



Full wwPDB EM Validation Report ⓘ

Nov 7, 2024 – 04:29 pm GMT

PDB ID : 8P5D
EMDB ID : EMD-17448
Title : Spraguea lophii ribosome in the closed conformation by cryo sub tomogram averaging
Authors : Gil Diez, P.; McLaren, M.; Isupov, M.N.; Daum, B.; Connors, R.; Williams, B.
Deposited on : 2023-05-23
Resolution : 10.80 Å(reported)

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

We welcome your comments at 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>.

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

EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

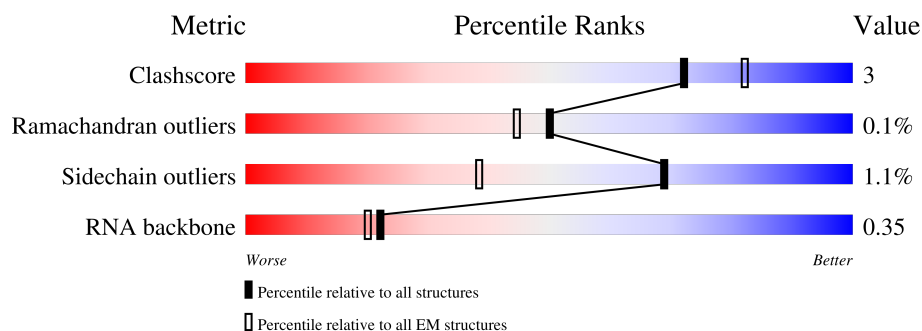
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 10.80 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 (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 210492 | 15764 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |
| RNA backbone | 6643 | 2191 |

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 ≥ 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 | L50 | 2618 | |
| 2 | L70 | 119 | |
| 3 | LA0 | 246 | |
| 4 | LAA | 147 | |
| 5 | LB0 | 392 | |
| 6 | LC0 | 328 | |
| 7 | LCC | 110 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 8 | LD0 | 291 | <div> <div>33%</div> <div>94%</div> <div>..</div> </div> |
| 9 | LDD | 110 | <div> <div>37%</div> <div>99%</div> <div>.</div> </div> |
| 10 | LE0 | 171 | <div> <div>63%</div> <div>91%</div> <div>...</div> </div> |
| 11 | LEE | 139 | <div> <div>38%</div> <div>94%</div> <div>..</div> </div> |
| 12 | LF0 | 235 | <div> <div>40%</div> <div>94%</div> <div>..</div> </div> |
| 13 | LFF | 111 | <div> <div>41%</div> <div>97%</div> <div>.</div> </div> |
| 14 | LG0 | 206 | <div> <div>42%</div> <div>94%</div> <div>..</div> </div> |
| 15 | LGG | 106 | <div> <div>32%</div> <div>93%</div> <div>...</div> </div> |
| 16 | LH0 | 187 | <div> <div>40%</div> <div>93%</div> <div>5% .</div> </div> |
| 17 | LHH | 119 | <div> <div>34%</div> <div>95%</div> <div>5%</div> </div> |
| 18 | LI0 | 218 | <div> <div>39%</div> <div>98%</div> <div>.</div> </div> |
| 19 | LII | 98 | <div> <div>38%</div> <div>95%</div> <div>..</div> </div> |
| 20 | LJ0 | 171 | <div> <div>43%</div> <div>92%</div> <div>6% .</div> </div> |
| 21 | LJJ | 92 | <div> <div>15%</div> <div>90%</div> <div>7% .</div> </div> |
| 22 | LL0 | 165 | <div> <div>36%</div> <div>92%</div> <div>8% .</div> </div> |
| 23 | LLL | 52 | <div> <div>40%</div> <div>98%</div> <div>.</div> </div> |
| 24 | LM0 | 115 | <div> <div>60%</div> <div>96%</div> <div>.</div> </div> |
| 25 | LMM | 127 | <div> <div>13%</div> <div>41%</div> <div>59%</div> </div> |
| 26 | LN0 | 204 | <div> <div>21%</div> <div>95%</div> <div>.</div> </div> |
| 27 | LO0 | 198 | <div> <div>40%</div> <div>97%</div> <div>.</div> </div> |
| 28 | LOO | 104 | <div> <div>35%</div> <div>92%</div> <div>..</div> </div> |
| 29 | LP0 | 167 | <div> <div>35%</div> <div>89%</div> <div>.. 8%</div> </div> |
| 30 | LPP | 89 | <div> <div>31%</div> <div>92%</div> <div>...</div> </div> |
| 31 | LQ0 | 183 | <div> <div>38%</div> <div>96%</div> <div>..</div> </div> |
| 32 | LR0 | 168 | <div> <div>45%</div> <div>96%</div> <div>..</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 33 | LS0 | 171 | <div> <div>43%</div> <div>96%</div> <div>..</div> </div> |
| 34 | LT0 | 158 | <div> <div>44%</div> <div>92%</div> <div>6% ..</div> </div> |
| 35 | LU0 | 113 | <div> <div>30%</div> <div>86%</div> <div>12%</div> </div> |
| 36 | LV0 | 142 | <div> <div>53%</div> <div>97%</div> <div>..</div> </div> |
| 37 | LW0 | 131 | <div> <div>50%</div> <div>67%</div> <div>10% . 22%</div> </div> |
| 38 | LX0 | 113 | <div> <div>47%</div> <div>96%</div> <div>..</div> </div> |
| 39 | LY0 | 131 | <div> <div>38%</div> <div>96%</div> <div>.</div> </div> |
| 40 | LZ0 | 153 | <div> <div>47%</div> <div>76%</div> <div>. 23%</div> </div> |
| 41 | MD1 | 151 | <div> <div>68%</div> <div>94%</div> <div>6%</div> </div> |
| 42 | S60 | 1368 | <div> <div>44%</div> <div>37%</div> <div>15% ..</div> </div> |
| 43 | SA0 | 233 | <div> <div>64%</div> <div>79%</div> <div>15% 6%</div> </div> |
| 44 | SAA | 102 | <div> <div>43%</div> <div>92%</div> <div>7% .</div> </div> |
| 45 | SB0 | 230 | <div> <div>51%</div> <div>88%</div> <div>. 11%</div> </div> |
| 46 | SBB | 82 | <div> <div>48%</div> <div>94%</div> <div>.. ..</div> </div> |
| 47 | SC0 | 248 | <div> <div>45%</div> <div>81%</div> <div>10% 9%</div> </div> |
| 48 | SCC | 65 | <div> <div>82%</div> <div>82%</div> <div>14% 5%</div> </div> |
| 49 | SD0 | 242 | <div> <div>58%</div> <div>82%</div> <div>7% 11%</div> </div> |
| 50 | SDD | 65 | <div> <div>40%</div> <div>86%</div> <div>14%</div> </div> |
| 51 | SE0 | 280 | <div> <div>48%</div> <div>85%</div> <div>8% 7%</div> </div> |
| 52 | SEE | 60 | <div> <div>55%</div> <div>90%</div> <div>. 7%</div> </div> |
| 53 | SF0 | 195 | <div> <div>43%</div> <div>86%</div> <div>12% ..</div> </div> |
| 54 | SFF | 150 | <div> <div>38%</div> <div>34%</div> <div>61%</div> </div> |
| 55 | SG0 | 230 | <div> <div>58%</div> <div>92%</div> <div>7%</div> </div> |
| 56 | SGG | 326 | <div> <div>61%</div> <div>94%</div> <div>..</div> </div> |
| 57 | SH0 | 164 | <div> <div>71%</div> <div>97%</div> <div>..</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 58 | SI0 | 173 | |
| 59 | SJ0 | 184 | |
| 60 | SK0 | 107 | |
| 61 | SL0 | 155 | |
| 62 | SM0 | 130 | |
| 63 | SN0 | 143 | |
| 64 | SO0 | 135 | |
| 65 | SP0 | 163 | |
| 66 | SQ0 | 143 | |
| 67 | SR0 | 120 | |
| 68 | SS0 | 160 | |
| 69 | ST0 | 143 | |
| 70 | SU0 | 119 | |
| 71 | SV0 | 67 | |
| 72 | SW0 | 128 | |
| 73 | SX0 | 141 | |
| 74 | SY0 | 146 | |
| 75 | SZ0 | 128 | |

2 Entry composition

There are 76 unique types of molecules in this entry. The entry contains 171817 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 RNA 28S.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 1 | L50 | 2499 | Total | C | N | O | P | 0 | 0 |
| | | | 53655 | 23950 | 9876 | 17330 | 2499 | | |

- Molecule 2 is a RNA chain called RNA 5S.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 2 | L70 | 119 | Total | C | N | O | P | 0 | 0 |
| | | | 2542 | 1136 | 459 | 828 | 119 | | |

- Molecule 3 is a protein called 60S ribosomal protein L8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3 | LA0 | 245 | Total | C | N | O | S | 0 | 0 |
| | | | 1889 | 1189 | 361 | 334 | 5 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| LA0 | 206 | ASN | THR | conflict | UNP S7W736 |

- Molecule 4 is a protein called uL15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4 | LAA | 147 | Total | C | N | O | S | 0 | 0 |
| | | | 1167 | 738 | 229 | 194 | 6 | | |

- Molecule 5 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5 | LB0 | 383 | Total | C | N | O | S | 0 | 0 |
| | | | 3039 | 1926 | 559 | 543 | 11 | | |

- Molecule 6 is a protein called 60S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6 | LC0 | 327 | Total | C | N | O | S | 0 | 0 |
| | | | 2604 | 1629 | 478 | 485 | 12 | | |

- Molecule 7 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7 | LCC | 99 | Total | C | N | O | S | 0 | 0 |
| | | | 781 | 504 | 126 | 148 | 3 | | |

- Molecule 8 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 8 | LD0 | 281 | Total | C | N | O | S | 0 | 0 |
| | | | 2298 | 1451 | 410 | 426 | 11 | | |

- Molecule 9 is a protein called 60S ribosomal protein L31.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9 | LDD | 109 | Total | C | N | O | S | 0 | 0 |
| | | | 895 | 575 | 163 | 154 | 3 | | |

- Molecule 10 is a protein called 60S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10 | LE0 | 165 | Total | C | N | O | S | 0 | 0 |
| | | | 1371 | 879 | 227 | 262 | 3 | | |

- Molecule 11 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11 | LEE | 135 | Total | C | N | O | S | 0 | 0 |
| | | | 1090 | 697 | 205 | 182 | 6 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 12 | LF0 | 231 | Total | C | N | O | S | 0 | 0 |
| | | | 1933 | 1234 | 342 | 350 | 7 | | |

- Molecule 13 is a protein called 60S ribosomal protein L35a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13 | LFF | 111 | Total | C | N | O | S | 0 | 0 |
| | | | 893 | 567 | 159 | 162 | 5 | | |

- Molecule 14 is a protein called 60S ribosomal protein L8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 14 | LG0 | 199 | Total | C | N | O | S | 0 | 0 |
| | | | 1590 | 1015 | 275 | 290 | 10 | | |

- Molecule 15 is a protein called Ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15 | LGG | 104 | Total | C | N | O | S | 0 | 0 |
| | | | 819 | 504 | 169 | 139 | 7 | | |

- Molecule 16 is a protein called 60S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16 | LH0 | 183 | Total | C | N | O | S | 0 | 0 |
| | | | 1477 | 951 | 252 | 266 | 8 | | |

- Molecule 17 is a protein called Ribosomal L29 protein (Fragment),Ribosomal L29 protein (Fragment),Ribosomal L29 protein (Fragment),Ribosomal L29 protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17 | LHH | 119 | Total | C | N | O | S | 0 | 0 |
| | | | 992 | 626 | 188 | 175 | 3 | | |

- Molecule 18 is a protein called S60 ribosomal protein L10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 18 | LI0 | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1750 | 1096 | 333 | 308 | 13 | | |

- Molecule 19 is a protein called 60S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19 | LII | 97 | Total | C | N | O | S | 0 | 0 |
| | | | 784 | 496 | 146 | 136 | 6 | | |

- Molecule 20 is a protein called 60S ribosomal protein L11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20 | LJ0 | 167 | Total | C | N | O | S | 0 | 0 |
| | | | 1332 | 847 | 242 | 236 | 7 | | |

- Molecule 21 is a protein called eL37.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 21 | LJJ | 89 | Total | C | N | O | S | 0 | 0 |
| | | | 701 | 427 | 146 | 118 | 10 | | |

- Molecule 22 is a protein called 60S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 22 | LL0 | 164 | Total | C | N | O | S | 0 | 0 |
| | | | 1353 | 857 | 252 | 232 | 12 | | |

- Molecule 23 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 23 | LLL | 51 | Total | C | N | O | S | 0 | 0 |
| | | | 427 | 272 | 87 | 65 | 3 | | |

- Molecule 24 is a protein called Transposase.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24 | LM0 | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 927 | 588 | 151 | 183 | 5 | | |

- Molecule 25 is a protein called Ubiquitin.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 25 | LMM | 52 | Total | C | N | O | S | 0 | 0 |
| | | | 427 | 264 | 89 | 70 | 4 | | |

- Molecule 26 is a protein called Ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 26 | LN0 | 203 | Total | C | N | O | S | 0 | 0 |
| | | | 1688 | 1055 | 346 | 276 | 11 | | |

- Molecule 27 is a protein called Ribosomal protein L13A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 27 | LO0 | 198 | Total | C | N | O | S | 0 | 0 |
| | | | 1598 | 1018 | 286 | 280 | 14 | | |

- Molecule 28 is a protein called 60S ribosomal protein L44.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28 | LOO | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 801 | 504 | 163 | 130 | 4 | | |

- Molecule 29 is a protein called 60S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29 | LP0 | 154 | Total | C | N | O | S | 0 | 0 |
| | | | 1238 | 794 | 225 | 213 | 6 | | |

- Molecule 30 is a protein called 60S ribosomal protein L37a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 30 | LPP | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 684 | 427 | 131 | 116 | 10 | | |

- Molecule 31 is a protein called 60S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31 | LQ0 | 182 | Total | C | N | O | S | 0 | 0 |
| | | | 1491 | 950 | 270 | 266 | 5 | | |

- Molecule 32 is a protein called 60S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32 | LR0 | 164 | Total | C | N | O | S | 0 | 0 |
| | | | 1336 | 832 | 261 | 236 | 7 | | |

- Molecule 33 is a protein called 60S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33 | LS0 | 170 | Total | C | N | O | S | 0 | 0 |
| | | | 1400 | 898 | 241 | 256 | 5 | | |

- Molecule 34 is a protein called 60s ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34 | LT0 | 156 | Total | C | N | O | S | 0 | 0 |
| | | | 1270 | 808 | 233 | 224 | 5 | | |

- Molecule 35 is a protein called 60S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35 | LU0 | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 810 | 526 | 135 | 147 | 2 | | |

- Molecule 36 is a protein called Ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36 | LV0 | 141 | Total | C | N | O | S | 0 | 0 |
| | | | 1057 | 663 | 200 | 189 | 5 | | |

- Molecule 37 is a protein called Ribosomal protein L24E.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37 | LW0 | 102 | Total | C | N | O | S | 0 | 0 |
| | | | 832 | 539 | 143 | 147 | 3 | | |

- Molecule 38 is a protein called 60S ribosomal protein L23a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38 | LX0 | 112 | Total | C | N | O | S | 0 | 0 |
| | | | 874 | 562 | 156 | 155 | 1 | | |

- Molecule 39 is a protein called 60S ribosomal protein L26.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39 | LY0 | 131 | Total | C | N | O | S | 0 | 0 |
| | | | 1048 | 658 | 197 | 186 | 7 | | |

- Molecule 40 is a protein called 60S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40 | LZ0 | 118 | Total | C | N | O | S | 0 | 0 |
| | | | 963 | 618 | 172 | 169 | 4 | | |

- Molecule 41 is a protein called DNL-type domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 41 | MD1 | 151 | Total | C | N | O | S | 0 | 0 |
| | | | 1229 | 776 | 201 | 241 | 11 | | |

- Molecule 42 is a RNA chain called RNA 16S.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|------|---------|-------|
| 42 | S60 | 1354 | Total | C | N | O | P | 0 | 0 |
| | | | 29181 | 13024 | 5463 | 9340 | 1354 | | |

- Molecule 43 is a protein called 40S ribosomal protein S0.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 43 | SA0 | 220 | Total | C | N | O | S | 0 | 0 |
| | | | 1725 | 1091 | 292 | 328 | 14 | | |

- Molecule 44 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44 | SAA | 101 | Total | C | N | O | S | 0 | 0 |
| | | | 827 | 513 | 163 | 145 | 6 | | |

- Molecule 45 is a protein called eS1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 45 | SB0 | 204 | Total | C | N | O | S | 0 | 0 |
| | | | 1609 | 1018 | 286 | 298 | 7 | | |

- Molecule 46 is a protein called eS27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46 | SBB | 81 | Total | C | N | O | S | 0 | 0 |
| | | | 627 | 394 | 108 | 116 | 9 | | |

- Molecule 47 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 47 | SC0 | 226 | Total | C | N | O | S | 0 | 0 |
| | | | 1727 | 1099 | 300 | 321 | 7 | | |

- Molecule 48 is a protein called eS28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 48 | SCC | 62 | Total | C | N | O | S | 0 | 0 |
| | | | 476 | 295 | 86 | 91 | 4 | | |

- Molecule 49 is a protein called 40S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 49 | SD0 | 216 | Total | C | N | O | S | 0 | 0 |
| | | | 1700 | 1085 | 300 | 307 | 8 | | |

- Molecule 50 is a protein called 40S ribosomal protein S29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 50 | SDD | 65 | Total | C | N | O | S | 0 | 0 |
| | | | 550 | 345 | 102 | 96 | 7 | | |

- Molecule 51 is a protein called 40S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 51 | SE0 | 260 | Total | C | N | O | S | 0 | 0 |
| | | | 2044 | 1297 | 361 | 379 | 7 | | |

- Molecule 52 is a protein called eS30.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 52 | SEE | 56 | Total | C | N | O | 0 | 0 |
| | | | 447 | 284 | 89 | 74 | | |

- Molecule 53 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53 | SF0 | 192 | Total | C | N | O | S | 0 | 0 |
| | | | 1509 | 953 | 275 | 275 | 6 | | |

- Molecule 54 is a protein called Ubiquitin/40s ribosomal protein S27a fusion.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 54 | SFF | 58 | Total | C | N | O | S | 0 | 0 |
| | | | 422 | 261 | 77 | 79 | 5 | | |

- Molecule 55 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 55 | SG0 | 229 | Total | C | N | O | S | 0 | 0 |
| | | | 1836 | 1179 | 325 | 328 | 4 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| SG0 | 171 | ALA | GLY | conflict | UNP S7WDE5 |
| SG0 | 173 | GLY | ASP | conflict | UNP S7WDE5 |

- Molecule 56 is a protein called Guanine nucleotide binding protein beta subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 56 | SGG | 319 | Total | C | N | O | S | 0 | 0 |
| | | | 2478 | 1558 | 411 | 494 | 15 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57 | SH0 | 163 | Total | C | N | O | S | 0 | 0 |
| | | | 1335 | 855 | 219 | 255 | 6 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 58 | SI0 | 167 | Total | C | N | O | S | 0 | 0 |
| | | | 1347 | 834 | 266 | 240 | 7 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 59 | SJ0 | 168 | Total | C | N | O | S | 0 | 0 |
| | | | 1379 | 880 | 252 | 243 | 4 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 60 | SK0 | 88 | Total | C | N | O | S | 0 | 0 |
| | | | 737 | 472 | 127 | 135 | 3 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 61 | SL0 | 150 | Total | C | N | O | S | 0 | 0 |
| | | | 1229 | 790 | 217 | 216 | 6 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 62 | SM0 | 113 | Total | C | N | O | S | 0 | 0 |
| | | | 876 | 553 | 156 | 162 | 5 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 63 | SN0 | 142 | Total | C | N | O | S | 0 | 0 |
| | | | 1130 | 728 | 196 | 202 | 4 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 64 | SO0 | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 983 | 606 | 191 | 183 | 3 | | |

- Molecule 65 is a protein called Ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 65 | SP0 | 117 | Total | C | N | O | S | 0 | 0 |
| | | | 950 | 598 | 172 | 173 | 7 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 66 | SQ0 | 142 | Total | C | N | O | S | 0 | 0 |
| | | | 1143 | 726 | 204 | 207 | 6 | | |

- Molecule 67 is a protein called eS17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 67 | SR0 | 119 | Total | C | N | O | S | 0 | 0 |
| | | | 974 | 613 | 172 | 186 | 3 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 68 | SS0 | 144 | Total | C | N | O | S | 0 | 0 |
| | | | 1150 | 720 | 220 | 207 | 3 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 69 | ST0 | 142 | Total | C | N | O | S | 0 | 0 |
| | | | 1161 | 741 | 208 | 211 | 1 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 70 | SU0 | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 809 | 515 | 144 | 143 | 7 | | |

- Molecule 71 is a protein called Ribosomal protein S21E.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 71 | SV0 | 65 | Total | C | N | O | S | 0 | 0 |
| | | | 521 | 319 | 96 | 101 | 5 | | |

- Molecule 72 is a protein called 40S ribosomal protein S15A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 72 | SW0 | 128 | Total | C | N | O | S | 0 | 0 |
| | | | 1022 | 639 | 195 | 180 | 8 | | |

- Molecule 73 is a protein called uS12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 73 | SX0 | 140 | Total | C | N | O | S | 0 | 0 |
| | | | 1098 | 692 | 216 | 186 | 4 | | |

- Molecule 74 is a protein called 40s ribosomal protein s24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 74 | SY0 | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 1118 | 693 | 215 | 204 | 6 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 75 | SZ0 | 76 | Total | C | N | O | S | 0 | 0 |
| | | | 633 | 403 | 116 | 113 | 1 | | |

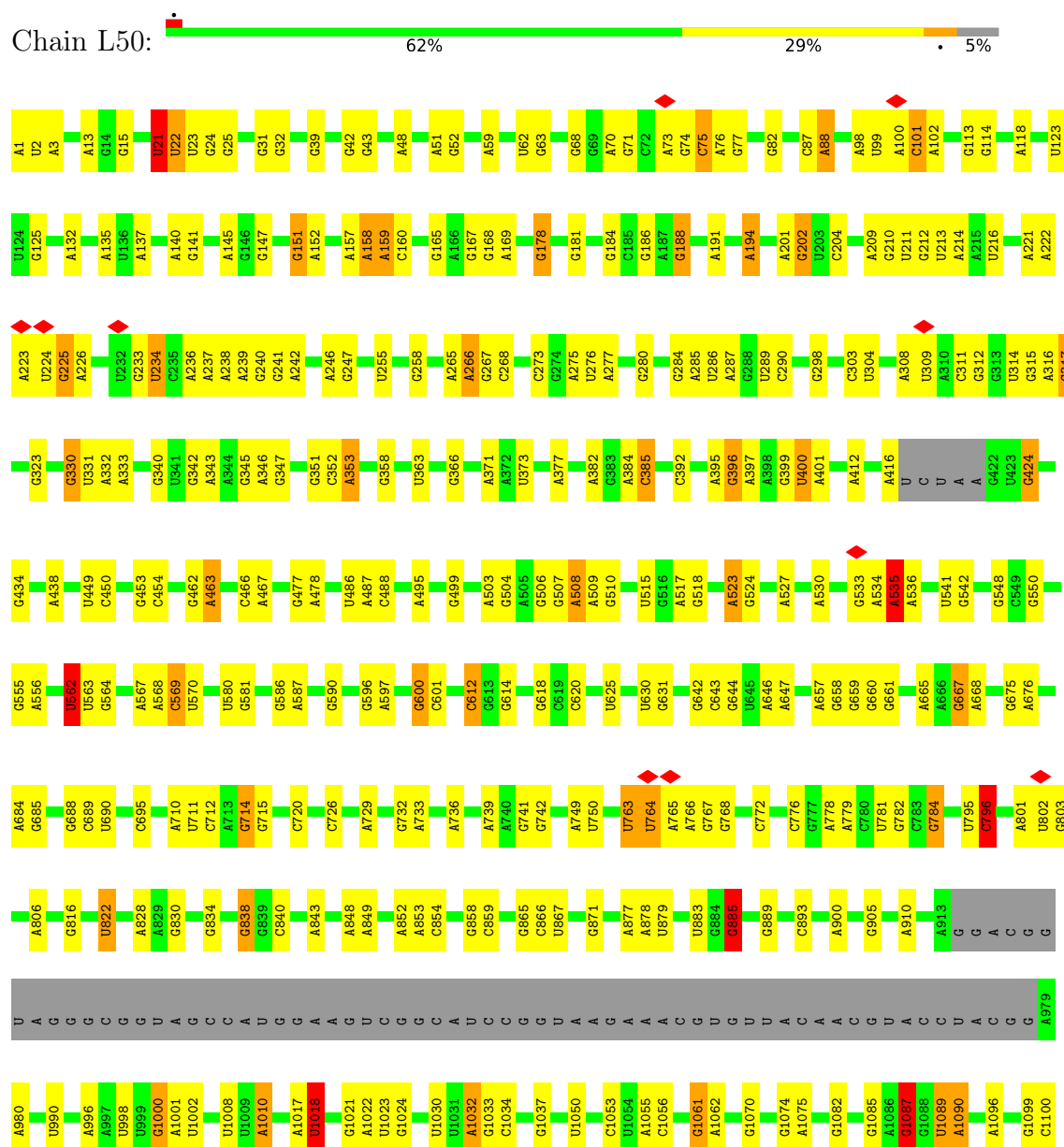
- Molecule 76 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 76 | LGG | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 76 | LJJ | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 76 | LMM | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 76 | LOO | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 76 | LPP | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 76 | SAA | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 76 | SBB | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 76 | SDD | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 76 | SFF | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

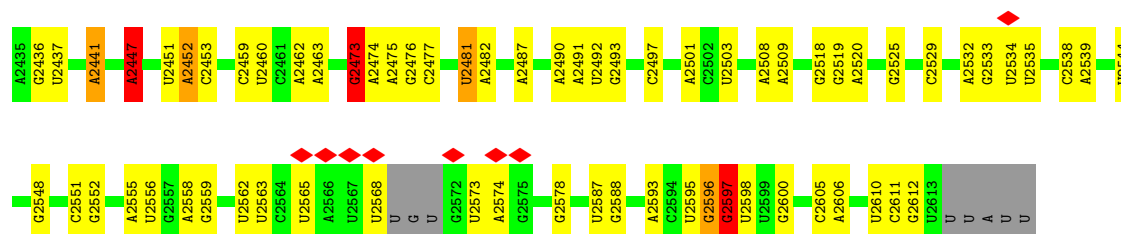
3 Residue-property plots

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.

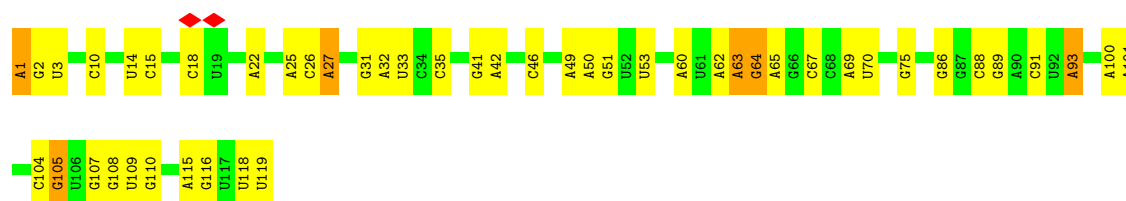
• Molecule 1: RNA 28S



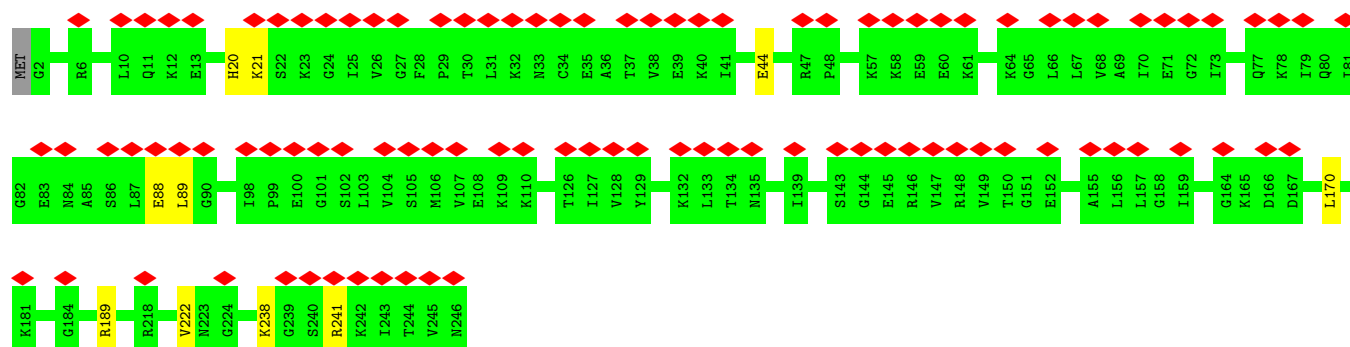
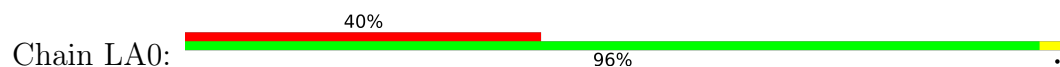




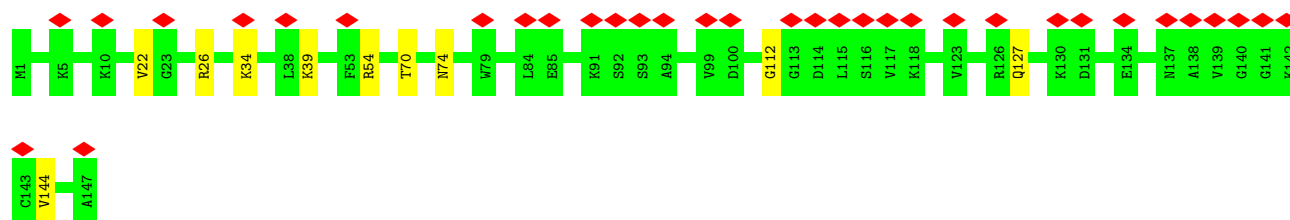
• Molecule 2: RNA 5S



• Molecule 3: 60S ribosomal protein L8

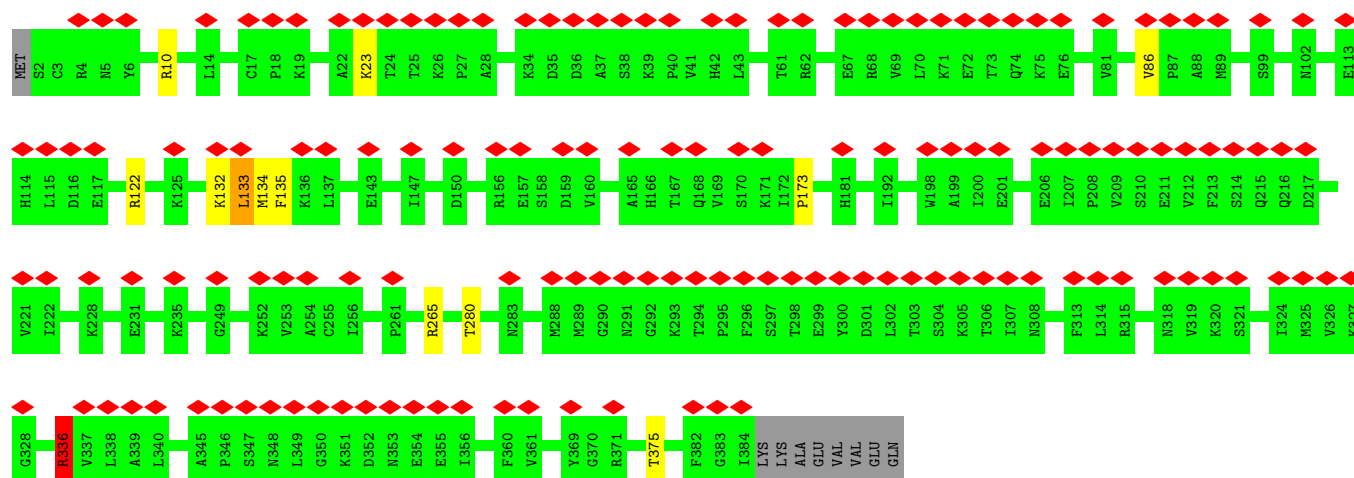


• Molecule 4: uL15

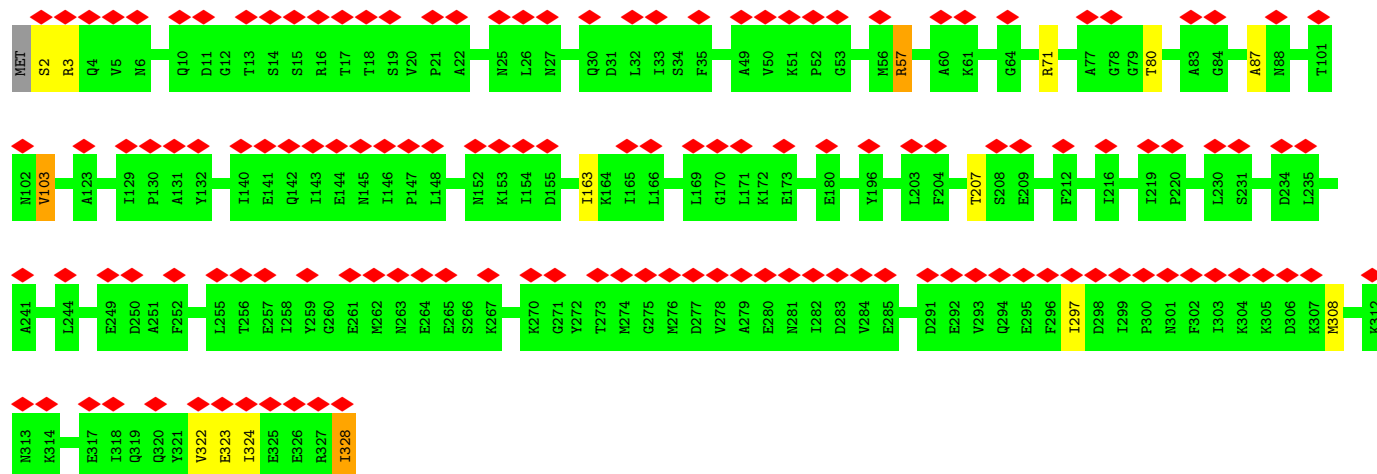
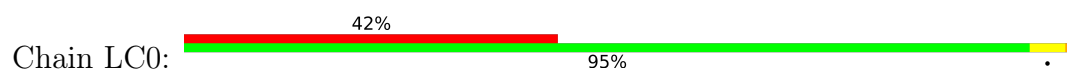


• Molecule 5: 60S ribosomal protein L3

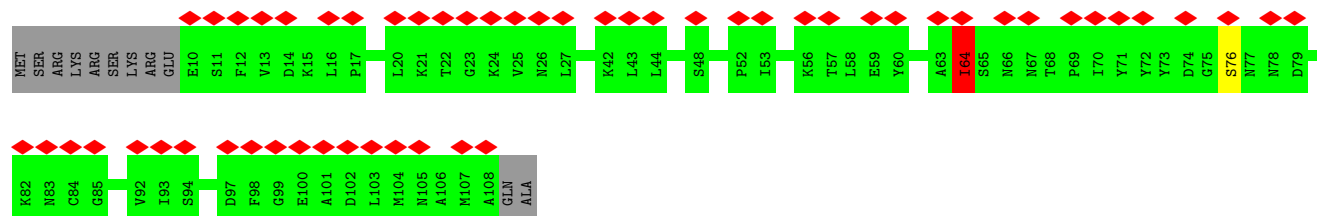
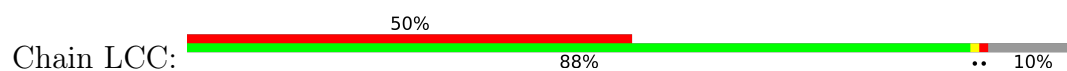




• Molecule 6: 60S ribosomal protein L4

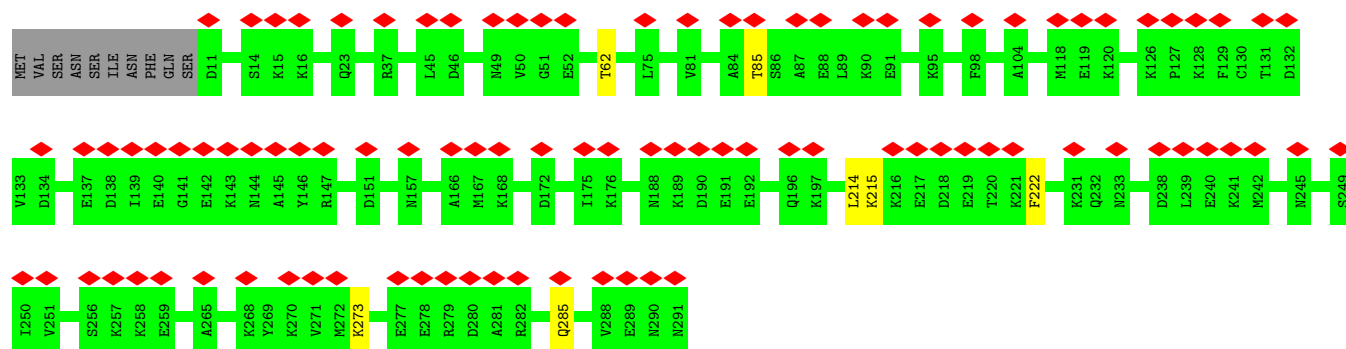


• Molecule 7: 60S ribosomal protein L3

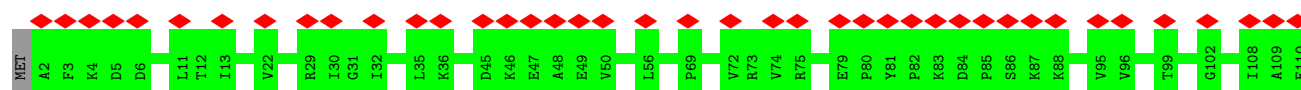


• Molecule 8: 60S ribosomal protein L5

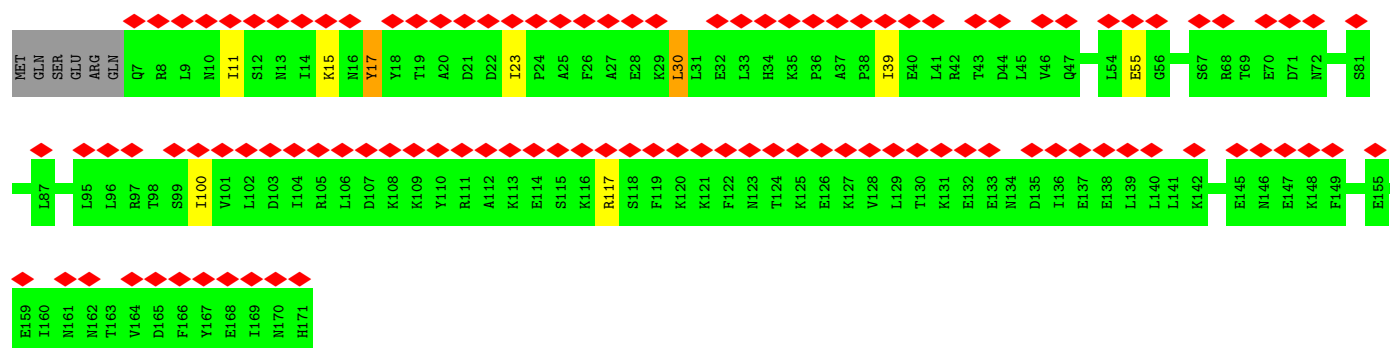




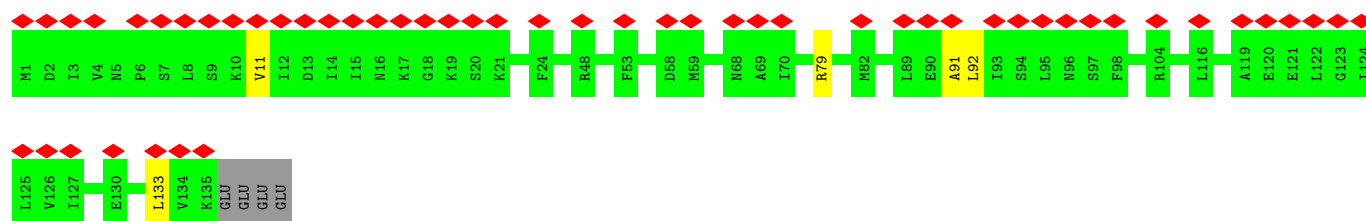
- Molecule 9: 60S ribosomal protein L31



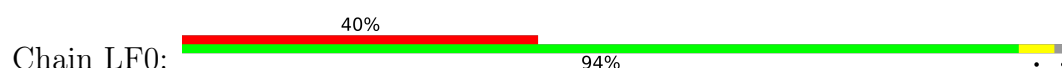
- Molecule 10: 60S ribosomal protein L6

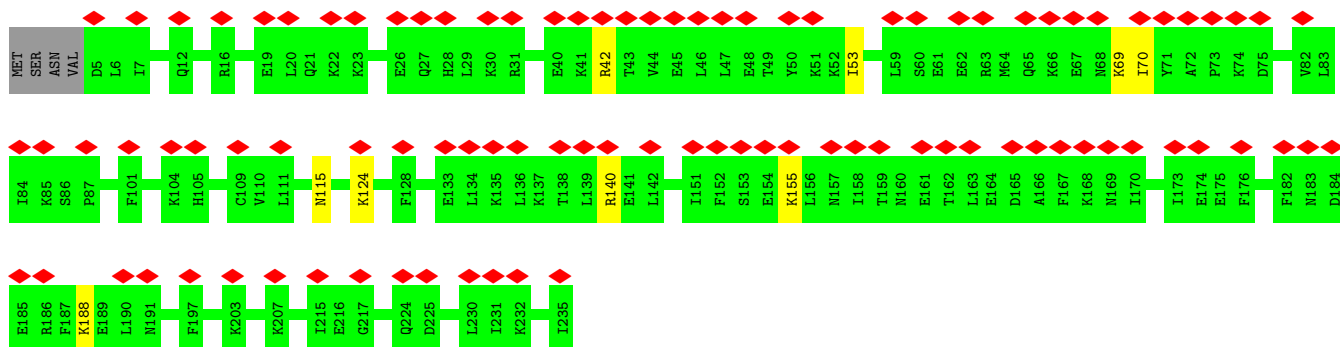


- Molecule 11: 60S ribosomal protein L32

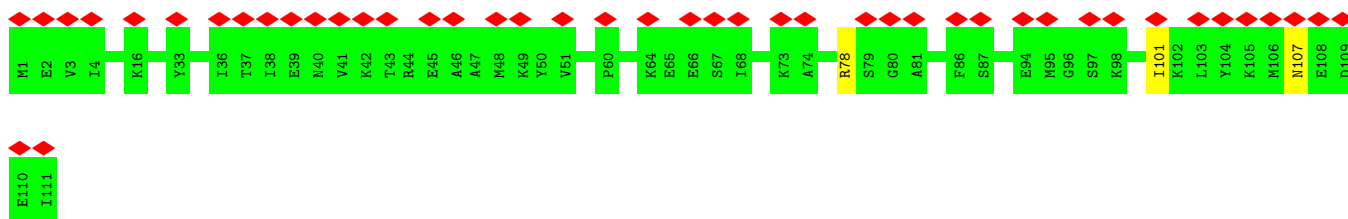
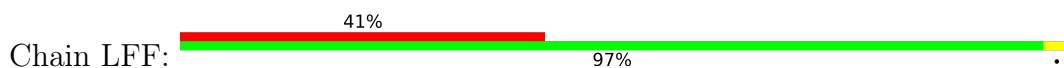


- Molecule 12: 60S ribosomal protein L7

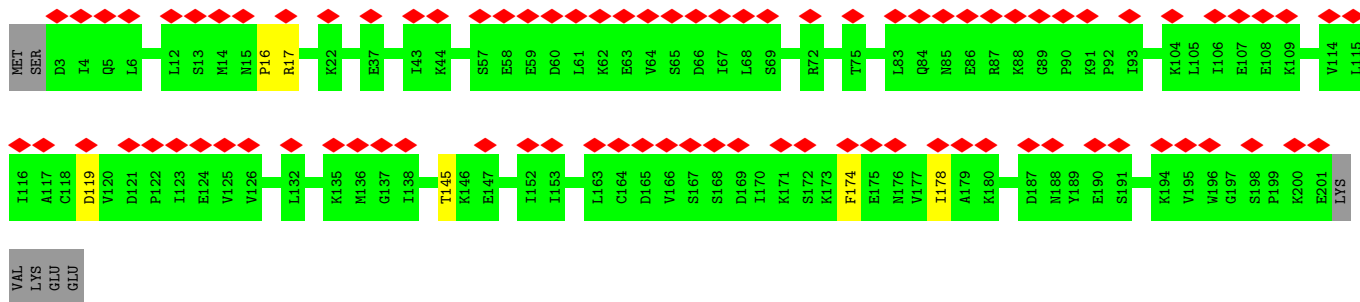
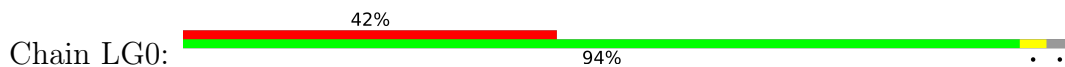




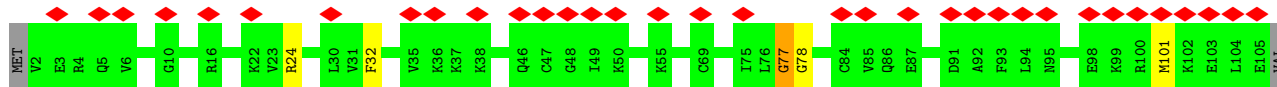
- Molecule 13: 60S ribosomal protein L35a



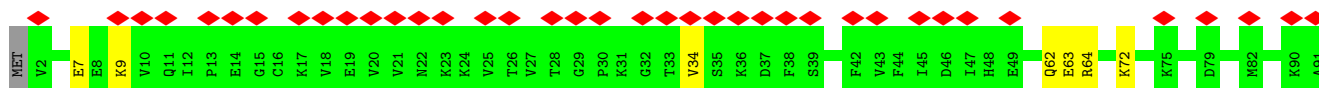
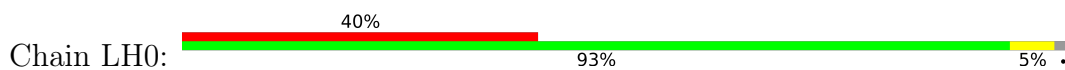
- Molecule 14: 60S ribosomal protein L8

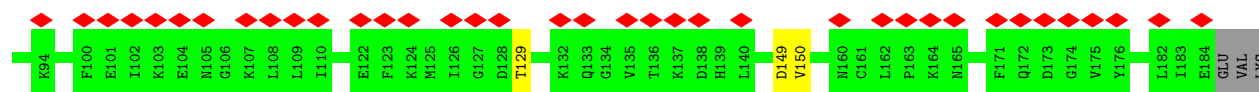


- Molecule 15: Ribosomal protein L34

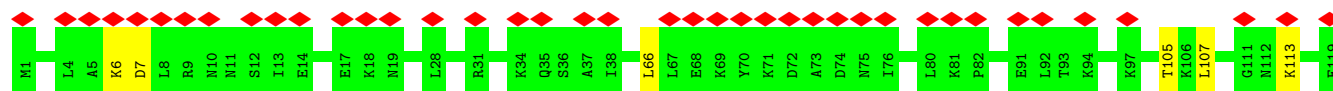


- Molecule 16: 60S ribosomal protein L9

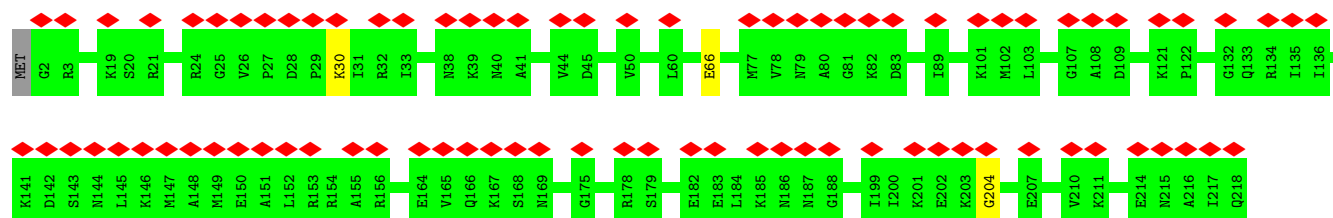




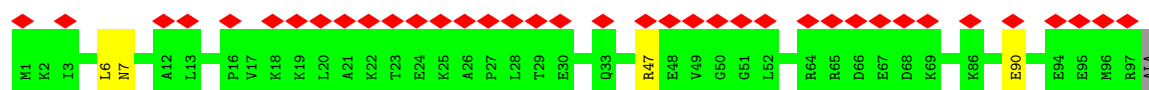
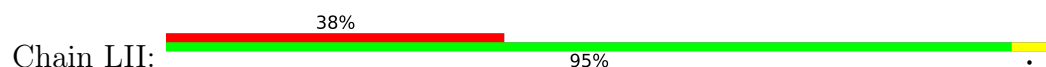
- Molecule 17: Ribosomal L29 protein (Fragment), Ribosomal L29 protein (Fragment), Ribosomal L29 protein (Fragment), Ribosomal L29 protein



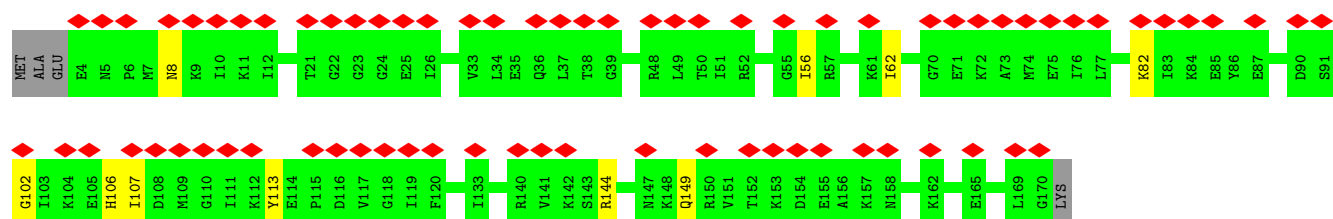
- Molecule 18: S60 ribosomal protein L10



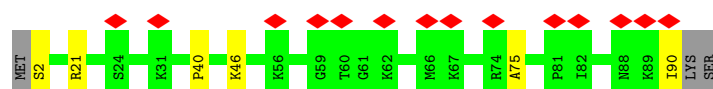
- Molecule 19: 60S ribosomal protein L36



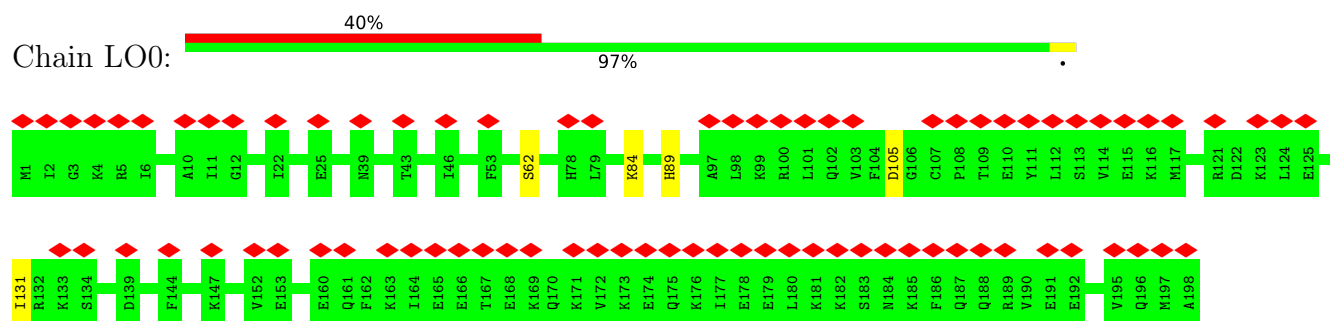
- Molecule 20: 60S ribosomal protein L11



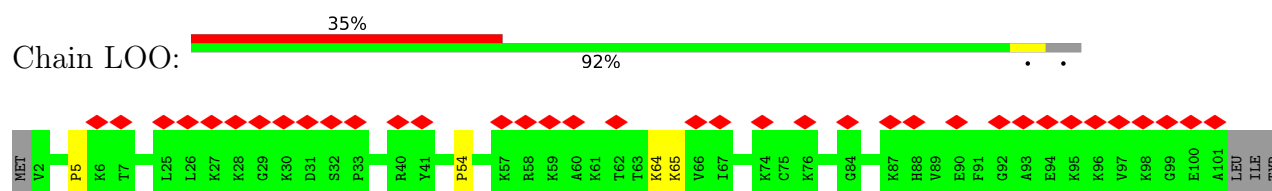
- Molecule 21: eL37



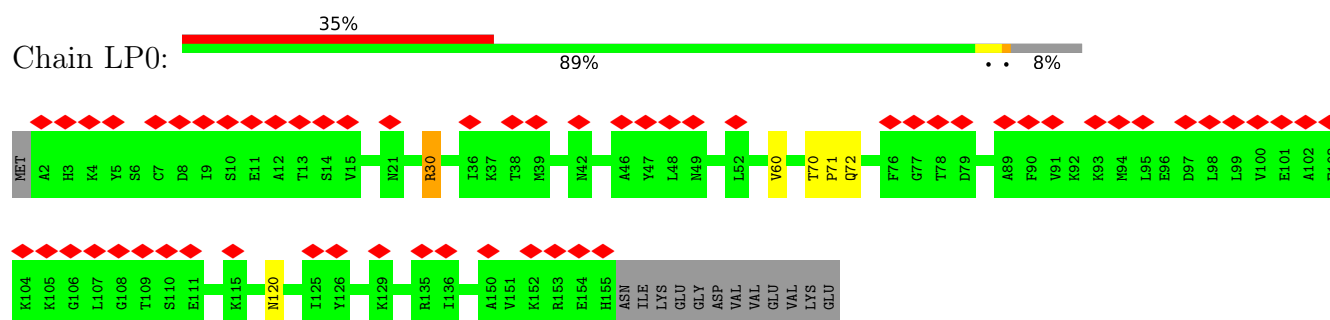
- Molecule 27: Ribosomal protein L13A



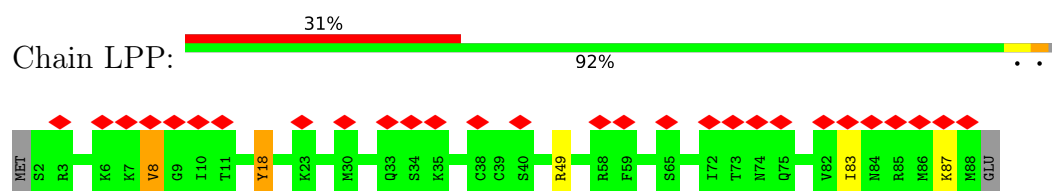
- Molecule 28: 60S ribosomal protein L44



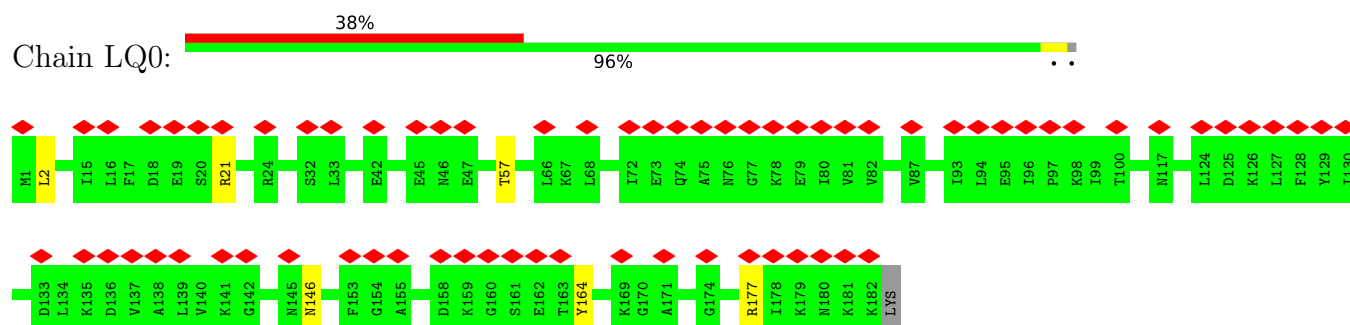
- Molecule 29: 60S ribosomal protein L17



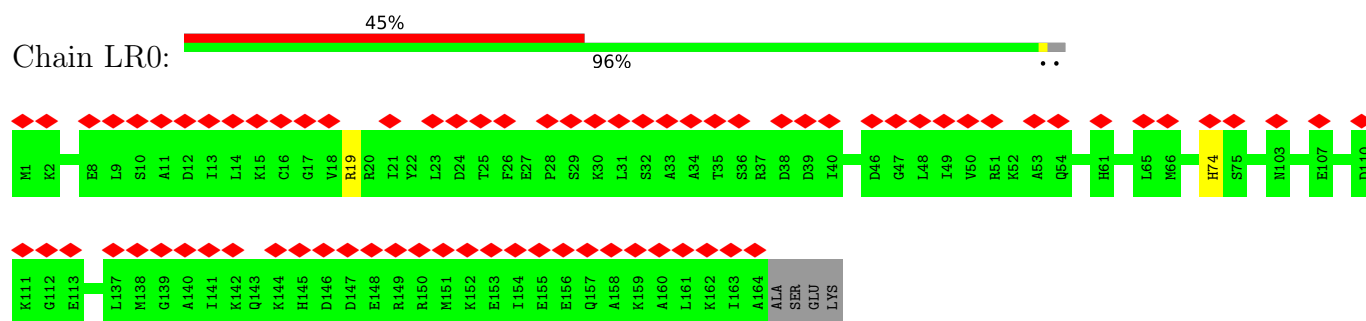
- Molecule 30: 60S ribosomal protein L37a



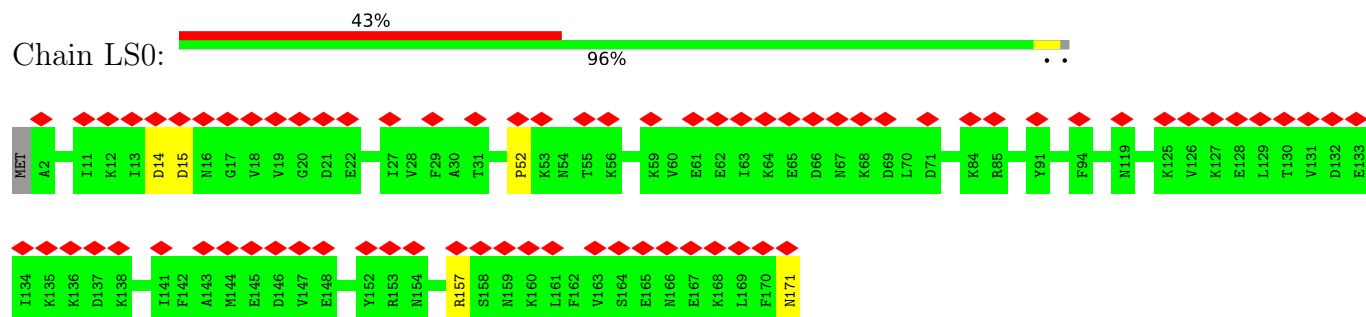
- Molecule 31: 60S ribosomal protein L18



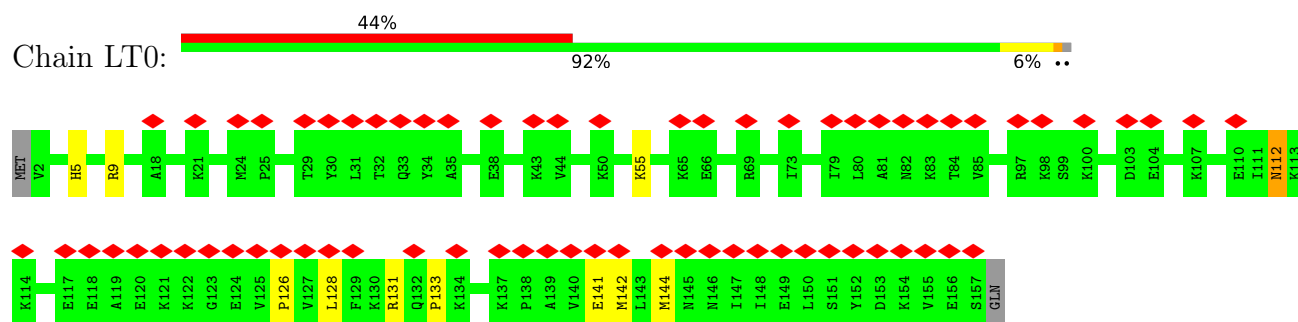
- Molecule 32: 60S ribosomal protein L19



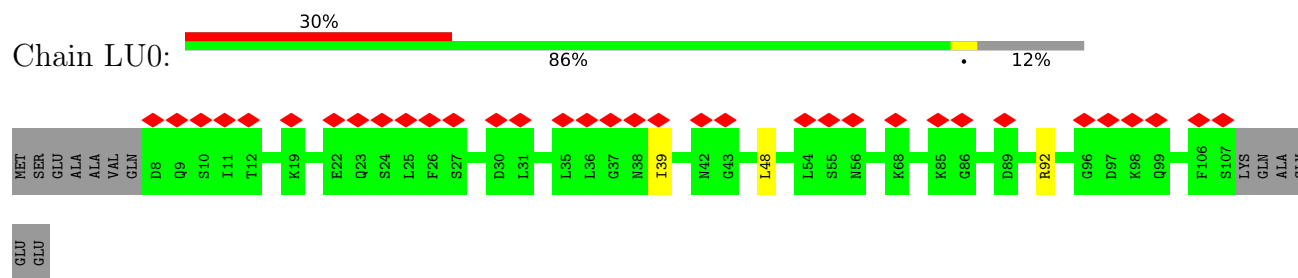
- Molecule 33: 60S ribosomal protein L20



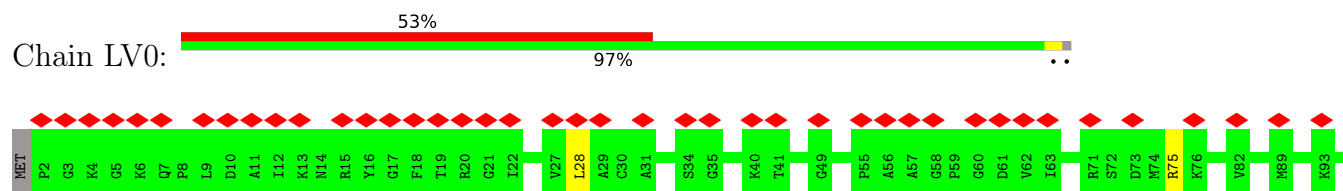
- Molecule 34: 60s ribosomal protein L21

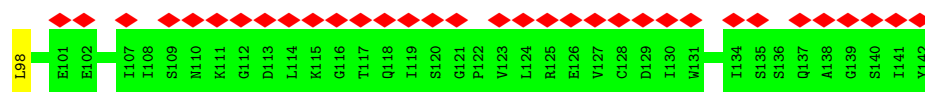


- Molecule 35: 60S ribosomal protein L22

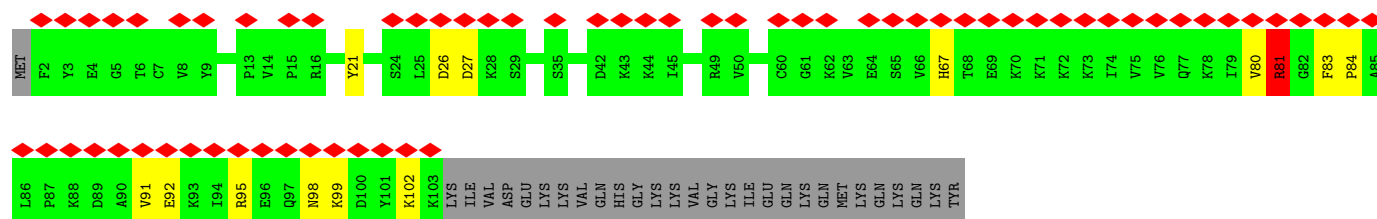
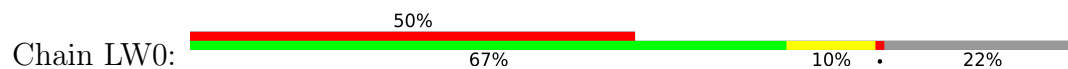


- Molecule 36: Ribosomal protein L23

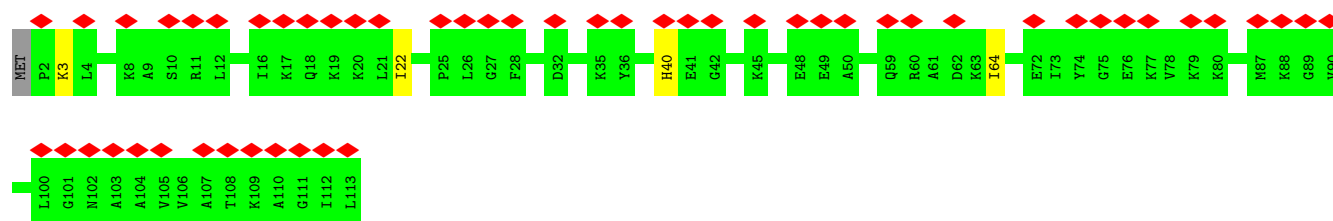




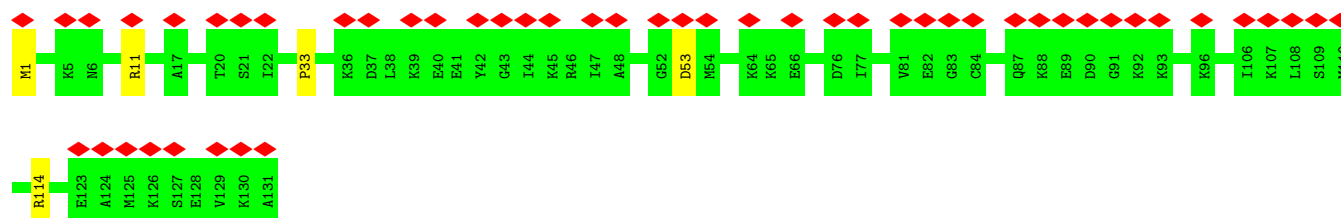
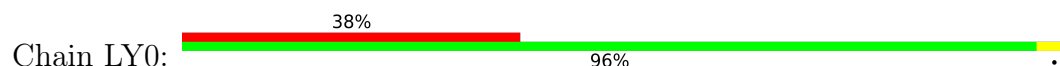
• Molecule 37: Ribosomal protein L24E



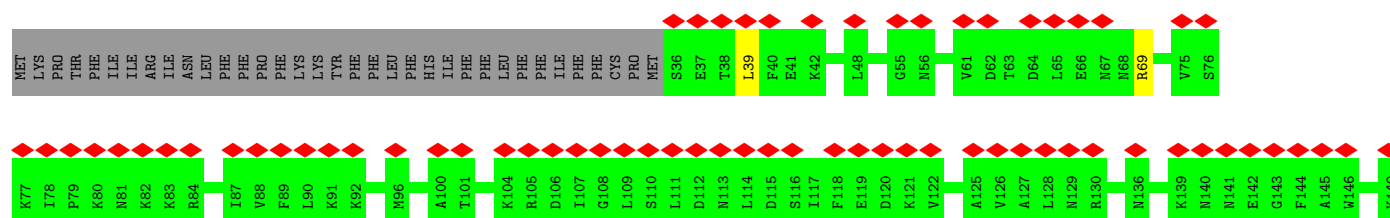
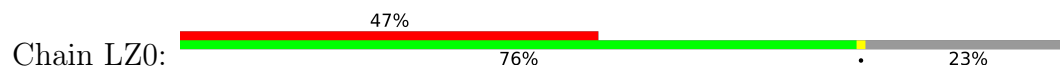
• Molecule 38: 60S ribosomal protein L23a

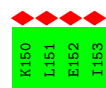


• Molecule 39: 60S ribosomal protein L26

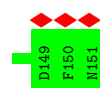
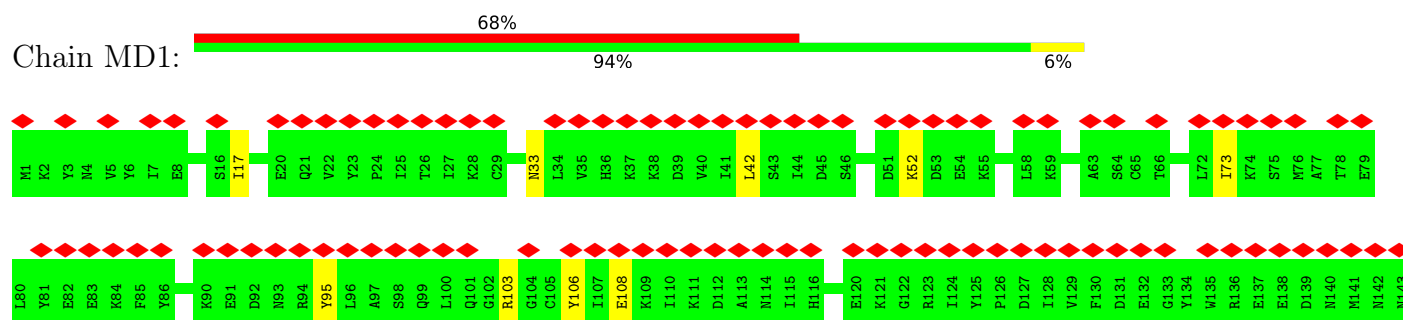


• Molecule 40: 60S ribosomal protein L27

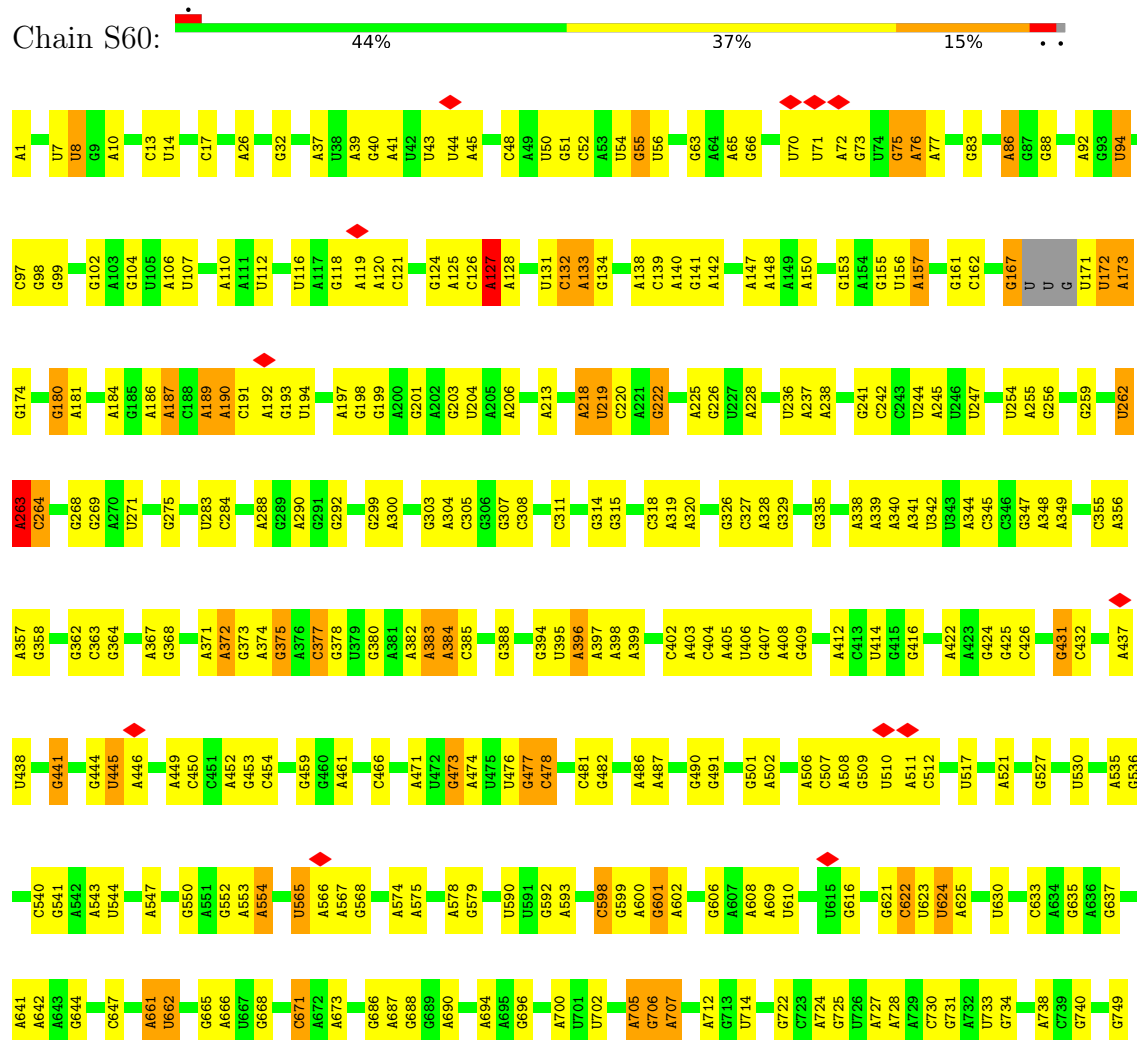


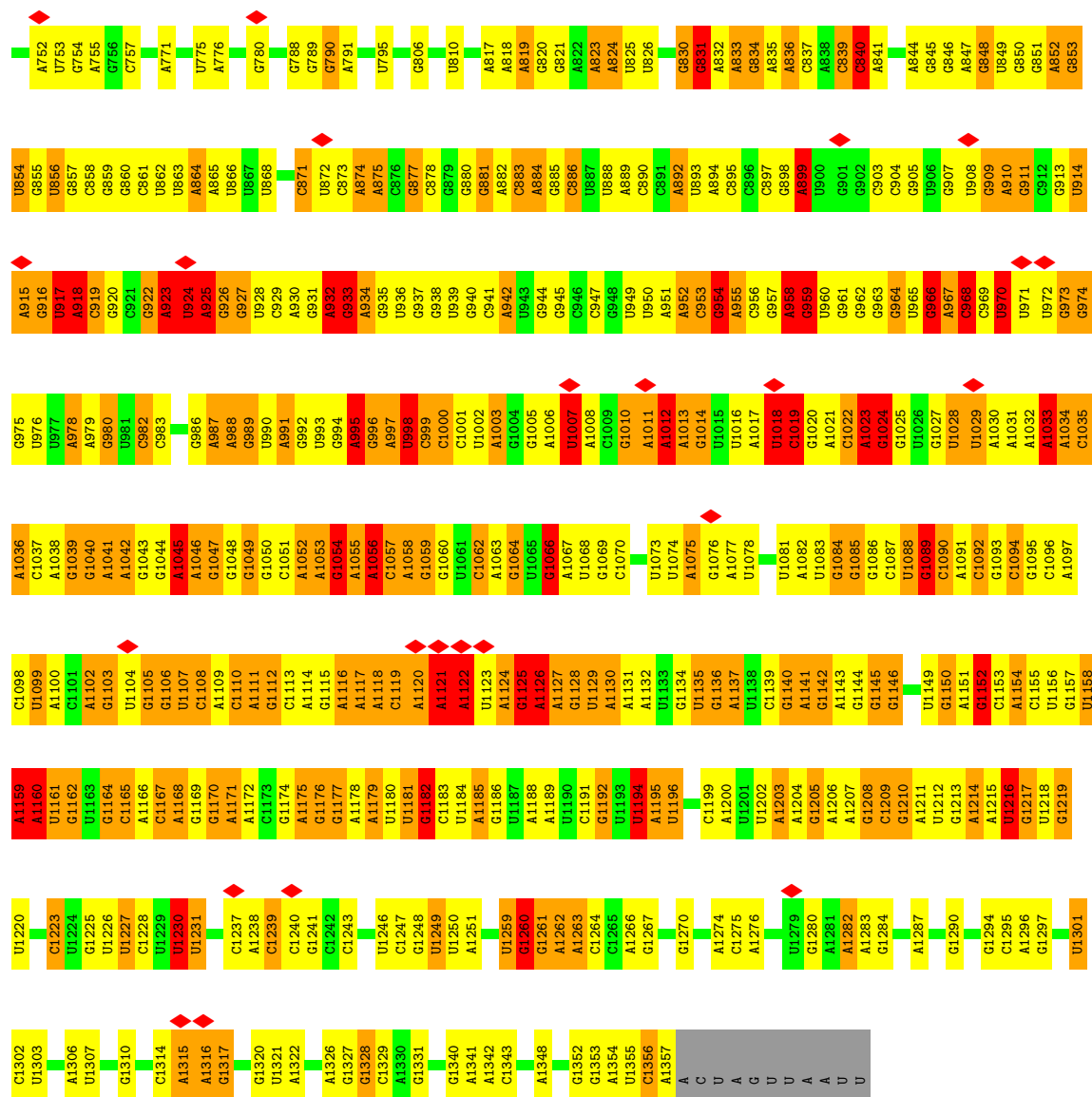


- Molecule 41: DNL-type domain-containing protein

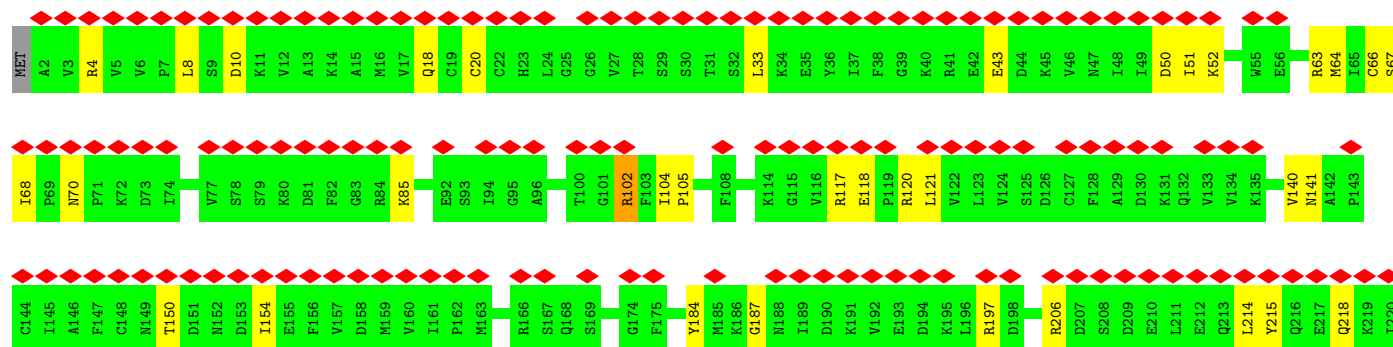
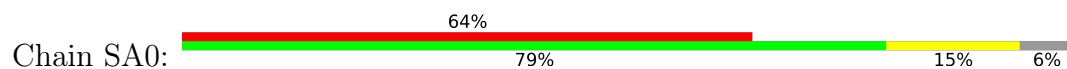


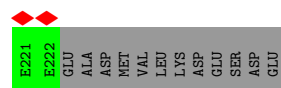
- Molecule 42: RNA 16S



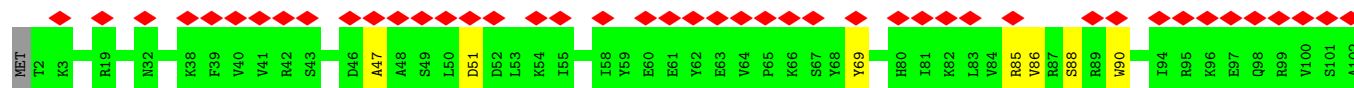


• Molecule 43: 40S ribosomal protein S0

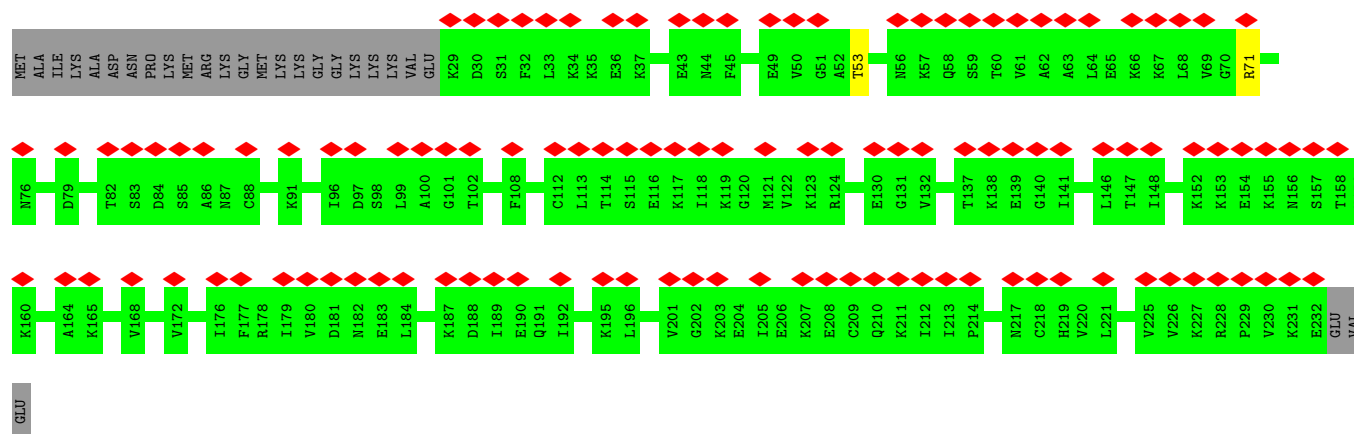




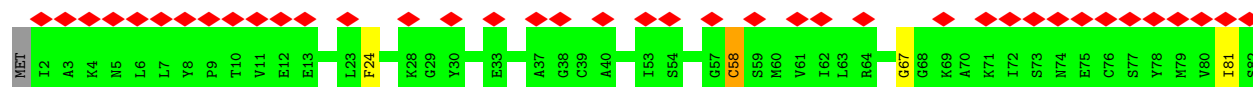
- Molecule 44: 40S ribosomal protein S26



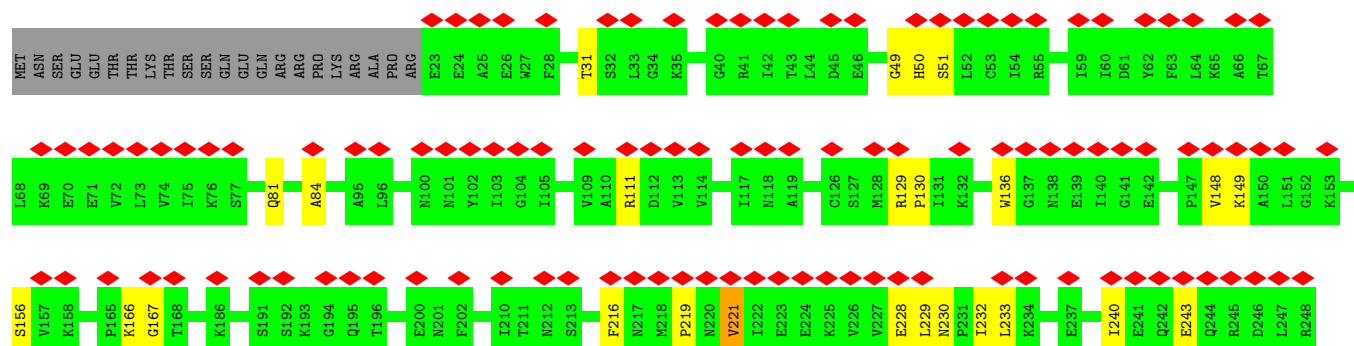
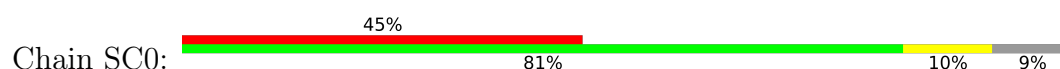
- Molecule 45: eS1



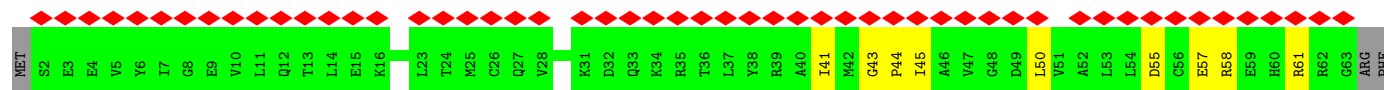
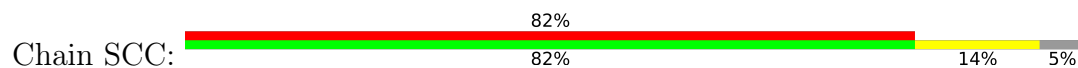
- Molecule 46: eS27



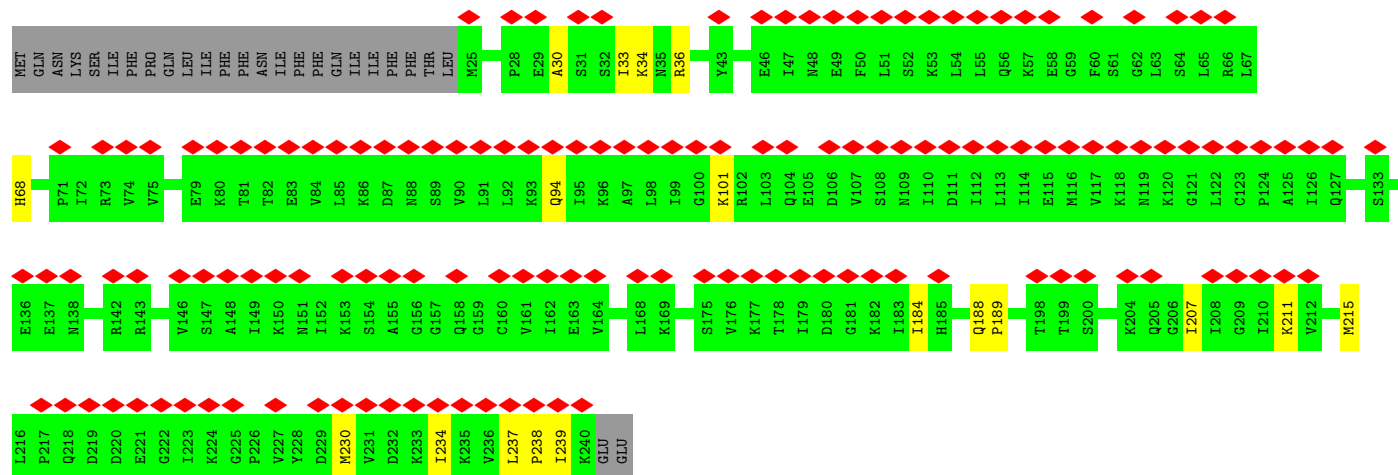
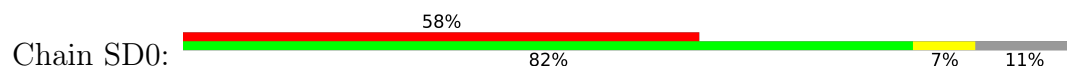
- Molecule 47: 40S ribosomal protein S2



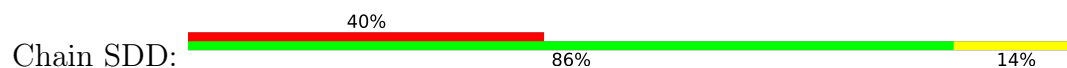
- Molecule 48: eS28



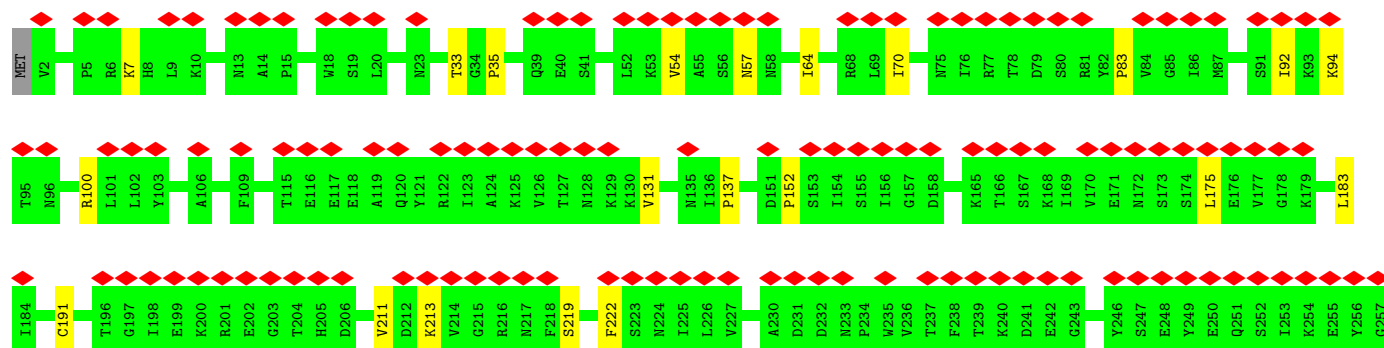
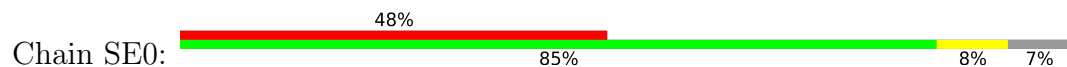
- Molecule 49: 40S ribosomal protein S3

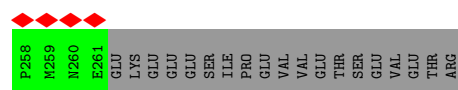


- Molecule 50: 40S ribosomal protein S29

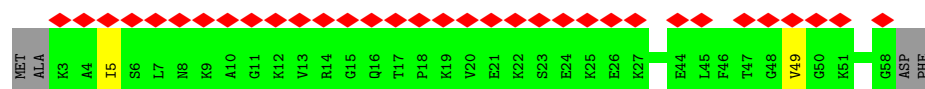


- Molecule 51: 40S ribosomal protein S4

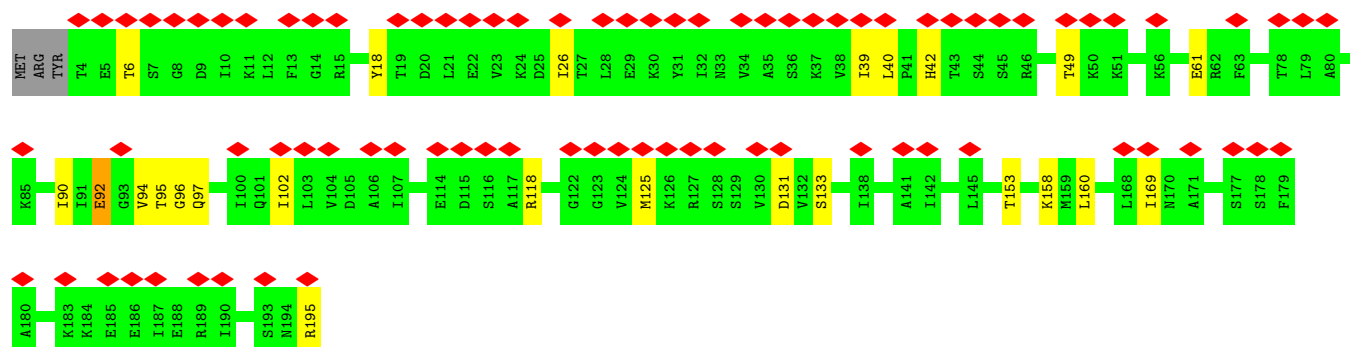
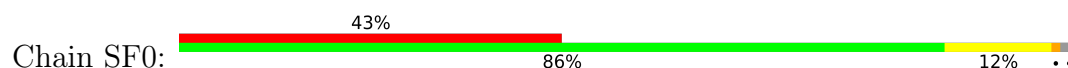




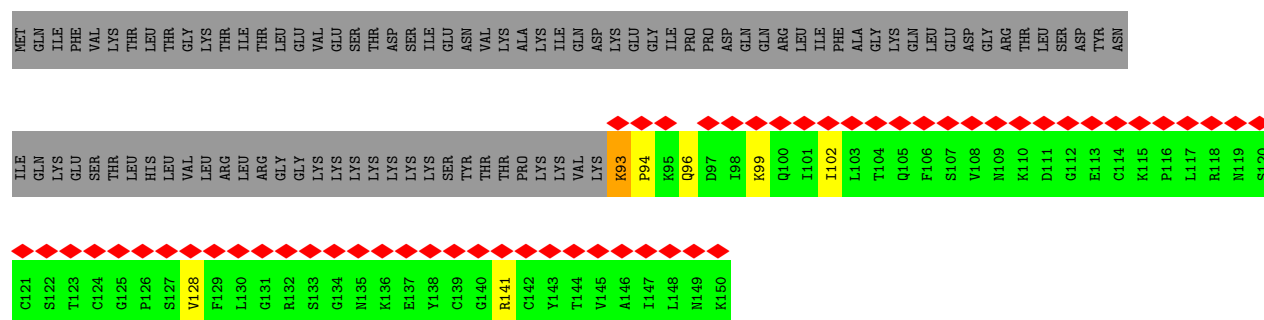
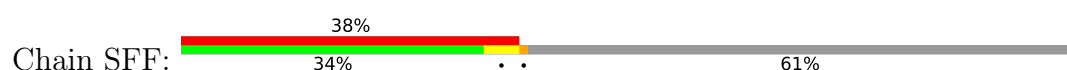
• Molecule 52: eS30



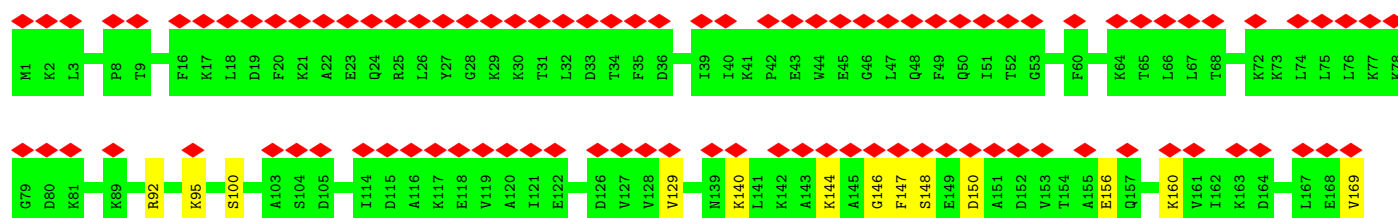
• Molecule 53: 40S ribosomal protein S5

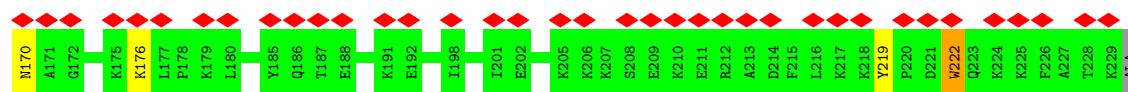


• Molecule 54: Ubiquitin/40s ribosomal protein S27a fusion



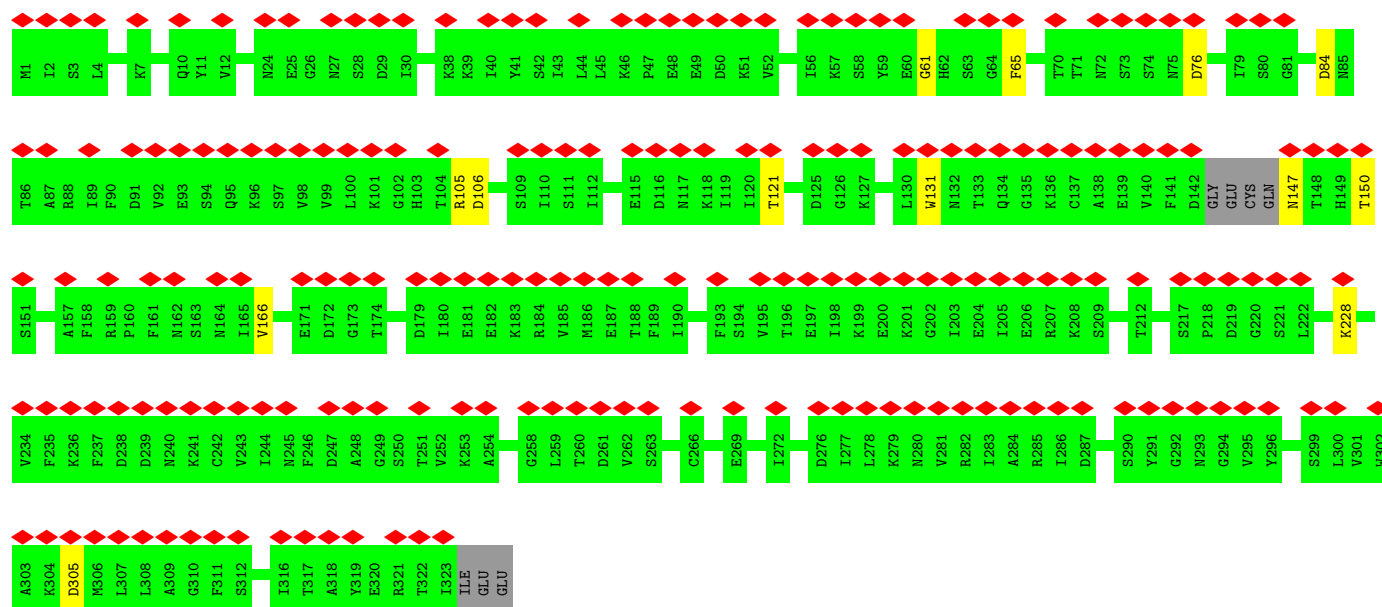
• Molecule 55: 40S ribosomal protein S6





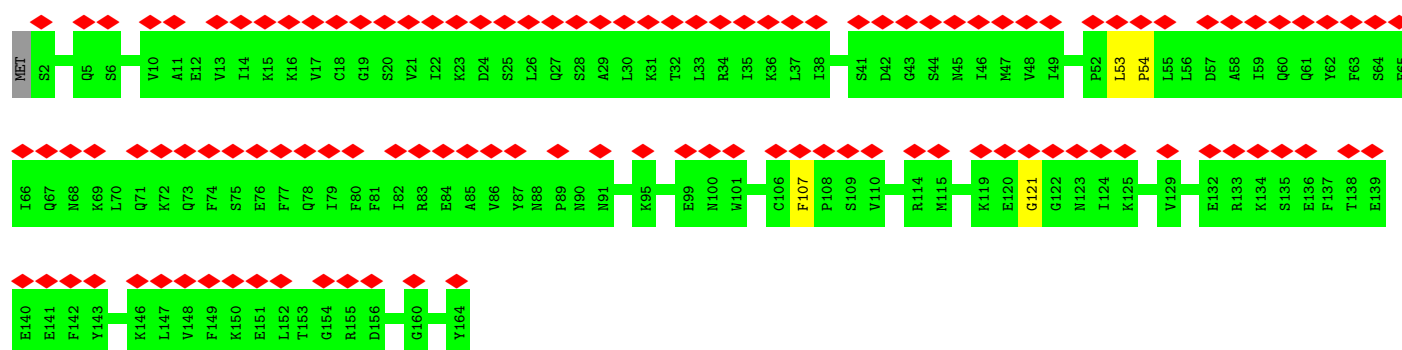
- Molecule 56: Guanine nucleotide binding protein beta subunit

Chain SGG:



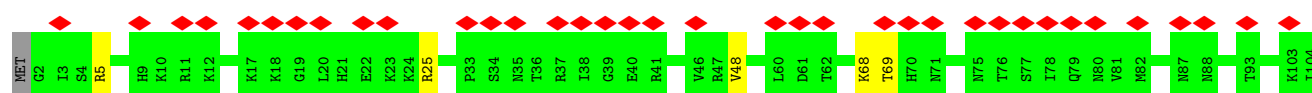
- Molecule 57: 40S ribosomal protein S7

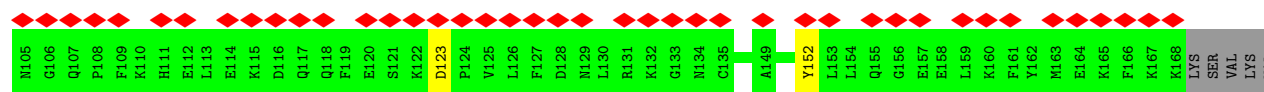
Chain SH0:



- Molecule 58: 40S ribosomal protein S8

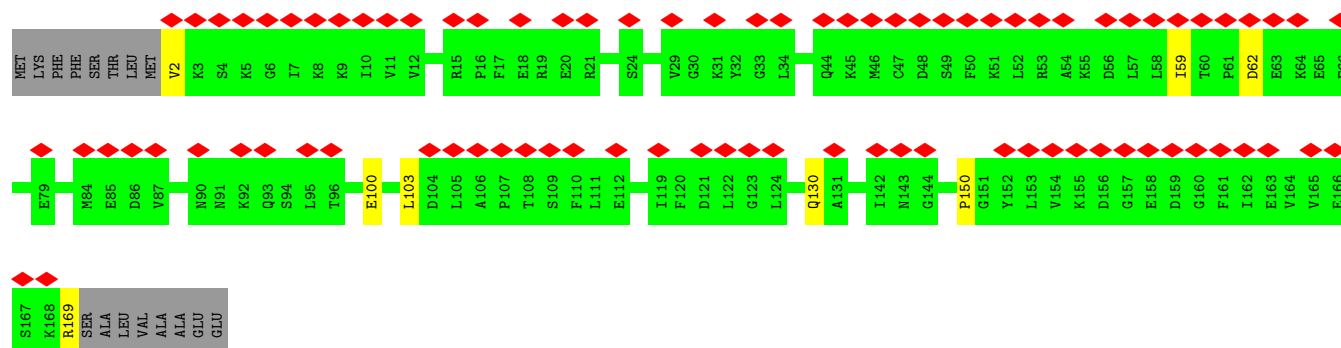
Chain SI0:





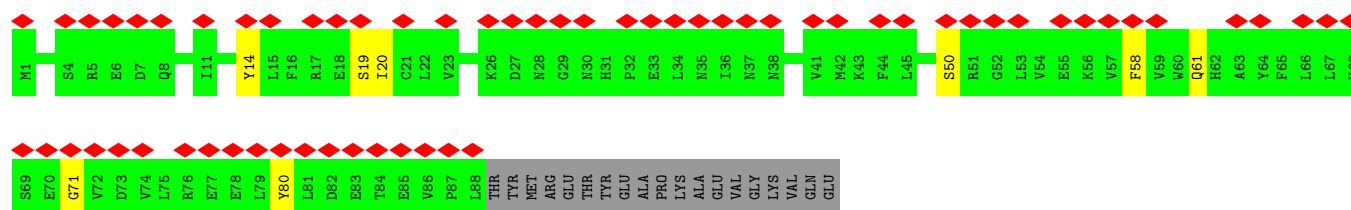
- Molecule 59: 40S ribosomal protein S9

Chain SJ0: 46% 87% 9%



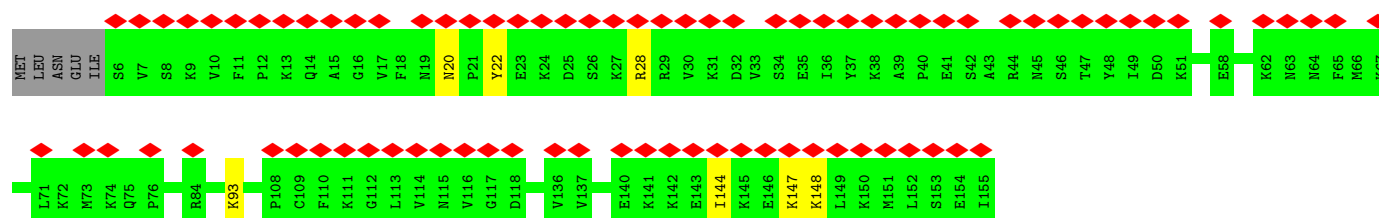
- Molecule 60: 40S ribosomal protein S10

Chain SK0: 59% 75% 7% 18%



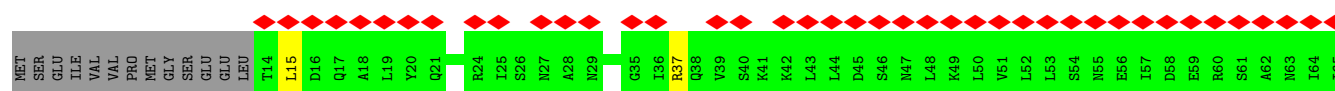
- Molecule 61: 40S ribosomal protein S11

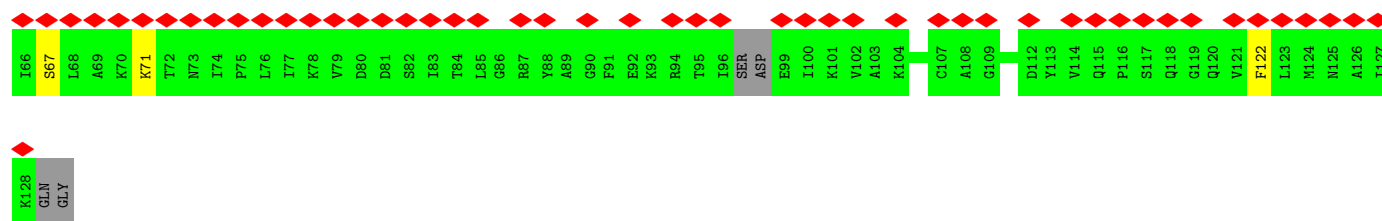
Chain SL0: 54% 92% 5%



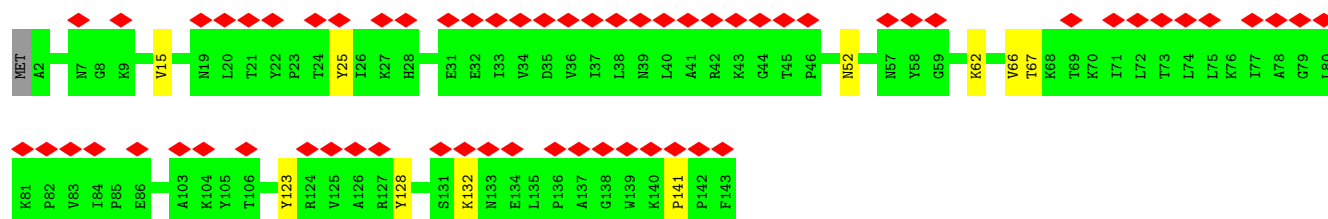
- Molecule 62: 40S ribosomal protein S12

Chain SM0: 70% 83% 13%

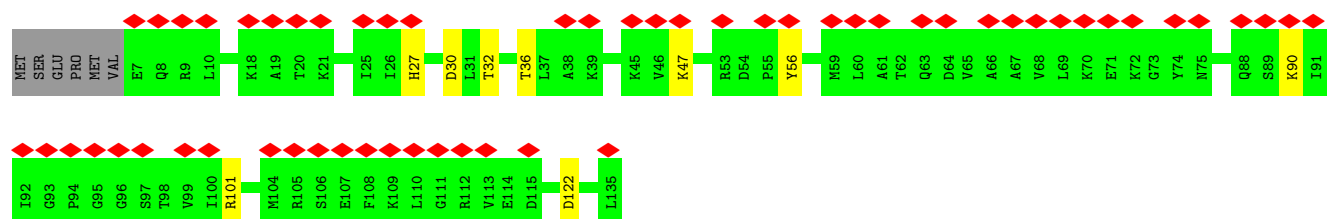
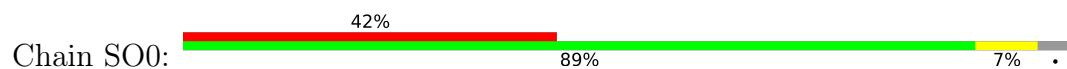




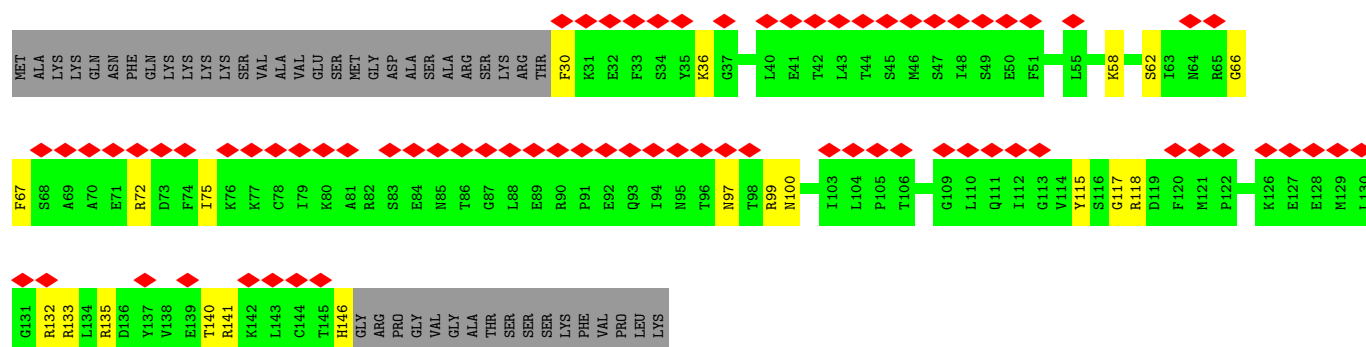
• Molecule 63: 40S ribosomal protein S13



• Molecule 64: 40S ribosomal protein S14

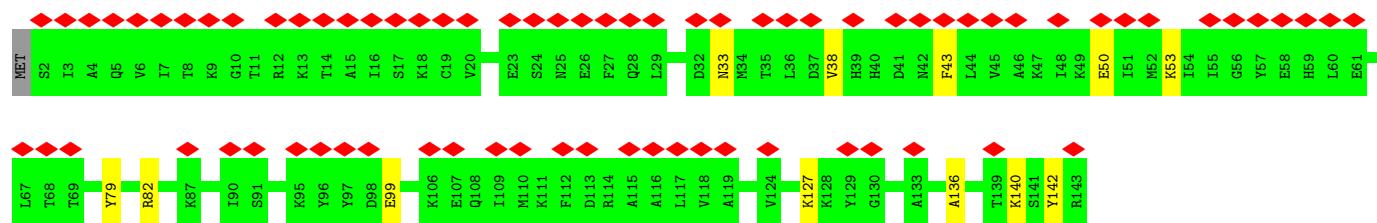


• Molecule 65: Ribosomal protein S19

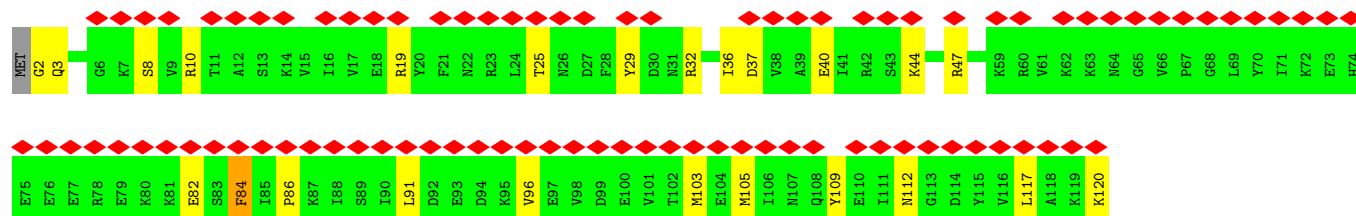
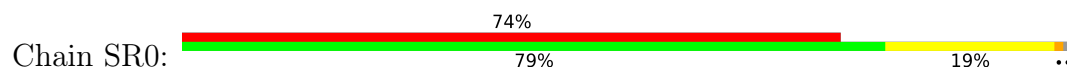


• Molecule 66: 40S ribosomal protein S16

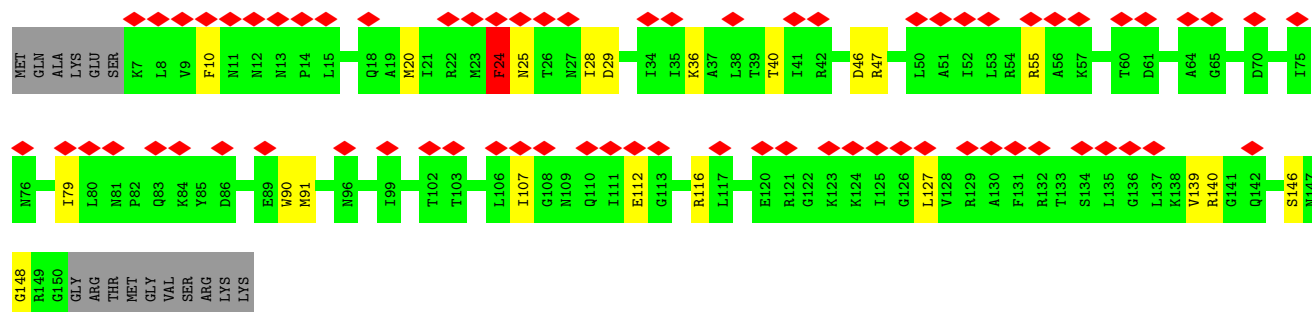
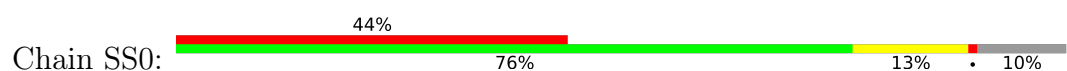




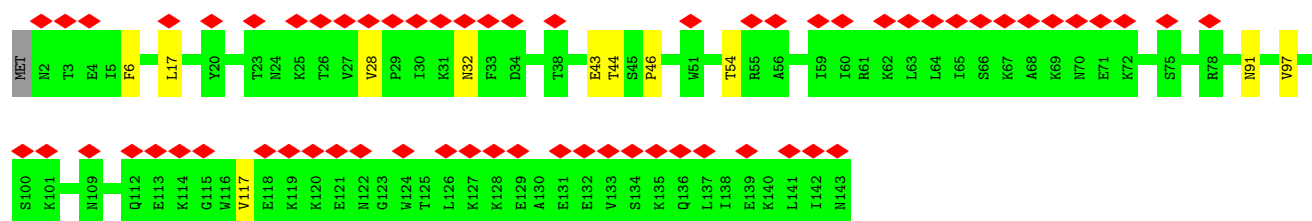
• Molecule 67: eS17



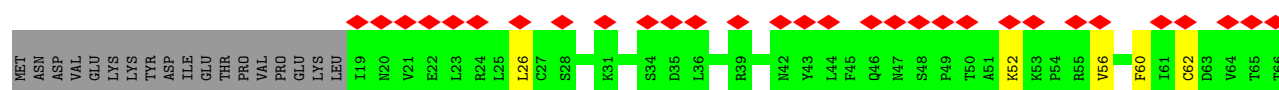
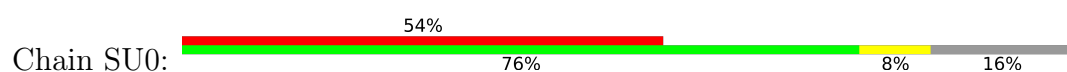
• Molecule 68: 40S ribosomal protein S18

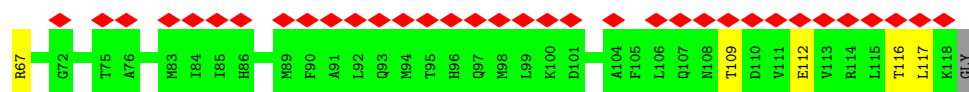


• Molecule 69: 40S Ribosomal protein S19

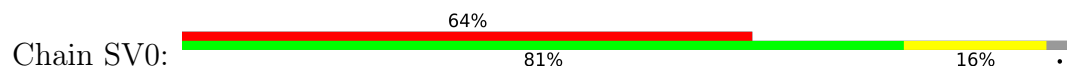


• Molecule 70: 40S ribosomal protein S20

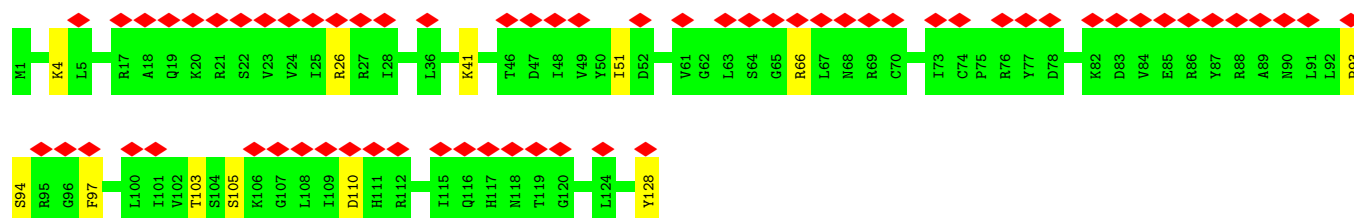




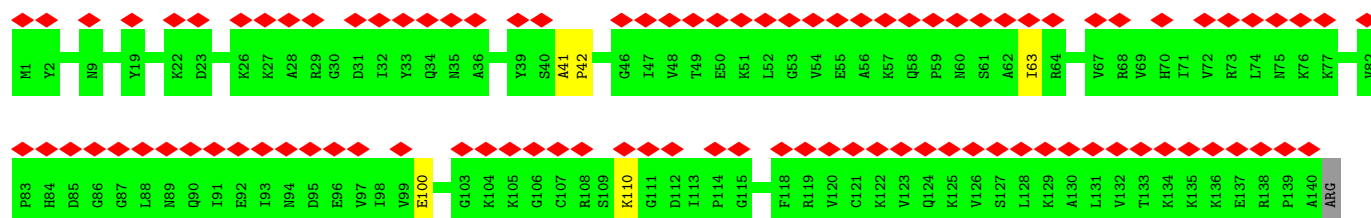
- Molecule 71: Ribosomal protein S21E



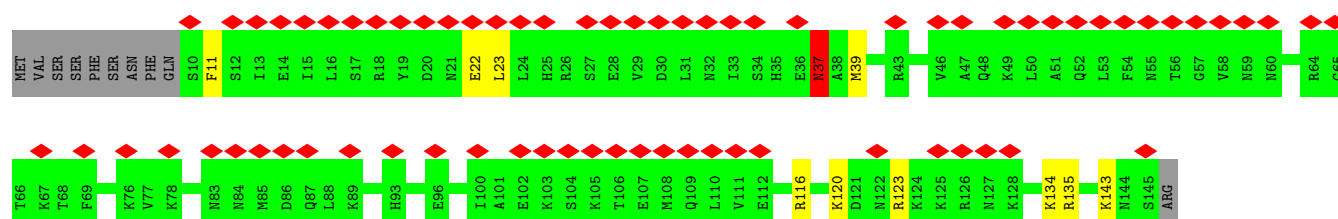
- Molecule 72: 40S ribosomal protein S15A



- Molecule 73: uS12

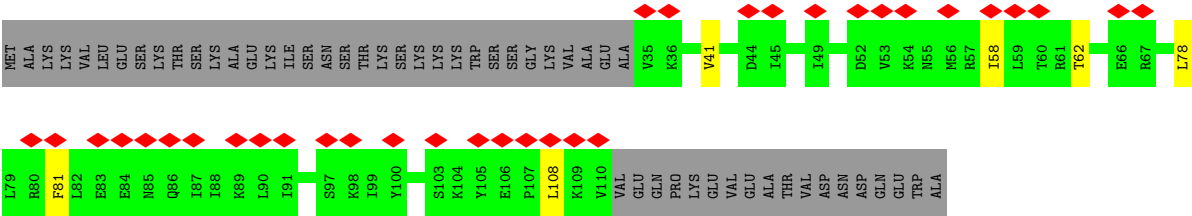


- Molecule 74: 40S ribosomal protein s24



- Molecule 75: 40S ribosomal protein S25





4 Experimental information

| Property | Value | Source |
|--------------------------------------|--|-----------|
| EM reconstruction method | SUBTOMOGRAM AVERAGING | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of subtomograms used | 1344 | 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 ($e^-/\text{\AA}^2$) | 120, 120 | Depositor |
| Minimum defocus (nm) | 2500 | Depositor |
| Maximum defocus (nm) | 6000 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k x 4k), GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value | 1.622 | Depositor |
| Minimum map value | -0.859 | Depositor |
| Average map value | 0.012 | Depositor |
| Map value standard deviation | 0.131 | Depositor |
| Recommended contour level | 0.39 | Depositor |
| Map size (\AA) | 453.00003, 453.00003, 453.00003 | wwPDB |
| Map dimensions | 100, 100, 100 | wwPDB |
| Map angles ($^\circ$) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (\AA) | 4.53, 4.53, 4.53 | Depositor |

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
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 | L50 | 0.75 | 1/60107 (0.0%) | 1.19 | 161/93753 (0.2%) |
| 2 | L70 | 0.75 | 1/2844 (0.0%) | 1.11 | 6/4429 (0.1%) |
| 3 | LA0 | 0.32 | 0/1926 | 0.74 | 0/2590 |
| 4 | LAA | 0.34 | 0/1191 | 0.66 | 0/1586 |
| 5 | LB0 | 0.32 | 0/3092 | 0.70 | 1/4144 (0.0%) |
| 6 | LC0 | 0.33 | 0/2646 | 0.75 | 1/3555 (0.0%) |
| 7 | LCC | 0.32 | 0/794 | 0.62 | 0/1067 |
| 8 | LD0 | 0.29 | 0/2328 | 0.67 | 0/3098 |
| 9 | LDD | 0.30 | 0/913 | 0.66 | 0/1223 |
| 10 | LE0 | 0.28 | 0/1394 | 0.65 | 0/1875 |
| 11 | LEE | 0.32 | 0/1108 | 0.69 | 0/1477 |
| 12 | LF0 | 0.30 | 0/1963 | 0.68 | 0/2618 |
| 13 | LFF | 0.33 | 0/906 | 0.70 | 0/1207 |
| 14 | LG0 | 0.28 | 0/1612 | 0.63 | 0/2163 |
| 15 | LGG | 0.34 | 0/825 | 0.78 | 1/1090 (0.1%) |
| 16 | LH0 | 0.30 | 0/1503 | 0.66 | 0/2018 |
| 17 | LHH | 0.28 | 0/999 | 0.66 | 0/1324 |
| 18 | LI0 | 0.32 | 0/1781 | 0.69 | 0/2382 |
| 19 | LII | 0.30 | 0/790 | 0.59 | 0/1041 |
| 20 | LJ0 | 0.30 | 0/1350 | 0.66 | 0/1797 |
| 21 | LJJ | 0.40 | 0/710 | 0.83 | 2/932 (0.2%) |
| 22 | LL0 | 0.30 | 0/1374 | 0.76 | 1/1827 (0.1%) |
| 23 | LLL | 0.34 | 0/435 | 0.72 | 0/576 |
| 24 | LM0 | 0.32 | 0/935 | 0.65 | 0/1251 |
| 25 | LMM | 0.41 | 0/431 | 0.68 | 0/568 |
| 26 | LN0 | 0.35 | 0/1722 | 0.74 | 1/2297 (0.0%) |
| 27 | LO0 | 0.30 | 0/1626 | 0.65 | 0/2168 |
| 28 | LOO | 0.34 | 0/811 | 0.70 | 0/1071 |
| 29 | LP0 | 0.32 | 0/1262 | 0.77 | 0/1689 |
| 30 | LPP | 0.40 | 0/693 | 0.78 | 2/918 (0.2%) |
| 31 | LQ0 | 0.30 | 0/1512 | 0.64 | 0/2014 |
| 32 | LR0 | 0.31 | 0/1352 | 0.65 | 1/1790 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 33 | LS0 | 0.30 | 0/1422 | 0.67 | 0/1898 |
| 34 | LT0 | 0.31 | 0/1294 | 0.68 | 0/1736 |
| 35 | LU0 | 0.30 | 0/826 | 0.67 | 0/1104 |
| 36 | LV0 | 0.31 | 0/1068 | 0.70 | 0/1429 |
| 37 | LW0 | 0.43 | 0/849 | 0.72 | 0/1129 |
| 38 | LX0 | 0.28 | 0/883 | 0.67 | 0/1175 |
| 39 | LY0 | 0.29 | 0/1058 | 0.69 | 1/1399 (0.1%) |
| 40 | LZ0 | 0.29 | 0/976 | 0.73 | 1/1302 (0.1%) |
| 41 | MD1 | 0.66 | 0/1249 | 0.87 | 1/1677 (0.1%) |
| 42 | S60 | 1.41 | 352/32725 (1.1%) | 1.41 | 375/51066 (0.7%) |
| 43 | SA0 | 0.36 | 1/1751 (0.1%) | 0.64 | 0/2358 |
| 44 | SAA | 0.38 | 0/839 | 0.73 | 0/1120 |
| 45 | SB0 | 0.29 | 0/1623 | 0.67 | 0/2169 |
| 46 | SBB | 0.47 | 1/634 (0.2%) | 0.65 | 0/844 |
| 47 | SC0 | 0.31 | 0/1751 | 0.69 | 2/2359 (0.1%) |
| 48 | SCC | 0.33 | 0/480 | 0.73 | 0/644 |
| 49 | SD0 | 0.30 | 0/1721 | 0.66 | 0/2304 |
| 50 | SDD | 0.40 | 0/559 | 0.75 | 1/742 (0.1%) |
| 51 | SE0 | 0.32 | 0/2080 | 0.72 | 2/2804 (0.1%) |
| 52 | SEE | 0.36 | 0/453 | 0.74 | 1/596 (0.2%) |
| 53 | SF0 | 0.31 | 0/1527 | 0.68 | 0/2045 |
| 54 | SFF | 0.43 | 0/427 | 0.68 | 0/573 |
| 55 | SG0 | 0.29 | 0/1864 | 0.68 | 0/2485 |
| 56 | SGG | 0.34 | 0/2517 | 0.71 | 1/3397 (0.0%) |
| 57 | SH0 | 0.31 | 0/1356 | 0.66 | 0/1820 |
| 58 | SI0 | 0.33 | 0/1369 | 0.68 | 0/1825 |
| 59 | SJ0 | 0.33 | 0/1403 | 0.68 | 0/1880 |
| 60 | SK0 | 0.29 | 0/750 | 0.71 | 0/1009 |
| 61 | SL0 | 0.32 | 0/1252 | 0.72 | 2/1672 (0.1%) |
| 62 | SM0 | 0.32 | 0/881 | 0.71 | 0/1182 |
| 63 | SN0 | 0.38 | 0/1154 | 0.78 | 0/1557 |
| 64 | SO0 | 0.33 | 0/993 | 0.72 | 0/1326 |
| 65 | SP0 | 0.33 | 0/964 | 0.71 | 0/1289 |
| 66 | SQ0 | 0.33 | 0/1163 | 0.74 | 3/1556 (0.2%) |
| 67 | SR0 | 0.64 | 0/985 | 0.96 | 2/1315 (0.2%) |
| 68 | SS0 | 0.34 | 0/1165 | 0.74 | 0/1566 |
| 69 | ST0 | 0.34 | 0/1181 | 0.75 | 1/1585 (0.1%) |
| 70 | SU0 | 0.33 | 0/824 | 0.74 | 2/1110 (0.2%) |
| 71 | SV0 | 0.33 | 0/525 | 0.66 | 0/700 |
| 72 | SW0 | 0.32 | 0/1037 | 0.71 | 0/1389 |
| 73 | SX0 | 0.31 | 0/1113 | 0.70 | 0/1486 |
| 74 | SY0 | 0.30 | 0/1131 | 0.72 | 1/1503 (0.1%) |
| 75 | SZ0 | 0.33 | 0/640 | 0.75 | 0/855 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| All | All | 0.78 | 356/183397 (0.2%) | 1.06 | 573/266518 (0.2%) |

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 |
|-----|-------|---------------------|---------------------|
| 6 | LC0 | 0 | 1 |
| 13 | LFF | 0 | 1 |
| 15 | LGG | 0 | 1 |
| All | All | 0 | 3 |

All (356) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 42 | S60 | 934 | A | P-O5' | 10.34 | 1.70 | 1.59 |
| 42 | S60 | 988 | A | N9-C4 | -8.57 | 1.32 | 1.37 |
| 43 | SA0 | 20 | CYS | C-N | 8.40 | 1.53 | 1.34 |
| 1 | L50 | 1 | A | OP3-P | -8.36 | 1.51 | 1.61 |
| 42 | S60 | 1049 | G | N7-C5 | -8.34 | 1.34 | 1.39 |
| 42 | S60 | 1052 | A | N9-C4 | -8.30 | 1.32 | 1.37 |
| 42 | S60 | 968 | C | N1-C6 | -8.24 | 1.32 | 1.37 |
| 42 | S60 | 835 | A | N7-C5 | -7.93 | 1.34 | 1.39 |
| 42 | S60 | 989 | G | N7-C5 | -7.77 | 1.34 | 1.39 |
| 42 | S60 | 979 | A | N7-C5 | -7.70 | 1.34 | 1.39 |
| 42 | S60 | 1011 | A | N7-C5 | -7.57 | 1.34 | 1.39 |
| 42 | S60 | 1178 | A | N9-C4 | -7.56 | 1.33 | 1.37 |
| 42 | S60 | 1045 | A | N3-C4 | -7.50 | 1.30 | 1.34 |
| 42 | S60 | 1 | A | OP3-P | -7.50 | 1.52 | 1.61 |
| 2 | L70 | 1 | A | OP3-P | -7.40 | 1.52 | 1.61 |
| 42 | S60 | 952 | A | N9-C4 | -7.34 | 1.33 | 1.37 |
| 42 | S60 | 978 | A | N9-C4 | -7.34 | 1.33 | 1.37 |
| 42 | S60 | 1089 | G | C8-N7 | 7.28 | 1.35 | 1.30 |
| 42 | S60 | 849 | U | C2-N3 | -7.28 | 1.32 | 1.37 |
| 42 | S60 | 1045 | A | N7-C5 | -7.24 | 1.34 | 1.39 |
| 42 | S60 | 847 | A | N3-C4 | -7.22 | 1.30 | 1.34 |
| 42 | S60 | 835 | A | N3-C4 | -7.21 | 1.30 | 1.34 |
| 42 | S60 | 1084 | G | C8-N7 | 7.21 | 1.35 | 1.30 |
| 42 | S60 | 951 | A | N9-C4 | -7.16 | 1.33 | 1.37 |
| 42 | S60 | 885 | G | N9-C8 | -7.13 | 1.32 | 1.37 |
| 42 | S60 | 1058 | A | N9-C4 | -7.12 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 42 | S60 | 987 | A | N9-C4 | -7.11 | 1.33 | 1.37 |
| 42 | S60 | 1036 | A | C5-C4 | -7.09 | 1.33 | 1.38 |
| 42 | S60 | 989 | G | C6-N1 | -7.05 | 1.34 | 1.39 |
| 42 | S60 | 963 | G | C5-C4 | -6.98 | 1.33 | 1.38 |
| 42 | S60 | 1164 | G | N7-C5 | 6.96 | 1.43 | 1.39 |
| 42 | S60 | 836 | A | N3-C4 | -6.92 | 1.30 | 1.34 |
| 42 | S60 | 1228 | C | C4-C5 | -6.90 | 1.37 | 1.43 |
| 42 | S60 | 848 | G | N9-C8 | -6.87 | 1.33 | 1.37 |
| 42 | S60 | 1028 | U | C2-N3 | -6.87 | 1.32 | 1.37 |
| 42 | S60 | 979 | A | N3-C4 | -6.87 | 1.30 | 1.34 |
| 42 | S60 | 1181 | U | C2-N3 | -6.86 | 1.32 | 1.37 |
| 42 | S60 | 1014 | G | N7-C5 | -6.86 | 1.35 | 1.39 |
| 42 | S60 | 1176 | G | N7-C5 | 6.84 | 1.43 | 1.39 |
| 42 | S60 | 851 | G | N7-C5 | 6.84 | 1.43 | 1.39 |
| 42 | S60 | 1121 | A | N9-C4 | 6.83 | 1.42 | 1.37 |
| 42 | S60 | 1038 | A | N9-C4 | -6.80 | 1.33 | 1.37 |
| 42 | S60 | 1027 | G | C5-C4 | -6.80 | 1.33 | 1.38 |
| 42 | S60 | 1053 | A | N3-C4 | 6.78 | 1.39 | 1.34 |
| 42 | S60 | 1154 | A | N9-C4 | 6.77 | 1.42 | 1.37 |
| 42 | S60 | 994 | G | N7-C5 | -6.77 | 1.35 | 1.39 |
| 42 | S60 | 877 | G | N9-C8 | -6.77 | 1.33 | 1.37 |
| 42 | S60 | 1182 | G | C8-N7 | -6.76 | 1.26 | 1.30 |
| 42 | S60 | 1086 | G | P-O5' | 6.72 | 1.66 | 1.59 |
| 42 | S60 | 1066 | G | N9-C8 | -6.71 | 1.33 | 1.37 |
| 42 | S60 | 1095 | G | C8-N7 | 6.70 | 1.34 | 1.30 |
| 42 | S60 | 884 | A | N9-C4 | 6.69 | 1.41 | 1.37 |
| 42 | S60 | 1022 | C | P-O5' | 6.65 | 1.66 | 1.59 |
| 42 | S60 | 877 | G | P-O5' | 6.64 | 1.66 | 1.59 |
| 42 | S60 | 1114 | A | P-O5' | 6.62 | 1.66 | 1.59 |
| 42 | S60 | 871 | C | N1-C6 | -6.61 | 1.33 | 1.37 |
| 42 | S60 | 1162 | G | C8-N7 | 6.61 | 1.34 | 1.30 |
| 42 | S60 | 1032 | A | C8-N7 | -6.57 | 1.26 | 1.31 |
| 42 | S60 | 1120 | A | N3-C4 | 6.55 | 1.38 | 1.34 |
| 42 | S60 | 1102 | A | N9-C4 | 6.54 | 1.41 | 1.37 |
| 42 | S60 | 1036 | A | C6-N6 | -6.54 | 1.28 | 1.33 |
| 42 | S60 | 859 | G | C8-N7 | 6.53 | 1.34 | 1.30 |
| 42 | S60 | 856 | U | P-O5' | 6.52 | 1.66 | 1.59 |
| 42 | S60 | 1067 | A | N7-C5 | 6.52 | 1.43 | 1.39 |
| 42 | S60 | 1183 | C | C4-C5 | -6.50 | 1.37 | 1.43 |
| 42 | S60 | 839 | C | C4-C5 | -6.49 | 1.37 | 1.43 |
| 42 | S60 | 1053 | A | N7-C5 | 6.49 | 1.43 | 1.39 |
| 42 | S60 | 1110 | C | C4-C5 | 6.47 | 1.48 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 42 | S60 | 1159 | A | N9-C4 | 6.47 | 1.41 | 1.37 |
| 42 | S60 | 1179 | A | N3-C4 | -6.44 | 1.30 | 1.34 |
| 42 | S60 | 885 | G | C6-N1 | -6.43 | 1.35 | 1.39 |
| 42 | S60 | 970 | U | C2-N3 | -6.42 | 1.33 | 1.37 |
| 42 | S60 | 978 | A | N7-C5 | -6.41 | 1.35 | 1.39 |
| 42 | S60 | 1050 | G | N9-C8 | -6.40 | 1.33 | 1.37 |
| 42 | S60 | 1174 | G | C2-N3 | 6.40 | 1.37 | 1.32 |
| 42 | S60 | 954 | G | N7-C5 | -6.39 | 1.35 | 1.39 |
| 42 | S60 | 1140 | G | N7-C5 | 6.39 | 1.43 | 1.39 |
| 42 | S60 | 1116 | A | N3-C4 | 6.37 | 1.38 | 1.34 |
| 42 | S60 | 1003 | A | C5-C4 | -6.37 | 1.34 | 1.38 |
| 42 | S60 | 983 | C | N1-C6 | -6.34 | 1.33 | 1.37 |
| 42 | S60 | 989 | G | N3-C4 | -6.34 | 1.31 | 1.35 |
| 42 | S60 | 892 | A | N3-C4 | 6.32 | 1.38 | 1.34 |
| 42 | S60 | 1111 | A | P-O5' | 6.29 | 1.66 | 1.59 |
| 42 | S60 | 1062 | C | N1-C6 | -6.28 | 1.33 | 1.37 |
| 42 | S60 | 850 | G | N9-C4 | -6.27 | 1.32 | 1.38 |
| 42 | S60 | 1106 | G | N7-C5 | 6.27 | 1.43 | 1.39 |
| 42 | S60 | 847 | A | N7-C5 | -6.25 | 1.35 | 1.39 |
| 42 | S60 | 1171 | A | N3-C4 | 6.25 | 1.38 | 1.34 |
| 42 | S60 | 892 | A | P-O5' | 6.24 | 1.66 | 1.59 |
| 42 | S60 | 1111 | A | N9-C4 | 6.22 | 1.41 | 1.37 |
| 42 | S60 | 1112 | G | P-O5' | 6.22 | 1.66 | 1.59 |
| 42 | S60 | 1058 | A | N7-C5 | -6.22 | 1.35 | 1.39 |
| 42 | S60 | 885 | G | N3-C4 | -6.19 | 1.31 | 1.35 |
| 42 | S60 | 1219 | G | C5-C4 | -6.19 | 1.34 | 1.38 |
| 42 | S60 | 1136 | G | P-O5' | 6.19 | 1.66 | 1.59 |
| 42 | S60 | 1113 | C | P-O5' | 6.19 | 1.66 | 1.59 |
| 42 | S60 | 1046 | A | C5-C4 | -6.17 | 1.34 | 1.38 |
| 42 | S60 | 835 | A | C6-N1 | -6.17 | 1.31 | 1.35 |
| 42 | S60 | 1155 | C | P-O5' | 6.17 | 1.66 | 1.59 |
| 42 | S60 | 877 | G | N3-C4 | -6.15 | 1.31 | 1.35 |
| 42 | S60 | 1064 | G | C8-N7 | 6.15 | 1.34 | 1.30 |
| 42 | S60 | 1046 | A | C6-N6 | -6.13 | 1.29 | 1.33 |
| 42 | S60 | 877 | G | C6-N1 | -6.12 | 1.35 | 1.39 |
| 42 | S60 | 877 | G | C8-N7 | 6.12 | 1.34 | 1.30 |
| 42 | S60 | 1045 | A | C6-N1 | -6.11 | 1.31 | 1.35 |
| 42 | S60 | 1053 | A | C6-N1 | 6.11 | 1.39 | 1.35 |
| 42 | S60 | 1177 | G | C8-N7 | -6.10 | 1.27 | 1.30 |
| 42 | S60 | 886 | C | C4-N4 | -6.10 | 1.28 | 1.33 |
| 42 | S60 | 865 | A | N9-C4 | 6.08 | 1.41 | 1.37 |
| 42 | S60 | 915 | A | N9-C4 | 6.08 | 1.41 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 42 | S60 | 1030 | A | N7-C5 | -6.08 | 1.35 | 1.39 |
| 42 | S60 | 1018 | U | C2-N3 | -6.08 | 1.33 | 1.37 |
| 42 | S60 | 1003 | A | N9-C4 | 6.07 | 1.41 | 1.37 |
| 42 | S60 | 847 | A | C6-N1 | -6.06 | 1.31 | 1.35 |
| 42 | S60 | 857 | G | P-O5' | 6.06 | 1.65 | 1.59 |
| 42 | S60 | 913 | G | C6-N1 | 6.05 | 1.43 | 1.39 |
| 42 | S60 | 875 | A | C5-C4 | -6.05 | 1.34 | 1.38 |
| 42 | S60 | 939 | U | P-O5' | 6.05 | 1.65 | 1.59 |
| 42 | S60 | 1067 | A | N3-C4 | 6.05 | 1.38 | 1.34 |
| 42 | S60 | 1116 | A | C6-N1 | 6.03 | 1.39 | 1.35 |
| 42 | S60 | 938 | G | P-O5' | 6.02 | 1.65 | 1.59 |
| 42 | S60 | 1049 | G | C6-N1 | -6.02 | 1.35 | 1.39 |
| 42 | S60 | 1161 | U | C2-N3 | -6.02 | 1.33 | 1.37 |
| 42 | S60 | 1120 | A | C6-N1 | 6.00 | 1.39 | 1.35 |
| 42 | S60 | 1129 | U | C2-N3 | -5.99 | 1.33 | 1.37 |
| 42 | S60 | 1048 | G | N9-C4 | -5.99 | 1.33 | 1.38 |
| 42 | S60 | 1086 | G | C6-N1 | 5.99 | 1.43 | 1.39 |
| 42 | S60 | 1092 | C | N3-C4 | 5.99 | 1.38 | 1.33 |
| 42 | S60 | 1103 | G | N3-C4 | 5.98 | 1.39 | 1.35 |
| 42 | S60 | 861 | C | P-O5' | 5.97 | 1.65 | 1.59 |
| 42 | S60 | 995 | A | C5-C4 | -5.97 | 1.34 | 1.38 |
| 42 | S60 | 1152 | G | C8-N7 | 5.96 | 1.34 | 1.30 |
| 42 | S60 | 1086 | G | N3-C4 | 5.94 | 1.39 | 1.35 |
| 42 | S60 | 1092 | C | P-O5' | 5.93 | 1.65 | 1.59 |
| 42 | S60 | 988 | A | N7-C5 | -5.92 | 1.35 | 1.39 |
| 42 | S60 | 1046 | A | N7-C5 | 5.92 | 1.42 | 1.39 |
| 42 | S60 | 1156 | U | P-O5' | 5.92 | 1.65 | 1.59 |
| 42 | S60 | 1165 | C | N3-C4 | 5.92 | 1.38 | 1.33 |
| 42 | S60 | 932 | A | N7-C5 | 5.91 | 1.42 | 1.39 |
| 42 | S60 | 863 | U | C2-N3 | 5.91 | 1.41 | 1.37 |
| 42 | S60 | 1171 | A | C6-N1 | 5.91 | 1.39 | 1.35 |
| 42 | S60 | 1174 | G | C8-N7 | 5.90 | 1.34 | 1.30 |
| 42 | S60 | 1086 | G | N7-C5 | 5.89 | 1.42 | 1.39 |
| 42 | S60 | 1154 | A | P-O5' | 5.89 | 1.65 | 1.59 |
| 42 | S60 | 1066 | G | C5-C4 | -5.89 | 1.34 | 1.38 |
| 42 | S60 | 885 | G | N7-C5 | -5.87 | 1.35 | 1.39 |
| 42 | S60 | 935 | G | C8-N7 | 5.87 | 1.34 | 1.30 |
| 42 | S60 | 938 | G | N7-C5 | 5.86 | 1.42 | 1.39 |
| 42 | S60 | 1051 | C | C4-N4 | -5.86 | 1.28 | 1.33 |
| 42 | S60 | 1067 | A | C6-N1 | 5.84 | 1.39 | 1.35 |
| 42 | S60 | 892 | A | C6-N1 | 5.83 | 1.39 | 1.35 |
| 42 | S60 | 1084 | G | C2-N3 | 5.80 | 1.37 | 1.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 42 | S60 | 1180 | U | C2-N3 | -5.80 | 1.33 | 1.37 |
| 42 | S60 | 899 | A | N9-C4 | 5.80 | 1.41 | 1.37 |
| 42 | S60 | 848 | G | C6-N1 | -5.80 | 1.35 | 1.39 |
| 42 | S60 | 1117 | A | N7-C5 | 5.79 | 1.42 | 1.39 |
| 42 | S60 | 1088 | U | P-O5' | 5.79 | 1.65 | 1.59 |
| 42 | S60 | 889 | A | P-O5' | 5.79 | 1.65 | 1.59 |
| 42 | S60 | 913 | G | N3-C4 | 5.79 | 1.39 | 1.35 |
| 42 | S60 | 1134 | G | N7-C5 | 5.78 | 1.42 | 1.39 |
| 42 | S60 | 973 | G | P-O5' | 5.77 | 1.65 | 1.59 |
| 42 | S60 | 932 | A | N9-C4 | 5.77 | 1.41 | 1.37 |
| 42 | S60 | 1122 | A | N9-C4 | 5.76 | 1.41 | 1.37 |
| 42 | S60 | 1207 | A | N9-C4 | 5.76 | 1.41 | 1.37 |
| 42 | S60 | 989 | G | N9-C8 | -5.76 | 1.33 | 1.37 |
| 42 | S60 | 1050 | G | C5-C4 | -5.75 | 1.34 | 1.38 |
| 42 | S60 | 836 | A | N7-C5 | -5.74 | 1.35 | 1.39 |
| 42 | S60 | 1117 | A | N3-C4 | 5.74 | 1.38 | 1.34 |
| 42 | S60 | 1027 | G | N1-C2 | -5.74 | 1.33 | 1.37 |
| 42 | S60 | 1040 | G | C5-C4 | -5.74 | 1.34 | 1.38 |
| 42 | S60 | 1030 | A | N3-C4 | -5.73 | 1.31 | 1.34 |
| 42 | S60 | 991 | A | C5-C4 | -5.73 | 1.34 | 1.38 |
| 42 | S60 | 860 | G | C2-N3 | 5.72 | 1.37 | 1.32 |
| 42 | S60 | 844 | A | N9-C4 | -5.71 | 1.34 | 1.37 |
| 42 | S60 | 969 | C | C4-N4 | -5.71 | 1.28 | 1.33 |
| 42 | S60 | 1117 | A | N9-C4 | 5.71 | 1.41 | 1.37 |
| 42 | S60 | 1209 | C | N1-C6 | 5.70 | 1.40 | 1.37 |
| 42 | S60 | 1092 | C | N1-C6 | 5.70 | 1.40 | 1.37 |
| 42 | S60 | 1141 | A | N7-C5 | 5.70 | 1.42 | 1.39 |
| 42 | S60 | 920 | G | C8-N7 | 5.69 | 1.34 | 1.30 |
| 42 | S60 | 952 | A | C5-C6 | -5.69 | 1.35 | 1.41 |
| 42 | S60 | 1203 | A | P-O5' | 5.69 | 1.65 | 1.59 |
| 42 | S60 | 1087 | C | N3-C4 | 5.68 | 1.38 | 1.33 |
| 42 | S60 | 1141 | A | N3-C4 | 5.66 | 1.38 | 1.34 |
| 42 | S60 | 1031 | A | C5-C4 | -5.66 | 1.34 | 1.38 |
| 42 | S60 | 852 | A | N3-C4 | 5.65 | 1.38 | 1.34 |
| 42 | S60 | 1051 | C | C2-N3 | -5.65 | 1.31 | 1.35 |
| 42 | S60 | 1052 | A | N7-C5 | -5.64 | 1.35 | 1.39 |
| 42 | S60 | 1206 | A | N3-C4 | -5.64 | 1.31 | 1.34 |
| 42 | S60 | 864 | A | N3-C4 | -5.64 | 1.31 | 1.34 |
| 42 | S60 | 954 | G | P-O5' | 5.61 | 1.65 | 1.59 |
| 42 | S60 | 1129 | U | P-O5' | 5.60 | 1.65 | 1.59 |
| 42 | S60 | 1073 | U | P-O5' | 5.60 | 1.65 | 1.59 |
| 42 | S60 | 1186 | G | C2'-C1' | -5.58 | 1.47 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 42 | S60 | 1051 | C | C5-C6 | -5.58 | 1.29 | 1.34 |
| 42 | S60 | 1185 | A | C8-N7 | -5.57 | 1.27 | 1.31 |
| 42 | S60 | 875 | A | C6-N6 | -5.56 | 1.29 | 1.33 |
| 42 | S60 | 907 | G | N7-C5 | 5.56 | 1.42 | 1.39 |
| 42 | S60 | 1047 | G | P-O5' | 5.55 | 1.65 | 1.59 |
| 42 | S60 | 1055 | A | N7-C5 | -5.55 | 1.35 | 1.39 |
| 42 | S60 | 1164 | G | C6-N1 | 5.54 | 1.43 | 1.39 |
| 42 | S60 | 1200 | A | P-O5' | 5.54 | 1.65 | 1.59 |
| 42 | S60 | 1195 | A | C8-N7 | 5.54 | 1.35 | 1.31 |
| 42 | S60 | 1016 | U | C2-N3 | -5.53 | 1.33 | 1.37 |
| 42 | S60 | 852 | A | P-O5' | 5.53 | 1.65 | 1.59 |
| 42 | S60 | 1160 | A | N9-C4 | 5.53 | 1.41 | 1.37 |
| 42 | S60 | 1002 | U | N1-C6 | -5.53 | 1.32 | 1.38 |
| 42 | S60 | 1230 | U | N1-C6 | -5.53 | 1.32 | 1.38 |
| 42 | S60 | 1059 | G | N7-C5 | 5.52 | 1.42 | 1.39 |
| 42 | S60 | 1165 | C | N1-C6 | 5.52 | 1.40 | 1.37 |
| 42 | S60 | 1174 | G | N9-C4 | 5.52 | 1.42 | 1.38 |
| 42 | S60 | 877 | G | C2-N3 | 5.52 | 1.37 | 1.32 |
| 42 | S60 | 1047 | G | C8-N7 | -5.51 | 1.27 | 1.30 |
| 42 | S60 | 1039 | G | N7-C5 | -5.51 | 1.35 | 1.39 |
| 42 | S60 | 1037 | C | C4-N4 | -5.50 | 1.28 | 1.33 |
| 42 | S60 | 1075 | A | P-O5' | 5.50 | 1.65 | 1.59 |
| 42 | S60 | 1029 | U | C2-N3 | -5.50 | 1.33 | 1.37 |
| 42 | S60 | 995 | A | N3-C4 | -5.49 | 1.31 | 1.34 |
| 42 | S60 | 1098 | C | P-O5' | 5.49 | 1.65 | 1.59 |
| 42 | S60 | 1049 | G | N3-C4 | -5.49 | 1.31 | 1.35 |
| 42 | S60 | 991 | A | N9-C8 | -5.48 | 1.33 | 1.37 |
| 42 | S60 | 1106 | G | P-O5' | 5.48 | 1.65 | 1.59 |
| 42 | S60 | 990 | U | N1-C6 | -5.47 | 1.33 | 1.38 |
| 42 | S60 | 1087 | C | N1-C6 | 5.47 | 1.40 | 1.37 |
| 42 | S60 | 1145 | G | C2'-C1' | -5.47 | 1.47 | 1.53 |
| 42 | S60 | 944 | G | C2-N3 | 5.47 | 1.37 | 1.32 |
| 42 | S60 | 886 | C | C5-C6 | -5.46 | 1.29 | 1.34 |
| 42 | S60 | 969 | C | C5-C6 | -5.44 | 1.29 | 1.34 |
| 42 | S60 | 833 | A | N9-C4 | -5.43 | 1.34 | 1.37 |
| 42 | S60 | 992 | G | C5-C4 | -5.42 | 1.34 | 1.38 |
| 42 | S60 | 1209 | C | N3-C4 | 5.42 | 1.37 | 1.33 |
| 42 | S60 | 953 | C | P-O5' | 5.42 | 1.65 | 1.59 |
| 42 | S60 | 1192 | G | C8-N7 | 5.42 | 1.34 | 1.30 |
| 42 | S60 | 1121 | A | N7-C5 | 5.42 | 1.42 | 1.39 |
| 42 | S60 | 1176 | G | C2-N3 | 5.42 | 1.37 | 1.32 |
| 42 | S60 | 968 | C | N3-C4 | -5.40 | 1.30 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 42 | S60 | 1137 | A | C5-C4 | 5.40 | 1.42 | 1.38 |
| 42 | S60 | 974 | G | C5-C4 | -5.39 | 1.34 | 1.38 |
| 42 | S60 | 857 | G | N3-C4 | 5.39 | 1.39 | 1.35 |
| 42 | S60 | 1028 | U | C4-O4 | -5.39 | 1.19 | 1.23 |
| 42 | S60 | 864 | A | N7-C5 | -5.38 | 1.36 | 1.39 |
| 42 | S60 | 1115 | G | C8-N7 | 5.38 | 1.34 | 1.30 |
| 42 | S60 | 1132 | A | C6-N1 | 5.38 | 1.39 | 1.35 |
| 42 | S60 | 1093 | G | P-O5' | 5.37 | 1.65 | 1.59 |
| 42 | S60 | 1220 | U | C2-N3 | -5.37 | 1.33 | 1.37 |
| 42 | S60 | 1117 | A | C6-N1 | 5.37 | 1.39 | 1.35 |
| 42 | S60 | 913 | G | P-O5' | 5.37 | 1.65 | 1.59 |
| 42 | S60 | 987 | A | C5-C6 | -5.37 | 1.36 | 1.41 |
| 42 | S60 | 1113 | C | N3-C4 | 5.37 | 1.37 | 1.33 |
| 42 | S60 | 1010 | G | N9-C4 | -5.36 | 1.33 | 1.38 |
| 42 | S60 | 1194 | U | N1-C2 | 5.36 | 1.43 | 1.38 |
| 42 | S60 | 975 | G | C8-N7 | -5.36 | 1.27 | 1.30 |
| 42 | S60 | 1097 | A | N7-C5 | 5.35 | 1.42 | 1.39 |
| 42 | S60 | 995 | A | N9-C8 | -5.35 | 1.33 | 1.37 |
| 42 | S60 | 1164 | G | P-O5' | 5.34 | 1.65 | 1.59 |
| 42 | S60 | 950 | U | P-O5' | 5.34 | 1.65 | 1.59 |
| 42 | S60 | 836 | A | N9-C8 | -5.33 | 1.33 | 1.37 |
| 42 | S60 | 1206 | A | N7-C5 | -5.33 | 1.36 | 1.39 |
| 42 | S60 | 969 | C | C2-N3 | -5.32 | 1.31 | 1.35 |
| 42 | S60 | 840 | C | N1-C6 | 5.32 | 1.40 | 1.37 |
| 42 | S60 | 1036 | A | N1-C2 | -5.31 | 1.29 | 1.34 |
| 42 | S60 | 1047 | G | N3-C4 | 5.31 | 1.39 | 1.35 |
| 42 | S60 | 1000 | C | C4-C5 | -5.31 | 1.38 | 1.43 |
| 42 | S60 | 1054 | G | N9-C8 | 5.30 | 1.41 | 1.37 |
| 42 | S60 | 1209 | C | P-O5' | 5.30 | 1.65 | 1.59 |
| 42 | S60 | 1161 | U | C4-O4 | -5.29 | 1.19 | 1.23 |
| 42 | S60 | 1165 | C | P-O5' | 5.29 | 1.65 | 1.59 |
| 42 | S60 | 1074 | U | C2-N3 | 5.29 | 1.41 | 1.37 |
| 42 | S60 | 1176 | G | N9-C4 | 5.28 | 1.42 | 1.38 |
| 42 | S60 | 979 | A | C6-N1 | -5.28 | 1.31 | 1.35 |
| 42 | S60 | 1066 | G | C2-N3 | 5.28 | 1.36 | 1.32 |
| 42 | S60 | 1179 | A | N7-C5 | -5.28 | 1.36 | 1.39 |
| 42 | S60 | 1131 | A | N3-C4 | 5.27 | 1.38 | 1.34 |
| 42 | S60 | 1059 | G | N3-C4 | 5.27 | 1.39 | 1.35 |
| 42 | S60 | 857 | G | C6-N1 | 5.27 | 1.43 | 1.39 |
| 42 | S60 | 837 | C | N1-C6 | -5.26 | 1.33 | 1.37 |
| 42 | S60 | 1127 | A | C5-C4 | -5.26 | 1.35 | 1.38 |
| 42 | S60 | 1182 | G | C5-C4 | -5.25 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 42 | S60 | 1120 | A | N7-C5 | 5.25 | 1.42 | 1.39 |
| 42 | S60 | 1140 | G | C6-N1 | 5.25 | 1.43 | 1.39 |
| 42 | S60 | 1118 | A | C5-C4 | 5.25 | 1.42 | 1.38 |
| 42 | S60 | 952 | A | C2-N3 | -5.25 | 1.28 | 1.33 |
| 42 | S60 | 1018 | U | C4-O4 | -5.25 | 1.19 | 1.23 |
| 42 | S60 | 1172 | A | P-O5' | 5.24 | 1.65 | 1.59 |
| 42 | S60 | 886 | C | C2-N3 | -5.24 | 1.31 | 1.35 |
| 42 | S60 | 935 | G | C2-N3 | 5.23 | 1.36 | 1.32 |
| 42 | S60 | 855 | G | C2-N3 | 5.23 | 1.36 | 1.32 |
| 42 | S60 | 847 | A | N9-C8 | -5.22 | 1.33 | 1.37 |
| 42 | S60 | 1085 | G | N7-C5 | 5.21 | 1.42 | 1.39 |
| 42 | S60 | 970 | U | C4-O4 | -5.21 | 1.19 | 1.23 |
| 46 | SBB | 58 | CYS | CB-SG | -5.21 | 1.73 | 1.81 |
| 42 | S60 | 884 | A | N7-C5 | 5.20 | 1.42 | 1.39 |
| 42 | S60 | 1141 | A | C6-N1 | 5.20 | 1.39 | 1.35 |
| 42 | S60 | 1085 | G | C2-N3 | 5.18 | 1.36 | 1.32 |
| 42 | S60 | 1226 | U | C2-N3 | -5.18 | 1.34 | 1.37 |
| 42 | S60 | 1081 | U | P-O5' | 5.18 | 1.65 | 1.59 |
| 42 | S60 | 955 | A | N9-C4 | -5.18 | 1.34 | 1.37 |
| 42 | S60 | 1142 | G | C2-N3 | 5.17 | 1.36 | 1.32 |
| 42 | S60 | 1164 | G | N3-C4 | 5.17 | 1.39 | 1.35 |
| 42 | S60 | 853 | G | C8-N7 | 5.16 | 1.34 | 1.30 |
| 42 | S60 | 1207 | A | C5-C4 | -5.16 | 1.35 | 1.38 |
| 42 | S60 | 1185 | A | C5-C4 | -5.16 | 1.35 | 1.38 |
| 42 | S60 | 963 | G | N1-C2 | -5.16 | 1.33 | 1.37 |
| 42 | S60 | 839 | C | P-O5' | 5.16 | 1.65 | 1.59 |
| 42 | S60 | 1175 | A | C5-C4 | 5.16 | 1.42 | 1.38 |
| 42 | S60 | 1116 | A | N7-C5 | 5.15 | 1.42 | 1.39 |
| 42 | S60 | 931 | G | N7-C5 | 5.15 | 1.42 | 1.39 |
| 42 | S60 | 963 | G | N9-C8 | -5.15 | 1.34 | 1.37 |
| 42 | S60 | 1227 | U | C2-N3 | -5.14 | 1.34 | 1.37 |
| 42 | S60 | 932 | A | N3-C4 | 5.14 | 1.38 | 1.34 |
| 42 | S60 | 1176 | G | N3-C4 | 5.14 | 1.39 | 1.35 |
| 42 | S60 | 1130 | A | N9-C4 | 5.13 | 1.41 | 1.37 |
| 42 | S60 | 836 | A | C6-N1 | -5.13 | 1.31 | 1.35 |
| 42 | S60 | 849 | U | C4-O4 | -5.13 | 1.19 | 1.23 |
| 42 | S60 | 862 | U | P-O5' | 5.12 | 1.64 | 1.59 |
| 42 | S60 | 892 | A | N7-C5 | 5.12 | 1.42 | 1.39 |
| 42 | S60 | 979 | A | N9-C8 | -5.12 | 1.33 | 1.37 |
| 42 | S60 | 1126 | A | N9-C4 | 5.12 | 1.41 | 1.37 |
| 42 | S60 | 1223 | C | P-O5' | 5.12 | 1.64 | 1.59 |
| 42 | S60 | 955 | A | N7-C5 | -5.11 | 1.36 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 42 | S60 | 1018 | U | P-O5' | 5.11 | 1.64 | 1.59 |
| 42 | S60 | 1011 | A | N3-C4 | -5.11 | 1.31 | 1.34 |
| 42 | S60 | 1095 | G | N7-C5 | -5.11 | 1.36 | 1.39 |
| 42 | S60 | 938 | G | N3-C4 | 5.10 | 1.39 | 1.35 |
| 42 | S60 | 853 | G | C5-C4 | 5.10 | 1.42 | 1.38 |
| 42 | S60 | 1137 | A | P-O5' | 5.10 | 1.64 | 1.59 |
| 42 | S60 | 1162 | G | C2-N3 | 5.10 | 1.36 | 1.32 |
| 42 | S60 | 1152 | G | C5-C4 | 5.09 | 1.42 | 1.38 |
| 42 | S60 | 1157 | G | C5-C4 | 5.08 | 1.42 | 1.38 |
| 42 | S60 | 1002 | U | N3-C4 | -5.08 | 1.33 | 1.38 |
| 42 | S60 | 1127 | A | C6-N6 | -5.07 | 1.29 | 1.33 |
| 42 | S60 | 855 | G | N9-C4 | 5.07 | 1.42 | 1.38 |
| 42 | S60 | 1057 | C | N1-C6 | -5.07 | 1.34 | 1.37 |
| 42 | S60 | 1120 | A | N9-C8 | 5.06 | 1.41 | 1.37 |
| 42 | S60 | 1122 | A | C8-N7 | 5.06 | 1.35 | 1.31 |
| 42 | S60 | 1178 | A | N7-C5 | -5.06 | 1.36 | 1.39 |
| 42 | S60 | 990 | U | N3-C4 | -5.06 | 1.33 | 1.38 |
| 42 | S60 | 840 | C | N3-C4 | 5.05 | 1.37 | 1.33 |
| 42 | S60 | 1106 | G | N3-C4 | 5.05 | 1.39 | 1.35 |
| 42 | S60 | 1206 | A | C6-N1 | -5.05 | 1.32 | 1.35 |
| 42 | S60 | 951 | A | P-O5' | 5.05 | 1.64 | 1.59 |
| 42 | S60 | 1186 | G | P-O5' | 5.05 | 1.64 | 1.59 |
| 42 | S60 | 1059 | G | C6-N1 | 5.05 | 1.43 | 1.39 |
| 42 | S60 | 1132 | A | N3-C4 | 5.04 | 1.37 | 1.34 |
| 42 | S60 | 1186 | G | N7-C5 | -5.04 | 1.36 | 1.39 |
| 42 | S60 | 953 | C | C4-N4 | -5.04 | 1.29 | 1.33 |
| 42 | S60 | 937 | G | N9-C4 | 5.03 | 1.42 | 1.38 |
| 42 | S60 | 1096 | C | N1-C6 | -5.03 | 1.34 | 1.37 |
| 42 | S60 | 931 | G | C2-N3 | 5.03 | 1.36 | 1.32 |
| 42 | S60 | 1047 | G | C6-N1 | 5.03 | 1.43 | 1.39 |
| 42 | S60 | 1129 | U | O3'-P | -5.03 | 1.55 | 1.61 |
| 42 | S60 | 1103 | G | N9-C8 | 5.03 | 1.41 | 1.37 |
| 42 | S60 | 949 | U | P-O5' | 5.02 | 1.64 | 1.59 |
| 42 | S60 | 1160 | A | N7-C5 | 5.01 | 1.42 | 1.39 |
| 42 | S60 | 1055 | A | N3-C4 | -5.00 | 1.31 | 1.34 |
| 42 | S60 | 982 | C | C4-C5 | -5.00 | 1.39 | 1.43 |

All (573) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 42 | S60 | 1356 | C | O5'-P-OP1 | -18.09 | 89.00 | 110.70 |
| 42 | S60 | 910 | A | P-O3'-C3' | -11.68 | 105.69 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 42 | S60 | 850 | G | C5-N7-C8 | -11.31 | 98.65 | 104.30 |
| 42 | S60 | 1034 | A | P-O3'-C3' | -11.29 | 106.16 | 119.70 |
| 42 | S60 | 904 | C | P-O3'-C3' | -10.87 | 106.66 | 119.70 |
| 1 | L50 | 330 | G | C2'-C3'-O3' | 10.38 | 132.33 | 109.50 |
| 42 | S60 | 917 | U | P-O3'-C3' | -10.32 | 107.31 | 119.70 |
| 42 | S60 | 1108 | C | P-O3'-C3' | -10.24 | 107.42 | 119.70 |
| 42 | S60 | 996 | G | P-O3'-C3' | -10.14 | 107.53 | 119.70 |
| 42 | S60 | 1261 | G | P-O3'-C3' | -9.97 | 107.73 | 119.70 |
| 42 | S60 | 1033 | A | P-O3'-C3' | -9.95 | 107.76 | 119.70 |
| 42 | S60 | 958 | A | P-O3'-C3' | -9.82 | 107.91 | 119.70 |
| 1 | L50 | 1265 | G | OP1-P-OP2 | -9.81 | 104.88 | 119.60 |
| 42 | S60 | 965 | U | P-O3'-C3' | -9.81 | 107.93 | 119.70 |
| 42 | S60 | 964 | G | P-O3'-C3' | -9.54 | 108.25 | 119.70 |
| 1 | L50 | 535 | A | P-O3'-C3' | 9.48 | 131.08 | 119.70 |
| 42 | S60 | 956 | C | P-O3'-C3' | -9.37 | 108.46 | 119.70 |
| 42 | S60 | 877 | G | N9-C4-C5 | 9.31 | 109.12 | 105.40 |
| 42 | S60 | 845 | G | P-O3'-C3' | -9.28 | 108.57 | 119.70 |
| 42 | S60 | 995 | A | P-O3'-C3' | -9.07 | 108.81 | 119.70 |
| 1 | L50 | 1395 | U | C2'-C3'-O3' | 9.06 | 129.43 | 109.50 |
| 42 | S60 | 1170 | G | C1'-O4'-C4' | -9.04 | 102.67 | 109.90 |
| 42 | S60 | 1260 | G | P-O3'-C3' | -9.02 | 108.87 | 119.70 |
| 42 | S60 | 998 | U | P-O3'-C3' | -8.98 | 108.93 | 119.70 |
| 42 | S60 | 850 | G | C4-C5-N7 | 8.96 | 114.38 | 110.80 |
| 42 | S60 | 923 | A | P-O3'-C3' | -8.91 | 109.01 | 119.70 |
| 1 | L50 | 1282 | C | N1-C2-O2 | 8.89 | 124.23 | 118.90 |
| 42 | S60 | 877 | G | C4-C5-N7 | -8.86 | 107.25 | 110.80 |
| 1 | L50 | 1959 | A | C2'-C3'-O3' | 8.84 | 128.94 | 109.50 |
| 42 | S60 | 824 | A | P-O3'-C3' | -8.81 | 109.12 | 119.70 |
| 1 | L50 | 1585 | U | P-O3'-C3' | -8.79 | 109.15 | 119.70 |
| 1 | L50 | 1148 | A | C4'-C3'-O3' | 8.77 | 130.55 | 113.00 |
| 42 | S60 | 961 | G | P-O3'-C3' | -8.71 | 109.25 | 119.70 |
| 42 | S60 | 1135 | U | C3'-C2'-C1' | -8.64 | 94.58 | 101.50 |
| 42 | S60 | 1125 | G | C3'-C2'-C1' | -8.48 | 94.72 | 101.50 |
| 42 | S60 | 394 | G | O5'-P-OP1 | -8.45 | 98.09 | 105.70 |
| 69 | ST0 | 117 | VAL | CA-CB-CG1 | 8.36 | 123.44 | 110.90 |
| 42 | S60 | 831 | G | P-O3'-C3' | -8.27 | 109.78 | 119.70 |
| 42 | S60 | 997 | A | P-O3'-C3' | -8.25 | 109.80 | 119.70 |
| 1 | L50 | 1709 | G | C1'-O4'-C4' | -8.20 | 103.34 | 109.90 |
| 42 | S60 | 1107 | U | P-O3'-C3' | -8.19 | 109.88 | 119.70 |
| 1 | L50 | 424 | G | O4'-C1'-N9 | 8.17 | 114.74 | 108.20 |
| 1 | L50 | 141 | G | O4'-C1'-N9 | 8.17 | 114.74 | 108.20 |
| 42 | S60 | 850 | G | N7-C8-N9 | 8.12 | 117.16 | 113.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 42 | S60 | 919 | C | N3-C4-C5 | -8.12 | 118.65 | 121.90 |
| 42 | S60 | 1150 | G | P-O3'-C3' | -8.10 | 109.98 | 119.70 |
| 1 | L50 | 2431 | C | O5'-P-OP1 | -8.06 | 98.44 | 105.70 |
| 42 | S60 | 848 | G | OP2-P-O3' | 8.06 | 122.94 | 105.20 |
| 1 | L50 | 1000 | G | C1'-O4'-C4' | -8.05 | 103.46 | 109.90 |
| 42 | S60 | 1168 | A | P-O3'-C3' | -8.05 | 110.04 | 119.70 |
| 42 | S60 | 1046 | A | C8-N9-C4 | 8.04 | 109.02 | 105.80 |
| 42 | S60 | 1167 | C | P-O3'-C3' | -8.04 | 110.06 | 119.70 |
| 1 | L50 | 2597 | G | C2'-C3'-O3' | 8.02 | 127.13 | 109.50 |
| 42 | S60 | 1174 | G | C3'-C2'-C1' | 8.01 | 107.91 | 101.50 |
| 42 | S60 | 1231 | U | P-O3'-C3' | -7.94 | 110.18 | 119.70 |
| 42 | S60 | 933 | G | O3'-P-O5' | 7.93 | 119.06 | 104.00 |
| 1 | L50 | 600 | G | O4'-C1'-N9 | 7.90 | 114.52 | 108.20 |
| 21 | LJJ | 21 | ARG | NE-CZ-NH2 | 7.90 | 124.25 | 120.30 |
| 42 | S60 | 262 | U | C2'-C3'-O3' | 7.89 | 126.85 | 109.50 |
| 42 | S60 | 989 | G | N9-C4-C5 | 7.88 | 108.55 | 105.40 |
| 1 | L50 | 1277 | G | C2'-C3'-O3' | 7.88 | 126.84 | 109.50 |
| 42 | S60 | 473 | G | C2'-C3'-O3' | 7.82 | 126.70 | 109.50 |
| 42 | S60 | 1066 | G | N3-C4-C5 | -7.76 | 124.72 | 128.60 |
| 1 | L50 | 1192 | A | C2'-C3'-O3' | 7.74 | 126.52 | 109.50 |
| 42 | S60 | 1023 | A | P-O3'-C3' | -7.71 | 110.45 | 119.70 |
| 42 | S60 | 127 | A | C2'-C3'-O3' | 7.70 | 126.45 | 109.50 |
| 42 | S60 | 383 | A | C2'-C3'-O3' | 7.66 | 126.34 | 109.50 |
| 42 | S60 | 1111 | A | N7-C8-N9 | -7.63 | 109.99 | 113.80 |
| 1 | L50 | 796 | C | O4'-C1'-N1 | 7.59 | 114.28 | 108.20 |
| 42 | S60 | 264 | C | O5'-P-OP1 | 7.59 | 119.81 | 110.70 |
| 42 | S60 | 1049 | G | C8-N9-C4 | -7.59 | 103.36 | 106.40 |
| 42 | S60 | 1001 | C | N3-C4-C5 | -7.58 | 118.87 | 121.90 |
| 42 | S60 | 180 | G | C4'-C3'-O3' | 7.58 | 128.15 | 113.00 |
| 42 | S60 | 1043 | G | P-O3'-C3' | -7.57 | 110.61 | 119.70 |
| 1 | L50 | 385 | C | O5'-P-OP1 | -7.57 | 98.89 | 105.70 |
| 42 | S60 | 1095 | G | N9-C4-C5 | 7.57 | 108.43 | 105.40 |
| 42 | S60 | 1041 | A | P-O3'-C3' | -7.56 | 110.63 | 119.70 |
| 42 | S60 | 819 | A | P-O3'-C3' | 7.55 | 128.76 | 119.70 |
| 1 | L50 | 1838 | G | O4'-C1'-C2' | -7.54 | 98.26 | 105.80 |
| 42 | S60 | 1216 | U | P-O3'-C3' | -7.52 | 110.67 | 119.70 |
| 56 | SGG | 166 | VAL | CA-CB-CG1 | 7.48 | 122.13 | 110.90 |
| 1 | L50 | 1966 | A | C2'-C3'-O3' | 7.48 | 125.95 | 109.50 |
| 42 | S60 | 1003 | A | C5-N7-C8 | 7.46 | 107.63 | 103.90 |
| 74 | SY0 | 37 | ASN | CB-CA-C | 7.46 | 125.31 | 110.40 |
| 1 | L50 | 463 | A | OP1-P-OP2 | -7.45 | 108.43 | 119.60 |
| 42 | S60 | 1186 | G | C3'-C2'-C1' | -7.40 | 95.58 | 101.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 42 | S60 | 1046 | A | C2-N3-C4 | 7.39 | 114.30 | 110.60 |
| 1 | L50 | 159 | A | OP1-P-OP2 | -7.38 | 108.53 | 119.60 |
| 42 | S60 | 994 | G | C4'-C3'-C2' | -7.37 | 95.23 | 102.60 |
| 42 | S60 | 1192 | G | C8-N9-C4 | -7.36 | 103.46 | 106.40 |
| 50 | SDD | 39 | VAL | CA-CB-CG1 | 7.36 | 121.94 | 110.90 |
| 42 | S60 | 598 | C | C2'-C3'-O3' | 7.34 | 125.66 | 109.50 |
| 42 | S60 | 944 | G | P-O3'-C3' | -7.34 | 110.89 | 119.70 |
| 42 | S60 | 960 | U | P-O3'-C3' | -7.33 | 110.90 | 119.70 |
| 1 | L50 | 1967 | A | C2'-C3'-O3' | 7.32 | 125.60 | 109.50 |
| 42 | S60 | 847 | A | N9-C4-C5 | 7.30 | 108.72 | 105.80 |
| 42 | S60 | 1066 | G | C4-C5-N7 | -7.30 | 107.88 | 110.80 |
| 42 | S60 | 848 | G | C4-C5-N7 | -7.26 | 107.89 | 110.80 |
| 42 | S60 | 966 | G | P-O3'-C3' | -7.24 | 111.01 | 119.70 |
| 1 | L50 | 644 | G | O5'-P-OP1 | 7.23 | 119.37 | 110.70 |
| 42 | S60 | 1089 | G | N9-C4-C5 | 7.18 | 108.27 | 105.40 |
| 1 | L50 | 1394 | U | C2'-C3'-O3' | 7.18 | 125.30 | 109.50 |
| 42 | S60 | 1055 | A | N9-C4-C5 | 7.18 | 108.67 | 105.80 |
| 1 | L50 | 586 | G | O4'-C1'-N9 | 7.17 | 113.94 | 108.20 |
| 42 | S60 | 1230 | U | P-O3'-C3' | -7.17 | 111.10 | 119.70 |
| 42 | S60 | 1195 | A | N9-C4-C5 | 7.14 | 108.66 | 105.80 |
| 42 | S60 | 933 | G | C4'-C3'-O3' | 7.12 | 127.23 | 113.00 |
| 42 | S60 | 1095 | G | C8-N9-C4 | -7.08 | 103.57 | 106.40 |
| 1 | L50 | 353 | A | O5'-P-OP1 | -7.08 | 99.33 | 105.70 |
| 1 | L50 | 21 | U | C2'-C3'-O3' | 7.05 | 125.01 | 109.50 |
| 42 | S60 | 830 | G | P-O3'-C3' | -7.03 | 111.27 | 119.70 |
| 52 | SEE | 49 | VAL | CA-CB-CG1 | 7.03 | 121.44 | 110.90 |
| 1 | L50 | 1182 | A | P-O3'-C3' | 6.97 | 128.07 | 119.70 |
| 42 | S60 | 864 | A | N9-C4-C5 | 6.97 | 108.59 | 105.80 |
| 42 | S60 | 1206 | A | N9-C4-C5 | 6.93 | 108.57 | 105.80 |
| 42 | S60 | 1048 | G | C4'-C3'-C2' | -6.91 | 95.69 | 102.60 |
| 42 | S60 | 1003 | A | C2-N3-C4 | 6.91 | 114.05 | 110.60 |
| 42 | S60 | 883 | C | C6-N1-C2 | 6.90 | 123.06 | 120.30 |
| 42 | S60 | 1051 | C | C6-N1-C2 | 6.89 | 123.06 | 120.30 |
| 42 | S60 | 894 | A | P-O3'-C3' | -6.88 | 111.44 | 119.70 |
| 42 | S60 | 859 | G | C8-N9-C4 | -6.88 | 103.65 | 106.40 |
| 42 | S60 | 1094 | C | N3-C4-C5 | -6.88 | 119.15 | 121.90 |
| 42 | S60 | 1062 | C | N3-C4-C5 | -6.85 | 119.16 | 121.90 |
| 42 | S60 | 1111 | A | C5-N7-C8 | 6.85 | 107.32 | 103.90 |
| 42 | S60 | 1046 | A | N7-C8-N9 | -6.84 | 110.38 | 113.80 |
| 42 | S60 | 1049 | G | N9-C4-C5 | 6.84 | 108.14 | 105.40 |
| 42 | S60 | 1134 | G | P-O3'-C3' | -6.83 | 111.50 | 119.70 |
| 42 | S60 | 1070 | C | N3-C4-C5 | -6.82 | 119.17 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | L50 | 562 | U | P-O5'-C5' | -6.81 | 110.00 | 120.90 |
| 42 | S60 | 918 | A | P-O3'-C3' | -6.81 | 111.53 | 119.70 |
| 42 | S60 | 1192 | G | N9-C4-C5 | 6.78 | 108.11 | 105.40 |
| 1 | L50 | 147 | G | P-O3'-C3' | -6.75 | 111.59 | 119.70 |
| 42 | S60 | 1182 | G | N9-C4-C5 | -6.75 | 102.70 | 105.40 |
| 67 | SR0 | 47 | ARG | NE-CZ-NH2 | 6.74 | 123.67 | 120.30 |
| 42 | S60 | 565 | U | C2'-C3'-O3' | 6.74 | 124.48 | 113.70 |
| 42 | S60 | 1011 | A | C8-N9-C4 | -6.74 | 103.10 | 105.80 |
| 42 | S60 | 1207 | A | C5-N7-C8 | 6.74 | 107.27 | 103.90 |
| 42 | S60 | 919 | C | C6-N1-C2 | -6.73 | 117.61 | 120.30 |
| 42 | S60 | 13 | C | OP1-P-OP2 | -6.73 | 109.51 | 119.60 |
| 42 | S60 | 963 | G | P-O3'-C3' | -6.73 | 111.63 | 119.70 |
| 1 | L50 | 1808 | A | C4'-C3'-O3' | 6.71 | 126.42 | 113.00 |
| 42 | S60 | 1014 | G | C8-N9-C4 | -6.71 | 103.72 | 106.40 |
| 42 | S60 | 1014 | G | N9-C4-C5 | 6.69 | 108.08 | 105.40 |
| 42 | S60 | 1207 | A | N7-C8-N9 | -6.68 | 110.46 | 113.80 |
| 1 | L50 | 1488 | U | O4'-C1'-N1 | 6.67 | 113.54 | 108.20 |
| 1 | L50 | 1317 | G | P-O3'-C3' | -6.67 | 111.70 | 119.70 |
| 1 | L50 | 600 | G | O4'-C1'-C2' | -6.66 | 99.14 | 105.80 |
| 1 | L50 | 1771 | G | P-O3'-C3' | 6.64 | 127.67 | 119.70 |
| 42 | S60 | 1185 | A | C8-N9-C4 | 6.64 | 108.46 | 105.80 |
| 1 | L50 | 1134 | A | C2'-C3'-O3' | 6.64 | 124.32 | 113.70 |
| 42 | S60 | 848 | G | N3-C4-C5 | -6.64 | 125.28 | 128.60 |
| 42 | S60 | 1053 | A | C8-N9-C4 | 6.60 | 108.44 | 105.80 |
| 1 | L50 | 667 | G | P-O3'-C3' | 6.59 | 127.61 | 119.70 |
| 42 | S60 | 954 | G | C8-N9-C4 | -6.58 | 103.77 | 106.40 |
| 42 | S60 | 875 | A | C2-N3-C4 | 6.57 | 113.88 | 110.60 |
| 42 | S60 | 1003 | A | N7-C8-N9 | -6.57 | 110.52 | 113.80 |
| 42 | S60 | 854 | U | P-O3'-C3' | -6.56 | 111.83 | 119.70 |
| 42 | S60 | 1356 | C | OP1-P-OP2 | 6.56 | 129.44 | 119.60 |
| 42 | S60 | 1179 | A | N9-C4-C5 | 6.55 | 108.42 | 105.80 |
| 1 | L50 | 1783 | A | P-O3'-C3' | -6.55 | 111.84 | 119.70 |
| 42 | S60 | 877 | G | N3-C4-C5 | -6.54 | 125.33 | 128.60 |
| 42 | S60 | 1212 | U | O4'-C1'-N1 | 6.54 | 113.43 | 108.20 |
| 42 | S60 | 213 | A | P-O3'-C3' | -6.53 | 111.86 | 119.70 |
| 42 | S60 | 874 | A | N9-C4-C5 | 6.53 | 108.41 | 105.80 |
| 42 | S60 | 1001 | C | C6-N1-C2 | -6.53 | 117.69 | 120.30 |
| 42 | S60 | 671 | C | O5'-P-OP1 | 6.52 | 118.52 | 110.70 |
| 42 | S60 | 857 | G | C4-C5-N7 | 6.51 | 113.41 | 110.80 |
| 41 | MD1 | 103 | ARG | NE-CZ-NH2 | 6.50 | 123.55 | 120.30 |
| 42 | S60 | 1153 | C | P-O3'-C3' | -6.50 | 111.90 | 119.70 |
| 42 | S60 | 1038 | A | C4'-C3'-C2' | -6.49 | 96.11 | 102.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | L50 | 2355 | A | OP1-P-OP2 | -6.48 | 109.88 | 119.60 |
| 42 | S60 | 1205 | G | C8-N9-C4 | -6.46 | 103.82 | 106.40 |
| 42 | S60 | 982 | C | N3-C4-C5 | -6.45 | 119.32 | 121.90 |
| 47 | SC0 | 221 | VAL | CA-CB-CG1 | 6.45 | 120.57 | 110.90 |
| 2 | L70 | 46 | C | P-O3'-C3' | -6.43 | 111.98 | 119.70 |
| 42 | S60 | 903 | C | P-O3'-C3' | -6.40 | 112.02 | 119.70 |
| 22 | LL0 | 67 | ARG | CG-CD-NE | 6.37 | 125.17 | 111.80 |
| 1 | L50 | 2114 | G | C4'-C3'-C2' | -6.37 | 96.23 | 102.60 |
| 1 | L50 | 548 | G | OP1-P-OP2 | -6.36 | 110.07 | 119.60 |
| 42 | S60 | 1066 | G | C5-N7-C8 | 6.36 | 107.48 | 104.30 |
| 1 | L50 | 400 | U | O5'-P-OP2 | -6.35 | 99.99 | 105.70 |
| 42 | S60 | 1052 | A | C5-N7-C8 | -6.31 | 100.75 | 103.90 |
| 42 | S60 | 1053 | A | N9-C4-C5 | -6.30 | 103.28 | 105.80 |
| 6 | LC0 | 57 | ARG | CG-CD-NE | -6.29 | 98.59 | 111.80 |
| 42 | S60 | 1177 | G | C4-C5-N7 | 6.27 | 113.31 | 110.80 |
| 1 | L50 | 371 | A | N7-C8-N9 | -6.26 | 110.67 | 113.80 |
| 5 | LB0 | 336 | ARG | CG-CD-NE | 6.25 | 124.92 | 111.80 |
| 26 | LN0 | 123 | GLN | CB-CA-C | -6.25 | 97.91 | 110.40 |
| 1 | L50 | 342 | G | P-O3'-C3' | -6.24 | 112.21 | 119.70 |
| 1 | L50 | 1102 | G | O4'-C1'-C2' | -6.24 | 99.56 | 105.80 |
| 1 | L50 | 1277 | G | C4'-C3'-O3' | 6.24 | 125.47 | 113.00 |
| 1 | L50 | 412 | A | OP1-P-OP2 | -6.22 | 110.27 | 119.60 |
| 42 | S60 | 1047 | G | N9-C4-C5 | -6.22 | 102.91 | 105.40 |
| 42 | S60 | 1127 | A | C8-N9-C4 | 6.22 | 108.29 | 105.80 |
| 42 | S60 | 1055 | A | C8-N9-C4 | -6.21 | 103.31 | 105.80 |
| 1 | L50 | 2481 | U | P-O3'-C3' | 6.19 | 127.13 | 119.70 |
| 42 | S60 | 201 | G | P-O3'-C3' | -6.18 | 112.28 | 119.70 |
| 42 | S60 | 1182 | G | C8-N9-C4 | 6.18 | 108.87 | 106.40 |
| 42 | S60 | 1195 | A | C8-N9-C4 | -6.17 | 103.33 | 105.80 |
| 42 | S60 | 1093 | G | C4-C5-N7 | 6.16 | 113.26 | 110.80 |
| 42 | S60 | 989 | G | C8-N9-C4 | -6.15 | 103.94 | 106.40 |
| 42 | S60 | 1089 | G | C8-N9-C4 | -6.15 | 103.94 | 106.40 |
| 42 | S60 | 1047 | G | C4-C5-N7 | 6.15 | 113.26 | 110.80 |
| 42 | S60 | 1048 | G | C5-N7-C8 | -6.15 | 101.22 | 104.30 |
| 42 | S60 | 973 | G | N9-C4-C5 | 6.15 | 107.86 | 105.40 |
| 1 | L50 | 462 | G | OP1-P-OP2 | -6.15 | 110.38 | 119.60 |
| 42 | S60 | 987 | A | C5-N7-C8 | -6.14 | 100.83 | 103.90 |
| 42 | S60 | 1103 | G | O4'-C1'-C2' | -6.14 | 99.66 | 105.80 |
| 1 | L50 | 125 | G | OP1-P-OP2 | -6.13 | 110.41 | 119.60 |
| 70 | SU0 | 67 | ARG | CG-CD-NE | 6.12 | 124.64 | 111.80 |
| 42 | S60 | 1050 | G | C4-C5-N7 | -6.11 | 108.36 | 110.80 |
| 42 | S60 | 885 | G | N9-C4-C5 | 6.10 | 107.84 | 105.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 42 | S60 | 877 | G | C8-N9-C4 | -6.09 | 103.97 | 106.40 |
| 47 | SC0 | 129 | ARG | CB-CA-C | -6.09 | 98.23 | 110.40 |
| 42 | S60 | 954 | G | N7-C8-N9 | 6.08 | 116.14 | 113.10 |
| 1 | L50 | 562 | U | C5'-C4'-C3' | -6.07 | 106.29 | 116.00 |
| 42 | S60 | 920 | G | N9-C4-C5 | 6.07 | 107.83 | 105.40 |
| 42 | S60 | 835 | A | C8-N9-C4 | -6.04 | 103.39 | 105.80 |
| 42 | S60 | 895 | C | P-O3'-C3' | -6.03 | 112.46 | 119.70 |
| 42 | S60 | 1119 | C | C2-N3-C4 | 6.03 | 122.92 | 119.90 |
| 42 | S60 | 858 | C | C2-N3-C4 | 6.03 | 122.92 | 119.90 |
| 42 | S60 | 262 | U | C4'-C3'-O3' | 6.03 | 125.05 | 113.00 |
| 1 | L50 | 1835 | G | C3'-C2'-C1' | 6.02 | 106.32 | 101.50 |
| 42 | S60 | 1046 | A | C5-C6-N1 | 6.02 | 120.71 | 117.70 |
| 1 | L50 | 477 | G | P-O3'-C3' | 6.02 | 126.92 | 119.70 |
| 1 | L50 | 140 | A | P-O3'-C3' | 6.01 | 126.92 | 119.70 |
| 42 | S60 | 953 | C | C6-N1-C2 | 6.01 | 122.70 | 120.30 |
| 1 | L50 | 1061 | G | O4'-C1'-N9 | 6.00 | 113.00 | 108.20 |
| 42 | S60 | 859 | G | N9-C4-C5 | 5.99 | 107.80 | 105.40 |
| 42 | S60 | 933 | G | C3'-C2'-C1' | -5.99 | 96.70 | 101.50 |
| 42 | S60 | 952 | A | C4-C5-N7 | 5.98 | 113.69 | 110.70 |
| 42 | S60 | 847 | A | C4-C5-C6 | 5.97 | 119.98 | 117.00 |
| 42 | S60 | 1019 | C | C3'-C2'-C1' | 5.96 | 106.27 | 101.50 |
| 42 | S60 | 885 | G | C4-C5-N7 | -5.96 | 108.42 | 110.80 |
| 21 | LJJ | 21 | ARG | NE-CZ-NH1 | -5.95 | 117.32 | 120.30 |
| 42 | S60 | 1056 | A | N9-C4-C5 | 5.95 | 108.18 | 105.80 |
| 42 | S60 | 1066 | G | C2-N3-C4 | 5.94 | 114.87 | 111.90 |
| 42 | S60 | 1067 | A | C8-N9-C4 | 5.94 | 108.17 | 105.80 |
| 42 | S60 | 180 | G | P-O3'-C3' | 5.94 | 126.82 | 119.70 |
| 42 | S60 | 924 | U | P-O3'-C3' | -5.94 | 112.58 | 119.70 |
| 42 | S60 | 884 | A | C3'-C2'-C1' | 5.93 | 106.24 | 101.50 |
| 2 | L70 | 31 | G | P-O3'-C3' | -5.92 | 112.59 | 119.70 |
| 42 | S60 | 853 | G | C8-N9-C4 | -5.91 | 104.03 | 106.40 |
| 42 | S60 | 1054 | G | C4-C5-N7 | 5.91 | 113.16 | 110.80 |
| 42 | S60 | 875 | A | N7-C8-N9 | -5.90 | 110.85 | 113.80 |
| 15 | LGG | 24 | ARG | CG-CD-NE | -5.89 | 99.42 | 111.80 |
| 42 | S60 | 1182 | G | C2-N3-C4 | 5.89 | 114.84 | 111.90 |
| 1 | L50 | 1277 | G | C3'-C2'-C1' | -5.89 | 96.79 | 101.50 |
| 42 | S60 | 1053 | A | N1-C2-N3 | -5.89 | 126.36 | 129.30 |
| 42 | S60 | 1208 | G | C2-N3-C4 | 5.88 | 114.84 | 111.90 |
| 42 | S60 | 848 | G | N9-C4-C5 | 5.88 | 107.75 | 105.40 |
| 42 | S60 | 1128 | G | C4-C5-N7 | 5.87 | 113.15 | 110.80 |
| 42 | S60 | 1176 | G | C2-N3-C4 | 5.87 | 114.83 | 111.90 |
| 42 | S60 | 874 | A | C4-C5-N7 | -5.84 | 107.78 | 110.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 42 | S60 | 1011 | A | C5-C6-N1 | -5.84 | 114.78 | 117.70 |
| 42 | S60 | 1182 | G | C5-C6-O6 | -5.84 | 125.10 | 128.60 |
| 42 | S60 | 959 | G | P-O3'-C3' | -5.83 | 112.70 | 119.70 |
| 42 | S60 | 969 | C | C6-N1-C2 | 5.83 | 122.63 | 120.30 |
| 1 | L50 | 317 | G | C3'-C2'-C1' | -5.83 | 96.83 | 101.50 |
| 1 | L50 | 523 | A | C1'-C2'-O2' | -5.83 | 93.11 | 110.60 |
| 42 | S60 | 952 | A | N1-C6-N6 | 5.83 | 122.10 | 118.60 |
| 42 | S60 | 1058 | A | C1'-O4'-C4' | -5.83 | 105.23 | 109.90 |
| 42 | S60 | 1186 | G | O4'-C1'-N9 | 5.82 | 112.86 | 108.20 |
| 42 | S60 | 1215 | A | C8-N9-C4 | 5.82 | 108.13 | 105.80 |
| 1 | L50 | 2235 | C | O5'-P-OP2 | -5.82 | 100.46 | 105.70 |
| 42 | S60 | 865 | A | C5-N7-C8 | 5.82 | 106.81 | 103.90 |
| 42 | S60 | 1010 | G | C1'-O4'-C4' | -5.82 | 105.25 | 109.90 |
| 42 | S60 | 942 | A | C8-N9-C4 | -5.81 | 103.47 | 105.80 |
| 42 | S60 | 1064 | G | N9-C4-C5 | 5.81 | 107.72 | 105.40 |
| 42 | S60 | 897 | C | P-O3'-C3' | -5.81 | 112.73 | 119.70 |
| 61 | SL0 | 28 | ARG | NE-CZ-NH1 | 5.80 | 123.20 | 120.30 |
| 1 | L50 | 1491 | U | P-O3'-C3' | 5.80 | 126.66 | 119.70 |
| 1 | L50 | 225 | G | C2'-C3'-O3' | 5.80 | 122.98 | 113.70 |
| 30 | LPP | 8 | VAL | CA-CB-CG1 | 5.79 | 119.59 | 110.90 |
| 42 | S60 | 864 | A | C8-N9-C4 | -5.79 | 103.48 | 105.80 |
| 42 | S60 | 954 | G | C2-N3-C4 | -5.79 | 109.00 | 111.90 |
| 42 | S60 | 947 | C | P-O3'-C3' | -5.79 | 112.75 | 119.70 |
| 42 | S60 | 1024 | G | P-O3'-C3' | -5.78 | 112.76 | 119.70 |
| 1 | L50 | 395 | A | C4'-C3'-O3' | -5.77 | 97.27 | 109.40 |
| 42 | S60 | 1177 | G | N9-C4-C5 | -5.77 | 103.09 | 105.40 |
| 51 | SE0 | 100 | ARG | NE-CZ-NH1 | -5.77 | 117.42 | 120.30 |
| 1 | L50 | 1838 | G | O5'-P-OP2 | -5.77 | 100.51 | 105.70 |
| 1 | L50 | 280 | G | C4'-C3'-C2' | -5.76 | 96.84 | 102.60 |
| 42 | S60 | 888 | U | C3'-C2'-C1' | -5.76 | 96.89 | 101.50 |
| 66 | SQ0 | 38 | VAL | CA-CB-CG1 | 5.76 | 119.54 | 110.90 |
| 1 | L50 | 1835 | G | P-O5'-C5' | -5.76 | 111.69 | 120.90 |
| 70 | SU0 | 56 | VAL | CA-CB-CG1 | 5.75 | 119.53 | 110.90 |
| 1 | L50 | 234 | U | O5'-P-OP2 | -5.75 | 100.53 | 105.70 |
| 42 | S60 | 1203 | A | C5-N7-C8 | 5.74 | 106.77 | 103.90 |
| 42 | S60 | 875 | A | C8-N9-C4 | 5.74 | 108.09 | 105.80 |
| 1 | L50 | 1102 | G | O5'-P-OP1 | 5.73 | 117.58 | 110.70 |
| 30 | LPP | 49 | ARG | CG-CD-NE | 5.73 | 123.83 | 111.80 |
| 1 | L50 | 2373 | G | C4'-C3'-C2' | -5.73 | 96.87 | 102.60 |
| 42 | S60 | 952 | A | N9-C4-C5 | -5.72 | 103.51 | 105.80 |
| 42 | S60 | 955 | A | C4'-C3'-C2' | -5.72 | 96.88 | 102.60 |
| 42 | S60 | 1106 | G | P-O3'-C3' | -5.71 | 112.84 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 42 | S60 | 1176 | G | O4'-C4'-C3' | 5.71 | 110.67 | 106.10 |
| 42 | S60 | 222 | G | C4'-C3'-C2' | -5.71 | 96.89 | 102.60 |
| 42 | S60 | 262 | U | O4'-C4'-C3' | -5.71 | 98.29 | 104.00 |
| 1 | L50 | 1303 | G | C4'-C3'-C2' | -5.71 | 96.89 | 102.60 |
| 42 | S60 | 871 | C | N3-C4-C5 | -5.71 | 119.62 | 121.90 |
| 42 | S60 | 960 | U | C4'-C3'-C2' | -5.71 | 96.89 | 102.60 |
| 61 | SL0 | 28 | ARG | NE-CZ-NH2 | -5.71 | 117.45 | 120.30 |
| 1 | L50 | 2452 | A | C4'-C3'-O3' | 5.70 | 124.39 | 113.00 |
| 42 | S60 | 1185 | A | N9-C4-C5 | -5.70 | 103.52 | 105.80 |
| 1 | L50 | 822 | U | P-O3'-C3' | -5.68 | 112.88 | 119.70 |
| 1 | L50 | 1733 | A | C4'-C3'-O3' | -5.68 | 97.47 | 109.40 |
| 42 | S60 | 1184 | U | C3'-C2'-C1' | -5.68 | 96.96 | 101.50 |
| 42 | S60 | 915 | A | P-O3'-C3' | -5.68 | 112.89 | 119.70 |
| 32 | LR0 | 74 | HIS | CB-CA-C | 5.67 | 121.74 | 110.40 |
| 42 | S60 | 1045 | A | N9-C4-C5 | 5.67 | 108.07 | 105.80 |
| 42 | S60 | 1048 | G | C6-C5-N7 | -5.67 | 127.00 | 130.40 |
| 42 | S60 | 1062 | C | C4-C5-C6 | 5.67 | 120.23 | 117.40 |
| 42 | S60 | 963 | G | C2-N3-C4 | 5.66 | 114.73 | 111.90 |
| 42 | S60 | 1146 | G | C3'-C2'-C1' | -5.66 | 96.97 | 101.50 |
| 42 | S60 | 840 | C | P-O3'-C3' | -5.66 | 112.91 | 119.70 |
| 42 | S60 | 848 | G | C5-N7-C8 | 5.66 | 107.13 | 104.30 |
| 1 | L50 | 1304 | A | P-O3'-C3' | -5.65 | 112.92 | 119.70 |
| 42 | S60 | 1207 | A | C2-N3-C4 | 5.65 | 113.43 | 110.60 |
| 42 | S60 | 1125 | G | C2'-C3'-O3' | 5.65 | 122.74 | 113.70 |
| 1 | L50 | 1277 | G | C4'-C3'-C2' | -5.64 | 96.96 | 102.60 |
| 42 | S60 | 922 | G | P-O3'-C3' | -5.64 | 112.94 | 119.70 |
| 42 | S60 | 1093 | G | C5-N7-C8 | -5.64 | 101.48 | 104.30 |
| 1 | L50 | 600 | G | N9-C1'-C2' | -5.63 | 105.81 | 112.00 |
| 42 | S60 | 920 | G | C4-C5-N7 | -5.62 | 108.55 | 110.80 |
| 42 | S60 | 1127 | A | C2-N3-C4 | 5.62 | 113.41 | 110.60 |
| 42 | S60 | 1259 | U | P-O3'-C3' | -5.62 | 112.96 | 119.70 |
| 42 | S60 | 919 | C | C2-N3-C4 | 5.61 | 122.70 | 119.90 |
| 42 | S60 | 1005 | G | C4'-C3'-C2' | -5.60 | 97.00 | 102.60 |
| 42 | S60 | 1094 | C | C2-N3-C4 | 5.59 | 122.70 | 119.90 |
| 42 | S60 | 1035 | C | P-O3'-C3' | -5.58 | 113.00 | 119.70 |
| 2 | L70 | 64 | G | OP1-P-OP2 | -5.58 | 111.24 | 119.60 |
| 1 | L50 | 2587 | U | C3'-C2'-C1' | -5.57 | 97.05 | 101.50 |
| 1 | L50 | 1832 | A | O5'-P-OP2 | -5.57 | 100.69 | 105.70 |
| 42 | S60 | 835 | A | N9-C4-C5 | 5.57 | 108.03 | 105.80 |
| 42 | S60 | 982 | C | C6-N1-C2 | -5.56 | 118.08 | 120.30 |
| 42 | S60 | 856 | U | C3'-C2'-C1' | -5.55 | 97.06 | 101.50 |
| 40 | LZ0 | 69 | ARG | CB-CG-CD | 5.55 | 126.03 | 111.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 42 | S60 | 944 | G | C4-C5-N7 | -5.54 | 108.58 | 110.80 |
| 42 | S60 | 1067 | A | N9-C4-C5 | -5.54 | 103.58 | 105.80 |
| 1 | L50 | 1282 | C | C2-N3-C4 | 5.54 | 122.67 | 119.90 |
| 42 | S60 | 973 | G | C4-C5-N7 | -5.54 | 108.58 | 110.80 |
| 42 | S60 | 1206 | A | C8-N9-C4 | -5.54 | 103.58 | 105.80 |
| 1 | L50 | 1471 | G | OP1-P-OP2 | -5.53 | 111.31 | 119.60 |
| 51 | SE0 | 100 | ARG | NE-CZ-NH2 | 5.53 | 123.06 | 120.30 |
| 42 | S60 | 886 | C | C6-N1-C2 | 5.53 | 122.51 | 120.30 |
| 42 | S60 | 839 | C | C2-N3-C4 | 5.53 | 122.66 | 119.90 |
| 42 | S60 | 1007 | U | O4'-C1'-N1 | 5.53 | 112.62 | 108.20 |
| 1 | L50 | 1485 | G | O4'-C1'-N9 | 5.52 | 112.62 | 108.20 |
| 42 | S60 | 951 | A | C5-N7-C8 | -5.52 | 101.14 | 103.90 |
| 42 | S60 | 871 | C | C4-C5-C6 | 5.52 | 120.16 | 117.40 |
| 42 | S60 | 1089 | G | C4-C5-N7 | -5.52 | 108.59 | 110.80 |
| 42 | S60 | 1106 | G | C8-N9-C4 | 5.51 | 108.61 | 106.40 |
| 42 | S60 | 1003 | A | C4-C5-N7 | -5.51 | 107.94 | 110.70 |
| 1 | L50 | 667 | G | OP1-P-OP2 | -5.51 | 111.34 | 119.60 |
| 42 | S60 | 1183 | C | C2-N3-C4 | 5.51 | 122.65 | 119.90 |
| 42 | S60 | 1195 | A | C4-C5-C6 | 5.51 | 119.75 | 117.00 |
| 42 | S60 | 1239 | C | O5'-P-OP2 | -5.51 | 100.74 | 105.70 |
| 42 | S60 | 622 | C | P-O3'-C3' | -5.50 | 113.09 | 119.70 |
| 42 | S60 | 1052 | A | N7-C8-N9 | 5.50 | 116.55 | 113.80 |
| 42 | S60 | 1127 | A | N7-C8-N9 | -5.50 | 111.05 | 113.80 |
| 1 | L50 | 178 | G | C5-C6-O6 | 5.50 | 131.90 | 128.60 |
| 1 | L50 | 714 | G | O5'-P-OP1 | 5.50 | 117.30 | 110.70 |
| 42 | S60 | 986 | G | C3'-C2'-C1' | 5.50 | 105.90 | 101.50 |
| 42 | S60 | 968 | C | O5'-P-OP2 | -5.50 | 100.75 | 105.70 |
| 42 | S60 | 865 | A | C4-C5-N7 | -5.49 | 107.95 | 110.70 |
| 42 | S60 | 1228 | C | C2-N3-C4 | 5.49 | 122.64 | 119.90 |
| 42 | S60 | 877 | G | C4-C5-C6 | 5.48 | 122.09 | 118.80 |
| 42 | S60 | 1182 | G | N1-C2-N3 | -5.47 | 120.62 | 123.90 |
| 1 | L50 | 1711 | A | O5'-P-OP2 | -5.47 | 100.78 | 105.70 |
| 42 | S60 | 839 | C | C5-C6-N1 | 5.46 | 123.73 | 121.00 |
| 42 | S60 | 1055 | A | C4-C5-C6 | 5.46 | 119.73 | 117.00 |
| 2 | L70 | 86 | G | C4'-C3'-C2' | -5.46 | 97.14 | 102.60 |
| 42 | S60 | 1084 | G | N9-C4-C5 | 5.45 | 107.58 | 105.40 |
| 1 | L50 | 1614 | G | O4'-C1'-N9 | 5.45 | 112.56 | 108.20 |
| 2 | L70 | 75 | G | C3'-C2'-C1' | -5.45 | 97.14 | 101.50 |
| 42 | S60 | 1056 | A | C4-C5-N7 | -5.45 | 107.98 | 110.70 |
| 1 | L50 | 838 | G | OP1-P-OP2 | -5.44 | 111.44 | 119.60 |
| 1 | L50 | 2441 | A | P-O3'-C3' | -5.44 | 113.17 | 119.70 |
| 42 | S60 | 1094 | C | C6-N1-C2 | -5.43 | 118.13 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 42 | S60 | 269 | G | OP1-P-OP2 | -5.43 | 111.45 | 119.60 |
| 42 | S60 | 1049 | G | C4-C5-C6 | 5.43 | 122.06 | 118.80 |
| 1 | L50 | 330 | G | C8-N9-C4 | -5.42 | 104.23 | 106.40 |
| 1 | L50 | 1074 | G | C2'-C3'-O3' | 5.42 | 122.37 | 113.70 |
| 42 | S60 | 944 | G | C5-N7-C8 | 5.42 | 107.01 | 104.30 |
| 42 | S60 | 836 | A | N9-C4-C5 | 5.42 | 107.97 | 105.80 |
| 67 | SR0 | 32 | ARG | NE-CZ-NH2 | 5.42 | 123.01 | 120.30 |
| 1 | L50 | 2473 | G | OP1-P-OP2 | -5.42 | 111.48 | 119.60 |
| 42 | S60 | 1205 | G | N7-C8-N9 | 5.41 | 115.81 | 113.10 |
| 42 | S60 | 1054 | G | C1'-O4'-C4' | -5.40 | 105.58 | 109.90 |
| 42 | S60 | 1328 | G | C3'-C2'-C1' | 5.39 | 105.81 | 101.50 |
| 42 | S60 | 1032 | A | N9-C4-C5 | -5.39 | 103.64 | 105.80 |
| 1 | L50 | 1808 | A | P-O3'-C3' | 5.39 | 126.16 | 119.70 |
| 1 | L50 | 1634 | C | C1'-O4'-C4' | -5.38 | 105.60 | 109.90 |
| 42 | S60 | 10 | A | P-O3'-C3' | -5.38 | 113.24 | 119.70 |
| 1 | L50 | 141 | G | C1'-O4'-C4' | -5.37 | 105.60 | 109.90 |
| 1 | L50 | 42 | G | C4'-C3'-C2' | -5.37 | 97.23 | 102.60 |
| 1 | L50 | 1282 | C | N3-C2-O2 | -5.36 | 118.15 | 121.90 |
| 1 | L50 | 141 | G | O4'-C1'-C2' | -5.35 | 100.45 | 105.80 |
| 1 | L50 | 518 | G | OP1-P-OP2 | -5.35 | 111.57 | 119.60 |
| 42 | S60 | 477 | G | C3'-C2'-C1' | 5.35 | 105.78 | 101.50 |
| 42 | S60 | 860 | G | N3-C4-C5 | -5.35 | 125.93 | 128.60 |
| 42 | S60 | 860 | G | C4-C5-N7 | -5.34 | 108.67 | 110.80 |
| 42 | S60 | 952 | A | C5-N7-C8 | -5.33 | 101.23 | 103.90 |
| 1 | L50 | 1466 | A | C3'-C2'-C1' | 5.33 | 105.76 | 101.50 |
| 42 | S60 | 864 | A | C4-C5-C6 | 5.33 | 119.67 | 117.00 |
| 42 | S60 | 1206 | A | C4-C5-C6 | 5.33 | 119.66 | 117.00 |
| 42 | S60 | 873 | C | C5-C6-N1 | -5.32 | 118.34 | 121.00 |
| 42 | S60 | 888 | U | OP1-P-OP2 | -5.32 | 111.62 | 119.60 |
| 42 | S60 | 954 | G | C5-C6-N1 | -5.32 | 108.84 | 111.50 |
| 42 | S60 | 1213 | G | C8-N9-C4 | 5.32 | 108.53 | 106.40 |
| 42 | S60 | 925 | A | P-O3'-C3' | -5.32 | 113.32 | 119.70 |
| 42 | S60 | 1118 | A | C5-C6-N1 | -5.31 | 115.05 | 117.70 |
| 42 | S60 | 1010 | G | C4-C5-N7 | 5.30 | 112.92 | 110.80 |
| 42 | S60 | 10 | A | O5'-P-OP2 | 5.30 | 117.06 | 110.70 |
| 42 | S60 | 979 | A | N9-C4-C5 | 5.30 | 107.92 | 105.80 |
| 42 | S60 | 1089 | G | C3'-C2'-C1' | 5.30 | 105.74 | 101.50 |
| 1 | L50 | 2332 | G | C4'-C3'-C2' | -5.29 | 97.31 | 102.60 |
| 42 | S60 | 847 | A | C4-C5-N7 | -5.29 | 108.05 | 110.70 |
| 42 | S60 | 849 | U | O5'-P-OP2 | -5.29 | 100.94 | 105.70 |
| 42 | S60 | 893 | U | P-O3'-C3' | -5.29 | 113.35 | 119.70 |
| 42 | S60 | 851 | G | C5-C6-O6 | -5.29 | 125.43 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 42 | S60 | 1128 | G | N9-C4-C5 | -5.29 | 103.29 | 105.40 |
| 42 | S60 | 1154 | A | P-O3'-C3' | -5.29 | 113.36 | 119.70 |
| 42 | S60 | 1052 | A | C5-C6-N1 | -5.28 | 115.06 | 117.70 |
| 42 | S60 | 1208 | G | C5-C6-N1 | 5.28 | 114.14 | 111.50 |
| 42 | S60 | 601 | G | C4'-C3'-C2' | -5.28 | 97.32 | 102.60 |
| 42 | S60 | 1010 | G | C5-N7-C8 | -5.27 | 101.66 | 104.30 |
| 1 | L50 | 2184 | G | P-O3'-C3' | 5.27 | 126.03 | 119.70 |
| 42 | S60 | 954 | G | C6-C5-N7 | -5.27 | 127.24 | 130.40 |
| 42 | S60 | 947 | C | N3-C4-C5 | -5.27 | 119.79 | 121.90 |
| 42 | S60 | 1003 | A | C5-C6-N1 | 5.27 | 120.33 | 117.70 |
| 42 | S60 | 1051 | C | N3-C4-C5 | 5.27 | 124.01 | 121.90 |
| 42 | S60 | 1054 | G | C5-N7-C8 | -5.26 | 101.67 | 104.30 |
| 42 | S60 | 834 | G | P-O3'-C3' | -5.25 | 113.40 | 119.70 |
| 42 | S60 | 954 | G | C5-N7-C8 | -5.25 | 101.68 | 104.30 |
| 42 | S60 | 1097 | A | C8-N9-C4 | 5.25 | 107.90 | 105.80 |
| 66 | SQ0 | 82 | ARG | NE-CZ-NH1 | -5.25 | 117.68 | 120.30 |
| 1 | L50 | 885 | G | P-O3'-C3' | -5.25 | 113.41 | 119.70 |
| 1 | L50 | 1605 | U | P-O3'-C3' | -5.24 | 113.41 | 119.70 |
| 42 | S60 | 1003 | A | C6-N1-C2 | -5.24 | 115.46 | 118.60 |
| 1 | L50 | 141 | G | C3'-C2'-C1' | -5.24 | 97.31 | 101.50 |
| 1 | L50 | 1010 | A | O5'-P-OP2 | -5.24 | 100.99 | 105.70 |
| 42 | S60 | 850 | G | C4'-C3'-C2' | -5.23 | 97.37 | 102.60 |
| 42 | S60 | 994 | G | C8-N9-C4 | -5.23 | 104.31 | 106.40 |
| 1 | L50 | 1839 | A | P-O3'-C3' | -5.23 | 113.43 | 119.70 |
| 42 | S60 | 993 | U | P-O3'-C3' | -5.23 | 113.43 | 119.70 |
| 42 | S60 | 1194 | U | C5-C6-N1 | -5.23 | 120.09 | 122.70 |
| 1 | L50 | 2447 | A | P-O5'-C5' | -5.23 | 112.54 | 120.90 |
| 42 | S60 | 1012 | A | C4'-C3'-C2' | -5.22 | 97.38 | 102.60 |
| 42 | S60 | 1218 | U | C3'-C2'-C1' | 5.22 | 105.68 | 101.50 |
| 1 | L50 | 515 | U | P-O3'-C3' | -5.22 | 113.44 | 119.70 |
| 1 | L50 | 1575 | G | C4'-C3'-C2' | -5.22 | 97.38 | 102.60 |
| 1 | L50 | 323 | G | C4'-C3'-C2' | -5.21 | 97.39 | 102.60 |
| 1 | L50 | 371 | A | C5-N7-C8 | 5.21 | 106.51 | 103.90 |
| 42 | S60 | 275 | G | C4'-C3'-C2' | -5.21 | 97.39 | 102.60 |
| 42 | S60 | 1161 | U | C6-N1-C2 | 5.21 | 124.13 | 121.00 |
| 42 | S60 | 1053 | A | C3'-C2'-C1' | -5.21 | 97.33 | 101.50 |
| 42 | S60 | 918 | A | C3'-C2'-C1' | -5.21 | 97.34 | 101.50 |
| 1 | L50 | 1513 | G | P-O3'-C3' | 5.20 | 125.94 | 119.70 |
| 1 | L50 | 2181 | A | O5'-P-OP1 | -5.20 | 101.02 | 105.70 |
| 42 | S60 | 1018 | U | N3-C4-C5 | 5.20 | 117.72 | 114.60 |
| 1 | L50 | 1499 | U | C2'-C3'-O3' | 5.19 | 122.01 | 113.70 |
| 42 | S60 | 1039 | G | C8-N9-C4 | -5.19 | 104.33 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | L50 | 1000 | G | C1'-C2'-O2' | -5.18 | 95.05 | 110.60 |
| 42 | S60 | 934 | A | P-O3'-C3' | -5.18 | 113.49 | 119.70 |
| 42 | S60 | 1203 | A | C2-N3-C4 | 5.18 | 113.19 | 110.60 |
| 42 | S60 | 963 | G | C4-C5-N7 | -5.17 | 108.73 | 110.80 |
| 42 | S60 | 1018 | U | C6-N1-C2 | 5.17 | 124.11 | 121.00 |
| 1 | L50 | 1160 | G | O4'-C1'-N9 | 5.17 | 112.34 | 108.20 |
| 1 | L50 | 2447 | A | O4'-C1'-N9 | 5.17 | 112.34 | 108.20 |
| 1 | L50 | 596 | G | C4'-C3'-C2' | -5.17 | 97.43 | 102.60 |
| 1 | L50 | 1165 | U | P-O3'-C3' | -5.17 | 113.50 | 119.70 |
| 42 | S60 | 861 | C | C6-N1-C2 | 5.17 | 122.37 | 120.30 |
| 42 | S60 | 1097 | A | C2-N3-C4 | 5.17 | 113.19 | 110.60 |
| 42 | S60 | 441 | G | C4'-C3'-C2' | -5.17 | 97.44 | 102.60 |
| 42 | S60 | 1189 | A | N7-C8-N9 | -5.17 | 111.22 | 113.80 |
| 1 | L50 | 1586 | G | OP1-P-OP2 | -5.16 | 111.85 | 119.60 |
| 42 | S60 | 1069 | G | C5-N7-C8 | -5.16 | 101.72 | 104.30 |
| 42 | S60 | 1208 | G | C5-N7-C8 | 5.16 | 106.88 | 104.30 |
| 1 | L50 | 462 | G | OP1-P-O3' | 5.16 | 116.55 | 105.20 |
| 1 | L50 | 690 | U | C4'-C3'-C2' | -5.16 | 97.44 | 102.60 |
| 1 | L50 | 1364 | U | P-O3'-C3' | -5.16 | 113.51 | 119.70 |
| 1 | L50 | 1602 | G | C4'-C3'-C2' | -5.16 | 97.44 | 102.60 |
| 42 | S60 | 1179 | A | C4-C5-N7 | -5.16 | 108.12 | 110.70 |
| 1 | L50 | 541 | U | P-O3'-C3' | -5.16 | 113.51 | 119.70 |
| 42 | S60 | 989 | G | C4-C5-N7 | -5.16 | 108.74 | 110.80 |
| 1 | L50 | 2315 | G | C4'-C3'-C2' | -5.15 | 97.45 | 102.60 |
| 42 | S60 | 459 | G | C4'-C3'-C2' | -5.15 | 97.45 | 102.60 |
| 42 | S60 | 1094 | C | C5-C6-N1 | 5.15 | 123.58 | 121.00 |
| 42 | S60 | 1001 | C | C2-N3-C4 | 5.15 | 122.47 | 119.90 |
| 1 | L50 | 2009 | U | O5'-P-OP2 | -5.14 | 101.07 | 105.70 |
| 2 | L70 | 93 | A | P-O3'-C3' | -5.14 | 113.53 | 119.70 |
| 42 | S60 | 1052 | A | C2-N3-C4 | -5.14 | 108.03 | 110.60 |
| 42 | S60 | 1118 | A | C8-N9-C4 | -5.14 | 103.75 | 105.80 |
| 39 | LY0 | 53 | ASP | CB-CA-C | 5.13 | 120.67 | 110.40 |
| 42 | S60 | 1176 | G | C5-C6-N1 | 5.13 | 114.07 | 111.50 |
| 42 | S60 | 1050 | G | N3-C4-C5 | -5.13 | 126.04 | 128.60 |
| 1 | L50 | 194 | A | OP1-P-OP2 | -5.13 | 111.91 | 119.60 |
| 1 | L50 | 1192 | A | OP1-P-OP2 | -5.12 | 111.91 | 119.60 |
| 42 | S60 | 952 | A | C6-N1-C2 | 5.12 | 121.67 | 118.60 |
| 42 | S60 | 1088 | U | C5-C6-N1 | -5.12 | 120.14 | 122.70 |
| 1 | L50 | 2452 | A | P-O3'-C3' | 5.12 | 125.84 | 119.70 |
| 1 | L50 | 614 | G | N3-C4-C5 | -5.12 | 126.04 | 128.60 |
| 1 | L50 | 330 | G | P-O3'-C3' | 5.12 | 125.84 | 119.70 |
| 42 | S60 | 995 | A | C5-N7-C8 | 5.11 | 106.46 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 42 | S60 | 858 | C | C5-C6-N1 | 5.11 | 123.56 | 121.00 |
| 42 | S60 | 263 | A | C5'-C4'-C3' | -5.11 | 107.83 | 116.00 |
| 1 | L50 | 590 | G | N3-C4-C5 | -5.10 | 126.05 | 128.60 |
| 42 | S60 | 1062 | C | C6-N1-C2 | -5.10 | 118.26 | 120.30 |
| 42 | S60 | 857 | G | N9-C4-C5 | -5.10 | 103.36 | 105.40 |
| 66 | SQ0 | 82 | ARG | NE-CZ-NH2 | 5.10 | 122.85 | 120.30 |
| 1 | L50 | 2341 | G | C4'-C3'-C2' | -5.09 | 97.51 | 102.60 |
| 42 | S60 | 883 | C | N3-C4-C5 | 5.09 | 123.94 | 121.90 |
| 42 | S60 | 1095 | G | C4-C5-C6 | 5.09 | 121.85 | 118.80 |
| 1 | L50 | 690 | U | OP1-P-O3' | 5.09 | 116.39 | 105.20 |
| 42 | S60 | 987 | A | C4-C5-N7 | 5.09 | 113.24 | 110.70 |
| 42 | S60 | 1208 | G | N7-C8-N9 | -5.09 | 110.56 | 113.10 |
| 1 | L50 | 569 | C | O5'-P-OP2 | -5.08 | 101.13 | 105.70 |
| 1 | L50 | 1018 | U | C1'-C2'-O2' | -5.08 | 95.35 | 110.60 |
| 1 | L50 | 1622 | G | C4'-C3'-C2' | -5.08 | 97.52 | 102.60 |
| 42 | S60 | 1059 | G | N9-C4-C5 | -5.08 | 103.37 | 105.40 |
| 1 | L50 | 2011 | A | P-O3'-C3' | -5.08 | 113.61 | 119.70 |
| 1 | L50 | 1182 | A | O5'-P-OP2 | 5.07 | 116.79 | 110.70 |
| 42 | S60 | 835 | A | C4-C5-C6 | 5.07 | 119.54 | 117.00 |
| 1 | L50 | 2145 | A | O5'-P-OP1 | -5.07 | 101.14 | 105.70 |
| 42 | S60 | 1000 | C | C2-N3-C4 | 5.07 | 122.44 | 119.90 |
| 42 | S60 | 881 | G | OP1-P-OP2 | -5.07 | 112.00 | 119.60 |
| 42 | S60 | 1064 | G | OP1-P-OP2 | -5.07 | 112.00 | 119.60 |
| 42 | S60 | 844 | A | P-O3'-C3' | -5.07 | 113.62 | 119.70 |
| 1 | L50 | 1614 | G | C1'-O4'-C4' | -5.07 | 105.85 | 109.90 |
| 1 | L50 | 2313 | G | O5'-P-OP1 | -5.07 | 101.14 | 105.70 |
| 42 | S60 | 162 | C | P-O3'-C3' | -5.07 | 113.62 | 119.70 |
| 42 | S60 | 1228 | C | C5-C6-N1 | 5.07 | 123.53 | 121.00 |
| 1 | L50 | 1625 | A | O5'-P-OP2 | -5.07 | 101.14 | 105.70 |
| 1 | L50 | 2167 | A | C3'-C2'-C1' | 5.07 | 105.55 | 101.50 |
| 42 | S60 | 975 | G | C4-C5-N7 | 5.07 | 112.83 | 110.80 |
| 42 | S60 | 1214 | A | P-O3'-C3' | -5.07 | 113.62 | 119.70 |
| 1 | L50 | 266 | A | O5'-P-OP1 | -5.06 | 101.14 | 105.70 |
| 42 | S60 | 951 | A | C4-C5-N7 | 5.06 | 113.23 | 110.70 |
| 42 | S60 | 989 | G | C4-C5-C6 | 5.06 | 121.83 | 118.80 |
| 42 | S60 | 308 | C | P-O3'-C3' | -5.06 | 113.63 | 119.70 |
| 42 | S60 | 1209 | C | C6-N1-C2 | 5.06 | 122.32 | 120.30 |
| 1 | L50 | 612 | C | OP1-P-OP2 | -5.05 | 112.02 | 119.60 |
| 42 | S60 | 8 | U | O5'-P-OP2 | -5.05 | 101.15 | 105.70 |
| 42 | S60 | 1111 | A | C8-N9-C4 | 5.05 | 107.82 | 105.80 |
| 42 | S60 | 859 | G | C4-C5-C6 | 5.05 | 121.83 | 118.80 |
| 42 | S60 | 1011 | A | N9-C4-C5 | 5.05 | 107.82 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 42 | S60 | 1161 | U | N3-C4-C5 | 5.05 | 117.63 | 114.60 |
| 42 | S60 | 1053 | A | C4-C5-C6 | -5.04 | 114.48 | 117.00 |
| 42 | S60 | 1086 | G | C3'-C2'-C1' | -5.04 | 97.47 | 101.50 |
| 42 | S60 | 1048 | G | N7-C8-N9 | 5.04 | 115.62 | 113.10 |
| 42 | S60 | 1011 | A | C4-C5-C6 | 5.04 | 119.52 | 117.00 |
| 42 | S60 | 1048 | G | C5-C6-N1 | -5.04 | 108.98 | 111.50 |
| 42 | S60 | 875 | A | C5-N7-C8 | 5.04 | 106.42 | 103.90 |
| 42 | S60 | 885 | G | C4'-C3'-C2' | -5.04 | 97.56 | 102.60 |
| 1 | L50 | 2556 | U | P-O3'-C3' | -5.03 | 113.67 | 119.70 |
| 1 | L50 | 1087 | G | C4'-C3'-C2' | -5.03 | 97.57 | 102.60 |
| 1 | L50 | 1484 | U | O5'-P-OP2 | 5.03 | 116.73 | 110.70 |
| 1 | L50 | 75 | C | C2'-C3'-O3' | 5.02 | 121.74 | 113.70 |
| 1 | L50 | 2019 | G | C4'-C3'-C2' | -5.02 | 97.58 | 102.60 |
| 42 | S60 | 833 | A | P-O3'-C3' | -5.02 | 113.67 | 119.70 |
| 1 | L50 | 1115 | G | C3'-C2'-C1' | -5.02 | 97.49 | 101.50 |
| 42 | S60 | 624 | U | P-O3'-C3' | -5.01 | 113.68 | 119.70 |
| 1 | L50 | 784 | G | P-O3'-C3' | -5.01 | 113.69 | 119.70 |
| 1 | L50 | 1018 | U | C1'-O4'-C4' | -5.01 | 105.89 | 109.90 |
| 1 | L50 | 1568 | G | OP1-P-OP2 | -5.01 | 112.09 | 119.60 |
| 1 | L50 | 1414 | U | P-O5'-C5' | -5.01 | 112.89 | 120.90 |
| 1 | L50 | 2154 | U | P-O3'-C3' | -5.01 | 113.69 | 119.70 |
| 42 | S60 | 987 | A | N1-C6-N6 | 5.01 | 121.61 | 118.60 |
| 1 | L50 | 151 | G | P-O3'-C3' | 5.01 | 125.71 | 119.70 |
| 1 | L50 | 1182 | A | OP1-P-OP2 | -5.00 | 112.09 | 119.60 |
| 42 | S60 | 882 | A | C5-N7-C8 | 5.00 | 106.40 | 103.90 |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 6 | LC0 | 87 | ALA | Peptide |
| 13 | LFF | 101 | ILE | Peptide |
| 15 | LGG | 77 | 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 | L50 | 53655 | 0 | 26955 | 118 | 0 |
| 2 | L70 | 2542 | 0 | 1282 | 8 | 0 |
| 3 | LA0 | 1889 | 0 | 1985 | 12 | 0 |
| 4 | LAA | 1167 | 0 | 1214 | 5 | 0 |
| 5 | LB0 | 3039 | 0 | 3183 | 6 | 0 |
| 6 | LC0 | 2604 | 0 | 2638 | 12 | 0 |
| 7 | LCC | 781 | 0 | 803 | 2 | 0 |
| 8 | LD0 | 2298 | 0 | 2384 | 6 | 0 |
| 9 | LDD | 895 | 0 | 948 | 0 | 0 |
| 10 | LE0 | 1371 | 0 | 1389 | 13 | 0 |
| 11 | LEE | 1090 | 0 | 1173 | 10 | 0 |
| 12 | LF0 | 1933 | 0 | 2011 | 11 | 0 |
| 13 | LFF | 893 | 0 | 945 | 2 | 0 |
| 14 | LG0 | 1590 | 0 | 1709 | 4 | 0 |
| 15 | LGG | 819 | 0 | 882 | 1 | 0 |
| 16 | LH0 | 1477 | 0 | 1528 | 4 | 0 |
| 17 | LHH | 992 | 0 | 1097 | 5 | 0 |
| 18 | LI0 | 1750 | 0 | 1797 | 2 | 0 |
| 19 | LII | 784 | 0 | 874 | 2 | 0 |
| 20 | LJ0 | 1332 | 0 | 1411 | 12 | 0 |
| 21 | LJJ | 701 | 0 | 753 | 4 | 0 |
| 22 | LL0 | 1353 | 0 | 1433 | 4 | 0 |
| 23 | LLL | 427 | 0 | 468 | 0 | 0 |
| 24 | LM0 | 927 | 0 | 961 | 5 | 0 |
| 25 | LMM | 427 | 0 | 461 | 0 | 0 |
| 26 | LN0 | 1688 | 0 | 1752 | 5 | 0 |
| 27 | LO0 | 1598 | 0 | 1681 | 3 | 0 |
| 28 | LOO | 801 | 0 | 886 | 4 | 0 |
| 29 | LP0 | 1238 | 0 | 1304 | 3 | 0 |
| 30 | LPP | 684 | 0 | 720 | 2 | 0 |
| 31 | LQ0 | 1491 | 0 | 1587 | 6 | 0 |
| 32 | LR0 | 1336 | 0 | 1430 | 0 | 0 |
| 33 | LS0 | 1400 | 0 | 1450 | 1 | 0 |
| 34 | LT0 | 1270 | 0 | 1321 | 15 | 0 |
| 35 | LU0 | 810 | 0 | 834 | 1 | 0 |
| 36 | LV0 | 1057 | 0 | 1139 | 2 | 0 |
| 37 | LW0 | 832 | 0 | 873 | 45 | 0 |
| 38 | LX0 | 874 | 0 | 956 | 5 | 0 |
| 39 | LY0 | 1048 | 0 | 1135 | 2 | 0 |
| 40 | LZ0 | 963 | 0 | 1022 | 2 | 0 |
| 41 | MD1 | 1229 | 0 | 1216 | 10 | 0 |
| 42 | S60 | 29181 | 0 | 14605 | 315 | 0 |
| 43 | SA0 | 1725 | 0 | 1750 | 137 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 44 | SAA | 827 | 0 | 859 | 18 | 0 |
| 45 | SB0 | 1609 | 0 | 1728 | 6 | 0 |
| 46 | SBB | 627 | 0 | 651 | 3 | 0 |
| 47 | SC0 | 1727 | 0 | 1802 | 90 | 0 |
| 48 | SCC | 476 | 0 | 488 | 18 | 0 |
| 49 | SD0 | 1700 | 0 | 1815 | 33 | 0 |
| 50 | SDD | 550 | 0 | 542 | 29 | 0 |
| 51 | SE0 | 2044 | 0 | 2116 | 26 | 0 |
| 52 | SEE | 447 | 0 | 483 | 1 | 0 |
| 53 | SF0 | 1509 | 0 | 1604 | 39 | 0 |
| 54 | SFF | 422 | 0 | 412 | 6 | 0 |
| 55 | SG0 | 1836 | 0 | 1972 | 38 | 0 |
| 56 | SGG | 2478 | 0 | 2458 | 22 | 0 |
| 57 | SH0 | 1335 | 0 | 1356 | 2 | 0 |
| 58 | SI0 | 1347 | 0 | 1379 | 9 | 0 |
| 59 | SJ0 | 1379 | 0 | 1436 | 15 | 0 |
| 60 | SK0 | 737 | 0 | 746 | 17 | 0 |
| 61 | SL0 | 1229 | 0 | 1302 | 5 | 0 |
| 62 | SM0 | 876 | 0 | 937 | 6 | 0 |
| 63 | SN0 | 1130 | 0 | 1189 | 10 | 0 |
| 64 | SO0 | 983 | 0 | 1028 | 14 | 0 |
| 65 | SP0 | 950 | 0 | 984 | 58 | 0 |
| 66 | SQ0 | 1143 | 0 | 1171 | 19 | 0 |
| 67 | SR0 | 974 | 0 | 1003 | 99 | 0 |
| 68 | SS0 | 1150 | 0 | 1207 | 32 | 0 |
| 69 | ST0 | 1161 | 0 | 1219 | 9 | 0 |
| 70 | SU0 | 809 | 0 | 838 | 14 | 0 |
| 71 | SV0 | 521 | 0 | 525 | 72 | 0 |
| 72 | SW0 | 1022 | 0 | 1052 | 18 | 0 |
| 73 | SX0 | 1098 | 0 | 1183 | 4 | 0 |
| 74 | SY0 | 1118 | 0 | 1166 | 12 | 0 |
| 75 | SZ0 | 633 | 0 | 678 | 13 | 0 |
| 76 | LGG | 1 | 0 | 0 | 0 | 0 |
| 76 | LJJ | 1 | 0 | 0 | 0 | 0 |
| 76 | LMM | 1 | 0 | 0 | 0 | 0 |
| 76 | LOO | 1 | 0 | 0 | 0 | 0 |
| 76 | LPP | 1 | 0 | 0 | 0 | 0 |
| 76 | SAA | 1 | 0 | 0 | 0 | 0 |
| 76 | SBB | 1 | 0 | 0 | 0 | 0 |
| 76 | SDD | 1 | 0 | 0 | 0 | 0 |
| 76 | SFF | 1 | 0 | 0 | 0 | 0 |
| All | All | 171817 | 0 | 133274 | 959 | 0 |

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

All (959) 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) |
|--------------------|---------------------|--------------------------|-------------------|
| 43:SA0:70:ASN:HB2 | 47:SC0:240:ILE:CD1 | 1.35 | 1.56 |
| 47:SC0:51:SER:HB2 | 71:SV0:6:ARG:NH2 | 1.30 | 1.44 |
| 49:SD0:238:PRO:C | 67:SR0:19:ARG:HH12 | 1.27 | 1.36 |
| 43:SA0:70:ASN:HB2 | 47:SC0:240:ILE:CG1 | 1.56 | 1.35 |
| 20:LJ0:82:LYS:HB3 | 65:SP0:30:PHE:CE2 | 1.62 | 1.34 |
| 43:SA0:70:ASN:CB | 47:SC0:240:ILE:HD11 | 1.59 | 1.30 |
| 43:SA0:141:ASN:O | 71:SV0:23:VAL:HG23 | 1.21 | 1.26 |
| 49:SD0:239:ILE:N | 67:SR0:19:ARG:HH12 | 1.35 | 1.24 |
| 3:LA0:241:ARG:NH1 | 42:S60:592:G:H4' | 1.51 | 1.22 |
| 50:SDD:8:TYR:CE2 | 65:SP0:72:ARG:HD2 | 1.75 | 1.21 |
| 49:SD0:238:PRO:C | 67:SR0:19:ARG:NH1 | 1.98 | 1.17 |
| 43:SA0:63:ARG:CZ | 71:SV0:30:LEU:HG | 1.75 | 1.16 |
| 47:SC0:51:SER:CB | 71:SV0:6:ARG:HH21 | 1.60 | 1.14 |
| 43:SA0:70:ASN:CB | 47:SC0:240:ILE:CD1 | 2.22 | 1.12 |
| 47:SC0:51:SER:CB | 71:SV0:6:ARG:NH2 | 2.11 | 1.11 |
| 37:LW0:99:LYS:HA | 37:LW0:102:LYS:HE2 | 1.30 | 1.09 |
| 20:LJ0:82:LYS:CB | 65:SP0:30:PHE:HE2 | 1.65 | 1.09 |
| 43:SA0:63:ARG:HG2 | 71:SV0:30:LEU:HD21 | 1.31 | 1.08 |
| 43:SA0:70:ASN:CG | 47:SC0:240:ILE:HG12 | 1.73 | 1.08 |
| 1:L50:1691:A:N6 | 42:S60:1248:G:H4' | 1.68 | 1.08 |
| 43:SA0:63:ARG:O | 71:SV0:28:VAL:HG22 | 1.55 | 1.07 |
| 47:SC0:219:PRO:HB3 | 72:SW0:66:ARG:NH2 | 1.68 | 1.07 |
| 74:SY0:22:GLU:O | 74:SY0:23:LEU:HG | 1.53 | 1.06 |
| 3:LA0:241:ARG:HH12 | 42:S60:592:G:C4' | 1.69 | 1.06 |
| 1:L50:535:A:O2' | 31:LQ0:146:ASN:HB3 | 1.55 | 1.05 |
| 43:SA0:187:GLY:HA2 | 71:SV0:35:ARG:NH2 | 1.71 | 1.05 |
| 43:SA0:64:MET:HB3 | 71:SV0:27:MET:HG2 | 1.38 | 1.05 |
| 43:SA0:141:ASN:C | 71:SV0:23:VAL:HG23 | 1.76 | 1.05 |
| 37:LW0:83:PHE:CD1 | 55:SG0:144:LYS:HG2 | 1.92 | 1.05 |
| 34:LT0:126:PRO:HB2 | 34:LT0:128:LEU:HG | 1.34 | 1.04 |
| 1:L50:1695:A:N1 | 42:S60:1249:U:C5' | 2.20 | 1.04 |
| 43:SA0:70:ASN:CB | 47:SC0:240:ILE:CG1 | 2.35 | 1.04 |
| 43:SA0:141:ASN:O | 71:SV0:23:VAL:CG2 | 2.05 | 1.04 |
| 50:SDD:12:LEU:HD21 | 65:SP0:67:PHE:CD2 | 1.92 | 1.03 |
| 47:SC0:136:TRP:HH2 | 59:SJ0:59:ILE:CG2 | 1.71 | 1.03 |
| 43:SA0:215:TYR:CD1 | 67:SR0:84:PHE:CE2 | 2.46 | 1.03 |
| 55:SG0:140:LYS:O | 55:SG0:144:LYS:HD3 | 1.58 | 1.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 37:LW0:83:PHE:CD1 | 55:SG0:144:LYS:CG | 2.41 | 1.02 |
| 49:SD0:239:ILE:N | 67:SR0:19:ARG:NH1 | 2.05 | 1.02 |
| 50:SDD:12:LEU:CD1 | 65:SP0:75:ILE:HG21 | 1.90 | 1.02 |
| 37:LW0:83:PHE:CD1 | 37:LW0:84:PRO:HD2 | 1.93 | 1.02 |
| 43:SA0:63:ARG:CG | 71:SV0:30:LEU:HD21 | 1.90 | 1.02 |
| 10:LE0:55:GLU:OE2 | 10:LE0:117:ARG:HG3 | 1.59 | 1.01 |
| 55:SG0:147:PHE:HZ | 55:SG0:160:LYS:HE2 | 1.22 | 1.01 |
| 43:SA0:117:ARG:HH12 | 47:SC0:243:GLU:CD | 1.64 | 1.00 |
| 1:L50:1695:A:N1 | 42:S60:1249:U:H5' | 1.76 | 1.00 |
| 1:L50:1695:A:C2 | 42:S60:1249:U:H5'' | 1.97 | 0.98 |
| 44:SAA:47:ALA:CB | 48:SCC:61:ARG:HE | 1.78 | 0.97 |
| 47:SC0:230:ASN:N | 71:SV0:24:GLN:HE22 | 1.61 | 0.97 |
| 3:LA0:241:ARG:HH12 | 42:S60:592:G:H4' | 1.13 | 0.96 |
| 43:SA0:215:TYR:HA | 67:SR0:84:PHE:CD2 | 2.01 | 0.96 |
| 47:SC0:51:SER:HB2 | 71:SV0:6:ARG:HH22 | 1.15 | 0.96 |
| 37:LW0:98:ASN:ND2 | 55:SG0:147:PHE:HA | 1.81 | 0.95 |
| 42:S60:973:G:H1 | 44:SAA:90:TRP:HZ2 | 1.09 | 0.95 |
| 43:SA0:70:ASN:HB2 | 47:SC0:240:ILE:HD11 | 0.95 | 0.95 |
| 43:SA0:63:ARG:NE | 71:SV0:30:LEU:HG | 1.81 | 0.94 |
| 56:SGG:65:PHE:CE2 | 67:SR0:29:TYR:CE2 | 2.55 | 0.94 |
| 43:SA0:51:ILE:HG13 | 67:SR0:105:MET:SD | 2.09 | 0.93 |
| 20:LJ0:82:LYS:HB3 | 65:SP0:30:PHE:CD2 | 2.03 | 0.93 |
| 42:S60:554:A:N3 | 72:SW0:103:THR:HG22 | 1.83 | 0.93 |
| 1:L50:1691:A:N6 | 42:S60:1248:G:C4' | 2.32 | 0.93 |
| 43:SA0:184:TYR:CD1 | 71:SV0:35:ARG:NH1 | 2.36 | 0.92 |
| 50:SDD:8:TYR:O | 65:SP0:67:PHE:N | 2.01 | 0.92 |
| 43:SA0:120:ARG:HE | 47:SC0:232:ILE:HG21 | 1.35 | 0.92 |
| 43:SA0:70:ASN:CA | 47:SC0:240:ILE:HD11 | 1.98 | 0.92 |
| 43:SA0:4:ARG:O | 71:SV0:30:LEU:HD12 | 1.69 | 0.92 |
| 10:LE0:100:ILE:HD11 | 24:LM0:102:PHE:HB2 | 1.49 | 0.91 |
| 50:SDD:8:TYR:CE2 | 65:SP0:72:ARG:CD | 2.54 | 0.91 |
| 37:LW0:99:LYS:CA | 37:LW0:102:LYS:HE2 | 2.00 | 0.91 |
| 43:SA0:70:ASN:CB | 47:SC0:240:ILE:HG12 | 1.99 | 0.91 |
| 42:S60:973:G:N1 | 44:SAA:90:TRP:CZ2 | 2.39 | 0.90 |
| 47:SC0:136:TRP:CH2 | 59:SJ0:59:ILE:CG2 | 2.54 | 0.90 |
| 42:S60:958:A:H3' | 42:S60:959:G:H21 | 1.37 | 0.90 |
| 43:SA0:184:TYR:O | 71:SV0:35:ARG:HD2 | 1.72 | 0.90 |
| 43:SA0:63:ARG:HD3 | 71:SV0:30:LEU:HD23 | 1.52 | 0.90 |
| 47:SC0:130:PRO:HB2 | 71:SV0:4:PHE:CZ | 2.07 | 0.90 |
| 48:SCC:58:ARG:HH12 | 64:SO0:101:ARG:HH22 | 1.19 | 0.90 |
| 20:LJ0:82:LYS:CB | 65:SP0:30:PHE:CE2 | 2.44 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 47:SC0:230:ASN:H | 71:SV0:24:GLN:HE22 | 0.91 | 0.89 |
| 43:SA0:70:ASN:ND2 | 47:SC0:240:ILE:HG12 | 1.88 | 0.89 |
| 43:SA0:63:ARG:HD3 | 71:SV0:30:LEU:CD2 | 2.03 | 0.89 |
| 43:SA0:67:SER:OG | 71:SV0:40:LEU:CD2 | 2.21 | 0.89 |
| 42:S60:203:G:N3 | 51:SE0:33:THR:HG21 | 1.88 | 0.88 |
| 43:SA0:51:ILE:HD12 | 67:SR0:105:MET:HG2 | 1.53 | 0.88 |
| 1:L50:1695:A:N1 | 42:S60:1249:U:H5' | 1.85 | 0.88 |
| 37:LW0:99:LYS:HA | 37:LW0:102:LYS:CE | 2.03 | 0.88 |
| 43:SA0:117:ARG:NH1 | 47:SC0:243:GLU:OE2 | 2.06 | 0.88 |
| 50:SDD:8:TYR:CD2 | 65:SP0:72:ARG:HD2 | 2.08 | 0.87 |
| 43:SA0:120:ARG:HE | 47:SC0:232:ILE:CG2 | 1.88 | 0.86 |
| 47:SC0:219:PRO:HB3 | 72:SW0:66:ARG:HH22 | 1.39 | 0.86 |
| 47:SC0:230:ASN:HB2 | 71:SV0:24:GLN:CD | 1.95 | 0.86 |
| 50:SDD:12:LEU:CD2 | 65:SP0:67:PHE:CD2 | 2.57 | 0.86 |
| 42:S60:973:G:N1 | 44:SAA:90:TRP:HZ2 | 1.72 | 0.86 |
| 50:SDD:8:TYR:CZ | 65:SP0:72:ARG:HD2 | 2.09 | 0.86 |
| 37:LW0:26:ASP:O | 37:LW0:27:ASP:OD1 | 1.94 | 0.86 |
| 47:SC0:230:ASN:H | 71:SV0:24:GLN:NE2 | 1.73 | 0.86 |
| 20:LJ0:82:LYS:HB3 | 65:SP0:30:PHE:HE2 | 1.06 | 0.86 |
| 42:S60:1084:G:N2 | 65:SP0:117:GLY:O | 2.09 | 0.85 |
| 43:SA0:67:SER:OG | 71:SV0:40:LEU:HD22 | 1.75 | 0.85 |
| 42:S60:995:A:H3' | 42:S60:996:G:H8 | 1.42 | 0.85 |
| 53:SF0:118:ARG:HD2 | 53:SF0:125:MET:HB3 | 1.58 | 0.85 |
| 42:S60:1149:U:OP1 | 68:SS0:139:VAL:N | 2.10 | 0.84 |
| 42:S60:826:U:O2' | 47:SC0:81:GLN:O | 1.94 | 0.84 |
| 42:S60:705:A:N3 | 42:S60:706:G:C6 | 2.46 | 0.84 |
| 42:S60:706:G:N3 | 42:S60:706:G:H2' | 1.92 | 0.83 |
| 41:MD1:52:LYS:HG3 | 42:S60:606:G:N2 | 1.93 | 0.83 |
| 50:SDD:12:LEU:HD11 | 65:SP0:75:ILE:HG21 | 1.59 | 0.83 |
| 3:LA0:241:ARG:NH1 | 42:S60:592:G:C4' | 2.33 | 0.82 |
| 43:SA0:63:ARG:CD | 71:SV0:30:LEU:CD2 | 2.57 | 0.82 |
| 42:S60:914:U:H3 | 42:S60:918:A:H61 | 1.23 | 0.82 |
| 43:SA0:215:TYR:O | 67:SR0:84:PHE:HE2 | 1.62 | 0.82 |
| 42:S60:1159:A:O2' | 65:SP0:100:ASN:ND2 | 2.11 | 0.82 |
| 42:S60:923:A:H4' | 42:S60:924:U:H2' | 1.61 | 0.81 |
| 53:SF0:39:ILE:HG21 | 66:SQ0:50:GLU:HB2 | 1.62 | 0.81 |
| 55:SG0:147:PHE:CZ | 55:SG0:160:LYS:HE2 | 2.13 | 0.81 |
| 42:S60:173:A:C8 | 51:SE0:131:VAL:CG1 | 2.64 | 0.81 |
| 43:SA0:63:ARG:HG2 | 71:SV0:30:LEU:CD2 | 2.11 | 0.81 |
| 49:SD0:234:ILE:HD12 | 67:SR0:8:SER:HB2 | 1.62 | 0.81 |
| 43:SA0:215:TYR:HA | 67:SR0:84:PHE:CE2 | 2.16 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 54:SFF:93:LYS:HB3 | 54:SFF:94:PRO:HD2 | 1.63 | 0.81 |
| 1:L50:1728:U:HO2' | 42:S60:1259:U:HO2' | 1.05 | 0.81 |
| 1:L50:1691:A:C6 | 42:S60:1248:G:O4' | 2.34 | 0.81 |
| 56:SGG:65:PHE:CZ | 67:SR0:29:TYR:CE2 | 2.69 | 0.81 |
| 42:S60:1055:A:O3' | 47:SC0:84:ALA:HB2 | 1.81 | 0.80 |
| 49:SD0:101:LYS:NZ | 60:SK0:14:TYR:OH | 2.13 | 0.80 |
| 47:SC0:136:TRP:HH2 | 59:SJ0:59:ILE:HG21 | 1.46 | 0.80 |
| 47:SC0:230:ASN:HB2 | 71:SV0:24:GLN:OE1 | 1.80 | 0.80 |
| 66:SQ0:33:ASN:ND2 | 69:ST0:6:PHE:CD2 | 2.50 | 0.80 |
| 10:LE0:23:ILE:HD11 | 11:LEE:79:ARG:HH12 | 1.46 | 0.80 |
| 54:SFF:99:LYS:HE2 | 54:SFF:102:ILE:HG12 | 1.64 | 0.80 |
| 56:SGG:65:PHE:HE2 | 67:SR0:29:TYR:CE2 | 1.96 | 0.79 |
| 53:SF0:96:GLY:O | 75:SZ0:108:LEU:CD2 | 2.31 | 0.79 |
| 37:LW0:83:PHE:CE1 | 55:SG0:144:LYS:HG2 | 2.17 | 0.79 |
| 43:SA0:67:SER:CA | 71:SV0:28:VAL:HG13 | 2.13 | 0.79 |
| 50:SDD:8:TYR:N | 65:SP0:67:PHE:O | 2.14 | 0.79 |
| 42:S60:973:G:H22 | 44:SAA:90:TRP:HH2 | 1.27 | 0.79 |
| 37:LW0:83:PHE:CD1 | 55:SG0:144:LYS:HG3 | 2.17 | 0.79 |
| 42:S60:988:A:O2' | 43:SA0:105:PRO:O | 2.00 | 0.79 |
| 43:SA0:215:TYR:HA | 67:SR0:84:PHE:HD2 | 1.48 | 0.79 |
| 47:SC0:166:LYS:HD2 | 59:SJ0:100:GLU:OE2 | 1.83 | 0.78 |
| 34:LT0:126:PRO:HB2 | 34:LT0:128:LEU:CG | 2.13 | 0.78 |
| 43:SA0:52:LYS:HB2 | 67:SR0:109:TYR:CZ | 2.19 | 0.78 |
| 37:LW0:83:PHE:CG | 37:LW0:84:PRO:HD2 | 2.18 | 0.78 |
| 53:SF0:39:ILE:CG2 | 66:SQ0:50:GLU:HB2 | 2.11 | 0.78 |
| 50:SDD:12:LEU:CD1 | 65:SP0:75:ILE:CG2 | 2.62 | 0.78 |
| 42:S60:1188:A:H5'' | 66:SQ0:136:ALA:HB2 | 1.65 | 0.77 |
| 42:S60:1045:A:OP2 | 67:SR0:2:GLY:N | 2.17 | 0.77 |
| 43:SA0:63:ARG:O | 71:SV0:28:VAL:CG2 | 2.32 | 0.77 |
| 43:SA0:206:ARG:NE | 67:SR0:86:PRO:HG2 | 1.99 | 0.77 |
| 42:S60:1055:A:O3' | 47:SC0:84:ALA:CB | 2.33 | 0.77 |
| 43:SA0:118:GLU:OE2 | 47:SC0:31:THR:HA | 1.84 | 0.77 |
| 43:SA0:187:GLY:HA2 | 71:SV0:35:ARG:CZ | 2.14 | 0.77 |
| 1:L50:796:C:H5'' | 34:LT0:131:ARG:H | 1.48 | 0.77 |
| 3:LA0:241:ARG:CZ | 42:S60:592:G:H4' | 2.15 | 0.77 |
| 53:SF0:6:THR:HG23 | 66:SQ0:53:LYS:NZ | 2.00 | 0.77 |
| 55:SG0:169:VAL:CG1 | 55:SG0:176:LYS:HE2 | 2.14 | 0.77 |
| 53:SF0:40:LEU:HD23 | 66:SQ0:43:PHE:CE1 | 2.20 | 0.77 |
| 43:SA0:102:ARG:H | 43:SA0:102:ARG:HD2 | 1.49 | 0.76 |
| 43:SA0:215:TYR:HD1 | 67:SR0:84:PHE:CD2 | 2.03 | 0.76 |
| 1:L50:2497:C:H5'' | 5:LB0:280:THR:HG21 | 1.68 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 43:SA0:67:SER:HA | 71:SV0:28:VAL:HG13 | 1.66 | 0.76 |
| 48:SCC:58:ARG:HH12 | 64:SO0:101:ARG:NH2 | 1.82 | 0.76 |
| 55:SG0:170:ASN:HD21 | 55:SG0:176:LYS:HD3 | 1.50 | 0.76 |
| 1:L50:1695:A:C2 | 42:S60:1249:U:C5' | 2.66 | 0.76 |
| 44:SAA:47:ALA:HB1 | 48:SCC:61:ARG:HE | 1.49 | 0.76 |
| 50:SDD:12:LEU:CD2 | 65:SP0:67:PHE:HD2 | 1.98 | 0.76 |
| 1:L50:883:U:H5'' | 24:LM0:35:ASN:ND2 | 2.01 | 0.76 |
| 43:SA0:70:ASN:N | 47:SC0:240:ILE:HD11 | 2.00 | 0.76 |
| 42:S60:982:C:H4' | 67:SR0:10:ARG:NH1 | 2.01 | 0.75 |
| 43:SA0:52:LYS:HB2 | 67:SR0:109:TYR:CE1 | 2.21 | 0.75 |
| 43:SA0:120:ARG:NE | 47:SC0:232:ILE:HG21 | 2.02 | 0.75 |
| 49:SD0:238:PRO:CA | 67:SR0:19:ARG:HH12 | 1.98 | 0.75 |
| 43:SA0:64:MET:CB | 71:SV0:27:MET:HG2 | 2.17 | 0.74 |
| 37:LW0:98:ASN:ND2 | 55:SG0:147:PHE:CA | 2.48 | 0.74 |
| 37:LW0:98:ASN:HD22 | 55:SG0:147:PHE:HA | 1.52 | 0.74 |
| 42:S60:982:C:O3' | 67:SR0:10:ARG:NH1 | 2.21 | 0.74 |
| 56:SGG:228:LYS:NZ | 67:SR0:25:THR:HG22 | 2.02 | 0.74 |
| 42:S60:840:C:H4' | 42:S60:1182:G:H5'' | 1.68 | 0.74 |
| 44:SAA:51:ASP:OD2 | 48:SCC:57:GLU:O | 2.06 | 0.74 |
| 1:L50:883:U:H5'' | 24:LM0:35:ASN:HD21 | 1.51 | 0.74 |
| 43:SA0:52:LYS:CB | 67:SR0:109:TYR:CZ | 2.70 | 0.74 |
| 56:SGG:228:LYS:HZ2 | 67:SR0:25:THR:HG22 | 1.51 | 0.74 |
| 5:LB0:336:ARG:HG3 | 5:LB0:336:ARG:HH11 | 1.51 | 0.74 |
| 45:SB0:53:THR:HG22 | 64:SO0:30:ASP:OD2 | 1.88 | 0.73 |
| 53:SF0:96:GLY:O | 75:SZ0:108:LEU:HD21 | 1.88 | 0.73 |
| 1:L50:2052:A:H5' | 20:LJ0:62:ILE:HD11 | 1.69 | 0.73 |
| 42:S60:173:A:H8 | 51:SE0:131:VAL:HG12 | 1.50 | 0.73 |
| 37:LW0:99:LYS:CB | 37:LW0:102:LYS:HE2 | 2.18 | 0.73 |
| 2:L70:27:A:OP2 | 8:LD0:62:THR:HG23 | 1.88 | 0.73 |
| 43:SA0:141:ASN:C | 71:SV0:23:VAL:CG2 | 2.55 | 0.73 |
| 43:SA0:184:TYR:CE2 | 71:SV0:35:ARG:HD3 | 2.24 | 0.73 |
| 42:S60:173:A:C8 | 51:SE0:131:VAL:HG12 | 2.23 | 0.72 |
| 43:SA0:215:TYR:CD1 | 67:SR0:84:PHE:CD2 | 2.76 | 0.72 |
| 49:SD0:36:ARG:NH1 | 70:SU0:112:GLU:OE2 | 2.21 | 0.72 |
| 42:S60:203:G:N3 | 51:SE0:33:THR:CG2 | 2.51 | 0.72 |
| 2:L70:3:U:H3 | 2:L70:116:G:H1 | 1.37 | 0.72 |
| 68:SS0:20:MET:HG2 | 68:SS0:29:ASP:HA | 1.71 | 0.72 |
| 43:SA0:184:TYR:O | 71:SV0:35:ARG:CD | 2.36 | 0.72 |
| 41:MD1:106:TYR:CE1 | 64:SO0:47:LYS:NZ | 2.54 | 0.72 |
| 1:L50:1691:A:N1 | 42:S60:1248:G:O4' | 2.23 | 0.71 |
| 7:LCC:64:ILE:HG22 | 40:LZ0:39:LEU:HD11 | 1.72 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 42:S60:705:A:C2 | 42:S60:706:G:O6 | 2.43 | 0.71 |
| 43:SA0:52:LYS:HD2 | 67:SR0:109:TYR:CE1 | 2.25 | 0.71 |
| 42:S60:995:A:H3' | 42:S60:996:G:C8 | 2.24 | 0.71 |
| 42:S60:1034:A:H2' | 42:S60:1035:C:C6 | 2.26 | 0.71 |
| 42:S60:237:A:H5' | 58:SI0:48:VAL:CG1 | 2.21 | 0.71 |
| 53:SF0:40:LEU:CD2 | 66:SQ0:43:PHE:CD1 | 2.74 | 0.71 |
| 2:L70:63:A:H2' | 18:LI0:204:GLY:O | 1.91 | 0.70 |
| 53:SF0:95:THR:HG21 | 53:SF0:102:ILE:HG12 | 1.72 | 0.70 |
| 42:S60:1315:A:H2' | 42:S60:1316:A:H8 | 1.54 | 0.70 |
| 48:SCC:41:ILE:HG23 | 53:SF0:131:ASP:O | 1.90 | 0.70 |
| 53:SF0:6:THR:HG23 | 66:SQ0:53:LYS:HZ1 | 1.54 | 0.70 |
| 42:S60:982:C:O2' | 67:SR0:10:ARG:NH1 | 2.22 | 0.70 |
| 42:S60:1040:G:N2 | 42:S60:1042:A:H3' | 2.06 | 0.70 |
| 42:S60:438:U:H4' | 73:SX0:110:LYS:HD2 | 1.72 | 0.70 |
| 47:SC0:136:TRP:CH2 | 59:SJ0:59:ILE:HG21 | 2.23 | 0.70 |
| 42:S60:237:A:H5' | 58:SI0:48:VAL:HG13 | 1.74 | 0.69 |
| 42:S60:1158:U:O2' | 50:SDD:7:LYS:NZ | 2.18 | 0.69 |
| 45:SB0:53:THR:HG21 | 64:SO0:32:THR:OG1 | 1.92 | 0.69 |
| 68:SS0:24:PHE:CZ | 68:SS0:107:ILE:HG21 | 2.27 | 0.69 |
| 42:S60:854:U:OP2 | 68:SS0:148:GLY:N | 2.24 | 0.69 |
| 47:SC0:49:GLY:O | 71:SV0:6:ARG:HB2 | 1.92 | 0.69 |
| 1:L50:796:C:H5'' | 34:LT0:131:ARG:N | 2.06 | 0.69 |
| 53:SF0:92:GLU:HG3 | 75:SZ0:108:LEU:HD12 | 1.73 | 0.69 |
| 14:LG0:119:ASP:OD1 | 14:LG0:145:THR:HA | 1.92 | 0.69 |
| 26:LN0:112:ASN:HD22 | 26:LN0:112:ASN:H | 1.40 | 0.69 |
| 43:SA0:120:ARG:HH11 | 47:SC0:232:ILE:HG21 | 1.57 | 0.69 |
| 42:S60:666:A:OP1 | 63:SN0:132:LYS:NZ | 2.25 | 0.69 |
| 47:SC0:219:PRO:CB | 72:SW0:66:ARG:NH2 | 2.51 | 0.69 |
| 52:SEE:5:ILE:HD12 | 73:SX0:63:ILE:HD12 | 1.74 | 0.68 |
| 43:SA0:67:SER:HA | 71:SV0:28:VAL:CG1 | 2.22 | 0.68 |
| 10:LE0:55:GLU:CD | 10:LE0:117:ARG:HG3 | 2.14 | 0.68 |
| 42:S60:1056:A:OP1 | 47:SC0:84:ALA:HB1 | 1.93 | 0.68 |
| 42:S60:1035:C:H2' | 42:S60:1036:A:C8 | 2.29 | 0.68 |
| 51:SE0:64:ILE:HD12 | 74:SY0:23:LEU:HD13 | 1.75 | 0.68 |
| 53:SF0:42:HIS:HD1 | 66:SQ0:79:TYR:HH | 1.41 | 0.68 |
| 42:S60:1315:A:H2' | 42:S60:1316:A:C8 | 2.28 | 0.68 |
| 37:LW0:98:ASN:ND2 | 55:SG0:147:PHE:N | 2.43 | 0.67 |
| 42:S60:173:A:H8 | 51:SE0:131:VAL:CG1 | 2.04 | 0.67 |
| 49:SD0:94:GLN:HE21 | 60:SK0:19:SER:HB3 | 1.59 | 0.67 |
| 36:LV0:98:LEU:HD23 | 37:LW0:21:TYR:HB2 | 1.75 | 0.67 |
| 42:S60:705:A:C2 | 42:S60:706:G:C6 | 2.82 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 43:SA0:51:ILE:CG1 | 67:SR0:105:MET:SD | 2.82 | 0.67 |
| 43:SA0:67:SER:CB | 71:SV0:28:VAL:HG13 | 2.24 | 0.67 |
| 50:SDD:12:LEU:HD23 | 65:SP0:67:PHE:HD2 | 1.59 | 0.67 |
| 56:SGG:65:PHE:HZ | 67:SR0:29:TYR:OH | 1.77 | 0.67 |
| 43:SA0:118:GLU:CD | 47:SC0:31:THR:HG1 | 1.98 | 0.67 |
| 56:SGG:65:PHE:CZ | 67:SR0:29:TYR:CZ | 2.83 | 0.67 |
| 47:SC0:130:PRO:HB2 | 71:SV0:4:PHE:CE1 | 2.29 | 0.67 |
| 67:SR0:103:MET:CE | 67:SR0:117:LEU:HG | 2.25 | 0.67 |
| 1:L50:2045:C:H5' | 20:LJ0:102:GLY:HA3 | 1.77 | 0.66 |
| 20:LJ0:107:ILE:HD11 | 20:LJ0:113:TYR:HD1 | 1.60 | 0.66 |
| 42:S60:1066:G:C5 | 60:SK0:58:PHE:CD1 | 2.83 | 0.66 |
| 43:SA0:63:ARG:CD | 71:SV0:30:LEU:HD21 | 2.24 | 0.66 |
| 45:SB0:71:ARG:HD3 | 64:SO0:32:THR:HG21 | 1.78 | 0.66 |
| 47:SC0:166:LYS:CD | 59:SJ0:100:GLU:OE2 | 2.43 | 0.66 |
| 42:S60:826:U:O2 | 47:SC0:81:GLN:HB3 | 1.96 | 0.66 |
| 42:S60:958:A:OP1 | 47:SC0:111:ARG:NH2 | 2.28 | 0.66 |
| 1:L50:535:A:O2' | 31:LQ0:146:ASN:CB | 2.38 | 0.65 |
| 1:L50:535:A:HO2' | 31:LQ0:146:ASN:HB3 | 1.61 | 0.65 |
| 1:L50:1191:U:H2' | 1:L50:1192:A:H5'' | 1.77 | 0.65 |
| 42:S60:823:A:H2' | 42:S60:824:A:C8 | 2.31 | 0.65 |
| 1:L50:2109:G:H5'' | 1:L50:2109:G:H8 | 1.59 | 0.65 |
| 10:LE0:30:LEU:HD22 | 11:LEE:11:VAL:CG1 | 2.26 | 0.65 |
| 42:S60:914:U:H3 | 42:S60:918:A:N6 | 1.94 | 0.65 |
| 48:SCC:55:ASP:OD2 | 53:SF0:195:ARG:HD3 | 1.96 | 0.65 |
| 1:L50:1018:U:O2' | 13:LFF:78:ARG:HD2 | 1.97 | 0.65 |
| 42:S60:1230:U:O2' | 44:SAA:88:SER:HB3 | 1.96 | 0.65 |
| 42:S60:982:C:H4' | 67:SR0:10:ARG:HH11 | 1.62 | 0.65 |
| 42:S60:1144:G:C2' | 42:S60:1145:G:H5' | 2.27 | 0.64 |
| 42:S60:661:A:H4' | 63:SN0:62:LYS:HE2 | 1.78 | 0.64 |
| 42:S60:840:C:O2' | 42:S60:1182:G:OP1 | 2.14 | 0.64 |
| 47:SC0:136:TRP:HH2 | 59:SJ0:59:ILE:HG23 | 1.60 | 0.64 |
| 42:S60:892:A:N3 | 65:SP0:115:TYR:OH | 2.29 | 0.64 |
| 42:S60:910:A:H62 | 42:S60:922:G:H21 | 1.44 | 0.64 |
| 55:SG0:169:VAL:HG11 | 55:SG0:176:LYS:HE2 | 1.79 | 0.64 |
| 56:SGG:105:ARG:HH22 | 67:SR0:37:ASP:CA | 2.11 | 0.64 |
| 68:SS0:139:VAL:O | 68:SS0:139:VAL:HG12 | 1.96 | 0.64 |
| 51:SE0:137:PRO:HG3 | 55:SG0:222:TRP:HE1 | 1.63 | 0.64 |
| 55:SG0:147:PHE:HZ | 55:SG0:160:LYS:CE | 2.02 | 0.64 |
| 37:LW0:99:LYS:HG2 | 37:LW0:102:LYS:NZ | 2.13 | 0.64 |
| 42:S60:1066:G:C6 | 60:SK0:58:PHE:CZ | 2.84 | 0.64 |
| 42:S60:1091:A:O4' | 65:SP0:146:HIS:HD2 | 1.81 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 56:SGG:65:PHE:HZ | 67:SR0:29:TYR:HH | 1.42 | 0.64 |
| 34:LT0:5:HIS:HA | 34:LT0:9:ARG:HD2 | 1.80 | 0.64 |
| 1:L50:1691:A:C6 | 42:S60:1248:G:C4' | 2.80 | 0.64 |
| 68:SS0:24:PHE:O | 68:SS0:25:ASN:OD1 | 2.15 | 0.64 |
| 48:SCC:50:LEU:CD1 | 53:SF0:26:ILE:HD12 | 2.28 | 0.63 |
| 48:SCC:50:LEU:HD13 | 53:SF0:26:ILE:HD12 | 1.80 | 0.63 |
| 53:SF0:96:GLY:O | 75:SZ0:108:LEU:HD23 | 1.97 | 0.63 |
| 20:LJ0:107:ILE:HD11 | 20:LJ0:113:TYR:CD1 | 2.33 | 0.63 |
| 37:LW0:99:LYS:HG2 | 37:LW0:102:LYS:HE2 | 1.80 | 0.63 |
| 41:MD1:52:LYS:HG3 | 42:S60:606:G:C2 | 2.32 | 0.63 |
| 1:L50:1694:U:O4 | 42:S60:1249:U:H4' | 1.98 | 0.63 |
| 43:SA0:140:VAL:O | 43:SA0:141:ASN:OD1 | 2.17 | 0.63 |
| 49:SD0:184:ILE:HD11 | 49:SD0:230:MET:SD | 2.39 | 0.63 |
| 43:SA0:70:ASN:ND2 | 47:SC0:240:ILE:CG1 | 2.61 | 0.63 |
| 43:SA0:206:ARG:NE | 67:SR0:86:PRO:CG | 2.62 | 0.63 |
| 68:SS0:24:PHE:CE1 | 68:SS0:107:ILE:HG21 | 2.34 | 0.63 |
| 42:S60:1085:G:H5'' | 65:SP0:140:THR:HG21 | 1.81 | 0.63 |
| 49:SD0:33:ILE:HG21 | 70:SU0:26:LEU:HD21 | 1.79 | 0.63 |
| 37:LW0:99:LYS:HA | 37:LW0:102:LYS:CD | 2.27 | 0.63 |
| 42:S60:1105:G:H5'' | 42:S60:1105:G:C8 | 2.34 | 0.63 |
| 56:SGG:65:PHE:HZ | 67:SR0:29:TYR:CZ | 2.17 | 0.62 |
| 42:S60:1158:U:H4' | 50:SDD:7:LYS:HE3 | 1.81 | 0.62 |
| 67:SR0:3:GLN:HG3 | 67:SR0:3:GLN:O | 1.99 | 0.62 |
| 37:LW0:99:LYS:O | 37:LW0:102:LYS:HG2 | 1.97 | 0.62 |
| 42:S60:1160:A:H2' | 65:SP0:58:LYS:HD3 | 1.80 | 0.62 |
| 42:S60:1181:U:OP1 | 66:SQ0:142:TYR:HE2 | 1.82 | 0.61 |
| 37:LW0:83:PHE:CE1 | 37:LW0:84:PRO:HD2 | 2.34 | 0.61 |
| 42:S60:982:C:C3' | 67:SR0:10:ARG:NH1 | 2.63 | 0.61 |
| 43:SA0:184:TYR:CE1 | 71:SV0:35:ARG:NH1 | 2.69 | 0.61 |
| 47:SC0:49:GLY:O | 71:SV0:6:ARG:HD2 | 1.99 | 0.61 |
| 49:SD0:94:GLN:HE21 | 60:SK0:19:SER:CB | 2.11 | 0.61 |
| 2:L70:26:C:OP1 | 8:LD0:62:THR:HG21 | 2.01 | 0.61 |
| 55:SG0:169:VAL:HG12 | 55:SG0:176:LYS:HE2 | 1.82 | 0.61 |
| 42:S60:1099:U:H1' | 69:ST0:91:ASN:OD1 | 2.01 | 0.61 |
| 43:SA0:4:ARG:O | 71:SV0:30:LEU:CD1 | 2.47 | 0.61 |
| 42:S60:924:U:H1' | 42:S60:925:A:N7 | 2.16 | 0.61 |
| 43:SA0:52:LYS:HB3 | 67:SR0:109:TYR:CZ | 2.35 | 0.61 |
| 48:SCC:58:ARG:NH1 | 64:SO0:101:ARG:NH2 | 2.49 | 0.61 |
| 42:S60:1166:A:O2' | 68:SS0:90:TRP:O | 2.19 | 0.61 |
| 43:SA0:118:GLU:OE2 | 47:SC0:31:THR:OG1 | 2.18 | 0.61 |
| 53:SF0:40:LEU:O | 53:SF0:42:HIS:N | 2.33 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 42:S60:1143:A:H5' | 68:SS0:36:LYS:HE3 | 1.84 | 0.60 |
| 43:SA0:52:LYS:CB | 67:SR0:109:TYR:CE1 | 2.84 | 0.60 |
| 43:SA0:120:ARG:NH1 | 47:SC0:232:ILE:HG21 | 2.15 | 0.60 |
| 53:SF0:40:LEU:CD2 | 66:SQ0:43:PHE:HD1 | 2.12 | 0.60 |
| 62:SM0:67:SER:O | 62:SM0:71:LYS:HG2 | 2.01 | 0.60 |
| 42:S60:856:U:O4 | 68:SS0:146:SER:HB3 | 2.02 | 0.60 |
| 42:S60:1034:A:H2' | 42:S60:1035:C:H6 | 1.63 | 0.60 |
| 1:L50:2042:A:H61 | 1:L50:2054:U:H3 | 1.48 | 0.60 |
| 12:LF0:115:ASN:HD21 | 34:LT0:133:PRO:HB2 | 1.66 | 0.60 |
| 21:LJJ:90:ILE:HG22 | 21:LJJ:90:ILE:O | 2.02 | 0.60 |
| 42:S60:705:A:N3 | 42:S60:706:G:O6 | 2.35 | 0.60 |
| 53:SF0:90:ILE:HG23 | 75:SZ0:58:ILE:CD1 | 2.32 | 0.60 |
| 62:SM0:15:LEU:HB3 | 62:SM0:122:PHE:HE2 | 1.67 | 0.60 |
| 42:S60:918:A:C8 | 42:S60:919:C:C5 | 2.90 | 0.59 |
| 43:SA0:102:ARG:H | 43:SA0:102:ARG:CD | 2.15 | 0.59 |
| 42:S60:988:A:H4' | 43:SA0:105:PRO:HG2 | 1.83 | 0.59 |
| 43:SA0:51:ILE:HG13 | 67:SR0:105:MET:CE | 2.30 | 0.59 |
| 43:SA0:215:TYR:O | 67:SR0:84:PHE:CE2 | 2.51 | 0.59 |
| 68:SS0:24:PHE:O | 68:SS0:25:ASN:CG | 2.41 | 0.59 |
| 42:S60:924:U:H1' | 42:S60:925:A:C5 | 2.36 | 0.59 |
| 42:S60:1144:G:H2' | 42:S60:1145:G:H5' | 1.84 | 0.59 |
| 49:SD0:94:GLN:HG2 | 60:SK0:20:ILE:HG23 | 1.84 | 0.59 |
| 50:SDD:12:LEU:HD11 | 65:SP0:75:ILE:HD13 | 1.84 | 0.59 |
| 10:LE0:23:ILE:CD1 | 11:LEE:79:ARG:HH12 | 2.16 | 0.59 |
| 42:S60:999:C:H2' | 42:S60:1000:C:C6 | 2.37 | 0.59 |
| 43:SA0:18:GLN:HE22 | 67:SR0:96:VAL:HB | 1.67 | 0.59 |
| 49:SD0:238:PRO:CA | 67:SR0:19:ARG:NH1 | 2.63 | 0.59 |
| 37:LW0:99:LYS:HG2 | 37:LW0:102:LYS:CE | 2.33 | 0.59 |
| 50:SDD:34:PHE:CE1 | 60:SK0:61:GLN:NE2 | 2.70 | 0.59 |
| 1:L50:733:A:O3' | 12:LF0:124:LYS:NZ | 2.35 | 0.59 |
| 43:SA0:67:SER:OG | 71:SV0:40:LEU:HD21 | 2.01 | 0.59 |
| 42:S60:403:A:H2' | 42:S60:404:C:C6 | 2.37 | 0.59 |
| 47:SC0:148:VAL:CG2 | 72:SW0:97:PHE:HE1 | 2.15 | 0.59 |
| 54:SFF:96:GLN:O | 54:SFF:96:GLN:HG2 | 2.02 | 0.59 |
| 42:S60:405:A:H2' | 42:S60:406:U:C6 | 2.38 | 0.59 |
| 47:SC0:148:VAL:CG2 | 72:SW0:97:PHE:CE1 | 2.86 | 0.59 |
| 50:SDD:8:TYR:CZ | 65:SP0:72:ARG:CD | 2.84 | 0.59 |
| 10:LE0:30:LEU:CD2 | 11:LEE:11:VAL:HG13 | 2.33 | 0.58 |
| 7:LCC:64:ILE:CG2 | 40:LZ0:39:LEU:HD11 | 2.32 | 0.58 |
| 37:LW0:83:PHE:CD1 | 37:LW0:84:PRO:CD | 2.81 | 0.58 |
| 43:SA0:63:ARG:NH1 | 71:SV0:30:LEU:HG | 2.17 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 43:SA0:70:ASN:CA | 47:SC0:240:ILE:CD1 | 2.68 | 0.58 |
| 51:SE0:64:ILE:CD1 | 74:SY0:23:LEU:HD13 | 2.33 | 0.58 |
| 55:SG0:170:ASN:HD21 | 55:SG0:176:LYS:CD | 2.15 | 0.58 |
| 42:S60:203:G:C2 | 51:SE0:33:THR:HG21 | 2.38 | 0.58 |
| 42:S60:945:G:OP1 | 49:SD0:211:LYS:HE3 | 2.03 | 0.58 |
| 12:LF0:188:LYS:HE3 | 31:LQ0:2:LEU:HD23 | 1.85 | 0.58 |
| 42:S60:999:C:H42 | 42:S60:1049:G:H1 | 1.52 | 0.58 |
| 42:S60:1007:U:C4 | 56:SGG:84:ASP:OD2 | 2.56 | 0.58 |
| 42:S60:187:A:H62 | 42:S60:194:U:H3 | 1.51 | 0.58 |
| 37:LW0:99:LYS:HA | 37:LW0:102:LYS:HG2 | 1.85 | 0.58 |
| 42:S60:554:A:N3 | 72:SW0:103:THR:CG2 | 2.62 | 0.58 |
| 43:SA0:63:ARG:NH1 | 71:SV0:30:LEU:H | 2.01 | 0.58 |
| 53:SF0:90:ILE:HG23 | 75:SZ0:58:ILE:HD13 | 1.86 | 0.58 |
| 37:LW0:99:LYS:CG | 37:LW0:102:LYS:HE2 | 2.34 | 0.57 |
| 43:SA0:206:ARG:CZ | 67:SR0:86:PRO:HG2 | 2.34 | 0.57 |
| 53:SF0:40:LEU:HD23 | 66:SQ0:43:PHE:CD1 | 2.38 | 0.57 |
| 68:SS0:55:ARG:HH22 | 69:ST0:32:ASN:HD22 | 1.51 | 0.57 |
| 42:S60:1107:U:H5'' | 69:ST0:43:GLU:HG2 | 1.86 | 0.57 |
| 42:S60:1125:G:H2' | 42:S60:1126:A:O4' | 2.03 | 0.57 |
| 43:SA0:102:ARG:HD2 | 43:SA0:102:ARG:N | 2.16 | 0.57 |
| 43:SA0:120:ARG:NH1 | 47:SC0:232:ILE:HD13 | 2.19 | 0.57 |
| 51:SE0:152:PRO:HD2 | 55:SG0:219:TYR:CE1 | 2.40 | 0.57 |
| 44:SAA:69:TYR:HE2 | 64:SO0:90:LYS:O | 1.86 | 0.57 |
| 37:LW0:95:ARG:HG2 | 37:LW0:99:LYS:HE3 | 1.85 | 0.57 |
| 43:SA0:197:ARG:HB3 | 67:SR0:91:LEU:CB | 2.34 | 0.57 |
| 42:S60:1091:A:O4' | 65:SP0:146:HIS:CD2 | 2.57 | 0.57 |
| 43:SA0:66:CYS:HB2 | 71:SV0:28:VAL:HG21 | 1.86 | 0.57 |
| 42:S60:1160:A:H5' | 65:SP0:133:ARG:NH2 | 2.20 | 0.56 |
| 42:S60:203:G:H21 | 51:SE0:33:THR:HG21 | 1.70 | 0.56 |
| 1:L50:2596:G:O2' | 5:LB0:173:PRO:HG2 | 2.04 | 0.56 |
| 42:S60:1108:C:H5'' | 69:ST0:44:THR:O | 2.05 | 0.56 |
| 42:S60:1230:U:H4' | 44:SAA:88:SER:HB3 | 1.88 | 0.56 |
| 43:SA0:51:ILE:N | 67:SR0:105:MET:SD | 2.77 | 0.56 |
| 42:S60:864:A:N7 | 65:SP0:118:ARG:NH2 | 2.53 | 0.56 |
| 42:S60:923:A:H5' | 42:S60:924:U:C4 | 2.40 | 0.56 |
| 42:S60:982:C:C4' | 67:SR0:10:ARG:NH1 | 2.68 | 0.56 |
| 1:L50:1405:G:H2' | 1:L50:1406:G:C8 | 2.39 | 0.56 |
| 37:LW0:98:ASN:HD22 | 55:SG0:146:GLY:C | 2.08 | 0.56 |
| 49:SD0:237:LEU:O | 67:SR0:19:ARG:CZ | 2.53 | 0.56 |
| 1:L50:1691:A:C6 | 42:S60:1248:G:C1' | 2.87 | 0.56 |
| 42:S60:1290:G:H8 | 42:S60:1290:G:H5'' | 1.70 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 43:SA0:52:LYS:CD | 67:SR0:109:TYR:CE1 | 2.87 | 0.56 |
| 43:SA0:63:ARG:NE | 71:SV0:30:LEU:CG | 2.64 | 0.56 |
| 43:SA0:206:ARG:CD | 67:SR0:86:PRO:HG2 | 2.35 | 0.56 |
| 53:SF0:118:ARG:HD2 | 53:SF0:125:MET:CB | 2.34 | 0.56 |
| 41:MD1:106:TYR:CE2 | 41:MD1:108:GLU:HA | 2.41 | 0.56 |
| 42:S60:1007:U:O4 | 56:SGG:84:ASP:OD2 | 2.23 | 0.56 |
| 43:SA0:215:TYR:CA | 67:SR0:84:PHE:CE2 | 2.87 | 0.56 |
| 50:SDD:12:LEU:HD21 | 65:SP0:67:PHE:CE2 | 2.41 | 0.56 |
| 42:S60:1066:G:C6 | 60:SK0:58:PHE:CE1 | 2.94 | 0.56 |
| 42:S60:852:A:H2' | 42:S60:853:G:C8 | 2.41 | 0.55 |
| 55:SG0:170:ASN:HD21 | 55:SG0:176:LYS:CE | 2.19 | 0.55 |
| 1:L50:796:C:H5' | 34:LT0:131:ARG:HE | 1.70 | 0.55 |
| 42:S60:171:U:H5' | 42:S60:172:U:H2' | 1.88 | 0.55 |
| 43:SA0:70:ASN:HB2 | 47:SC0:240:ILE:HG13 | 1.76 | 0.55 |
| 42:S60:856:U:O4 | 68:SS0:146:SER:CB | 2.54 | 0.55 |
| 42:S60:1066:G:C5 | 60:SK0:58:PHE:CE1 | 2.95 | 0.55 |
| 42:S60:1055:A:O3' | 47:SC0:84:ALA:HB1 | 2.07 | 0.55 |
| 42:S60:1160:A:OP1 | 65:SP0:133:ARG:NH1 | 2.39 | 0.55 |
| 47:SC0:230:ASN:HB2 | 71:SV0:24:GLN:NE2 | 2.20 | 0.55 |
| 42:S60:932:A:H2' | 42:S60:933:G:C8 | 2.42 | 0.55 |
| 42:S60:1084:G:O3' | 65:SP0:99:ARG:HD3 | 2.06 | 0.55 |
| 50:SDD:12:LEU:HD12 | 65:SP0:75:ILE:HG21 | 1.86 | 0.55 |
| 42:S60:958:A:H3' | 42:S60:959:G:N2 | 2.16 | 0.55 |
| 42:S60:1089:G:O4' | 65:SP0:141:ARG:HD3 | 2.06 | 0.55 |
| 43:SA0:67:SER:HB2 | 71:SV0:28:VAL:HG13 | 1.88 | 0.55 |
| 51:SE0:54:VAL:HG22 | 74:SY0:23:LEU:HD11 | 1.88 | 0.55 |
| 42:S60:1150:G:H2' | 42:S60:1151:A:C8 | 2.42 | 0.55 |
| 43:SA0:68:ILE:HD12 | 43:SA0:121:LEU:HD22 | 1.89 | 0.55 |
| 47:SC0:130:PRO:HG2 | 71:SV0:4:PHE:CE1 | 2.42 | 0.55 |
| 47:SC0:229:LEU:HD12 | 71:SV0:42:ILE:HG12 | 1.89 | 0.55 |
| 37:LW0:83:PHE:CG | 55:SG0:144:LYS:HG3 | 2.42 | 0.54 |
| 43:SA0:10:ASP:CG | 67:SR0:112:ASN:HD21 | 2.10 | 0.54 |
| 48:SCC:44:PRO:O | 53:SF0:133:SER:CB | 2.55 | 0.54 |
| 50:SDD:7:LYS:HA | 65:SP0:67:PHE:O | 2.07 | 0.54 |
| 4:LAA:70:THR:HG21 | 19:LII:6:LEU:HG | 1.88 | 0.54 |
| 43:SA0:197:ARG:CB | 67:SR0:91:LEU:CB | 2.86 | 0.54 |
| 53:SF0:153:THR:HG21 | 53:SF0:160:LEU:HD13 | 1.88 | 0.54 |
| 42:S60:1181:U:OP1 | 66:SQ0:142:TYR:CE2 | 2.61 | 0.54 |
| 1:L50:1940:C:H2' | 1:L50:1941:A:C8 | 2.42 | 0.54 |
| 2:L70:60:A:H5' | 8:LD0:273:LYS:HG2 | 1.88 | 0.54 |
| 43:SA0:67:SER:HG | 71:SV0:40:LEU:HD22 | 1.71 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:L50:275:A:N6 | 6:LC0:163:ILE:CD1 | 2.71 | 0.54 |
| 37:LW0:83:PHE:CG | 55:SG0:144:LYS:HB3 | 2.43 | 0.54 |
| 42:S60:1056:A:H5' | 47:SC0:84:ALA:HA | 1.89 | 0.54 |
| 42:S60:1208:G:OP2 | 66:SQ0:127:LYS:HE3 | 2.07 | 0.54 |
| 10:LE0:30:LEU:HD22 | 11:LEE:11:VAL:HG13 | 1.89 | 0.54 |
| 42:S60:932:A:H3' | 42:S60:933:G:H8 | 1.73 | 0.54 |
| 50:SDD:34:PHE:CZ | 60:SK0:61:GLN:HG2 | 2.43 | 0.54 |
| 63:SN0:123:TYR:OH | 63:SN0:141:PRO:HG2 | 2.07 | 0.54 |
| 68:SS0:24:PHE:CZ | 68:SS0:107:ILE:HG12 | 2.42 | 0.54 |
| 42:S60:288:A:H5'' | 58:SI0:25:ARG:NH2 | 2.23 | 0.54 |
| 43:SA0:117:ARG:NH1 | 47:SC0:243:GLU:CD | 2.48 | 0.54 |
| 67:SR0:103:MET:HE1 | 67:SR0:117:LEU:HG | 1.90 | 0.54 |
| 42:S60:1066:G:N7 | 60:SK0:58:PHE:CG | 2.76 | 0.54 |
| 44:SAA:47:ALA:CB | 48:SCC:61:ARG:NE | 2.61 | 0.54 |
| 49:SD0:188:GLN:N | 49:SD0:189:PRO:HD2 | 2.23 | 0.54 |
| 42:S60:982:C:C3' | 67:SR0:10:ARG:HH11 | 2.22 | 0.53 |
| 37:LW0:83:PHE:CG | 55:SG0:144:LYS:CG | 2.90 | 0.53 |
| 42:S60:982:C:C4' | 67:SR0:10:ARG:HH11 | 2.21 | 0.53 |
| 42:S60:1010:G:OP1 | 70:SU0:52:LYS:NZ | 2.39 | 0.53 |
| 49:SD0:237:LEU:HD21 | 67:SR0:40:GLU:OE2 | 2.08 | 0.53 |
| 49:SD0:36:ARG:NH1 | 70:SU0:112:GLU:CD | 2.62 | 0.53 |
| 49:SD0:94:GLN:NE2 | 60:SK0:19:SER:OG | 2.42 | 0.53 |
| 24:LM0:70:ASP:O | 24:LM0:71:ILE:HG12 | 2.09 | 0.53 |
| 43:SA0:51:ILE:HG13 | 67:SR0:105:MET:HE3 | 1.91 | 0.53 |
| 47:SC0:130:PRO:HG2 | 71:SV0:4:PHE:HE1 | 1.74 | 0.53 |
| 74:SY0:116:ARG:NH2 | 74:SY0:120:LYS:HZ1 | 2.06 | 0.53 |
| 42:S60:1007:U:C5 | 56:SGG:84:ASP:OD2 | 2.62 | 0.53 |
| 68:SS0:28:ILE:CD1 | 68:SS0:40:THR:HB | 2.39 | 0.53 |
| 1:L50:2198:G:H1 | 1:L50:2226:U:H3 | 1.54 | 0.53 |
| 37:LW0:98:ASN:HD22 | 55:SG0:147:PHE:CA | 2.15 | 0.53 |
| 1:L50:22:U:OP2 | 39:LY0:11:ARG:NH1 | 2.39 | 0.53 |
| 1:L50:1738:G:N3 | 42:S60:1306:A:H2 | 2.06 | 0.53 |
| 1:L50:1880:U:H3 | 1:L50:1938:A:H61 | 1.56 | 0.53 |
| 42:S60:132:C:H3' | 42:S60:133:A:H8 | 1.72 | 0.53 |
| 20:LJ0:82:LYS:HB2 | 65:SP0:30:PHE:HE2 | 1.65 | 0.53 |
| 37:LW0:83:PHE:CD2 | 55:SG0:144:LYS:HB3 | 2.44 | 0.53 |
| 42:S60:918:A:N7 | 42:S60:919:C:C4 | 2.77 | 0.53 |
| 42:S60:1023:A:P | 67:SR0:3:GLN:CD | 2.87 | 0.53 |
| 42:S60:1023:A:H5'' | 67:SR0:3:GLN:HG2 | 1.90 | 0.53 |
| 43:SA0:51:ILE:HD12 | 67:SR0:105:MET:CG | 2.32 | 0.53 |
| 42:S60:1108:C:H4' | 69:ST0:46:PRO:HA | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 56:SGG:105:ARG:HH21 | 67:SR0:36:ILE:HG22 | 1.73 | 0.53 |
| 1:L50:1169:C:H1' | 1:L50:1170:A:H8 | 1.73 | 0.52 |
| 42:S60:1090:C:O2 | 65:SP0:146:HIS:CE1 | 2.62 | 0.52 |
| 42:S60:1160:A:OP1 | 65:SP0:62:SER:OG | 2.22 | 0.52 |
| 42:S60:1167:C:H2' | 42:S60:1168:A:O4' | 2.08 | 0.52 |
| 43:SA0:120:ARG:CZ | 47:SC0:232:ILE:HG21 | 2.39 | 0.52 |
| 42:S60:372:A:C4 | 59:SJ0:2:VAL:HG21 | 2.45 | 0.52 |
| 48:SCC:43:GLY:HA3 | 53:SF0:133:SER:OG | 2.09 | 0.52 |
| 1:L50:796:C:H4' | 34:LT0:131:ARG:O | 2.10 | 0.52 |
| 37:LW0:98:ASN:ND2 | 55:SG0:146:GLY:C | 2.63 | 0.52 |
| 42:S60:167:G:H21 | 42:S60:173:A:H2 | 1.55 | 0.52 |
| 42:S60:244:U:H2' | 42:S60:245:A:C8 | 2.44 | 0.52 |
| 42:S60:932:A:H3' | 42:S60:933:G:C8 | 2.44 | 0.52 |
| 42:S60:886:C:O2' | 50:SDD:26:THR:HB | 2.08 | 0.52 |
| 51:SE0:137:PRO:HG3 | 55:SG0:222:TRP:NE1 | 2.23 | 0.52 |
| 68:SS0:24:PHE:CE1 | 68:SS0:107:ILE:CG2 | 2.92 | 0.52 |
| 10:LE0:11:ILE:HD11 | 11:LEE:92:LEU:HD23 | 1.90 | 0.52 |
| 42:S60:203:G:N2 | 51:SE0:33:THR:HG21 | 2.25 | 0.52 |
| 48:SCC:44:PRO:O | 53:SF0:133:SER:HB2 | 2.09 | 0.52 |
| 53:SF0:40:LEU:HD23 | 66:SQ0:43:PHE:HE1 | 1.73 | 0.52 |
| 55:SG0:176:LYS:HD2 | 55:SG0:176:LYS:N | 2.25 | 0.52 |
| 68:SS0:139:VAL:O | 68:SS0:139:VAL:CG1 | 2.57 | 0.52 |
| 12:LF0:69:LYS:HD3 | 34:LT0:141:GLU:HG2 | 1.91 | 0.52 |
| 42:S60:864:A:C8 | 65:SP0:118:ARG:NH2 | 2.77 | 0.52 |
| 12:LF0:70:ILE:HG12 | 34:LT0:144:MET:HG3 | 1.92 | 0.52 |
| 37:LW0:81:ARG:HH12 | 55:SG0:148:SER:HB2 | 1.74 | 0.52 |
| 42:S60:1181:U:H4' | 66:SQ0:140:LYS:O | 2.09 | 0.52 |
| 53:SF0:92:GLU:HG3 | 75:SZ0:108:LEU:CD1 | 2.40 | 0.52 |
| 64:SO0:27:HIS:CE1 | 64:SO0:36:THR:HG23 | 2.45 | 0.52 |
| 3:LA0:89:LEU:HD13 | 30:LPP:83:ILE:CD1 | 2.39 | 0.52 |
| 37:LW0:83:PHE:CG | 37:LW0:84:PRO:CD | 2.92 | 0.52 |
| 42:S60:1056:A:P | 47:SC0:84:ALA:HB1 | 2.49 | 0.52 |
| 37:LW0:99:LYS:C | 37:LW0:102:LYS:HG2 | 2.30 | 0.52 |
| 43:SA0:184:TYR:CZ | 71:SV0:35:ARG:HD3 | 2.44 | 0.52 |
| 1:L50:290:C:O3' | 39:LY0:33:PRO:HG3 | 2.09 | 0.52 |
| 1:L50:401:A:N1 | 6:LC0:80:THR:HG22 | 2.24 | 0.52 |
| 2:L70:27:A:OP2 | 8:LD0:62:THR:CG2 | 2.57 | 0.52 |
| 1:L50:2596:G:H5' | 1:L50:2597:G:H5'' | 1.92 | 0.51 |
| 12:LF0:115:ASN:ND2 | 34:LT0:133:PRO:HB2 | 2.24 | 0.51 |
| 1:L50:555:G:H1' | 6:LC0:71:ARG:HH11 | 1.75 | 0.51 |
| 43:SA0:18:GLN:HE22 | 67:SR0:96:VAL:CB | 2.23 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 43:SA0:63:ARG:CD | 71:SV0:30:LEU:HG | 2.39 | 0.51 |
| 50:SDD:12:LEU:HD13 | 65:SP0:75:ILE:CG2 | 2.41 | 0.51 |
| 59:SJ0:100:GLU:OE1 | 59:SJ0:103:LEU:HD12 | 2.11 | 0.51 |
| 43:SA0:215:TYR:C | 67:SR0:84:PHE:HE2 | 2.14 | 0.51 |
| 53:SF0:40:LEU:HD21 | 66:SQ0:43:PHE:HD1 | 1.76 | 0.51 |
| 1:L50:1942:U:H2' | 1:L50:1943:C:C5 | 2.46 | 0.51 |
| 34:LT0:112:ASN:C | 34:LT0:112:ASN:HD22 | 2.12 | 0.51 |
| 42:S60:823:A:H2' | 42:S60:824:A:H8 | 1.73 | 0.51 |
| 1:L50:1131:U:H3 | 1:L50:1135:G:H1 | 1.57 | 0.51 |
| 37:LW0:99:LYS:HA | 37:LW0:102:LYS:CG | 2.40 | 0.51 |
| 41:MD1:42:LEU:HG | 41:MD1:73:ILE:HD11 | 1.91 | 0.51 |
| 42:S60:1143:A:C4 | 68:SS0:36:LYS:HB2 | 2.46 | 0.51 |
| 42:S60:1152:G:OP1 | 65:SP0:36:LYS:NZ | 2.37 | 0.51 |
| 1:L50:2544:U:OP1 | 5:LB0:375:THR:HG22 | 2.11 | 0.51 |
| 4:LAA:74:ASN:HD22 | 4:LAA:112:GLY:H | 1.59 | 0.51 |
| 42:S60:966:G:H2' | 42:S60:967:A:C8 | 2.46 | 0.51 |
| 33:LS0:14:ASP:CG | 33:LS0:15:ASP:H | 2.15 | 0.50 |
| 41:MD1:33:ASN:ND2 | 64:SO0:56:TYR:CE2 | 2.80 | 0.50 |
| 42:S60:995:A:H2' | 42:S60:996:G:O4' | 2.10 | 0.50 |
| 42:S60:1315:A:C2 | 42:S60:1316:A:N6 | 2.79 | 0.50 |
| 43:SA0:51:ILE:CD1 | 67:SR0:105:MET:CE | 2.89 | 0.50 |
| 45:SB0:53:THR:CG2 | 64:SO0:32:THR:OG1 | 2.58 | 0.50 |
| 56:SGG:65:PHE:CE2 | 67:SR0:29:TYR:CZ | 2.99 | 0.50 |
| 1:L50:1328:A:H62 | 1:L50:1367:A:H61 | 1.59 | 0.50 |
| 53:SF0:92:GLU:CG | 75:SZ0:108:LEU:HD12 | 2.41 | 0.50 |
| 56:SGG:105:ARG:HH22 | 67:SR0:37:ASP:CB | 2.24 | 0.50 |
| 1:L50:396:G:N3 | 1:L50:396:G:H5'' | 2.26 | 0.50 |
| 42:S60:139:C:O3' | 55:SG0:95:LYS:NZ | 2.45 | 0.50 |
| 42:S60:1066:G:N7 | 60:SK0:58:PHE:CD1 | 2.79 | 0.50 |
| 51:SE0:70:ILE:HD13 | 51:SE0:92:ILE:HG12 | 1.92 | 0.50 |
| 1:L50:562:U:H5'' | 1:L50:562:U:H6 | 1.76 | 0.50 |
| 42:S60:834:G:H5' | 44:SAA:85:ARG:HD2 | 1.93 | 0.50 |
| 47:SC0:216:PHE:HZ | 72:SW0:128:TYR:HD1 | 1.59 | 0.50 |
| 68:SS0:10:PHE:HD1 | 75:SZ0:81:PHE:CD2 | 2.30 | 0.50 |
| 45:SB0:71:ARG:HB3 | 64:SO0:32:THR:HG21 | 1.93 | 0.50 |
| 1:L50:1089:U:H2' | 1:L50:1090:A:C8 | 2.47 | 0.50 |
| 42:S60:923:A:H5' | 42:S60:924:U:N3 | 2.27 | 0.50 |
| 42:S60:926:G:H2' | 42:S60:927:G:N7 | 2.26 | 0.50 |
| 42:S60:1167:C:H4' | 68:SS0:91:MET:O | 2.12 | 0.50 |
| 43:SA0:52:LYS:HD2 | 67:SR0:109:TYR:CD1 | 2.47 | 0.50 |
| 3:LA0:88:GLU:HG2 | 30:LPP:87:LYS:HE2 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 42:S60:55:G:H5' | 74:SY0:123:ARG:HH11 | 1.77 | 0.50 |
| 42:S60:832:A:H2' | 42:S60:833:A:C8 | 2.47 | 0.50 |
| 55:SG0:170:ASN:ND2 | 55:SG0:176:LYS:HD3 | 2.22 | 0.50 |
| 56:SGG:65:PHE:HE2 | 67:SR0:29:TYR:CD2 | 2.29 | 0.50 |
| 1:L50:1601:A:H4' | 3:LA0:170:LEU:O | 2.11 | 0.49 |
| 37:LW0:99:LYS:CA | 37:LW0:102:LYS:HG2 | 2.42 | 0.49 |
| 42:S60:1149:U:C5 | 68:SS0:140:ARG:NH2 | 2.79 | 0.49 |
| 42:S60:1216:U:H2' | 42:S60:1217:G:C8 | 2.47 | 0.49 |
| 42:S60:1019:C:H2' | 42:S60:1020:G:C8 | 2.47 | 0.49 |
| 47:SC0:229:LEU:HB2 | 71:SV0:42:ILE:HD11 | 1.94 | 0.49 |
| 10:LE0:23:ILE:HD11 | 11:LEE:79:ARG:NH1 | 2.21 | 0.49 |
| 53:SF0:90:ILE:O | 53:SF0:94:VAL:HG23 | 2.12 | 0.49 |
| 1:L50:2473:G:OP1 | 16:LH0:72:LYS:HG3 | 2.12 | 0.49 |
| 42:S60:1124:A:H2' | 42:S60:1125:G:C8 | 2.46 | 0.49 |
| 42:S60:1160:A:C2' | 65:SP0:58:LYS:HD3 | 2.41 | 0.49 |
| 1:L50:1441:U:H4' | 38:LX0:64:ILE:HD11 | 1.95 | 0.49 |
| 1:L50:2051:C:C6 | 20:LJ0:56:ILE:HD11 | 2.48 | 0.49 |
| 67:SR0:36:ILE:HD11 | 67:SR0:44:LYS:NZ | 2.27 | 0.49 |
| 70:SU0:116:THR:C | 70:SU0:117:LEU:HG | 2.32 | 0.49 |
| 49:SD0:34:LYS:HE3 | 70:SU0:60:PHE:HB3 | 1.93 | 0.49 |
| 42:S60:1083:U:O2' | 65:SP0:97:ASN:ND2 | 2.46 | 0.49 |
| 49:SD0:237:LEU:O | 67:SR0:19:ARG:NH1 | 2.45 | 0.49 |
| 53:SF0:6:THR:CG2 | 66:SQ0:53:LYS:HZ1 | 2.23 | 0.49 |
| 53:SF0:158:LYS:HA | 75:SZ0:62:THR:HG21 | 1.95 | 0.49 |
| 1:L50:2108:U:H6 | 1:L50:2108:U:H5'' | 1.78 | 0.49 |
| 42:S60:917:U:H5' | 42:S60:918:A:N3 | 2.27 | 0.49 |
| 42:S60:1066:G:O6 | 60:SK0:58:PHE:CE2 | 2.66 | 0.49 |
| 54:SFF:99:LYS:HE2 | 54:SFF:102:ILE:CG1 | 2.40 | 0.49 |
| 56:SGG:105:ARG:HH22 | 67:SR0:37:ASP:HB2 | 1.78 | 0.49 |
| 56:SGG:121:THR:HG21 | 56:SGG:131:TRP:CH2 | 2.47 | 0.49 |
| 42:S60:999:C:H2' | 42:S60:1000:C:H6 | 1.76 | 0.49 |
| 16:LH0:63:GLU:OE2 | 27:LO0:131:ILE:HG21 | 2.13 | 0.49 |
| 1:L50:2447:A:H5'' | 1:L50:2447:A:H8 | 1.78 | 0.48 |
| 42:S60:65:A:H62 | 42:S60:75:G:H21 | 1.60 | 0.48 |
| 42:S60:377:C:OP1 | 59:SJ0:150:PRO:HD2 | 2.13 | 0.48 |
| 42:S60:995:A:C2' | 42:S60:996:G:H5' | 2.43 | 0.48 |
| 42:S60:1126:A:H8 | 42:S60:1164:G:H21 | 1.61 | 0.48 |
| 56:SGG:105:ARG:NH2 | 67:SR0:36:ILE:HG22 | 2.28 | 0.48 |
| 1:L50:399:G:O6 | 6:LC0:57:ARG:NH1 | 2.46 | 0.48 |
| 1:L50:486:U:H2' | 1:L50:487:A:C8 | 2.48 | 0.48 |
| 14:LG0:17:ARG:NH1 | 26:LN0:32:GLN:HE22 | 2.11 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 42:S60:237:A:C5' | 58:SI0:48:VAL:HG13 | 2.43 | 0.48 |
| 42:S60:899:A:O2' | 60:SK0:50:SER:OG | 2.18 | 0.48 |
| 45:SB0:71:ARG:HB3 | 64:SO0:32:THR:CG2 | 2.43 | 0.48 |
| 47:SC0:166:LYS:CE | 59:SJ0:100:GLU:OE2 | 2.61 | 0.48 |
| 51:SE0:92:ILE:HG22 | 51:SE0:94:LYS:O | 2.13 | 0.48 |
| 75:SZ0:41:VAL:HG21 | 75:SZ0:78:LEU:HD22 | 1.93 | 0.48 |
| 1:L50:1691:A:C2 | 42:S60:1317:G:N2 | 2.81 | 0.48 |
| 3:LA0:238:LYS:HZ3 | 42:S60:714:U:P | 2.37 | 0.48 |
| 42:S60:126:C:H2' | 42:S60:127:A:C8 | 2.48 | 0.48 |
| 42:S60:236:U:O2 | 58:SI0:5:ARG:NH1 | 2.46 | 0.48 |
| 42:S60:1091:A:C8 | 65:SP0:146:HIS:CD2 | 3.01 | 0.48 |
| 1:L50:1424:A:H5' | 15:LGG:77:GLY:HA3 | 1.94 | 0.48 |
| 53:SF0:96:GLY:C | 75:SZ0:108:LEU:HD21 | 2.34 | 0.48 |
| 1:L50:1643:G:H1 | 1:L50:1672:A:H61 | 1.61 | 0.48 |
| 42:S60:1208:G:C2' | 42:S60:1209:C:H5' | 2.44 | 0.48 |
| 42:S60:404:C:H4' | 74:SY0:37:ASN:HA | 1.95 | 0.48 |
| 44:SAA:47:ALA:HB2 | 48:SCC:61:ARG:HE | 1.71 | 0.48 |
| 16:LH0:7:GLU:OE2 | 16:LH0:9:LYS:HE3 | 2.13 | 0.48 |
| 42:S60:1209:C:H2' | 42:S60:1210:G:C8 | 2.49 | 0.48 |
| 42:S60:1262:A:H3' | 42:S60:1263:A:H8 | 1.79 | 0.48 |
| 68:SS0:46:ASP:OD1 | 68:SS0:47:ARG:N | 2.43 | 0.48 |
| 42:S60:1165:C:H2' | 42:S60:1166:A:C8 | 2.48 | 0.48 |
| 53:SF0:6:THR:CG2 | 66:SQ0:53:LYS:NZ | 2.74 | 0.48 |
| 42:S60:125:A:H2' | 42:S60:126:C:C6 | 2.49 | 0.48 |
| 42:S60:662:U:H1' | 63:SN0:52:ASN:ND2 | 2.29 | 0.48 |
| 42:S60:1260:G:H1 | 42:S60:1303:U:H3 | 1.61 | 0.48 |
| 1:L50:1325:G:H22 | 1:L50:1370:U:H3 | 1.62 | 0.47 |
| 41:MD1:52:LYS:HG3 | 42:S60:606:G:H22 | 1.78 | 0.47 |
| 42:S60:911:G:H8 | 42:S60:911:G:OP2 | 1.97 | 0.47 |
| 50:SDD:8:TYR:CE2 | 65:SP0:72:ARG:NE | 2.82 | 0.47 |
| 42:S60:1068:U:H5' | 49:SD0:207:ILE:HD11 | 1.96 | 0.47 |
| 43:SA0:215:TYR:CA | 67:SR0:84:PHE:HE2 | 2.26 | 0.47 |
| 47:SC0:230:ASN:N | 71:SV0:24:GLN:NE2 | 2.45 | 0.47 |
| 1:L50:1609:G:N2 | 1:L50:1614:G:O2' | 2.47 | 0.47 |
| 42:S60:1151:A:C2 | 42:S60:1152:G:H1' | 2.49 | 0.47 |
| 43:SA0:52:LYS:HB2 | 67:SR0:109:TYR:CE2 | 2.49 | 0.47 |
| 49:SD0:68:HIS:NE2 | 70:SU0:109:THR:O | 2.47 | 0.47 |
| 50:SDD:43:TYR:CE2 | 70:SU0:62:CYS:HB2 | 2.49 | 0.47 |
| 42:S60:999:C:H2' | 42:S60:1000:C:O4' | 2.14 | 0.47 |
| 1:L50:1878:G:H2' | 1:L50:1879:A:C8 | 2.50 | 0.47 |
| 42:S60:997:A:H3' | 42:S60:998:U:C5 | 2.50 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 8:LD0:215:LYS:HE2 | 8:LD0:222:PHE:CE2 | 2.49 | 0.47 |
| 42:S60:1140:G:H5' | 42:S60:1143:A:N7 | 2.29 | 0.47 |
| 43:SA0:215:TYR:CD1 | 67:SR0:84:PHE:CZ | 3.01 | 0.47 |
| 47:SC0:216:PHE:HZ | 72:SW0:128:TYR:CD1 | 2.33 | 0.47 |
| 47:SC0:233:LEU:HD13 | 71:SV0:26:ASN:ND2 | 2.30 | 0.47 |
| 55:SG0:144:LYS:N | 55:SG0:144:LYS:HD2 | 2.30 | 0.47 |
| 68:SS0:112:GLU:O | 68:SS0:116:ARG:HG2 | 2.15 | 0.47 |
| 1:L50:2060:A:N3 | 1:L50:2060:A:H2' | 2.30 | 0.47 |
| 1:L50:2116:A:H2' | 1:L50:2117:A:C8 | 2.49 | 0.47 |
| 42:S60:932:A:C6 | 42:S60:933:G:C6 | 3.03 | 0.47 |
| 43:SA0:10:ASP:CB | 67:SR0:112:ASN:HD21 | 2.28 | 0.47 |
| 43:SA0:118:GLU:CD | 47:SC0:31:THR:OG1 | 2.51 | 0.47 |
| 47:SC0:50:HIS:O | 71:SV0:6:ARG:NH2 | 2.48 | 0.47 |
| 1:L50:1869:A:H5' | 26:LN0:24:ARG:HD2 | 1.96 | 0.47 |
| 1:L50:2109:G:H5'' | 1:L50:2109:G:C8 | 2.45 | 0.47 |
| 3:LA0:238:LYS:HD3 | 42:S60:714:U:H5' | 1.96 | 0.47 |
| 20:LJ0:8:ASN:HD22 | 20:LJ0:149:GLN:HE22 | 1.61 | 0.47 |
| 42:S60:916:G:H5' | 42:S60:916:G:H8 | 1.80 | 0.47 |
| 42:S60:967:A:O5' | 42:S60:967:A:H8 | 1.97 | 0.47 |
| 42:S60:1168:A:H3' | 42:S60:1169:G:H8 | 1.79 | 0.47 |
| 37:LW0:95:ARG:O | 37:LW0:99:LYS:HG3 | 2.14 | 0.47 |
| 42:S60:1110:C:H5' | 69:ST0:54:THR:HG22 | 1.97 | 0.47 |
| 46:SBB:24:PHE:CZ | 72:SW0:51:ILE:HG23 | 2.49 | 0.47 |
| 68:SS0:10:PHE:CD1 | 75:SZ0:81:PHE:CD2 | 3.03 | 0.47 |
| 42:S60:349:A:OP1 | 51:SE0:57:ASN:ND2 | 2.48 | 0.46 |
| 42:S60:384:A:C2 | 59:SJ0:169:ARG:HB2 | 2.50 | 0.46 |
| 42:S60:910:A:H62 | 42:S60:922:G:N2 | 2.11 | 0.46 |
| 49:SD0:36:ARG:NH1 | 70:SU0:112:GLU:OE1 | 2.48 | 0.46 |
| 37:LW0:98:ASN:CG | 55:SG0:147:PHE:HA | 2.35 | 0.46 |
| 42:S60:909:G:O6 | 62:SM0:37:ARG:HB3 | 2.15 | 0.46 |
| 42:S60:1018:U:H4' | 42:S60:1019:C:OP2 | 2.15 | 0.46 |
| 1:L50:303:C:H2' | 1:L50:304:U:C6 | 2.51 | 0.46 |
| 42:S60:995:A:C8 | 42:S60:996:G:C8 | 3.03 | 0.46 |
| 42:S60:1012:A:HO2' | 42:S60:1013:A:H8 | 1.61 | 0.46 |
| 42:S60:1035:C:H2' | 42:S60:1036:A:H8 | 1.74 | 0.46 |
| 43:SA0:120:ARG:HE | 47:SC0:232:ILE:HG22 | 1.75 | 0.46 |
| 47:SC0:233:LEU:HD13 | 71:SV0:26:ASN:CG | 2.35 | 0.46 |
| 31:LQ0:21:ARG:HB3 | 31:LQ0:57:THR:HG21 | 1.98 | 0.46 |
| 10:LE0:39:ILE:HG22 | 13:LFF:107:ASN:ND2 | 2.30 | 0.46 |
| 42:S60:507:C:H2' | 42:S60:508:A:C8 | 2.50 | 0.46 |
| 42:S60:958:A:OP1 | 47:SC0:111:ARG:CZ | 2.63 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 42:S60:970:U:H5'' | 42:S60:970:U:H6 | 1.80 | 0.46 |
| 42:S60:997:A:C2 | 42:S60:998:U:H1' | 2.50 | 0.46 |
| 54:SFF:128:VAL:HG21 | 54:SFF:141:ARG:HE | 1.80 | 0.46 |
| 42:S60:86:A:H1' | 51:SE0:7:LYS:HD2 | 1.97 | 0.46 |
| 42:S60:131:U:H2' | 42:S60:132:C:C6 | 2.51 | 0.46 |
| 1:L50:2140:A:O2' | 1:L50:2141:U:H2' | 2.15 | 0.46 |
| 42:S60:396:A:H2' | 42:S60:397:A:C8 | 2.51 | 0.46 |
| 42:S60:964:G:N2 | 42:S60:966:G:H3' | 2.31 | 0.46 |
| 42:S60:1085:G:C5' | 65:SP0:140:THR:HG21 | 2.44 | 0.46 |
| 43:SA0:10:ASP:HB3 | 67:SR0:112:ASN:OD1 | 2.16 | 0.46 |
| 51:SE0:183:LEU:HD22 | 51:SE0:191:CYS:HB2 | 1.98 | 0.46 |
| 57:SH0:121:GLY:HA3 | 72:SW0:41:LYS:HG3 | 1.96 | 0.46 |
| 22:LL0:25:GLN:HB3 | 22:LL0:26:PRO:HD3 | 1.97 | 0.46 |
| 42:S60:466:C:H4' | 73:SX0:100:GLU:HG2 | 1.97 | 0.46 |
| 42:S60:1194:U:H2' | 42:S60:1196:U:C5 | 2.51 | 0.46 |
| 37:LW0:99:LYS:O | 37:LW0:102:LYS:CG | 2.64 | 0.46 |
| 41:MD1:52:LYS:CG | 42:S60:606:G:N2 | 2.74 | 0.46 |
| 42:S60:1085:G:H4' | 65:SP0:140:THR:CG2 | 2.46 | 0.46 |
| 42:S60:244:U:H2' | 42:S60:245:A:H8 | 1.81 | 0.45 |
| 42:S60:517:U:H5' | 51:SE0:219:SER:O | 2.15 | 0.45 |
| 42:S60:989:G:H5' | 43:SA0:104:ILE:HG23 | 1.98 | 0.45 |
| 63:SN0:66:VAL:HG23 | 63:SN0:67:THR:HG23 | 1.97 | 0.45 |
| 68:SS0:20:MET:CE | 68:SS0:29:ASP:OD1 | 2.63 | 0.45 |
| 1:L50:1308:A:H61 | 1:L50:2434:A:H2 | 1.63 | 0.45 |
| 6:LC0:322:VAL:O | 12:LF0:140:ARG:NH2 | 2.49 | 0.45 |
| 29:LP0:30:ARG:HD3 | 29:LP0:30:ARG:C | 2.36 | 0.45 |
| 42:S60:706:G:N3 | 42:S60:706:G:C2' | 2.74 | 0.45 |
| 42:S60:864:A:N1 | 65:SP0:118:ARG:HB2 | 2.31 | 0.45 |
| 42:S60:864:A:C4 | 65:SP0:118:ARG:HD3 | 2.52 | 0.45 |
| 43:SA0:63:ARG:CG | 71:SV0:30:LEU:CD2 | 2.67 | 0.45 |
| 68:SS0:24:PHE:CE2 | 68:SS0:107:ILE:HG12 | 2.52 | 0.45 |
| 68:SS0:55:ARG:HH22 | 69:ST0:32:ASN:ND2 | 2.13 | 0.45 |
| 2:L70:1:A:H61 | 2:L70:118:U:H3 | 1.63 | 0.45 |
| 4:LAA:127:GLN:HE22 | 19:LII:7:ASN:H | 1.63 | 0.45 |
| 6:LC0:103:VAL:HG13 | 22:LL0:23:PHE:CZ | 2.52 | 0.45 |
| 10:LE0:11:ILE:HD12 | 11:LEE:91:ALA:HB1 | 1.99 | 0.45 |
| 37:LW0:83:PHE:HB2 | 55:SG0:144:LYS:HG3 | 1.97 | 0.45 |
| 42:S60:63:G:H2' | 42:S60:76:A:C2 | 2.50 | 0.45 |
| 42:S60:864:A:C2 | 65:SP0:118:ARG:HB2 | 2.52 | 0.45 |
| 1:L50:2267:C:O2 | 1:L50:2267:C:O4' | 2.33 | 0.45 |
| 42:S60:705:A:C2 | 42:S60:706:G:N1 | 2.83 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 42:S60:1109:A:H2' | 42:S60:1110:C:C6 | 2.52 | 0.45 |
| 43:SA0:85:LYS:NZ | 67:SR0:82:GLU:OE2 | 2.48 | 0.45 |
| 49:SD0:239:ILE:CA | 67:SR0:19:ARG:NH1 | 2.77 | 0.45 |
| 1:L50:1691:A:H61 | 42:S60:1248:G:C4' | 2.25 | 0.45 |
| 42:S60:1010:G:OP1 | 70:SU0:52:LYS:CE | 2.65 | 0.45 |
| 43:SA0:197:ARG:HD3 | 67:SR0:91:LEU:CB | 2.46 | 0.45 |
| 42:S60:55:G:H5' | 74:SY0:123:ARG:NH1 | 2.32 | 0.45 |
| 47:SC0:148:VAL:HG21 | 72:SW0:97:PHE:CE1 | 2.51 | 0.45 |
| 1:L50:1032:A:H8 | 1:L50:1032:A:H5'' | 1.82 | 0.45 |
| 29:LP0:70:THR:HG22 | 29:LP0:72:GLN:H | 1.81 | 0.45 |
| 43:SA0:52:LYS:HB2 | 67:SR0:109:TYR:CD1 | 2.51 | 0.45 |
| 54:SFF:96:GLN:N | 54:SFF:96:GLN:OE1 | 2.50 | 0.45 |
| 65:SP0:132:ARG:NH2 | 68:SS0:127:LEU:HD22 | 2.32 | 0.45 |
| 42:S60:171:U:H5' | 42:S60:172:U:H6 | 1.82 | 0.45 |
| 42:S60:1121:A:H3' | 42:S60:1122:A:H8 | 1.82 | 0.45 |
| 49:SD0:34:LYS:HD3 | 70:SU0:62:CYS:HB3 | 1.98 | 0.45 |
| 1:L50:188:G:OP2 | 4:LAA:34:LYS:HG2 | 2.17 | 0.45 |
| 42:S60:661:A:H5' | 63:SN0:15:VAL:O | 2.17 | 0.45 |
| 43:SA0:64:MET:HB3 | 71:SV0:27:MET:CG | 2.28 | 0.45 |
| 47:SC0:50:HIS:HA | 71:SV0:6:ARG:HD2 | 1.98 | 0.45 |
| 1:L50:202:G:O2' | 17:LHH:105:THR:HG22 | 2.16 | 0.44 |
| 2:L70:70:U:H3 | 2:L70:105:G:H1 | 1.65 | 0.44 |
| 34:LT0:126:PRO:HB2 | 34:LT0:128:LEU:CD2 | 2.47 | 0.44 |
| 42:S60:1082:A:H2' | 42:S60:1083:U:C6 | 2.52 | 0.44 |
| 43:SA0:218:GLN:HB3 | 67:SR0:84:PHE:CE2 | 2.51 | 0.44 |
| 48:SCC:45:ILE:HG12 | 53:SF0:133:SER:HB3 | 1.99 | 0.44 |
| 51:SE0:175:LEU:HD22 | 51:SE0:222:PHE:CD1 | 2.52 | 0.44 |
| 42:S60:478:C:O2 | 61:SL0:93:LYS:HE2 | 2.17 | 0.44 |
| 43:SA0:117:ARG:CZ | 47:SC0:243:GLU:OE2 | 2.65 | 0.44 |
| 74:SY0:116:ARG:CZ | 74:SY0:120:LYS:NZ | 2.80 | 0.44 |
| 12:LF0:69:LYS:HG3 | 34:LT0:142:MET:O | 2.17 | 0.44 |
| 24:LM0:71:ILE:O | 24:LM0:71:ILE:HG13 | 2.18 | 0.44 |
| 42:S60:997:A:H3' | 42:S60:998:U:C6 | 2.53 | 0.44 |
| 42:S60:1167:C:H4' | 68:SS0:91:MET:C | 2.38 | 0.44 |
| 47:SC0:130:PRO:CB | 71:SV0:4:PHE:CE1 | 2.98 | 0.44 |
| 35:LU0:39:ILE:HG23 | 35:LU0:48:LEU:HD21 | 2.00 | 0.44 |
| 47:SC0:148:VAL:HG21 | 72:SW0:97:PHE:CZ | 2.53 | 0.44 |
| 64:SO0:27:HIS:HE1 | 64:SO0:36:THR:HG23 | 1.82 | 0.44 |
| 1:L50:1885:G:H1 | 1:L50:1933:C:H42 | 1.66 | 0.44 |
| 42:S60:431:G:H2' | 42:S60:445:U:N3 | 2.32 | 0.44 |
| 42:S60:662:U:H1' | 63:SN0:52:ASN:HD21 | 1.83 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:L50:2416:G:H5'' | 1:L50:2416:G:H8 | 1.82 | 0.44 |
| 6:LC0:328:ILE:HG13 | 12:LF0:53:ILE:HG22 | 1.99 | 0.44 |
| 43:SA0:214:LEU:HD13 | 67:SR0:86:PRO:HG3 | 2.00 | 0.44 |
| 50:SDD:16:PHE:HE1 | 65:SP0:66:GLY:HA3 | 1.82 | 0.44 |
| 58:SI0:69:THR:HG21 | 61:SL0:22:TYR:CE2 | 2.52 | 0.44 |
| 1:L50:158:A:N6 | 1:L50:168:G:H1' | 2.32 | 0.44 |
| 5:LB0:133:LEU:H | 5:LB0:133:LEU:HG | 1.69 | 0.44 |
| 42:S60:1144:G:O2' | 42:S60:1145:G:H5' | 2.17 | 0.44 |
| 42:S60:1199:C:OP2 | 50:SDD:41:ARG:NH2 | 2.47 | 0.44 |
| 1:L50:2551:C:H2' | 1:L50:2552:G:O4' | 2.18 | 0.43 |
| 17:LHH:113:LYS:HE2 | 22:LL0:46:ASN:HD22 | 1.83 | 0.43 |
| 41:MD1:17:ILE:HD12 | 41:MD1:95:TYR:CD2 | 2.53 | 0.43 |
| 43:SA0:63:ARG:CD | 71:SV0:30:LEU:CG | 2.95 | 0.43 |
| 67:SR0:36:ILE:HD11 | 67:SR0:44:LYS:HZ2 | 1.83 | 0.43 |
| 26:LN0:14:LYS:HE2 | 26:LN0:120:TRP:CZ3 | 2.53 | 0.43 |
| 41:MD1:106:TYR:HE2 | 41:MD1:108:GLU:HA | 1.83 | 0.43 |
| 42:S60:1107:U:H2' | 42:S60:1108:C:C6 | 2.53 | 0.43 |
| 42:S60:1230:U:O3' | 44:SAA:88:SER:HA | 2.18 | 0.43 |
| 3:LA0:238:LYS:NZ | 42:S60:714:U:H5'' | 2.32 | 0.43 |
| 27:LO0:84:LYS:HE2 | 27:LO0:89:HIS:CD2 | 2.54 | 0.43 |
| 42:S60:1085:G:OP1 | 65:SP0:99:ARG:NE | 2.46 | 0.43 |
| 42:S60:1149:U:C5 | 68:SS0:140:ARG:CZ | 3.00 | 0.43 |
| 47:SC0:148:VAL:HG22 | 72:SW0:94:SER:HB2 | 2.00 | 0.43 |
| 47:SC0:167:GLY:HA3 | 59:SJ0:103:LEU:O | 2.17 | 0.43 |
| 49:SD0:30:ALA:HB2 | 70:SU0:60:PHE:CE2 | 2.53 | 0.43 |
| 68:SS0:24:PHE:CE2 | 68:SS0:79:ILE:HG21 | 2.53 | 0.43 |
| 70:SU0:116:THR:O | 70:SU0:117:LEU:HG | 2.18 | 0.43 |
| 1:L50:2525:G:H5' | 29:LP0:71:PRO:HD3 | 2.00 | 0.43 |
| 1:L50:2462:A:H2' | 1:L50:2463:A:C8 | 2.54 | 0.43 |
| 37:LW0:98:ASN:HD22 | 55:SG0:147:PHE:N | 2.10 | 0.43 |
| 42:S60:50:U:H2' | 42:S60:51:G:C8 | 2.54 | 0.43 |
| 42:S60:94:U:H3' | 42:S60:263:A:H61 | 1.83 | 0.43 |
| 42:S60:933:G:H8 | 42:S60:933:G:O5' | 2.02 | 0.43 |
| 72:SW0:26:ARG:O | 72:SW0:26:ARG:HG2 | 2.18 | 0.43 |
| 74:SY0:116:ARG:NH1 | 74:SY0:120:LYS:HZ2 | 2.16 | 0.43 |
| 11:LEE:133:LEU:HG | 11:LEE:133:LEU:O | 2.19 | 0.43 |
| 14:LG0:174:PHE:CE2 | 14:LG0:178:ILE:HD11 | 2.53 | 0.43 |
| 44:SAA:51:ASP:OD2 | 48:SCC:57:GLU:C | 2.57 | 0.43 |
| 42:S60:914:U:C5 | 42:S60:916:G:C5 | 3.06 | 0.43 |
| 42:S60:916:G:O3' | 42:S60:917:U:O2 | 2.37 | 0.43 |
| 43:SA0:50:ASP:OD1 | 67:SR0:109:TYR:OH | 2.33 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:SE0:54:VAL:CG2 | 74:SY0:23:LEU:HD11 | 2.47 | 0.43 |
| 58:SI0:123:ASP:HB2 | 61:SL0:22:TYR:HE1 | 1.84 | 0.43 |
| 1:L50:21:U:H5' | 1:L50:1087:G:OP1 | 2.19 | 0.43 |
| 1:L50:88:A:H5' | 21:LJJ:75:ALA:HB2 | 2.01 | 0.43 |
| 1:L50:1089:U:H2' | 1:L50:1090:A:H8 | 1.84 | 0.43 |
| 1:L50:1875:G:H2' | 1:L50:1876:A:C8 | 2.53 | 0.43 |
| 42:S60:926:G:H2' | 42:S60:927:G:C8 | 2.54 | 0.43 |
| 1:L50:555:G:H1' | 6:LC0:71:ARG:NH1 | 2.34 | 0.43 |
| 6:LC0:2:SER:O | 6:LC0:3:ARG:HG2 | 2.19 | 0.43 |
| 42:S60:173:A:N7 | 51:SE0:131:VAL:CG1 | 2.82 | 0.43 |
| 42:S60:218:A:H4' | 42:S60:219:U:H5'' | 2.00 | 0.43 |
| 42:S60:1033:A:H2' | 42:S60:1034:A:H5' | 2.00 | 0.43 |
| 43:SA0:43:GLU:HG2 | 67:SR0:120:LYS:HE2 | 2.01 | 0.43 |
| 49:SD0:94:GLN:NE2 | 60:SK0:19:SER:HB3 | 2.32 | 0.43 |
| 58:SI0:69:THR:HG22 | 61:SL0:20:ASN:OD1 | 2.18 | 0.43 |
| 43:SA0:50:ASP:OD1 | 67:SR0:109:TYR:CE2 | 2.72 | 0.43 |
| 1:L50:597:A:H4' | 63:SN0:123:TYR:CD1 | 2.53 | 0.42 |
| 4:LAA:144:VAL:HG21 | 22:LL0:163:TYR:O | 2.19 | 0.42 |
| 47:SC0:166:LYS:O | 59:SJ0:103:LEU:HB3 | 2.18 | 0.42 |
| 58:SI0:68:LYS:HE2 | 58:SI0:152:TYR:CD2 | 2.54 | 0.42 |
| 62:SM0:15:LEU:CB | 62:SM0:122:PHE:HE2 | 2.31 | 0.42 |
| 1:L50:1933:C:H2' | 1:L50:1934:C:C6 | 2.55 | 0.42 |
| 12:LF0:69:LYS:HD3 | 34:LT0:141:GLU:CG | 2.49 | 0.42 |
| 37:LW0:67:HIS:HB2 | 42:S60:1282:A:N3 | 2.34 | 0.42 |
| 42:S60:705:A:H2' | 42:S60:707:A:N7 | 2.34 | 0.42 |
| 1:L50:1325:G:H1 | 1:L50:1370:U:H3 | 1.67 | 0.42 |
| 1:L50:1441:U:H4' | 38:LX0:64:ILE:CD1 | 2.49 | 0.42 |
| 5:LB0:265:ARG:NH1 | 27:LO0:62:SER:OG | 2.53 | 0.42 |
| 42:S60:1107:U:H2' | 42:S60:1108:C:H6 | 1.84 | 0.42 |
| 42:S60:1208:G:H2' | 42:S60:1209:C:H5' | 2.01 | 0.42 |
| 43:SA0:33:LEU:HD13 | 43:SA0:150:THR:HA | 2.00 | 0.42 |
| 49:SD0:94:GLN:NE2 | 60:SK0:19:SER:CB | 2.81 | 0.42 |
| 67:SR0:103:MET:SD | 67:SR0:117:LEU:HG | 2.59 | 0.42 |
| 1:L50:1691:A:H62 | 42:S60:1248:G:H4' | 1.71 | 0.42 |
| 42:S60:517:U:C5' | 51:SE0:219:SER:O | 2.66 | 0.42 |
| 42:S60:790:G:H5'' | 42:S60:790:G:H8 | 1.84 | 0.42 |
| 49:SD0:34:LYS:CE | 70:SU0:60:PHE:HB3 | 2.49 | 0.42 |
| 74:SY0:116:ARG:CZ | 74:SY0:120:LYS:HZ2 | 2.33 | 0.42 |
| 42:S60:189:A:H2' | 42:S60:190:A:H4' | 2.01 | 0.42 |
| 42:S60:502:A:O3' | 72:SW0:4:LYS:NZ | 2.52 | 0.42 |
| 42:S60:696:G:H1 | 42:S60:712:A:H2 | 1.68 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 42:S60:1160:A:P | 65:SP0:62:SER:HG | 2.41 | 0.42 |
| 42:S60:1262:A:C8 | 42:S60:1262:A:H5'' | 2.54 | 0.42 |
| 42:S60:1023:A:P | 67:SR0:3:GLN:OE1 | 2.78 | 0.42 |
| 1:L50:145:A:H5'' | 21:LJJ:46:LYS:HD2 | 2.01 | 0.42 |
| 1:L50:1298:A:H5' | 1:L50:1299:A:OP2 | 2.20 | 0.42 |
| 1:L50:2170:A:C8 | 28:LOO:54:PRO:HB3 | 2.55 | 0.42 |
| 17:LHH:6:LYS:HG3 | 17:LHH:7:ASP:OD1 | 2.19 | 0.42 |
| 42:S60:954:G:H5' | 42:S60:980:G:OP1 | 2.20 | 0.42 |
| 47:SC0:130:PRO:CG | 71:SV0:4:PHE:CE1 | 3.03 | 0.42 |
| 42:S60:1024:G:C2 | 42:S60:1025:G:C8 | 3.08 | 0.42 |
| 42:S60:1230:U:O3' | 44:SAA:88:SER:CB | 2.68 | 0.42 |
| 43:SA0:215:TYR:CE1 | 67:SR0:84:PHE:CZ | 3.08 | 0.42 |
| 56:SGG:147:ASN:N | 56:SGG:147:ASN:HD22 | 2.17 | 0.42 |
| 1:L50:32:G:H21 | 1:L50:377:A:H62 | 1.66 | 0.42 |
| 1:L50:1698:A:H1' | 42:S60:1247:C:H1' | 2.01 | 0.42 |
| 1:L50:1936:U:HO2' | 1:L50:1937:G:H8 | 1.66 | 0.42 |
| 1:L50:2160:G:H5'' | 28:LOO:65:LYS:HD2 | 2.02 | 0.42 |
| 1:L50:2492:U:H2' | 1:L50:2493:G:C8 | 2.55 | 0.42 |
| 1:L50:2573:U:H2' | 1:L50:2574:A:C8 | 2.55 | 0.42 |
| 42:S60:864:A:C6 | 65:SP0:118:ARG:HB2 | 2.55 | 0.42 |
| 42:S60:1231:U:H4' | 44:SAA:86:VAL:CG1 | 2.50 | 0.42 |
| 50:SDD:7:LYS:CA | 65:SP0:67:PHE:O | 2.68 | 0.42 |
| 57:SH0:53:LEU:HB3 | 57:SH0:54:PRO:HD3 | 2.02 | 0.42 |
| 63:SN0:128:TYR:HE1 | 63:SN0:132:LYS:HZ2 | 1.66 | 0.42 |
| 1:L50:1691:A:C2 | 42:S60:1248:G:H1' | 2.55 | 0.42 |
| 17:LHH:66:LEU:HD12 | 38:LX0:22:ILE:HD11 | 2.01 | 0.42 |
| 31:LQ0:164:TYR:CE2 | 31:LQ0:177:ARG:HD2 | 2.55 | 0.42 |
| 47:SC0:228:GLU:O | 71:SV0:42:ILE:HG21 | 2.20 | 0.42 |
| 1:L50:2610:U:H2' | 1:L50:2611:C:C6 | 2.55 | 0.41 |
| 42:S60:132:C:H3' | 42:S60:133:A:C8 | 2.53 | 0.41 |
| 42:S60:995:A:C3' | 42:S60:996:G:H8 | 2.23 | 0.41 |
| 43:SA0:10:ASP:CB | 67:SR0:112:ASN:OD1 | 2.67 | 0.41 |
| 28:LOO:64:LYS:HB3 | 28:LOO:64:LYS:HE2 | 1.92 | 0.41 |
| 42:S60:375:G:H8 | 42:S60:375:G:H5'' | 1.86 | 0.41 |
| 42:S60:1054:G:H2' | 42:S60:1055:A:O4' | 2.21 | 0.41 |
| 47:SC0:149:LYS:HB3 | 72:SW0:93:PRO:HA | 2.01 | 0.41 |
| 65:SP0:132:ARG:CZ | 68:SS0:127:LEU:HD22 | 2.50 | 0.41 |
| 1:L50:1296:C:H6 | 1:L50:1296:C:H5'' | 1.85 | 0.41 |
| 18:LI0:30:LYS:HE2 | 18:LI0:66:GLU:HG2 | 2.02 | 0.41 |
| 42:S60:830:G:O3' | 42:S60:831:G:H8 | 2.02 | 0.41 |
| 42:S60:995:A:H2' | 42:S60:996:G:H5' | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 42:S60:996:G:H2' | 42:S60:997:A:O4' | 2.20 | 0.41 |
| 42:S60:1108:C:H5' | 69:ST0:44:THR:OG1 | 2.20 | 0.41 |
| 49:SD0:184:ILE:HD12 | 49:SD0:215:MET:CE | 2.50 | 0.41 |
| 42:S60:552:G:O2' | 72:SW0:105:SER:HB3 | 2.20 | 0.41 |
| 42:S60:1262:A:H61 | 42:S60:1301:U:H3 | 1.68 | 0.41 |
| 53:SF0:49:THR:O | 53:SF0:49:THR:HG22 | 2.20 | 0.41 |
| 61:SL0:144:ILE:HD13 | 61:SL0:147:LYS:HE2 | 2.03 | 0.41 |
| 62:SM0:15:LEU:C | 62:SM0:15:LEU:HD12 | 2.41 | 0.41 |
| 1:L50:2026:G:C2 | 28:LOO:5:PRO:HG2 | 2.55 | 0.41 |
| 42:S60:924:U:H1' | 42:S60:925:A:C8 | 2.55 | 0.41 |
| 43:SA0:184:TYR:CD2 | 71:SV0:35:ARG:HD3 | 2.54 | 0.41 |
| 1:L50:222:A:H2' | 1:L50:223:A:C8 | 2.55 | 0.41 |
| 8:LD0:214:LEU:HD23 | 8:LD0:214:LEU:HA | 1.94 | 0.41 |
| 42:S60:574:A:H1' | 46:SBB:67:GLY:CA | 2.51 | 0.41 |
| 42:S60:1168:A:H3' | 42:S60:1169:G:C8 | 2.55 | 0.41 |
| 62:SM0:15:LEU:HB3 | 62:SM0:122:PHE:CE2 | 2.52 | 0.41 |
| 1:L50:1642:G:H2' | 1:L50:1643:G:C8 | 2.56 | 0.41 |
| 1:L50:2211:A:H5'' | 1:L50:2212:G:N2 | 2.35 | 0.41 |
| 42:S60:156:U:H2' | 42:S60:157:A:C8 | 2.55 | 0.41 |
| 1:L50:885:G:H5'' | 1:L50:885:G:H8 | 1.86 | 0.41 |
| 6:LC0:323:GLU:HG2 | 6:LC0:324:ILE:N | 2.36 | 0.41 |
| 10:LE0:17:TYR:CE1 | 11:LEE:79:ARG:HD3 | 2.56 | 0.41 |
| 21:LJJ:40:PRO:O | 38:LX0:3:LYS:HE3 | 2.21 | 0.41 |
| 37:LW0:102:LYS:HB3 | 55:SG0:150:ASP:HB3 | 2.03 | 0.41 |
| 42:S60:999:C:O2' | 42:S60:1000:C:H5' | 2.20 | 0.41 |
| 46:SBB:81:ILE:CD1 | 63:SN0:25:TYR:HB2 | 2.51 | 0.41 |
| 49:SD0:184:ILE:HD12 | 49:SD0:215:MET:HE3 | 2.03 | 0.41 |
| 1:L50:506:G:H2' | 1:L50:508:A:N7 | 2.36 | 0.41 |
| 1:L50:1133:C:H4' | 1:L50:1134:A:H5' | 2.02 | 0.41 |
| 42:S60:967:A:H5'' | 42:S60:968:C:C6 | 2.55 | 0.41 |
| 42:S60:999:C:C4 | 42:S60:1000:C:C4 | 3.09 | 0.41 |
| 47:SC0:166:LYS:CB | 59:SJ0:100:GLU:OE2 | 2.69 | 0.41 |
| 51:SE0:35:PRO:HD2 | 51:SE0:83:PRO:HG2 | 2.03 | 0.41 |
| 56:SGG:65:PHE:HZ | 67:SR0:29:TYR:CE2 | 2.27 | 0.41 |
| 1:L50:763:U:H2' | 1:L50:764:U:O4' | 2.21 | 0.40 |
| 1:L50:2473:G:H2' | 1:L50:2474:A:O4' | 2.21 | 0.40 |
| 17:LHH:66:LEU:CD1 | 38:LX0:22:ILE:HD11 | 2.51 | 0.40 |
| 42:S60:933:G:C8 | 42:S60:933:G:O5' | 2.74 | 0.40 |
| 73:SX0:41:ALA:HA | 73:SX0:42:PRO:HD3 | 1.98 | 0.40 |
| 42:S60:1090:C:O2 | 65:SP0:146:HIS:HE1 | 2.02 | 0.40 |
| 44:SAA:51:ASP:OD2 | 48:SCC:58:ARG:HA | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 47:SC0:230:ASN:CB | 71:SV0:24:GLN:NE2 | 2.84 | 0.40 |
| 55:SG0:156:GLU:O | 55:SG0:160:LYS:HG3 | 2.20 | 0.40 |
| 1:L50:158:A:H61 | 1:L50:168:G:H1' | 1.87 | 0.40 |
| 1:L50:1940:C:H2' | 1:L50:1941:A:H8 | 1.86 | 0.40 |
| 36:LV0:75:ARG:HH22 | 42:S60:1261:G:H5' | 1.86 | 0.40 |
| 42:S60:1022:C:N3 | 42:S60:1024:G:C8 | 2.89 | 0.40 |
| 43:SA0:118:GLU:OE2 | 47:SC0:31:THR:CA | 2.61 | 0.40 |
| 1:L50:885:G:H5'' | 1:L50:885:G:C8 | 2.56 | 0.40 |
| 14:LG0:16:PRO:HG2 | 26:LN0:32:GLN:HE21 | 1.86 | 0.40 |
| 16:LH0:129:THR:HG22 | 16:LH0:150:VAL:HG22 | 2.04 | 0.40 |
| 42:S60:405:A:H2' | 42:S60:406:U:H6 | 1.84 | 0.40 |
| 42:S60:1023:A:H5'' | 67:SR0:3:GLN:CG | 2.52 | 0.40 |
| 43:SA0:51:ILE:CG1 | 67:SR0:105:MET:CE | 2.99 | 0.40 |
| 43:SA0:215:TYR:CG | 67:SR0:84:PHE:CE2 | 3.05 | 0.40 |
| 53:SF0:95:THR:CG2 | 53:SF0:169:ILE:HG12 | 2.52 | 0.40 |
| 1:L50:101:C:H2' | 1:L50:102:A:C8 | 2.56 | 0.40 |
| 1:L50:401:A:N1 | 6:LC0:80:THR:CG2 | 2.84 | 0.40 |
| 3:LA0:20:HIS:CD2 | 3:LA0:21:LYS:HG3 | 2.57 | 0.40 |
| 6:LC0:308:MET:HE3 | 12:LF0:155:LYS:HB3 | 2.02 | 0.40 |
| 42:S60:641:A:H2' | 42:S60:642:A:C8 | 2.57 | 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 | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 3 | LA0 | 243/246 (99%) | 236 (97%) | 7 (3%) | 0 | 100 | 100 |
| 4 | LAA | 145/147 (99%) | 142 (98%) | 3 (2%) | 0 | 100 | 100 |
| 5 | LB0 | 381/392 (97%) | 372 (98%) | 9 (2%) | 0 | 100 | 100 |
| 6 | LC0 | 325/328 (99%) | 313 (96%) | 11 (3%) | 1 (0%) | 37 | 73 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 7 | LCC | 97/110 (88%) | 94 (97%) | 2 (2%) | 1 (1%) | 13 | 49 |
| 8 | LD0 | 279/291 (96%) | 274 (98%) | 5 (2%) | 0 | 100 | 100 |
| 9 | LDD | 107/110 (97%) | 104 (97%) | 3 (3%) | 0 | 100 | 100 |
| 10 | LE0 | 163/171 (95%) | 154 (94%) | 9 (6%) | 0 | 100 | 100 |
| 11 | LEE | 133/139 (96%) | 127 (96%) | 6 (4%) | 0 | 100 | 100 |
| 12 | LF0 | 229/235 (97%) | 224 (98%) | 5 (2%) | 0 | 100 | 100 |
| 13 | LFF | 109/111 (98%) | 106 (97%) | 3 (3%) | 0 | 100 | 100 |
| 14 | LG0 | 197/206 (96%) | 194 (98%) | 3 (2%) | 0 | 100 | 100 |
| 15 | LGG | 102/106 (96%) | 96 (94%) | 5 (5%) | 1 (1%) | 13 | 49 |
| 16 | LH0 | 181/187 (97%) | 177 (98%) | 4 (2%) | 0 | 100 | 100 |
| 17 | LHH | 117/119 (98%) | 109 (93%) | 8 (7%) | 0 | 100 | 100 |
| 18 | LI0 | 215/218 (99%) | 214 (100%) | 1 (0%) | 0 | 100 | 100 |
| 19 | LII | 95/98 (97%) | 91 (96%) | 4 (4%) | 0 | 100 | 100 |
| 20 | LJ0 | 165/171 (96%) | 155 (94%) | 10 (6%) | 0 | 100 | 100 |
| 21 | LJJ | 87/92 (95%) | 86 (99%) | 1 (1%) | 0 | 100 | 100 |
| 22 | LL0 | 162/165 (98%) | 155 (96%) | 6 (4%) | 1 (1%) | 22 | 60 |
| 23 | LLL | 49/52 (94%) | 48 (98%) | 1 (2%) | 0 | 100 | 100 |
| 24 | LM0 | 113/115 (98%) | 106 (94%) | 6 (5%) | 1 (1%) | 14 | 52 |
| 25 | LMM | 50/127 (39%) | 50 (100%) | 0 | 0 | 100 | 100 |
| 26 | LN0 | 201/204 (98%) | 195 (97%) | 6 (3%) | 0 | 100 | 100 |
| 27 | LO0 | 196/198 (99%) | 193 (98%) | 3 (2%) | 0 | 100 | 100 |
| 28 | LOO | 98/104 (94%) | 96 (98%) | 2 (2%) | 0 | 100 | 100 |
| 29 | LP0 | 152/167 (91%) | 145 (95%) | 7 (5%) | 0 | 100 | 100 |
| 30 | LPP | 85/89 (96%) | 80 (94%) | 4 (5%) | 1 (1%) | 11 | 44 |
| 31 | LQ0 | 180/183 (98%) | 175 (97%) | 5 (3%) | 0 | 100 | 100 |
| 32 | LR0 | 162/168 (96%) | 160 (99%) | 2 (1%) | 0 | 100 | 100 |
| 33 | LS0 | 168/171 (98%) | 159 (95%) | 9 (5%) | 0 | 100 | 100 |
| 34 | LT0 | 154/158 (98%) | 145 (94%) | 9 (6%) | 0 | 100 | 100 |
| 35 | LU0 | 98/113 (87%) | 93 (95%) | 5 (5%) | 0 | 100 | 100 |
| 36 | LV0 | 139/142 (98%) | 137 (99%) | 2 (1%) | 0 | 100 | 100 |
| 37 | LW0 | 100/131 (76%) | 93 (93%) | 6 (6%) | 1 (1%) | 13 | 49 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 38 | LX0 | 110/113 (97%) | 106 (96%) | 4 (4%) | 0 | 100 | 100 |
| 39 | LY0 | 129/131 (98%) | 123 (95%) | 6 (5%) | 0 | 100 | 100 |
| 40 | LZ0 | 116/153 (76%) | 116 (100%) | 0 | 0 | 100 | 100 |
| 41 | MD1 | 149/151 (99%) | 144 (97%) | 5 (3%) | 0 | 100 | 100 |
| 43 | SA0 | 218/233 (94%) | 206 (94%) | 12 (6%) | 0 | 100 | 100 |
| 44 | SAA | 99/102 (97%) | 98 (99%) | 1 (1%) | 0 | 100 | 100 |
| 45 | SB0 | 202/230 (88%) | 197 (98%) | 5 (2%) | 0 | 100 | 100 |
| 46 | SBB | 79/82 (96%) | 77 (98%) | 2 (2%) | 0 | 100 | 100 |
| 47 | SC0 | 224/248 (90%) | 220 (98%) | 4 (2%) | 0 | 100 | 100 |
| 48 | SCC | 60/65 (92%) | 57 (95%) | 3 (5%) | 0 | 100 | 100 |
| 49 | SD0 | 214/242 (88%) | 212 (99%) | 2 (1%) | 0 | 100 | 100 |
| 50 | SDD | 63/65 (97%) | 58 (92%) | 5 (8%) | 0 | 100 | 100 |
| 51 | SE0 | 258/280 (92%) | 247 (96%) | 11 (4%) | 0 | 100 | 100 |
| 52 | SEE | 54/60 (90%) | 53 (98%) | 1 (2%) | 0 | 100 | 100 |
| 53 | SF0 | 190/195 (97%) | 180 (95%) | 10 (5%) | 0 | 100 | 100 |
| 54 | SFF | 56/150 (37%) | 52 (93%) | 4 (7%) | 0 | 100 | 100 |
| 55 | SG0 | 227/230 (99%) | 214 (94%) | 13 (6%) | 0 | 100 | 100 |
| 56 | SGG | 315/326 (97%) | 295 (94%) | 19 (6%) | 1 (0%) | 37 | 73 |
| 57 | SH0 | 161/164 (98%) | 156 (97%) | 4 (2%) | 1 (1%) | 22 | 60 |
| 58 | SI0 | 165/173 (95%) | 161 (98%) | 4 (2%) | 0 | 100 | 100 |
| 59 | SJ0 | 166/184 (90%) | 165 (99%) | 1 (1%) | 0 | 100 | 100 |
| 60 | SK0 | 86/107 (80%) | 81 (94%) | 4 (5%) | 1 (1%) | 11 | 44 |
| 61 | SL0 | 148/155 (96%) | 141 (95%) | 7 (5%) | 0 | 100 | 100 |
| 62 | SM0 | 109/130 (84%) | 106 (97%) | 3 (3%) | 0 | 100 | 100 |
| 63 | SN0 | 140/143 (98%) | 134 (96%) | 6 (4%) | 0 | 100 | 100 |
| 64 | SO0 | 127/135 (94%) | 120 (94%) | 7 (6%) | 0 | 100 | 100 |
| 65 | SP0 | 115/163 (71%) | 113 (98%) | 2 (2%) | 0 | 100 | 100 |
| 66 | SQ0 | 140/143 (98%) | 134 (96%) | 6 (4%) | 0 | 100 | 100 |
| 67 | SR0 | 117/120 (98%) | 113 (97%) | 4 (3%) | 0 | 100 | 100 |
| 68 | SS0 | 142/160 (89%) | 137 (96%) | 4 (3%) | 1 (1%) | 19 | 57 |
| 69 | ST0 | 140/143 (98%) | 140 (100%) | 0 | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 70 | SU0 | 98/119 (82%) | 94 (96%) | 4 (4%) | 0 | 100 | 100 |
| 71 | SV0 | 63/67 (94%) | 62 (98%) | 1 (2%) | 0 | 100 | 100 |
| 72 | SW0 | 126/128 (98%) | 124 (98%) | 2 (2%) | 0 | 100 | 100 |
| 73 | SX0 | 138/141 (98%) | 136 (99%) | 2 (1%) | 0 | 100 | 100 |
| 74 | SY0 | 134/146 (92%) | 122 (91%) | 10 (8%) | 2 (2%) | 8 | 40 |
| 75 | SZ0 | 74/128 (58%) | 69 (93%) | 5 (7%) | 0 | 100 | 100 |
| All | All | 10629/11469 (93%) | 10261 (96%) | 355 (3%) | 13 (0%) | 50 | 83 |

All (13) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15 | LGG | 78 | GLY |
| 74 | SY0 | 134 | LYS |
| 30 | LPP | 18 | TYR |
| 37 | LW0 | 81 | ARG |
| 68 | SS0 | 24 | PHE |
| 74 | SY0 | 37 | ASN |
| 56 | SGG | 61 | GLY |
| 24 | LM0 | 48 | GLY |
| 57 | SH0 | 107 | PHE |
| 60 | SK0 | 71 | GLY |
| 7 | LCC | 64 | ILE |
| 22 | LL0 | 8 | PRO |
| 6 | LC0 | 297 | ILE |

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 | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 3 | LA0 | 202/203 (100%) | 199 (98%) | 3 (2%) | 60 | 75 |
| 4 | LAA | 123/123 (100%) | 119 (97%) | 4 (3%) | 33 | 52 |
| 5 | LB0 | 328/336 (98%) | 319 (97%) | 9 (3%) | 40 | 58 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 6 | LC0 | 277/278 (100%) | 274 (99%) | 3 (1%) | 70 | 80 |
| 7 | LCC | 87/97 (90%) | 85 (98%) | 2 (2%) | 45 | 64 |
| 8 | LD0 | 251/261 (96%) | 249 (99%) | 2 (1%) | 79 | 85 |
| 9 | LDD | 99/100 (99%) | 99 (100%) | 0 | 100 | 100 |
| 10 | LE0 | 153/159 (96%) | 150 (98%) | 3 (2%) | 50 | 68 |
| 11 | LEE | 118/122 (97%) | 118 (100%) | 0 | 100 | 100 |
| 12 | LF0 | 212/216 (98%) | 211 (100%) | 1 (0%) | 86 | 89 |
| 13 | LFF | 98/98 (100%) | 98 (100%) | 0 | 100 | 100 |
| 14 | LG0 | 183/190 (96%) | 183 (100%) | 0 | 100 | 100 |
| 15 | LGG | 88/90 (98%) | 86 (98%) | 2 (2%) | 45 | 64 |
| 16 | LH0 | 165/169 (98%) | 161 (98%) | 4 (2%) | 44 | 62 |
| 17 | LHH | 110/110 (100%) | 109 (99%) | 1 (1%) | 75 | 83 |
| 18 | LI0 | 188/189 (100%) | 188 (100%) | 0 | 100 | 100 |
| 19 | LII | 84/84 (100%) | 82 (98%) | 2 (2%) | 44 | 62 |
| 20 | LJ0 | 146/149 (98%) | 144 (99%) | 2 (1%) | 62 | 75 |
| 21 | LJJ | 78/81 (96%) | 77 (99%) | 1 (1%) | 65 | 77 |
| 22 | LL0 | 148/149 (99%) | 142 (96%) | 6 (4%) | 26 | 47 |
| 23 | LLL | 46/47 (98%) | 46 (100%) | 0 | 100 | 100 |
| 24 | LM0 | 110/110 (100%) | 110 (100%) | 0 | 100 | 100 |
| 25 | LMM | 46/112 (41%) | 46 (100%) | 0 | 100 | 100 |
| 26 | LN0 | 175/176 (99%) | 171 (98%) | 4 (2%) | 45 | 64 |
| 27 | LO0 | 178/178 (100%) | 177 (99%) | 1 (1%) | 84 | 88 |
| 28 | LOO | 85/89 (96%) | 85 (100%) | 0 | 100 | 100 |
| 29 | LP0 | 135/147 (92%) | 132 (98%) | 3 (2%) | 47 | 65 |
| 30 | LPP | 75/77 (97%) | 73 (97%) | 2 (3%) | 40 | 58 |
| 31 | LQ0 | 165/166 (99%) | 165 (100%) | 0 | 100 | 100 |
| 32 | LR0 | 142/145 (98%) | 141 (99%) | 1 (1%) | 81 | 87 |
| 33 | LS0 | 155/156 (99%) | 152 (98%) | 3 (2%) | 52 | 69 |
| 34 | LT0 | 140/142 (99%) | 138 (99%) | 2 (1%) | 62 | 75 |
| 35 | LU0 | 89/98 (91%) | 88 (99%) | 1 (1%) | 70 | 80 |
| 36 | LV0 | 113/114 (99%) | 112 (99%) | 1 (1%) | 75 | 83 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 37 | LW0 | 93/120 (78%) | 89 (96%) | 4 (4%) | 25 | 46 |
| 38 | LX0 | 92/93 (99%) | 91 (99%) | 1 (1%) | 70 | 80 |
| 39 | LY0 | 116/116 (100%) | 114 (98%) | 2 (2%) | 56 | 72 |
| 40 | LZ0 | 106/141 (75%) | 106 (100%) | 0 | 100 | 100 |
| 41 | MD1 | 139/139 (100%) | 139 (100%) | 0 | 100 | 100 |
| 43 | SA0 | 194/206 (94%) | 191 (98%) | 3 (2%) | 60 | 75 |
| 44 | SAA | 92/93 (99%) | 92 (100%) | 0 | 100 | 100 |
| 45 | SB0 | 182/203 (90%) | 182 (100%) | 0 | 100 | 100 |
| 46 | SBB | 72/73 (99%) | 71 (99%) | 1 (1%) | 62 | 75 |
| 47 | SC0 | 187/209 (90%) | 185 (99%) | 2 (1%) | 70 | 80 |
| 48 | SCC | 51/54 (94%) | 51 (100%) | 0 | 100 | 100 |
| 49 | SD0 | 189/215 (88%) | 189 (100%) | 0 | 100 | 100 |
| 50 | SDD | 57/57 (100%) | 57 (100%) | 0 | 100 | 100 |
| 51 | SE0 | 231/251 (92%) | 229 (99%) | 2 (1%) | 75 | 83 |
| 52 | SEE | 44/47 (94%) | 44 (100%) | 0 | 100 | 100 |
| 53 | SF0 | 167/170 (98%) | 163 (98%) | 4 (2%) | 44 | 62 |
| 54 | SFF | 46/136 (34%) | 45 (98%) | 1 (2%) | 47 | 65 |
| 55 | SG0 | 199/199 (100%) | 195 (98%) | 4 (2%) | 50 | 68 |
| 56 | SGG | 282/288 (98%) | 278 (99%) | 4 (1%) | 62 | 75 |
| 57 | SH0 | 153/154 (99%) | 153 (100%) | 0 | 100 | 100 |
| 58 | SI0 | 147/153 (96%) | 147 (100%) | 0 | 100 | 100 |
| 59 | SJ0 | 152/165 (92%) | 150 (99%) | 2 (1%) | 65 | 77 |
| 60 | SK0 | 83/99 (84%) | 82 (99%) | 1 (1%) | 67 | 78 |
| 61 | SL0 | 140/145 (97%) | 139 (99%) | 1 (1%) | 81 | 87 |
| 62 | SM0 | 99/114 (87%) | 99 (100%) | 0 | 100 | 100 |
| 63 | SN0 | 126/127 (99%) | 126 (100%) | 0 | 100 | 100 |
| 64 | SO0 | 102/108 (94%) | 101 (99%) | 1 (1%) | 73 | 82 |
| 65 | SP0 | 107/144 (74%) | 106 (99%) | 1 (1%) | 75 | 83 |
| 66 | SQ0 | 120/121 (99%) | 119 (99%) | 1 (1%) | 79 | 85 |
| 67 | SR0 | 109/111 (98%) | 108 (99%) | 1 (1%) | 75 | 83 |
| 68 | SS0 | 125/138 (91%) | 124 (99%) | 1 (1%) | 79 | 85 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|-------------|-----|
| 69 | ST0 | 129/130 (99%) | 126 (98%) | 3 (2%) | 45 | 64 |
| 70 | SU0 | 92/110 (84%) | 92 (100%) | 0 | 100 | 100 |
| 71 | SV0 | 61/63 (97%) | 61 (100%) | 0 | 100 | 100 |
| 72 | SW0 | 111/111 (100%) | 110 (99%) | 1 (1%) | 75 | 83 |
| 73 | SX0 | 115/116 (99%) | 115 (100%) | 0 | 100 | 100 |
| 74 | SY0 | 126/136 (93%) | 121 (96%) | 5 (4%) | 27 | 47 |
| 75 | SZ0 | 73/118 (62%) | 73 (100%) | 0 | 100 | 100 |
| All | All | 9501/10134 (94%) | 9392 (99%) | 109 (1%) | 69 | 80 |

All (109) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | LA0 | 44 | GLU |
| 3 | LA0 | 189 | ARG |
| 3 | LA0 | 222 | VAL |
| 4 | LAA | 22 | VAL |
| 4 | LAA | 26 | ARG |
| 4 | LAA | 39 | LYS |
| 4 | LAA | 54 | ARG |
| 5 | LB0 | 10 | ARG |
| 5 | LB0 | 23 | LYS |
| 5 | LB0 | 86 | VAL |
| 5 | LB0 | 122 | ARG |
| 5 | LB0 | 132 | LYS |
| 5 | LB0 | 133 | LEU |
| 5 | LB0 | 134 | MET |
| 5 | LB0 | 135 | PHE |
| 5 | LB0 | 336 | ARG |
| 6 | LC0 | 103 | VAL |
| 6 | LC0 | 207 | THR |
| 6 | LC0 | 328 | ILE |
| 7 | LCC | 64 | ILE |
| 7 | LCC | 76 | SER |
| 8 | LD0 | 85 | THR |
| 8 | LD0 | 285 | GLN |
| 10 | LE0 | 15 | LYS |
| 10 | LE0 | 17 | TYR |
| 10 | LE0 | 30 | LEU |
| 12 | LF0 | 42 | ARG |
| 15 | LGG | 32 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15 | LGG | 101 | MET |
| 16 | LH0 | 34 | VAL |
| 16 | LH0 | 62 | GLN |
| 16 | LH0 | 64 | ARG |
| 16 | LH0 | 149 | ASP |
| 17 | LHH | 107 | LEU |
| 19 | LII | 47 | ARG |
| 19 | LII | 90 | GLU |
| 20 | LJ0 | 106 | HIS |
| 20 | LJ0 | 144 | ARG |
| 21 | LJJ | 2 | SER |
| 22 | LL0 | 5 | GLN |
| 22 | LL0 | 30 | LEU |
| 22 | LL0 | 44 | TYR |
| 22 | LL0 | 90 | VAL |
| 22 | LL0 | 97 | ARG |
| 22 | LL0 | 98 | ARG |
| 26 | LN0 | 65 | ARG |
| 26 | LN0 | 112 | ASN |
| 26 | LN0 | 135 | VAL |
| 26 | LN0 | 155 | VAL |
| 27 | LO0 | 105 | ASP |
| 29 | LP0 | 30 | ARG |
| 29 | LP0 | 60 | VAL |
| 29 | LP0 | 120 | ASN |
| 30 | LPP | 8 | VAL |
| 30 | LPP | 18 | TYR |
| 32 | LR0 | 19 | ARG |
| 33 | LS0 | 52 | PRO |
| 33 | LS0 | 157 | ARG |
| 33 | LS0 | 171 | ASN |
| 34 | LT0 | 55 | LYS |
| 34 | LT0 | 112 | ASN |
| 35 | LU0 | 92 | ARG |
| 36 | LV0 | 28 | LEU |
| 37 | LW0 | 80 | VAL |
| 37 | LW0 | 81 | ARG |
| 37 | LW0 | 91 | VAL |
| 37 | LW0 | 92 | GLU |
| 38 | LX0 | 40 | HIS |
| 39 | LY0 | 1 | MET |
| 39 | LY0 | 114 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 43 | SA0 | 8 | LEU |
| 43 | SA0 | 102 | ARG |
| 43 | SA0 | 154 | ILE |
| 46 | SBB | 58 | CYS |
| 47 | SC0 | 156 | SER |
| 47 | SC0 | 221 | VAL |
| 51 | SE0 | 211 | VAL |
| 51 | SE0 | 213 | LYS |
| 53 | SF0 | 18 | TYR |
| 53 | SF0 | 61 | GLU |
| 53 | SF0 | 92 | GLU |
| 53 | SF0 | 97 | GLN |
| 54 | SFF | 93 | LYS |
| 55 | SG0 | 92 | ARG |
| 55 | SG0 | 100 | SER |
| 55 | SG0 | 129 | VAL |
| 55 | SG0 | 222 | TRP |
| 56 | SGG | 76 | ASP |
| 56 | SGG | 106 | ASP |
| 56 | SGG | 150 | THR |
| 56 | SGG | 305 | ASP |
| 59 | SJ0 | 62 | ASP |
| 59 | SJ0 | 130 | GLN |
| 60 | SK0 | 80 | TYR |
| 61 | SL0 | 148 | LYS |
| 64 | SO0 | 122 | ASP |
| 65 | SP0 | 135 | ARG |
| 66 | SQ0 | 99 | GLU |
| 67 | SR0 | 84 | PHE |
| 68 | SS0 | 24 | PHE |
| 69 | ST0 | 17 | LEU |
| 69 | ST0 | 28 | VAL |
| 69 | ST0 | 97 | VAL |
| 72 | SW0 | 110 | ASP |
| 74 | SY0 | 11 | PHE |
| 74 | SY0 | 37 | ASN |
| 74 | SY0 | 39 | MET |
| 74 | SY0 | 135 | ARG |
| 74 | SY0 | 143 | LYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | L50 | 2494/2618 (95%) | 736 (29%) | 103 (4%) |
| 2 | L70 | 118/119 (99%) | 36 (30%) | 4 (3%) |
| 42 | S60 | 1352/1368 (98%) | 518 (38%) | 70 (5%) |
| All | All | 3964/4105 (96%) | 1290 (32%) | 177 (4%) |

All (1290) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L50 | 2 | U |
| 1 | L50 | 3 | A |
| 1 | L50 | 13 | A |
| 1 | L50 | 15 | G |
| 1 | L50 | 21 | U |
| 1 | L50 | 22 | U |
| 1 | L50 | 23 | U |
| 1 | L50 | 24 | G |
| 1 | L50 | 25 | G |
| 1 | L50 | 31 | G |
| 1 | L50 | 39 | G |
| 1 | L50 | 43 | G |
| 1 | L50 | 48 | A |
| 1 | L50 | 51 | A |
| 1 | L50 | 52 | G |
| 1 | L50 | 59 | A |
| 1 | L50 | 62 | U |
| 1 | L50 | 63 | G |
| 1 | L50 | 68 | G |
| 1 | L50 | 70 | A |
| 1 | L50 | 71 | G |
| 1 | L50 | 73 | A |
| 1 | L50 | 74 | G |
| 1 | L50 | 75 | C |
| 1 | L50 | 76 | A |
| 1 | L50 | 77 | G |
| 1 | L50 | 82 | G |
| 1 | L50 | 87 | C |
| 1 | L50 | 88 | A |
| 1 | L50 | 98 | A |
| 1 | L50 | 99 | U |
| 1 | L50 | 100 | A |
| 1 | L50 | 101 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L50 | 113 | G |
| 1 | L50 | 114 | G |
| 1 | L50 | 118 | A |
| 1 | L50 | 123 | U |
| 1 | L50 | 132 | A |
| 1 | L50 | 135 | A |
| 1 | L50 | 137 | A |
| 1 | L50 | 151 | G |
| 1 | L50 | 152 | A |
| 1 | L50 | 157 | A |
| 1 | L50 | 158 | A |
| 1 | L50 | 159 | A |
| 1 | L50 | 160 | C |
| 1 | L50 | 165 | G |
| 1 | L50 | 167 | G |
| 1 | L50 | 169 | A |
| 1 | L50 | 178 | G |
| 1 | L50 | 181 | G |
| 1 | L50 | 184 | G |
| 1 | L50 | 186 | G |
| 1 | L50 | 188 | G |
| 1 | L50 | 191 | A |
| 1 | L50 | 194 | A |
| 1 | L50 | 201 | A |
| 1 | L50 | 202 | G |
| 1 | L50 | 204 | C |
| 1 | L50 | 209 | A |
| 1 | L50 | 210 | G |
| 1 | L50 | 211 | U |
| 1 | L50 | 212 | G |
| 1 | L50 | 213 | U |
| 1 | L50 | 214 | A |
| 1 | L50 | 216 | U |
| 1 | L50 | 221 | A |
| 1 | L50 | 224 | U |
| 1 | L50 | 225 | G |
| 1 | L50 | 226 | A |
| 1 | L50 | 233 | G |
| 1 | L50 | 234 | U |
| 1 | L50 | 237 | A |
| 1 | L50 | 238 | A |
| 1 | L50 | 239 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L50 | 240 | G |
| 1 | L50 | 241 | G |
| 1 | L50 | 242 | A |
| 1 | L50 | 246 | A |
| 1 | L50 | 247 | G |
| 1 | L50 | 255 | U |
| 1 | L50 | 258 | G |
| 1 | L50 | 266 | A |
| 1 | L50 | 267 | G |
| 1 | L50 | 268 | C |
| 1 | L50 | 273 | C |
| 1 | L50 | 276 | U |
| 1 | L50 | 277 | A |
| 1 | L50 | 284 | G |
| 1 | L50 | 285 | A |
| 1 | L50 | 286 | U |
| 1 | L50 | 287 | A |
| 1 | L50 | 289 | U |
| 1 | L50 | 298 | G |
| 1 | L50 | 309 | U |
| 1 | L50 | 311 | C |
| 1 | L50 | 312 | G |
| 1 | L50 | 314 | U |
| 1 | L50 | 315 | G |
| 1 | L50 | 316 | A |
| 1 | L50 | 317 | G |
| 1 | L50 | 330 | G |
| 1 | L50 | 331 | U |
| 1 | L50 | 332 | A |
| 1 | L50 | 333 | A |
| 1 | L50 | 340 | G |
| 1 | L50 | 343 | A |
| 1 | L50 | 345 | G |
| 1 | L50 | 346 | A |
| 1 | L50 | 347 | G |
| 1 | L50 | 352 | C |
| 1 | L50 | 353 | A |
| 1 | L50 | 358 | G |
| 1 | L50 | 366 | G |
| 1 | L50 | 373 | U |
| 1 | L50 | 382 | A |
| 1 | L50 | 384 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L50 | 385 | C |
| 1 | L50 | 392 | C |
| 1 | L50 | 396 | G |
| 1 | L50 | 397 | A |
| 1 | L50 | 400 | U |
| 1 | L50 | 416 | A |
| 1 | L50 | 434 | G |
| 1 | L50 | 438 | A |
| 1 | L50 | 449 | U |
| 1 | L50 | 450 | C |
| 1 | L50 | 453 | G |
| 1 | L50 | 454 | C |
| 1 | L50 | 467 | A |
| 1 | L50 | 478 | A |
| 1 | L50 | 488 | C |
| 1 | L50 | 495 | A |
| 1 | L50 | 499 | G |
| 1 | L50 | 503 | A |
| 1 | L50 | 504 | G |
| 1 | L50 | 507 | G |
| 1 | L50 | 508 | A |
| 1 | L50 | 509 | A |
| 1 | L50 | 510 | G |
| 1 | L50 | 517 | A |
| 1 | L50 | 523 | A |
| 1 | L50 | 524 | G |
| 1 | L50 | 527 | A |
| 1 | L50 | 530 | A |
| 1 | L50 | 533 | G |
| 1 | L50 | 534 | A |
| 1 | L50 | 535 | A |
| 1 | L50 | 536 | A |
| 1 | L50 | 542 | G |
| 1 | L50 | 556 | A |
| 1 | L50 | 562 | U |
| 1 | L50 | 563 | U |
| 1 | L50 | 564 | G |
| 1 | L50 | 567 | A |
| 1 | L50 | 568 | A |
| 1 | L50 | 569 | C |
| 1 | L50 | 570 | U |
| 1 | L50 | 580 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L50 | 581 | G |
| 1 | L50 | 587 | A |
| 1 | L50 | 601 | C |
| 1 | L50 | 612 | C |
| 1 | L50 | 618 | G |
| 1 | L50 | 620 | C |
| 1 | L50 | 625 | U |
| 1 | L50 | 630 | U |
| 1 | L50 | 631 | G |
| 1 | L50 | 642 | G |
| 1 | L50 | 643 | C |
| 1 | L50 | 646 | A |
| 1 | L50 | 647 | A |
| 1 | L50 | 658 | G |
| 1 | L50 | 659 | G |
| 1 | L50 | 660 | G |
| 1 | L50 | 661 | G |
| 1 | L50 | 665 | A |
| 1 | L50 | 667 | G |
| 1 | L50 | 668 | A |
| 1 | L50 | 675 | G |
| 1 | L50 | 676 | A |
| 1 | L50 | 684 | A |
| 1 | L50 | 685 | G |
| 1 | L50 | 688 | G |
| 1 | L50 | 689 | C |
| 1 | L50 | 695 | C |
| 1 | L50 | 710 | A |
| 1 | L50 | 711 | U |
| 1 | L50 | 714 | G |
| 1 | L50 | 715 | G |
| 1 | L50 | 720 | C |
| 1 | L50 | 726 | C |
| 1 | L50 | 729 | A |
| 1 | L50 | 732 | G |
| 1 | L50 | 736 | A |
| 1 | L50 | 739 | A |
| 1 | L50 | 742 | G |
| 1 | L50 | 749 | A |
| 1 | L50 | 750 | U |
| 1 | L50 | 763 | U |
| 1 | L50 | 764 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L50 | 765 | A |
| 1 | L50 | 766 | A |
| 1 | L50 | 767 | G |
| 1 | L50 | 768 | G |
| 1 | L50 | 772 | C |
| 1 | L50 | 776 | C |
| 1 | L50 | 778 | A |
| 1 | L50 | 779 | A |
| 1 | L50 | 781 | U |
| 1 | L50 | 782 | G |
| 1 | L50 | 784 | G |
| 1 | L50 | 795 | U |
| 1 | L50 | 796 | C |
| 1 | L50 | 801 | A |
| 1 | L50 | 802 | U |
| 1 | L50 | 803 | G |
| 1 | L50 | 806 | A |
| 1 | L50 | 816 | G |
| 1 | L50 | 822 | U |
| 1 | L50 | 828 | A |
| 1 | L50 | 830 | G |
| 1 | L50 | 834 | G |
| 1 | L50 | 838 | G |
| 1 | L50 | 840 | C |
| 1 | L50 | 843 | A |
| 1 | L50 | 848 | A |
| 1 | L50 | 849 | A |
| 1 | L50 | 852 | A |
| 1 | L50 | 854 | C |
| 1 | L50 | 858 | G |
| 1 | L50 | 859 | C |
| 1 | L50 | 865 | G |
| 1 | L50 | 866 | C |
| 1 | L50 | 867 | U |
| 1 | L50 | 871 | G |
| 1 | L50 | 877 | A |
| 1 | L50 | 878 | A |
| 1 | L50 | 879 | U |
| 1 | L50 | 885 | G |
| 1 | L50 | 889 | G |
| 1 | L50 | 893 | C |
| 1 | L50 | 900 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | L50 | 905 | G |
| 1 | L50 | 910 | A |
| 1 | L50 | 980 | A |
| 1 | L50 | 990 | U |
| 1 | L50 | 998 | U |
| 1 | L50 | 1001 | A |
| 1 | L50 | 1002 | U |
| 1 | L50 | 1010 | A |
| 1 | L50 | 1017 | A |
| 1 | L50 | 1018 | U |
| 1 | L50 | 1021 | G |
| 1 | L50 | 1022 | A |
| 1 | L50 | 1023 | U |
| 1 | L50 | 1024 | G |
| 1 | L50 | 1030 | U |
| 1 | L50 | 1032 | A |
| 1 | L50 | 1033 | G |
| 1 | L50 | 1034 | C |
| 1 | L50 | 1037 | G |
| 1 | L50 | 1050 | U |
| 1 | L50 | 1053 | C |
| 1 | L50 | 1055 | A |
| 1 | L50 | 1056 | C |
| 1 | L50 | 1061 | G |
| 1 | L50 | 1062 | A |
| 1 | L50 | 1070 | G |
| 1 | L50 | 1075 | A |
| 1 | L50 | 1082 | G |
| 1 | L50 | 1085 | G |
| 1 | L50 | 1087 | G |
| 1 | L50 | 1089 | U |
| 1 | L50 | 1090 | A |
| 1 | L50 | 1096 | A |
| 1 | L50 | 1099 | G |
| 1 | L50 | 1100 | C |
| 1 | L50 | 1102 | G |
| 1 | L50 | 1105 | C |
| 1 | L50 | 1111 | G |
| 1 | L50 | 1117 | A |
| 1 | L50 | 1118 | G |
| 1 | L50 | 1120 | G |
| 1 | L50 | 1121 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | L50 | 1123 | A |
| 1 | L50 | 1124 | A |
| 1 | L50 | 1130 | C |
| 1 | L50 | 1131 | U |
| 1 | L50 | 1133 | C |
| 1 | L50 | 1134 | A |
| 1 | L50 | 1135 | G |
| 1 | L50 | 1136 | C |
| 1 | L50 | 1142 | A |
| 1 | L50 | 1144 | A |
| 1 | L50 | 1148 | A |
| 1 | L50 | 1149 | G |
| 1 | L50 | 1150 | G |
| 1 | L50 | 1151 | A |
| 1 | L50 | 1155 | G |
| 1 | L50 | 1163 | U |
| 1 | L50 | 1169 | C |
| 1 | L50 | 1170 | A |
| 1 | L50 | 1171 | U |
| 1 | L50 | 1172 | A |
| 1 | L50 | 1173 | A |
| 1 | L50 | 1175 | A |
| 1 | L50 | 1177 | G |
| 1 | L50 | 1181 | G |
| 1 | L50 | 1182 | A |
| 1 | L50 | 1183 | G |
| 1 | L50 | 1189 | U |
| 1 | L50 | 1191 | U |
| 1 | L50 | 1192 | A |
| 1 | L50 | 1193 | A |
| 1 | L50 | 1194 | G |
| 1 | L50 | 1196 | G |
| 1 | L50 | 1213 | A |
| 1 | L50 | 1217 | A |
| 1 | L50 | 1218 | A |
| 1 | L50 | 1221 | A |
| 1 | L50 | 1224 | A |
| 1 | L50 | 1231 | U |
| 1 | L50 | 1232 | G |
| 1 | L50 | 1233 | A |
| 1 | L50 | 1235 | A |
| 1 | L50 | 1236 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | L50 | 1237 | U |
| 1 | L50 | 1243 | G |
| 1 | L50 | 1247 | G |
| 1 | L50 | 1250 | C |
| 1 | L50 | 1252 | G |
| 1 | L50 | 1254 | C |
| 1 | L50 | 1256 | U |
| 1 | L50 | 1257 | A |
| 1 | L50 | 1264 | C |
| 1 | L50 | 1267 | G |
| 1 | L50 | 1268 | U |
| 1 | L50 | 1269 | A |
| 1 | L50 | 1270 | U |
| 1 | L50 | 1274 | C |
| 1 | L50 | 1277 | G |
| 1 | L50 | 1278 | U |
| 1 | L50 | 1282 | C |
| 1 | L50 | 1283 | A |
| 1 | L50 | 1284 | C |
| 1 | L50 | 1296 | C |
| 1 | L50 | 1299 | A |
| 1 | L50 | 1304 | A |
| 1 | L50 | 1305 | A |
| 1 | L50 | 1308 | A |
| 1 | L50 | 1309 | C |
| 1 | L50 | 1317 | G |
| 1 | L50 | 1318 | U |
| 1 | L50 | 1327 | A |
| 1 | L50 | 1332 | G |
| 1 | L50 | 1333 | A |
| 1 | L50 | 1340 | A |
| 1 | L50 | 1341 | G |
| 1 | L50 | 1342 | A |
| 1 | L50 | 1346 | A |
| 1 | L50 | 1350 | U |
| 1 | L50 | 1355 | C |
| 1 | L50 | 1356 | G |
| 1 | L50 | 1359 | G |
| 1 | L50 | 1361 | G |
| 1 | L50 | 1362 | G |
| 1 | L50 | 1374 | U |
| 1 | L50 | 1375 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | L50 | 1384 | U |
| 1 | L50 | 1385 | G |
| 1 | L50 | 1386 | A |
| 1 | L50 | 1387 | G |
| 1 | L50 | 1395 | U |
| 1 | L50 | 1396 | G |
| 1 | L50 | 1402 | G |
| 1 | L50 | 1411 | C |
| 1 | L50 | 1412 | C |
| 1 | L50 | 1414 | U |
| 1 | L50 | 1416 | A |
| 1 | L50 | 1427 | A |
| 1 | L50 | 1429 | A |
| 1 | L50 | 1430 | U |
| 1 | L50 | 1431 | G |
| 1 | L50 | 1432 | G |
| 1 | L50 | 1440 | G |
| 1 | L50 | 1447 | C |
| 1 | L50 | 1449 | A |
| 1 | L50 | 1450 | A |
| 1 | L50 | 1453 | G |
| 1 | L50 | 1455 | A |
| 1 | L50 | 1457 | C |
| 1 | L50 | 1458 | A |
| 1 | L50 | 1466 | A |
| 1 | L50 | 1467 | A |
| 1 | L50 | 1468 | G |
| 1 | L50 | 1474 | G |
| 1 | L50 | 1475 | A |
| 1 | L50 | 1479 | U |
| 1 | L50 | 1485 | G |
| 1 | L50 | 1486 | G |
| 1 | L50 | 1488 | U |
| 1 | L50 | 1489 | G |
| 1 | L50 | 1490 | U |
| 1 | L50 | 1491 | U |
| 1 | L50 | 1492 | U |
| 1 | L50 | 1499 | U |
| 1 | L50 | 1513 | G |
| 1 | L50 | 1524 | G |
| 1 | L50 | 1527 | U |
| 1 | L50 | 1533 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | L50 | 1534 | G |
| 1 | L50 | 1535 | G |
| 1 | L50 | 1536 | G |
| 1 | L50 | 1538 | G |
| 1 | L50 | 1547 | G |
| 1 | L50 | 1554 | U |
| 1 | L50 | 1555 | G |
| 1 | L50 | 1556 | U |
| 1 | L50 | 1557 | G |
| 1 | L50 | 1563 | A |
| 1 | L50 | 1564 | U |
| 1 | L50 | 1565 | U |
| 1 | L50 | 1566 | G |
| 1 | L50 | 1568 | G |
| 1 | L50 | 1569 | A |
| 1 | L50 | 1571 | A |
| 1 | L50 | 1573 | G |
| 1 | L50 | 1574 | G |
| 1 | L50 | 1575 | G |
| 1 | L50 | 1583 | A |
| 1 | L50 | 1591 | G |
| 1 | L50 | 1592 | U |
| 1 | L50 | 1602 | G |
| 1 | L50 | 1610 | A |
| 1 | L50 | 1611 | A |
| 1 | L50 | 1612 | G |
| 1 | L50 | 1613 | A |
| 1 | L50 | 1614 | G |
| 1 | L50 | 1617 | A |
| 1 | L50 | 1619 | G |
| 1 | L50 | 1624 | G |
| 1 | L50 | 1626 | G |
| 1 | L50 | 1638 | G |
| 1 | L50 | 1643 | G |
| 1 | L50 | 1644 | U |
| 1 | L50 | 1645 | C |
| 1 | L50 | 1646 | G |
| 1 | L50 | 1649 | A |
| 1 | L50 | 1651 | A |
| 1 | L50 | 1653 | G |
| 1 | L50 | 1665 | A |
| 1 | L50 | 1668 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | L50 | 1674 | G |
| 1 | L50 | 1675 | G |
| 1 | L50 | 1680 | A |
| 1 | L50 | 1682 | G |
| 1 | L50 | 1685 | G |
| 1 | L50 | 1686 | G |
| 1 | L50 | 1689 | G |
| 1 | L50 | 1692 | A |
| 1 | L50 | 1693 | C |
| 1 | L50 | 1697 | G |
| 1 | L50 | 1698 | A |
| 1 | L50 | 1699 | C |
| 1 | L50 | 1705 | U |
| 1 | L50 | 1708 | G |
| 1 | L50 | 1709 | G |
| 1 | L50 | 1710 | U |
| 1 | L50 | 1711 | A |
| 1 | L50 | 1717 | A |
| 1 | L50 | 1718 | C |
| 1 | L50 | 1720 | C |
| 1 | L50 | 1724 | G |
| 1 | L50 | 1733 | A |
| 1 | L50 | 1735 | G |
| 1 | L50 | 1739 | A |
| 1 | L50 | 1742 | C |
| 1 | L50 | 1743 | G |
| 1 | L50 | 1746 | U |
| 1 | L50 | 1749 | A |
| 1 | L50 | 1751 | G |
| 1 | L50 | 1755 | U |
| 1 | L50 | 1760 | A |
| 1 | L50 | 1770 | U |
| 1 | L50 | 1772 | U |
| 1 | L50 | 1797 | A |
| 1 | L50 | 1799 | U |
| 1 | L50 | 1800 | U |
| 1 | L50 | 1801 | C |
| 1 | L50 | 1808 | A |
| 1 | L50 | 1809 | A |
| 1 | L50 | 1810 | C |
| 1 | L50 | 1811 | G |
| 1 | L50 | 1820 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | L50 | 1821 | G |
| 1 | L50 | 1822 | G |
| 1 | L50 | 1828 | G |
| 1 | L50 | 1832 | A |
| 1 | L50 | 1833 | A |
| 1 | L50 | 1835 | G |
| 1 | L50 | 1836 | A |
| 1 | L50 | 1837 | A |
| 1 | L50 | 1838 | G |
| 1 | L50 | 1839 | A |
| 1 | L50 | 1846 | U |
| 1 | L50 | 1854 | A |
| 1 | L50 | 1858 | U |
| 1 | L50 | 1860 | G |
| 1 | L50 | 1868 | A |
| 1 | L50 | 1869 | A |
| 1 | L50 | 1870 | G |
| 1 | L50 | 1872 | U |
| 1 | L50 | 1873 | G |
| 1 | L50 | 1874 | U |
| 1 | L50 | 1881 | U |
| 1 | L50 | 1883 | A |
| 1 | L50 | 1885 | G |
| 1 | L50 | 1887 | G |
| 1 | L50 | 1888 | A |
| 1 | L50 | 1931 | C |
| 1 | L50 | 1934 | C |
| 1 | L50 | 1935 | A |
| 1 | L50 | 1937 | G |
| 1 | L50 | 1938 | A |
| 1 | L50 | 1939 | U |
| 1 | L50 | 1940 | C |
| 1 | L50 | 1941 | A |
| 1 | L50 | 1942 | U |
| 1 | L50 | 1943 | C |
| 1 | L50 | 1946 | G |
| 1 | L50 | 1949 | A |
| 1 | L50 | 1950 | C |
| 1 | L50 | 1955 | G |
| 1 | L50 | 1956 | U |
| 1 | L50 | 1957 | U |
| 1 | L50 | 1958 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | L50 | 1959 | A |
| 1 | L50 | 1960 | A |
| 1 | L50 | 1961 | G |
| 1 | L50 | 1963 | A |
| 1 | L50 | 1966 | A |
| 1 | L50 | 1967 | A |
| 1 | L50 | 1968 | G |
| 1 | L50 | 1973 | G |
| 1 | L50 | 1977 | G |
| 1 | L50 | 1978 | G |
| 1 | L50 | 1985 | G |
| 1 | L50 | 1991 | G |
| 1 | L50 | 1995 | G |
| 1 | L50 | 1997 | A |
| 1 | L50 | 2007 | A |
| 1 | L50 | 2008 | A |
| 1 | L50 | 2011 | A |
| 1 | L50 | 2013 | A |
| 1 | L50 | 2019 | G |
| 1 | L50 | 2020 | U |
| 1 | L50 | 2022 | G |
| 1 | L50 | 2023 | A |
| 1 | L50 | 2027 | A |
| 1 | L50 | 2030 | G |
| 1 | L50 | 2031 | U |
| 1 | L50 | 2032 | A |
| 1 | L50 | 2036 | A |
| 1 | L50 | 2037 | C |
| 1 | L50 | 2039 | G |
| 1 | L50 | 2042 | A |
| 1 | L50 | 2043 | G |
| 1 | L50 | 2045 | C |
| 1 | L50 | 2046 | G |
| 1 | L50 | 2047 | A |
| 1 | L50 | 2048 | G |
| 1 | L50 | 2049 | A |
| 1 | L50 | 2052 | A |
| 1 | L50 | 2057 | U |
| 1 | L50 | 2059 | U |
| 1 | L50 | 2060 | A |
| 1 | L50 | 2061 | G |
| 1 | L50 | 2062 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | L50 | 2063 | G |
| 1 | L50 | 2065 | A |
| 1 | L50 | 2067 | A |
| 1 | L50 | 2073 | U |
| 1 | L50 | 2075 | A |
| 1 | L50 | 2076 | A |
| 1 | L50 | 2077 | G |
| 1 | L50 | 2078 | A |
| 1 | L50 | 2085 | G |
| 1 | L50 | 2087 | G |
| 1 | L50 | 2093 | G |
| 1 | L50 | 2096 | C |
| 1 | L50 | 2097 | U |
| 1 | L50 | 2098 | A |
| 1 | L50 | 2099 | C |
| 1 | L50 | 2108 | U |
| 1 | L50 | 2109 | G |
| 1 | L50 | 2110 | A |
| 1 | L50 | 2111 | G |
| 1 | L50 | 2114 | G |
| 1 | L50 | 2122 | G |
| 1 | L50 | 2124 | C |
| 1 | L50 | 2130 | G |
| 1 | L50 | 2131 | A |
| 1 | L50 | 2136 | A |
| 1 | L50 | 2140 | A |
| 1 | L50 | 2141 | U |
| 1 | L50 | 2142 | A |
| 1 | L50 | 2145 | A |
| 1 | L50 | 2146 | G |
| 1 | L50 | 2149 | A |
| 1 | L50 | 2150 | C |
| 1 | L50 | 2152 | U |
| 1 | L50 | 2160 | G |
| 1 | L50 | 2162 | G |
| 1 | L50 | 2164 | G |
| 1 | L50 | 2167 | A |
| 1 | L50 | 2168 | G |
| 1 | L50 | 2169 | A |
| 1 | L50 | 2170 | A |
| 1 | L50 | 2171 | A |
| 1 | L50 | 2177 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | L50 | 2178 | C |
| 1 | L50 | 2185 | A |
| 1 | L50 | 2189 | C |
| 1 | L50 | 2211 | A |
| 1 | L50 | 2212 | G |
| 1 | L50 | 2213 | A |
| 1 | L50 | 2217 | C |
| 1 | L50 | 2221 | G |
| 1 | L50 | 2224 | G |
| 1 | L50 | 2228 | U |
| 1 | L50 | 2229 | U |
| 1 | L50 | 2234 | U |
| 1 | L50 | 2235 | C |
| 1 | L50 | 2239 | G |
| 1 | L50 | 2241 | U |
| 1 | L50 | 2243 | U |
| 1 | L50 | 2253 | C |
| 1 | L50 | 2254 | U |
| 1 | L50 | 2255 | A |
| 1 | L50 | 2257 | C |
| 1 | L50 | 2260 | G |
| 1 | L50 | 2262 | C |
| 1 | L50 | 2266 | G |
| 1 | L50 | 2272 | G |
| 1 | L50 | 2275 | G |
| 1 | L50 | 2279 | A |
| 1 | L50 | 2286 | G |
| 1 | L50 | 2291 | U |
| 1 | L50 | 2293 | C |
| 1 | L50 | 2296 | C |
| 1 | L50 | 2303 | C |
| 1 | L50 | 2304 | A |
| 1 | L50 | 2306 | G |
| 1 | L50 | 2309 | A |
| 1 | L50 | 2310 | C |
| 1 | L50 | 2313 | G |
| 1 | L50 | 2319 | G |
| 1 | L50 | 2322 | U |
| 1 | L50 | 2323 | U |
| 1 | L50 | 2325 | G |
| 1 | L50 | 2337 | A |
| 1 | L50 | 2339 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | L50 | 2340 | G |
| 1 | L50 | 2345 | G |
| 1 | L50 | 2347 | U |
| 1 | L50 | 2351 | U |
| 1 | L50 | 2355 | A |
| 1 | L50 | 2358 | G |
| 1 | L50 | 2364 | A |
| 1 | L50 | 2376 | A |
| 1 | L50 | 2377 | G |
| 1 | L50 | 2379 | G |
| 1 | L50 | 2394 | A |
| 1 | L50 | 2399 | A |
| 1 | L50 | 2401 | C |
| 1 | L50 | 2410 | A |
| 1 | L50 | 2412 | C |
| 1 | L50 | 2413 | U |
| 1 | L50 | 2416 | G |
| 1 | L50 | 2419 | G |
| 1 | L50 | 2420 | C |
| 1 | L50 | 2423 | C |
| 1 | L50 | 2424 | G |
| 1 | L50 | 2432 | G |
| 1 | L50 | 2434 | A |
| 1 | L50 | 2436 | G |
| 1 | L50 | 2437 | U |
| 1 | L50 | 2441 | A |
| 1 | L50 | 2447 | A |
| 1 | L50 | 2451 | U |
| 1 | L50 | 2452 | A |
| 1 | L50 | 2453 | C |
| 1 | L50 | 2459 | C |
| 1 | L50 | 2460 | U |
| 1 | L50 | 2473 | G |
| 1 | L50 | 2475 | A |
| 1 | L50 | 2476 | G |
| 1 | L50 | 2477 | C |
| 1 | L50 | 2482 | A |
| 1 | L50 | 2487 | A |
| 1 | L50 | 2490 | A |
| 1 | L50 | 2491 | A |
| 1 | L50 | 2501 | A |
| 1 | L50 | 2503 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | L50 | 2508 | A |
| 1 | L50 | 2509 | A |
| 1 | L50 | 2518 | G |
| 1 | L50 | 2519 | G |
| 1 | L50 | 2520 | A |
| 1 | L50 | 2529 | C |
| 1 | L50 | 2532 | A |
| 1 | L50 | 2533 | G |
| 1 | L50 | 2534 | U |
| 1 | L50 | 2535 | U |
| 1 | L50 | 2538 | C |
| 1 | L50 | 2539 | A |
| 1 | L50 | 2548 | G |
| 1 | L50 | 2555 | A |
| 1 | L50 | 2558 | A |
| 1 | L50 | 2559 | G |
| 1 | L50 | 2562 | U |
| 1 | L50 | 2563 | U |
| 1 | L50 | 2565 | U |
| 1 | L50 | 2568 | U |
| 1 | L50 | 2578 | G |
| 1 | L50 | 2588 | G |
| 1 | L50 | 2593 | A |
| 1 | L50 | 2595 | U |
| 1 | L50 | 2596 | G |
| 1 | L50 | 2597 | G |
| 1 | L50 | 2598 | U |
| 1 | L50 | 2600 | G |
| 1 | L50 | 2605 | C |
| 1 | L50 | 2606 | A |
| 1 | L50 | 2612 | G |
| 2 | L70 | 2 | G |
| 2 | L70 | 10 | C |
| 2 | L70 | 14 | U |
| 2 | L70 | 15 | C |
| 2 | L70 | 18 | C |
| 2 | L70 | 22 | A |
| 2 | L70 | 25 | A |
| 2 | L70 | 27 | A |
| 2 | L70 | 32 | A |
| 2 | L70 | 33 | U |
| 2 | L70 | 35 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | L70 | 41 | G |
| 2 | L70 | 42 | A |
| 2 | L70 | 49 | A |
| 2 | L70 | 50 | A |
| 2 | L70 | 51 | G |
| 2 | L70 | 53 | U |
| 2 | L70 | 63 | A |
| 2 | L70 | 64 | G |
| 2 | L70 | 65 | A |
| 2 | L70 | 67 | C |
| 2 | L70 | 69 | A |
| 2 | L70 | 88 | C |
| 2 | L70 | 89 | G |
| 2 | L70 | 91 | C |
| 2 | L70 | 93 | A |
| 2 | L70 | 100 | A |
| 2 | L70 | 101 | A |
| 2 | L70 | 104 | C |
| 2 | L70 | 105 | G |
| 2 | L70 | 107 | G |
| 2 | L70 | 108 | G |
| 2 | L70 | 109 | U |
| 2 | L70 | 110 | G |
| 2 | L70 | 115 | A |
| 2 | L70 | 119 | U |
| 42 | S60 | 7 | U |
| 42 | S60 | 8 | U |
| 42 | S60 | 14 | U |
| 42 | S60 | 17 | C |
| 42 | S60 | 26 | A |
| 42 | S60 | 32 | G |
| 42 | S60 | 37 | A |
| 42 | S60 | 39 | A |
| 42 | S60 | 40 | G |
| 42 | S60 | 41 | A |
| 42 | S60 | 43 | U |
| 42 | S60 | 44 | U |
| 42 | S60 | 45 | A |
| 42 | S60 | 48 | C |
| 42 | S60 | 52 | C |
| 42 | S60 | 54 | U |
| 42 | S60 | 55 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42 | S60 | 56 | U |
| 42 | S60 | 66 | G |
| 42 | S60 | 70 | U |
| 42 | S60 | 71 | U |
| 42 | S60 | 72 | A |
| 42 | S60 | 73 | G |
| 42 | S60 | 75 | G |
| 42 | S60 | 76 | A |
| 42 | S60 | 77 | A |
| 42 | S60 | 83 | G |
| 42 | S60 | 86 | A |
| 42 | S60 | 88 | G |
| 42 | S60 | 92 | A |
| 42 | S60 | 94 | U |
| 42 | S60 | 97 | C |
| 42 | S60 | 98 | G |
| 42 | S60 | 99 | G |
| 42 | S60 | 102 | G |
| 42 | S60 | 104 | G |
| 42 | S60 | 106 | A |
| 42 | S60 | 107 | U |
| 42 | S60 | 110 | A |
| 42 | S60 | 112 | U |
| 42 | S60 | 116 | U |
| 42 | S60 | 118 | G |
| 42 | S60 | 119 | A |
| 42 | S60 | 120 | A |
| 42 | S60 | 121 | C |
| 42 | S60 | 124 | G |
| 42 | S60 | 127 | A |
| 42 | S60 | 128 | A |
| 42 | S60 | 132 | C |
| 42 | S60 | 133 | A |
| 42 | S60 | 134 | G |
| 42 | S60 | 138 | A |
| 42 | S60 | 140 | A |
| 42 | S60 | 141 | G |
| 42 | S60 | 142 | A |
| 42 | S60 | 147 | A |
| 42 | S60 | 148 | A |
| 42 | S60 | 150 | A |
| 42 | S60 | 153 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42 | S60 | 155 | G |
| 42 | S60 | 157 | A |
| 42 | S60 | 161 | G |
| 42 | S60 | 167 | G |
| 42 | S60 | 172 | U |
| 42 | S60 | 173 | A |
| 42 | S60 | 174 | G |
| 42 | S60 | 180 | G |
| 42 | S60 | 181 | A |
| 42 | S60 | 184 | A |
| 42 | S60 | 186 | A |
| 42 | S60 | 187 | A |
| 42 | S60 | 189 | A |
| 42 | S60 | 190 | A |
| 42 | S60 | 191 | C |
| 42 | S60 | 192 | A |
| 42 | S60 | 193 | G |
| 42 | S60 | 197 | A |
| 42 | S60 | 198 | G |
| 42 | S60 | 199 | G |
| 42 | S60 | 204 | U |
| 42 | S60 | 206 | A |
| 42 | S60 | 219 | U |
| 42 | S60 | 220 | C |
| 42 | S60 | 222 | G |
| 42 | S60 | 226 | G |
| 42 | S60 | 228 | A |
| 42 | S60 | 238 | A |
| 42 | S60 | 241 | G |
| 42 | S60 | 242 | C |
| 42 | S60 | 247 | U |
| 42 | S60 | 254 | U |
| 42 | S60 | 255 | A |
| 42 | S60 | 256 | G |
| 42 | S60 | 259 | G |
| 42 | S60 | 262 | U |
| 42 | S60 | 263 | A |
| 42 | S60 | 264 | C |
| 42 | S60 | 268 | G |
| 42 | S60 | 271 | U |
| 42 | S60 | 283 | U |
| 42 | S60 | 284 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42 | S60 | 290 | A |
| 42 | S60 | 292 | G |
| 42 | S60 | 299 | G |
| 42 | S60 | 300 | A |
| 42 | S60 | 303 | G |
| 42 | S60 | 304 | A |
| 42 | S60 | 305 | C |
| 42 | S60 | 307 | G |
| 42 | S60 | 311 | C |
| 42 | S60 | 314 | G |
| 42 | S60 | 315 | G |
| 42 | S60 | 318 | C |
| 42 | S60 | 319 | A |
| 42 | S60 | 320 | A |
| 42 | S60 | 326 | G |
| 42 | S60 | 327 | C |
| 42 | S60 | 328 | A |
| 42 | S60 | 329 | G |
| 42 | S60 | 335 | G |
| 42 | S60 | 338 | A |
| 42 | S60 | 340 | A |
| 42 | S60 | 341 | A |
| 42 | S60 | 342 | U |
| 42 | S60 | 344 | A |
| 42 | S60 | 345 | C |
| 42 | S60 | 347 | G |
| 42 | S60 | 348 | A |
| 42 | S60 | 355 | C |
| 42 | S60 | 356 | A |
| 42 | S60 | 357 | A |
| 42 | S60 | 358 | G |
| 42 | S60 | 362 | G |
| 42 | S60 | 363 | C |
| 42 | S60 | 364 | G |
| 42 | S60 | 367 | A |
| 42 | S60 | 368 | G |
| 42 | S60 | 371 | A |
| 42 | S60 | 372 | A |
| 42 | S60 | 373 | G |
| 42 | S60 | 374 | A |
| 42 | S60 | 375 | G |
| 42 | S60 | 377 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42 | S60 | 378 | G |
| 42 | S60 | 380 | G |
| 42 | S60 | 382 | A |
| 42 | S60 | 383 | A |
| 42 | S60 | 384 | A |
| 42 | S60 | 385 | C |
| 42 | S60 | 388 | G |
| 42 | S60 | 395 | U |
| 42 | S60 | 396 | A |
| 42 | S60 | 398 | A |
| 42 | S60 | 399 | A |
| 42 | S60 | 402 | C |
| 42 | S60 | 407 | G |
| 42 | S60 | 408 | A |
| 42 | S60 | 409 | G |
| 42 | S60 | 412 | A |
| 42 | S60 | 414 | U |
| 42 | S60 | 416 | G |
| 42 | S60 | 422 | A |
| 42 | S60 | 424 | G |
| 42 | S60 | 425 | G |
| 42 | S60 | 426 | C |
| 42 | S60 | 431 | G |
| 42 | S60 | 432 | C |
| 42 | S60 | 437 | A |
| 42 | S60 | 441 | G |
| 42 | S60 | 444 | G |
| 42 | S60 | 445 | U |
| 42 | S60 | 446 | A |
| 42 | S60 | 449 | A |
| 42 | S60 | 450 | C |
| 42 | S60 | 452 | A |
| 42 | S60 | 453 | G |
| 42 | S60 | 454 | C |
| 42 | S60 | 461 | A |
| 42 | S60 | 471 | A |
| 42 | S60 | 473 | G |
| 42 | S60 | 474 | A |
| 42 | S60 | 476 | U |
| 42 | S60 | 477 | G |
| 42 | S60 | 478 | C |
| 42 | S60 | 481 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42 | S60 | 482 | G |
| 42 | S60 | 486 | A |
| 42 | S60 | 487 | A |
| 42 | S60 | 490 | G |
| 42 | S60 | 491 | G |
| 42 | S60 | 501 | G |
| 42 | S60 | 506 | A |
| 42 | S60 | 509 | G |
| 42 | S60 | 510 | U |
| 42 | S60 | 511 | A |
| 42 | S60 | 512 | C |
| 42 | S60 | 521 | A |
| 42 | S60 | 527 | G |
| 42 | S60 | 530 | U |
| 42 | S60 | 535 | A |
| 42 | S60 | 536 | G |
| 42 | S60 | 540 | C |
| 42 | S60 | 541 | G |
| 42 | S60 | 543 | A |
| 42 | S60 | 544 | U |
| 42 | S60 | 547 | A |
| 42 | S60 | 550 | G |
| 42 | S60 | 553 | A |
| 42 | S60 | 554 | A |
| 42 | S60 | 565 | U |
| 42 | S60 | 566 | A |
| 42 | S60 | 567 | A |
| 42 | S60 | 568 | G |
| 42 | S60 | 575 | A |
| 42 | S60 | 578 | A |
| 42 | S60 | 579 | G |
| 42 | S60 | 590 | U |
| 42 | S60 | 593 | A |
| 42 | S60 | 598 | C |
| 42 | S60 | 599 | G |
| 42 | S60 | 600 | A |
| 42 | S60 | 601 | G |
| 42 | S60 | 602 | A |
| 42 | S60 | 608 | A |
| 42 | S60 | 609 | A |
| 42 | S60 | 610 | U |
| 42 | S60 | 616 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42 | S60 | 621 | G |
| 42 | S60 | 622 | C |
| 42 | S60 | 623 | U |
| 42 | S60 | 624 | U |
| 42 | S60 | 625 | A |
| 42 | S60 | 630 | U |
| 42 | S60 | 633 | C |
| 42 | S60 | 635 | G |
| 42 | S60 | 637 | G |
| 42 | S60 | 644 | G |
| 42 | S60 | 647 | C |
| 42 | S60 | 661 | A |
| 42 | S60 | 662 | U |
| 42 | S60 | 665 | G |
| 42 | S60 | 668 | G |
| 42 | S60 | 671 | C |
| 42 | S60 | 673 | A |
| 42 | S60 | 686 | G |
| 42 | S60 | 687 | A |
| 42 | S60 | 688 | G |
| 42 | S60 | 690 | A |
| 42 | S60 | 694 | A |
| 42 | S60 | 700 | A |
| 42 | S60 | 702 | U |
| 42 | S60 | 705 | A |
| 42 | S60 | 706 | G |
| 42 | S60 | 707 | A |
| 42 | S60 | 722 | G |
| 42 | S60 | 724 | A |
| 42 | S60 | 725 | G |
| 42 | S60 | 727 | A |
| 42 | S60 | 728 | A |
| 42 | S60 | 730 | C |
| 42 | S60 | 731 | G |
| 42 | S60 | 733 | U |
| 42 | S60 | 734 | G |
| 42 | S60 | 738 | A |
| 42 | S60 | 740 | G |
| 42 | S60 | 749 | G |
| 42 | S60 | 752 | A |
| 42 | S60 | 753 | U |
| 42 | S60 | 754 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42 | S60 | 755 | A |
| 42 | S60 | 757 | C |
| 42 | S60 | 771 | A |
| 42 | S60 | 775 | U |
| 42 | S60 | 776 | A |
| 42 | S60 | 780 | G |
| 42 | S60 | 789 | G |
| 42 | S60 | 790 | G |
| 42 | S60 | 791 | A |
| 42 | S60 | 795 | U |
| 42 | S60 | 806 | G |
| 42 | S60 | 810 | U |
| 42 | S60 | 817 | A |
| 42 | S60 | 818 | A |
| 42 | S60 | 820 | G |
| 42 | S60 | 821 | G |
| 42 | S60 | 823 | A |
| 42 | S60 | 825 | U |
| 42 | S60 | 831 | G |
| 42 | S60 | 836 | A |
| 42 | S60 | 839 | C |
| 42 | S60 | 840 | C |
| 42 | S60 | 841 | A |
| 42 | S60 | 846 | G |
| 42 | S60 | 848 | G |
| 42 | S60 | 866 | U |
| 42 | S60 | 868 | U |
| 42 | S60 | 871 | C |
| 42 | S60 | 872 | U |
| 42 | S60 | 874 | A |
| 42 | S60 | 875 | A |
| 42 | S60 | 877 | G |
| 42 | S60 | 878 | C |
| 42 | S60 | 880 | G |
| 42 | S60 | 881 | G |
| 42 | S60 | 883 | C |
| 42 | S60 | 884 | A |
| 42 | S60 | 890 | C |
| 42 | S60 | 898 | G |
| 42 | S60 | 899 | A |
| 42 | S60 | 905 | G |
| 42 | S60 | 908 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42 | S60 | 909 | G |
| 42 | S60 | 911 | G |
| 42 | S60 | 915 | A |
| 42 | S60 | 916 | G |
| 42 | S60 | 917 | U |
| 42 | S60 | 918 | A |
| 42 | S60 | 924 | U |
| 42 | S60 | 925 | A |
| 42 | S60 | 926 | G |
| 42 | S60 | 927 | G |
| 42 | S60 | 928 | U |
| 42 | S60 | 929 | C |
| 42 | S60 | 930 | A |
| 42 | S60 | 932 | A |
| 42 | S60 | 933 | G |
| 42 | S60 | 934 | A |
| 42 | S60 | 936 | U |
| 42 | S60 | 940 | G |
| 42 | S60 | 941 | C |
| 42 | S60 | 942 | A |
| 42 | S60 | 952 | A |
| 42 | S60 | 953 | C |
| 42 | S60 | 955 | A |
| 42 | S60 | 957 | G |
| 42 | S60 | 958 | A |
| 42 | S60 | 959 | G |
| 42 | S60 | 962 | G |
| 42 | S60 | 966 | G |
| 42 | S60 | 967 | A |
| 42 | S60 | 968 | C |
| 42 | S60 | 970 | U |
| 42 | S60 | 971 | U |
| 42 | S60 | 972 | U |
| 42 | S60 | 974 | G |
| 42 | S60 | 976 | U |
| 42 | S60 | 978 | A |
| 42 | S60 | 980 | G |
| 42 | S60 | 987 | A |
| 42 | S60 | 991 | A |
| 42 | S60 | 995 | A |
| 42 | S60 | 998 | U |
| 42 | S60 | 999 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 42 | S60 | 1003 | A |
| 42 | S60 | 1006 | A |
| 42 | S60 | 1007 | U |
| 42 | S60 | 1008 | A |
| 42 | S60 | 1011 | A |
| 42 | S60 | 1012 | A |
| 42 | S60 | 1013 | A |
| 42 | S60 | 1014 | G |
| 42 | S60 | 1017 | A |
| 42 | S60 | 1018 | U |
| 42 | S60 | 1019 | C |
| 42 | S60 | 1021 | A |
| 42 | S60 | 1023 | A |
| 42 | S60 | 1024 | G |
| 42 | S60 | 1028 | U |
| 42 | S60 | 1029 | U |
| 42 | S60 | 1033 | A |
| 42 | S60 | 1039 | G |
| 42 | S60 | 1041 | A |
| 42 | S60 | 1042 | A |
| 42 | S60 | 1044 | G |
| 42 | S60 | 1045 | A |
| 42 | S60 | 1046 | A |
| 42 | S60 | 1047 | G |
| 42 | S60 | 1052 | A |
| 42 | S60 | 1053 | A |
| 42 | S60 | 1054 | G |
| 42 | S60 | 1056 | A |
| 42 | S60 | 1057 | C |
| 42 | S60 | 1058 | A |
| 42 | S60 | 1059 | G |
| 42 | S60 | 1060 | G |
| 42 | S60 | 1062 | C |
| 42 | S60 | 1063 | A |
| 42 | S60 | 1064 | G |
| 42 | S60 | 1066 | G |
| 42 | S60 | 1075 | A |
| 42 | S60 | 1076 | G |
| 42 | S60 | 1077 | A |
| 42 | S60 | 1078 | U |
| 42 | S60 | 1088 | U |
| 42 | S60 | 1089 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 42 | S60 | 1090 | C |
| 42 | S60 | 1092 | C |
| 42 | S60 | 1094 | C |
| 42 | S60 | 1099 | U |
| 42 | S60 | 1100 | A |
| 42 | S60 | 1102 | A |
| 42 | S60 | 1103 | G |
| 42 | S60 | 1104 | U |
| 42 | S60 | 1105 | G |
| 42 | S60 | 1106 | G |
| 42 | S60 | 1111 | A |
| 42 | S60 | 1112 | G |
| 42 | S60 | 1116 | A |
| 42 | S60 | 1117 | A |
| 42 | S60 | 1118 | A |
| 42 | S60 | 1119 | C |
| 42 | S60 | 1120 | A |
| 42 | S60 | 1121 | A |
| 42 | S60 | 1122 | A |
| 42 | S60 | 1123 | U |
| 42 | S60 | 1124 | A |
| 42 | S60 | 1125 | G |
| 42 | S60 | 1126 | A |
| 42 | S60 | 1127 | A |
| 42 | S60 | 1128 | G |
| 42 | S60 | 1129 | U |
| 42 | S60 | 1130 | A |
| 42 | S60 | 1135 | U |
| 42 | S60 | 1136 | G |
| 42 | S60 | 1137 | A |
| 42 | S60 | 1139 | C |
| 42 | S60 | 1141 | A |
| 42 | S60 | 1142 | G |
| 42 | S60 | 1146 | G |
| 42 | S60 | 1152 | G |
| 42 | S60 | 1154 | A |
| 42 | S60 | 1158 | U |
| 42 | S60 | 1159 | A |
| 42 | S60 | 1160 | A |
| 42 | S60 | 1161 | U |
| 42 | S60 | 1162 | G |
| 42 | S60 | 1170 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 42 | S60 | 1171 | A |
| 42 | S60 | 1175 | A |
| 42 | S60 | 1176 | G |
| 42 | S60 | 1177 | G |
| 42 | S60 | 1179 | A |
| 42 | S60 | 1182 | G |
| 42 | S60 | 1185 | A |
| 42 | S60 | 1191 | C |
| 42 | S60 | 1192 | G |
| 42 | S60 | 1194 | U |
| 42 | S60 | 1195 | A |
| 42 | S60 | 1196 | U |
| 42 | S60 | 1202 | U |
| 42 | S60 | 1203 | A |
| 42 | S60 | 1204 | A |
| 42 | S60 | 1205 | G |
| 42 | S60 | 1210 | G |
| 42 | S60 | 1211 | A |
| 42 | S60 | 1214 | A |
| 42 | S60 | 1216 | U |
| 42 | S60 | 1217 | G |
| 42 | S60 | 1219 | G |
| 42 | S60 | 1223 | C |
| 42 | S60 | 1225 | G |
| 42 | S60 | 1227 | U |
| 42 | S60 | 1230 | U |
| 42 | S60 | 1237 | C |
| 42 | S60 | 1238 | A |
| 42 | S60 | 1239 | C |
| 42 | S60 | 1240 | C |
| 42 | S60 | 1241 | G |
| 42 | S60 | 1243 | C |
| 42 | S60 | 1246 | U |
| 42 | S60 | 1249 | U |
| 42 | S60 | 1250 | U |
| 42 | S60 | 1251 | A |
| 42 | S60 | 1260 | G |
| 42 | S60 | 1262 | A |
| 42 | S60 | 1263 | A |
| 42 | S60 | 1264 | C |
| 42 | S60 | 1266 | A |
| 42 | S60 | 1267 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 42 | S60 | 1270 | G |
| 42 | S60 | 1274 | A |
| 42 | S60 | 1275 | C |
| 42 | S60 | 1276 | A |
| 42 | S60 | 1280 | G |
| 42 | S60 | 1282 | A |
| 42 | S60 | 1283 | A |
| 42 | S60 | 1284 | G |
| 42 | S60 | 1287 | A |
| 42 | S60 | 1294 | G |
| 42 | S60 | 1295 | C |
| 42 | S60 | 1296 | A |
| 42 | S60 | 1297 | G |
| 42 | S60 | 1301 | U |
| 42 | S60 | 1302 | C |
| 42 | S60 | 1307 | U |
| 42 | S60 | 1310 | G |
| 42 | S60 | 1314 | C |
| 42 | S60 | 1315 | A |
| 42 | S60 | 1316 | A |
| 42 | S60 | 1317 | G |
| 42 | S60 | 1320 | G |
| 42 | S60 | 1322 | A |
| 42 | S60 | 1326 | A |
| 42 | S60 | 1327 | G |
| 42 | S60 | 1328 | G |
| 42 | S60 | 1329 | C |
| 42 | S60 | 1331 | G |
| 42 | S60 | 1340 | G |
| 42 | S60 | 1341 | A |
| 42 | S60 | 1342 | A |
| 42 | S60 | 1343 | C |
| 42 | S60 | 1348 | A |
| 42 | S60 | 1352 | G |
| 42 | S60 | 1353 | G |
| 42 | S60 | 1354 | A |
| 42 | S60 | 1355 | U |
| 42 | S60 | 1356 | C |
| 42 | S60 | 1357 | A |

All (177) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | L50 | 2 | U |
| 1 | L50 | 3 | A |
| 1 | L50 | 21 | U |
| 1 | L50 | 22 | U |
| 1 | L50 | 73 | A |
| 1 | L50 | 75 | C |
| 1 | L50 | 135 | A |
| 1 | L50 | 211 | U |
| 1 | L50 | 214 | A |
| 1 | L50 | 225 | G |
| 1 | L50 | 236 | A |
| 1 | L50 | 265 | A |
| 1 | L50 | 276 | U |
| 1 | L50 | 308 | A |
| 1 | L50 | 330 | G |
| 1 | L50 | 351 | G |
| 1 | L50 | 363 | U |
| 1 | L50 | 396 | G |
| 1 | L50 | 424 | G |
| 1 | L50 | 463 | A |
| 1 | L50 | 466 | C |
| 1 | L50 | 523 | A |
| 1 | L50 | 535 | A |
| 1 | L50 | 550 | G |
| 1 | L50 | 563 | U |
| 1 | L50 | 567 | A |
| 1 | L50 | 600 | G |
| 1 | L50 | 657 | A |
| 1 | L50 | 659 | G |
| 1 | L50 | 667 | G |
| 1 | L50 | 710 | A |
| 1 | L50 | 712 | C |
| 1 | L50 | 732 | G |
| 1 | L50 | 741 | G |
| 1 | L50 | 778 | A |
| 1 | L50 | 782 | G |
| 1 | L50 | 853 | A |
| 1 | L50 | 996 | A |
| 1 | L50 | 1000 | G |
| 1 | L50 | 1008 | U |
| 1 | L50 | 1017 | A |
| 1 | L50 | 1018 | U |
| 1 | L50 | 1032 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | L50 | 1061 | G |
| 1 | L50 | 1089 | U |
| 1 | L50 | 1134 | A |
| 1 | L50 | 1148 | A |
| 1 | L50 | 1172 | A |
| 1 | L50 | 1182 | A |
| 1 | L50 | 1256 | U |
| 1 | L50 | 1277 | G |
| 1 | L50 | 1384 | U |
| 1 | L50 | 1394 | U |
| 1 | L50 | 1395 | U |
| 1 | L50 | 1449 | A |
| 1 | L50 | 1454 | U |
| 1 | L50 | 1474 | G |
| 1 | L50 | 1485 | G |
| 1 | L50 | 1491 | U |
| 1 | L50 | 1564 | U |
| 1 | L50 | 1596 | A |
| 1 | L50 | 1611 | A |
| 1 | L50 | 1614 | G |
| 1 | L50 | 1644 | U |
| 1 | L50 | 1697 | G |
| 1 | L50 | 1709 | G |
| 1 | L50 | 1717 | A |
| 1 | L50 | 1743 | G |
| 1 | L50 | 1749 | A |
| 1 | L50 | 1798 | U |
| 1 | L50 | 1800 | U |
| 1 | L50 | 1808 | A |
| 1 | L50 | 1809 | A |
| 1 | L50 | 1835 | G |
| 1 | L50 | 1838 | G |
| 1 | L50 | 1931 | C |
| 1 | L50 | 1942 | U |
| 1 | L50 | 1945 | C |
| 1 | L50 | 1959 | A |
| 1 | L50 | 1966 | A |
| 1 | L50 | 1967 | A |
| 1 | L50 | 2015 | C |
| 1 | L50 | 2036 | A |
| 1 | L50 | 2051 | C |
| 1 | L50 | 2060 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | L50 | 2075 | A |
| 1 | L50 | 2212 | G |
| 1 | L50 | 2240 | A |
| 1 | L50 | 2254 | U |
| 1 | L50 | 2255 | A |
| 1 | L50 | 2347 | U |
| 1 | L50 | 2351 | U |
| 1 | L50 | 2363 | A |
| 1 | L50 | 2419 | G |
| 1 | L50 | 2420 | C |
| 1 | L50 | 2447 | A |
| 1 | L50 | 2452 | A |
| 1 | L50 | 2476 | G |
| 1 | L50 | 2481 | U |
| 1 | L50 | 2519 | G |
| 1 | L50 | 2532 | A |
| 1 | L50 | 2596 | G |
| 1 | L50 | 2597 | G |
| 2 | L70 | 32 | A |
| 2 | L70 | 41 | G |
| 2 | L70 | 62 | A |
| 2 | L70 | 109 | U |
| 42 | S60 | 71 | U |
| 42 | S60 | 76 | A |
| 42 | S60 | 118 | G |
| 42 | S60 | 127 | A |
| 42 | S60 | 180 | G |
| 42 | S60 | 186 | A |
| 42 | S60 | 190 | A |
| 42 | S60 | 191 | C |
| 42 | S60 | 218 | A |
| 42 | S60 | 225 | A |
| 42 | S60 | 226 | G |
| 42 | S60 | 256 | G |
| 42 | S60 | 262 | U |
| 42 | S60 | 283 | U |
| 42 | S60 | 303 | G |
| 42 | S60 | 328 | A |
| 42 | S60 | 339 | A |
| 42 | S60 | 355 | C |
| 42 | S60 | 372 | A |
| 42 | S60 | 383 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 42 | S60 | 407 | G |
| 42 | S60 | 408 | A |
| 42 | S60 | 424 | G |
| 42 | S60 | 425 | G |
| 42 | S60 | 445 | U |
| 42 | S60 | 473 | G |
| 42 | S60 | 509 | G |
| 42 | S60 | 511 | A |
| 42 | S60 | 553 | A |
| 42 | S60 | 565 | U |
| 42 | S60 | 598 | C |
| 42 | S60 | 661 | A |
| 42 | S60 | 724 | A |
| 42 | S60 | 753 | U |
| 42 | S60 | 776 | A |
| 42 | S60 | 788 | G |
| 42 | S60 | 819 | A |
| 42 | S60 | 877 | G |
| 42 | S60 | 914 | U |
| 42 | S60 | 916 | G |
| 42 | S60 | 917 | U |
| 42 | S60 | 918 | A |
| 42 | S60 | 923 | A |
| 42 | S60 | 925 | A |
| 42 | S60 | 927 | G |
| 42 | S60 | 934 | A |
| 42 | S60 | 954 | G |
| 42 | S60 | 970 | U |
| 42 | S60 | 980 | G |
| 42 | S60 | 1007 | U |
| 42 | S60 | 1018 | U |
| 42 | S60 | 1021 | A |
| 42 | S60 | 1023 | A |
| 42 | S60 | 1045 | A |
| 42 | S60 | 1057 | C |
| 42 | S60 | 1077 | A |
| 42 | S60 | 1088 | U |
| 42 | S60 | 1089 | G |
| 42 | S60 | 1103 | G |
| 42 | S60 | 1105 | G |
| 42 | S60 | 1125 | G |
| 42 | S60 | 1135 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 42 | S60 | 1141 | A |
| 42 | S60 | 1175 | A |
| 42 | S60 | 1176 | G |
| 42 | S60 | 1262 | A |
| 42 | S60 | 1314 | C |
| 42 | S60 | 1321 | U |
| 42 | S60 | 1328 | G |
| 42 | S60 | 1356 | C |

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 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

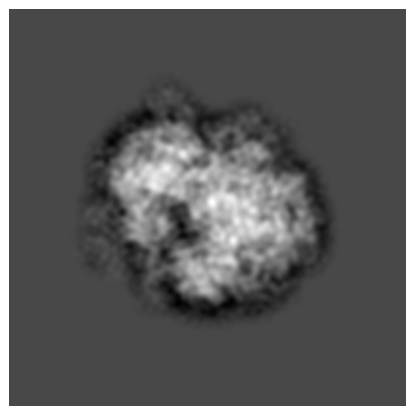
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17448. These allow visual inspection of the internal detail of the map and identification of artifacts.

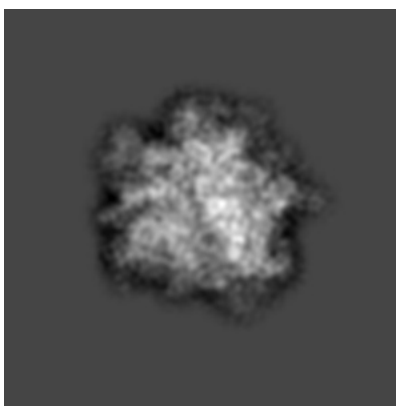
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

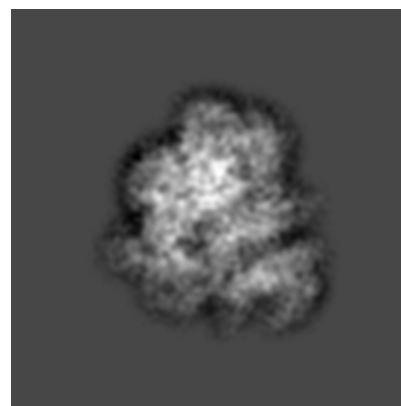
6.1.1 Primary map



X

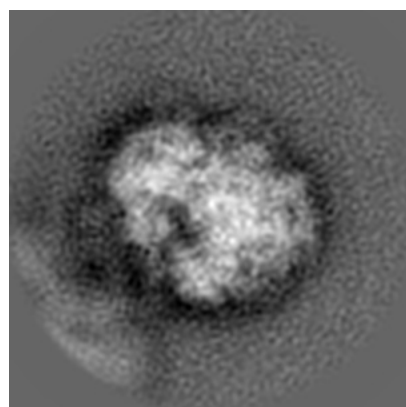


Y

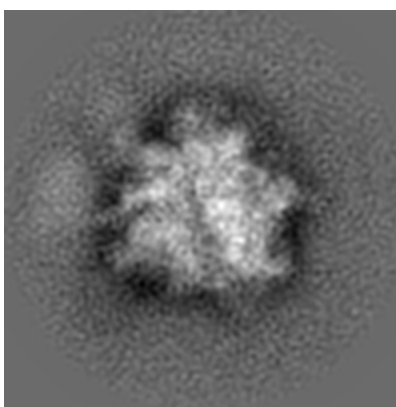


Z

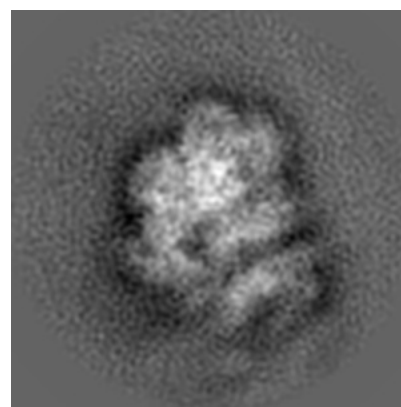
6.1.2 Raw map



X



Y

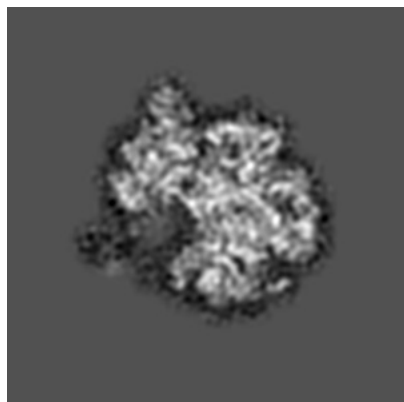


Z

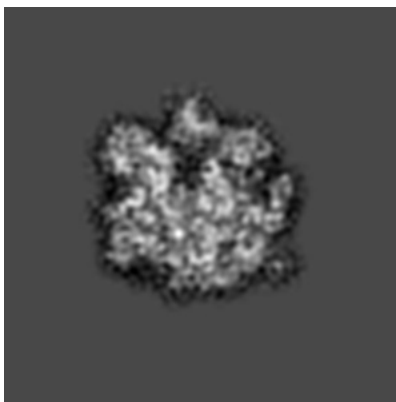
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

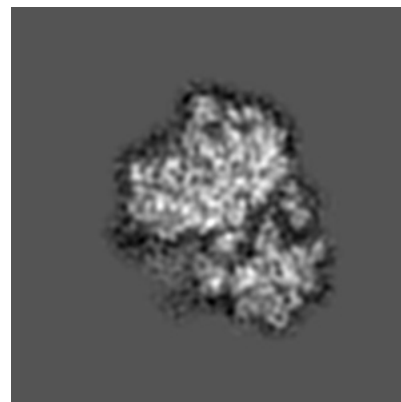
6.2.1 Primary map



X Index: 50

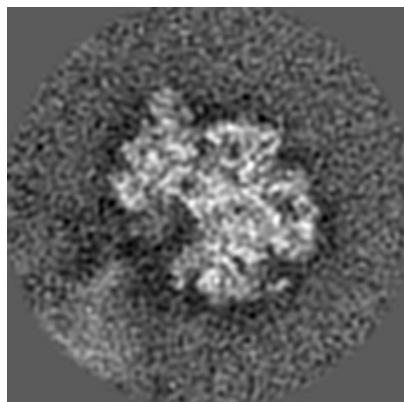


Y Index: 50

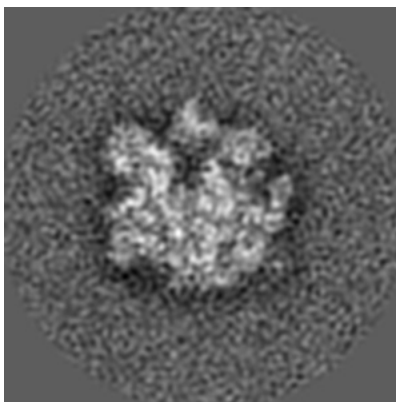


Z Index: 50

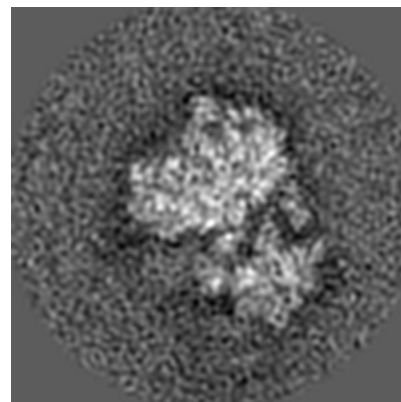
6.2.2 Raw map



X Index: 50



Y Index: 50

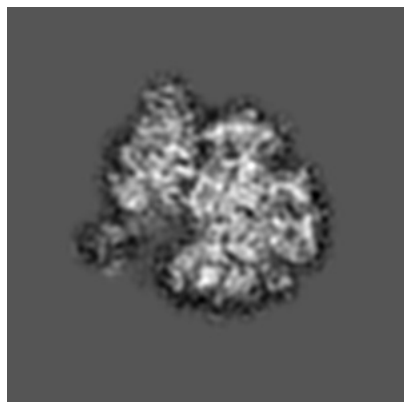


Z Index: 50

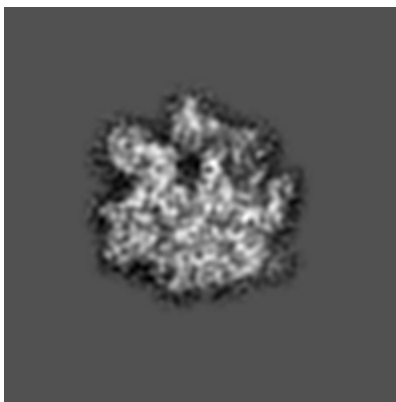
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

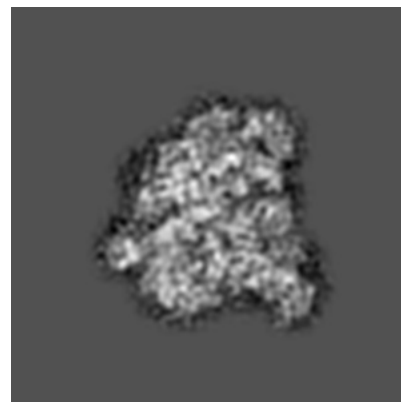
6.3.1 Primary map



X Index: 51

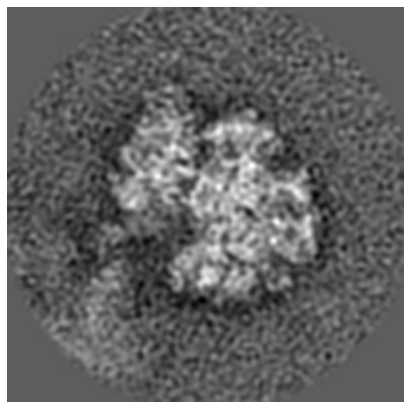


Y Index: 51

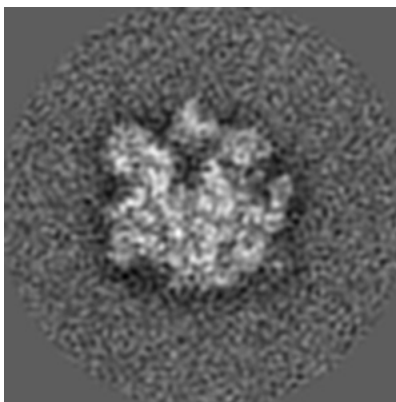


Z Index: 57

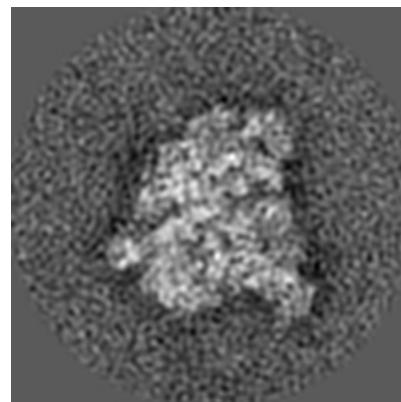
6.3.2 Raw map



X Index: 51



Y Index: 50

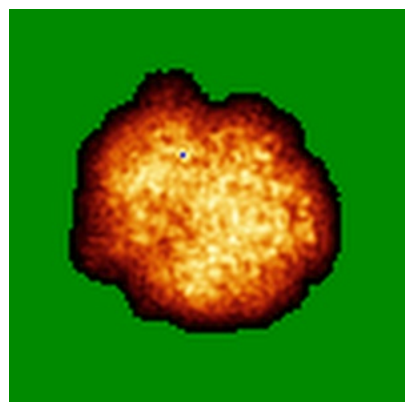


Z Index: 57

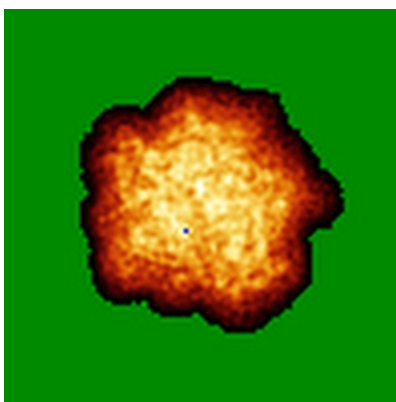
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

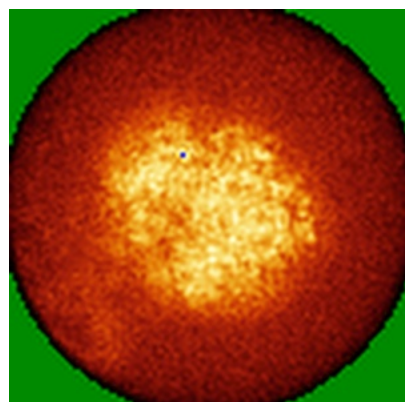


Y

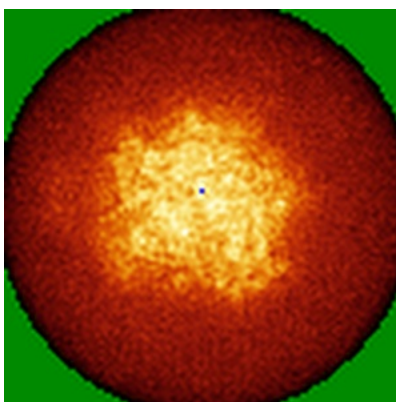


Z

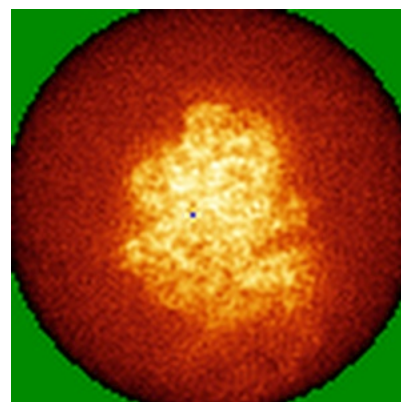
6.4.2 Raw map



X



Y

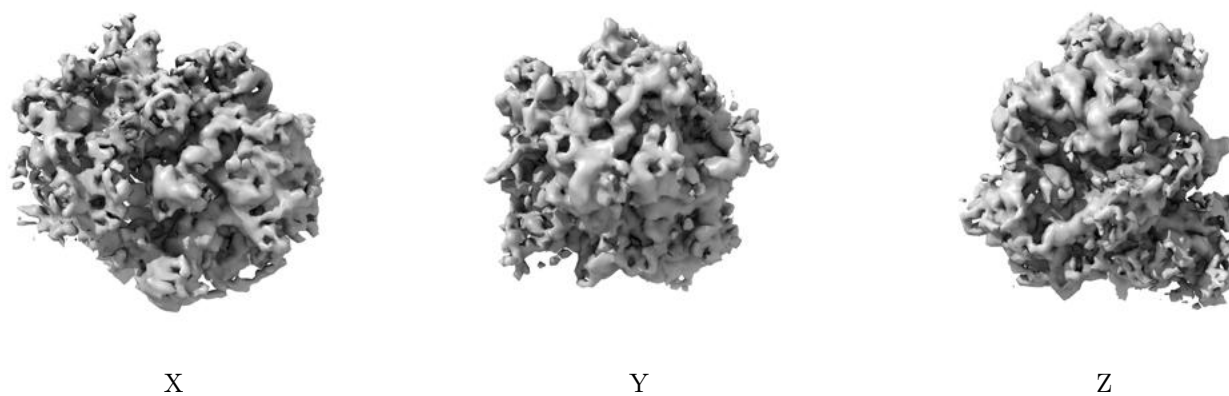


Z

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.

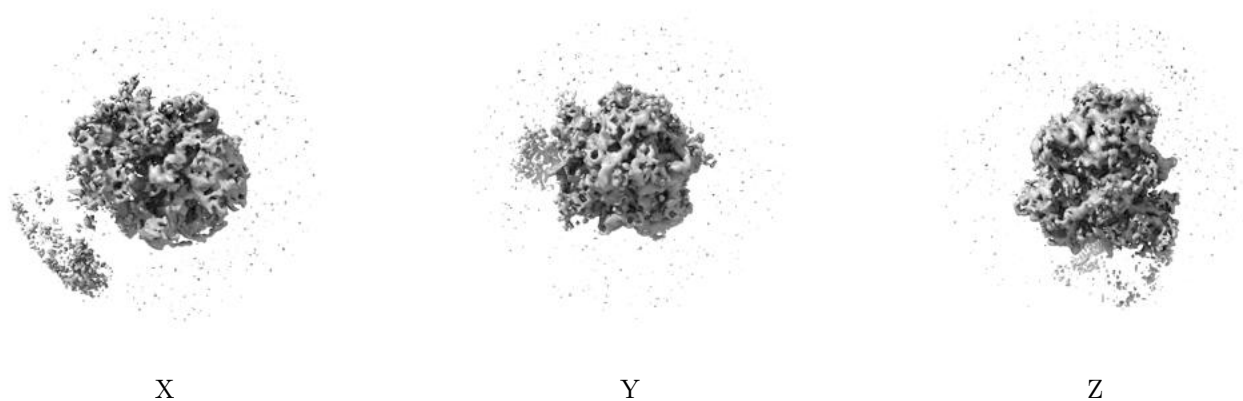
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.39. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

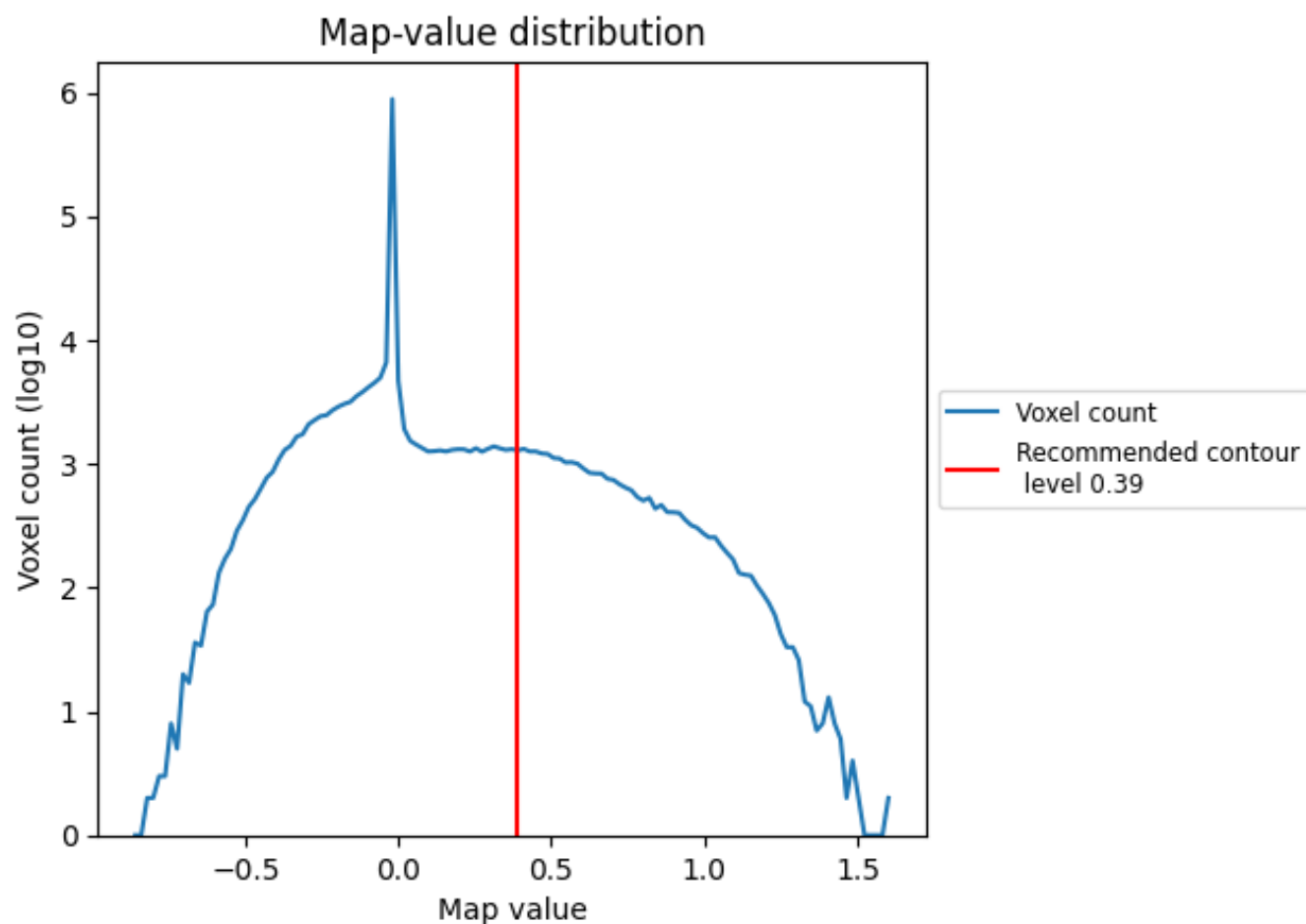
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

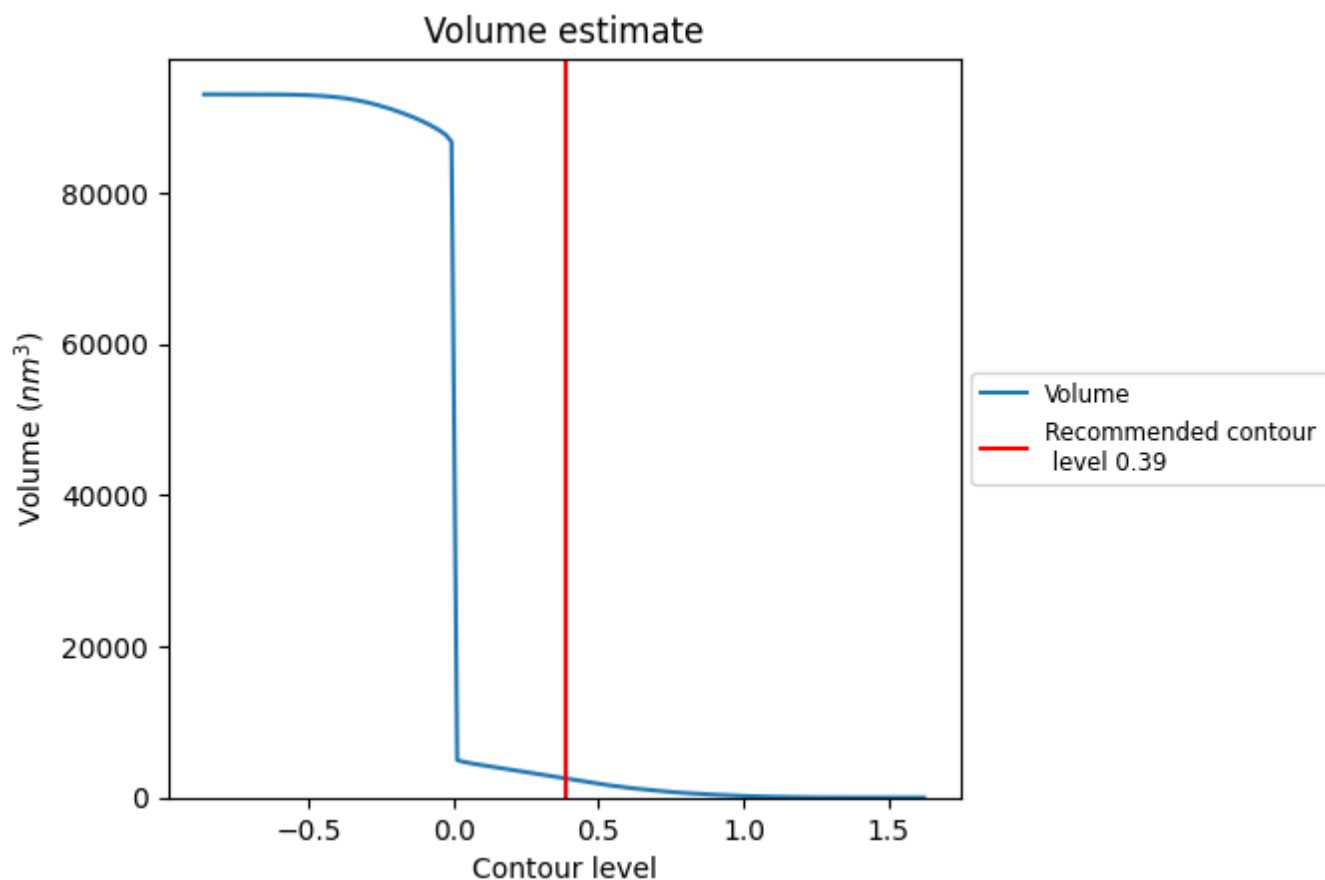
This section contains the results of statistical analysis of the map.

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.

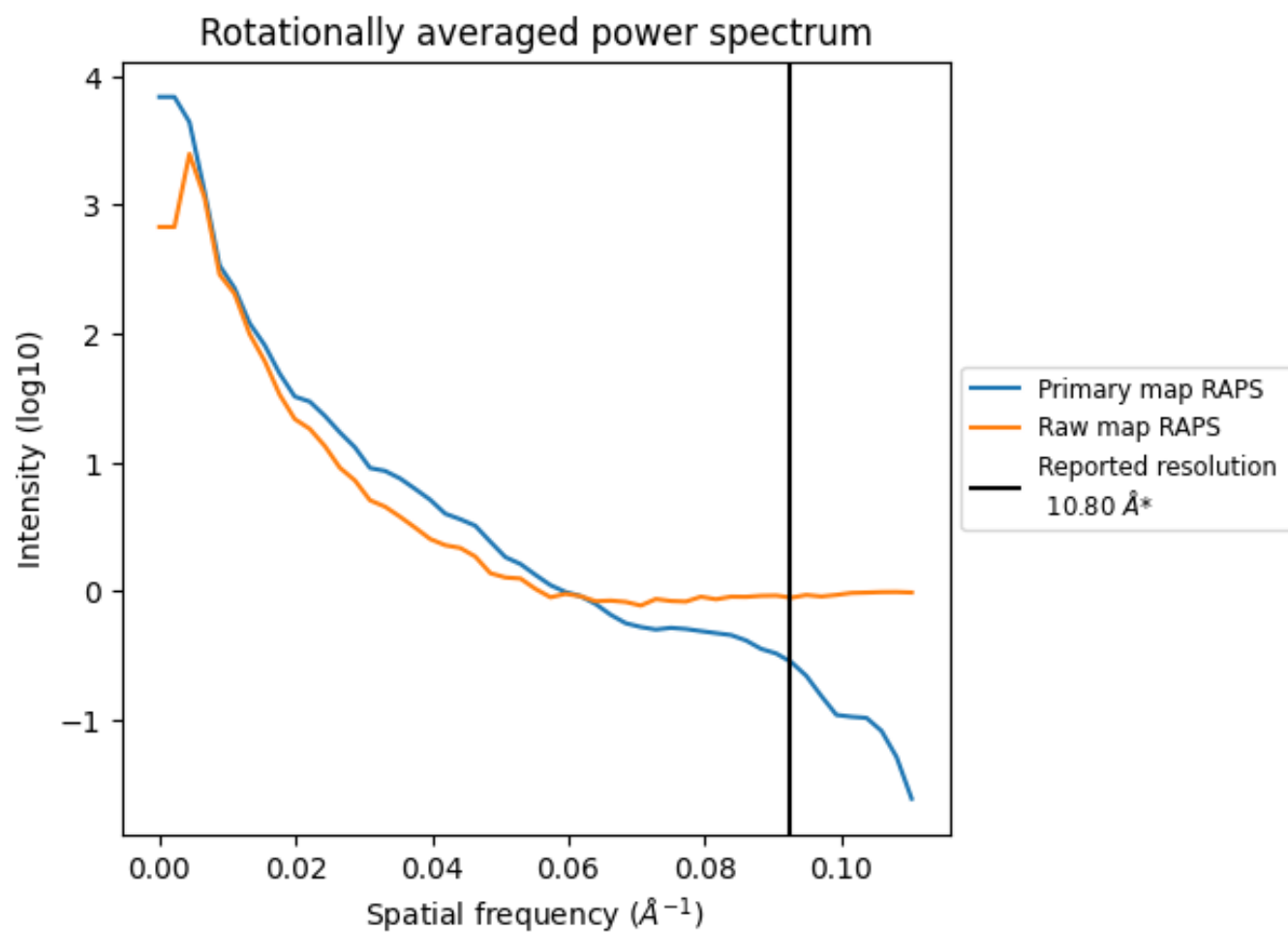
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2482 nm³; this corresponds to an approximate mass of 2242 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 ⓘ

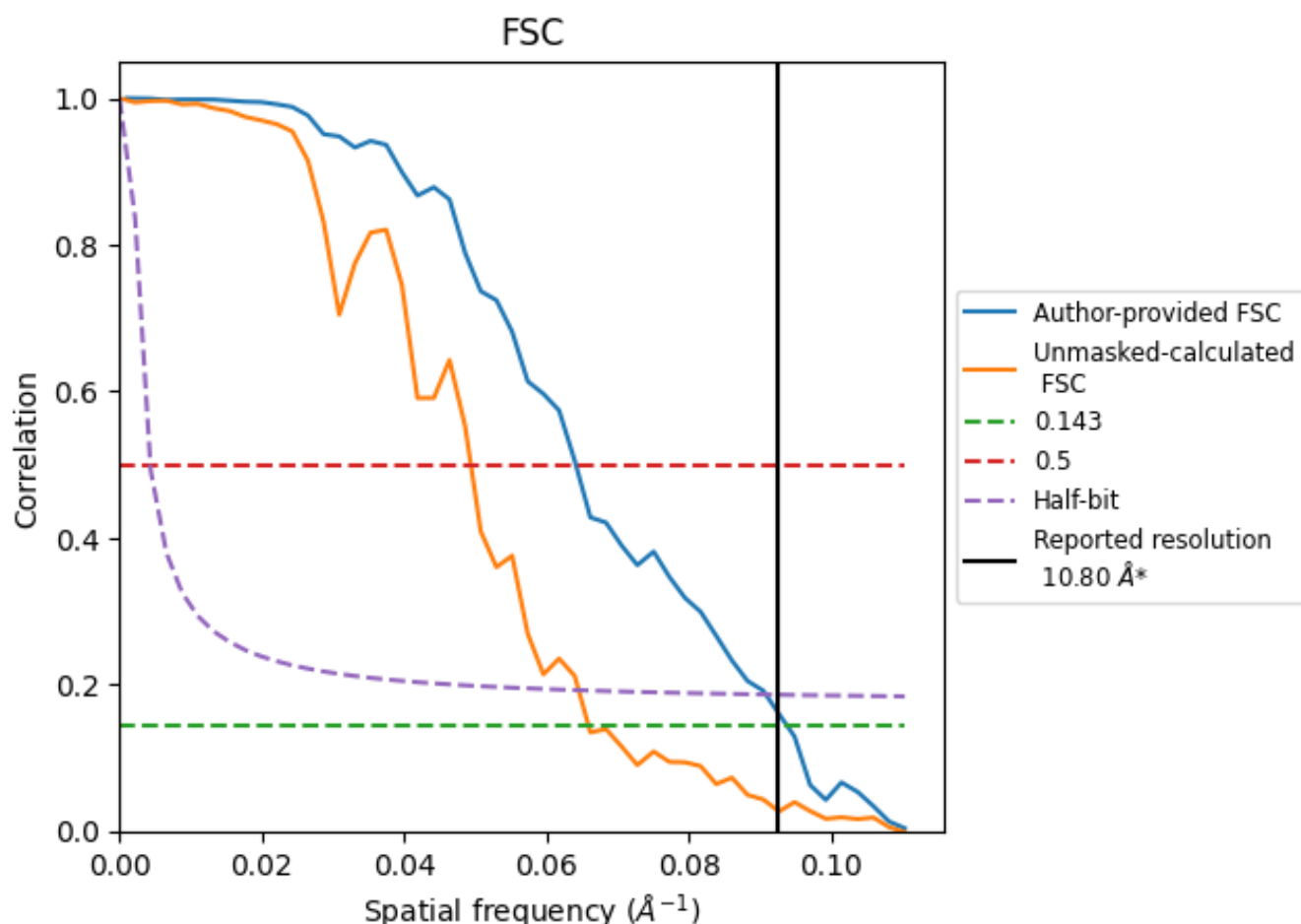


*Reported resolution corresponds to spatial frequency of 0.093 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.093 \AA^{-1}

8.2 Resolution estimates [i](#)

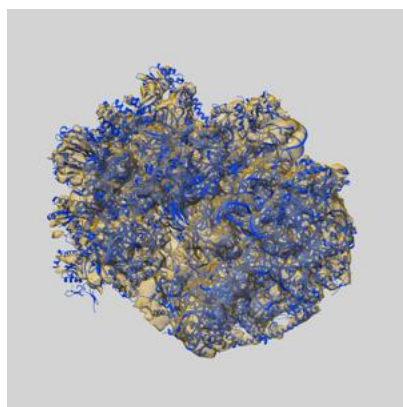
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|-------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 10.80 | - | - |
| Author-provided FSC curve | 10.65 | 15.58 | 11.00 |
| Unmasked-calculated* | 15.15 | 20.24 | 15.48 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 15.15 differs from the reported value 10.8 by more than 10 %

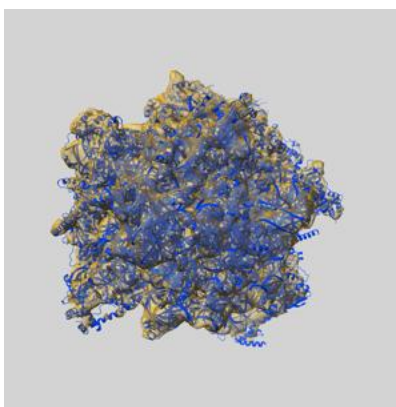
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17448 and PDB model 8P5D. Per-residue inclusion information can be found in section [3](#) on page [18](#).

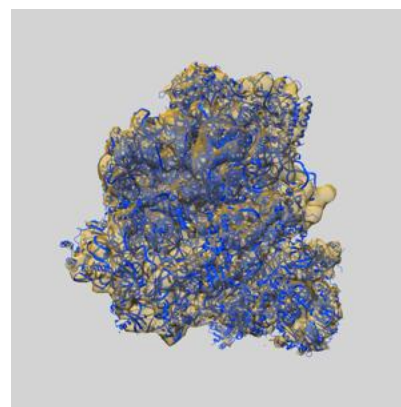
9.1 Map-model overlay [i](#)



X



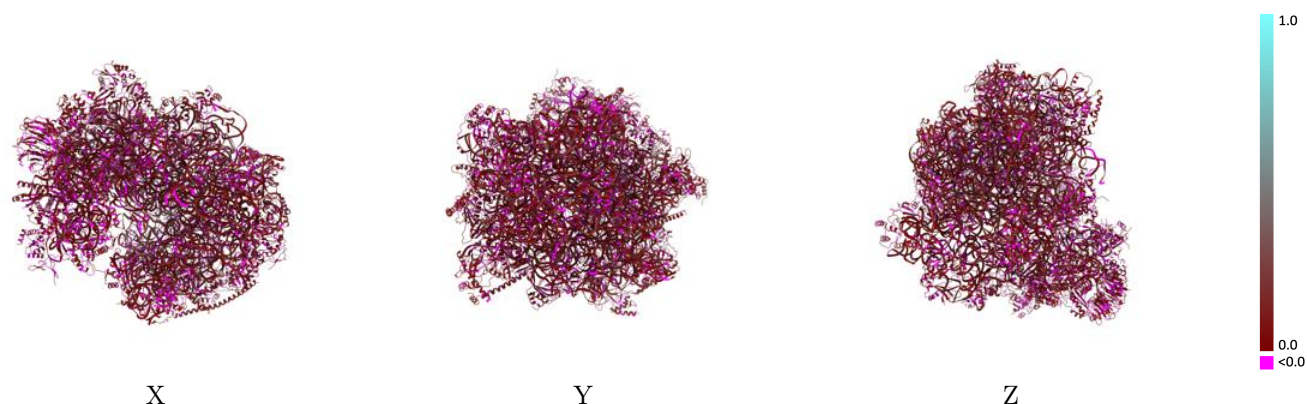
Y



Z

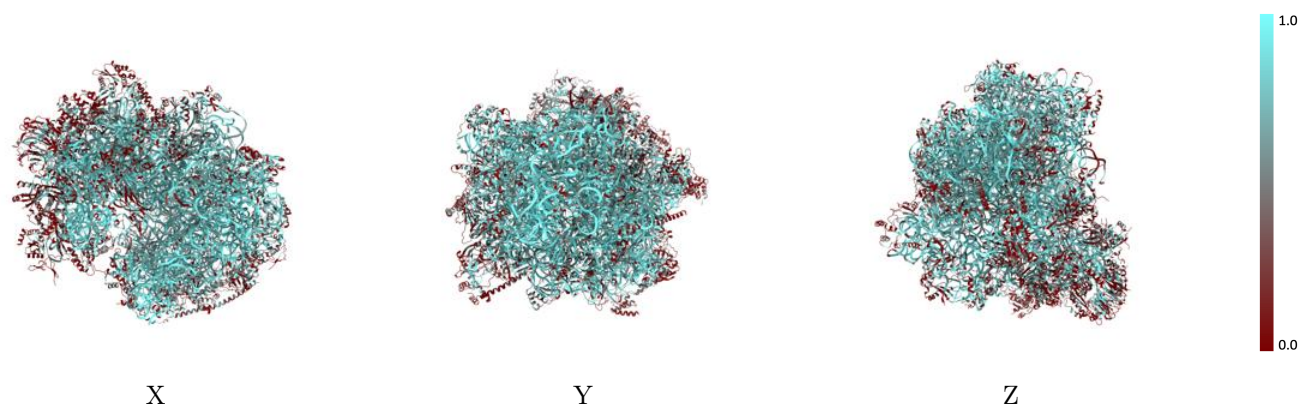
The images above show the 3D surface view of the map at the recommended contour level 0.39 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



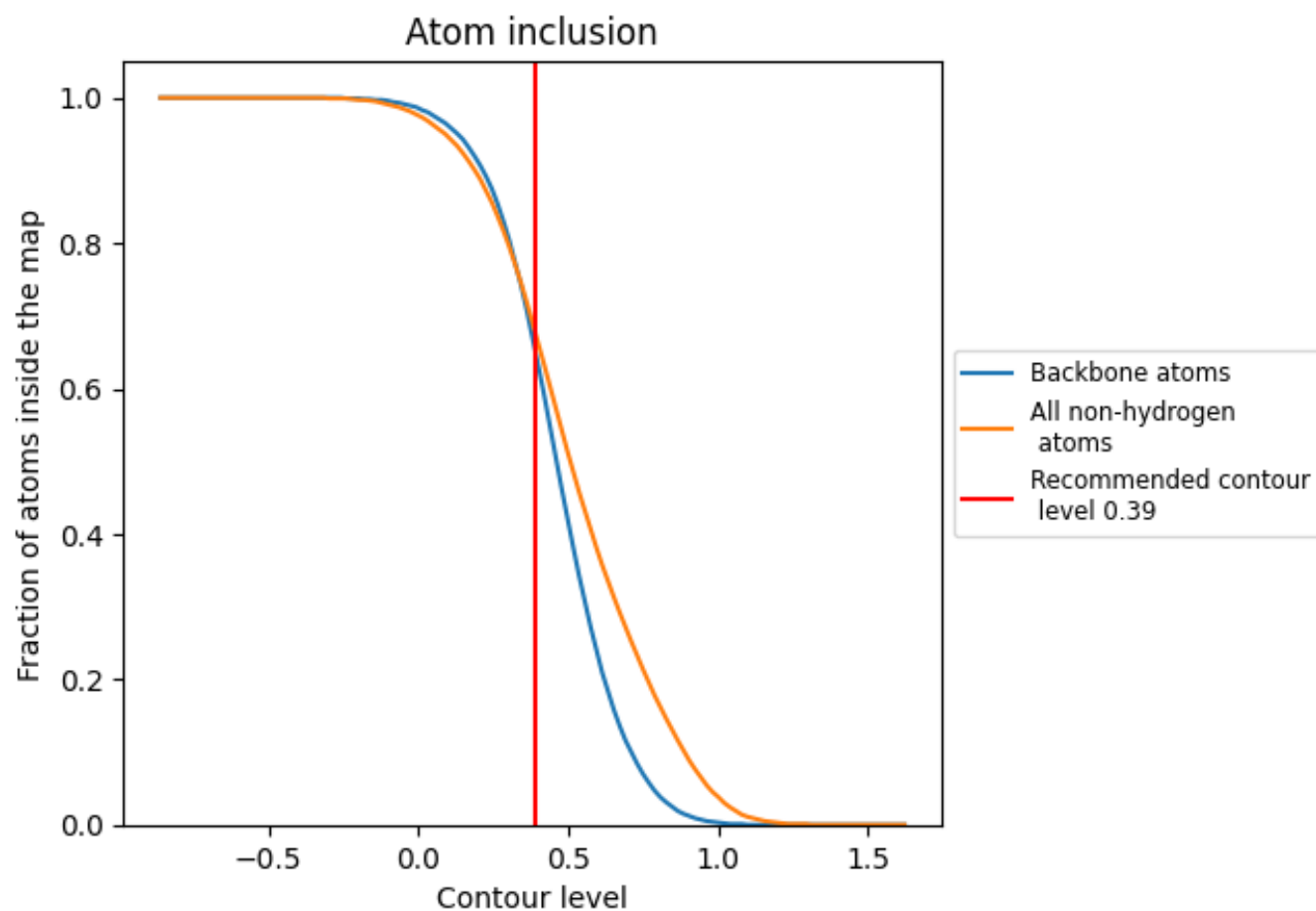
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.39).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 68% 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 (0.39) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.6780 |  0.0880 |
| L50 |  0.9150 |  0.1100 |
| L70 |  0.9040 |  0.1200 |
| LA0 |  0.5280 |  0.0500 |
| LAA |  0.7060 |  0.0460 |
| LB0 |  0.5470 |  0.0550 |
| LC0 |  0.5060 |  0.0530 |
| LCC |  0.4150 |  0.0890 |
| LD0 |  0.5650 |  0.0600 |
| LDD |  0.5200 |  0.0830 |
| LE0 |  0.3100 |  0.0940 |
| LEE |  0.5220 |  0.0490 |
| LF0 |  0.4930 |  0.0820 |
| LFF |  0.5130 |  0.0670 |
| LG0 |  0.4810 |  0.0950 |
| LGG |  0.5720 |  0.0420 |
| LH0 |  0.4950 |  0.0810 |
| LHH |  0.5640 |  0.0950 |
| LI0 |  0.5460 |  0.0630 |
| LII |  0.5210 |  0.0730 |
| LJ0 |  0.5060 |  0.0720 |
| LJJ |  0.7270 |  0.0670 |
| LL0 |  0.5870 |  0.0660 |
| LLL |  0.5270 |  0.0420 |
| LM0 |  0.3300 |  0.0970 |
| LMM |  0.6050 |  0.0700 |
| LN0 |  0.7350 |  0.0210 |
| LO0 |  0.4870 |  0.0860 |
| LOO |  0.5920 |  0.0590 |
| LP0 |  0.5630 |  0.0720 |
| LPP |  0.5880 |  0.0790 |
| LQ0 |  0.5240 |  0.0650 |
| LR0 |  0.4620 |  0.0860 |
| LS0 |  0.4650 |  0.0850 |
| LT0 |  0.5090 |  0.0430 |



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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| LU0 |  0.5760 |  0.0960 |
| LV0 |  0.3960 |  0.0630 |
| LW0 |  0.2860 |  0.0700 |
| LX0 |  0.4370 |  0.0780 |
| LY0 |  0.5510 |  0.0880 |
| LZ0 |  0.3690 |  0.0760 |
| MD1 |  0.2650 |  0.0630 |
| S60 |  0.8810 |  0.1040 |
| SA0 |  0.2730 |  0.0810 |
| SAA |  0.4940 |  0.0590 |
| SB0 |  0.3950 |  0.0660 |
| SBB |  0.4690 |  0.0830 |
| SC0 |  0.4390 |  0.0860 |
| SCC |  0.1420 |  0.0520 |
| SD0 |  0.2890 |  0.0880 |
| SDD |  0.5110 |  0.0520 |
| SE0 |  0.4240 |  0.0690 |
| SEE |  0.3990 |  0.0730 |
| SF0 |  0.4840 |  0.0640 |
| SFF |  0.0260 |  0.0160 |
| SG0 |  0.3730 |  0.0740 |
| SGG |  0.3450 |  0.0650 |
| SH0 |  0.2640 |  0.0870 |
| SI0 |  0.4300 |  0.0500 |
| SJ0 |  0.4350 |  0.0830 |
| SK0 |  0.2860 |  0.0660 |
| SL0 |  0.3800 |  0.0780 |
| SM0 |  0.1760 |  0.0430 |
| SN0 |  0.4590 |  0.0740 |
| SO0 |  0.5000 |  0.0440 |
| SP0 |  0.3270 |  0.0440 |
| SQ0 |  0.4240 |  0.0520 |
| SR0 |  0.2240 |  0.0710 |
| SS0 |  0.4530 |  0.0570 |
| ST0 |  0.4690 |  0.0750 |
| SU0 |  0.3330 |  0.0770 |
| SV0 |  0.3190 |  0.0940 |
| SW0 |  0.4180 |  0.0710 |
| SX0 |  0.2580 |  0.0350 |
| SY0 |  0.4020 |  0.0650 |
| SZ0 |  0.4930 |  0.0580 |