



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 02:15 AM UTC

PDB ID : 4V53 / pdb_00004v53
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with gentamicin.
Authors : Borovinskaya, M.A.; Pai, R.D.; Zhang, W.; Schuwirth, B.-S.; Holton, J.M.; Hirokawa, G.; Kaji, H.; Kaji, A.; Cate, J.H.D.
Deposited on : 2007-06-16
Resolution : 3.54 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : **FAILED**
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.48.1

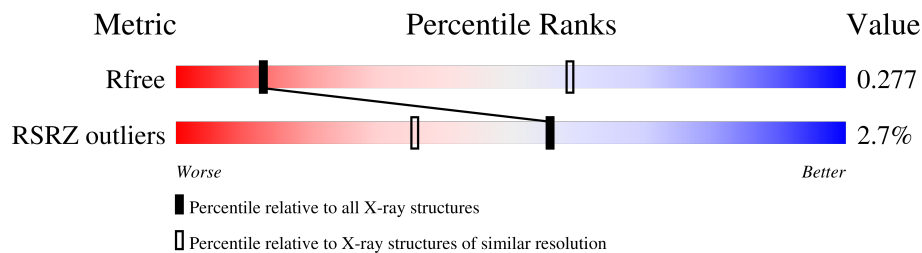
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.54 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) | Similar resolution (#Entries, resolution range(Å)) |
|---------------|-----------------------------|---|
| R_{free} | 164625 | 1272 (3.60-3.48) |
| RSRZ outliers | 164620 | 1271 (3.60-3.48) |

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

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 284252 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|----------------|------------|-----------|------------|-----------|---------|---------|-------|
| | | | Total | C | N | O | P | | | |
| 1 | AA | 1530 | Total 32831 | C 14642 | N 6024 | O 10635 | P 1530 | 0 | 0 | 0 |
| 1 | CA | 1530 | Total 32831 | C 14642 | N 6024 | O 10635 | P 1530 | 0 | 0 | 0 |

- Molecule 2 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 2 | AC | 206 | Total 1624 | C 1028 | N 305 | O 288 | S 3 | 0 | 0 | 0 |
| 2 | CC | 206 | Total 1624 | C 1028 | N 305 | O 288 | S 3 | 0 | 0 | 0 |

- Molecule 3 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 3 | AD | 205 | Total 1643 | C 1026 | N 315 | O 298 | S 4 | 0 | 0 | 0 |
| 3 | CD | 205 | Total 1643 | C 1026 | N 315 | O 298 | S 4 | 0 | 0 | 0 |

- Molecule 4 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 4 | AE | 150 | Total 1105 | C 687 | N 211 | O 201 | S 6 | 0 | 0 | 0 |
| 4 | CE | 150 | Total 1105 | C 687 | N 211 | O 201 | S 6 | 0 | 0 | 0 |

- Molecule 5 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | AF | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 817 | 515 | 148 | 148 | 6 | | | |
| 5 | CF | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 817 | 515 | 148 | 148 | 6 | | | |

- Molecule 6 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | AG | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1174 | 730 | 226 | 214 | 4 | | | |
| 6 | CG | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1196 | 745 | 230 | 217 | 4 | | | |

- Molecule 7 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | AH | 129 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 979 | 616 | 173 | 184 | 6 | | | |
| 7 | CH | 129 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 979 | 616 | 173 | 184 | 6 | | | |

- Molecule 8 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | AI | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1022 | 634 | 206 | 179 | 3 | | | |
| 8 | CI | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1022 | 634 | 206 | 179 | 3 | | | |

- Molecule 9 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9 | AJ | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 786 | 493 | 150 | 142 | 1 | | | |
| 9 | CJ | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 786 | 493 | 150 | 142 | 1 | | | |

- Molecule 10 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | AK | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 877 | 540 | 174 | 160 | 3 | | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | CK | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 877 | 540 | 174 | 160 | 3 | | | |

- Molecule 11 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | AL | 123 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 955 | 590 | 196 | 165 | 4 | | | |
| 11 | CL | 123 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 955 | 590 | 196 | 165 | 4 | | | |

- Molecule 12 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | AM | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 883 | 546 | 178 | 156 | 3 | | | |
| 12 | CM | 113 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 876 | 541 | 177 | 155 | 3 | | | |

- Molecule 13 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | AN | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 774 | 483 | 160 | 128 | 3 | | | |
| 13 | CN | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 774 | 483 | 160 | 128 | 3 | | | |

- Molecule 14 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14 | AO | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 714 | 439 | 144 | 130 | 1 | | | |
| 14 | CO | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 714 | 439 | 144 | 130 | 1 | | | |

- Molecule 15 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15 | AP | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 649 | 406 | 128 | 114 | 1 | | | |
| 15 | CP | 80 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 638 | 400 | 126 | 111 | 1 | | | |

- Molecule 16 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | AQ | 80 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 648 | 411 | 121 | 113 | 3 | | | |
| 16 | CQ | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 657 | 417 | 122 | 115 | 3 | | | |

- Molecule 17 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 17 | AR | 55 | Total | C | N | O | 0 | 0 | 0 |
| | | | 455 | 288 | 86 | 81 | | | |
| 17 | CR | 55 | Total | C | N | O | 0 | 0 | 0 |
| | | | 455 | 288 | 86 | 81 | | | |

- Molecule 18 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 18 | AS | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 637 | 408 | 120 | 107 | 2 | | | |
| 18 | CS | 80 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 644 | 413 | 121 | 108 | 2 | | | |

- Molecule 19 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | AT | 85 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 665 | 411 | 137 | 114 | 3 | | | |
| 19 | CT | 85 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 665 | 411 | 137 | 114 | 3 | | | |

- Molecule 20 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 20 | AB | 218 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1704 | 1081 | 305 | 311 | 7 | | | |
| 20 | CB | 218 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1704 | 1081 | 305 | 311 | 7 | | | |

- Molecule 21 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 21 | AU | 51 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 425 | 265 | 86 | 73 | 1 | | | |
| 21 | CU | 51 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 425 | 265 | 86 | 73 | 1 | | | |

- Molecule 22 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 22 | BA | 117 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2507 | 1116 | 459 | 815 | 117 | | | |
| 22 | DA | 117 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2507 | 1116 | 459 | 815 | 117 | | | |

- Molecule 23 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 23 | BB | 2841 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 60995 | 27210 | 11229 | 19715 | 2841 | | | |
| 23 | DB | 2841 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 60995 | 27210 | 11229 | 19715 | 2841 | | | |

- Molecule 24 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 24 | BI | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1032 | 651 | 179 | 196 | 6 | | | |
| 24 | DI | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1032 | 651 | 179 | 196 | 6 | | | |

- Molecule 25 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 25 | BC | 271 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2082 | 1288 | 423 | 364 | 7 | | | |
| 25 | DC | 271 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2082 | 1288 | 423 | 364 | 7 | | | |

- Molecule 26 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26 | BD | 209 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1565 | 979 | 288 | 294 | 4 | | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26 | DD | 209 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1565 | 979 | 288 | 294 | 4 | | | |

- Molecule 27 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 27 | BK | 121 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 930 | 582 | 179 | 164 | 5 | | | |
| 27 | DK | 121 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 930 | 582 | 179 | 164 | 5 | | | |

- Molecule 28 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28 | BP | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 917 | 574 | 179 | 163 | 1 | | | |
| 28 | DP | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 917 | 574 | 179 | 163 | 1 | | | |

- Molecule 29 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 29 | BE | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1552 | 974 | 283 | 290 | 5 | | | |
| 29 | DE | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1552 | 974 | 283 | 290 | 5 | | | |

- Molecule 30 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 30 | BY | 58 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 449 | 281 | 87 | 79 | 2 | | | |
| 30 | DY | 58 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 449 | 281 | 87 | 79 | 2 | | | |

- Molecule 31 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 31 | B0 | 56 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 444 | 269 | 94 | 80 | 1 | | | |
| 31 | D0 | 56 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 444 | 269 | 94 | 80 | 1 | | | |

- Molecule 32 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 32 | B4 | 38 | Total 302 | C 185 | N 65 | O 48 | S 4 | 0 | 0 | 0 |
| 32 | D4 | 38 | Total 302 | C 185 | N 65 | O 48 | S 4 | 0 | 0 | 0 |

- Molecule 33 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 33 | B1 | 50 | Total 409 | C 263 | N 75 | O 71 | 0 | 0 | 0 |
| 33 | D1 | 50 | Total 409 | C 263 | N 75 | O 71 | 0 | 0 | 0 |

- Molecule 34 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|---------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 34 | B3 | 64 | Total 504 | C 323 | N 105 | O 74 | S 2 | 0 | 0 | 0 |
| 34 | D3 | 64 | Total 504 | C 323 | N 105 | O 74 | S 2 | 0 | 0 | 0 |

- Molecule 35 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 35 | BV | 94 | Total 753 | C 479 | N 137 | O 134 | S 3 | 0 | 0 | 0 |
| 35 | DV | 94 | Total 753 | C 479 | N 137 | O 134 | S 3 | 0 | 0 | 0 |

- Molecule 36 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 36 | B2 | 46 | Total 377 | C 228 | N 90 | O 57 | S 2 | 0 | 0 | 0 |
| 36 | D2 | 46 | Total 377 | C 228 | N 90 | O 57 | S 2 | 0 | 0 | 0 |

- Molecule 37 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37 | BL | 143 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1045 | 649 | 206 | 189 | 1 | | | |
| 37 | DL | 143 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1045 | 649 | 206 | 189 | 1 | | | |

- Molecule 38 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38 | BM | 136 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1074 | 686 | 205 | 177 | 6 | | | |
| 38 | DM | 136 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1074 | 686 | 205 | 177 | 6 | | | |

- Molecule 39 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 39 | BX | 63 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 509 | 313 | 99 | 95 | 2 | | | |
| 39 | DX | 63 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 509 | 313 | 99 | 95 | 2 | | | |

- Molecule 40 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40 | BH | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1111 | 699 | 197 | 214 | 1 | | | |
| 40 | DH | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1111 | 699 | 197 | 214 | 1 | | | |

- Molecule 41 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41 | BJ | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1129 | 714 | 212 | 199 | 4 | | | |
| 41 | DJ | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1129 | 714 | 212 | 199 | 4 | | | |

- Molecule 42 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42 | BN | 120 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 960 | 593 | 196 | 166 | 5 | | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42 | DN | 120 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 960 | 593 | 196 | 166 | 5 | | | |

- Molecule 43 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 43 | BO | 116 | Total | C | N | O | 0 | 0 | 0 |
| | | | 892 | 552 | 178 | 162 | | | |
| 43 | DO | 116 | Total | C | N | O | 0 | 0 | 0 |
| | | | 892 | 552 | 178 | 162 | | | |

- Molecule 44 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 44 | BQ | 117 | Total | C | N | O | 0 | 0 | 0 |
| | | | 947 | 604 | 192 | 151 | | | |
| 44 | DQ | 117 | Total | C | N | O | 0 | 0 | 0 |
| | | | 947 | 604 | 192 | 151 | | | |

- Molecule 45 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45 | BS | 110 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 857 | 532 | 166 | 156 | 3 | | | |
| 45 | DS | 110 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 857 | 532 | 166 | 156 | 3 | | | |

- Molecule 46 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 46 | BU | 102 | Total | C | N | O | 0 | 0 | 0 |
| | | | 779 | 492 | 146 | 141 | | | |
| 46 | DU | 102 | Total | C | N | O | 0 | 0 | 0 |
| | | | 779 | 492 | 146 | 141 | | | |

- Molecule 47 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47 | BF | 178 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1420 | 905 | 251 | 258 | 6 | | | |
| 47 | DF | 178 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1420 | 905 | 251 | 258 | 6 | | | |

- Molecule 48 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 48 | BG | 176 | Total 1323 | C 832 | N 243 | O 246 | S 2 | 0 | 0 | 0 |
| 48 | DG | 176 | Total 1323 | C 832 | N 243 | O 246 | S 2 | 0 | 0 | 0 |

- Molecule 49 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 49 | BR | 103 | Total 816 | C 516 | N 153 | O 145 | S 2 | 0 | 0 | 0 |
| 49 | DR | 103 | Total 816 | C 516 | N 153 | O 145 | S 2 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 50 | BT | 93 | Total 738 | C 466 | N 139 | O 131 | S 2 | 0 | 0 | 0 |
| 50 | DT | 93 | Total 738 | C 466 | N 139 | O 131 | S 2 | 0 | 0 | 0 |

- Molecule 51 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 51 | BZ | 77 | Total 625 | C 388 | N 129 | O 106 | S 2 | 0 | 0 | 0 |
| 51 | DZ | 77 | Total 625 | C 388 | N 129 | O 106 | S 2 | 0 | 0 | 0 |

- Molecule 52 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 52 | BW | 79 | Total 596 | C 367 | N 120 | O 108 | S 1 | 0 | 0 | 0 |
| 52 | DW | 79 | Total 596 | C 367 | N 120 | O 108 | S 1 | 0 | 0 | 0 |

- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| | | | Total | C | N | O | | |
| 54 | CA | 1 | 31 | 19 | 5 | 7 | 0 | 0 |
| 54 | CA | 1 | 31 | 19 | 5 | 7 | 0 | 0 |
| 54 | DB | 1 | 31 | 19 | 5 | 7 | 0 | 0 |

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| | | | Total | Zn | | |
| 55 | B4 | 1 | 1 | 1 | 0 | 0 |
| 55 | D4 | 1 | 1 | 1 | 0 | 0 |

- Molecule 56 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| | | | Total | O | | |
| 56 | AA | 292 | 292 | 292 | 0 | 0 |
| 56 | AE | 1 | 1 | 1 | 0 | 0 |
| 56 | AK | 1 | 1 | 1 | 0 | 0 |
| 56 | AL | 2 | 2 | 2 | 0 | 0 |
| 56 | AN | 2 | 2 | 2 | 0 | 0 |
| 56 | AT | 2 | 2 | 2 | 0 | 0 |
| 56 | BB | 492 | 492 | 492 | 0 | 0 |
| 56 | BC | 7 | 7 | 7 | 0 | 0 |
| 56 | BE | 3 | 3 | 3 | 0 | 0 |
| 56 | B2 | 1 | 1 | 1 | 0 | 0 |
| 56 | BL | 3 | 3 | 3 | 0 | 0 |
| 56 | BH | 1 | 1 | 1 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 56 | CA | 297 | Total O 297 297 | 0 | 0 |
| 56 | CE | 2 | Total O 2 2 | 0 | 0 |
| 56 | CK | 1 | Total O 1 1 | 0 | 0 |
| 56 | CL | 2 | Total O 2 2 | 0 | 0 |
| 56 | CN | 4 | Total O 4 4 | 0 | 0 |
| 56 | CT | 2 | Total O 2 2 | 0 | 0 |
| 56 | DB | 502 | Total O 502 502 | 0 | 0 |
| 56 | DC | 4 | Total O 4 4 | 0 | 0 |
| 56 | DE | 2 | Total O 2 2 | 0 | 0 |
| 56 | DL | 4 | Total O 4 4 | 0 | 0 |

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

3 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 208.85Å 379.20Å 739.28Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 70.00 – 3.54 70.00 – 3.55 | Depositor EDS |
| % Data completeness (in resolution range) | 88.8 (70.00-3.54) 89.8 (70.00-3.55) | Depositor EDS |
| R_{merge} | 0.10 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.69 (at 3.58Å) | Xtrriage |
| Refinement program | CNS | Depositor |
| R, R_{free} | 0.281 , 0.320 0.245 , 0.277 | Depositor DCC |
| R_{free} test set | 30217 reflections (4.81%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 125.1 | Xtrriage |
| Anisotropy | 0.234 | Xtrriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.28 , 41.9 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$ | Xtrriage |
| Estimated twinning fraction | No twinning to report. | Xtrriage |
| F_o, F_c correlation | 0.93 | EDS |
| Total number of atoms | 284252 | wwPDB-VP |
| Average B, all atoms (Å ²) | 66.0 | wwPDB-VP |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 353 ligands modelled in this entry, 345 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 54 | LLL | CA | 2062 | - | 31,33,33 | 2.53 | 14 (45%) | 33,49,49 | 1.27 | 3 (9%) |
| 54 | LLL | CA | 2064 | - | 31,33,33 | 2.47 | 13 (41%) | 33,49,49 | 1.26 | 3 (9%) |
| 54 | LLL | CA | 2063 | - | 31,33,33 | 2.60 | 16 (51%) | 33,49,49 | 1.30 | 4 (12%) |
| 54 | LLL | AA | 2063 | - | 31,33,33 | 2.49 | 14 (45%) | 33,49,49 | 1.41 | 3 (9%) |
| 54 | LLL | BB | 3111 | - | 31,33,33 | 2.57 | 15 (48%) | 33,49,49 | 1.28 | 5 (15%) |
| 54 | LLL | DB | 3112 | - | 31,33,33 | 2.57 | 15 (48%) | 33,49,49 | 1.25 | 3 (9%) |
| 54 | LLL | AA | 2061 | - | 31,33,33 | 2.52 | 12 (38%) | 33,49,49 | 1.34 | 4 (12%) |
| 54 | LLL | AA | 2062 | - | 31,33,33 | 2.60 | 17 (54%) | 33,49,49 | 1.33 | 4 (12%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 54 | LLL | CA | 2062 | - | - | 1/11/65/65 | 0/3/3/3 |
| 54 | LLL | CA | 2064 | - | - | 1/11/65/65 | 0/3/3/3 |
| 54 | LLL | CA | 2063 | - | - | 5/11/65/65 | 0/3/3/3 |
| 54 | LLL | AA | 2063 | - | - | 2/11/65/65 | 0/3/3/3 |
| 54 | LLL | BB | 3111 | - | - | 2/11/65/65 | 0/3/3/3 |
| 54 | LLL | DB | 3112 | - | - | 1/11/65/65 | 0/3/3/3 |
| 54 | LLL | AA | 2061 | - | - | 1/11/65/65 | 0/3/3/3 |
| 54 | LLL | AA | 2062 | - | - | 2/11/65/65 | 0/3/3/3 |

All (116) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 54 | CA | 2063 | LLL | O53-C53 | 6.75 | 1.52 | 1.43 |
| 54 | AA | 2062 | LLL | O53-C53 | 6.63 | 1.52 | 1.43 |
| 54 | DB | 3112 | LLL | O53-C53 | 6.59 | 1.52 | 1.43 |
| 54 | BB | 3111 | LLL | O53-C53 | 6.58 | 1.52 | 1.43 |
| 54 | AA | 2061 | LLL | O53-C53 | 6.52 | 1.52 | 1.43 |
| 54 | CA | 2062 | LLL | O53-C53 | 6.51 | 1.52 | 1.43 |
| 54 | AA | 2063 | LLL | O53-C53 | 6.47 | 1.51 | 1.43 |
| 54 | CA | 2064 | LLL | O53-C53 | 6.42 | 1.51 | 1.43 |
| 54 | AA | 2063 | LLL | O53-C13 | 4.92 | 1.52 | 1.41 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 54 | CA | 2063 | LLL | O53-C13 | 4.87 | 1.52 | 1.41 |
| 54 | CA | 2062 | LLL | O53-C13 | 4.81 | 1.51 | 1.41 |
| 54 | AA | 2062 | LLL | O53-C13 | 4.78 | 1.51 | 1.41 |
| 54 | CA | 2064 | LLL | O53-C13 | 4.70 | 1.51 | 1.41 |
| 54 | BB | 3111 | LLL | O53-C13 | 4.70 | 1.51 | 1.41 |
| 54 | DB | 3112 | LLL | O53-C13 | 4.64 | 1.51 | 1.41 |
| 54 | AA | 2061 | LLL | O53-C13 | 4.63 | 1.51 | 1.41 |
| 54 | CA | 2062 | LLL | C53-C43 | 4.62 | 1.56 | 1.52 |
| 54 | DB | 3112 | LLL | C53-C43 | 4.59 | 1.56 | 1.52 |
| 54 | BB | 3111 | LLL | C53-C43 | 4.56 | 1.56 | 1.52 |
| 54 | AA | 2061 | LLL | C53-C43 | 4.55 | 1.56 | 1.52 |
| 54 | AA | 2062 | LLL | C53-C43 | 4.40 | 1.56 | 1.52 |
| 54 | CA | 2064 | LLL | C53-C43 | 4.39 | 1.56 | 1.52 |
| 54 | CA | 2063 | LLL | C53-C43 | 4.21 | 1.56 | 1.52 |
| 54 | BB | 3111 | LLL | C33-N33 | 3.98 | 1.50 | 1.45 |
| 54 | CA | 2063 | LLL | C33-N33 | 3.95 | 1.50 | 1.45 |
| 54 | DB | 3112 | LLL | C33-N33 | 3.90 | 1.50 | 1.45 |
| 54 | AA | 2062 | LLL | C33-N33 | 3.89 | 1.50 | 1.45 |
| 54 | AA | 2061 | LLL | C33-N33 | 3.72 | 1.50 | 1.45 |
| 54 | CA | 2064 | LLL | C33-N33 | 3.70 | 1.50 | 1.45 |
| 54 | DB | 3112 | LLL | O51-C11 | 3.68 | 1.51 | 1.41 |
| 54 | BB | 3111 | LLL | O51-C11 | 3.68 | 1.51 | 1.41 |
| 54 | AA | 2061 | LLL | C41-C51 | 3.67 | 1.60 | 1.51 |
| 54 | CA | 2063 | LLL | O51-C11 | 3.66 | 1.51 | 1.41 |
| 54 | CA | 2062 | LLL | C33-N33 | 3.61 | 1.50 | 1.45 |
| 54 | CA | 2062 | LLL | O51-C11 | 3.59 | 1.51 | 1.41 |
| 54 | AA | 2062 | LLL | O51-C11 | 3.56 | 1.51 | 1.41 |
| 54 | AA | 2063 | LLL | O51-C11 | 3.56 | 1.51 | 1.41 |
| 54 | AA | 2063 | LLL | C23-C33 | 3.54 | 1.60 | 1.53 |
| 54 | CA | 2062 | LLL | C41-C51 | 3.54 | 1.60 | 1.51 |
| 54 | BB | 3111 | LLL | C41-C51 | 3.52 | 1.60 | 1.51 |
| 54 | AA | 2062 | LLL | C41-C51 | 3.50 | 1.60 | 1.51 |
| 54 | AA | 2063 | LLL | C41-C51 | 3.49 | 1.60 | 1.51 |
| 54 | CA | 2064 | LLL | C41-C51 | 3.48 | 1.60 | 1.51 |
| 54 | CA | 2063 | LLL | C41-C51 | 3.47 | 1.60 | 1.51 |
| 54 | DB | 3112 | LLL | C41-C51 | 3.47 | 1.60 | 1.51 |
| 54 | AA | 2063 | LLL | C33-N33 | 3.44 | 1.50 | 1.45 |
| 54 | CA | 2064 | LLL | O51-C11 | 3.41 | 1.50 | 1.41 |
| 54 | AA | 2062 | LLL | C23-C33 | 3.33 | 1.60 | 1.53 |
| 54 | AA | 2063 | LLL | C53-C43 | 3.28 | 1.55 | 1.52 |
| 54 | CA | 2063 | LLL | C23-C33 | 3.25 | 1.60 | 1.53 |
| 54 | CA | 2062 | LLL | C23-C33 | 3.24 | 1.60 | 1.53 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 54 | BB | 3111 | LLL | C23-C33 | 3.23 | 1.60 | 1.53 |
| 54 | DB | 3112 | LLL | C23-C33 | 3.22 | 1.60 | 1.53 |
| 54 | AA | 2063 | LLL | C42-C32 | 3.18 | 1.60 | 1.53 |
| 54 | AA | 2061 | LLL | C23-C33 | 3.17 | 1.60 | 1.53 |
| 54 | AA | 2061 | LLL | O51-C11 | 3.14 | 1.49 | 1.41 |
| 54 | CA | 2064 | LLL | C42-C32 | 3.14 | 1.59 | 1.53 |
| 54 | CA | 2063 | LLL | C42-C32 | 3.14 | 1.59 | 1.53 |
| 54 | DB | 3112 | LLL | C42-C32 | 3.12 | 1.59 | 1.53 |
| 54 | AA | 2062 | LLL | C42-C32 | 3.07 | 1.59 | 1.53 |
| 54 | BB | 3111 | LLL | C42-C32 | 3.04 | 1.59 | 1.53 |
| 54 | CA | 2062 | LLL | C42-C32 | 2.99 | 1.59 | 1.53 |
| 54 | CA | 2063 | LLL | C52-C42 | 2.98 | 1.60 | 1.52 |
| 54 | CA | 2064 | LLL | C23-C33 | 2.96 | 1.59 | 1.53 |
| 54 | AA | 2061 | LLL | C22-C32 | 2.89 | 1.59 | 1.53 |
| 54 | DB | 3112 | LLL | C52-C42 | 2.87 | 1.60 | 1.52 |
| 54 | AA | 2061 | LLL | C42-C32 | 2.84 | 1.59 | 1.53 |
| 54 | AA | 2063 | LLL | C22-C32 | 2.81 | 1.59 | 1.53 |
| 54 | AA | 2061 | LLL | C52-C42 | 2.73 | 1.59 | 1.52 |
| 54 | BB | 3111 | LLL | C52-C42 | 2.72 | 1.59 | 1.52 |
| 54 | AA | 2062 | LLL | C22-C32 | 2.69 | 1.59 | 1.53 |
| 54 | AA | 2062 | LLL | C52-C42 | 2.66 | 1.59 | 1.52 |
| 54 | CA | 2063 | LLL | C22-C32 | 2.64 | 1.59 | 1.53 |
| 54 | DB | 3112 | LLL | C22-C32 | 2.62 | 1.59 | 1.53 |
| 54 | CA | 2062 | LLL | C52-C42 | 2.61 | 1.59 | 1.52 |
| 54 | BB | 3111 | LLL | C22-C32 | 2.59 | 1.59 | 1.53 |
| 54 | CA | 2064 | LLL | C22-C32 | 2.58 | 1.59 | 1.53 |
| 54 | CA | 2062 | LLL | C22-C32 | 2.57 | 1.59 | 1.53 |
| 54 | AA | 2063 | LLL | C52-C42 | 2.56 | 1.59 | 1.52 |
| 54 | AA | 2062 | LLL | C52-C62 | 2.45 | 1.58 | 1.52 |
| 54 | BB | 3111 | LLL | C52-C62 | 2.37 | 1.58 | 1.52 |
| 54 | CA | 2063 | LLL | C52-C62 | 2.36 | 1.58 | 1.52 |
| 54 | CA | 2064 | LLL | C52-C42 | 2.36 | 1.58 | 1.52 |
| 54 | DB | 3112 | LLL | C52-C62 | 2.35 | 1.58 | 1.52 |
| 54 | AA | 2062 | LLL | O43-C43 | -2.31 | 1.40 | 1.44 |
| 54 | AA | 2063 | LLL | C52-C62 | 2.26 | 1.58 | 1.52 |
| 54 | AA | 2061 | LLL | C52-C62 | 2.26 | 1.58 | 1.52 |
| 54 | BB | 3111 | LLL | O51-C51 | 2.19 | 1.47 | 1.44 |
| 54 | CA | 2063 | LLL | C41-C31 | 2.18 | 1.58 | 1.52 |
| 54 | DB | 3112 | LLL | O51-C51 | 2.17 | 1.47 | 1.44 |
| 54 | AA | 2062 | LLL | O51-C51 | 2.15 | 1.47 | 1.44 |
| 54 | CA | 2063 | LLL | O51-C51 | 2.15 | 1.47 | 1.44 |
| 54 | BB | 3111 | LLL | C31-C21 | 2.15 | 1.59 | 1.53 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 54 | DB | 3112 | LLL | C31-C21 | 2.14 | 1.59 | 1.53 |
| 54 | AA | 2062 | LLL | C31-C21 | 2.14 | 1.59 | 1.53 |
| 54 | BB | 3111 | LLL | C41-C31 | 2.13 | 1.58 | 1.52 |
| 54 | DB | 3112 | LLL | C41-C31 | 2.13 | 1.58 | 1.52 |
| 54 | AA | 2062 | LLL | C22-C12 | 2.13 | 1.58 | 1.53 |
| 54 | CA | 2062 | LLL | C41-C31 | 2.13 | 1.58 | 1.52 |
| 54 | AA | 2063 | LLL | C41-C31 | 2.12 | 1.58 | 1.52 |
| 54 | AA | 2061 | LLL | C41-C31 | 2.11 | 1.58 | 1.52 |
| 54 | AA | 2062 | LLL | O62-C13 | 2.11 | 1.47 | 1.41 |
| 54 | CA | 2062 | LLL | C31-C21 | 2.11 | 1.59 | 1.53 |
| 54 | CA | 2064 | LLL | C41-C31 | 2.10 | 1.58 | 1.52 |
| 54 | CA | 2063 | LLL | C31-C21 | 2.09 | 1.59 | 1.53 |
| 54 | CA | 2062 | LLL | O51-C51 | 2.09 | 1.47 | 1.44 |
| 54 | AA | 2062 | LLL | C41-C31 | 2.09 | 1.58 | 1.52 |
| 54 | AA | 2063 | LLL | O51-C51 | 2.08 | 1.47 | 1.44 |
| 54 | DB | 3112 | LLL | C22-C12 | 2.08 | 1.58 | 1.53 |
| 54 | CA | 2063 | LLL | C22-C12 | 2.06 | 1.58 | 1.53 |
| 54 | CA | 2063 | LLL | O62-C13 | 2.06 | 1.47 | 1.41 |
| 54 | CA | 2062 | LLL | C52-C62 | 2.04 | 1.57 | 1.52 |
| 54 | CA | 2064 | LLL | C52-C62 | 2.03 | 1.57 | 1.52 |
| 54 | BB | 3111 | LLL | C22-C12 | 2.03 | 1.57 | 1.53 |
| 54 | CA | 2064 | LLL | C31-C21 | 2.01 | 1.58 | 1.53 |
| 54 | AA | 2063 | LLL | O62-C13 | 2.00 | 1.47 | 1.41 |

All (29) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54 | AA | 2063 | LLL | C53-O53-C13 | 4.54 | 118.52 | 111.53 |
| 54 | CA | 2063 | LLL | C53-O53-C13 | 4.24 | 118.06 | 111.53 |
| 54 | AA | 2062 | LLL | C53-O53-C13 | 4.14 | 117.90 | 111.53 |
| 54 | CA | 2062 | LLL | C53-O53-C13 | 4.11 | 117.85 | 111.53 |
| 54 | BB | 3111 | LLL | C53-O53-C13 | 4.05 | 117.76 | 111.53 |
| 54 | DB | 3112 | LLL | C53-O53-C13 | 3.96 | 117.63 | 111.53 |
| 54 | CA | 2064 | LLL | C53-O53-C13 | 3.86 | 117.48 | 111.53 |
| 54 | AA | 2061 | LLL | C53-O53-C13 | 3.83 | 117.42 | 111.53 |
| 54 | AA | 2061 | LLL | C13-O62-C62 | 2.98 | 125.03 | 117.98 |
| 54 | AA | 2063 | LLL | C13-O62-C62 | 2.92 | 124.91 | 117.98 |
| 54 | AA | 2062 | LLL | O43-C43-C83 | -2.77 | 102.07 | 108.08 |
| 54 | AA | 2062 | LLL | C13-O62-C62 | 2.72 | 124.42 | 117.98 |
| 54 | CA | 2064 | LLL | O43-C43-C83 | -2.64 | 102.36 | 108.08 |
| 54 | AA | 2061 | LLL | O43-C43-C83 | -2.64 | 102.36 | 108.08 |
| 54 | CA | 2063 | LLL | O43-C43-C83 | -2.63 | 102.38 | 108.08 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54 | BB | 3111 | LLL | O43-C43-C83 | -2.57 | 102.51 | 108.08 |
| 54 | DB | 3112 | LLL | O43-C43-C83 | -2.57 | 102.51 | 108.08 |
| 54 | AA | 2063 | LLL | O43-C43-C83 | -2.52 | 102.61 | 108.08 |
| 54 | CA | 2062 | LLL | O43-C43-C83 | -2.49 | 102.68 | 108.08 |
| 54 | CA | 2062 | LLL | C13-O62-C62 | 2.44 | 123.76 | 117.98 |
| 54 | CA | 2063 | LLL | C13-O62-C62 | 2.22 | 123.24 | 117.98 |
| 54 | BB | 3111 | LLL | C13-O62-C62 | 2.17 | 123.13 | 117.98 |
| 54 | DB | 3112 | LLL | C13-O62-C62 | 2.16 | 123.10 | 117.98 |
| 54 | CA | 2064 | LLL | C13-O62-C62 | 2.15 | 123.08 | 117.98 |
| 54 | BB | 3111 | LLL | C11-O51-C51 | 2.09 | 115.45 | 113.13 |
| 54 | AA | 2062 | LLL | C93-N33-C33 | 2.06 | 117.30 | 114.47 |
| 54 | BB | 3111 | LLL | C93-N33-C33 | 2.05 | 117.28 | 114.47 |
| 54 | AA | 2061 | LLL | O51-C51-C41 | 2.04 | 112.06 | 109.91 |
| 54 | CA | 2063 | LLL | C93-N33-C33 | 2.04 | 117.27 | 114.47 |

There are no chirality outliers.

All (15) torsion outliers are listed below:

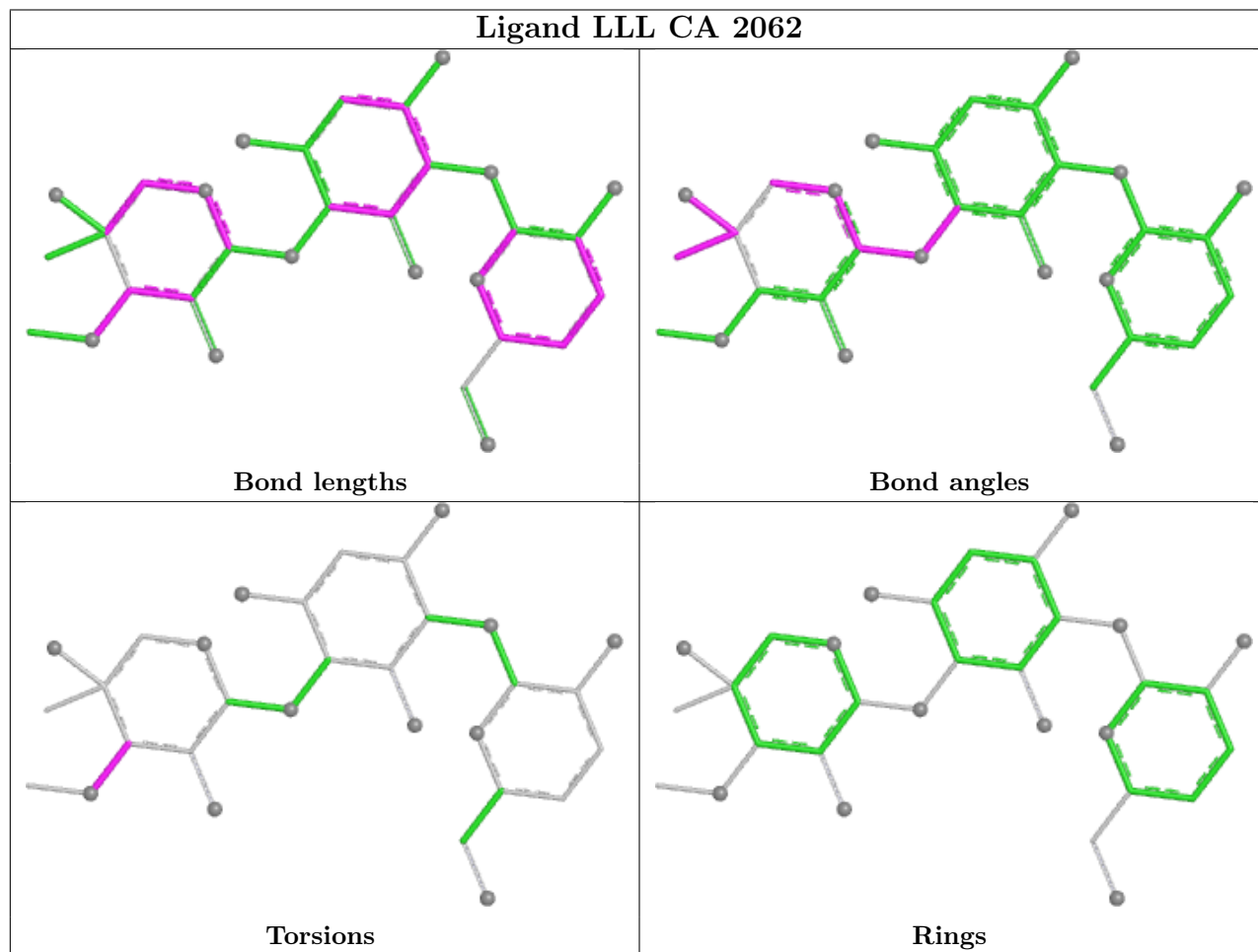
| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 54 | AA | 2062 | LLL | C23-C33-N33-C93 |
| 54 | CA | 2062 | LLL | C23-C33-N33-C93 |
| 54 | CA | 2064 | LLL | C23-C33-N33-C93 |
| 54 | DB | 3112 | LLL | C23-C33-N33-C93 |
| 54 | AA | 2063 | LLL | O53-C13-O62-C62 |
| 54 | CA | 2063 | LLL | O53-C13-O62-C62 |
| 54 | CA | 2063 | LLL | C23-C13-O62-C62 |
| 54 | CA | 2063 | LLL | C52-C42-O11-C11 |
| 54 | AA | 2061 | LLL | C23-C33-N33-C93 |
| 54 | AA | 2063 | LLL | C23-C33-N33-C93 |
| 54 | BB | 3111 | LLL | C23-C33-N33-C93 |
| 54 | CA | 2063 | LLL | C23-C33-N33-C93 |
| 54 | AA | 2062 | LLL | C21-C11-O11-C42 |
| 54 | BB | 3111 | LLL | C21-C11-O11-C42 |
| 54 | CA | 2063 | LLL | O51-C11-O11-C42 |

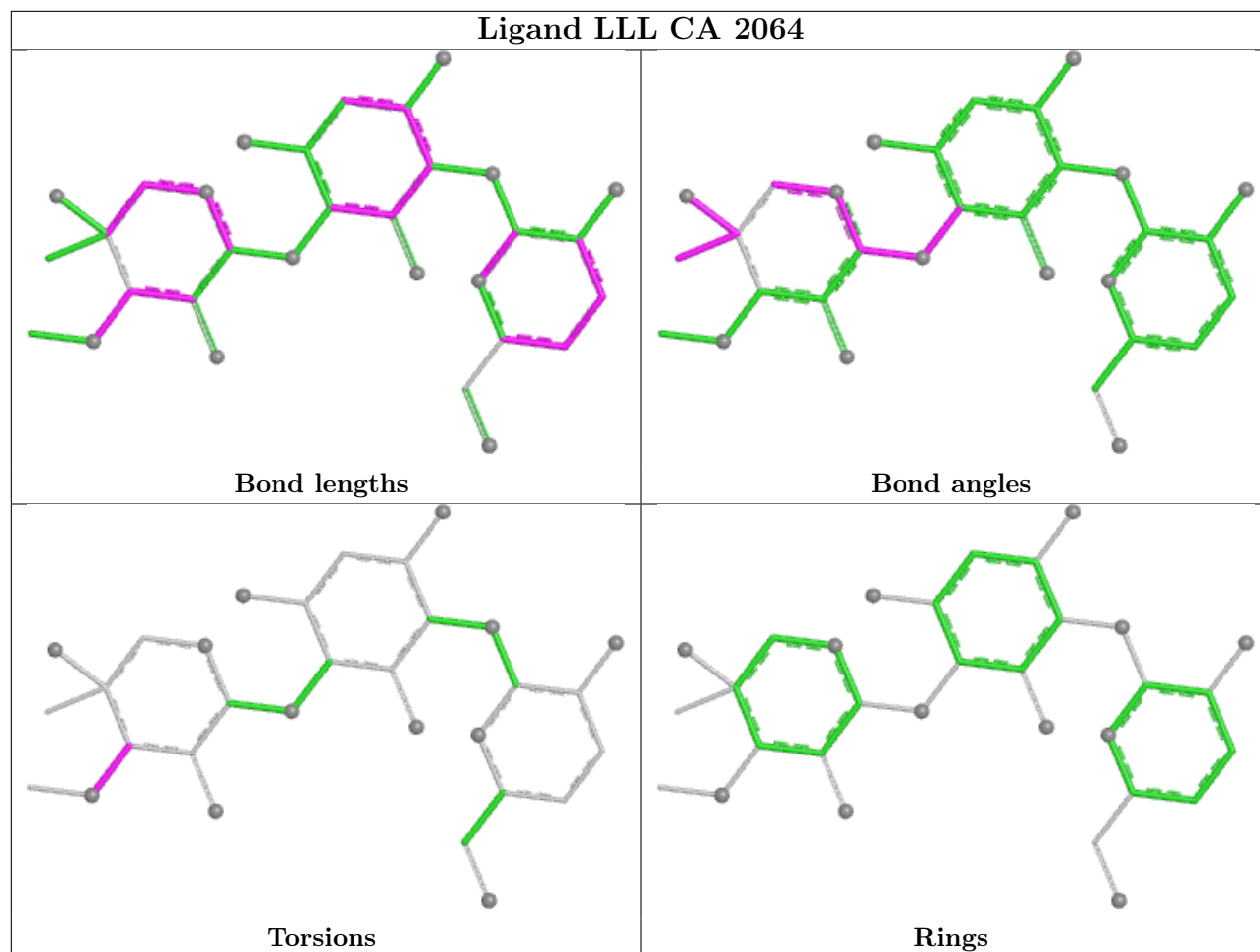
There are no ring outliers.

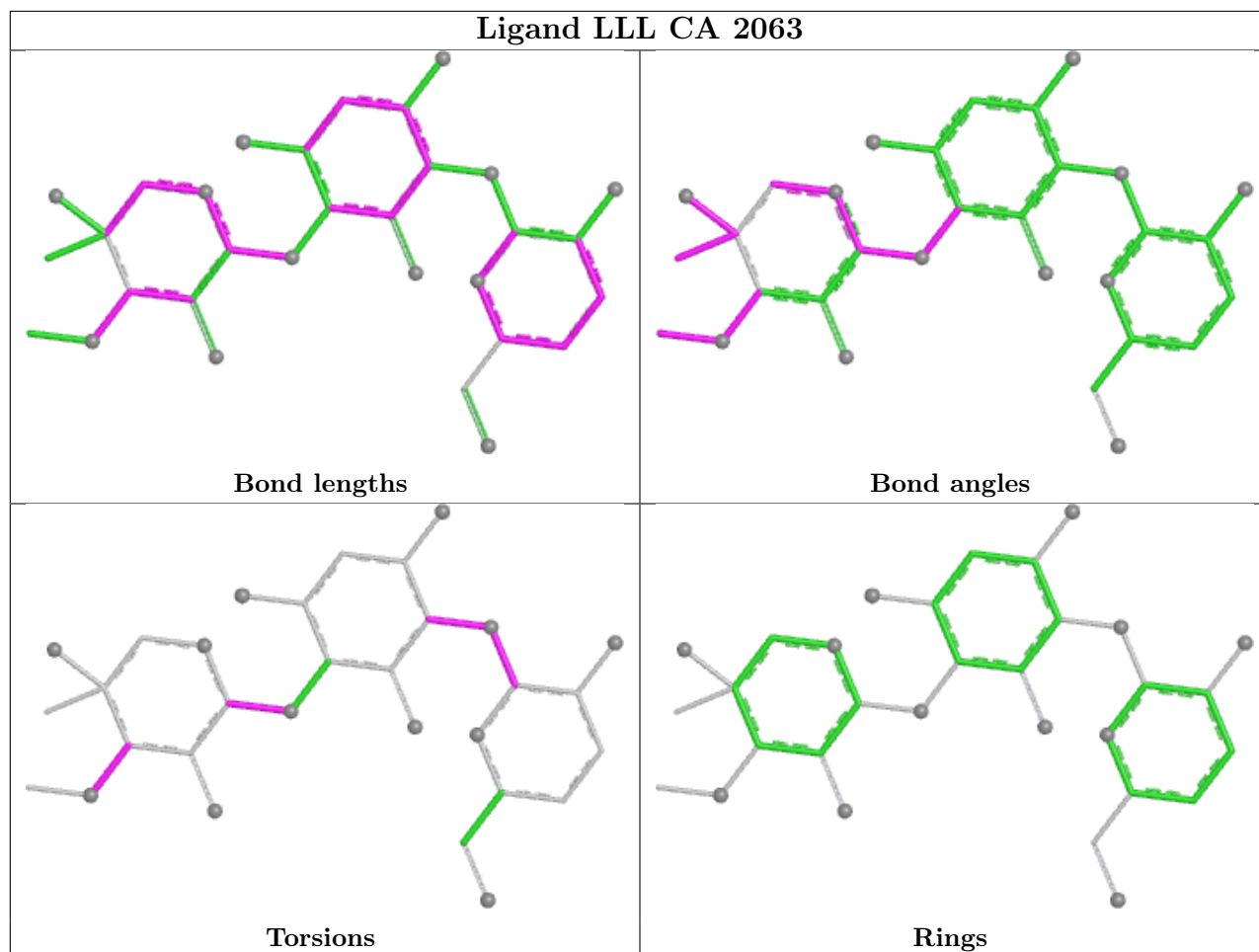
No monomer is involved in short contacts.

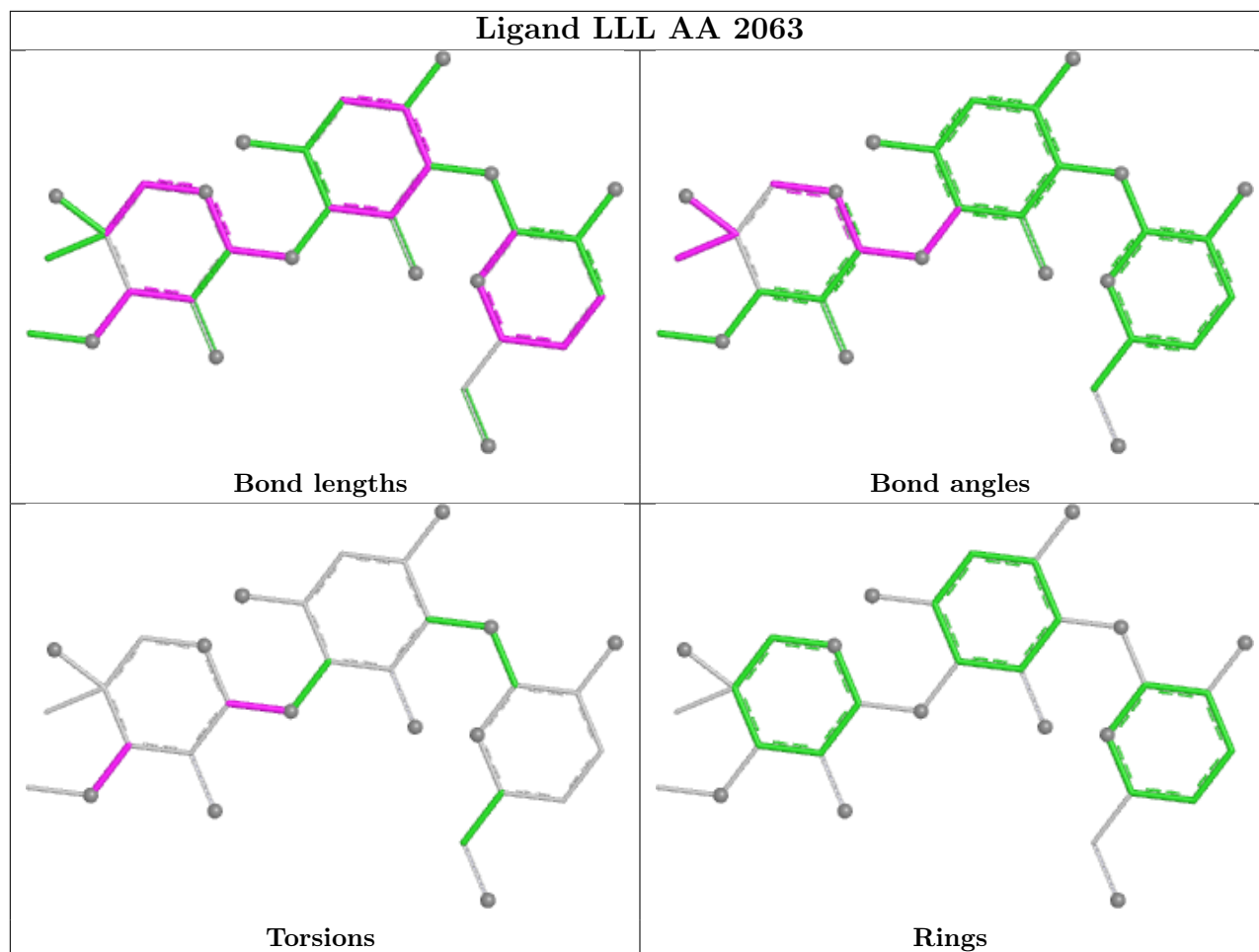
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

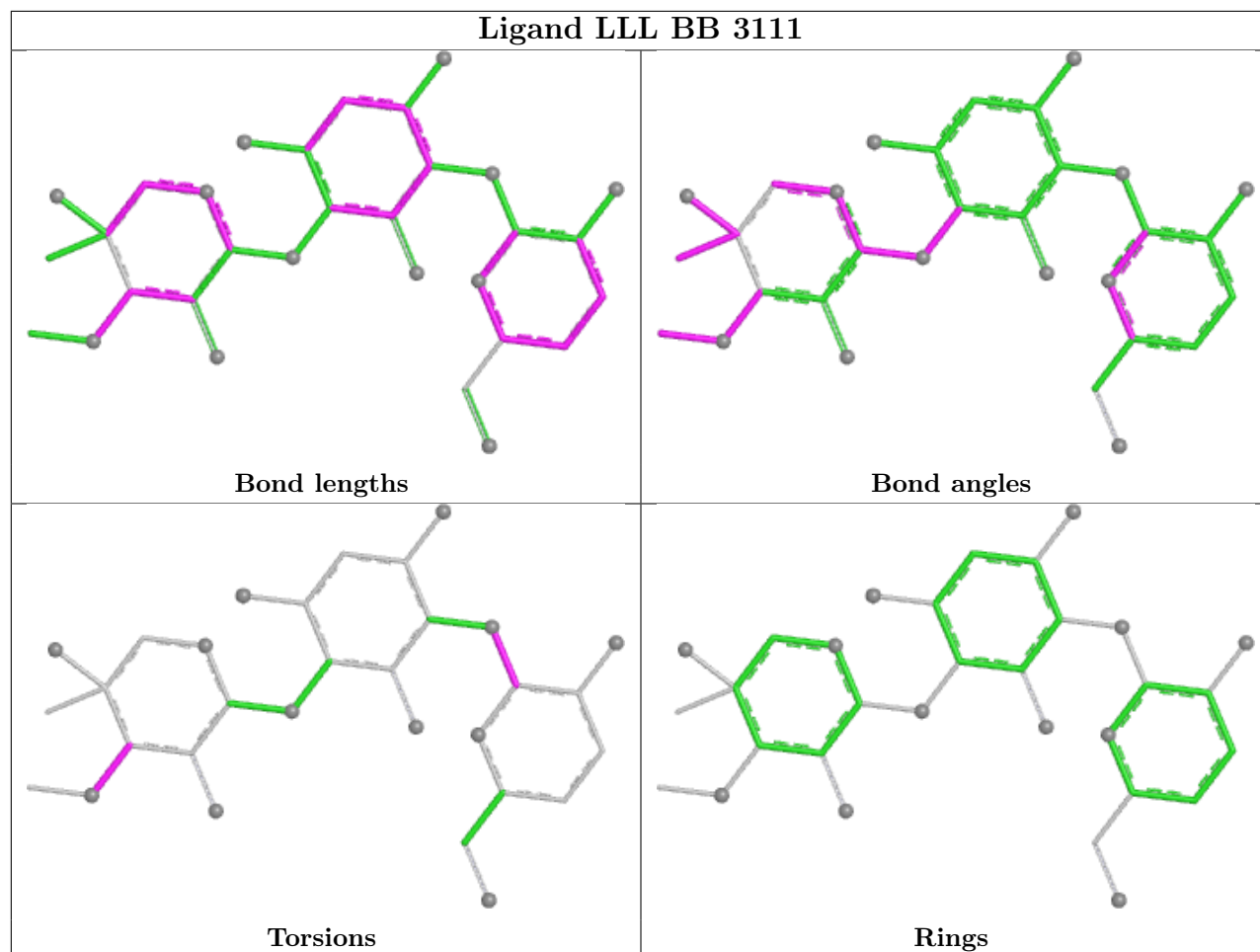
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

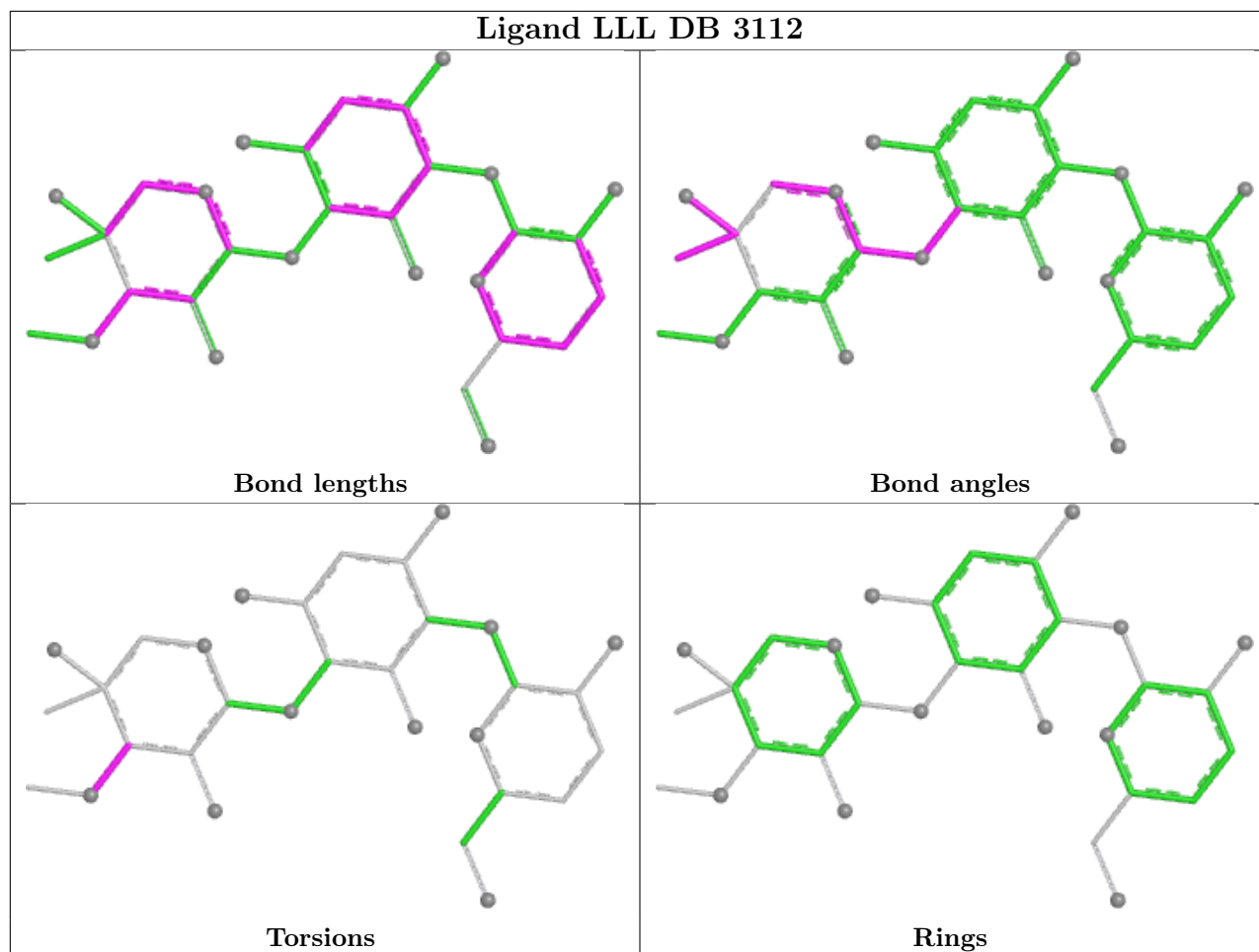


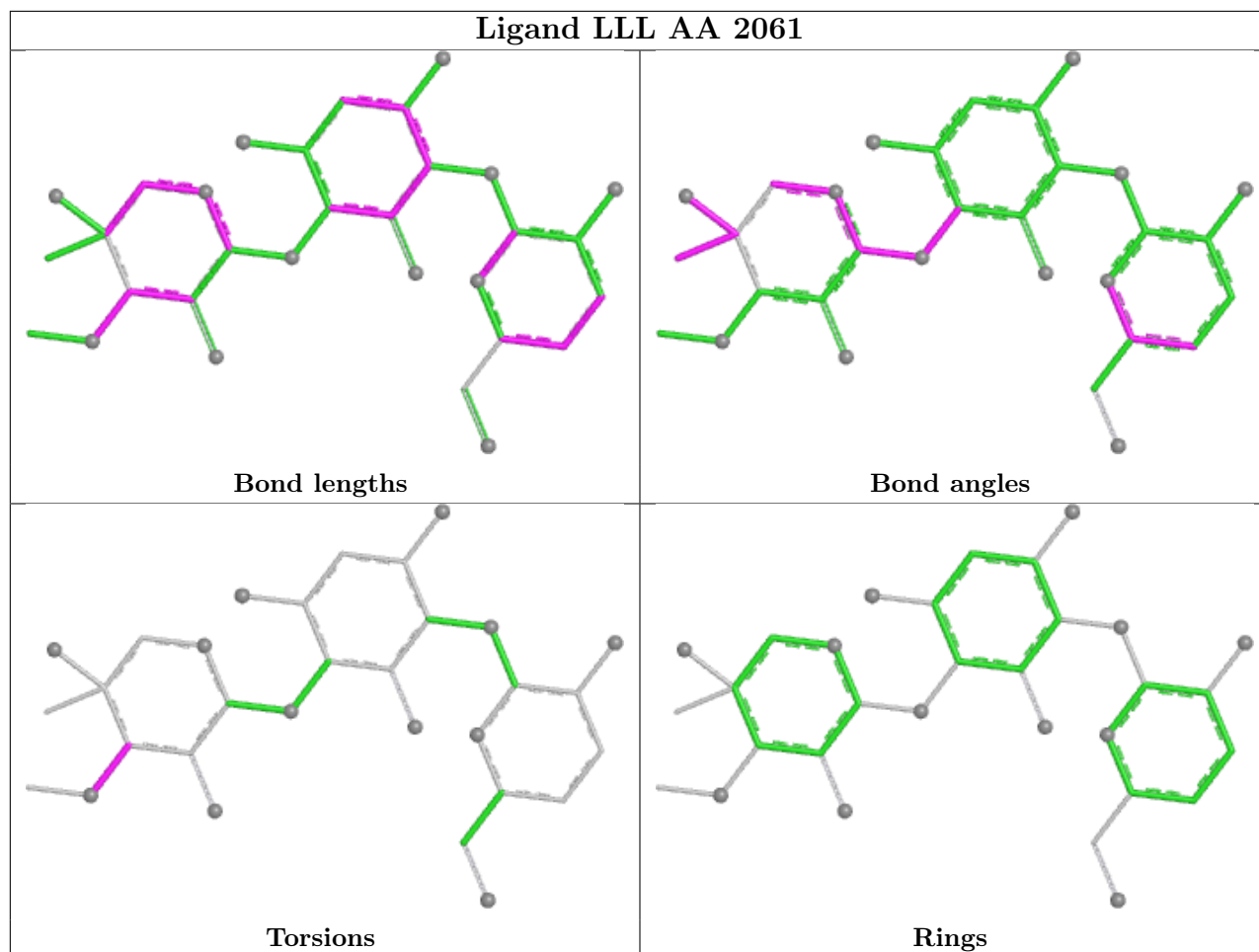


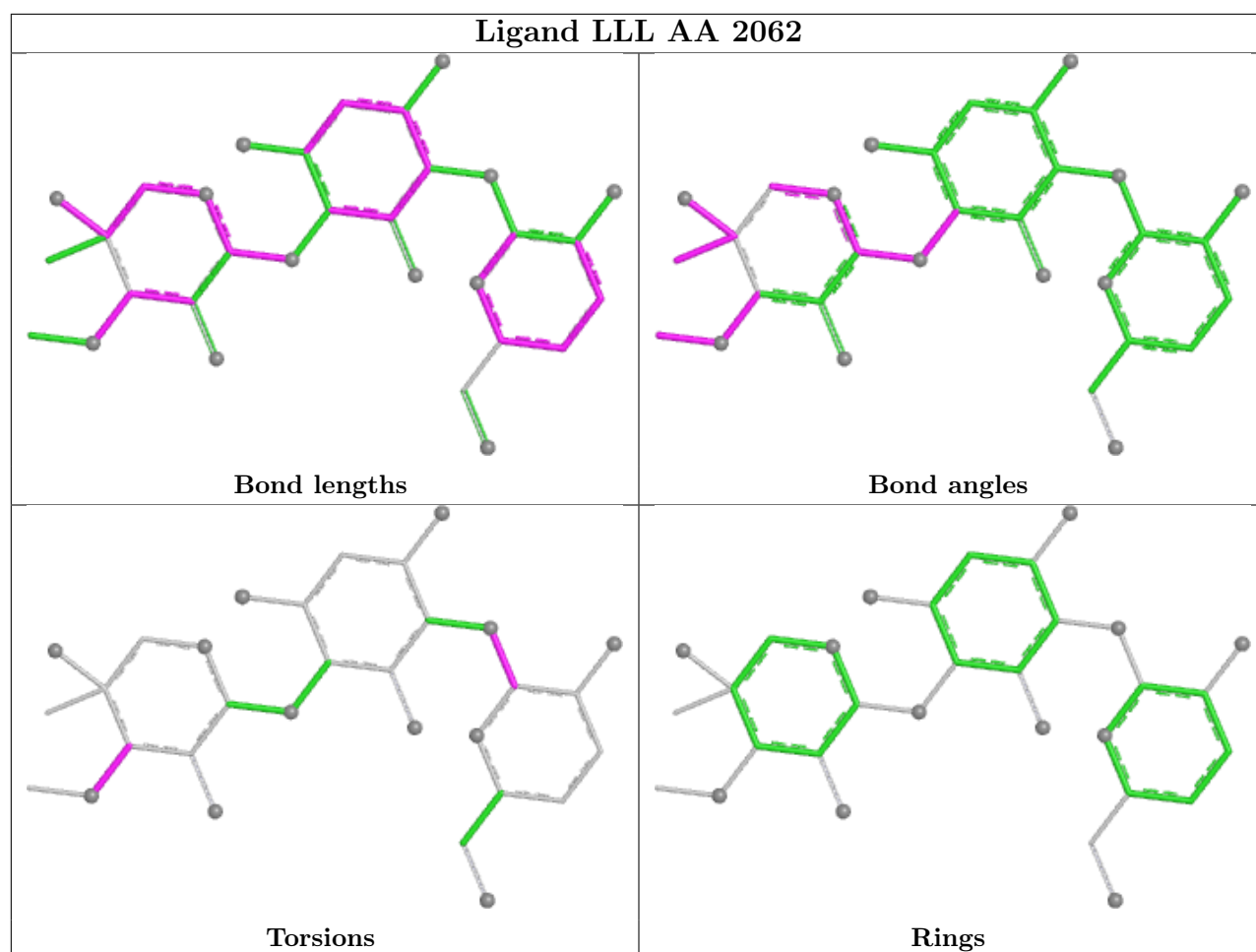












4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 23 | BB | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | BB | 2322:A | O3' | 2323:G | P | 1.78 |

5 Fit of model and data i

5.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | AA | 1530/1542 (99%) | -0.28 | 20 (1%) 74 53 | 22, 85, 131, 156 | 0 |
| 1 | CA | 1530/1542 (99%) | -0.43 | 10 (0%) 84 66 | 5, 60, 120, 167 | 0 |
| 2 | AC | 206/232 (88%) | -0.14 | 4 (1%) 66 44 | 14, 72, 111, 136 | 0 |
| 2 | CC | 206/232 (88%) | -0.21 | 4 (1%) 66 44 | 5, 74, 103, 160 | 0 |
| 3 | AD | 205/205 (100%) | 0.21 | 5 (2%) 59 39 | 21, 87, 115, 135 | 0 |
| 3 | CD | 205/205 (100%) | -0.03 | 2 (0%) 79 59 | 8, 65, 107, 121 | 0 |
| 4 | AE | 150/166 (90%) | 0.11 | 4 (2%) 56 35 | 6, 74, 105, 134 | 0 |
| 4 | CE | 150/166 (90%) | -0.06 | 6 (4%) 43 27 | 5, 59, 96, 125 | 0 |
| 5 | AF | 100/135 (74%) | -0.28 | 1 (1%) 79 59 | 22, 72, 114, 148 | 0 |
| 5 | CF | 100/135 (74%) | -0.24 | 0 100 100 | 12, 72, 109, 123 | 0 |
| 6 | AG | 150/178 (84%) | -0.02 | 5 (3%) 49 31 | 47, 89, 116, 152 | 0 |
| 6 | CG | 152/178 (85%) | -0.40 | 1 (0%) 84 66 | 29, 80, 115, 134 | 0 |
| 7 | AH | 129/129 (100%) | -0.14 | 4 (3%) 51 33 | 31, 80, 112, 136 | 0 |
| 7 | CH | 129/129 (100%) | -0.09 | 4 (3%) 51 33 | 5, 56, 91, 112 | 0 |
| 8 | AI | 127/129 (98%) | 0.12 | 6 (4%) 37 24 | 31, 83, 118, 143 | 0 |
| 8 | CI | 127/129 (98%) | 0.34 | 12 (9%) 15 11 | 35, 84, 118, 157 | 0 |
| 9 | AJ | 98/103 (95%) | 0.22 | 6 (6%) 28 19 | 22, 87, 121, 135 | 0 |
| 9 | CJ | 98/103 (95%) | 0.45 | 6 (6%) 28 19 | 33, 84, 110, 125 | 0 |
| 10 | AK | 117/128 (91%) | -0.25 | 2 (1%) 69 47 | 5, 67, 102, 117 | 0 |
| 10 | CK | 117/128 (91%) | -0.34 | 2 (1%) 69 47 | 5, 56, 101, 119 | 0 |
| 11 | AL | 123/123 (100%) | 0.42 | 13 (10%) 13 9 | 22, 75, 110, 146 | 0 |
| 11 | CL | 123/123 (100%) | 0.28 | 7 (5%) 30 20 | 5, 47, 103, 123 | 0 |
| 12 | AM | 114/117 (97%) | -0.16 | 1 (0%) 81 61 | 58, 96, 124, 147 | 0 |
| 12 | CM | 113/117 (96%) | -0.16 | 1 (0%) 81 61 | 48, 89, 116, 135 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 13 | AN | 96/100 (96%) | 0.36 | 5 (5%) 34 22 | 27, 85, 121, 154 | 0 |
| 13 | CN | 96/100 (96%) | 0.33 | 3 (3%) 51 33 | 40, 87, 114, 142 | 0 |
| 14 | AO | 88/89 (98%) | -0.16 | 1 (1%) 77 56 | 38, 80, 109, 133 | 0 |
| 14 | CO | 88/89 (98%) | 0.02 | 5 (5%) 30 20 | 5, 56, 107, 128 | 0 |
| 15 | AP | 82/82 (100%) | 0.54 | 7 (8%) 18 12 | 48, 88, 121, 135 | 0 |
| 15 | CP | 80/82 (97%) | 0.54 | 6 (7%) 22 15 | 11, 59, 109, 147 | 0 |
| 16 | AQ | 80/83 (96%) | -0.12 | 1 (1%) 74 53 | 31, 87, 117, 124 | 0 |
| 16 | CQ | 81/83 (97%) | -0.22 | 0 100 100 | 9, 58, 99, 121 | 0 |
| 17 | AR | 55/74 (74%) | -0.06 | 2 (3%) 46 29 | 19, 76, 118, 138 | 0 |
| 17 | CR | 55/74 (74%) | -0.17 | 2 (3%) 46 29 | 19, 68, 119, 131 | 0 |
| 18 | AS | 79/91 (86%) | 0.03 | 1 (1%) 74 53 | 68, 100, 124, 136 | 0 |
| 18 | CS | 80/91 (87%) | 0.07 | 4 (5%) 35 23 | 48, 94, 127, 153 | 0 |
| 19 | AT | 85/86 (98%) | 0.12 | 3 (3%) 47 30 | 39, 92, 123, 144 | 0 |
| 19 | CT | 85/86 (98%) | 0.21 | 7 (8%) 19 13 | 19, 61, 106, 125 | 0 |
| 20 | AB | 218/240 (90%) | -0.28 | 2 (0%) 81 61 | 20, 87, 113, 132 | 0 |
| 20 | CB | 218/240 (90%) | -0.31 | 0 100 100 | 29, 89, 118, 144 | 0 |
| 21 | AU | 51/70 (72%) | 0.66 | 4 (7%) 20 14 | 36, 89, 126, 134 | 0 |
| 21 | CU | 51/70 (72%) | 0.58 | 7 (13%) 8 7 | 46, 78, 116, 132 | 0 |
| 22 | BA | 117/120 (97%) | -0.35 | 2 (1%) 69 47 | 47, 78, 117, 140 | 0 |
| 22 | DA | 117/120 (97%) | -0.02 | 3 (2%) 57 37 | 30, 80, 115, 155 | 0 |
| 23 | BB | 2841/2904 (97%) | -0.38 | 29 (1%) 79 59 | 9, 58, 127, 165 | 0 |
| 23 | DB | 2841/2904 (97%) | -0.45 | 18 (0%) 85 69 | 5, 45, 124, 163 | 0 |
| 24 | BI | 141/141 (100%) | 0.34 | 4 (2%) 55 35 | 59, 117, 149, 158 | 0 |
| 24 | DI | 141/141 (100%) | 0.12 | 4 (2%) 55 35 | 70, 117, 148, 160 | 0 |
| 25 | BC | 271/272 (99%) | 0.37 | 16 (5%) 29 20 | 5, 47, 88, 105 | 0 |
| 25 | DC | 271/272 (99%) | 0.31 | 13 (4%) 36 24 | 5, 32, 80, 112 | 0 |
| 26 | BD | 209/209 (100%) | 0.22 | 16 (7%) 21 15 | 12, 71, 107, 141 | 0 |
| 26 | DD | 209/209 (100%) | 0.35 | 14 (6%) 25 17 | 5, 49, 98, 135 | 0 |
| 27 | BK | 121/123 (98%) | 0.24 | 1 (0%) 82 64 | 16, 67, 106, 134 | 0 |
| 27 | DK | 121/123 (98%) | 0.12 | 5 (4%) 42 26 | 5, 37, 90, 130 | 0 |
| 28 | BP | 114/114 (100%) | 0.31 | 7 (6%) 28 19 | 25, 81, 113, 131 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 28 | DP | 114/114 (100%) | 0.10 | 3 (2%) 57 37 | 7, 49, 94, 112 | 0 |
| 29 | BE | 201/201 (100%) | -0.02 | 7 (3%) 47 30 | 5, 65, 104, 147 | 0 |
| 29 | DE | 201/201 (100%) | -0.02 | 6 (2%) 52 33 | 5, 62, 107, 138 | 0 |
| 30 | BY | 58/58 (100%) | -0.21 | 1 (1%) 69 47 | 26, 69, 107, 137 | 0 |
| 30 | DY | 58/58 (100%) | -0.01 | 1 (1%) 69 47 | 6, 64, 110, 117 | 0 |
| 31 | B0 | 56/56 (100%) | 0.27 | 2 (3%) 46 29 | 5, 71, 113, 136 | 0 |
| 31 | D0 | 56/56 (100%) | 0.11 | 2 (3%) 46 29 | 10, 43, 99, 104 | 0 |
| 32 | B4 | 38/38 (100%) | 0.91 | 6 (15%) 6 5 | 33, 76, 108, 125 | 0 |
| 32 | D4 | 38/38 (100%) | 0.49 | 1 (2%) 57 37 | 15, 65, 94, 105 | 0 |
| 33 | B1 | 50/54 (92%) | -0.24 | 1 (2%) 64 43 | 50, 75, 102, 115 | 0 |
| 33 | D1 | 50/54 (92%) | -0.48 | 0 100 100 | 27, 74, 105, 118 | 0 |
| 34 | B3 | 64/64 (100%) | 0.74 | 10 (15%) 6 5 | 9, 55, 82, 106 | 0 |
| 34 | D3 | 64/64 (100%) | 0.76 | 8 (12%) 9 7 | 5, 39, 84, 101 | 0 |
| 35 | BV | 94/94 (100%) | -0.33 | 1 (1%) 77 56 | 31, 86, 115, 129 | 0 |
| 35 | DV | 94/94 (100%) | -0.24 | 0 100 100 | 8, 79, 108, 125 | 0 |
| 36 | B2 | 46/46 (100%) | 0.55 | 3 (6%) 26 18 | 8, 40, 81, 113 | 0 |
| 36 | D2 | 46/46 (100%) | 0.36 | 4 (8%) 17 12 | 5, 28, 68, 113 | 0 |
| 37 | BL | 143/144 (99%) | 0.16 | 3 (2%) 63 42 | 9, 63, 99, 134 | 0 |
| 37 | DL | 143/144 (99%) | 0.15 | 4 (2%) 55 35 | 5, 55, 95, 123 | 0 |
| 38 | BM | 136/136 (100%) | 0.11 | 6 (4%) 39 25 | 5, 65, 100, 131 | 0 |
| 38 | DM | 136/136 (100%) | 0.34 | 7 (5%) 34 23 | 5, 55, 94, 134 | 0 |
| 39 | BX | 63/63 (100%) | -0.15 | 0 100 100 | 18, 76, 110, 123 | 0 |
| 39 | DX | 63/63 (100%) | -0.39 | 0 100 100 | 36, 82, 107, 142 | 0 |
| 40 | BH | 149/149 (100%) | 0.28 | 2 (1%) 74 53 | 25, 98, 122, 146 | 0 |
| 40 | DH | 149/149 (100%) | -0.05 | 1 (0%) 84 66 | 18, 88, 112, 141 | 0 |
| 41 | BJ | 142/142 (100%) | 0.53 | 17 (11%) 10 8 | 16, 70, 106, 118 | 0 |
| 41 | DJ | 142/142 (100%) | 0.40 | 7 (4%) 36 23 | 5, 60, 101, 131 | 0 |
| 42 | BN | 120/127 (94%) | 0.13 | 5 (4%) 41 26 | 14, 65, 101, 145 | 0 |
| 42 | DN | 120/127 (94%) | 0.26 | 7 (5%) 30 20 | 5, 42, 75, 118 | 0 |
| 43 | BO | 116/117 (99%) | 0.03 | 4 (3%) 48 30 | 40, 78, 104, 128 | 0 |
| 43 | DO | 116/117 (99%) | 0.25 | 10 (8%) 18 12 | 5, 73, 106, 157 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 44 | BQ | 117/117 (100%) | 0.15 | 4 (3%) 48 30 | 5, 60, 95, 109 | 0 |
| 44 | DQ | 117/117 (100%) | 0.39 | 9 (7%) 21 15 | 5, 50, 92, 120 | 0 |
| 45 | BS | 110/110 (100%) | 0.01 | 4 (3%) 46 29 | 6, 56, 98, 118 | 0 |
| 45 | DS | 110/110 (100%) | 0.19 | 6 (5%) 32 21 | 5, 48, 95, 128 | 0 |
| 46 | BU | 102/103 (99%) | -0.09 | 1 (0%) 79 59 | 9, 71, 105, 123 | 0 |
| 46 | DU | 102/103 (99%) | -0.05 | 2 (1%) 64 43 | 34, 80, 112, 130 | 0 |
| 47 | BF | 178/178 (100%) | -0.13 | 2 (1%) 77 56 | 40, 95, 125, 140 | 0 |
| 47 | DF | 178/178 (100%) | 0.16 | 10 (5%) 31 20 | 38, 85, 125, 138 | 0 |
| 48 | BG | 176/176 (100%) | -0.22 | 1 (0%) 85 69 | 37, 88, 114, 146 | 0 |
| 48 | DG | 176/176 (100%) | -0.02 | 3 (1%) 69 47 | 17, 82, 110, 133 | 0 |
| 49 | BR | 103/103 (100%) | -0.11 | 2 (1%) 66 44 | 13, 78, 112, 120 | 0 |
| 49 | DR | 103/103 (100%) | 0.27 | 5 (4%) 36 23 | 15, 72, 111, 128 | 0 |
| 50 | BT | 93/100 (93%) | 0.23 | 7 (7%) 22 15 | 14, 70, 112, 124 | 0 |
| 50 | DT | 93/100 (93%) | 0.24 | 4 (4%) 40 26 | 8, 66, 108, 120 | 0 |
| 51 | BZ | 77/78 (98%) | 0.38 | 4 (5%) 34 22 | 5, 54, 93, 115 | 0 |
| 51 | DZ | 77/78 (98%) | 0.29 | 2 (2%) 57 37 | 5, 43, 87, 114 | 0 |
| 52 | BW | 79/84 (94%) | 0.97 | 14 (17%) 4 4 | 8, 75, 111, 136 | 0 |
| 52 | DW | 79/84 (94%) | 0.99 | 15 (18%) 4 4 | 12, 65, 103, 122 | 0 |
| All | All | 20417/21046 (97%) | -0.11 | 542 (2%) 56 35 | 5, 68, 120, 167 | 0 |

All (542) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 8 | CI | 129 | ARG | 12.3 |
| 22 | DA | 88 | C | 11.9 |
| 1 | AA | 79 | G | 8.6 |
| 26 | DD | 118 | PHE | 8.1 |
| 22 | BA | 88 | C | 7.8 |
| 8 | CI | 118 | ARG | 7.7 |
| 1 | AA | 78 | A | 7.7 |
| 22 | DA | 52 | A | 7.3 |
| 11 | CL | 24 | GLU | 7.0 |
| 9 | CJ | 84 | VAL | 6.3 |
| 26 | BD | 118 | PHE | 6.2 |
| 15 | CP | 52 | LEU | 6.0 |
| 52 | DW | 18 | LYS | 5.8 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 11 | CL | 22 | ALA | 5.7 |
| 11 | AL | 13 | ARG | 5.7 |
| 34 | B3 | 24 | LYS | 5.5 |
| 28 | BP | 99 | LEU | 5.5 |
| 11 | AL | 11 | ARG | 5.4 |
| 41 | BJ | 111 | LYS | 5.4 |
| 1 | AA | 86 | G | 5.4 |
| 10 | AK | 128 | VAL | 5.4 |
| 25 | DC | 250 | GLN | 5.3 |
| 36 | B2 | 1 | MET | 5.2 |
| 25 | BC | 5 | CYS | 5.2 |
| 23 | BB | 140 | C | 5.2 |
| 25 | DC | 109 | LEU | 5.1 |
| 52 | DW | 19 | ARG | 5.0 |
| 23 | BB | 139 | U | 5.0 |
| 11 | CL | 14 | LYS | 5.0 |
| 43 | BO | 12 | THR | 4.9 |
| 26 | DD | 131 | ASP | 4.9 |
| 41 | DJ | 44 | TYR | 4.9 |
| 1 | AA | 80 | A | 4.9 |
| 19 | CT | 63 | LYS | 4.8 |
| 25 | BC | 3 | VAL | 4.8 |
| 11 | AL | 25 | ALA | 4.8 |
| 1 | CA | 1362 | A | 4.7 |
| 11 | CL | 12 | ALA | 4.7 |
| 1 | AA | 1362 | A | 4.7 |
| 25 | BC | 17 | LYS | 4.7 |
| 28 | BP | 106 | ALA | 4.7 |
| 23 | BB | 1176 | U | 4.7 |
| 43 | DO | 3 | LYS | 4.6 |
| 15 | CP | 28 | ARG | 4.5 |
| 52 | BW | 45 | HIS | 4.5 |
| 44 | DQ | 90 | ASP | 4.5 |
| 52 | DW | 43 | LYS | 4.5 |
| 11 | AL | 3 | VAL | 4.5 |
| 36 | B2 | 46 | LYS | 4.4 |
| 23 | BB | 715 | A | 4.3 |
| 11 | CL | 123 | ALA | 4.3 |
| 41 | DJ | 42 | ALA | 4.3 |
| 52 | BW | 33 | GLY | 4.3 |
| 11 | CL | 13 | ARG | 4.2 |
| 8 | CI | 127 | SER | 4.2 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 8 | AI | 129 | ARG | 4.1 |
| 41 | BJ | 54 | ILE | 4.1 |
| 36 | D2 | 1 | MET | 4.1 |
| 43 | DO | 2 | ASP | 4.1 |
| 21 | CU | 35 | GLU | 4.1 |
| 25 | DC | 201 | LEU | 4.0 |
| 11 | AL | 12 | ALA | 4.0 |
| 11 | AL | 22 | ALA | 3.9 |
| 1 | AA | 1080 | A | 3.9 |
| 11 | AL | 1 | ALA | 3.9 |
| 34 | B3 | 58 | ILE | 3.8 |
| 42 | DN | 15 | SER | 3.8 |
| 32 | B4 | 7 | VAL | 3.8 |
| 52 | DW | 33 | GLY | 3.8 |
| 29 | BE | 60 | TRP | 3.8 |
| 25 | BC | 209 | ALA | 3.8 |
| 52 | BW | 17 | ALA | 3.8 |
| 34 | D3 | 51 | LYS | 3.8 |
| 52 | DW | 36 | ILE | 3.8 |
| 52 | BW | 36 | ILE | 3.7 |
| 50 | BT | 76 | ARG | 3.7 |
| 52 | BW | 62 | ALA | 3.7 |
| 28 | DP | 91 | VAL | 3.7 |
| 42 | BN | 17 | ARG | 3.7 |
| 41 | DJ | 80 | HIS | 3.7 |
| 49 | DR | 67 | GLY | 3.7 |
| 23 | BB | 2320 | U | 3.7 |
| 25 | BC | 20 | ASN | 3.7 |
| 26 | BD | 151 | THR | 3.7 |
| 26 | DD | 168 | GLU | 3.7 |
| 25 | DC | 34 | GLU | 3.6 |
| 42 | BN | 12 | ARG | 3.6 |
| 8 | AI | 127 | SER | 3.6 |
| 23 | DB | 2134 | A | 3.6 |
| 52 | DW | 17 | ALA | 3.6 |
| 47 | DF | 124 | ARG | 3.6 |
| 8 | CI | 119 | LYS | 3.6 |
| 45 | BS | 74 | ILE | 3.6 |
| 41 | BJ | 44 | TYR | 3.6 |
| 11 | AL | 14 | LYS | 3.6 |
| 52 | BW | 74 | LYS | 3.6 |
| 1 | AA | 83 | C | 3.5 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 11 | CL | 25 | ALA | 3.5 |
| 47 | DF | 169 | LEU | 3.5 |
| 26 | BD | 140 | HIS | 3.5 |
| 19 | CT | 5 | SER | 3.5 |
| 21 | AU | 15 | LEU | 3.5 |
| 8 | CI | 122 | ARG | 3.5 |
| 10 | CK | 128 | VAL | 3.5 |
| 23 | DB | 139 | U | 3.5 |
| 42 | BN | 21 | PHE | 3.4 |
| 27 | DK | 35 | VAL | 3.4 |
| 52 | BW | 14 | ASP | 3.4 |
| 29 | BE | 146 | VAL | 3.4 |
| 42 | DN | 12 | ARG | 3.4 |
| 24 | DI | 84 | GLY | 3.4 |
| 8 | AI | 128 | LYS | 3.3 |
| 14 | CO | 47 | LYS | 3.3 |
| 38 | BM | 93 | VAL | 3.3 |
| 45 | DS | 32 | ALA | 3.3 |
| 41 | BJ | 86 | GLN | 3.3 |
| 32 | B4 | 29 | ALA | 3.3 |
| 23 | BB | 2213 | U | 3.3 |
| 25 | DC | 11 | GLY | 3.3 |
| 7 | CH | 62 | LEU | 3.3 |
| 23 | BB | 878 | A | 3.3 |
| 4 | AE | 109 | ALA | 3.3 |
| 8 | CI | 128 | LYS | 3.3 |
| 3 | CD | 190 | LEU | 3.2 |
| 46 | BU | 14 | THR | 3.2 |
| 37 | DL | 58 | TYR | 3.2 |
| 23 | DB | 2157 | G | 3.2 |
| 19 | CT | 3 | ILE | 3.2 |
| 24 | DI | 23 | VAL | 3.2 |
| 11 | AL | 27 | PRO | 3.2 |
| 34 | B3 | 10 | ALA | 3.2 |
| 19 | AT | 5 | SER | 3.2 |
| 38 | DM | 95 | LEU | 3.2 |
| 23 | BB | 1459 | G | 3.2 |
| 23 | BB | 1175 | A | 3.2 |
| 34 | B3 | 14 | LYS | 3.2 |
| 43 | DO | 28 | VAL | 3.2 |
| 6 | AG | 78 | ARG | 3.2 |
| 41 | BJ | 81 | ILE | 3.1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 27 | DK | 45 | GLU | 3.1 |
| 1 | AA | 1079 | G | 3.1 |
| 48 | BG | 167 | VAL | 3.1 |
| 42 | BN | 10 | LEU | 3.1 |
| 8 | CI | 126 | PHE | 3.1 |
| 48 | DG | 88 | LEU | 3.1 |
| 29 | DE | 57 | LYS | 3.1 |
| 41 | BJ | 113 | PRO | 3.1 |
| 19 | CT | 66 | ILE | 3.1 |
| 32 | B4 | 3 | VAL | 3.1 |
| 10 | AK | 125 | LYS | 3.1 |
| 13 | AN | 97 | LYS | 3.1 |
| 13 | CN | 46 | LYS | 3.1 |
| 25 | BC | 6 | LYS | 3.1 |
| 15 | CP | 41 | PRO | 3.1 |
| 21 | CU | 36 | PHE | 3.1 |
| 25 | DC | 264 | LYS | 3.1 |
| 38 | BM | 67 | VAL | 3.1 |
| 25 | DC | 33 | LEU | 3.0 |
| 41 | BJ | 43 | GLU | 3.0 |
| 26 | DD | 140 | HIS | 3.0 |
| 44 | BQ | 21 | LYS | 3.0 |
| 1 | CA | 1397 | C | 3.0 |
| 19 | CT | 14 | GLU | 3.0 |
| 21 | CU | 43 | GLU | 3.0 |
| 23 | DB | 1099 | G | 3.0 |
| 3 | AD | 159 | GLU | 3.0 |
| 45 | DS | 12 | SER | 3.0 |
| 52 | DW | 12 | GLY | 3.0 |
| 26 | BD | 148 | GLN | 3.0 |
| 32 | B4 | 26 | ILE | 3.0 |
| 50 | BT | 69 | ARG | 3.0 |
| 9 | AJ | 59 | LYS | 3.0 |
| 47 | DF | 8 | LYS | 3.0 |
| 25 | BC | 85 | ASN | 3.0 |
| 18 | AS | 7 | GLY | 3.0 |
| 49 | DR | 50 | GLY | 3.0 |
| 28 | BP | 91 | VAL | 3.0 |
| 43 | BO | 106 | LEU | 3.0 |
| 29 | DE | 65 | THR | 3.0 |
| 8 | CI | 123 | ARG | 3.0 |
| 21 | CU | 46 | ARG | 3.0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 41 | DJ | 86 | GLN | 3.0 |
| 47 | DF | 24 | VAL | 2.9 |
| 43 | DO | 16 | ARG | 2.9 |
| 34 | B3 | 28 | LEU | 2.9 |
| 1 | AA | 82 | G | 2.9 |
| 23 | DB | 2133 | G | 2.9 |
| 1 | AA | 87 | C | 2.9 |
| 36 | D2 | 46 | LYS | 2.9 |
| 25 | DC | 64 | VAL | 2.9 |
| 26 | BD | 111 | GLY | 2.9 |
| 38 | DM | 118 | LYS | 2.9 |
| 3 | CD | 202 | LEU | 2.9 |
| 8 | CI | 117 | LEU | 2.9 |
| 38 | DM | 124 | LEU | 2.9 |
| 38 | BM | 103 | TYR | 2.9 |
| 45 | DS | 105 | VAL | 2.9 |
| 23 | DB | 359 | G | 2.9 |
| 23 | DB | 919 | U | 2.9 |
| 52 | BW | 42 | THR | 2.9 |
| 13 | AN | 35 | ALA | 2.9 |
| 42 | DN | 14 | SER | 2.9 |
| 23 | DB | 645 | C | 2.9 |
| 19 | AT | 12 | GLN | 2.9 |
| 9 | AJ | 63 | ASP | 2.8 |
| 26 | BD | 128 | ARG | 2.8 |
| 42 | DN | 70 | THR | 2.8 |
| 1 | AA | 412 | A | 2.8 |
| 23 | BB | 62 | U | 2.8 |
| 45 | BS | 82 | MET | 2.8 |
| 15 | AP | 22 | ALA | 2.8 |
| 23 | DB | 1459 | G | 2.8 |
| 14 | CO | 40 | GLN | 2.8 |
| 24 | DI | 27 | LEU | 2.8 |
| 23 | BB | 2146 | C | 2.8 |
| 32 | D4 | 15 | LYS | 2.8 |
| 49 | DR | 73 | LYS | 2.8 |
| 3 | AD | 4 | LEU | 2.8 |
| 23 | DB | 548 | G | 2.8 |
| 37 | BL | 37 | GLY | 2.8 |
| 4 | AE | 22 | LYS | 2.8 |
| 29 | BE | 94 | GLN | 2.8 |
| 49 | DR | 86 | GLN | 2.8 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 44 | DQ | 108 | LEU | 2.8 |
| 7 | CH | 39 | LEU | 2.8 |
| 13 | AN | 65 | GLN | 2.8 |
| 23 | DB | 62 | U | 2.8 |
| 47 | DF | 27 | VAL | 2.8 |
| 11 | AL | 9 | LYS | 2.8 |
| 23 | BB | 2145 | C | 2.7 |
| 49 | BR | 86 | GLN | 2.7 |
| 2 | AC | 167 | TYR | 2.7 |
| 34 | D3 | 58 | ILE | 2.7 |
| 19 | CT | 65 | LEU | 2.7 |
| 25 | BC | 201 | LEU | 2.7 |
| 29 | BE | 143 | LEU | 2.7 |
| 6 | CG | 78 | ARG | 2.7 |
| 38 | BM | 129 | THR | 2.7 |
| 37 | DL | 77 | ILE | 2.7 |
| 1 | AA | 108 | G | 2.7 |
| 11 | AL | 123 | ALA | 2.7 |
| 24 | DI | 6 | ALA | 2.7 |
| 38 | DM | 42 | THR | 2.7 |
| 45 | DS | 77 | ASP | 2.7 |
| 26 | BD | 144 | GLY | 2.7 |
| 34 | B3 | 19 | GLY | 2.7 |
| 41 | BJ | 112 | GLY | 2.7 |
| 41 | BJ | 67 | ASN | 2.7 |
| 14 | CO | 48 | LYS | 2.7 |
| 43 | DO | 33 | ARG | 2.7 |
| 21 | AU | 35 | GLU | 2.7 |
| 28 | DP | 67 | GLU | 2.7 |
| 41 | DJ | 46 | PRO | 2.7 |
| 23 | DB | 100 | U | 2.7 |
| 12 | CM | 44 | ILE | 2.7 |
| 36 | B2 | 31 | LEU | 2.7 |
| 8 | CI | 114 | LYS | 2.7 |
| 18 | CS | 7 | GLY | 2.7 |
| 29 | BE | 59 | PRO | 2.7 |
| 26 | BD | 186 | LEU | 2.7 |
| 47 | DF | 174 | PHE | 2.7 |
| 40 | DH | 12 | LEU | 2.6 |
| 41 | DJ | 45 | THR | 2.6 |
| 4 | CE | 31 | SER | 2.6 |
| 47 | DF | 171 | ALA | 2.6 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 52 | DW | 31 | LEU | 2.6 |
| 29 | DE | 59 | PRO | 2.6 |
| 25 | DC | 4 | LYS | 2.6 |
| 41 | BJ | 72 | LYS | 2.6 |
| 26 | BD | 142 | VAL | 2.6 |
| 50 | BT | 67 | VAL | 2.6 |
| 3 | AD | 26 | ALA | 2.6 |
| 42 | DN | 98 | LEU | 2.6 |
| 34 | D3 | 31 | ILE | 2.6 |
| 23 | BB | 978 | G | 2.6 |
| 26 | DD | 113 | SER | 2.6 |
| 15 | CP | 20 | VAL | 2.6 |
| 5 | AF | 52 | ASN | 2.6 |
| 1 | AA | 81 | A | 2.6 |
| 34 | D3 | 13 | PHE | 2.6 |
| 36 | D2 | 43 | THR | 2.6 |
| 52 | BW | 50 | VAL | 2.6 |
| 23 | BB | 1171 | G | 2.6 |
| 1 | CA | 121 | U | 2.6 |
| 23 | BB | 138 | U | 2.6 |
| 25 | BC | 4 | LYS | 2.6 |
| 47 | DF | 155 | ILE | 2.6 |
| 43 | DO | 7 | ARG | 2.6 |
| 25 | BC | 22 | GLU | 2.6 |
| 18 | CS | 15 | LEU | 2.6 |
| 8 | AI | 12 | LYS | 2.6 |
| 38 | DM | 81 | ARG | 2.6 |
| 8 | CI | 116 | GLY | 2.6 |
| 25 | BC | 11 | GLY | 2.6 |
| 34 | B3 | 13 | PHE | 2.6 |
| 44 | DQ | 25 | GLY | 2.6 |
| 21 | AU | 23 | GLU | 2.5 |
| 1 | CA | 765 | G | 2.5 |
| 41 | BJ | 73 | VAL | 2.5 |
| 37 | BL | 15 | ALA | 2.5 |
| 11 | AL | 19 | ASN | 2.5 |
| 27 | DK | 81 | GLY | 2.5 |
| 29 | BE | 54 | GLY | 2.5 |
| 52 | DW | 6 | GLY | 2.5 |
| 9 | CJ | 47 | GLU | 2.5 |
| 23 | DB | 546 | U | 2.5 |
| 23 | DB | 140 | C | 2.5 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 28 | DP | 101 | GLU | 2.5 |
| 29 | BE | 155 | GLU | 2.5 |
| 8 | AI | 119 | LYS | 2.5 |
| 24 | BI | 27 | LEU | 2.5 |
| 26 | BD | 114 | LYS | 2.5 |
| 6 | AG | 4 | ARG | 2.5 |
| 25 | BC | 12 | ARG | 2.5 |
| 9 | CJ | 52 | LEU | 2.5 |
| 52 | BW | 39 | GLN | 2.5 |
| 15 | CP | 38 | PHE | 2.5 |
| 23 | BB | 2148 | G | 2.5 |
| 29 | DE | 60 | TRP | 2.5 |
| 40 | BH | 85 | GLY | 2.5 |
| 10 | CK | 125 | LYS | 2.5 |
| 2 | CC | 167 | TYR | 2.5 |
| 26 | BD | 27 | ILE | 2.5 |
| 50 | DT | 72 | GLN | 2.5 |
| 52 | DW | 42 | THR | 2.5 |
| 28 | BP | 58 | PHE | 2.5 |
| 34 | D3 | 21 | PHE | 2.5 |
| 23 | BB | 1172 | C | 2.5 |
| 7 | AH | 81 | GLY | 2.5 |
| 14 | CO | 46 | HIS | 2.5 |
| 1 | CA | 1074 | G | 2.4 |
| 43 | DO | 97 | PHE | 2.4 |
| 1 | AA | 562 | U | 2.4 |
| 38 | DM | 37 | GLY | 2.4 |
| 50 | DT | 11 | LEU | 2.4 |
| 23 | BB | 1727 | C | 2.4 |
| 42 | DN | 21 | PHE | 2.4 |
| 41 | BJ | 37 | ARG | 2.4 |
| 1 | CA | 85 | U | 2.4 |
| 4 | CE | 117 | ALA | 2.4 |
| 46 | DU | 32 | LYS | 2.4 |
| 38 | BM | 42 | THR | 2.4 |
| 15 | AP | 6 | LEU | 2.4 |
| 26 | DD | 77 | ARG | 2.4 |
| 49 | DR | 40 | MET | 2.4 |
| 23 | BB | 508 | A | 2.4 |
| 21 | CU | 39 | LYS | 2.4 |
| 49 | BR | 73 | LYS | 2.4 |
| 25 | DC | 202 | ARG | 2.4 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | CA | 240 | G | 2.4 |
| 24 | BI | 58 | ILE | 2.4 |
| 22 | BA | 52 | A | 2.4 |
| 2 | AC | 151 | GLU | 2.4 |
| 2 | CC | 165 | GLU | 2.4 |
| 4 | CE | 124 | ALA | 2.4 |
| 38 | DM | 111 | GLU | 2.4 |
| 25 | DC | 263 | ASP | 2.4 |
| 23 | BB | 2104 | C | 2.4 |
| 26 | BD | 26 | VAL | 2.3 |
| 44 | DQ | 97 | ILE | 2.3 |
| 23 | BB | 2154 | A | 2.3 |
| 23 | DB | 1808 | A | 2.3 |
| 4 | CE | 28 | ARG | 2.3 |
| 9 | CJ | 81 | GLU | 2.3 |
| 23 | DB | 2213 | U | 2.3 |
| 34 | B3 | 30 | HIS | 2.3 |
| 50 | BT | 72 | GLN | 2.3 |
| 34 | D3 | 53 | ASP | 2.3 |
| 7 | AH | 125 | ILE | 2.3 |
| 21 | AU | 13 | VAL | 2.3 |
| 50 | BT | 16 | VAL | 2.3 |
| 6 | AG | 81 | GLY | 2.3 |
| 26 | BD | 112 | THR | 2.3 |
| 31 | D0 | 22 | THR | 2.3 |
| 15 | AP | 81 | ALA | 2.3 |
| 32 | B4 | 36 | ARG | 2.3 |
| 38 | BM | 81 | ARG | 2.3 |
| 1 | CA | 1534 | A | 2.3 |
| 26 | DD | 200 | ASP | 2.3 |
| 48 | DG | 161 | VAL | 2.3 |
| 23 | BB | 546 | U | 2.3 |
| 25 | BC | 126 | GLY | 2.3 |
| 15 | AP | 5 | ARG | 2.3 |
| 52 | BW | 40 | ARG | 2.3 |
| 15 | AP | 43 | ALA | 2.3 |
| 17 | AR | 19 | GLU | 2.3 |
| 1 | AA | 134 | G | 2.3 |
| 6 | AG | 76 | SER | 2.3 |
| 20 | AB | 161 | PHE | 2.3 |
| 26 | BD | 131 | ASP | 2.3 |
| 26 | DD | 112 | THR | 2.3 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | AA | 208 | U | 2.3 |
| 45 | BS | 78 | GLU | 2.3 |
| 7 | AH | 128 | VAL | 2.3 |
| 24 | BI | 4 | VAL | 2.3 |
| 44 | BQ | 90 | ASP | 2.3 |
| 51 | BZ | 17 | ASN | 2.3 |
| 51 | DZ | 78 | TYR | 2.3 |
| 13 | CN | 41 | TRP | 2.3 |
| 43 | DO | 37 | ALA | 2.3 |
| 23 | BB | 979 | A | 2.3 |
| 52 | DW | 68 | PHE | 2.3 |
| 41 | BJ | 75 | TYR | 2.3 |
| 26 | DD | 126 | ASN | 2.3 |
| 43 | DO | 4 | LYS | 2.2 |
| 28 | BP | 102 | ARG | 2.2 |
| 44 | DQ | 10 | ARG | 2.2 |
| 42 | DN | 83 | LEU | 2.2 |
| 4 | CE | 109 | ALA | 2.2 |
| 26 | BD | 129 | THR | 2.2 |
| 15 | AP | 80 | LYS | 2.2 |
| 34 | D3 | 27 | ASN | 2.2 |
| 51 | BZ | 60 | ASP | 2.2 |
| 34 | B3 | 31 | ILE | 2.2 |
| 7 | CH | 71 | VAL | 2.2 |
| 31 | B0 | 2 | VAL | 2.2 |
| 2 | CC | 130 | ARG | 2.2 |
| 19 | CT | 67 | HIS | 2.2 |
| 33 | B1 | 7 | LYS | 2.2 |
| 41 | BJ | 39 | LYS | 2.2 |
| 25 | DC | 43 | ASN | 2.2 |
| 43 | BO | 8 | ILE | 2.2 |
| 44 | BQ | 28 | SER | 2.2 |
| 2 | AC | 90 | VAL | 2.2 |
| 26 | DD | 170 | VAL | 2.2 |
| 1 | CA | 412 | A | 2.2 |
| 3 | AD | 72 | ARG | 2.2 |
| 22 | DA | 53 | A | 2.2 |
| 25 | DC | 174 | ARG | 2.2 |
| 45 | BS | 75 | PHE | 2.2 |
| 20 | AB | 100 | LEU | 2.2 |
| 26 | DD | 162 | ALA | 2.2 |
| 27 | BK | 104 | THR | 2.2 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 18 | CS | 4 | LEU | 2.2 |
| 44 | DQ | 4 | LYS | 2.2 |
| 8 | CI | 109 | GLN | 2.2 |
| 23 | BB | 1808 | A | 2.2 |
| 41 | BJ | 42 | ALA | 2.2 |
| 42 | BN | 70 | THR | 2.2 |
| 43 | DO | 9 | ARG | 2.2 |
| 44 | DQ | 12 | ARG | 2.2 |
| 47 | DF | 157 | THR | 2.2 |
| 23 | DB | 141 | G | 2.2 |
| 29 | DE | 58 | LYS | 2.2 |
| 37 | DL | 65 | GLY | 2.2 |
| 50 | DT | 71 | GLY | 2.2 |
| 30 | DY | 54 | VAL | 2.2 |
| 44 | DQ | 105 | PHE | 2.2 |
| 51 | DZ | 51 | VAL | 2.2 |
| 1 | AA | 209 | U | 2.2 |
| 23 | BB | 405 | U | 2.2 |
| 28 | BP | 30 | TRP | 2.2 |
| 23 | BB | 2147 | A | 2.2 |
| 50 | DT | 89 | GLU | 2.1 |
| 9 | AJ | 8 | ILE | 2.1 |
| 13 | CN | 35 | ALA | 2.1 |
| 44 | BQ | 19 | GLN | 2.1 |
| 4 | CE | 136 | VAL | 2.1 |
| 17 | CR | 66 | LEU | 2.1 |
| 6 | AG | 73 | GLU | 2.1 |
| 9 | AJ | 60 | ASP | 2.1 |
| 17 | CR | 19 | GLU | 2.1 |
| 23 | DB | 653 | U | 2.1 |
| 1 | AA | 1081 | A | 2.1 |
| 27 | DK | 17 | ARG | 2.1 |
| 25 | BC | 250 | GLN | 2.1 |
| 46 | DU | 33 | VAL | 2.1 |
| 9 | AJ | 52 | LEU | 2.1 |
| 26 | DD | 154 | LYS | 2.1 |
| 34 | D3 | 1 | PRO | 2.1 |
| 45 | DS | 83 | LYS | 2.1 |
| 2 | CC | 154 | GLY | 2.1 |
| 43 | BO | 107 | ALA | 2.1 |
| 52 | DW | 32 | ALA | 2.1 |
| 15 | CP | 36 | VAL | 2.1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 21 | CU | 53 | LYS | 2.1 |
| 1 | AA | 77 | A | 2.1 |
| 23 | BB | 2516 | A | 2.1 |
| 9 | CJ | 44 | THR | 2.1 |
| 37 | BL | 5 | THR | 2.1 |
| 4 | AE | 53 | ARG | 2.1 |
| 7 | CH | 35 | ILE | 2.1 |
| 26 | BD | 30 | GLU | 2.1 |
| 30 | BY | 10 | ARG | 2.1 |
| 50 | BT | 18 | GLU | 2.1 |
| 52 | BW | 16 | GLU | 2.1 |
| 37 | DL | 45 | GLY | 2.1 |
| 47 | DF | 125 | GLY | 2.1 |
| 52 | BW | 75 | ASN | 2.1 |
| 52 | DW | 13 | ARG | 2.1 |
| 25 | BC | 2 | VAL | 2.1 |
| 40 | BH | 142 | VAL | 2.1 |
| 41 | DJ | 105 | VAL | 2.1 |
| 1 | CA | 1353 | G | 2.1 |
| 8 | AI | 118 | ARG | 2.1 |
| 9 | CJ | 45 | ARG | 2.1 |
| 41 | BJ | 84 | ILE | 2.1 |
| 16 | AQ | 33 | TYR | 2.1 |
| 4 | AE | 124 | ALA | 2.1 |
| 13 | AN | 1 | ALA | 2.1 |
| 44 | DQ | 26 | ALA | 2.1 |
| 51 | BZ | 16 | ASN | 2.1 |
| 2 | AC | 199 | VAL | 2.1 |
| 18 | CS | 26 | ASP | 2.1 |
| 21 | CU | 15 | LEU | 2.1 |
| 36 | D2 | 29 | GLN | 2.1 |
| 24 | BI | 53 | PRO | 2.1 |
| 41 | BJ | 110 | PRO | 2.1 |
| 45 | DS | 92 | ARG | 2.1 |
| 51 | BZ | 18 | ARG | 2.1 |
| 26 | DD | 121 | THR | 2.1 |
| 47 | BF | 155 | ILE | 2.1 |
| 13 | AN | 91 | GLU | 2.1 |
| 26 | DD | 144 | GLY | 2.1 |
| 11 | AL | 16 | ALA | 2.1 |
| 32 | B4 | 20 | ASP | 2.0 |
| 25 | BC | 141 | HIS | 2.0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | AA | 1534 | A | 2.0 |
| 19 | AT | 27 | MET | 2.0 |
| 23 | BB | 1093 | G | 2.0 |
| 14 | CO | 58 | ARG | 2.0 |
| 31 | B0 | 54 | ILE | 2.0 |
| 12 | AM | 26 | LYS | 2.0 |
| 47 | BF | 102 | LEU | 2.0 |
| 7 | AH | 71 | VAL | 2.0 |
| 14 | AO | 44 | ALA | 2.0 |
| 29 | DE | 172 | ALA | 2.0 |
| 50 | BT | 65 | GLY | 2.0 |
| 9 | AJ | 54 | SER | 2.0 |
| 15 | AP | 28 | ARG | 2.0 |
| 27 | DK | 71 | ARG | 2.0 |
| 28 | BP | 47 | ILE | 2.0 |
| 17 | AR | 28 | LEU | 2.0 |
| 52 | BW | 20 | LEU | 2.0 |
| 48 | DG | 160 | GLY | 2.0 |
| 3 | AD | 162 | GLU | 2.0 |
| 23 | BB | 1177 | G | 2.0 |
| 52 | DW | 40 | ARG | 2.0 |
| 52 | DW | 45 | HIS | 2.0 |
| 31 | D0 | 54 | ILE | 2.0 |
| 35 | BV | 83 | LYS | 2.0 |
| 34 | B3 | 21 | PHE | 2.0 |

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

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 53 | MG | AA | 2025 | 1/1 | 0.07 | 0.13 | 50,50,50,50 | 1 |
| 53 | MG | CA | 2027 | 1/1 | 0.23 | 0.18 | 55,55,55,55 | 1 |
| 53 | MG | CA | 2029 | 1/1 | 0.40 | 0.20 | 57,57,57,57 | 1 |
| 53 | MG | AA | 2023 | 1/1 | 0.41 | 0.37 | 44,44,44,44 | 1 |
| 53 | MG | AA | 2059 | 1/1 | 0.41 | 0.34 | 102,102,102,102 | 0 |
| 53 | MG | AA | 2022 | 1/1 | 0.52 | 0.25 | 100,100,100,100 | 0 |
| 53 | MG | AA | 2039 | 1/1 | 0.59 | 0.29 | 92,92,92,92 | 0 |
| 53 | MG | AA | 2026 | 1/1 | 0.63 | 0.27 | 51,51,51,51 | 1 |
| 53 | MG | CA | 2026 | 1/1 | 0.72 | 0.34 | 40,40,40,40 | 1 |
| 53 | MG | DB | 3095 | 1/1 | 0.76 | 0.07 | 96,96,96,96 | 0 |
| 53 | MG | BB | 3033 | 1/1 | 0.80 | 0.20 | 90,90,90,90 | 0 |
| 53 | MG | DB | 3066 | 1/1 | 0.81 | 0.17 | 100,100,100,100 | 0 |
| 53 | MG | AA | 2002 | 1/1 | 0.81 | 0.15 | 100,100,100,100 | 0 |
| 53 | MG | AA | 2047 | 1/1 | 0.82 | 0.26 | 73,73,73,73 | 0 |
| 53 | MG | DB | 3058 | 1/1 | 0.83 | 0.35 | 96,96,96,96 | 0 |
| 53 | MG | AA | 2056 | 1/1 | 0.85 | 0.16 | 103,103,103,103 | 0 |
| 54 | LLL | AA | 2063 | 31/31 | 0.85 | 0.26 | 62,62,62,62 | 31 |
| 54 | LLL | CA | 2064 | 31/31 | 0.85 | 0.16 | 41,41,41,41 | 31 |
| 53 | MG | BB | 3093 | 1/1 | 0.86 | 0.15 | 80,80,80,80 | 0 |
| 53 | MG | CA | 2020 | 1/1 | 0.86 | 0.35 | 85,85,85,85 | 0 |
| 53 | MG | AA | 2037 | 1/1 | 0.86 | 0.29 | 87,87,87,87 | 0 |
| 54 | LLL | AA | 2062 | 31/31 | 0.86 | 0.27 | 73,73,73,73 | 31 |
| 53 | MG | BB | 3057 | 1/1 | 0.86 | 0.11 | 72,72,72,72 | 0 |
| 53 | MG | BB | 3063 | 1/1 | 0.86 | 0.10 | 51,51,51,51 | 0 |
| 54 | LLL | DB | 3112 | 31/31 | 0.86 | 0.14 | 54,54,54,54 | 0 |
| 53 | MG | CA | 2035 | 1/1 | 0.87 | 0.11 | 85,85,85,85 | 0 |
| 53 | MG | BB | 3090 | 1/1 | 0.88 | 0.09 | 60,60,60,60 | 0 |
| 53 | MG | AA | 2057 | 1/1 | 0.88 | 0.20 | 80,80,80,80 | 0 |
| 53 | MG | BB | 3100 | 1/1 | 0.88 | 0.10 | 105,105,105,105 | 0 |
| 53 | MG | AA | 2046 | 1/1 | 0.89 | 0.07 | 95,95,95,95 | 0 |
| 54 | LLL | CA | 2063 | 31/31 | 0.89 | 0.14 | 70,70,70,70 | 0 |
| 54 | LLL | BB | 3111 | 31/31 | 0.90 | 0.28 | 67,67,67,67 | 31 |
| 53 | MG | DB | 3030 | 1/1 | 0.90 | 0.13 | 26,26,26,26 | 0 |
| 53 | MG | CA | 2036 | 1/1 | 0.91 | 0.10 | 74,74,74,74 | 0 |
| 53 | MG | AA | 2050 | 1/1 | 0.91 | 0.05 | 103,103,103,103 | 0 |
| 53 | MG | BB | 3072 | 1/1 | 0.91 | 0.07 | 57,57,57,57 | 0 |
| 53 | MG | DB | 3059 | 1/1 | 0.91 | 0.10 | 100,100,100,100 | 0 |
| 53 | MG | DB | 3013 | 1/1 | 0.92 | 0.10 | 37,37,37,37 | 0 |
| 53 | MG | AA | 2012 | 1/1 | 0.92 | 0.07 | 70,70,70,70 | 0 |
| 53 | MG | BB | 3034 | 1/1 | 0.92 | 0.16 | 52,52,52,52 | 0 |
| 53 | MG | BB | 3047 | 1/1 | 0.92 | 0.06 | 77,77,77,77 | 0 |
| 53 | MG | CA | 2022 | 1/1 | 0.93 | 0.08 | 105,105,105,105 | 0 |
| 53 | MG | CA | 2057 | 1/1 | 0.93 | 0.11 | 61,61,61,61 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 54 | LLL | AA | 2061 | 31/31 | 0.93 | 0.08 | 20,20,20,20 | 0 |
| 53 | MG | AA | 2015 | 1/1 | 0.94 | 0.10 | 78,78,78,78 | 0 |
| 53 | MG | AA | 2019 | 1/1 | 0.94 | 0.10 | 87,87,87,87 | 0 |
| 53 | MG | CA | 2021 | 1/1 | 0.94 | 0.06 | 70,70,70,70 | 0 |
| 53 | MG | DB | 3034 | 1/1 | 0.94 | 0.10 | 74,74,74,74 | 0 |
| 53 | MG | CA | 2047 | 1/1 | 0.94 | 0.09 | 74,74,74,74 | 0 |
| 53 | MG | CA | 2011 | 1/1 | 0.95 | 0.07 | 82,82,82,82 | 0 |
| 53 | MG | CA | 2015 | 1/1 | 0.95 | 0.08 | 108,108,108,108 | 0 |
| 53 | MG | BB | 3050 | 1/1 | 0.95 | 0.05 | 18,18,18,18 | 0 |
| 53 | MG | DB | 3052 | 1/1 | 0.95 | 0.14 | 62,62,62,62 | 0 |
| 53 | MG | AA | 2035 | 1/1 | 0.95 | 0.07 | 71,71,71,71 | 0 |
| 53 | MG | BB | 3010 | 1/1 | 0.95 | 0.05 | 73,73,73,73 | 0 |
| 53 | MG | AA | 2005 | 1/1 | 0.95 | 0.05 | 72,72,72,72 | 0 |
| 53 | MG | DB | 3092 | 1/1 | 0.95 | 0.04 | 76,76,76,76 | 0 |
| 53 | MG | BB | 3078 | 1/1 | 0.95 | 0.16 | 67,67,67,67 | 0 |
| 53 | MG | CA | 2028 | 1/1 | 0.95 | 0.09 | 77,77,77,77 | 0 |
| 53 | MG | BB | 3081 | 1/1 | 0.95 | 0.09 | 40,40,40,40 | 0 |
| 53 | MG | AA | 2014 | 1/1 | 0.95 | 0.08 | 72,72,72,72 | 0 |
| 53 | MG | BB | 3043 | 1/1 | 0.95 | 0.17 | 86,86,86,86 | 0 |
| 54 | LLL | CA | 2062 | 31/31 | 0.95 | 0.07 | 9,9,9,9 | 0 |
| 53 | MG | BB | 3097 | 1/1 | 0.95 | 0.16 | 56,56,56,56 | 0 |
| 53 | MG | CA | 2048 | 1/1 | 0.95 | 0.15 | 65,65,65,65 | 0 |
| 53 | MG | AA | 2030 | 1/1 | 0.95 | 0.08 | 88,88,88,88 | 0 |
| 53 | MG | AA | 2058 | 1/1 | 0.96 | 0.04 | 94,94,94,94 | 0 |
| 53 | MG | DB | 3057 | 1/1 | 0.96 | 0.05 | 53,53,53,53 | 0 |
| 53 | MG | AA | 2032 | 1/1 | 0.96 | 0.15 | 67,67,67,67 | 0 |
| 53 | MG | BB | 3094 | 1/1 | 0.96 | 0.05 | 69,69,69,69 | 0 |
| 53 | MG | BB | 3008 | 1/1 | 0.96 | 0.04 | 80,80,80,80 | 0 |
| 53 | MG | DB | 3083 | 1/1 | 0.96 | 0.11 | 56,56,56,56 | 0 |
| 53 | MG | DB | 3084 | 1/1 | 0.96 | 0.06 | 25,25,25,25 | 0 |
| 53 | MG | BB | 3099 | 1/1 | 0.96 | 0.06 | 56,56,56,56 | 0 |
| 53 | MG | BB | 3009 | 1/1 | 0.96 | 0.06 | 70,70,70,70 | 0 |
| 53 | MG | AA | 2051 | 1/1 | 0.96 | 0.11 | 66,66,66,66 | 0 |
| 53 | MG | AA | 2027 | 1/1 | 0.96 | 0.07 | 56,56,56,56 | 0 |
| 53 | MG | CA | 2018 | 1/1 | 0.96 | 0.11 | 60,60,60,60 | 0 |
| 53 | MG | AA | 2024 | 1/1 | 0.96 | 0.19 | 73,73,73,73 | 0 |
| 53 | MG | DB | 3018 | 1/1 | 0.96 | 0.06 | 48,48,48,48 | 0 |
| 53 | MG | DB | 3029 | 1/1 | 0.96 | 0.06 | 66,66,66,66 | 0 |
| 53 | MG | BB | 3042 | 1/1 | 0.96 | 0.03 | 96,96,96,96 | 0 |
| 53 | MG | BB | 3089 | 1/1 | 0.96 | 0.05 | 63,63,63,63 | 0 |
| 53 | MG | BB | 3077 | 1/1 | 0.97 | 0.05 | 44,44,44,44 | 0 |
| 53 | MG | BB | 3032 | 1/1 | 0.97 | 0.07 | 36,36,36,36 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 53 | MG | BB | 3080 | 1/1 | 0.97 | 0.07 | 56,56,56,56 | 0 |
| 53 | MG | AA | 2008 | 1/1 | 0.97 | 0.17 | 81,81,81,81 | 0 |
| 53 | MG | BB | 3087 | 1/1 | 0.97 | 0.08 | 73,73,73,73 | 0 |
| 53 | MG | CA | 2025 | 1/1 | 0.97 | 0.06 | 72,72,72,72 | 0 |
| 53 | MG | AA | 2034 | 1/1 | 0.97 | 0.08 | 42,42,42,42 | 0 |
| 53 | MG | AA | 2020 | 1/1 | 0.97 | 0.04 | 91,91,91,91 | 0 |
| 53 | MG | BB | 3091 | 1/1 | 0.97 | 0.05 | 34,34,34,34 | 0 |
| 53 | MG | AA | 2049 | 1/1 | 0.97 | 0.04 | 93,93,93,93 | 0 |
| 53 | MG | DB | 3085 | 1/1 | 0.97 | 0.05 | 5,5,5,5 | 0 |
| 53 | MG | DB | 3089 | 1/1 | 0.97 | 0.14 | 52,52,52,52 | 0 |
| 53 | MG | DB | 3090 | 1/1 | 0.97 | 0.06 | 57,57,57,57 | 0 |
| 53 | MG | AA | 2036 | 1/1 | 0.97 | 0.04 | 62,62,62,62 | 0 |
| 53 | MG | AA | 2001 | 1/1 | 0.97 | 0.10 | 27,27,27,27 | 0 |
| 53 | MG | DB | 3111 | 1/1 | 0.97 | 0.08 | 43,43,43,43 | 0 |
| 53 | MG | CA | 2037 | 1/1 | 0.97 | 0.04 | 69,69,69,69 | 0 |
| 53 | MG | CA | 2041 | 1/1 | 0.97 | 0.08 | 69,69,69,69 | 0 |
| 53 | MG | AA | 2055 | 1/1 | 0.97 | 0.08 | 57,57,57,57 | 0 |
| 53 | MG | BB | 3013 | 1/1 | 0.97 | 0.06 | 41,41,41,41 | 0 |
| 53 | MG | CA | 2006 | 1/1 | 0.97 | 0.07 | 73,73,73,73 | 0 |
| 53 | MG | CA | 2058 | 1/1 | 0.97 | 0.16 | 63,63,63,63 | 0 |
| 53 | MG | CA | 2010 | 1/1 | 0.97 | 0.04 | 59,59,59,59 | 0 |
| 53 | MG | BB | 3022 | 1/1 | 0.97 | 0.07 | 44,44,44,44 | 0 |
| 55 | ZN | B4 | 101 | 1/1 | 0.97 | 0.04 | 82,82,82,82 | 0 |
| 55 | ZN | D4 | 101 | 1/1 | 0.97 | 0.04 | 45,45,45,45 | 0 |
| 53 | MG | CN | 201 | 1/1 | 0.98 | 0.04 | 50,50,50,50 | 0 |
| 53 | MG | BB | 3004 | 1/1 | 0.98 | 0.09 | 43,43,43,43 | 0 |
| 53 | MG | DB | 3015 | 1/1 | 0.98 | 0.03 | 50,50,50,50 | 0 |
| 53 | MG | CA | 2019 | 1/1 | 0.98 | 0.04 | 63,63,63,63 | 0 |
| 53 | MG | DB | 3024 | 1/1 | 0.98 | 0.04 | 53,53,53,53 | 0 |
| 53 | MG | BB | 3068 | 1/1 | 0.98 | 0.13 | 37,37,37,37 | 0 |
| 53 | MG | BB | 3092 | 1/1 | 0.98 | 0.04 | 40,40,40,40 | 0 |
| 53 | MG | BB | 3071 | 1/1 | 0.98 | 0.04 | 63,63,63,63 | 0 |
| 53 | MG | DB | 3035 | 1/1 | 0.98 | 0.04 | 54,54,54,54 | 0 |
| 53 | MG | DB | 3036 | 1/1 | 0.98 | 0.04 | 26,26,26,26 | 0 |
| 53 | MG | DB | 3051 | 1/1 | 0.98 | 0.07 | 57,57,57,57 | 0 |
| 53 | MG | CA | 2023 | 1/1 | 0.98 | 0.04 | 54,54,54,54 | 0 |
| 53 | MG | AA | 2028 | 1/1 | 0.98 | 0.04 | 53,53,53,53 | 0 |
| 53 | MG | BB | 3095 | 1/1 | 0.98 | 0.04 | 59,59,59,59 | 0 |
| 53 | MG | BB | 3038 | 1/1 | 0.98 | 0.10 | 77,77,77,77 | 0 |
| 53 | MG | DB | 3060 | 1/1 | 0.98 | 0.04 | 79,79,79,79 | 0 |
| 53 | MG | DB | 3061 | 1/1 | 0.98 | 0.09 | 58,58,58,58 | 0 |
| 53 | MG | AA | 2044 | 1/1 | 0.98 | 0.06 | 48,48,48,48 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 53 | MG | DB | 3070 | 1/1 | 0.98 | 0.10 | 43,43,43,43 | 0 |
| 53 | MG | DB | 3073 | 1/1 | 0.98 | 0.04 | 33,33,33,33 | 0 |
| 53 | MG | DB | 3077 | 1/1 | 0.98 | 0.04 | 50,50,50,50 | 0 |
| 53 | MG | DB | 3078 | 1/1 | 0.98 | 0.03 | 48,48,48,48 | 0 |
| 53 | MG | DB | 3082 | 1/1 | 0.98 | 0.05 | 42,42,42,42 | 0 |
| 53 | MG | AA | 2007 | 1/1 | 0.98 | 0.03 | 70,70,70,70 | 0 |
| 53 | MG | CA | 2030 | 1/1 | 0.98 | 0.06 | 31,31,31,31 | 0 |
| 53 | MG | BB | 3106 | 1/1 | 0.98 | 0.06 | 31,31,31,31 | 0 |
| 53 | MG | BB | 3110 | 1/1 | 0.98 | 0.05 | 74,74,74,74 | 0 |
| 53 | MG | AA | 2031 | 1/1 | 0.98 | 0.04 | 49,49,49,49 | 0 |
| 53 | MG | DB | 3091 | 1/1 | 0.98 | 0.07 | 45,45,45,45 | 0 |
| 53 | MG | CA | 2038 | 1/1 | 0.98 | 0.10 | 77,77,77,77 | 0 |
| 53 | MG | CA | 2008 | 1/1 | 0.98 | 0.04 | 86,86,86,86 | 0 |
| 53 | MG | DB | 3104 | 1/1 | 0.98 | 0.08 | 55,55,55,55 | 0 |
| 53 | MG | DB | 3106 | 1/1 | 0.98 | 0.04 | 37,37,37,37 | 0 |
| 53 | MG | CA | 2042 | 1/1 | 0.98 | 0.04 | 66,66,66,66 | 0 |
| 53 | MG | CA | 2044 | 1/1 | 0.98 | 0.03 | 67,67,67,67 | 0 |
| 53 | MG | BB | 3084 | 1/1 | 0.98 | 0.12 | 67,67,67,67 | 0 |
| 53 | MG | AA | 2017 | 1/1 | 0.98 | 0.07 | 76,76,76,76 | 0 |
| 53 | MG | CA | 2049 | 1/1 | 0.98 | 0.07 | 63,63,63,63 | 0 |
| 53 | MG | CA | 2052 | 1/1 | 0.98 | 0.05 | 66,66,66,66 | 0 |
| 53 | MG | CA | 2054 | 1/1 | 0.98 | 0.03 | 91,91,91,91 | 0 |
| 53 | MG | CA | 2014 | 1/1 | 0.98 | 0.05 | 72,72,72,72 | 0 |
| 53 | MG | AA | 2038 | 1/1 | 0.98 | 0.06 | 45,45,45,45 | 0 |
| 53 | MG | CA | 2059 | 1/1 | 0.98 | 0.07 | 51,51,51,51 | 0 |
| 53 | MG | CA | 2060 | 1/1 | 0.98 | 0.07 | 55,55,55,55 | 0 |
| 53 | MG | AA | 2021 | 1/1 | 0.99 | 0.12 | 23,23,23,23 | 0 |
| 53 | MG | AA | 2029 | 1/1 | 0.99 | 0.03 | 50,50,50,50 | 0 |
| 53 | MG | BB | 3051 | 1/1 | 0.99 | 0.03 | 43,43,43,43 | 0 |
| 53 | MG | BB | 3052 | 1/1 | 0.99 | 0.11 | 26,26,26,26 | 0 |
| 53 | MG | BB | 3053 | 1/1 | 0.99 | 0.03 | 59,59,59,59 | 0 |
| 53 | MG | CA | 2031 | 1/1 | 0.99 | 0.03 | 37,37,37,37 | 0 |
| 53 | MG | CA | 2033 | 1/1 | 0.99 | 0.06 | 57,57,57,57 | 0 |
| 53 | MG | CA | 2034 | 1/1 | 0.99 | 0.03 | 15,15,15,15 | 0 |
| 53 | MG | BB | 3054 | 1/1 | 0.99 | 0.04 | 39,39,39,39 | 0 |
| 53 | MG | BB | 3055 | 1/1 | 0.99 | 0.07 | 40,40,40,40 | 0 |
| 53 | MG | AA | 2011 | 1/1 | 0.99 | 0.04 | 41,41,41,41 | 0 |
| 53 | MG | BB | 3058 | 1/1 | 0.99 | 0.04 | 32,32,32,32 | 0 |
| 53 | MG | BB | 3059 | 1/1 | 0.99 | 0.03 | 39,39,39,39 | 0 |
| 53 | MG | BB | 3061 | 1/1 | 0.99 | 0.05 | 45,45,45,45 | 0 |
| 53 | MG | CA | 2043 | 1/1 | 0.99 | 0.07 | 31,31,31,31 | 0 |
| 53 | MG | AA | 2040 | 1/1 | 0.99 | 0.09 | 65,65,65,65 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 53 | MG | CA | 2045 | 1/1 | 0.99 | 0.07 | 77,77,77,77 | 0 |
| 53 | MG | CA | 2046 | 1/1 | 0.99 | 0.03 | 70,70,70,70 | 0 |
| 53 | MG | BB | 3064 | 1/1 | 0.99 | 0.06 | 37,37,37,37 | 0 |
| 53 | MG | BB | 3065 | 1/1 | 0.99 | 0.03 | 44,44,44,44 | 0 |
| 53 | MG | BB | 3067 | 1/1 | 0.99 | 0.04 | 40,40,40,40 | 0 |
| 53 | MG | CA | 2051 | 1/1 | 0.99 | 0.02 | 38,38,38,38 | 0 |
| 53 | MG | AA | 2041 | 1/1 | 0.99 | 0.03 | 57,57,57,57 | 0 |
| 53 | MG | AA | 2060 | 1/1 | 0.99 | 0.03 | 46,46,46,46 | 0 |
| 53 | MG | CA | 2056 | 1/1 | 0.99 | 0.04 | 32,32,32,32 | 0 |
| 53 | MG | BB | 3003 | 1/1 | 0.99 | 0.09 | 17,17,17,17 | 0 |
| 53 | MG | BB | 3073 | 1/1 | 0.99 | 0.04 | 33,33,33,33 | 0 |
| 53 | MG | BB | 3075 | 1/1 | 0.99 | 0.09 | 33,33,33,33 | 0 |
| 53 | MG | BB | 3076 | 1/1 | 0.99 | 0.04 | 23,23,23,23 | 0 |
| 53 | MG | AA | 2042 | 1/1 | 0.99 | 0.04 | 28,28,28,28 | 0 |
| 53 | MG | DB | 3001 | 1/1 | 0.99 | 0.04 | 5,5,5,5 | 0 |
| 53 | MG | DB | 3003 | 1/1 | 0.99 | 0.03 | 17,17,17,17 | 0 |
| 53 | MG | DB | 3004 | 1/1 | 0.99 | 0.06 | 21,21,21,21 | 0 |
| 53 | MG | DB | 3011 | 1/1 | 0.99 | 0.07 | 35,35,35,35 | 0 |
| 53 | MG | BB | 3007 | 1/1 | 0.99 | 0.03 | 60,60,60,60 | 0 |
| 53 | MG | BB | 3079 | 1/1 | 0.99 | 0.03 | 52,52,52,52 | 0 |
| 53 | MG | AA | 2043 | 1/1 | 0.99 | 0.02 | 44,44,44,44 | 0 |
| 53 | MG | DB | 3020 | 1/1 | 0.99 | 0.09 | 5,5,5,5 | 0 |
| 53 | MG | DB | 3022 | 1/1 | 0.99 | 0.04 | 23,23,23,23 | 0 |
| 53 | MG | AA | 2016 | 1/1 | 0.99 | 0.02 | 36,36,36,36 | 0 |
| 53 | MG | DB | 3026 | 1/1 | 0.99 | 0.06 | 33,33,33,33 | 0 |
| 53 | MG | DB | 3027 | 1/1 | 0.99 | 0.03 | 12,12,12,12 | 0 |
| 53 | MG | DB | 3028 | 1/1 | 0.99 | 0.08 | 37,37,37,37 | 0 |
| 53 | MG | AA | 2045 | 1/1 | 0.99 | 0.15 | 48,48,48,48 | 0 |
| 53 | MG | AA | 2004 | 1/1 | 0.99 | 0.03 | 35,35,35,35 | 0 |
| 53 | MG | DB | 3031 | 1/1 | 0.99 | 0.03 | 8,8,8,8 | 0 |
| 53 | MG | DB | 3032 | 1/1 | 0.99 | 0.05 | 45,45,45,45 | 0 |
| 53 | MG | DB | 3033 | 1/1 | 0.99 | 0.02 | 18,18,18,18 | 0 |
| 53 | MG | BB | 3088 | 1/1 | 0.99 | 0.03 | 26,26,26,26 | 0 |
| 53 | MG | BB | 3014 | 1/1 | 0.99 | 0.06 | 39,39,39,39 | 0 |
| 53 | MG | BB | 3016 | 1/1 | 0.99 | 0.06 | 43,43,43,43 | 0 |
| 53 | MG | DB | 3039 | 1/1 | 0.99 | 0.09 | 36,36,36,36 | 0 |
| 53 | MG | DB | 3041 | 1/1 | 0.99 | 0.04 | 41,41,41,41 | 0 |
| 53 | MG | DB | 3042 | 1/1 | 0.99 | 0.03 | 22,22,22,22 | 0 |
| 53 | MG | DB | 3043 | 1/1 | 0.99 | 0.05 | 5,5,5,5 | 0 |
| 53 | MG | DB | 3044 | 1/1 | 0.99 | 0.05 | 18,18,18,18 | 0 |
| 53 | MG | DB | 3045 | 1/1 | 0.99 | 0.03 | 66,66,66,66 | 0 |
| 53 | MG | DB | 3048 | 1/1 | 0.99 | 0.06 | 36,36,36,36 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 53 | MG | DB | 3050 | 1/1 | 0.99 | 0.05 | 73,73,73,73 | 0 |
| 53 | MG | BB | 3019 | 1/1 | 0.99 | 0.03 | 49,49,49,49 | 0 |
| 53 | MG | BB | 3020 | 1/1 | 0.99 | 0.07 | 13,13,13,13 | 0 |
| 53 | MG | DB | 3053 | 1/1 | 0.99 | 0.06 | 66,66,66,66 | 0 |
| 53 | MG | BB | 3021 | 1/1 | 0.99 | 0.04 | 22,22,22,22 | 0 |
| 53 | MG | AA | 2033 | 1/1 | 0.99 | 0.03 | 69,69,69,69 | 0 |
| 53 | MG | BB | 3023 | 1/1 | 0.99 | 0.03 | 11,11,11,11 | 0 |
| 53 | MG | BB | 3096 | 1/1 | 0.99 | 0.04 | 44,44,44,44 | 0 |
| 53 | MG | BB | 3024 | 1/1 | 0.99 | 0.11 | 21,21,21,21 | 0 |
| 53 | MG | DB | 3062 | 1/1 | 0.99 | 0.04 | 43,43,43,43 | 0 |
| 53 | MG | DB | 3063 | 1/1 | 0.99 | 0.03 | 21,21,21,21 | 0 |
| 53 | MG | BB | 3098 | 1/1 | 0.99 | 0.02 | 43,43,43,43 | 0 |
| 53 | MG | BB | 3026 | 1/1 | 0.99 | 0.04 | 24,24,24,24 | 0 |
| 53 | MG | DB | 3071 | 1/1 | 0.99 | 0.03 | 34,34,34,34 | 0 |
| 53 | MG | DB | 3072 | 1/1 | 0.99 | 0.04 | 25,25,25,25 | 0 |
| 53 | MG | BB | 3027 | 1/1 | 0.99 | 0.05 | 24,24,24,24 | 0 |
| 53 | MG | BB | 3103 | 1/1 | 0.99 | 0.07 | 5,5,5,5 | 0 |
| 53 | MG | BB | 3104 | 1/1 | 0.99 | 0.03 | 18,18,18,18 | 0 |
| 53 | MG | DB | 3079 | 1/1 | 0.99 | 0.04 | 43,43,43,43 | 0 |
| 53 | MG | BB | 3105 | 1/1 | 0.99 | 0.03 | 34,34,34,34 | 0 |
| 53 | MG | BB | 3028 | 1/1 | 0.99 | 0.05 | 16,16,16,16 | 0 |
| 53 | MG | BB | 3107 | 1/1 | 0.99 | 0.04 | 41,41,41,41 | 0 |
| 53 | MG | BB | 3030 | 1/1 | 0.99 | 0.05 | 53,53,53,53 | 0 |
| 53 | MG | DB | 3086 | 1/1 | 0.99 | 0.06 | 24,24,24,24 | 0 |
| 53 | MG | CA | 2003 | 1/1 | 0.99 | 0.02 | 44,44,44,44 | 0 |
| 53 | MG | CA | 2004 | 1/1 | 0.99 | 0.10 | 13,13,13,13 | 0 |
| 53 | MG | BB | 3031 | 1/1 | 0.99 | 0.07 | 32,32,32,32 | 0 |
| 53 | MG | CA | 2007 | 1/1 | 0.99 | 0.04 | 47,47,47,47 | 0 |
| 53 | MG | AA | 2048 | 1/1 | 0.99 | 0.03 | 48,48,48,48 | 0 |
| 53 | MG | DB | 3097 | 1/1 | 0.99 | 0.05 | 42,42,42,42 | 0 |
| 53 | MG | DB | 3099 | 1/1 | 0.99 | 0.04 | 5,5,5,5 | 0 |
| 53 | MG | CA | 2009 | 1/1 | 0.99 | 0.04 | 84,84,84,84 | 0 |
| 53 | MG | AA | 2018 | 1/1 | 0.99 | 0.04 | 76,76,76,76 | 0 |
| 53 | MG | DB | 3107 | 1/1 | 0.99 | 0.04 | 15,15,15,15 | 0 |
| 53 | MG | DB | 3108 | 1/1 | 0.99 | 0.06 | 5,5,5,5 | 0 |
| 53 | MG | AA | 2013 | 1/1 | 0.99 | 0.03 | 70,70,70,70 | 0 |
| 53 | MG | CA | 2012 | 1/1 | 0.99 | 0.04 | 49,49,49,49 | 0 |
| 53 | MG | BB | 3035 | 1/1 | 0.99 | 0.03 | 35,35,35,35 | 0 |
| 53 | MG | BB | 3036 | 1/1 | 0.99 | 0.05 | 57,57,57,57 | 0 |
| 53 | MG | BB | 3037 | 1/1 | 0.99 | 0.03 | 29,29,29,29 | 0 |
| 53 | MG | AA | 2006 | 1/1 | 0.99 | 0.03 | 57,57,57,57 | 0 |
| 53 | MG | BB | 3039 | 1/1 | 0.99 | 0.04 | 35,35,35,35 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 53 | MG | BB | 3040 | 1/1 | 0.99 | 0.07 | 40,40,40,40 | 0 |
| 53 | MG | AA | 2053 | 1/1 | 0.99 | 0.04 | 58,58,58,58 | 0 |
| 53 | MG | AA | 2054 | 1/1 | 0.99 | 0.03 | 66,66,66,66 | 0 |
| 53 | MG | BB | 3044 | 1/1 | 0.99 | 0.03 | 55,55,55,55 | 0 |
| 53 | MG | CA | 2024 | 1/1 | 1.00 | 0.06 | 23,23,23,23 | 0 |
| 53 | MG | BB | 3062 | 1/1 | 1.00 | 0.03 | 29,29,29,29 | 0 |
| 53 | MG | BB | 3025 | 1/1 | 1.00 | 0.02 | 51,51,51,51 | 0 |
| 53 | MG | BB | 3041 | 1/1 | 1.00 | 0.02 | 18,18,18,18 | 0 |
| 53 | MG | BB | 3012 | 1/1 | 1.00 | 0.04 | 31,31,31,31 | 0 |
| 53 | MG | BB | 3066 | 1/1 | 1.00 | 0.03 | 37,37,37,37 | 0 |
| 53 | MG | AA | 2010 | 1/1 | 1.00 | 0.04 | 45,45,45,45 | 0 |
| 53 | MG | AA | 2003 | 1/1 | 1.00 | 0.02 | 29,29,29,29 | 0 |
| 53 | MG | CA | 2032 | 1/1 | 1.00 | 0.04 | 22,22,22,22 | 0 |
| 53 | MG | BB | 3069 | 1/1 | 1.00 | 0.07 | 5,5,5,5 | 0 |
| 53 | MG | BB | 3101 | 1/1 | 1.00 | 0.06 | 11,11,11,11 | 0 |
| 53 | MG | DB | 3037 | 1/1 | 1.00 | 0.07 | 5,5,5,5 | 0 |
| 53 | MG | DB | 3038 | 1/1 | 1.00 | 0.03 | 17,17,17,17 | 0 |
| 53 | MG | BB | 3102 | 1/1 | 1.00 | 0.01 | 16,16,16,16 | 0 |
| 53 | MG | DB | 3040 | 1/1 | 1.00 | 0.04 | 5,5,5,5 | 0 |
| 53 | MG | BB | 3070 | 1/1 | 1.00 | 0.01 | 24,24,24,24 | 0 |
| 53 | MG | BB | 3045 | 1/1 | 1.00 | 0.04 | 19,19,19,19 | 0 |
| 53 | MG | BB | 3046 | 1/1 | 1.00 | 0.02 | 50,50,50,50 | 0 |
| 53 | MG | CA | 2039 | 1/1 | 1.00 | 0.04 | 19,19,19,19 | 0 |
| 53 | MG | CA | 2040 | 1/1 | 1.00 | 0.03 | 12,12,12,12 | 0 |
| 53 | MG | DB | 3046 | 1/1 | 1.00 | 0.02 | 5,5,5,5 | 0 |
| 53 | MG | DB | 3047 | 1/1 | 1.00 | 0.04 | 5,5,5,5 | 0 |
| 53 | MG | BB | 3029 | 1/1 | 1.00 | 0.03 | 5,5,5,5 | 0 |
| 53 | MG | DB | 3049 | 1/1 | 1.00 | 0.05 | 5,5,5,5 | 0 |
| 53 | MG | BB | 3074 | 1/1 | 1.00 | 0.03 | 9,9,9,9 | 0 |
| 53 | MG | BB | 3108 | 1/1 | 1.00 | 0.02 | 12,12,12,12 | 0 |
| 53 | MG | BB | 3109 | 1/1 | 1.00 | 0.03 | 37,37,37,37 | 0 |
| 53 | MG | BB | 3048 | 1/1 | 1.00 | 0.03 | 22,22,22,22 | 0 |
| 53 | MG | DB | 3054 | 1/1 | 1.00 | 0.05 | 13,13,13,13 | 0 |
| 53 | MG | DB | 3055 | 1/1 | 1.00 | 0.10 | 11,11,11,11 | 0 |
| 53 | MG | DB | 3056 | 1/1 | 1.00 | 0.01 | 5,5,5,5 | 0 |
| 53 | MG | CA | 2001 | 1/1 | 1.00 | 0.06 | 5,5,5,5 | 0 |
| 53 | MG | CA | 2002 | 1/1 | 1.00 | 0.02 | 27,27,27,27 | 0 |
| 53 | MG | BB | 3049 | 1/1 | 1.00 | 0.02 | 20,20,20,20 | 0 |
| 53 | MG | BB | 3015 | 1/1 | 1.00 | 0.08 | 5,5,5,5 | 0 |
| 53 | MG | CA | 2050 | 1/1 | 1.00 | 0.01 | 5,5,5,5 | 0 |
| 53 | MG | CA | 2005 | 1/1 | 1.00 | 0.02 | 10,10,10,10 | 0 |
| 53 | MG | BB | 3005 | 1/1 | 1.00 | 0.01 | 5,5,5,5 | 0 |

Continued on next page...

Continued from previous page...

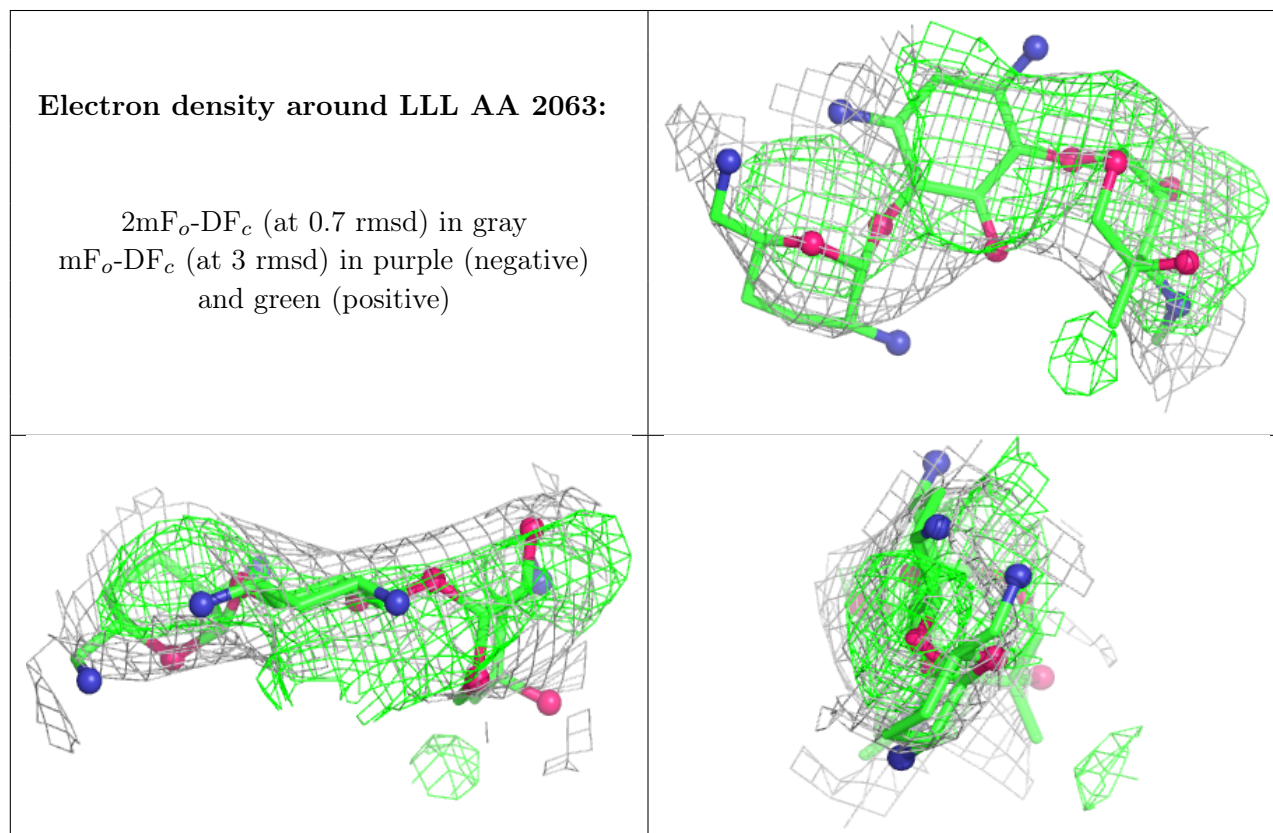
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 53 | MG | DB | 3064 | 1/1 | 1.00 | 0.09 | 11,11,11,11 | 0 |
| 53 | MG | DB | 3065 | 1/1 | 1.00 | 0.13 | 16,16,16,16 | 0 |
| 53 | MG | CA | 2053 | 1/1 | 1.00 | 0.07 | 51,51,51,51 | 0 |
| 53 | MG | DB | 3067 | 1/1 | 1.00 | 0.03 | 5,5,5,5 | 0 |
| 53 | MG | DB | 3068 | 1/1 | 1.00 | 0.03 | 5,5,5,5 | 0 |
| 53 | MG | DB | 3069 | 1/1 | 1.00 | 0.03 | 21,21,21,21 | 0 |
| 53 | MG | BB | 3017 | 1/1 | 1.00 | 0.05 | 16,16,16,16 | 0 |
| 53 | MG | CA | 2055 | 1/1 | 1.00 | 0.02 | 31,31,31,31 | 0 |
| 53 | MG | BB | 3018 | 1/1 | 1.00 | 0.07 | 54,54,54,54 | 0 |
| 53 | MG | BB | 3006 | 1/1 | 1.00 | 0.01 | 19,19,19,19 | 0 |
| 53 | MG | DB | 3074 | 1/1 | 1.00 | 0.02 | 5,5,5,5 | 0 |
| 53 | MG | DB | 3075 | 1/1 | 1.00 | 0.03 | 41,41,41,41 | 0 |
| 53 | MG | DB | 3076 | 1/1 | 1.00 | 0.02 | 43,43,43,43 | 0 |
| 53 | MG | BB | 3082 | 1/1 | 1.00 | 0.04 | 5,5,5,5 | 0 |
| 53 | MG | BB | 3083 | 1/1 | 1.00 | 0.05 | 33,33,33,33 | 0 |
| 53 | MG | AA | 2009 | 1/1 | 1.00 | 0.03 | 27,27,27,27 | 0 |
| 53 | MG | DB | 3080 | 1/1 | 1.00 | 0.02 | 5,5,5,5 | 0 |
| 53 | MG | DB | 3081 | 1/1 | 1.00 | 0.03 | 5,5,5,5 | 0 |
| 53 | MG | CA | 2061 | 1/1 | 1.00 | 0.03 | 25,25,25,25 | 0 |
| 53 | MG | CA | 2013 | 1/1 | 1.00 | 0.03 | 48,48,48,48 | 0 |
| 53 | MG | BB | 3085 | 1/1 | 1.00 | 0.03 | 59,59,59,59 | 0 |
| 53 | MG | DB | 3002 | 1/1 | 1.00 | 0.01 | 12,12,12,12 | 0 |
| 53 | MG | BB | 3086 | 1/1 | 1.00 | 0.03 | 5,5,5,5 | 0 |
| 53 | MG | DB | 3087 | 1/1 | 1.00 | 0.06 | 63,63,63,63 | 0 |
| 53 | MG | DB | 3088 | 1/1 | 1.00 | 0.07 | 18,18,18,18 | 0 |
| 53 | MG | CA | 2016 | 1/1 | 1.00 | 0.04 | 10,10,10,10 | 0 |
| 53 | MG | DB | 3005 | 1/1 | 1.00 | 0.04 | 6,6,6,6 | 0 |
| 53 | MG | DB | 3006 | 1/1 | 1.00 | 0.06 | 5,5,5,5 | 0 |
| 53 | MG | DB | 3007 | 1/1 | 1.00 | 0.05 | 18,18,18,18 | 0 |
| 53 | MG | DB | 3093 | 1/1 | 1.00 | 0.02 | 7,7,7,7 | 0 |
| 53 | MG | DB | 3094 | 1/1 | 1.00 | 0.06 | 14,14,14,14 | 0 |
| 53 | MG | DB | 3008 | 1/1 | 1.00 | 0.02 | 8,8,8,8 | 0 |
| 53 | MG | DB | 3096 | 1/1 | 1.00 | 0.05 | 5,5,5,5 | 0 |
| 53 | MG | DB | 3009 | 1/1 | 1.00 | 0.06 | 5,5,5,5 | 0 |
| 53 | MG | DB | 3098 | 1/1 | 1.00 | 0.07 | 23,23,23,23 | 0 |
| 53 | MG | DB | 3010 | 1/1 | 1.00 | 0.02 | 14,14,14,14 | 0 |
| 53 | MG | DB | 3100 | 1/1 | 1.00 | 0.02 | 5,5,5,5 | 0 |
| 53 | MG | DB | 3101 | 1/1 | 1.00 | 0.07 | 26,26,26,26 | 0 |
| 53 | MG | DB | 3102 | 1/1 | 1.00 | 0.01 | 16,16,16,16 | 0 |
| 53 | MG | DB | 3103 | 1/1 | 1.00 | 0.03 | 7,7,7,7 | 0 |
| 53 | MG | CA | 2017 | 1/1 | 1.00 | 0.10 | 5,5,5,5 | 0 |
| 53 | MG | DB | 3105 | 1/1 | 1.00 | 0.02 | 30,30,30,30 | 0 |

Continued on next page...

Continued from previous page...

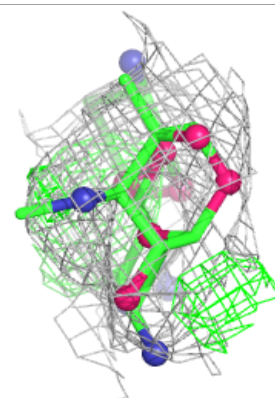
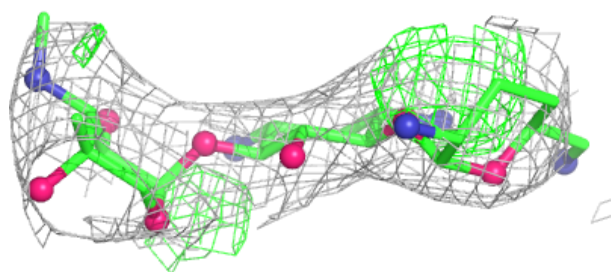
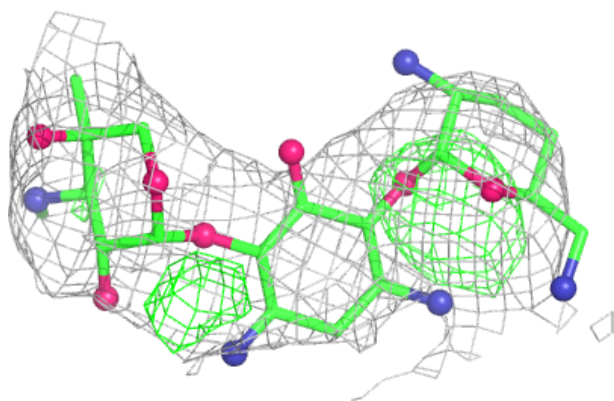
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 53 | MG | DB | 3012 | 1/1 | 1.00 | 0.01 | 14,14,14,14 | 0 |
| 53 | MG | BB | 3056 | 1/1 | 1.00 | 0.04 | 22,22,22,22 | 0 |
| 53 | MG | DB | 3014 | 1/1 | 1.00 | 0.07 | 13,13,13,13 | 0 |
| 53 | MG | DB | 3109 | 1/1 | 1.00 | 0.01 | 28,28,28,28 | 0 |
| 53 | MG | DB | 3110 | 1/1 | 1.00 | 0.08 | 29,29,29,29 | 0 |
| 53 | MG | AA | 2052 | 1/1 | 1.00 | 0.02 | 69,69,69,69 | 0 |
| 53 | MG | DB | 3016 | 1/1 | 1.00 | 0.05 | 17,17,17,17 | 0 |
| 53 | MG | DB | 3017 | 1/1 | 1.00 | 0.03 | 5,5,5,5 | 0 |
| 53 | MG | BB | 3001 | 1/1 | 1.00 | 0.12 | 8,8,8,8 | 0 |
| 53 | MG | DB | 3019 | 1/1 | 1.00 | 0.07 | 6,6,6,6 | 0 |
| 53 | MG | BB | 3002 | 1/1 | 1.00 | 0.04 | 5,5,5,5 | 0 |
| 53 | MG | DB | 3021 | 1/1 | 1.00 | 0.02 | 5,5,5,5 | 0 |
| 53 | MG | BB | 3060 | 1/1 | 1.00 | 0.05 | 59,59,59,59 | 0 |
| 53 | MG | DB | 3023 | 1/1 | 1.00 | 0.05 | 13,13,13,13 | 0 |
| 53 | MG | BB | 3011 | 1/1 | 1.00 | 0.04 | 21,21,21,21 | 0 |
| 53 | MG | DB | 3025 | 1/1 | 1.00 | 0.03 | 5,5,5,5 | 0 |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

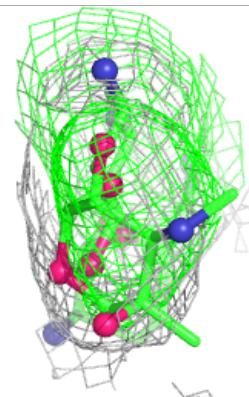
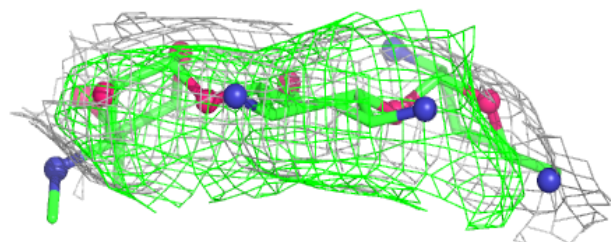
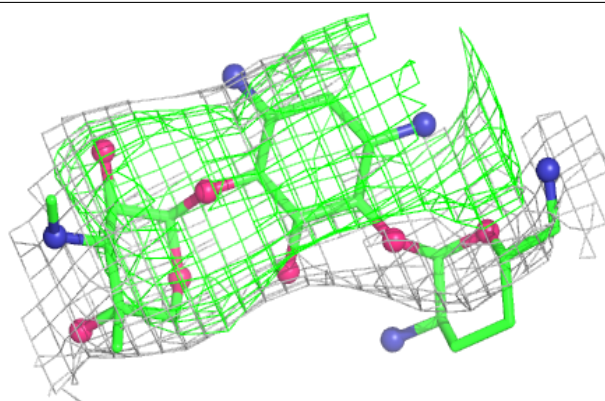


Electron density around LLL CA 2064:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

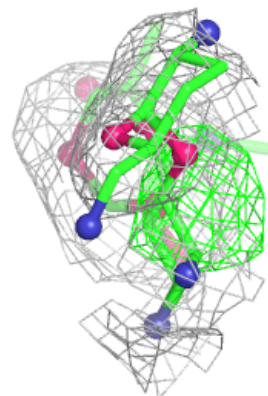
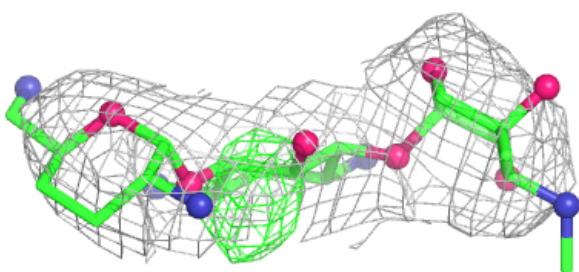
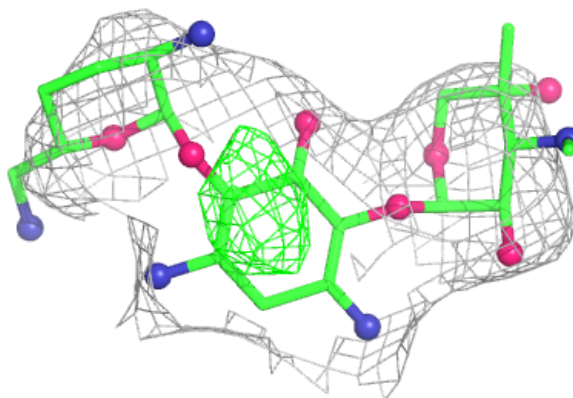
**Electron density around LLL AA 2062:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

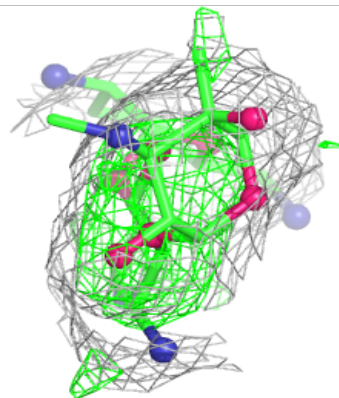
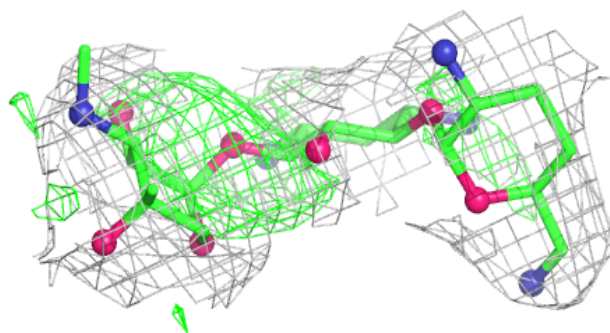
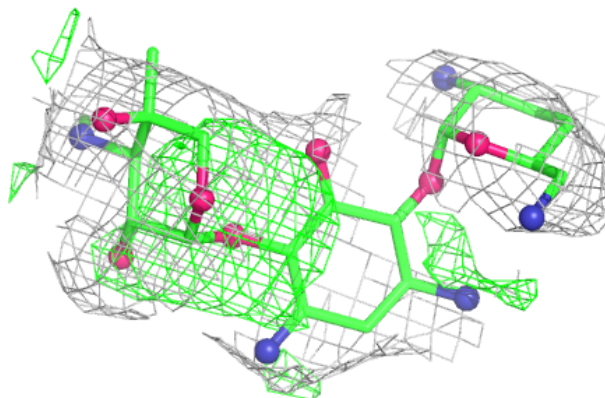


Electron density around LLL DB 3112:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

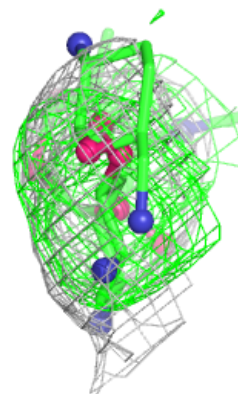
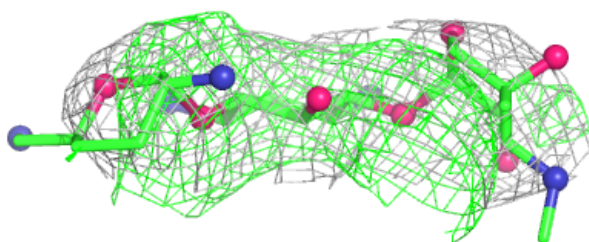
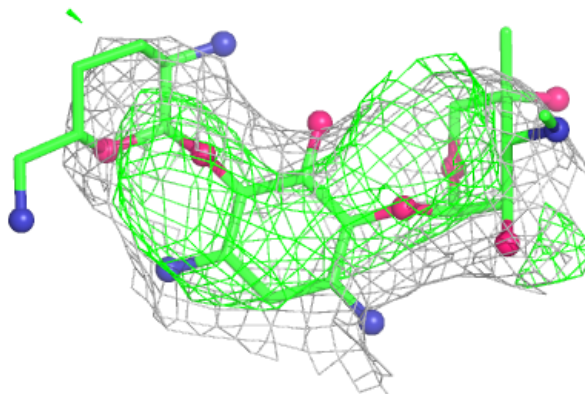
**Electron density around LLL CA 2063:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

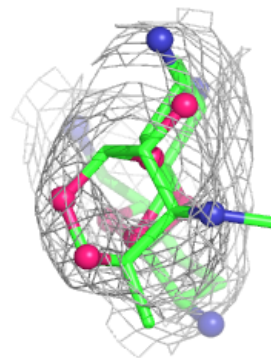
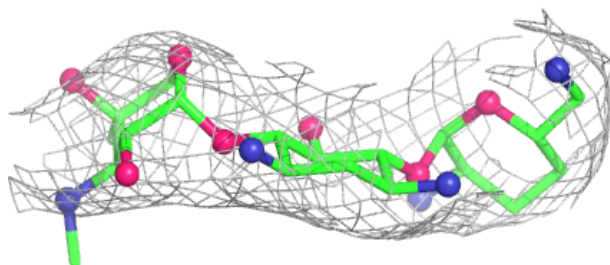
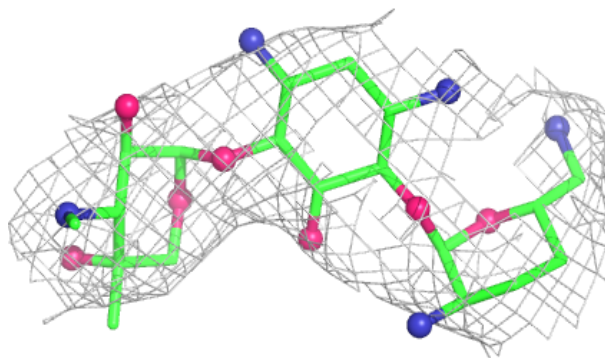


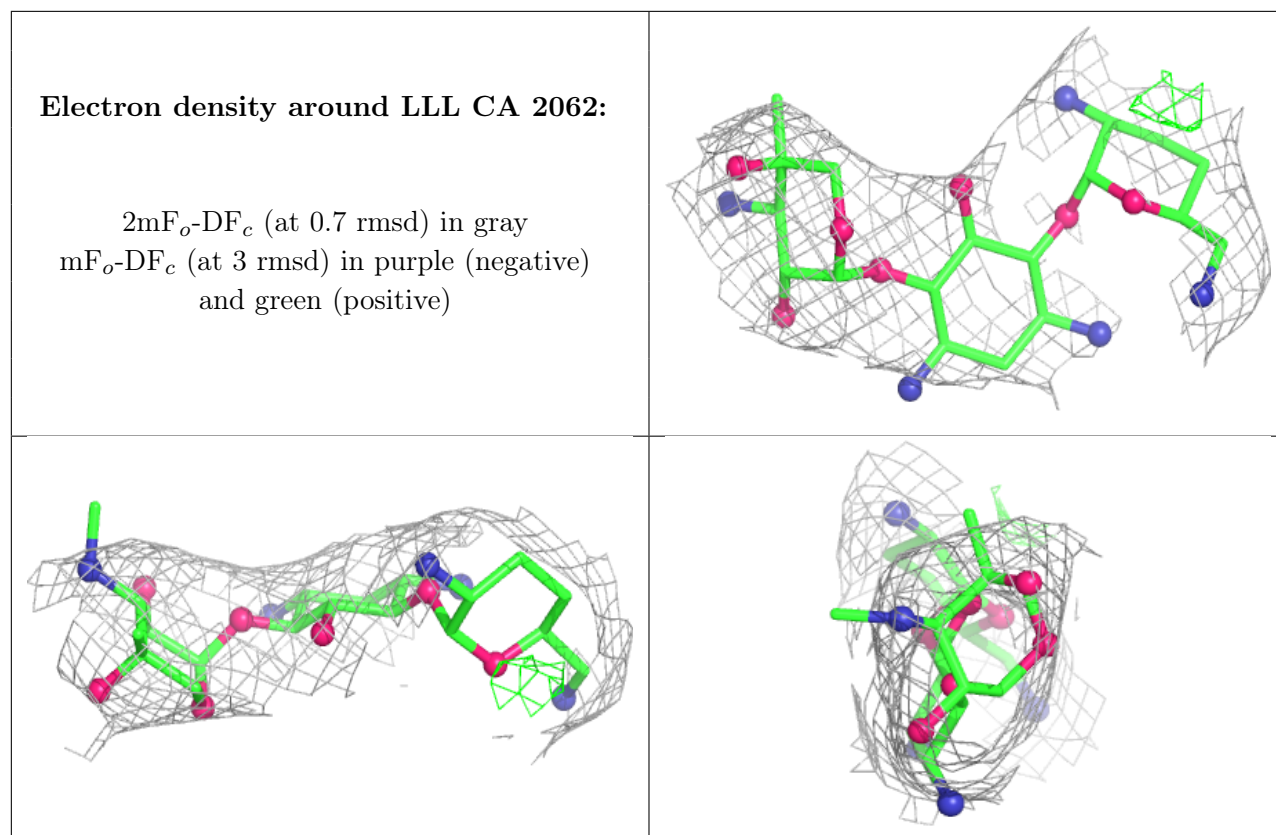
Electron density around LLL BB 3111:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around LLL AA 2061:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





5.5 Other polymers [i](#)

There are no such residues in this entry.