    | 615 | C    |
| 49  | S2    | 627 | U    |
| 49  | S2    | 633 | C    |
| 49  | S2    | 634 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49  | S2    | 643 | A    |
| 49  | S2    | 645 | C    |
| 49  | S2    | 655 | A    |
| 49  | S2    | 658 | U    |
| 49  | S2    | 660 | C    |
| 49  | S2    | 668 | A    |
| 49  | S2    | 669 | A    |
| 49  | S2    | 671 | A    |
| 49  | S2    | 672 | A    |
| 49  | S2    | 673 | G    |
| 49  | S2    | 687 | C    |
| 49  | S2    | 689 | U    |
| 49  | S2    | 690 | G    |
| 49  | S2    | 691 | G    |
| 49  | S2    | 692 | G    |
| 49  | S2    | 693 | A    |
| 49  | S2    | 694 | G    |
| 49  | S2    | 746 | C    |
| 49  | S2    | 747 | U    |
| 49  | S2    | 748 | C    |
| 49  | S2    | 749 | U    |
| 49  | S2    | 751 | G    |
| 49  | S2    | 752 | G    |
| 49  | S2    | 753 | C    |
| 49  | S2    | 790 | C    |
| 49  | S2    | 791 | C    |
| 49  | S2    | 792 | C    |
| 49  | S2    | 793 | G    |
| 49  | S2    | 795 | A    |
| 49  | S2    | 796 | G    |
| 49  | S2    | 797 | C    |
| 49  | S2    | 798 | A    |
| 49  | S2    | 799 | U    |
| 49  | S2    | 808 | A    |
| 49  | S2    | 810 | A    |
| 49  | S2    | 811 | A    |
| 49  | S2    | 812 | A    |
| 49  | S2    | 821 | G    |
| 49  | S2    | 822 | U    |
| 49  | S2    | 823 | U    |
| 49  | S2    | 830 | A    |
| 49  | S2    | 834 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49  | S2    | 835 | C    |
| 49  | S2    | 836 | G    |
| 49  | S2    | 837 | A    |
| 49  | S2    | 838 | G    |
| 49  | S2    | 839 | C    |
| 49  | S2    | 840 | C    |
| 49  | S2    | 841 | G    |
| 49  | S2    | 842 | C    |
| 49  | S2    | 847 | A    |
| 49  | S2    | 853 | C    |
| 49  | S2    | 856 | C    |
| 49  | S2    | 869 | A    |
| 49  | S2    | 870 | A    |
| 49  | S2    | 872 | A    |
| 49  | S2    | 874 | G    |
| 49  | S2    | 878 | G    |
| 49  | S2    | 879 | C    |
| 49  | S2    | 880 | G    |
| 49  | S2    | 881 | G    |
| 49  | S2    | 882 | U    |
| 49  | S2    | 883 | U    |
| 49  | S2    | 886 | A    |
| 49  | S2    | 888 | U    |
| 49  | S2    | 889 | U    |
| 49  | S2    | 890 | U    |
| 49  | S2    | 891 | G    |
| 49  | S2    | 893 | U    |
| 49  | S2    | 895 | G    |
| 49  | S2    | 896 | U    |
| 49  | S2    | 897 | U    |
| 49  | S2    | 898 | U    |
| 49  | S2    | 899 | U    |
| 49  | S2    | 900 | C    |
| 49  | S2    | 901 | G    |
| 49  | S2    | 903 | A    |
| 49  | S2    | 904 | A    |
| 49  | S2    | 906 | U    |
| 49  | S2    | 909 | G    |
| 49  | S2    | 912 | C    |
| 49  | S2    | 913 | A    |
| 49  | S2    | 917 | U    |
| 49  | S2    | 920 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 49  | S2    | 922  | A    |
| 49  | S2    | 932  | G    |
| 49  | S2    | 933  | G    |
| 49  | S2    | 934  | G    |
| 49  | S2    | 945  | U    |
| 49  | S2    | 950  | C    |
| 49  | S2    | 955  | A    |
| 49  | S2    | 956  | G    |
| 49  | S2    | 958  | G    |
| 49  | S2    | 963  | A    |
| 49  | S2    | 970  | G    |
| 49  | S2    | 971  | G    |
| 49  | S2    | 972  | A    |
| 49  | S2    | 978  | G    |
| 49  | S2    | 986  | G    |
| 49  | S2    | 990  | A    |
| 49  | S2    | 992  | A    |
| 49  | S2    | 995  | G    |
| 49  | S2    | 999  | G    |
| 49  | S2    | 1002 | U    |
| 49  | S2    | 1008 | A    |
| 49  | S2    | 1017 | U    |
| 49  | S2    | 1023 | A    |
| 49  | S2    | 1027 | A    |
| 49  | S2    | 1042 | A    |
| 49  | S2    | 1043 | G    |
| 49  | S2    | 1045 | U    |
| 49  | S2    | 1060 | A    |
| 49  | S2    | 1061 | U    |
| 49  | S2    | 1062 | A    |
| 49  | S2    | 1083 | A    |
| 49  | S2    | 1085 | C    |
| 49  | S2    | 1108 | G    |
| 49  | S2    | 1109 | C    |
| 49  | S2    | 1110 | G    |
| 49  | S2    | 1114 | U    |
| 49  | S2    | 1116 | C    |
| 49  | S2    | 1118 | C    |
| 49  | S2    | 1132 | C    |
| 49  | S2    | 1133 | A    |
| 49  | S2    | 1153 | C    |
| 49  | S2    | 1154 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 49  | S2    | 1157 | G    |
| 49  | S2    | 1166 | G    |
| 49  | S2    | 1168 | G    |
| 49  | S2    | 1183 | A    |
| 49  | S2    | 1186 | U    |
| 49  | S2    | 1195 | A    |
| 49  | S2    | 1201 | U    |
| 49  | S2    | 1207 | G    |
| 49  | S2    | 1208 | A    |
| 49  | S2    | 1212 | G    |
| 49  | S2    | 1215 | C    |
| 49  | S2    | 1217 | A    |
| 49  | S2    | 1221 | G    |
| 49  | S2    | 1224 | G    |
| 49  | S2    | 1242 | U    |
| 49  | S2    | 1243 | U    |
| 49  | S2    | 1251 | A    |
| 49  | S2    | 1253 | A    |
| 49  | S2    | 1254 | C    |
| 49  | S2    | 1256 | G    |
| 49  | S2    | 1257 | G    |
| 49  | S2    | 1259 | A    |
| 49  | S2    | 1265 | A    |
| 49  | S2    | 1269 | G    |
| 49  | S2    | 1271 | C    |
| 49  | S2    | 1274 | G    |
| 49  | S2    | 1275 | G    |
| 49  | S2    | 1281 | G    |
| 49  | S2    | 1284 | A    |
| 49  | S2    | 1285 | G    |
| 49  | S2    | 1295 | A    |
| 49  | S2    | 1298 | G    |
| 49  | S2    | 1301 | A    |
| 49  | S2    | 1302 | G    |
| 49  | S2    | 1308 | U    |
| 49  | S2    | 1309 | C    |
| 49  | S2    | 1312 | G    |
| 49  | S2    | 1318 | G    |
| 49  | S2    | 1330 | G    |
| 49  | S2    | 1332 | A    |
| 49  | S2    | 1333 | U    |
| 49  | S2    | 1341 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 49  | S2    | 1342 | U    |
| 49  | S2    | 1364 | U    |
| 49  | S2    | 1371 | U    |
| 49  | S2    | 1372 | U    |
| 49  | S2    | 1373 | C    |
| 49  | S2    | 1378 | A    |
| 49  | S2    | 1396 | A    |
| 49  | S2    | 1397 | U    |
| 49  | S2    | 1401 | A    |
| 49  | S2    | 1402 | A    |
| 49  | S2    | 1403 | C    |
| 49  | S2    | 1404 | U    |
| 49  | S2    | 1405 | A    |
| 49  | S2    | 1407 | U    |
| 49  | S2    | 1408 | U    |
| 49  | S2    | 1409 | A    |
| 49  | S2    | 1415 | C    |
| 49  | S2    | 1417 | C    |
| 49  | S2    | 1419 | C    |
| 49  | S2    | 1420 | G    |
| 49  | S2    | 1421 | A    |
| 49  | S2    | 1422 | G    |
| 49  | S2    | 1423 | C    |
| 49  | S2    | 1424 | G    |
| 49  | S2    | 1425 | G    |
| 49  | S2    | 1426 | U    |
| 49  | S2    | 1427 | C    |
| 49  | S2    | 1428 | G    |
| 49  | S2    | 1431 | G    |
| 49  | S2    | 1433 | C    |
| 49  | S2    | 1434 | C    |
| 49  | S2    | 1435 | C    |
| 49  | S2    | 1436 | C    |
| 49  | S2    | 1438 | A    |
| 49  | S2    | 1447 | G    |
| 49  | S2    | 1449 | G    |
| 49  | S2    | 1450 | G    |
| 49  | S2    | 1452 | A    |
| 49  | S2    | 1454 | A    |
| 49  | S2    | 1462 | U    |
| 49  | S2    | 1463 | U    |
| 49  | S2    | 1464 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 49  | S2    | 1465 | A    |
| 49  | S2    | 1476 | A    |
| 49  | S2    | 1478 | U    |
| 49  | S2    | 1487 | A    |
| 49  | S2    | 1488 | C    |
| 49  | S2    | 1489 | A    |
| 49  | S2    | 1490 | G    |
| 49  | S2    | 1494 | U    |
| 49  | S2    | 1495 | G    |
| 49  | S2    | 1497 | G    |
| 49  | S2    | 1498 | A    |
| 49  | S2    | 1507 | G    |
| 49  | S2    | 1508 | A    |
| 49  | S2    | 1509 | U    |
| 49  | S2    | 1513 | C    |
| 49  | S2    | 1514 | G    |
| 49  | S2    | 1515 | G    |
| 49  | S2    | 1522 | A    |
| 49  | S2    | 1523 | C    |
| 49  | S2    | 1526 | G    |
| 49  | S2    | 1527 | C    |
| 49  | S2    | 1528 | G    |
| 49  | S2    | 1533 | A    |
| 49  | S2    | 1534 | C    |
| 49  | S2    | 1536 | G    |
| 49  | S2    | 1539 | U    |
| 49  | S2    | 1543 | U    |
| 49  | S2    | 1544 | C    |
| 49  | S2    | 1545 | A    |
| 49  | S2    | 1546 | G    |
| 49  | S2    | 1548 | G    |
| 49  | S2    | 1552 | G    |
| 49  | S2    | 1553 | C    |
| 49  | S2    | 1555 | U    |
| 49  | S2    | 1556 | A    |
| 49  | S2    | 1568 | C    |
| 49  | S2    | 1569 | A    |
| 49  | S2    | 1570 | G    |
| 49  | S2    | 1574 | C    |
| 49  | S2    | 1575 | G    |
| 49  | S2    | 1578 | U    |
| 49  | S2    | 1579 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 49  | S2    | 1580 | A    |
| 49  | S2    | 1581 | C    |
| 49  | S2    | 1585 | U    |
| 49  | S2    | 1586 | U    |
| 49  | S2    | 1587 | G    |
| 49  | S2    | 1588 | A    |
| 49  | S2    | 1589 | A    |
| 49  | S2    | 1598 | G    |
| 49  | S2    | 1601 | A    |
| 49  | S2    | 1602 | U    |
| 49  | S2    | 1607 | A    |
| 49  | S2    | 1612 | G    |
| 49  | S2    | 1614 | A    |
| 49  | S2    | 1621 | U    |
| 49  | S2    | 1622 | U    |
| 49  | S2    | 1623 | A    |
| 49  | S2    | 1624 | U    |
| 49  | S2    | 1630 | A    |
| 49  | S2    | 1631 | U    |
| 49  | S2    | 1632 | G    |
| 49  | S2    | 1635 | C    |
| 49  | S2    | 1636 | G    |
| 49  | S2    | 1637 | A    |
| 49  | S2    | 1639 | G    |
| 49  | S2    | 1647 | A    |
| 49  | S2    | 1648 | G    |
| 49  | S2    | 1654 | G    |
| 49  | S2    | 1661 | A    |
| 49  | S2    | 1663 | A    |
| 49  | S2    | 1665 | G    |
| 49  | S2    | 1671 | G    |
| 49  | S2    | 1672 | U    |
| 49  | S2    | 1680 | G    |
| 49  | S2    | 1683 | C    |
| 49  | S2    | 1695 | A    |
| 49  | S2    | 1698 | C    |
| 49  | S2    | 1699 | A    |
| 49  | S2    | 1702 | G    |
| 49  | S2    | 1719 | A    |
| 49  | S2    | 1721 | U    |
| 49  | S2    | 1722 | G    |
| 49  | S2    | 1735 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 49  | S2    | 1736 | G    |
| 49  | S2    | 1742 | C    |
| 49  | S2    | 1744 | G    |
| 49  | S2    | 1745 | A    |
| 49  | S2    | 1748 | G    |
| 49  | S2    | 1753 | C    |
| 49  | S2    | 1754 | G    |
| 49  | S2    | 1755 | C    |
| 49  | S2    | 1756 | C    |
| 49  | S2    | 1758 | G    |
| 49  | S2    | 1780 | G    |
| 49  | S2    | 1782 | G    |
| 49  | S2    | 1783 | C    |
| 49  | S2    | 1784 | G    |
| 49  | S2    | 1785 | C    |
| 49  | S2    | 1786 | U    |
| 49  | S2    | 1813 | A    |
| 49  | S2    | 1821 | U    |
| 49  | S2    | 1824 | A    |
| 49  | S2    | 1825 | A    |
| 49  | S2    | 1826 | G    |
| 49  | S2    | 1829 | G    |
| 49  | S2    | 1831 | A    |
| 49  | S2    | 1835 | A    |
| 49  | S2    | 1838 | U    |
| 49  | S2    | 1849 | G    |
| 49  | S2    | 1851 | A    |
| 49  | S2    | 1852 | C    |
| 49  | S2    | 1861 | G    |
| 49  | S2    | 1862 | G    |
| 49  | S2    | 1863 | A    |
| 49  | S2    | 1865 | C    |
| 49  | S2    | 1866 | A    |
| 49  | S2    | 1869 | A    |

All (32) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | L5    | 406  | C    |
| 4   | L5    | 504  | G    |
| 4   | L5    | 914  | U    |
| 4   | L5    | 1082 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | L5    | 1757 | U    |
| 4   | L5    | 2019 | C    |
| 4   | L5    | 2117 | G    |
| 4   | L5    | 2416 | G    |
| 4   | L5    | 2675 | G    |
| 4   | L5    | 2760 | G    |
| 4   | L5    | 3614 | G    |
| 4   | L5    | 3673 | C    |
| 4   | L5    | 4699 | U    |
| 4   | L5    | 4913 | G    |
| 6   | L8    | 87   | G    |
| 49  | S2    | 21   | U    |
| 49  | S2    | 32   | U    |
| 49  | S2    | 42   | A    |
| 49  | S2    | 77   | A    |
| 49  | S2    | 420  | G    |
| 49  | S2    | 465  | A    |
| 49  | S2    | 588  | G    |
| 49  | S2    | 591  | U    |
| 49  | S2    | 604  | A    |
| 49  | S2    | 688  | U    |
| 49  | S2    | 811  | A    |
| 49  | S2    | 1395 | C    |
| 49  | S2    | 1434 | C    |
| 49  | S2    | 1606 | G    |
| 49  | S2    | 1622 | U    |
| 49  | S2    | 1664 | A    |
| 49  | S2    | 1860 | A    |

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 80 ligands modelled in this entry, 79 are monoatomic - leaving 1 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 84  | 3HE  | L5    | 5101 | -    | 21,21,21     | 0.92 | 2 (9%)      | 23,30,30    | 2.27 | 8 (34%)     |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 84  | 3HE  | L5    | 5101 | -    | -       | 6/8/36/36 | 0/2/2/2 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 84  | L5    | 5101 | 3HE  | C12-N | -2.62 | 1.33        | 1.37     |
| 84  | L5    | 5101 | 3HE  | C11-N | -2.51 | 1.33        | 1.37     |

All (8) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 84  | L5    | 5101 | 3HE  | C10-C11-N  | 5.00  | 121.99      | 115.92   |
| 84  | L5    | 5101 | 3HE  | C9-C13-C12 | -4.80 | 106.38      | 114.46   |
| 84  | L5    | 5101 | 3HE  | C13-C12-N  | 3.93  | 120.69      | 115.92   |
| 84  | L5    | 5101 | 3HE  | C11-N-C12  | -3.59 | 121.55      | 125.87   |
| 84  | L5    | 5101 | 3HE  | C9-C8-C7   | -2.98 | 109.36      | 116.64   |
| 84  | L5    | 5101 | 3HE  | C9-C10-C11 | -2.83 | 109.69      | 114.46   |
| 84  | L5    | 5101 | 3HE  | C14-C3-C2  | -2.33 | 107.76      | 111.51   |
| 84  | L5    | 5101 | 3HE  | C14-C3-C4  | -2.15 | 110.08      | 112.48   |

There are no chirality outliers.

All (6) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 84  | L5    | 5101 | 3HE  | C4-C5-C7-C8 |

*Continued on next page...*

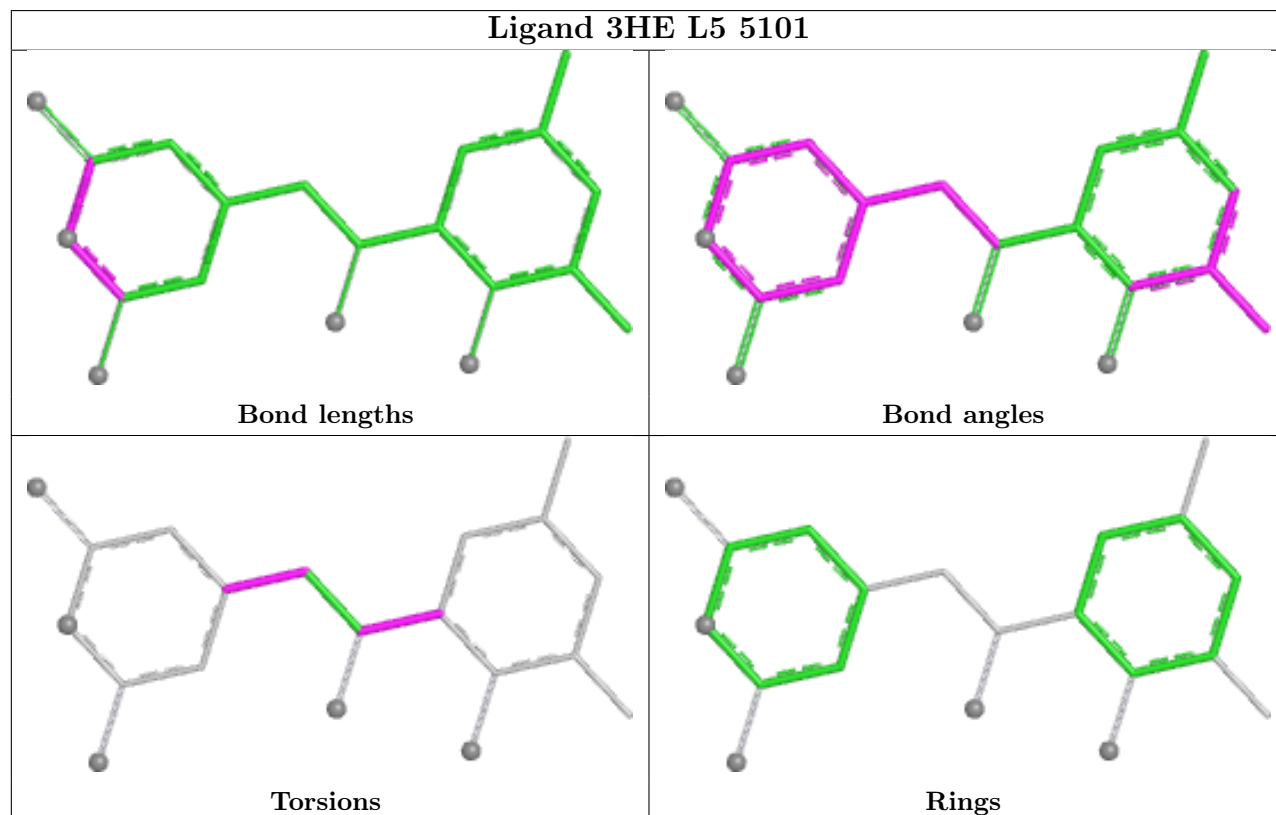
*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms        |
|-----|-------|------|------|--------------|
| 84  | L5    | 5101 | 3HE  | C4-C5-C7-O3  |
| 84  | L5    | 5101 | 3HE  | C6-C5-C7-C8  |
| 84  | L5    | 5101 | 3HE  | C6-C5-C7-O3  |
| 84  | L5    | 5101 | 3HE  | C7-C8-C9-C10 |
| 84  | L5    | 5101 | 3HE  | C7-C8-C9-C13 |

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

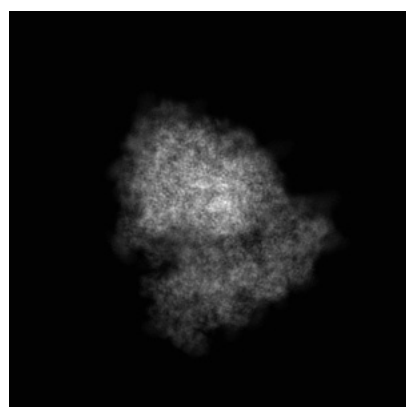
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10668. These allow visual inspection of the internal detail of the map and identification of artifacts.

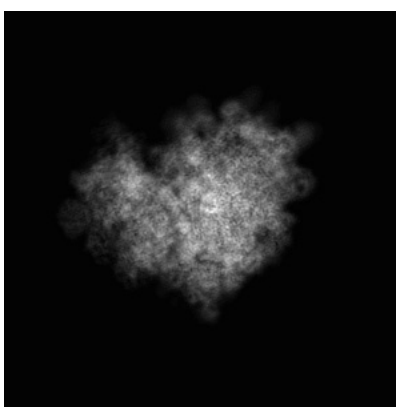
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

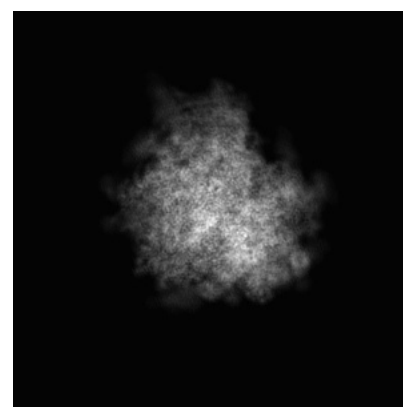
#### 6.1.1 Primary map



X



Y

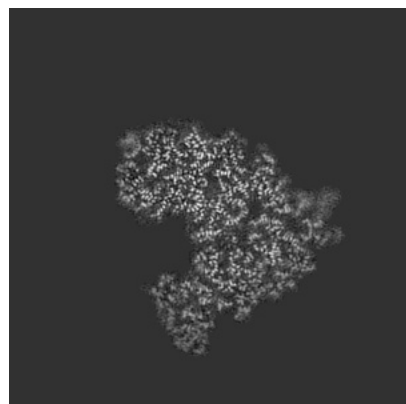


Z

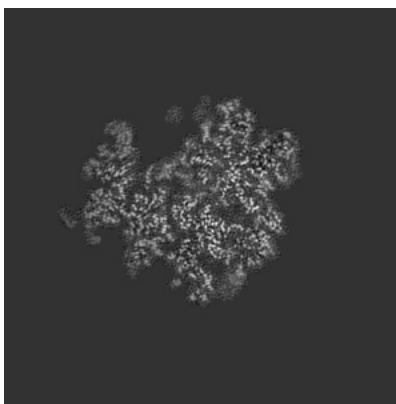
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

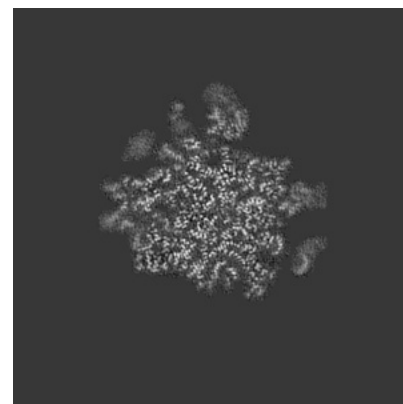
#### 6.2.1 Primary map



X Index: 275



Y Index: 275

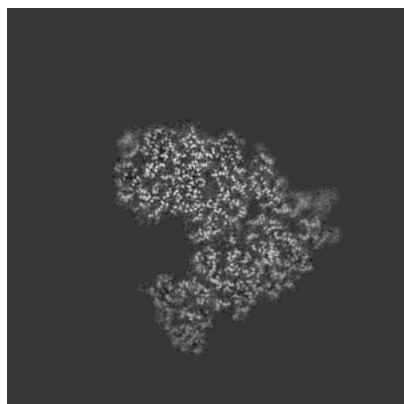


Z Index: 275

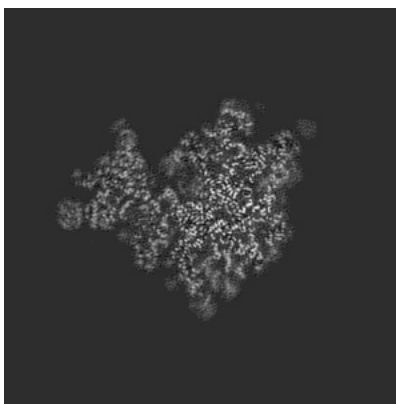
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

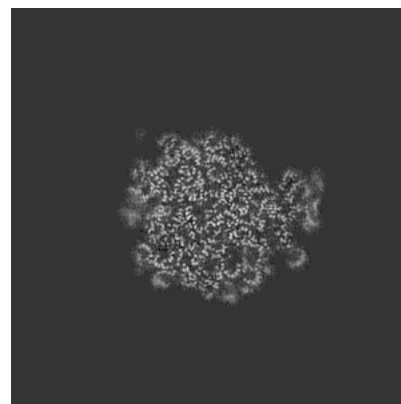
### 6.3.1 Primary map



X Index: 276



Y Index: 265

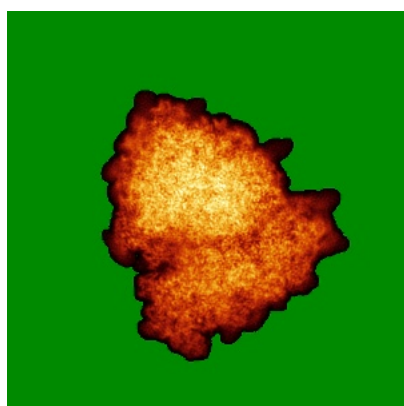


Z Index: 308

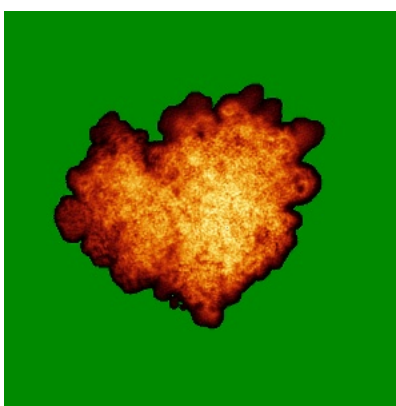
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

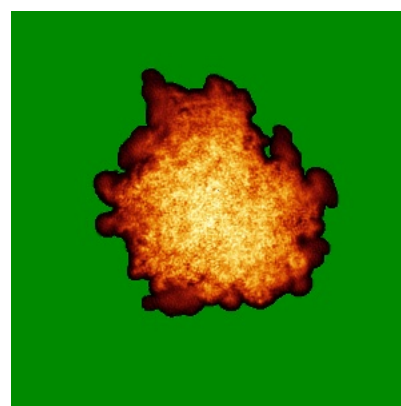
### 6.4.1 Primary map



X



Y

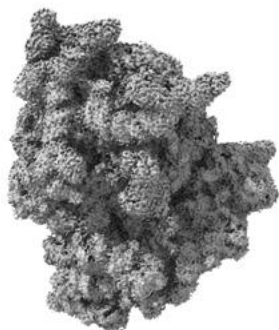


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

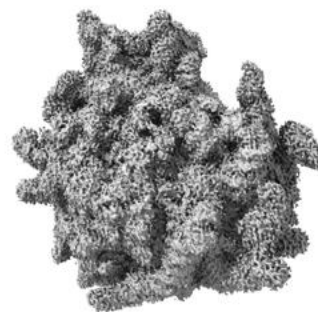
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0092. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

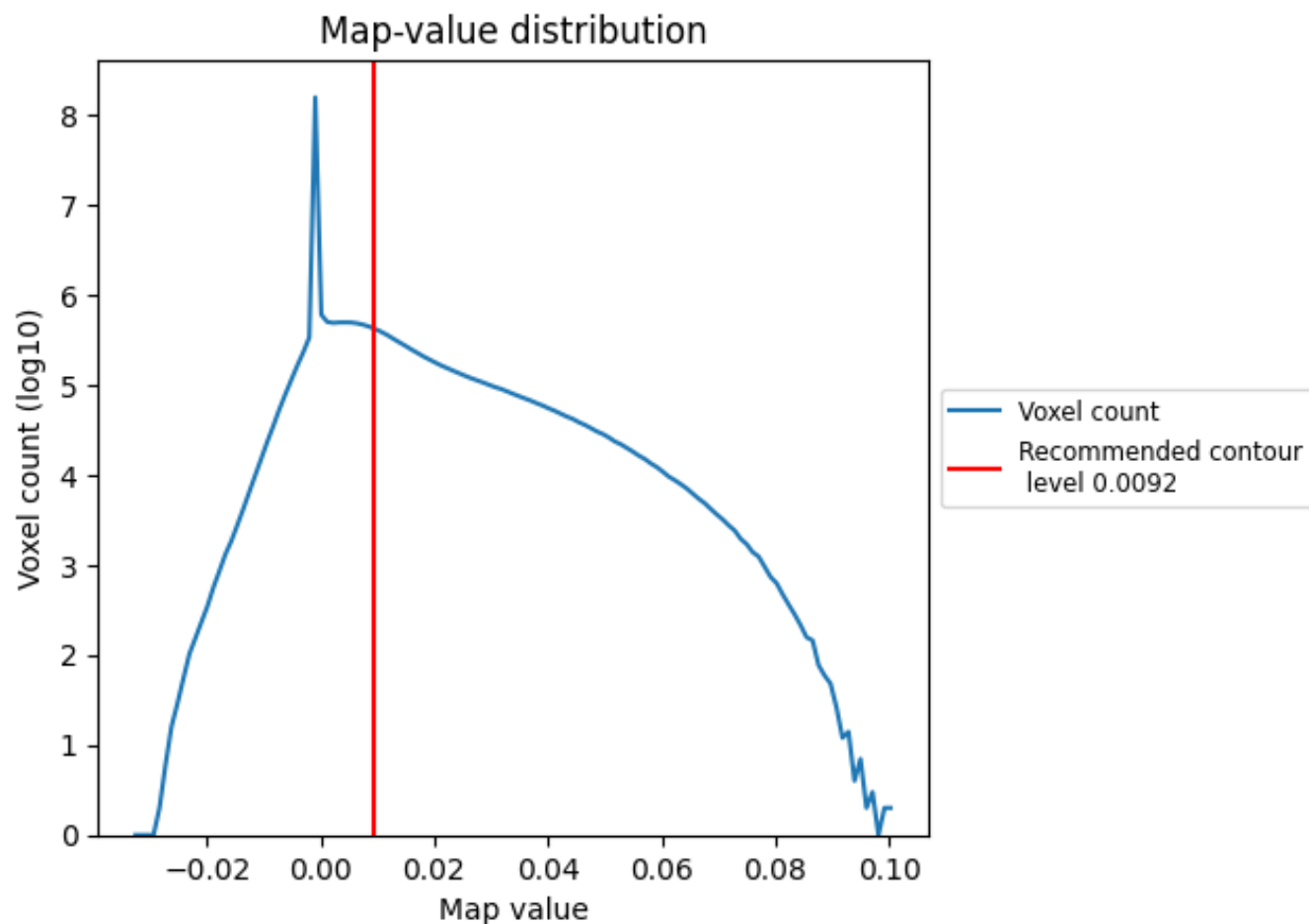
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

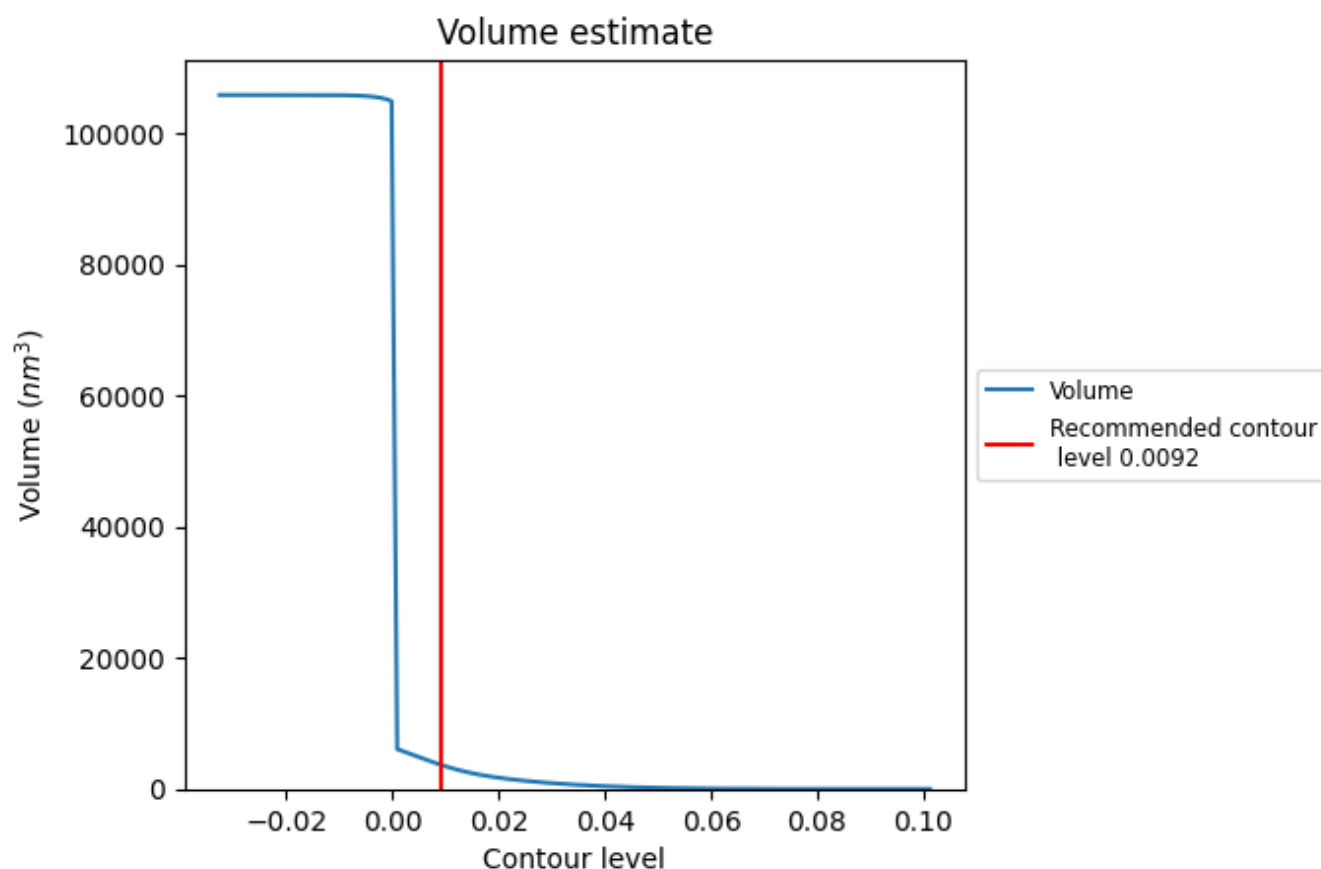
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

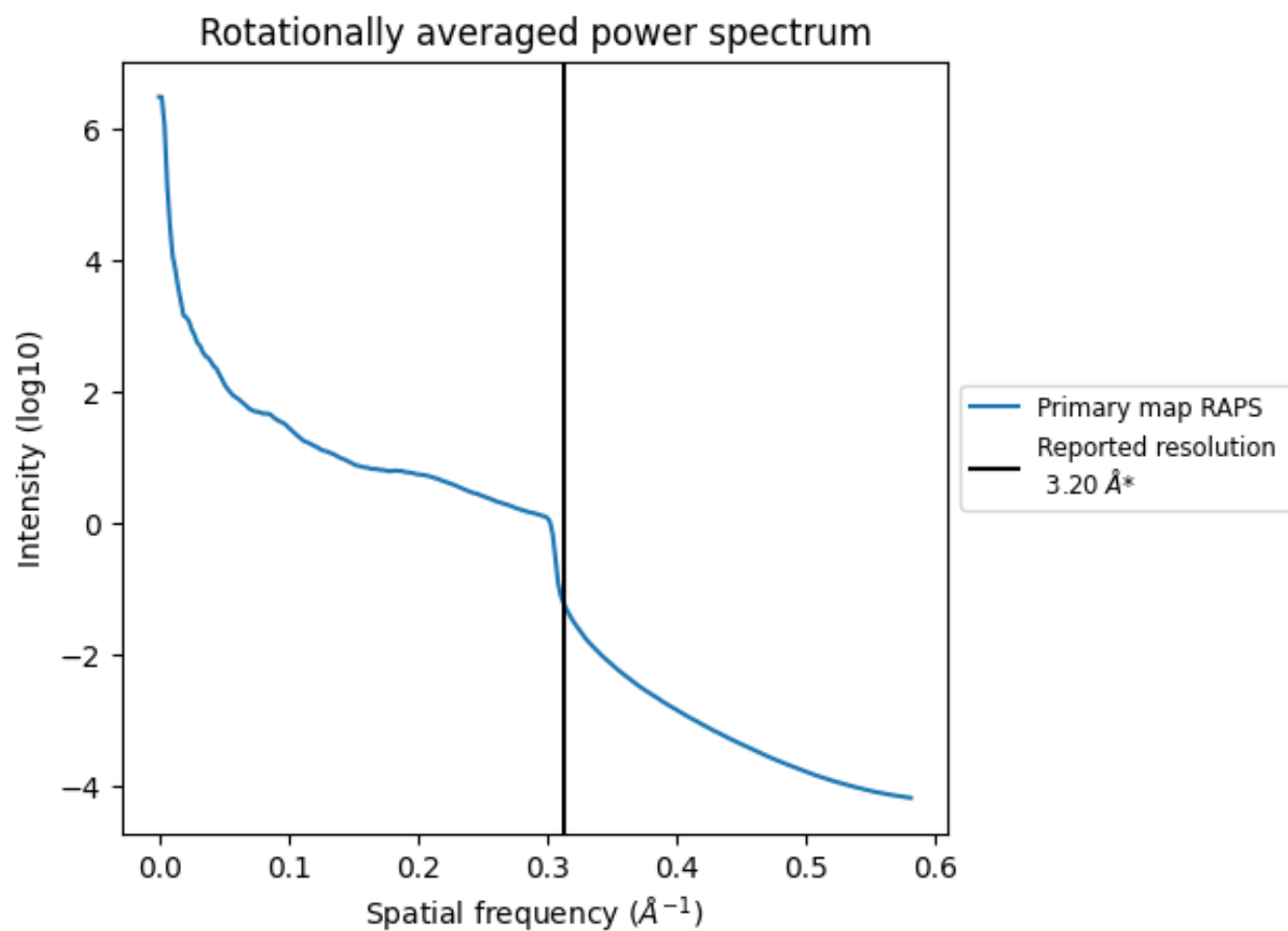
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3664  $\text{nm}^3$ ; this corresponds to an approximate mass of 3310 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

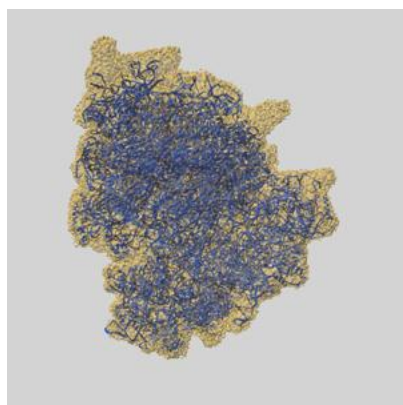
## 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

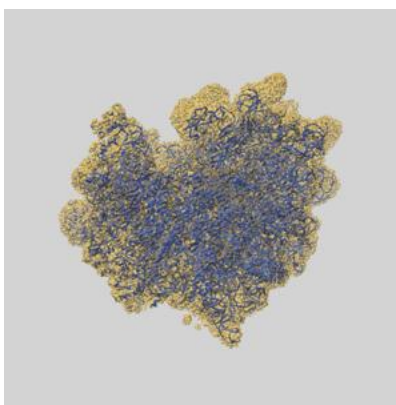
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10668 and PDB model 6Y0G. Per-residue inclusion information can be found in section 3 on page 21.

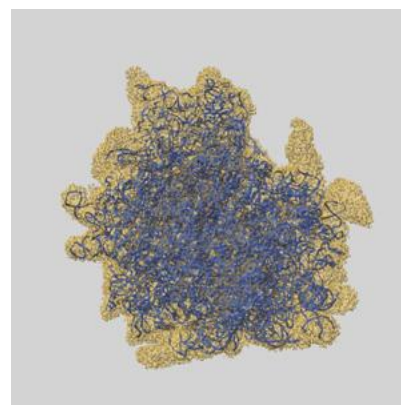
### 9.1 Map-model overlay [i](#)



X



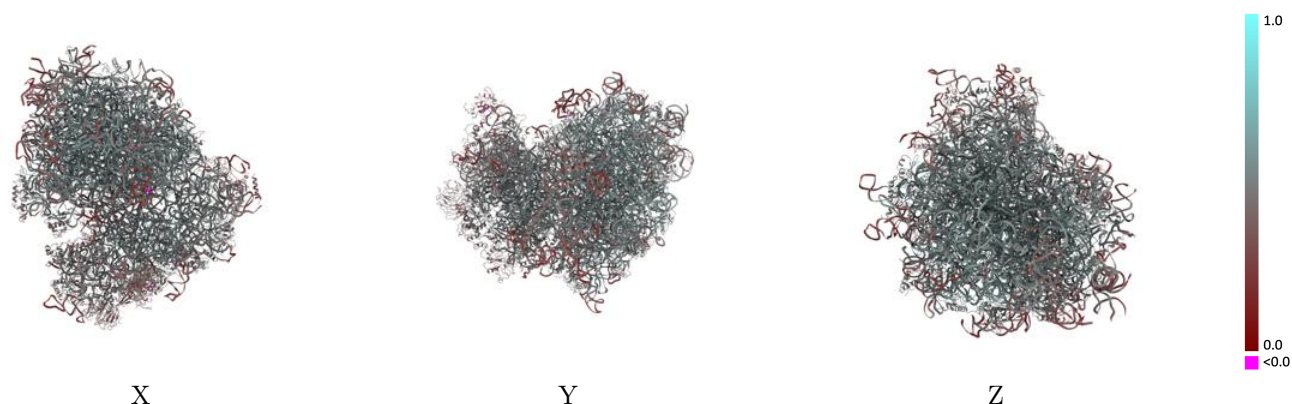
Y



Z

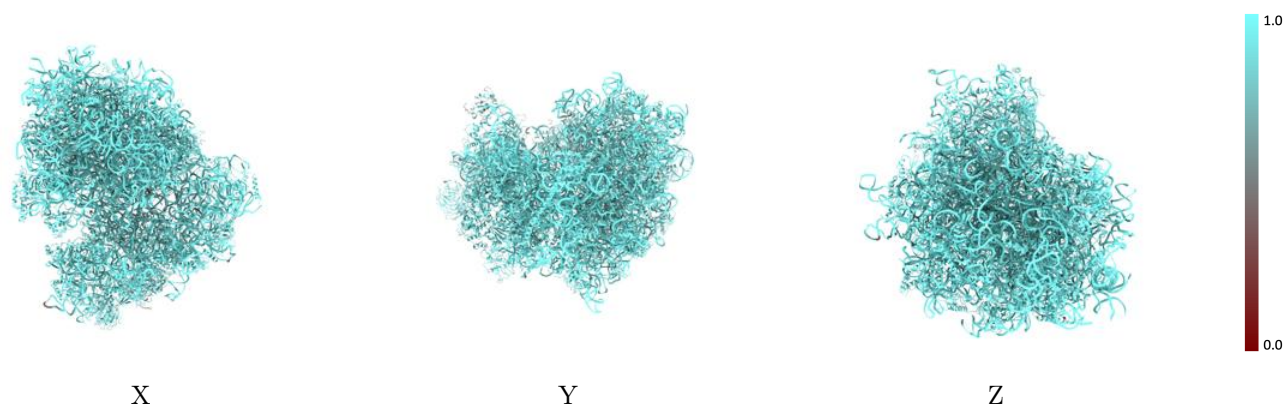
The images above show the 3D surface view of the map at the recommended contour level 0.0092 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



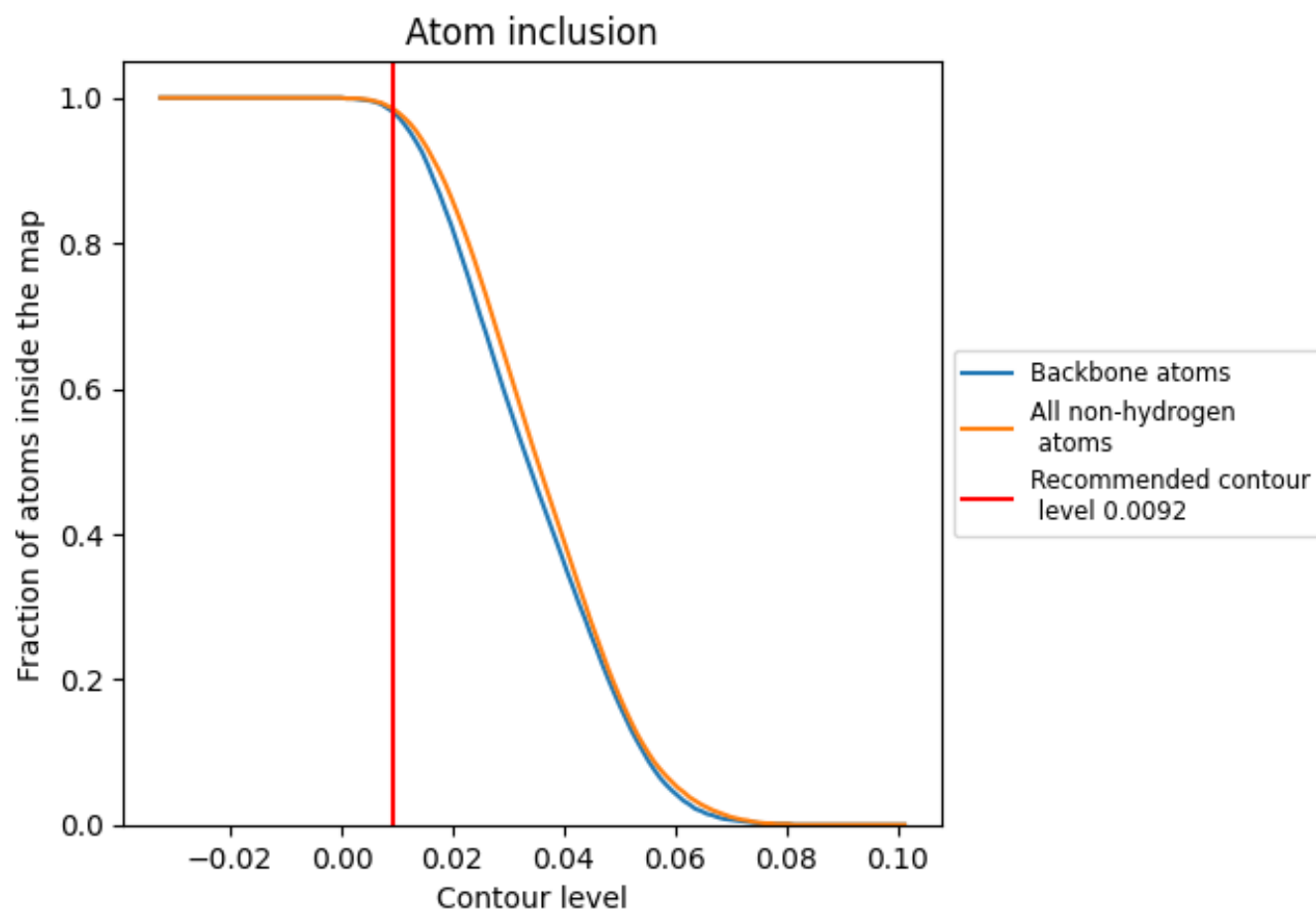
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0092).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0092) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9850   |  0.4880   |
| A4    |  0.9910   |  0.4220   |
| B4    |  0.9910   |  0.4330   |
| C4    |  0.9000   |  0.0840   |
| D4    |  0.9890   |  0.4320   |
| L5    |  0.9960   |  0.4950   |
| L7    |  0.9990   |  0.5120   |
| L8    |  0.9970   |  0.5200   |
| LA    |  0.9960   |  0.5530   |
| LB    |  0.9890   |  0.5280   |
| LC    |  0.9960   |  0.5420   |
| LD    |  0.9900   |  0.4850   |
| LE    |  0.9950   |  0.5000   |
| LF    |  0.9960   |  0.5360   |
| LG    |  0.9810  |  0.5040  |
| LH    |  0.9930 |  0.5030 |
| LI    |  0.9890 |  0.5150 |
| LJ    |  0.9660 |  0.4420 |
| LL    |  0.9860 |  0.5230 |
| LM    |  0.9880 |  0.5130 |
| LN    |  0.9950 |  0.5600 |
| LO    |  0.9890 |  0.5290 |
| LP    |  0.9970 |  0.5470 |
| LQ    |  0.9950 |  0.5490 |
| LR    |  0.9780 |  0.5110 |
| LS    |  0.9960 |  0.5400 |
| LT    |  0.9910 |  0.5270 |
| LU    |  0.9930 |  0.4750 |
| LV    |  0.9840 |  0.5360 |
| LW    |  0.9600 |  0.4340 |
| LX    |  0.9910 |  0.5230 |
| LY    |  0.9970 |  0.5310 |
| LZ    |  0.9900 |  0.5080 |
| La    |  0.9930 |  0.5480 |
| Lb    |  0.9640 |  0.5000 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| Lc    |  0.9710   |  0.4960   |
| Ld    |  0.9910   |  0.5280   |
| Le    |  0.9960   |  0.5550   |
| Lf    |  0.9940   |  0.5560   |
| Lg    |  0.9830   |  0.5210   |
| Lh    |  0.9830   |  0.5170   |
| Li    |  0.9880   |  0.5050   |
| Lj    |  1.0000   |  0.5580   |
| Lk    |  0.9840   |  0.4890   |
| Ll    |  0.9950   |  0.5460   |
| Lm    |  0.9900   |  0.5280   |
| Ln    |  0.9900   |  0.5330   |
| Lo    |  0.9900   |  0.5240   |
| Lp    |  0.9870   |  0.5320   |
| Lr    |  0.9960   |  0.5420   |
| S2    |  0.9930   |  0.4690   |
| SA    |  0.9330   |  0.4480   |
| SB    |  0.9690  |  0.4310  |
| SC    |  0.9730 |  0.4920 |
| SD    |  0.9630 |  0.4510 |
| SE    |  0.9820 |  0.4890 |
| SF    |  0.9630 |  0.4350 |
| SG    |  0.9790 |  0.4410 |
| SH    |  0.9020 |  0.4010 |
| SI    |  0.9860 |  0.4780 |
| SJ    |  0.9800 |  0.4660 |
| SK    |  0.9670 |  0.4400 |
| SL    |  0.9800 |  0.5010 |
| SM    |  0.6590 |  0.3060 |
| SN    |  0.9750 |  0.4770 |
| SO    |  0.9710 |  0.4380 |
| SP    |  0.9840 |  0.4580 |
| SQ    |  0.9550 |  0.4430 |
| SR    |  0.8870 |  0.4100 |
| SS    |  0.9720 |  0.4510 |
| ST    |  0.9790 |  0.4450 |
| SU    |  0.9180 |  0.4310 |
| SV    |  0.9570 |  0.4570 |
| SW    |  0.9730 |  0.5050 |
| SX    |  0.9920 |  0.5330 |
| SY    |  0.9820 |  0.4540 |
| SZ    |  0.9370 |  0.4160 |

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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| Sa    |  0.9910 |  0.4880 |
| Sb    |  0.9560 |  0.4540 |
| Sc    |  0.9510 |  0.4420 |
| Sd    |  0.9830 |  0.4850 |
| Se    |  0.9840 |  0.4910 |
| Sf    |  0.7530 |  0.3380 |
| Sg    |  0.9180 |  0.3600 |