



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2025 – 01:46 PM EST

PDB ID : 4X66
Title : Crystal Structure of 30S ribosomal subunit from *Thermus thermophilus*
Authors : Demirci, H.; Chen, J.; Choi, J.; Soltis, M.; Puglisi, J.D.
Deposited on : 2014-12-06
Resolution : 3.45 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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.21
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

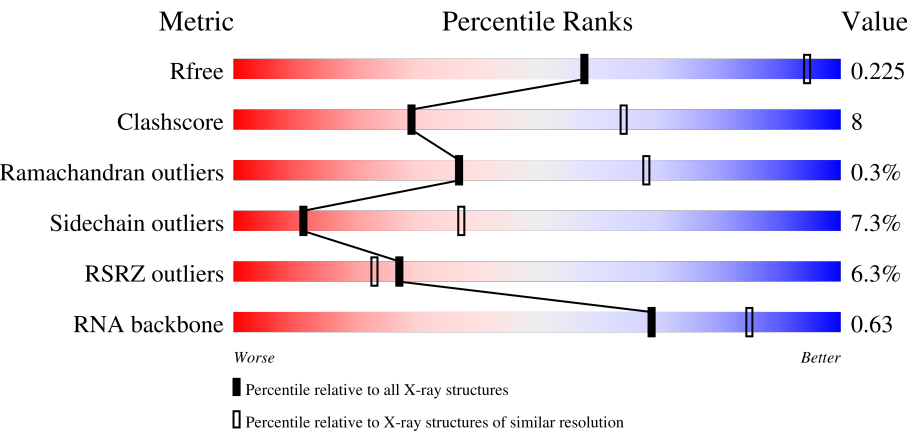
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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.





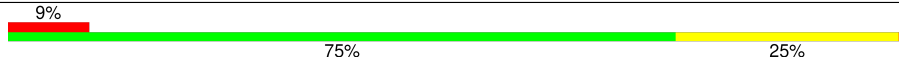
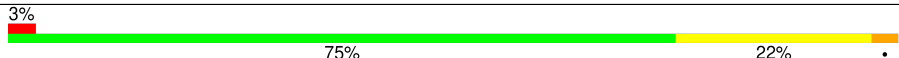
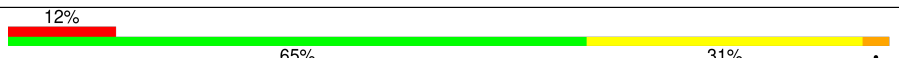
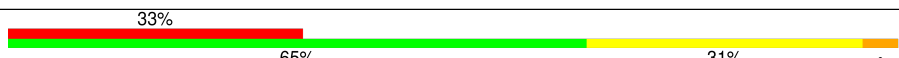
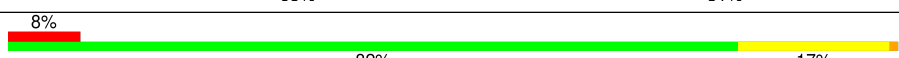
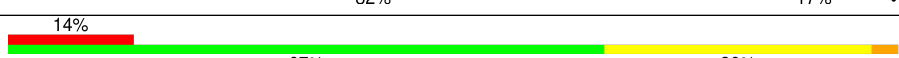
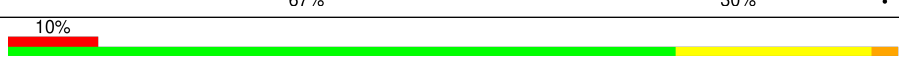

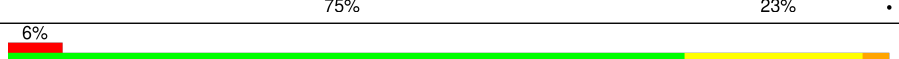
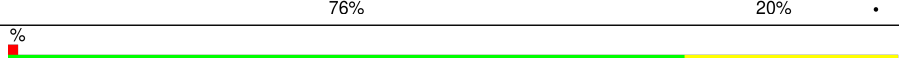

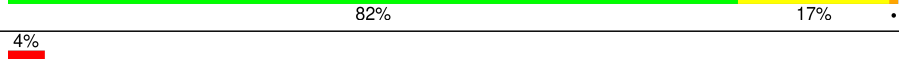
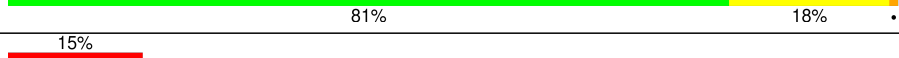

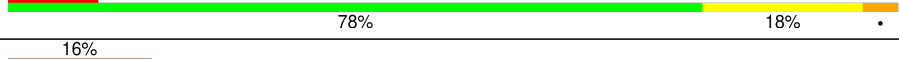

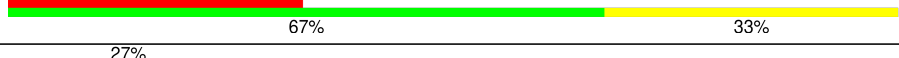
| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R _{free} | 164625 | 1587 (3.50-3.38) |
| Clashscore | 180529 | 1676 (3.50-3.38) |
| Ramachandran outliers | 177936 | 1665 (3.50-3.38) |
| Sidechain outliers | 177891 | 1666 (3.50-3.38) |
| RSRZ outliers | 164620 | 1587 (3.50-3.38) |
| RNA backbone | 3690 | 1044 (3.88-3.00) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 1522 | <div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>54%37%8%</div></div> |
| 2 | B | 236 | <div><div>8%</div><div><div></div><div></div><div></div><div></div></div><div>77%23%</div></div> |
| 3 | C | 207 | <div><div>8%</div><div><div></div><div></div><div></div><div></div></div><div>77%21%</div></div> |
| 4 | D | 208 | <div><div>9%</div><div><div></div><div></div><div></div><div></div></div><div>80%18%</div></div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 5 | E | 151 |  |
| 6 | F | 101 |  |
| 7 | G | 155 |  |
| 8 | H | 138 |  |
| 9 | I | 127 |  |
| 10 | J | 99 |  |
| 11 | K | 119 |  |
| 12 | L | 125 |  |
| 13 | M | 118 |  |
| 14 | N | 60 |  |
| 15 | O | 88 |  |
| 16 | P | 84 |  |
| 17 | Q | 99 |  |
| 18 | R | 73 |  |
| 19 | S | 81 |  |
| 20 | T | 99 |  |
| 21 | U | 25 |  |
| 22 | a | 6 |  |
| 23 | b | 11 |  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 25 | MG | A | 1727 | - | - | - | X |
| 25 | MG | A | 1775 | - | - | - | X |
| 25 | MG | A | 1819 | - | - | - | X |
| 25 | MG | A | 1828 | - | - | - | X |
| 25 | MG | A | 1830 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 26 | K | A | 1897 | - | - | - | X |
| 26 | K | A | 1904 | - | - | - | X |
| 26 | K | G | 202 | - | - | - | X |

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 52822 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 |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1 | A | 1512 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32504 | 14477 | 6011 | 10505 | 1511 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|-------------|
| A | 1534 | C | A | conflict | GB 55771382 |
| A | 1535 | A | C | conflict | GB 55771382 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | B | 236 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1874 | 1195 | 336 | 338 | 5 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | C | 207 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1613 | 1016 | 315 | 281 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4 | D | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1703 | 1066 | 339 | 291 | 7 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | E | 151 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1147 | 724 | 218 | 201 | 4 | | | |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | G | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1257 | 781 | 252 | 218 | 6 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | H | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1116 | 705 | 215 | 193 | 3 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 9 | I | 127 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1010 | 639 | 197 | 174 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | J | 99 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 793 | 498 | 157 | 137 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | K | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 885 | 549 | 168 | 165 | 3 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | L | 125 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 973 | 612 | 196 | 163 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | M | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 937 | 579 | 193 | 163 | 2 | | | |

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | P | 84 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 701 | 443 | 140 | 117 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17 | Q | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 823 | 528 | 151 | 142 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 18 | R | 73 | Total | C | N | O | 0 | 0 | 0 |
| | | | 598 | 381 | 118 | 99 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | S | 81 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 648 | 414 | 120 | 112 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | T | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 763 | 470 | 162 | 129 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 21 | U | 25 | Total | C | N | O | 0 | 0 | 1 |
| | | | 209 | 128 | 51 | 30 | | | |

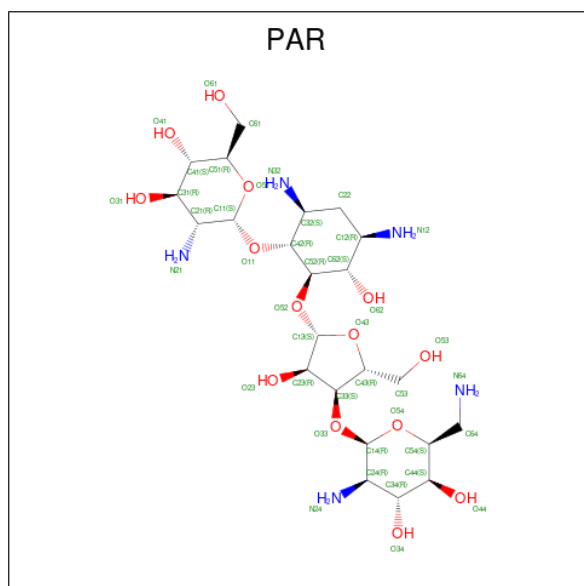
- Molecule 22 is a RNA chain called RNA (5'-D(*AP*AP*(MA6)P*UP*UP*U)-3').

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 22 | a | 6 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 124 | 58 | 21 | 40 | 5 | | | |

- Molecule 23 is a RNA chain called RNA (5'-D(P*GP*AP*CP*UP*(70U)P*UP*UP*(12A)P*AP*(PSU)P*C)-3').

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---|---------|---------|-------|
| 23 | b | 11 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 247 | 112 | 37 | 85 | 11 | 2 | | | |

- Molecule 24 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---------|---------|
| 24 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---------|---------|
| 24 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 24 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 24 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 24 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 24 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |

- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 25 | A | 280 | Total | Mg | 0 | 0 |
| | | | 280 | 280 | | |
| 25 | C | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 25 | D | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 25 | E | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 25 | F | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 25 | G | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 25 | H | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 25 | L | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 25 | P | 4 | Total | Mg | 0 | 0 |
| | | | 4 | 4 | | |
| 25 | Q | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 25 | S | 3 | Total | Mg | 0 | 0 |
| | | | 3 | 3 | | |
| 25 | T | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 25 | a | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 25 | b | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 26 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 26 | A | 44 | Total K 44 44 | 0 | 0 |
| 26 | E | 1 | Total K 1 1 | 0 | 0 |
| 26 | G | 1 | Total K 1 1 | 0 | 0 |

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 27 | D | 1 | Total Zn 1 1 | 0 | 0 |
| 27 | N | 1 | Total Zn 1 1 | 0 | 0 |

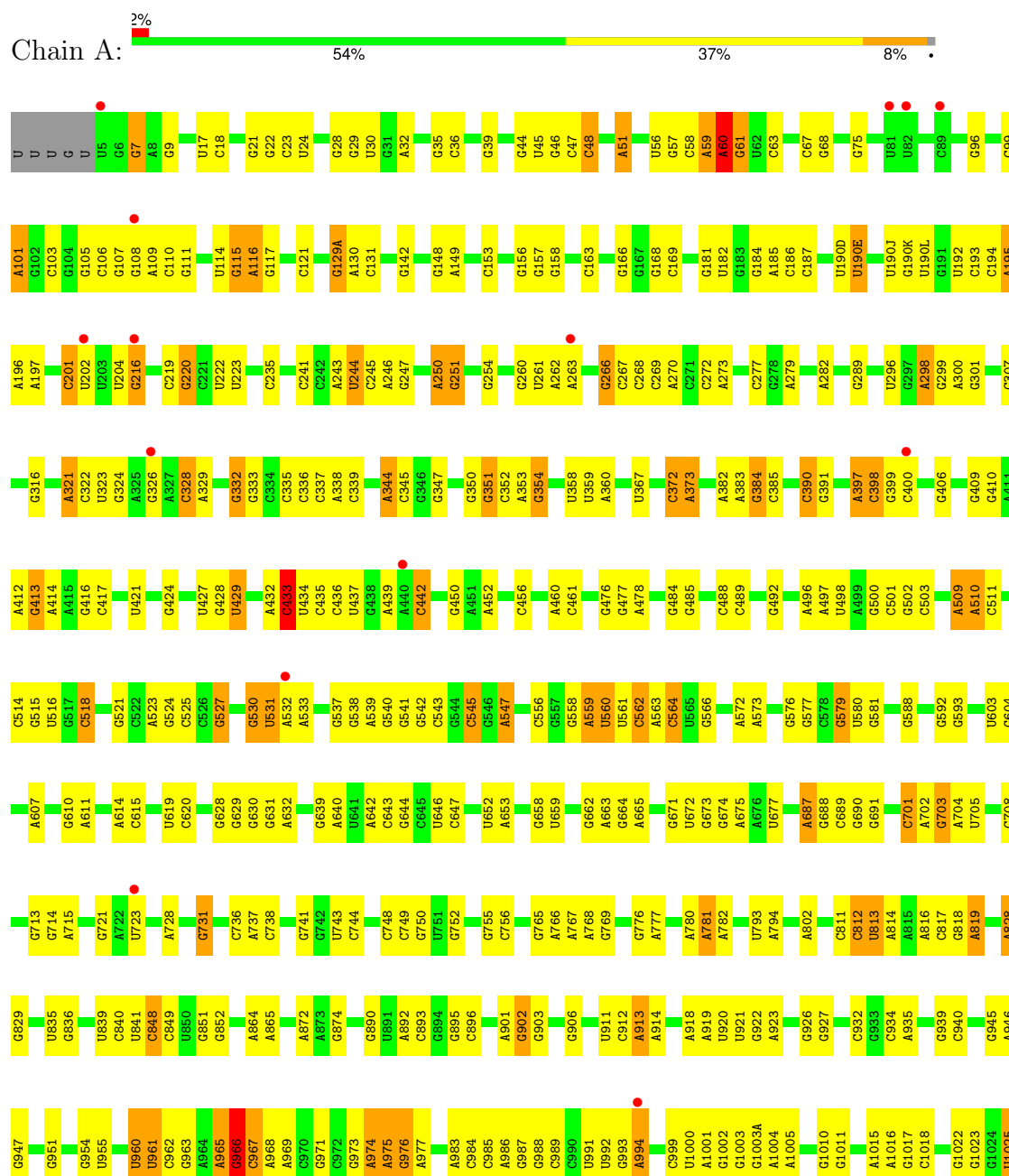
- Molecule 28 is water.

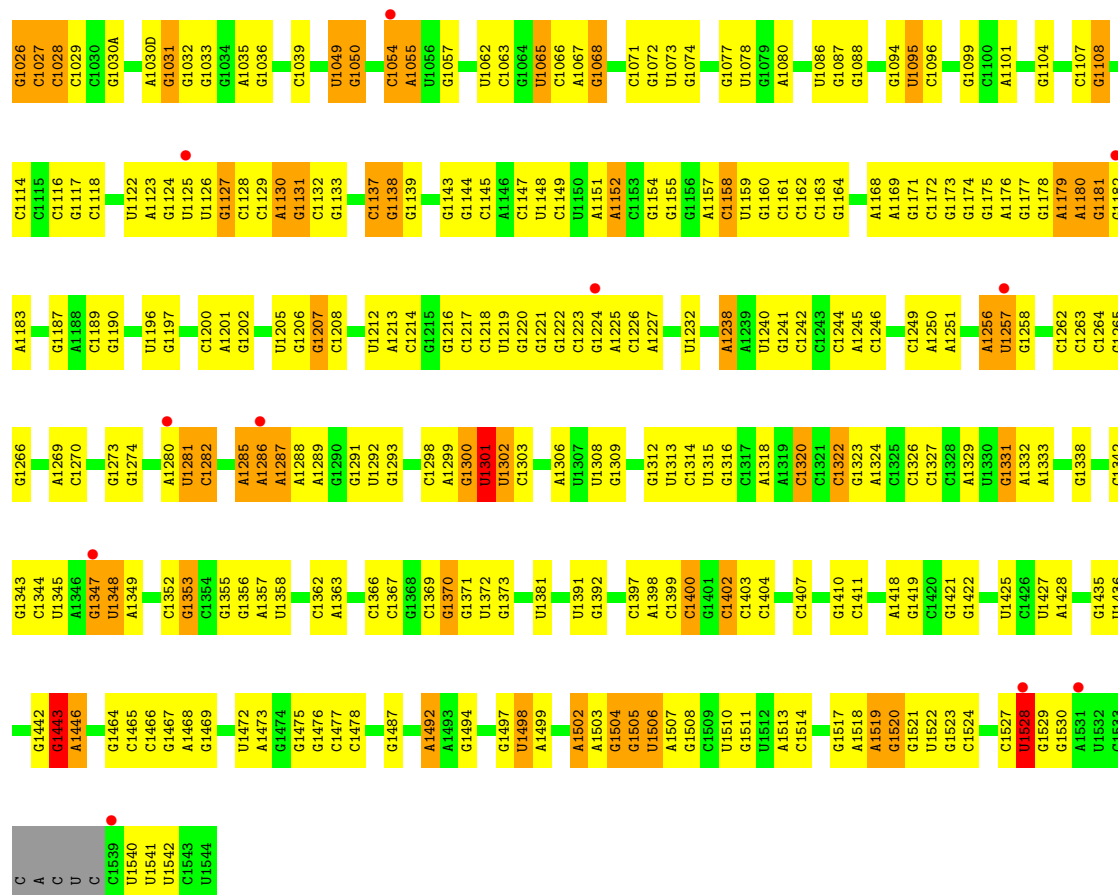
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 28 | A | 212 | Total O 212 212 | 0 | 0 |
| 28 | D | 2 | Total O 2 2 | 0 | 0 |
| 28 | E | 5 | Total O 5 5 | 0 | 0 |
| 28 | K | 1 | Total O 1 1 | 0 | 0 |
| 28 | L | 4 | Total O 4 4 | 0 | 0 |
| 28 | O | 1 | Total O 1 1 | 0 | 0 |
| 28 | T | 1 | Total O 1 1 | 0 | 0 |
| 28 | a | 1 | Total O 1 1 | 0 | 0 |

3 Residue-property plots

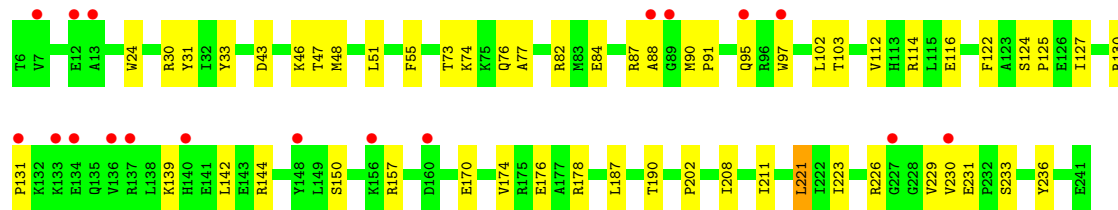
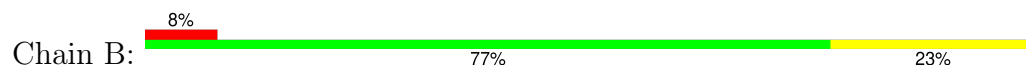
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 16S rRNA

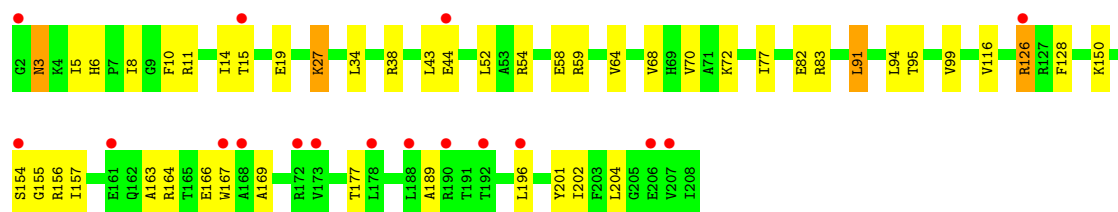
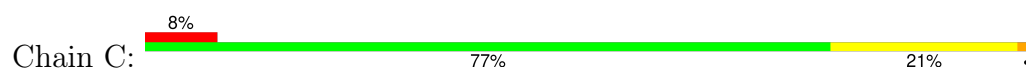




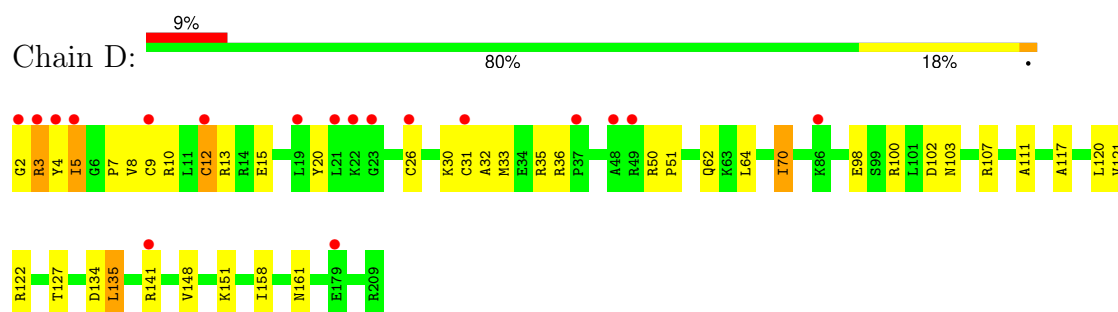
• Molecule 2: 30S ribosomal protein S2



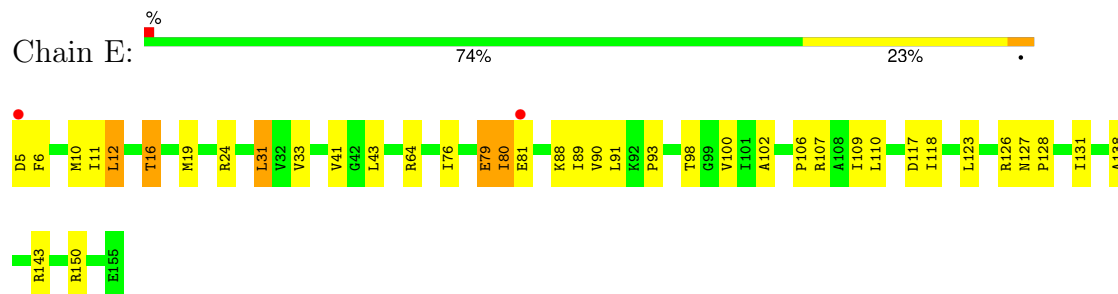
• Molecule 3: 30S ribosomal protein S3



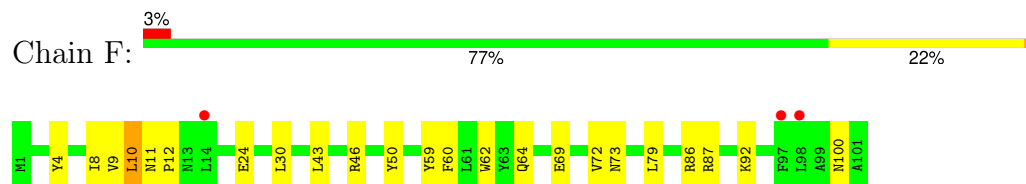
• Molecule 4: 30S ribosomal protein S4



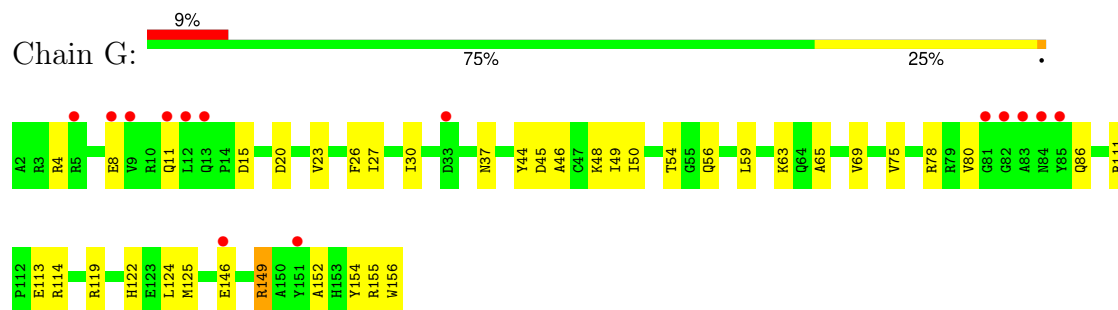
- Molecule 5: 30S ribosomal protein S5



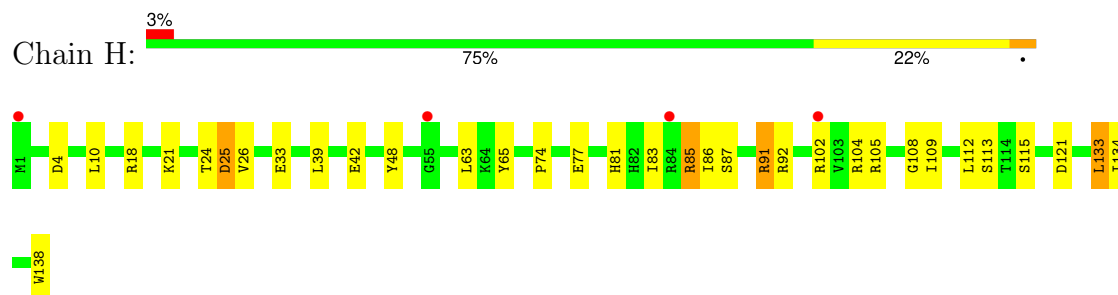
- Molecule 6: 30S ribosomal protein S6



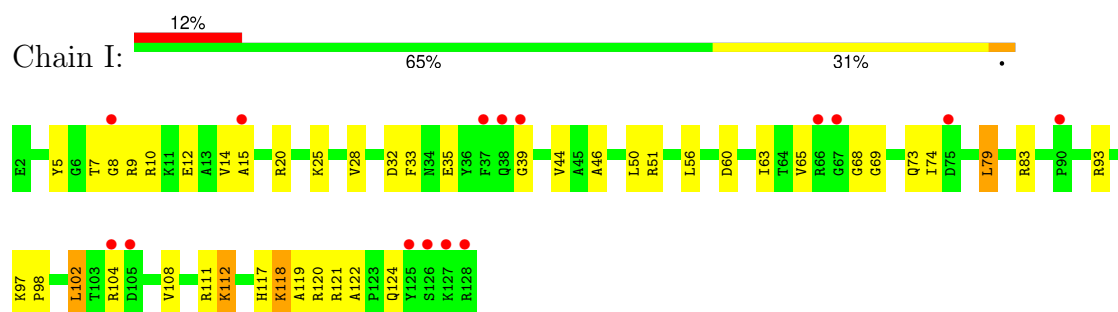
- Molecule 7: 30S ribosomal protein S7



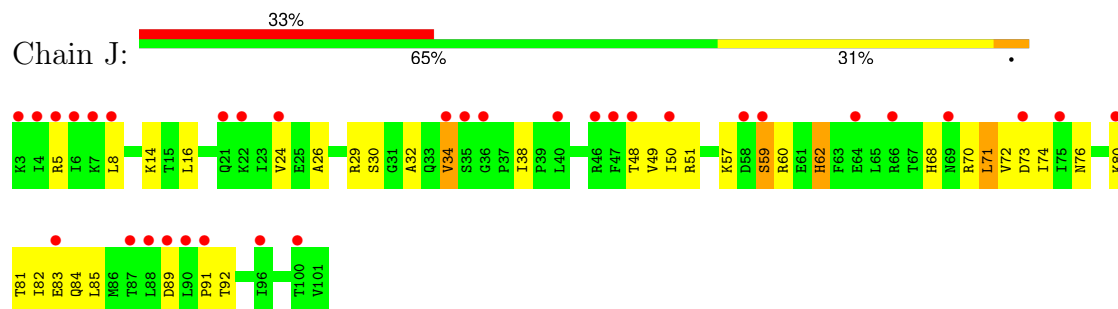
- Molecule 8: 30S ribosomal protein S8



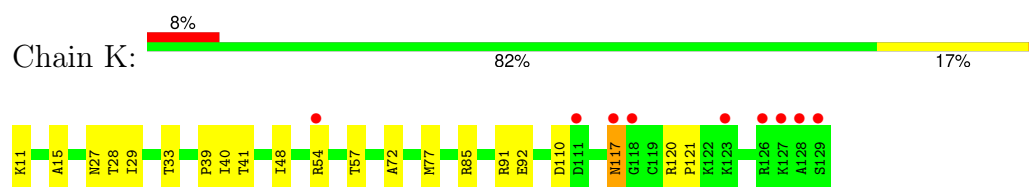
- Molecule 9: 30S ribosomal protein S9



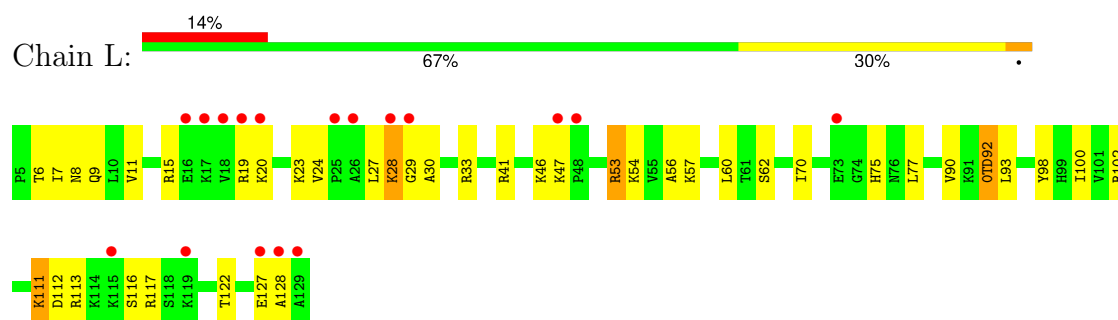
- Molecule 10: 30S ribosomal protein S10



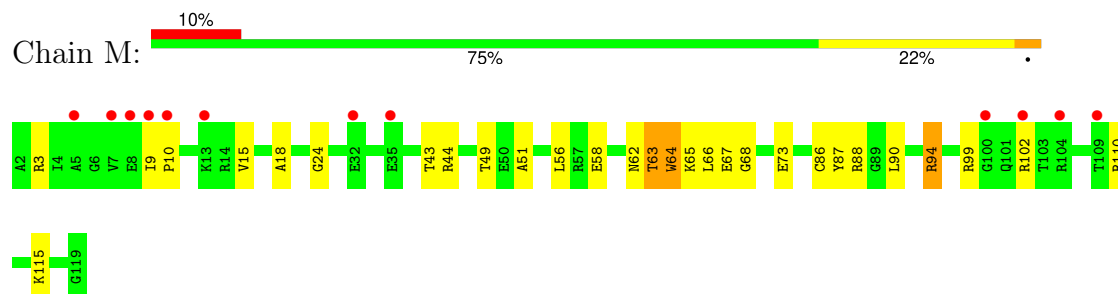
- Molecule 11: 30S ribosomal protein S11



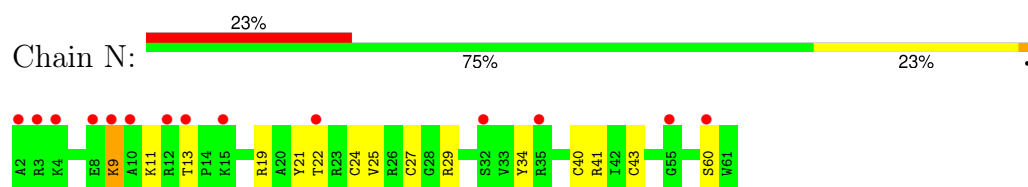
- Molecule 12: 30S ribosomal protein S12



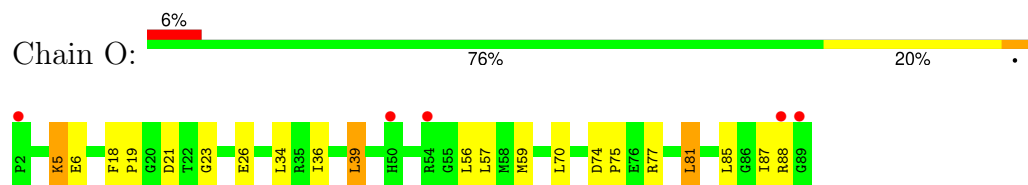
- Molecule 13: 30S ribosomal protein S13



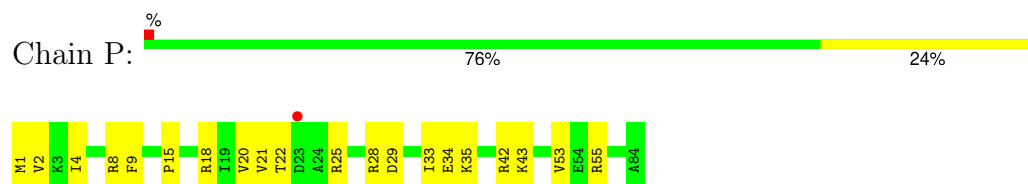
- Molecule 14: 30S ribosomal protein S14 type Z



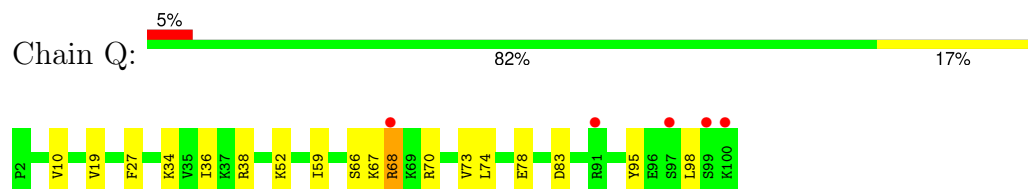
- Molecule 15: 30S ribosomal protein S15



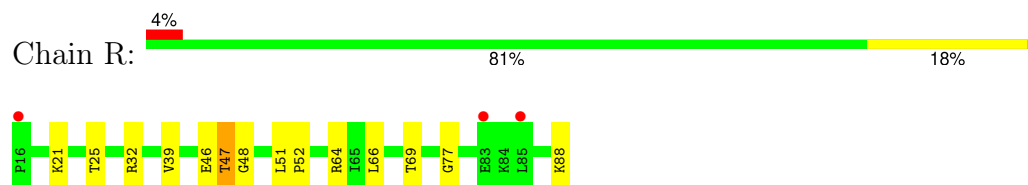
- Molecule 16: 30S ribosomal protein S16



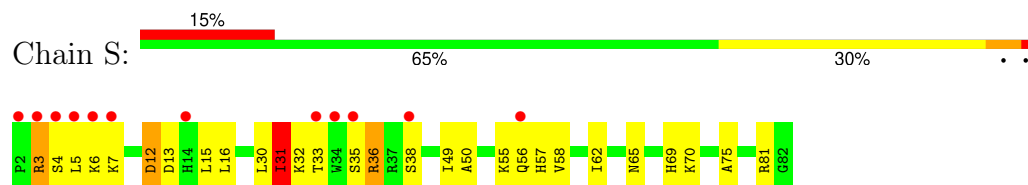
- Molecule 17: 30S ribosomal protein S17



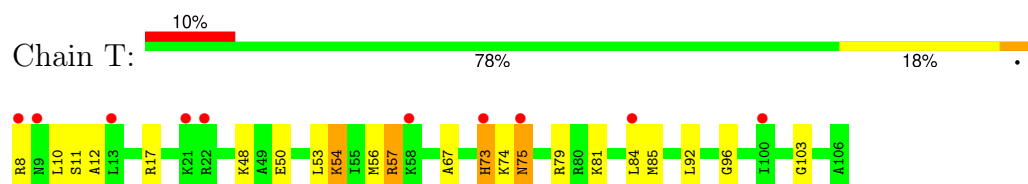
- Molecule 18: 30S ribosomal protein S18



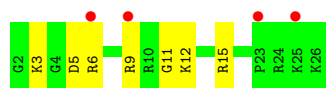
- Molecule 19: 30S ribosomal protein S19



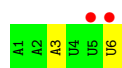
- Molecule 20: 30S ribosomal protein S20



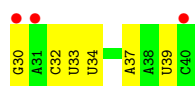
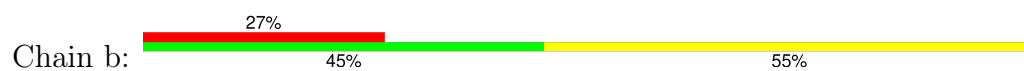
- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: RNA (5'-D(*AP*AP*(MA6)P*UP*UP*U)-3')



- Molecule 23: RNA (5'-D(P*GP*AP*CP*UP*(70U)P*UP*UP*(12A)P*AP*(PSU)P*C)-3')



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 41 21 2 | Depositor |
| Cell constants a, b, c, α , β , γ | 401.32Å 401.32Å 175.65Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 49.78 – 3.45 49.78 – 3.45 | Depositor EDS |
| % Data completeness (in resolution range) | 96.4 (49.78-3.45) 90.7 (49.78-3.45) | Depositor EDS |
| R_{merge} | 0.19 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.58 (at 3.48Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: dev_1938) | Depositor |
| R, R_{free} | 0.194 , 0.227 0.194 , 0.225 | Depositor DCC |
| R_{free} test set | 9121 reflections (5.05%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 82.3 | Xtriage |
| Anisotropy | 0.114 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.26 , 68.7 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.92 | EDS |
| Total number of atoms | 52822 | wwPDB-VP |
| Average B, all atoms (Å ²) | 91.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% 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.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: M2G, PSU, PAR, 4OC, MG, 5MC, 70U, 6MZ, 7MG, 0TD, K, ZN, 12A, MA6, 2MG, UR3

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|-----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | A | 0.48 | 0/36037 | 0.83 | 13/56239 (0.0%) |
| 2 | B | 0.25 | 0/1909 | 0.40 | 0/2579 |
| 3 | C | 0.28 | 0/1637 | 0.43 | 0/2207 |
| 4 | D | 0.31 | 0/1733 | 0.45 | 1/2318 (0.0%) |
| 5 | E | 0.33 | 0/1163 | 0.50 | 0/1566 |
| 6 | F | 0.25 | 0/856 | 0.40 | 0/1154 |
| 7 | G | 0.27 | 0/1276 | 0.43 | 0/1709 |
| 8 | H | 0.36 | 0/1136 | 0.44 | 0/1527 |
| 9 | I | 0.27 | 0/1029 | 0.44 | 0/1379 |
| 10 | J | 0.27 | 0/806 | 0.48 | 0/1084 |
| 11 | K | 0.32 | 0/900 | 0.47 | 0/1213 |
| 12 | L | 0.33 | 0/978 | 0.50 | 0/1308 |
| 13 | M | 0.27 | 0/947 | 0.43 | 0/1270 |
| 14 | N | 0.31 | 0/501 | 0.41 | 0/664 |
| 15 | O | 0.26 | 0/745 | 0.41 | 0/992 |
| 16 | P | 0.34 | 0/717 | 0.46 | 0/965 |
| 17 | Q | 0.35 | 0/836 | 0.47 | 0/1117 |
| 18 | R | 0.28 | 0/604 | 0.41 | 0/801 |
| 19 | S | 0.25 | 0/662 | 0.49 | 0/892 |
| 20 | T | 0.29 | 0/765 | 0.50 | 0/1007 |
| 21 | U | 0.26 | 0/213 | 0.42 | 0/279 |
| 22 | a | 0.32 | 0/111 | 0.80 | 0/168 |
| 23 | b | 0.82 | 1/184 (0.5%) | 0.78 | 0/277 |
| All | All | 0.42 | 1/55745 (0.0%) | 0.73 | 14/82715 (0.0%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 23 | b | 30 | G | OP3-P | -10.52 | 1.48 | 1.61 |

All (14) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | A | 254 | G | O5'-P-OP1 | -7.51 | 98.94 | 105.70 |
| 1 | A | 1301 | U | P-O3'-C3' | 6.86 | 127.94 | 119.70 |
| 1 | A | 60 | A | P-O3'-C3' | 6.17 | 127.11 | 119.70 |
| 1 | A | 1528 | U | P-O3'-C3' | 5.93 | 126.82 | 119.70 |
| 1 | A | 328 | C | C2-N1-C1' | 5.61 | 124.97 | 118.80 |
| 4 | D | 12 | CYS | CA-CB-SG | 5.49 | 123.88 | 114.00 |
| 1 | A | 913 | A | P-O3'-C3' | 5.42 | 126.20 | 119.70 |
| 1 | A | 328 | C | P-O3'-C3' | 5.36 | 126.14 | 119.70 |
| 1 | A | 812 | C | P-O3'-C3' | 5.25 | 126.00 | 119.70 |
| 1 | A | 433 | C | C2-N1-C1' | 5.24 | 124.56 | 118.80 |
| 1 | A | 1285 | A | P-O3'-C3' | 5.09 | 125.81 | 119.70 |
| 1 | A | 1065 | U | P-O3'-C3' | 5.08 | 125.79 | 119.70 |
| 1 | A | 108 | G | O4'-C1'-N9 | 5.06 | 112.25 | 108.20 |
| 1 | A | 1443 | G | P-O3'-C3' | 5.03 | 125.73 | 119.70 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 32504 | 0 | 16434 | 455 | 0 |
| 2 | B | 1874 | 0 | 1887 | 29 | 0 |
| 3 | C | 1613 | 0 | 1677 | 33 | 0 |
| 4 | D | 1703 | 0 | 1763 | 25 | 0 |
| 5 | E | 1147 | 0 | 1207 | 25 | 0 |
| 6 | F | 843 | 0 | 857 | 10 | 0 |
| 7 | G | 1257 | 0 | 1296 | 20 | 0 |
| 8 | H | 1116 | 0 | 1177 | 22 | 0 |
| 9 | I | 1010 | 0 | 1037 | 34 | 0 |
| 10 | J | 793 | 0 | 835 | 25 | 0 |
| 11 | K | 885 | 0 | 904 | 10 | 0 |
| 12 | L | 973 | 0 | 1058 | 31 | 0 |
| 13 | M | 937 | 0 | 995 | 15 | 0 |
| 14 | N | 492 | 0 | 529 | 13 | 0 |
| 15 | O | 734 | 0 | 771 | 11 | 0 |
| 16 | P | 701 | 0 | 720 | 12 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 17 | Q | 823 | 0 | 891 | 12 | 0 |
| 18 | R | 598 | 0 | 670 | 9 | 0 |
| 19 | S | 648 | 0 | 672 | 18 | 0 |
| 20 | T | 763 | 0 | 861 | 12 | 0 |
| 21 | U | 209 | 0 | 221 | 5 | 0 |
| 22 | a | 124 | 0 | 67 | 0 | 0 |
| 23 | b | 247 | 0 | 129 | 0 | 0 |
| 24 | A | 252 | 0 | 270 | 13 | 0 |
| 25 | A | 280 | 0 | 0 | 0 | 0 |
| 25 | C | 1 | 0 | 0 | 0 | 0 |
| 25 | D | 1 | 0 | 0 | 0 | 0 |
| 25 | E | 1 | 0 | 0 | 0 | 0 |
| 25 | F | 1 | 0 | 0 | 0 | 0 |
| 25 | G | 1 | 0 | 0 | 0 | 0 |
| 25 | H | 2 | 0 | 0 | 0 | 0 |
| 25 | L | 2 | 0 | 0 | 0 | 0 |
| 25 | P | 4 | 0 | 0 | 0 | 0 |
| 25 | Q | 2 | 0 | 0 | 0 | 0 |
| 25 | S | 3 | 0 | 0 | 0 | 0 |
| 25 | T | 1 | 0 | 0 | 0 | 0 |
| 25 | a | 1 | 0 | 0 | 0 | 0 |
| 25 | b | 1 | 0 | 0 | 0 | 0 |
| 26 | A | 44 | 0 | 0 | 0 | 0 |
| 26 | E | 1 | 0 | 0 | 0 | 0 |
| 26 | G | 1 | 0 | 0 | 0 | 0 |
| 27 | D | 1 | 0 | 0 | 0 | 0 |
| 27 | N | 1 | 0 | 0 | 0 | 0 |
| 28 | A | 212 | 0 | 0 | 3 | 0 |
| 28 | D | 2 | 0 | 0 | 1 | 0 |
| 28 | E | 5 | 0 | 0 | 0 | 0 |
| 28 | K | 1 | 0 | 0 | 0 | 0 |
| 28 | L | 4 | 0 | 0 | 0 | 0 |
| 28 | O | 1 | 0 | 0 | 0 | 0 |
| 28 | T | 1 | 0 | 0 | 0 | 0 |
| 28 | a | 1 | 0 | 0 | 0 | 0 |
| All | All | 52822 | 0 | 36928 | 740 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (740) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1028:C:H42 | 1:A:1033:G:H1 | 1.13 | 0.96 |
| 1:A:153:C:H42 | 1:A:168:G:H1 | 1.20 | 0.89 |
| 1:A:235:C:H5' | 17:Q:70:ARG:HG2 | 1.53 | 0.88 |
| 1:A:48:C:OP1 | 24:A:1603:PAR:N12 | 2.07 | 0.87 |
| 1:A:664:G:H22 | 1:A:741:G:H1 | 1.22 | 0.86 |
| 1:A:1306:A:H61 | 1:A:1331:G:H1' | 1.39 | 0.85 |
| 11:K:15:ALA:HA | 11:K:77:MET:HA | 1.61 | 0.82 |
| 1:A:1422:G:N2 | 1:A:1478:C:N3 | 2.32 | 0.78 |
| 1:A:442:C:H42 | 1:A:492:G:H1 | 1.30 | 0.77 |
| 1:A:1391:U:H2' | 1:A:1392:G:C8 | 2.19 | 0.77 |
| 1:A:677:U:H3 | 1:A:713:G:H22 | 1.32 | 0.76 |
| 1:A:1028:C:N4 | 1:A:1033:G:H1 | 1.84 | 0.75 |
| 1:A:103:C:OP1 | 20:T:17:ARG:NH1 | 2.19 | 0.74 |
| 2:B:223:ILE:HD13 | 2:B:230:VAL:H | 1.52 | 0.74 |
| 20:T:10:LEU:HG | 20:T:12:ALA:H | 1.53 | 0.74 |
| 13:M:88:ARG:HH11 | 19:S:3:ARG:HH21 | 1.33 | 0.73 |
| 19:S:33:THR:HG22 | 19:S:35:SER:H | 1.50 | 0.73 |
| 1:A:951:G:OP2 | 13:M:102:ARG:NH2 | 2.22 | 0.73 |
| 1:A:537:G:OP1 | 12:L:113:ARG:NH2 | 2.21 | 0.72 |
| 1:A:975:A:H4' | 1:A:976:G:H5'' | 1.71 | 0.72 |
| 7:G:146:GLU:HA | 7:G:149:ARG:HG2 | 1.73 | 0.71 |
| 10:J:82:ILE:HA | 10:J:85:LEU:HB2 | 1.72 | 0.71 |
| 9:I:46:ALA:HB2 | 9:I:74:ILE:HG23 | 1.74 | 0.70 |
| 1:A:501:C:OP1 | 12:L:117:ARG:NH2 | 2.24 | 0.70 |
| 9:I:44:VAL:HG12 | 9:I:51:ARG:HH22 | 1.55 | 0.70 |
| 1:A:413:G:N2 | 1:A:429:U:OP2 | 2.24 | 0.70 |
| 1:A:409:G:H1 | 1:A:433:C:H42 | 1.40 | 0.69 |
| 10:J:8:LEU:HB2 | 10:J:70:ARG:HB2 | 1.75 | 0.69 |
| 3:C:14:ILE:HG22 | 3:C:15:THR:HG23 | 1.73 | 0.69 |
| 1:A:673:G:H2' | 1:A:674:G:C8 | 2.27 | 0.69 |
| 1:A:153:C:N4 | 1:A:168:G:H1 | 1.89 | 0.69 |
| 1:A:974:A:OP2 | 14:N:41:ARG:NH1 | 2.26 | 0.69 |
| 1:A:1502:A:H2 | 1:A:1505:G:H1 | 1.39 | 0.69 |
| 1:A:713:G:H2' | 1:A:714:G:C8 | 2.28 | 0.69 |
| 1:A:1162:C:H42 | 1:A:1174:G:H1 | 1.39 | 0.69 |
| 1:A:1435:G:H2' | 1:A:1436:U:C6 | 2.29 | 0.68 |
| 1:A:1391:U:H2' | 1:A:1392:G:H8 | 1.59 | 0.68 |
| 1:A:1249:C:O2' | 9:I:73:GLN:NE2 | 2.26 | 0.68 |
| 9:I:51:ARG:HG3 | 9:I:56:LEU:HD21 | 1.73 | 0.68 |
| 4:D:32:ALA:HA | 4:D:35:ARG:HG2 | 1.75 | 0.68 |
| 8:H:10:LEU:HD22 | 8:H:83:ILE:HD11 | 1.74 | 0.68 |
| 13:M:10:PRO:HB2 | 13:M:18:ALA:HB1 | 1.74 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-------------------|--------------------------|-------------------|
| 1:A:1004:A:OP1 | 1:A:1025:U:N3 | 2.25 | 0.68 |
| 1:A:1422:G:H1 | 1:A:1478:C:H42 | 1.40 | 0.67 |
| 4:D:102:ASP:OD1 | 4:D:103:ASN:N | 2.26 | 0.67 |
| 19:S:36:ARG:NH2 | 19:S:75:ALA:O | 2.28 | 0.66 |
| 1:A:1086:U:H3 | 1:A:1099:G:H22 | 1.42 | 0.66 |
| 3:C:156:ARG:H | 3:C:163:ALA:HA | 1.60 | 0.66 |
| 5:E:80:ILE:HD12 | 5:E:91:LEU:HB2 | 1.76 | 0.66 |
| 1:A:1306:A:N6 | 1:A:1331:G:H1' | 2.08 | 0.66 |
| 1:A:60:A:H4' | 1:A:61:G:O5' | 1.96 | 0.66 |
| 3:C:64:VAL:HB | 3:C:99:VAL:HG21 | 1.78 | 0.65 |
| 1:A:1200:C:O2' | 1:A:1205:U:O4 | 2.13 | 0.65 |
| 1:A:1427:U:H2' | 1:A:1428:A:H8 | 1.61 | 0.65 |
| 4:D:7:PRO:HB2 | 4:D:10:ARG:HD2 | 1.78 | 0.65 |
| 1:A:21:G:H2' | 1:A:22:G:C8 | 2.31 | 0.65 |
| 3:C:11:ARG:NH1 | 3:C:177:THR:O | 2.29 | 0.65 |
| 1:A:1152:A:OP1 | 10:J:68:HIS:ND1 | 2.30 | 0.65 |
| 1:A:1250:A:H2' | 1:A:1251:A:C8 | 2.32 | 0.64 |
| 17:Q:66:SER:O | 17:Q:70:ARG:NH1 | 2.31 | 0.64 |
| 6:F:10:LEU:HD12 | 6:F:59:TYR:HB3 | 1.80 | 0.64 |
| 14:N:11:LYS:HG3 | 14:N:13:THR:H | 1.61 | 0.64 |
| 1:A:984:C:H42 | 1:A:1221:G:H1 | 1.46 | 0.64 |
| 1:A:1347:G:O6 | 9:I:10:ARG:NH2 | 2.28 | 0.64 |
| 10:J:48:THR:HA | 10:J:62:HIS:HB3 | 1.80 | 0.64 |
| 1:A:756:C:N4 | 28:A:2075:HOH:O | 2.30 | 0.64 |
| 1:A:1345:U:OP1 | 9:I:120:ARG:NH1 | 2.31 | 0.64 |
| 9:I:9:ARG:HG2 | 9:I:14:VAL:HG12 | 1.78 | 0.64 |
| 12:L:53:ARG:NH1 | 12:L:92:OTD:OD2 | 2.31 | 0.64 |
| 16:P:4:ILE:HG12 | 16:P:21:VAL:HG22 | 1.80 | 0.63 |
| 3:C:70:VAL:HG12 | 3:C:72:LYS:H | 1.63 | 0.63 |
| 1:A:201:C:H42 | 1:A:216:G:H1 | 1.46 | 0.62 |
| 1:A:652:U:O4 | 1:A:752:G:O2' | 2.17 | 0.62 |
| 1:A:1281:U:H5'' | 1:A:1282:C:H5 | 1.64 | 0.62 |
| 1:A:674:G:H2' | 1:A:675:A:H8 | 1.64 | 0.62 |
| 3:C:64:VAL:HG23 | 3:C:99:VAL:HG11 | 1.81 | 0.62 |
| 1:A:1026:G:H3' | 1:A:1027:C:H5'' | 1.81 | 0.62 |
| 1:A:1147:C:O2' | 9:I:5:TYR:OH | 2.17 | 0.62 |
| 1:A:662:G:N7 | 24:A:1604:PAR:N12 | 2.48 | 0.62 |
| 13:M:65:LYS:NZ | 13:M:73:GLU:OE2 | 2.33 | 0.62 |
| 1:A:1286:A:H2' | 1:A:1287:A:H4' | 1.81 | 0.62 |
| 1:A:269:C:H2' | 1:A:270:A:H8 | 1.65 | 0.61 |
| 8:H:86:ILE:HD12 | 8:H:133:LEU:HD22 | 1.82 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:A:1122:U:O4 | 1:A:1123:A:N6 | 2.33 | 0.61 |
| 1:A:542:G:OP1 | 4:D:10:ARG:NH2 | 2.33 | 0.61 |
| 1:A:1137:C:H4' | 1:A:1138:G:C2 | 2.35 | 0.61 |
| 5:E:81:GLU:HG3 | 5:E:90:VAL:HG22 | 1.81 | 0.61 |
| 7:G:54:THR:HG22 | 7:G:56:GLN:H | 1.64 | 0.61 |
| 9:I:25:LYS:N | 9:I:60:ASP:OD1 | 2.34 | 0.61 |
| 1:A:1301:U:HO2' | 1:A:1302:U:P | 2.23 | 0.61 |
| 1:A:201:C:N3 | 1:A:216:G:N2 | 2.37 | 0.60 |
| 1:A:1003:G:N2 | 1:A:1039:C:O2 | 2.34 | 0.60 |
| 1:A:1301:U:O2' | 1:A:1302:U:O5' | 2.18 | 0.60 |
| 24:A:1602:PAR:H23 | 24:A:1602:PAR:HN21 | 1.67 | 0.60 |
| 9:I:97:LYS:HA | 9:I:102:LEU:HD11 | 1.84 | 0.60 |
| 10:J:49:VAL:HG23 | 14:N:41:ARG:HB2 | 1.82 | 0.60 |
| 19:S:50:ALA:HB1 | 19:S:57:HIS:HB3 | 1.83 | 0.60 |
| 2:B:48:MET:HA | 2:B:51:LEU:HB2 | 1.81 | 0.60 |
| 1:A:51:A:OP2 | 24:A:1603:PAR:N24 | 2.35 | 0.60 |
| 3:C:189:ALA:HB3 | 3:C:196:LEU:HB2 | 1.83 | 0.60 |
| 1:A:427:U:OP1 | 4:D:13:ARG:NH2 | 2.33 | 0.60 |
| 1:A:1356:G:H2' | 1:A:1357:A:C8 | 2.37 | 0.60 |
| 20:T:75:ASN:OD1 | 20:T:75:ASN:N | 2.34 | 0.60 |
| 1:A:1313:U:O4 | 19:S:4:SER:OG | 2.18 | 0.60 |
| 1:A:1435:G:H2' | 1:A:1436:U:H6 | 1.66 | 0.60 |
| 1:A:714:G:H2' | 1:A:715:A:C8 | 2.37 | 0.59 |
| 1:A:243:A:H4' | 1:A:244:U:H5' | 1.84 | 0.59 |
| 1:A:1402:4OC:HM22 | 1:A:1403:C:H5' | 1.84 | 0.59 |
| 19:S:55:LYS:HG2 | 19:S:56:GLN:HG3 | 1.84 | 0.59 |
| 2:B:77:ALA:HB2 | 2:B:211:ILE:HD13 | 1.84 | 0.59 |
| 5:E:33:VAL:HG22 | 5:E:43:LEU:HD23 | 1.83 | 0.59 |
| 15:O:87:ILE:HG22 | 15:O:88:ARG:H | 1.67 | 0.59 |
| 3:C:44:GLU:HG2 | 3:C:52:LEU:HD11 | 1.84 | 0.59 |
| 1:A:1323:G:H2' | 1:A:1324:A:C8 | 2.38 | 0.59 |
| 1:A:442:C:N4 | 1:A:492:G:H1 | 2.00 | 0.58 |
| 1:A:1010:G:H2' | 1:A:1011:G:H8 | 1.68 | 0.58 |
| 1:A:1222:G:OP2 | 1:A:1322:C:N4 | 2.31 | 0.58 |
| 15:O:26:GLU:HA | 15:O:81:LEU:HD11 | 1.85 | 0.58 |
| 1:A:279:A:OP2 | 17:Q:95:TYR:OH | 2.19 | 0.58 |
| 1:A:1504:G:OP1 | 1:A:1507:A:H4' | 2.03 | 0.58 |
| 10:J:89:ASP:HB2 | 10:J:91:PRO:HD2 | 1.86 | 0.58 |
| 1:A:28:G:O2' | 1:A:296:U:OP1 | 2.21 | 0.58 |
| 3:C:157:ILE:HD13 | 3:C:166:GLU:HB2 | 1.85 | 0.58 |
| 6:F:9:VAL:HB | 6:F:87:ARG:HB2 | 1.84 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1520:G:H2' | 1:A:1521:G:H8 | 1.69 | 0.57 |
| 7:G:78:ARG:NH1 | 7:G:154:TYR:O | 2.37 | 0.57 |
| 17:Q:67:LYS:HA | 17:Q:70:ARG:HH12 | 1.69 | 0.57 |
| 1:A:390:C:H2' | 1:A:391:G:C8 | 2.39 | 0.57 |
| 5:E:98:THR:HB | 5:E:117:ASP:HB3 | 1.85 | 0.57 |
| 1:A:250:A:H4' | 1:A:251:G:O5' | 2.03 | 0.57 |
| 1:A:1143:G:H2' | 1:A:1144:G:C8 | 2.38 | 0.57 |
| 1:A:1392:G:H21 | 1:A:1502:A:H8 | 1.50 | 0.57 |
| 20:T:10:LEU:HD12 | 20:T:11:SER:H | 1.69 | 0.57 |
| 1:A:241:C:H4' | 12:L:19:ARG:HH22 | 1.70 | 0.57 |
| 1:A:266:G:H5' | 1:A:268:C:H41 | 1.68 | 0.57 |
| 7:G:122:HIS:HA | 7:G:125:MET:HE2 | 1.86 | 0.57 |
| 1:A:1343:G:H2' | 1:A:1344:C:C6 | 2.40 | 0.57 |
| 4:D:141:ARG:NH2 | 28:D:401:HOH:O | 2.36 | 0.57 |
| 5:E:12:LEU:HD13 | 5:E:31:LEU:HB2 | 1.86 | 0.57 |
| 1:A:1250:A:H4' | 9:I:68:GLY:N | 2.20 | 0.57 |
| 3:C:155:GLY:HA2 | 3:C:164:ARG:H | 1.70 | 0.57 |
| 1:A:765:G:N2 | 1:A:813:U:OP2 | 2.36 | 0.56 |
| 1:A:811:C:O2' | 1:A:901:A:N1 | 2.37 | 0.56 |
| 1:A:946:A:H2' | 1:A:947:G:C8 | 2.40 | 0.56 |
| 1:A:1124:G:N7 | 1:A:1145:C:O2' | 2.30 | 0.56 |
| 1:A:1291:G:H4' | 9:I:39:GLY:HA3 | 1.86 | 0.56 |
| 4:D:98:GLU:OE2 | 4:D:107:ARG:NE | 2.30 | 0.56 |
| 3:C:6:HIS:HD2 | 3:C:8:ILE:H | 1.51 | 0.56 |
| 1:A:1494:G:OP1 | 24:A:1601:PAR:N32 | 2.39 | 0.56 |
| 8:H:42:GLU:HG3 | 8:H:109:ILE:HD13 | 1.87 | 0.56 |
| 1:A:646:U:H2' | 1:A:647:C:C6 | 2.40 | 0.56 |
| 1:A:114:U:H5'' | 24:A:1603:PAR:H52 | 1.86 | 0.56 |
| 2:B:174:VAL:O | 2:B:178:ARG:HG2 | 2.05 | 0.56 |
| 3:C:19:GLU:HG2 | 3:C:54:ARG:HE | 1.71 | 0.56 |
| 5:E:80:ILE:HD13 | 5:E:138:ALA:HB1 | 1.87 | 0.56 |
| 2:B:88:ALA:HB1 | 2:B:226:ARG:HH21 | 1.71 | 0.56 |
| 3:C:3:ASN:OD1 | 3:C:3:ASN:N | 2.38 | 0.56 |
| 5:E:102:ALA:O | 5:E:107:ARG:NH1 | 2.38 | 0.55 |
| 17:Q:68:ARG:O | 17:Q:68:ARG:HG3 | 2.06 | 0.55 |
| 1:A:17:U:H2' | 1:A:18:C:C6 | 2.41 | 0.55 |
| 1:A:619:U:N3 | 4:D:134:ASP:OD1 | 2.27 | 0.55 |
| 11:K:110:ASP:OD2 | 18:R:88:LYS:NZ | 2.39 | 0.55 |
| 1:A:372:C:H4' | 1:A:373:A:O5' | 2.06 | 0.55 |
| 1:A:1071:C:H42 | 1:A:1104:G:H1 | 1.54 | 0.55 |
| 1:A:1510:U:H2' | 1:A:1511:G:C8 | 2.42 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 12:L:56:ALA:HB2 | 12:L:70:ILE:HD11 | 1.87 | 0.55 |
| 1:A:390:C:O3' | 16:P:28:ARG:NH2 | 2.40 | 0.55 |
| 10:J:57:LYS:HE2 | 10:J:60:ARG:NH2 | 2.21 | 0.55 |
| 1:A:975:A:H5' | 1:A:975:A:H8 | 1.72 | 0.55 |
| 1:A:1326:C:OP1 | 21:U:12:LYS:NZ | 2.39 | 0.55 |
| 4:D:111:ALA:HB2 | 4:D:120:LEU:HD12 | 1.88 | 0.55 |
| 10:J:57:LYS:HG3 | 10:J:60:ARG:HH21 | 1.72 | 0.55 |
| 1:A:523:A:N6 | 12:L:92:0TD:OD1 | 2.40 | 0.55 |
| 1:A:918:A:H2' | 1:A:919:A:C8 | 2.42 | 0.55 |
| 20:T:67:ALA:O | 20:T:73:HIS:ND1 | 2.40 | 0.55 |
| 1:A:1287:A:H2' | 1:A:1288:A:C8 | 2.41 | 0.54 |
| 13:M:88:ARG:NH1 | 19:S:3:ARG:HH21 | 2.04 | 0.54 |
| 13:M:49:THR:HG22 | 13:M:51:ALA:H | 1.72 | 0.54 |
| 18:R:32:ARG:HA | 18:R:69:THR:HG21 | 1.89 | 0.54 |
| 1:A:864:A:H2' | 1:A:865:A:C8 | 2.42 | 0.54 |
| 12:L:75:HIS:HA | 12:L:102:ARG:HH22 | 1.72 | 0.54 |
| 1:A:1057:G:H5'' | 3:C:154:SER:HB2 | 1.90 | 0.54 |
| 2:B:33:TYR:HB2 | 2:B:43:ASP:HA | 1.89 | 0.54 |
| 1:A:983:A:O2' | 1:A:1050:G:OP2 | 2.26 | 0.54 |
| 1:A:1392:G:N2 | 1:A:1502:A:H8 | 2.05 | 0.54 |
| 5:E:110:LEU:HD13 | 5:E:118:ILE:HG21 | 1.89 | 0.54 |
| 13:M:63:THR:HG23 | 13:M:64:TRP:H | 1.73 | 0.54 |
| 1:A:1049:U:H4' | 1:A:1050:G:O5' | 2.07 | 0.54 |
| 10:J:51:ARG:HB2 | 10:J:59:SER:HB2 | 1.90 | 0.54 |
| 14:N:27:CYS:SG | 14:N:29:ARG:HB2 | 2.48 | 0.54 |
| 3:C:58:GLU:HB3 | 10:J:92:THR:HG21 | 1.90 | 0.53 |
| 8:H:18:ARG:NH2 | 8:H:81:HIS:O | 2.42 | 0.53 |
| 1:A:1266:G:N2 | 1:A:1269:A:OP2 | 2.35 | 0.53 |
| 12:L:24:VAL:HG13 | 12:L:98:TYR:HE1 | 1.72 | 0.53 |
| 1:A:559:A:OP1 | 5:E:126:ARG:NH2 | 2.34 | 0.53 |
| 9:I:28:VAL:HG22 | 9:I:63:ILE:HB | 1.90 | 0.53 |
| 1:A:262:A:H2' | 1:A:263:A:C8 | 2.44 | 0.53 |
| 1:A:580:U:H2' | 1:A:581:G:O4' | 2.09 | 0.53 |
| 1:A:390:C:H2' | 1:A:391:G:H8 | 1.72 | 0.53 |
| 1:A:1187:G:O2' | 9:I:111:ARG:NH1 | 2.42 | 0.53 |
| 1:A:1349:A:OP2 | 9:I:118:LYS:NZ | 2.42 | 0.53 |
| 7:G:15:ASP:HB3 | 7:G:20:ASP:H | 1.75 | 0.52 |
| 1:A:1288:A:H2' | 1:A:1289:A:C8 | 2.45 | 0.52 |
| 5:E:79:GLU:O | 8:H:104:ARG:NH1 | 2.41 | 0.52 |
| 1:A:1314:C:H2' | 1:A:1315:U:H6 | 1.75 | 0.52 |
| 1:A:835:U:OP1 | 18:R:64:ARG:NH2 | 2.38 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1035:A:H2' | 1:A:1036:G:H8 | 1.73 | 0.52 |
| 5:E:79:GLU:HG3 | 5:E:93:PRO:HD2 | 1.91 | 0.52 |
| 14:N:9:LYS:HD3 | 14:N:21:TYR:O | 2.09 | 0.52 |
| 1:A:190(J):U:H2' | 1:A:190(K):G:H8 | 1.74 | 0.52 |
| 14:N:24:CYS:SG | 14:N:40:CYS:N | 2.82 | 0.52 |
| 1:A:35:G:H2' | 1:A:36:C:C6 | 2.45 | 0.52 |
| 1:A:477:G:H2' | 1:A:478:A:H8 | 1.75 | 0.52 |
| 1:A:1425:U:H3 | 1:A:1475:G:H1 | 1.58 | 0.52 |
| 24:A:1601:PAR:O44 | 24:A:1601:PAR:N64 | 2.42 | 0.52 |
| 8:H:85:ARG:NE | 8:H:87:SER:O | 2.43 | 0.52 |
| 1:A:1016:A:H2' | 1:A:1017:G:O4' | 2.10 | 0.52 |
| 1:A:1163:C:H2' | 1:A:1164:G:H8 | 1.75 | 0.52 |
| 1:A:1062:U:H2' | 1:A:1063:C:C6 | 2.44 | 0.52 |
| 1:A:1128:C:N3 | 1:A:1144:G:N2 | 2.58 | 0.51 |
| 1:A:1245:A:H2' | 1:A:1246:C:C6 | 2.45 | 0.51 |
| 1:A:1371:G:O3' | 9:I:69:GLY:HA3 | 2.10 | 0.51 |
| 7:G:15:ASP:OD1 | 7:G:44:TYR:OH | 2.26 | 0.51 |
| 7:G:113:GLU:HB2 | 7:G:119:ARG:HG3 | 1.91 | 0.51 |
| 8:H:21:LYS:O | 8:H:65:TYR:OH | 2.17 | 0.51 |
| 12:L:41:ARG:HH21 | 12:L:57:LYS:NZ | 2.08 | 0.51 |
| 1:A:1162:C:N4 | 1:A:1174:G:H1 | 2.07 | 0.51 |
| 5:E:88:LYS:HB3 | 5:E:123:LEU:HB2 | 1.91 | 0.51 |
| 1:A:1015:A:H2' | 1:A:1016:A:C8 | 2.46 | 0.51 |
| 1:A:524:G:H2' | 1:A:525:C:C6 | 2.45 | 0.51 |
| 1:A:116:A:H5'' | 28:A:2018:HOH:O | 2.10 | 0.51 |
| 1:A:501:C:H2' | 1:A:502:G:H8 | 1.75 | 0.51 |
| 16:P:22:THR:HA | 16:P:33:ILE:HG13 | 1.92 | 0.51 |
| 1:A:1095:U:H2' | 1:A:1096:C:C6 | 2.46 | 0.51 |
| 2:B:84:GLU:OE2 | 2:B:233:SER:OG | 2.20 | 0.51 |
| 2:B:122:PHE:HA | 2:B:127:ILE:HG12 | 1.91 | 0.51 |
| 2:B:124:SER:HB2 | 2:B:125:PRO:HD2 | 1.93 | 0.51 |
| 7:G:75:VAL:HG21 | 7:G:86:GLN:HB3 | 1.93 | 0.51 |
| 10:J:26:ALA:O | 10:J:84:GLN:NE2 | 2.44 | 0.51 |
| 1:A:1262:C:H42 | 1:A:1273:G:H1 | 1.59 | 0.51 |
| 1:A:24:U:OP1 | 12:L:23:LYS:NZ | 2.37 | 0.51 |
| 1:A:750:G:N3 | 15:O:23:GLY:HA3 | 2.26 | 0.51 |
| 1:A:999:C:H2' | 1:A:1000:U:C6 | 2.46 | 0.51 |
| 1:A:1505:G:O2' | 1:A:1506:U:OP2 | 2.27 | 0.51 |
| 9:I:8:GLY:HA2 | 9:I:79:LEU:HD13 | 1.92 | 0.51 |
| 1:A:976:G:H5' | 1:A:1358:U:O2' | 2.10 | 0.50 |
| 1:A:1443:G:H4' | 1:A:1446:A:O5' | 2.10 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:73:THR:HG23 | 2:B:95:GLN:O | 2.11 | 0.50 |
| 5:E:102:ALA:HB1 | 5:E:106:PRO:HG2 | 1.93 | 0.50 |
| 7:G:46:ALA:O | 7:G:50:ILE:HG12 | 2.11 | 0.50 |
| 1:A:1475:G:H2' | 1:A:1476:G:H8 | 1.76 | 0.50 |
| 1:A:1498:UR3:OP2 | 1:A:1542:U:O2' | 2.27 | 0.50 |
| 3:C:64:VAL:H | 3:C:99:VAL:HB | 1.77 | 0.50 |
| 5:E:98:THR:N | 5:E:117:ASP:OD2 | 2.44 | 0.50 |
| 1:A:192:U:H2' | 1:A:193:C:H6 | 1.77 | 0.50 |
| 1:A:192:U:H1' | 20:T:103:GLY:HA2 | 1.92 | 0.50 |
| 1:A:359:U:H2' | 1:A:360:A:H8 | 1.76 | 0.50 |
| 10:J:24:VAL:HG13 | 10:J:34:VAL:HG11 | 1.93 | 0.50 |
| 1:A:190(K):G:H2' | 1:A:190(L):U:H6 | 1.75 | 0.50 |
| 2:B:97:TRP:HZ2 | 2:B:102:LEU:HD13 | 1.77 | 0.50 |
| 9:I:112:LYS:HE3 | 9:I:117:HIS:O | 2.11 | 0.50 |
| 10:J:29:ARG:NH1 | 10:J:84:GLN:OE1 | 2.44 | 0.50 |
| 19:S:13:ASP:HA | 19:S:16:LEU:HB3 | 1.93 | 0.50 |
| 1:A:241:C:H4' | 12:L:19:ARG:NH2 | 2.26 | 0.50 |
| 1:A:639:G:H2' | 1:A:640:A:H8 | 1.75 | 0.50 |
| 1:A:973:G:H3' | 1:A:974:A:H5'' | 1.94 | 0.50 |
| 2:B:223:ILE:HD13 | 2:B:230:VAL:N | 2.24 | 0.50 |
| 8:H:24:THR:HG22 | 8:H:63:LEU:HD21 | 1.94 | 0.50 |
| 1:A:603:U:H2' | 1:A:604:G:H8 | 1.77 | 0.50 |
| 1:A:646:U:H2' | 1:A:647:C:H6 | 1.75 | 0.50 |
| 1:A:1513:A:H2' | 1:A:1514:C:C6 | 2.47 | 0.50 |
| 11:K:27:ASN:OD1 | 11:K:28:THR:N | 2.45 | 0.50 |
| 13:M:86:CYS:SG | 13:M:87:TYR:N | 2.84 | 0.50 |
| 1:A:1002:G:H2' | 1:A:1003:G:C8 | 2.47 | 0.50 |
| 5:E:143:ARG:NH1 | 8:H:77:GLU:OE2 | 2.43 | 0.50 |
| 10:J:32:ALA:HB2 | 10:J:76:ASN:HB2 | 1.94 | 0.50 |
| 1:A:1132:C:H2' | 1:A:1133:G:H8 | 1.77 | 0.49 |
| 1:A:1352:C:OP1 | 21:U:3:LYS:NZ | 2.29 | 0.49 |
| 3:C:34:LEU:HG | 14:N:25:VAL:HG21 | 1.93 | 0.49 |
| 1:A:1287:A:H2 | 1:A:1353:G:H1' | 1.77 | 0.49 |
| 24:A:1602:PAR:H23 | 24:A:1602:PAR:N21 | 2.27 | 0.49 |
| 8:H:25:ASP:N | 8:H:25:ASP:OD1 | 2.44 | 0.49 |
| 1:A:736:C:H2' | 1:A:737:A:C8 | 2.47 | 0.49 |
| 13:M:90:LEU:O | 13:M:94:ARG:HG2 | 2.13 | 0.49 |
| 1:A:1343:G:H4' | 9:I:122:ALA:HB3 | 1.94 | 0.49 |
| 10:J:48:THR:O | 14:N:34:TYR:OH | 2.30 | 0.49 |
| 1:A:976:G:OP2 | 1:A:1358:U:O2' | 2.26 | 0.49 |
| 5:E:80:ILE:HG23 | 8:H:104:ARG:HH22 | 1.78 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:272:C:H2' | 1:A:273:A:H8 | 1.78 | 0.49 |
| 1:A:501:C:H2' | 1:A:502:G:C8 | 2.47 | 0.49 |
| 1:A:558:G:OP2 | 1:A:559:A:O2' | 2.28 | 0.49 |
| 1:A:614:A:H2' | 1:A:615:C:C6 | 2.48 | 0.49 |
| 1:A:1178:G:OP1 | 9:I:93:ARG:NH1 | 2.45 | 0.49 |
| 1:A:335:C:H2' | 1:A:336:C:C6 | 2.48 | 0.49 |
| 2:B:47:THR:HA | 2:B:202:PRO:HG2 | 1.94 | 0.49 |
| 15:O:39:LEU:HD13 | 15:O:56:LEU:HB2 | 1.94 | 0.49 |
| 1:A:743:U:H2' | 1:A:744:C:C6 | 2.48 | 0.49 |
| 1:A:1157:A:C2 | 1:A:1181:G:C4 | 3.00 | 0.49 |
| 1:A:1219:U:P | 14:N:19:ARG:HH22 | 2.36 | 0.49 |
| 2:B:73:THR:N | 2:B:170:GLU:OE1 | 2.37 | 0.49 |
| 3:C:5:ILE:HD13 | 3:C:10:PHE:HB2 | 1.94 | 0.49 |
| 3:C:38:ARG:HB3 | 3:C:94:LEU:HD21 | 1.94 | 0.49 |
| 12:L:41:ARG:HH21 | 12:L:57:LYS:HZ1 | 1.61 | 0.49 |
| 1:A:851:G:H2' | 1:A:852:G:H8 | 1.77 | 0.49 |
| 1:A:1256:A:HO2' | 1:A:1257:U:P | 2.36 | 0.49 |
| 8:H:108:GLY:HA3 | 8:H:138:TRP:HB3 | 1.94 | 0.49 |
| 1:A:45:U:H2' | 1:A:46:G:C8 | 2.48 | 0.48 |
| 1:A:920:U:H2' | 1:A:921:U:C6 | 2.47 | 0.48 |
| 1:A:1189:C:OP1 | 10:J:51:ARG:NH2 | 2.34 | 0.48 |
| 17:Q:83:ASP:OD1 | 17:Q:83:ASP:N | 2.46 | 0.48 |
| 1:A:59:A:H1' | 1:A:354:G:N2 | 2.28 | 0.48 |
| 24:A:1604:PAR:O53 | 24:A:1604:PAR:N21 | 2.43 | 0.48 |
| 8:H:121:ASP:OD1 | 8:H:121:ASP:N | 2.44 | 0.48 |
| 10:J:51:ARG:HG3 | 10:J:60:ARG:O | 2.14 | 0.48 |
| 1:A:186:C:H2' | 1:A:187:C:C6 | 2.48 | 0.48 |
| 1:A:186:C:H2' | 1:A:187:C:H6 | 1.78 | 0.48 |
| 1:A:737:A:H2' | 1:A:738:C:H6 | 1.78 | 0.48 |
| 1:A:1218:C:H2' | 1:A:1219:U:C6 | 2.49 | 0.48 |
| 1:A:1288:A:H2' | 1:A:1289:A:H8 | 1.78 | 0.48 |
| 1:A:1298:C:H4' | 1:A:1299:A:C4 | 2.49 | 0.48 |
| 1:A:1347:G:O2' | 1:A:1348:U:P | 2.71 | 0.48 |
| 9:I:50:LEU:HB3 | 9:I:56:LEU:H | 1.79 | 0.48 |
| 1:A:456:C:H42 | 1:A:476:G:H1 | 1.61 | 0.48 |
| 1:A:538:G:H2' | 1:A:539:A:H8 | 1.77 | 0.48 |
| 3:C:59:ARG:HG2 | 3:C:64:VAL:HG22 | 1.96 | 0.48 |
| 21:U:6:ARG:HB2 | 21:U:15:ARG:NH1 | 2.28 | 0.48 |
| 1:A:105:G:H2' | 1:A:106:C:C6 | 2.48 | 0.48 |
| 7:G:23:VAL:O | 7:G:27:ILE:HG12 | 2.13 | 0.48 |
| 1:A:737:A:H2' | 1:A:738:C:C6 | 2.48 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1001:A:H2' | 1:A:1002:G:C8 | 2.49 | 0.48 |
| 1:A:1072:G:H2' | 1:A:1073:U:C6 | 2.48 | 0.48 |
| 1:A:523:A:H61 | 12:L:92:0TD:CG | 2.27 | 0.48 |
| 1:A:966:M2G:H8 | 1:A:966:M2G:OP2 | 1.97 | 0.48 |
| 1:A:427:U:OP2 | 4:D:36:ARG:NH2 | 2.40 | 0.48 |
| 1:A:767:A:O2' | 1:A:1524:C:O2 | 2.27 | 0.48 |
| 3:C:116:VAL:HG21 | 3:C:202:ILE:HD11 | 1.96 | 0.48 |
| 4:D:70:ILE:HD11 | 4:D:100:ARG:CZ | 2.44 | 0.48 |
| 19:S:3:ARG:HH22 | 19:S:69:HIS:CE1 | 2.32 | 0.48 |
| 1:A:344:A:H5' | 1:A:345:C:C5 | 2.49 | 0.47 |
| 1:A:434:U:H2' | 1:A:435:C:C6 | 2.49 | 0.47 |
| 1:A:1028:C:H2' | 1:A:1029:C:H6 | 1.78 | 0.47 |
| 3:C:27:LYS:HD3 | 3:C:27:LYS:H | 1.79 | 0.47 |
| 6:F:8:ILE:HD11 | 6:F:79:LEU:HD13 | 1.96 | 0.47 |
| 1:A:360:A:N6 | 24:A:1603:PAR:H44 | 2.30 | 0.47 |
| 1:A:190(K):G:H2' | 1:A:190(L):U:C6 | 2.49 | 0.47 |
| 1:A:642:A:C8 | 8:H:115:SER:HA | 2.50 | 0.47 |
| 10:J:5:ARG:HA | 10:J:73:ASP:OD1 | 2.14 | 0.47 |
| 1:A:382:A:H2' | 1:A:383:A:C8 | 2.49 | 0.47 |
| 1:A:610:G:OP1 | 24:A:1605:PAR:N64 | 2.48 | 0.47 |
| 1:A:1320:C:O2 | 19:S:36:ARG:NH1 | 2.47 | 0.47 |
| 8:H:113:SER:HB2 | 8:H:134:ILE:HD11 | 1.96 | 0.47 |
| 9:I:32:ASP:OD1 | 9:I:33:PHE:N | 2.47 | 0.47 |
| 11:K:72:ALA:HB1 | 11:K:77:MET:HE2 | 1.96 | 0.47 |
| 1:A:384:G:H2' | 1:A:385:C:C6 | 2.50 | 0.47 |
| 1:A:1154:G:H2' | 1:A:1155:G:H8 | 1.79 | 0.47 |
| 1:A:1520:G:H2' | 1:A:1521:G:C8 | 2.49 | 0.47 |
| 9:I:15:ALA:HB2 | 9:I:65:VAL:HG13 | 1.96 | 0.47 |
| 16:P:34:GLU:OE2 | 16:P:55:ARG:HD3 | 2.15 | 0.47 |
| 1:A:1131:G:H2' | 1:A:1132:C:C6 | 2.49 | 0.47 |
| 1:A:1179:A:O2' | 1:A:1180:A:OP1 | 2.33 | 0.47 |
| 4:D:121:VAL:O | 4:D:134:ASP:HA | 2.15 | 0.47 |
| 1:A:266:G:O3' | 17:Q:67:LYS:HB2 | 2.15 | 0.47 |
| 1:A:1028:C:N3 | 1:A:1033:G:N2 | 2.50 | 0.47 |
| 1:A:776:G:N2 | 1:A:802:A:OP2 | 2.39 | 0.47 |
| 1:A:1292:U:H2' | 1:A:1293:G:C8 | 2.50 | 0.47 |
| 1:A:1399:C:C2 | 1:A:1502:A:N6 | 2.83 | 0.47 |
| 4:D:9:CYS:O | 4:D:12:CYS:HB2 | 2.15 | 0.47 |
| 1:A:975:A:H5' | 1:A:975:A:C8 | 2.49 | 0.47 |
| 1:A:1399:C:H4' | 1:A:1400:5MC:H5'' | 1.97 | 0.47 |
| 1:A:1466:C:H2' | 1:A:1467:G:O4' | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 18:R:46:GLU:CD | 18:R:46:GLU:H | 2.17 | 0.47 |
| 1:A:1168:A:H2' | 1:A:1169:A:C8 | 2.49 | 0.46 |
| 1:A:1427:U:H2' | 1:A:1428:A:C8 | 2.45 | 0.46 |
| 10:J:32:ALA:O | 10:J:34:VAL:HG23 | 2.16 | 0.46 |
| 1:A:359:U:H2' | 1:A:360:A:C8 | 2.50 | 0.46 |
| 1:A:545:C:OP2 | 4:D:62:GLN:NE2 | 2.48 | 0.46 |
| 1:A:560:U:H5' | 1:A:566:G:C2 | 2.50 | 0.46 |
| 1:A:1148:U:H2' | 1:A:1149:C:O4' | 2.16 | 0.46 |
| 1:A:1369:C:H2' | 1:A:1370:G:C8 | 2.50 | 0.46 |
| 15:O:26:GLU:OE1 | 15:O:77:ARG:HD2 | 2.14 | 0.46 |
| 19:S:31:ILE:HG22 | 19:S:49:ILE:HA | 1.98 | 0.46 |
| 1:A:190(J):U:H2' | 1:A:190(K):G:C8 | 2.50 | 0.46 |
| 1:A:399:G:H2' | 1:A:400:C:C6 | 2.51 | 0.46 |
| 14:N:27:CYS:HB3 | 14:N:43:CYS:SG | 2.54 | 0.46 |
| 18:R:47:THR:HG22 | 18:R:48:GLY:H | 1.81 | 0.46 |
| 1:A:44:G:N2 | 1:A:399:G:C4 | 2.83 | 0.46 |
| 1:A:1238:A:N7 | 1:A:1303:C:H1' | 2.30 | 0.46 |
| 1:A:1367:C:OP2 | 9:I:112:LYS:NZ | 2.47 | 0.46 |
| 1:A:1372:U:H2' | 1:A:1373:G:O4' | 2.15 | 0.46 |
| 1:A:1477:C:H2' | 1:A:1478:C:H6 | 1.80 | 0.46 |
| 4:D:148:VAL:HG11 | 4:D:158:ILE:HD13 | 1.97 | 0.46 |
| 5:E:33:VAL:HG11 | 5:E:109:ILE:HA | 1.96 | 0.46 |
| 18:R:51:LEU:HA | 18:R:52:PRO:HD3 | 1.80 | 0.46 |
| 1:A:148:G:H2' | 1:A:149:A:C8 | 2.50 | 0.46 |
| 1:A:662:G:H2' | 1:A:663:A:C8 | 2.50 | 0.46 |
| 1:A:1118:C:H1' | 1:A:1179:A:C5 | 2.51 | 0.46 |
| 2:B:103:THR:HG23 | 2:B:176:GLU:OE1 | 2.16 | 0.46 |
| 21:U:5:ASP:O | 21:U:11:GLY:HA3 | 2.16 | 0.46 |
| 1:A:321:A:H2' | 1:A:322:C:H6 | 1.81 | 0.46 |
| 1:A:509:A:N3 | 1:A:543:C:O2' | 2.42 | 0.46 |
| 1:A:851:G:H2' | 1:A:852:G:C8 | 2.51 | 0.46 |
| 1:A:895:G:H2' | 1:A:896:C:C6 | 2.49 | 0.46 |
| 1:A:1086:U:H3 | 1:A:1099:G:N2 | 2.12 | 0.46 |
| 3:C:155:GLY:HA3 | 3:C:163:ALA:HB1 | 1.98 | 0.46 |
| 1:A:337:C:H2' | 1:A:338:A:H8 | 1.81 | 0.46 |
| 1:A:708:C:OP1 | 11:K:85:ARG:NH2 | 2.41 | 0.46 |
| 1:A:1264:C:H2' | 1:A:1265:G:H8 | 1.81 | 0.46 |
| 1:A:1507:A:H2' | 1:A:1508:G:C8 | 2.51 | 0.46 |
| 9:I:8:GLY:HA3 | 9:I:79:LEU:HB3 | 1.97 | 0.46 |
| 19:S:30:LEU:HB3 | 19:S:31:ILE:H | 1.41 | 0.46 |
| 1:A:530:G:HO2' | 1:A:531:U:P | 2.38 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:547:A:OP2 | 4:D:2:GLY:N | 2.48 | 0.46 |
| 2:B:55:PHE:HD2 | 2:B:221:LEU:HG | 1.80 | 0.46 |
| 4:D:151:LYS:H | 4:D:151:LYS:HD2 | 1.80 | 0.46 |
| 5:E:100:VAL:O | 5:E:107:ARG:NH2 | 2.47 | 0.46 |
| 1:A:450:G:OP1 | 16:P:43:LYS:NZ | 2.49 | 0.46 |
| 1:A:984:C:N4 | 1:A:1221:G:H1 | 2.13 | 0.46 |
| 3:C:68:VAL:HG12 | 3:C:70:VAL:HG23 | 1.97 | 0.46 |
| 4:D:3:ARG:NH2 | 4:D:5:ILE:HD11 | 2.31 | 0.46 |
| 1:A:848:C:H2' | 1:A:849:C:H6 | 1.80 | 0.46 |
| 1:A:1292:U:H2' | 1:A:1293:G:H8 | 1.80 | 0.46 |
| 17:Q:10:VAL:HG13 | 17:Q:19:VAL:HB | 1.98 | 0.46 |
| 1:A:658:G:H2' | 1:A:659:U:H6 | 1.80 | 0.45 |
| 6:F:50:TYR:CE2 | 18:R:77:GLY:HA2 | 2.52 | 0.45 |
| 21:U:6:ARG:HB2 | 21:U:15:ARG:HH12 | 1.82 | 0.45 |
| 1:A:190(D):U:O2' | 1:A:190(E):U:H5' | 2.16 | 0.45 |
| 1:A:620:C:C2 | 4:D:135:LEU:HD22 | 2.51 | 0.45 |
| 1:A:965:A:H4' | 1:A:966:M2G:OP1 | 2.14 | 0.45 |
| 1:A:56:U:H2' | 1:A:57:G:H8 | 1.80 | 0.45 |
| 1:A:954:G:H2' | 1:A:955:U:C6 | 2.51 | 0.45 |
| 1:A:1190:G:OP1 | 3:C:5:ILE:HG13 | 2.16 | 0.45 |
| 1:A:1244:C:H42 | 1:A:1293:G:H1 | 1.63 | 0.45 |
| 3:C:150:LYS:HB3 | 3:C:201:TYR:HB2 | 1.97 | 0.45 |
| 8:H:4:ASP:OD2 | 8:H:85:ARG:NH1 | 2.50 | 0.45 |
| 9:I:7:THR:HB | 9:I:83:ARG:HH11 | 1.82 | 0.45 |
| 1:A:922:G:C6 | 1:A:923:A:C6 | 3.05 | 0.45 |
| 1:A:1342:C:H2' | 1:A:1343:G:C8 | 2.51 | 0.45 |
| 15:O:56:LEU:HA | 15:O:59:MET:HE2 | 1.98 | 0.45 |
| 1:A:219:C:C4 | 1:A:220:G:C8 | 3.04 | 0.45 |
| 1:A:769:G:H4' | 1:A:1513:A:H4' | 1.98 | 0.45 |
| 1:A:1073:U:C2 | 1:A:1074:G:C8 | 3.04 | 0.45 |
| 1:A:1219:U:OP1 | 14:N:19:ARG:NH2 | 2.33 | 0.45 |
| 3:C:70:VAL:HG12 | 3:C:72:LYS:N | 2.30 | 0.45 |
| 4:D:111:ALA:HA | 4:D:161:ASN:ND2 | 2.31 | 0.45 |
| 7:G:78:ARG:HG2 | 7:G:80:VAL:HG23 | 1.99 | 0.45 |
| 15:O:85:LEU:HD23 | 15:O:85:LEU:HA | 1.81 | 0.45 |
| 1:A:110:C:O2' | 16:P:25:ARG:O | 2.34 | 0.45 |
| 1:A:316:G:OP2 | 1:A:351:G:O2' | 2.35 | 0.45 |
| 1:A:436:C:H2' | 1:A:437:U:H6 | 1.82 | 0.45 |
| 1:A:538:G:H2' | 1:A:539:A:C8 | 2.52 | 0.45 |
| 1:A:628:G:H2' | 1:A:629:G:C8 | 2.51 | 0.45 |
| 1:A:1342:C:H2' | 1:A:1343:G:H8 | 1.82 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 19:S:50:ALA:HA | 19:S:58:VAL:O | 2.17 | 0.45 |
| 1:A:360:A:H61 | 24:A:1603:PAR:H44 | 1.81 | 0.45 |
| 1:A:539:A:H2' | 1:A:540:G:C8 | 2.52 | 0.45 |
| 6:F:62:TRP:CH2 | 6:F:64:GLN:HB2 | 2.52 | 0.45 |
| 19:S:12:ASP:HB2 | 19:S:38:SER:HB3 | 1.99 | 0.45 |
| 20:T:53:LEU:O | 20:T:57:ARG:HD2 | 2.17 | 0.45 |
| 1:A:939:G:H2' | 1:A:940:C:C6 | 2.52 | 0.45 |
| 7:G:26:PHE:CE2 | 7:G:30:ILE:HD11 | 2.52 | 0.45 |
| 9:I:8:GLY:H | 9:I:83:ARG:NH1 | 2.15 | 0.45 |
| 1:A:902:G:H2' | 1:A:903:G:H8 | 1.82 | 0.45 |
| 2:B:178:ARG:NH2 | 8:H:74:PRO:HB3 | 2.32 | 0.45 |
| 16:P:8:ARG:NH2 | 16:P:15:PRO:HB3 | 2.31 | 0.45 |
| 1:A:384:G:H2' | 1:A:385:C:H6 | 1.80 | 0.44 |
| 1:A:434:U:H2' | 1:A:435:C:H6 | 1.82 | 0.44 |
| 1:A:999:C:H2' | 1:A:1000:U:H6 | 1.82 | 0.44 |
| 1:A:1074:G:O2' | 2:B:103:THR:OG1 | 2.35 | 0.44 |
| 1:A:1320:C:N3 | 19:S:36:ARG:HD3 | 2.31 | 0.44 |
| 6:F:4:TYR:CZ | 6:F:72:VAL:HG21 | 2.51 | 0.44 |
| 7:G:45:ASP:O | 7:G:49:ILE:HG13 | 2.17 | 0.44 |
| 9:I:118:LYS:O | 9:I:120:ARG:N | 2.45 | 0.44 |
| 1:A:261:U:OP2 | 20:T:79:ARG:NH2 | 2.51 | 0.44 |
| 1:A:1224:G:O2' | 1:A:1322:C:OP1 | 2.29 | 0.44 |
| 1:A:1355:G:H2' | 1:A:1356:G:C8 | 2.52 | 0.44 |
| 4:D:20:TYR:HD2 | 4:D:26:CYS:HB3 | 1.83 | 0.44 |
| 17:Q:59:ILE:HD13 | 17:Q:73:VAL:HA | 1.99 | 0.44 |
| 1:A:960:U:H1' | 1:A:1223:C:H5' | 1.98 | 0.44 |
| 1:A:1028:C:H2' | 1:A:1029:C:C6 | 2.53 | 0.44 |
| 1:A:1127:G:H21 | 1:A:1147:C:N4 | 2.14 | 0.44 |
| 2:B:231:GLU:CD | 2:B:231:GLU:H | 2.21 | 0.44 |
| 5:E:5:ASP:OD1 | 5:E:5:ASP:N | 2.50 | 0.44 |
| 13:M:67:GLU:HB3 | 13:M:68:GLY:H | 1.44 | 0.44 |
| 1:A:277:C:OP1 | 17:Q:68:ARG:NH2 | 2.25 | 0.44 |
| 1:A:537:G:H2' | 1:A:538:G:C8 | 2.53 | 0.44 |
| 1:A:1035:A:H2' | 1:A:1036:G:C8 | 2.53 | 0.44 |
| 1:A:1172:C:H2' | 1:A:1173:G:H8 | 1.82 | 0.44 |
| 1:A:1240:U:OP1 | 7:G:119:ARG:NH1 | 2.49 | 0.44 |
| 18:R:21:LYS:O | 18:R:25:THR:OG1 | 2.31 | 0.44 |
| 20:T:92:LEU:O | 20:T:96:GLY:N | 2.49 | 0.44 |
| 1:A:129(A):G:N2 | 1:A:190(E):U:H5'' | 2.33 | 0.44 |
| 12:L:60:LEU:HB3 | 12:L:62:SER:H | 1.83 | 0.44 |
| 1:A:260:G:H2' | 1:A:261:U:C6 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1163:C:H2' | 1:A:1164:G:C8 | 2.52 | 0.44 |
| 1:A:1316:G:N2 | 1:A:1318:A:H3' | 2.32 | 0.44 |
| 5:E:11:ILE:HB | 5:E:31:LEU:HB3 | 2.00 | 0.44 |
| 12:L:127:GLU:HB2 | 12:L:128:ALA:H | 1.57 | 0.44 |
| 1:A:142:G:O2' | 1:A:196:A:N1 | 2.46 | 0.44 |
| 12:L:70:ILE:HD13 | 12:L:77:LEU:HD12 | 2.00 | 0.44 |
| 1:A:503:C:OP2 | 12:L:116:SER:OG | 2.23 | 0.44 |
| 1:A:610:G:C4 | 1:A:611:A:C8 | 3.05 | 0.44 |
| 1:A:643:C:C2 | 1:A:644:G:C8 | 3.06 | 0.44 |
| 1:A:1031:G:H2' | 1:A:1032:G:H8 | 1.83 | 0.44 |
| 1:A:1300:G:O2' | 1:A:1301:U:O5' | 2.35 | 0.44 |
| 1:A:1521:G:H2' | 1:A:1522:U:C6 | 2.53 | 0.44 |
| 2:B:87:ARG:CZ | 2:B:233:SER:HB2 | 2.47 | 0.44 |
| 3:C:91:LEU:HD21 | 3:C:99:VAL:HG22 | 1.98 | 0.44 |
| 4:D:117:ALA:O | 4:D:121:VAL:HG23 | 2.18 | 0.44 |
| 1:A:358:U:H2' | 1:A:359:U:C6 | 2.53 | 0.44 |
| 1:A:1323:G:H2' | 1:A:1324:A:H8 | 1.82 | 0.44 |
| 2:B:90:MET:HA | 2:B:91:PRO:HD3 | 1.80 | 0.44 |
| 13:M:3:ARG:HA | 13:M:9:ILE:HG13 | 2.00 | 0.44 |
| 1:A:321:A:H2' | 1:A:322:C:C6 | 2.53 | 0.43 |
| 1:A:542:G:H2' | 1:A:543:C:H6 | 1.82 | 0.43 |
| 1:A:603:U:H2' | 1:A:604:G:C8 | 2.53 | 0.43 |
| 1:A:872:A:C4 | 1:A:874:G:N7 | 2.86 | 0.43 |
| 1:A:1077:G:N2 | 1:A:1080:A:OP2 | 2.46 | 0.43 |
| 1:A:1315:U:H2' | 1:A:1316:G:O4' | 2.18 | 0.43 |
| 1:A:114:U:O2' | 1:A:115:G:H5' | 2.19 | 0.43 |
| 1:A:350:G:O2' | 1:A:351:G:H5' | 2.18 | 0.43 |
| 1:A:690:G:H2' | 1:A:691:G:C8 | 2.54 | 0.43 |
| 1:A:731:G:OP1 | 1:A:766:A:H1' | 2.19 | 0.43 |
| 1:A:1418:A:H2' | 1:A:1419:G:O4' | 2.18 | 0.43 |
| 10:J:30:SER:HB2 | 10:J:81:THR:HA | 2.00 | 0.43 |
| 1:A:7:G:H5' | 1:A:298:A:O4' | 2.17 | 0.43 |
| 1:A:57:G:H2' | 1:A:58:C:C6 | 2.53 | 0.43 |
| 1:A:109:A:C6 | 1:A:326:G:C6 | 3.07 | 0.43 |
| 1:A:1072:G:H2' | 1:A:1073:U:H6 | 1.84 | 0.43 |
| 1:A:1128:C:H42 | 1:A:1143:G:H1 | 1.65 | 0.43 |
| 20:T:50:GLU:O | 20:T:54:LYS:HB2 | 2.18 | 0.43 |
| 1:A:168:G:C2 | 1:A:169:C:C5 | 3.06 | 0.43 |
| 1:A:399:G:H2' | 1:A:400:C:H6 | 1.83 | 0.43 |
| 1:A:562:C:H1' | 12:L:15:ARG:HG3 | 2.01 | 0.43 |
| 1:A:946:A:O2' | 1:A:1333:A:N3 | 2.43 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1160:G:C6 | 1:A:1161:C:C5 | 3.07 | 0.43 |
| 5:E:131:ILE:HD13 | 5:E:131:ILE:HA | 1.92 | 0.43 |
| 10:J:49:VAL:HG23 | 14:N:41:ARG:HD2 | 2.00 | 0.43 |
| 11:K:33:THR:HA | 11:K:39:PRO:HA | 2.00 | 0.43 |
| 1:A:56:U:H2' | 1:A:57:G:C8 | 2.54 | 0.43 |
| 1:A:323:U:H2' | 1:A:324:G:O4' | 2.18 | 0.43 |
| 1:A:921:U:O2 | 5:E:19:MET:HB2 | 2.19 | 0.43 |
| 1:A:1220:G:H2' | 1:A:1221:G:C8 | 2.53 | 0.43 |
| 1:A:1527:C:O2' | 1:A:1528:U:H5' | 2.19 | 0.43 |
| 12:L:54:LYS:HD2 | 12:L:54:LYS:N | 2.34 | 0.43 |
| 13:M:65:LYS:O | 13:M:66:LEU:HD23 | 2.18 | 0.43 |
| 1:A:768:A:H4' | 1:A:1523:G:N2 | 2.33 | 0.43 |
| 1:A:1003(A):G:H2' | 1:A:1004:A:H4' | 2.01 | 0.43 |
| 1:A:1256:A:O2' | 1:A:1257:U:O5' | 2.36 | 0.43 |
| 4:D:31:CYS:C | 4:D:33:MET:H | 2.22 | 0.43 |
| 11:K:54:ARG:O | 11:K:57:THR:OG1 | 2.27 | 0.43 |
| 12:L:46:LYS:HG3 | 12:L:92:OTD:H5 | 2.00 | 0.43 |
| 1:A:29:G:O2' | 1:A:30:U:H5' | 2.19 | 0.43 |
| 1:A:335:C:H2' | 1:A:336:C:H6 | 1.82 | 0.43 |
| 1:A:1017:G:H2' | 1:A:1018:C:C6 | 2.53 | 0.43 |
| 1:A:1068:G:H8 | 1:A:1068:G:OP2 | 2.01 | 0.43 |
| 7:G:65:ALA:O | 7:G:69:VAL:HG23 | 2.19 | 0.43 |
| 1:A:296:U:O2' | 1:A:556:C:O2 | 2.35 | 0.43 |
| 1:A:518:C:H2' | 1:A:530:G:N3 | 2.34 | 0.43 |
| 1:A:818:G:H3' | 1:A:819:A:H5'' | 2.00 | 0.43 |
| 1:A:1087:G:H2' | 1:A:1088:G:H8 | 1.84 | 0.43 |
| 15:O:18:PHE:HB2 | 15:O:19:PRO:HD2 | 2.00 | 0.43 |
| 16:P:34:GLU:HG2 | 16:P:35:LYS:N | 2.34 | 0.43 |
| 1:A:222:U:H2' | 1:A:223:U:H6 | 1.84 | 0.43 |
| 1:A:736:C:H2' | 1:A:737:A:H8 | 1.84 | 0.43 |
| 1:A:743:U:H2' | 1:A:744:C:H6 | 1.82 | 0.43 |
| 10:J:50:ILE:H | 10:J:50:ILE:HG13 | 1.68 | 0.43 |
| 12:L:7:ILE:O | 12:L:11:VAL:HG23 | 2.19 | 0.43 |
| 15:O:36:ILE:HG12 | 15:O:59:MET:HE3 | 2.01 | 0.43 |
| 1:A:67:C:H2' | 1:A:68:G:C8 | 2.54 | 0.43 |
| 1:A:246:A:C2 | 1:A:282:A:C5 | 3.07 | 0.43 |
| 1:A:397:A:H5' | 1:A:398:C:OP1 | 2.17 | 0.43 |
| 1:A:836:G:C6 | 1:A:851:G:C6 | 3.07 | 0.43 |
| 1:A:1189:C:H5'' | 3:C:5:ILE:HG12 | 2.01 | 0.43 |
| 1:A:1521:G:H2' | 1:A:1522:U:H6 | 1.84 | 0.43 |
| 1:A:129(A):G:C2 | 1:A:190(E):U:H5'' | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:658:G:H2' | 1:A:659:U:C6 | 2.54 | 0.42 |
| 1:A:895:G:H2' | 1:A:896:C:H6 | 1.84 | 0.42 |
| 1:A:1031:G:H2' | 1:A:1032:G:C8 | 2.54 | 0.42 |
| 3:C:150:LYS:HG3 | 3:C:169:ALA:HB2 | 2.01 | 0.42 |
| 1:A:110:C:H2' | 1:A:111:G:O4' | 2.18 | 0.42 |
| 1:A:780:A:O2' | 1:A:781:A:H5'' | 2.19 | 0.42 |
| 1:A:848:C:H2' | 1:A:849:C:C6 | 2.54 | 0.42 |
| 1:A:983:A:H5' | 1:A:984:C:OP2 | 2.19 | 0.42 |
| 1:A:1130:A:OP1 | 9:I:20:ARG:NH2 | 2.52 | 0.42 |
| 1:A:1157:A:H4' | 1:A:1158:C:O5' | 2.19 | 0.42 |
| 1:A:1410:G:H2' | 1:A:1411:C:C6 | 2.55 | 0.42 |
| 9:I:65:VAL:HG11 | 9:I:73:GLN:HB3 | 2.01 | 0.42 |
| 12:L:8:ASN:OD1 | 17:Q:34:LYS:HE2 | 2.19 | 0.42 |
| 12:L:24:VAL:HG13 | 12:L:98:TYR:CE1 | 2.52 | 0.42 |
| 16:P:15:PRO:HD2 | 16:P:42:ARG:HD3 | 2.01 | 0.42 |
| 1:A:192:U:C1' | 20:T:103:GLY:HA2 | 2.48 | 0.42 |
| 1:A:332:G:C2 | 1:A:333:G:C8 | 3.07 | 0.42 |
| 1:A:509:A:O2' | 1:A:510:A:OP1 | 2.35 | 0.42 |
| 1:A:1114:C:H1' | 14:N:60:SER:OG | 2.19 | 0.42 |
| 6:F:46:ARG:HB2 | 6:F:60:PHE:CE2 | 2.55 | 0.42 |
| 13:M:15:VAL:HG23 | 13:M:43:THR:O | 2.19 | 0.42 |
| 15:O:5:LYS:H | 15:O:5:LYS:HD2 | 1.84 | 0.42 |
| 1:A:156:G:C6 | 1:A:166:G:C6 | 3.08 | 0.42 |
| 1:A:235:C:N4 | 28:A:2086:HOH:O | 2.52 | 0.42 |
| 1:A:560:U:H4' | 1:A:561:U:H5'' | 1.99 | 0.42 |
| 1:A:945:G:C2 | 1:A:946:A:C8 | 3.07 | 0.42 |
| 1:A:1216:G:H2' | 1:A:1217:C:H6 | 1.85 | 0.42 |
| 7:G:59:LEU:HD11 | 7:G:63:LYS:HE3 | 2.00 | 0.42 |
| 1:A:45:U:OP1 | 1:A:307:C:O2' | 2.36 | 0.42 |
| 1:A:1017:G:H2' | 1:A:1018:C:H6 | 1.83 | 0.42 |
| 1:A:1175:G:H2' | 1:A:1176:A:H8 | 1.83 | 0.42 |
| 1:A:1177:G:O5' | 9:I:97:LYS:NZ | 2.52 | 0.42 |
| 3:C:77:ILE:O | 3:C:83:ARG:HB3 | 2.19 | 0.42 |
| 10:J:16:LEU:HD12 | 10:J:68:HIS:HB2 | 2.01 | 0.42 |
| 1:A:542:G:H2' | 1:A:543:C:C6 | 2.54 | 0.42 |
| 1:A:1273:G:H2' | 1:A:1274:G:O4' | 2.19 | 0.42 |
| 2:B:130:ARG:HB3 | 2:B:131:PRO:HD2 | 2.01 | 0.42 |
| 12:L:117:ARG:HB3 | 12:L:122:THR:O | 2.19 | 0.42 |
| 13:M:24:GLY:HA3 | 13:M:66:LEU:HD22 | 2.02 | 0.42 |
| 1:A:514:C:H2' | 1:A:515:G:H8 | 1.83 | 0.42 |
| 1:A:642:A:H2' | 1:A:643:C:H6 | 1.85 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:704:A:C5 | 1:A:705:U:C5 | 3.08 | 0.42 |
| 1:A:828:A:H2' | 1:A:829:G:O4' | 2.20 | 0.42 |
| 1:A:974:A:H8 | 1:A:974:A:OP1 | 2.03 | 0.42 |
| 1:A:1206:G:C6 | 1:A:1207:2MG:C5 | 3.07 | 0.42 |
| 1:A:1475:G:H2' | 1:A:1476:G:C8 | 2.54 | 0.42 |
| 5:E:127:ASN:HA | 5:E:128:PRO:HD3 | 1.94 | 0.42 |
| 7:G:111:ARG:HB2 | 7:G:119:ARG:HG2 | 2.02 | 0.42 |
| 1:A:184:G:H2' | 1:A:185:A:H8 | 1.84 | 0.42 |
| 1:A:477:G:H2' | 1:A:478:A:C8 | 2.54 | 0.42 |
| 1:A:1472:U:H2' | 1:A:1473:A:H8 | 1.84 | 0.42 |
| 1:A:1492:A:OP1 | 12:L:47:LYS:N | 2.53 | 0.42 |
| 4:D:50:ARG:HA | 4:D:51:PRO:HD3 | 1.80 | 0.42 |
| 11:K:40:ILE:HG22 | 11:K:41:THR:HG23 | 2.00 | 0.42 |
| 12:L:6:THR:OG1 | 12:L:9:GLN:HG3 | 2.19 | 0.42 |
| 12:L:90:VAL:HG12 | 12:L:92:0TD:OD1 | 2.18 | 0.42 |
| 1:A:192:U:H2' | 1:A:193:C:C6 | 2.55 | 0.42 |
| 1:A:1366:C:H2' | 1:A:1367:C:C6 | 2.55 | 0.42 |
| 7:G:152:ALA:O | 7:G:155:ARG:NH1 | 2.52 | 0.42 |
| 1:A:194:C:H2' | 1:A:195:A:H5'' | 2.02 | 0.42 |
| 1:A:911:U:H2' | 1:A:912:C:C6 | 2.55 | 0.42 |
| 1:A:986:A:H2' | 1:A:987:G:C8 | 2.55 | 0.42 |
| 1:A:1054:C:H2' | 1:A:1055:A:H5'' | 2.02 | 0.42 |
| 3:C:126:ARG:HE | 3:C:128:PHE:HD1 | 1.67 | 0.42 |
| 1:A:671:G:H2' | 1:A:672:U:O4' | 2.20 | 0.41 |
| 1:A:932:C:H4' | 7:G:4:ARG:NH2 | 2.35 | 0.41 |
| 12:L:111:LYS:HE3 | 12:L:112:ASP:H | 1.85 | 0.41 |
| 1:A:962:C:H2' | 1:A:963:G:O4' | 2.20 | 0.41 |
| 1:A:1464:G:H2' | 1:A:1465:C:C6 | 2.55 | 0.41 |
| 19:S:5:LEU:O | 19:S:6:LYS:HB2 | 2.20 | 0.41 |
| 1:A:372:C:H1' | 1:A:373:A:OP2 | 2.20 | 0.41 |
| 1:A:592:G:H2' | 1:A:593:G:H8 | 1.85 | 0.41 |
| 1:A:1080:A:H5'' | 5:E:16:THR:HG21 | 2.03 | 0.41 |
| 11:K:120:ARG:HA | 11:K:121:PRO:HD3 | 1.89 | 0.41 |
| 12:L:28:LYS:HB3 | 12:L:30:ALA:HB2 | 2.02 | 0.41 |
| 12:L:127:GLU:OE1 | 12:L:128:ALA:N | 2.53 | 0.41 |
| 1:A:674:G:H2' | 1:A:675:A:C8 | 2.49 | 0.41 |
| 1:A:987:G:H2' | 1:A:988:G:C8 | 2.56 | 0.41 |
| 1:A:1291:G:OP1 | 7:G:37:ASN:ND2 | 2.52 | 0.41 |
| 1:A:1498:UR3:O4' | 1:A:1519:MA6:H2 | 2.21 | 0.41 |
| 11:K:117:ASN:OD1 | 11:K:117:ASN:N | 2.53 | 0.41 |
| 17:Q:27:PHE:CE2 | 17:Q:36:ILE:HD11 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:22:G:H2' | 1:A:23:C:C6 | 2.55 | 0.41 |
| 1:A:57:G:H2' | 1:A:58:C:H6 | 1.85 | 0.41 |
| 1:A:99:C:H2' | 1:A:101:A:O4' | 2.21 | 0.41 |
| 1:A:338:A:H2' | 1:A:339:C:H6 | 1.86 | 0.41 |
| 1:A:488:C:H2' | 1:A:489:C:H6 | 1.85 | 0.41 |
| 1:A:687:A:C2 | 1:A:704:A:C5 | 3.08 | 0.41 |
| 1:A:741:G:OP2 | 24:A:1604:PAR:O41 | 2.36 | 0.41 |
| 1:A:1035:A:C2 | 1:A:1036:G:C5 | 3.09 | 0.41 |
| 1:A:1151:A:C2 | 1:A:1152:A:C5 | 3.09 | 0.41 |
| 1:A:1207:2MG:H2' | 1:A:1208:C:H6 | 1.86 | 0.41 |
| 1:A:1262:C:H2' | 1:A:1263:C:H6 | 1.86 | 0.41 |
| 1:A:1370:G:C2 | 1:A:1371:G:C8 | 3.08 | 0.41 |
| 1:A:299:G:H2' | 1:A:300:A:C8 | 2.56 | 0.41 |
| 1:A:540:G:H2' | 1:A:541:G:O4' | 2.20 | 0.41 |
| 1:A:579:G:H5' | 1:A:728:A:H1' | 2.01 | 0.41 |
| 1:A:890:G:O2' | 1:A:906:G:O6 | 2.28 | 0.41 |
| 1:A:1030(A):G:N2 | 1:A:1030(D):A:OP2 | 2.52 | 0.41 |
| 1:A:1241:G:H2' | 1:A:1242:C:C6 | 2.55 | 0.41 |
| 3:C:5:ILE:HG13 | 3:C:5:ILE:H | 1.70 | 0.41 |
| 5:E:31:LEU:HD23 | 5:E:31:LEU:HA | 1.83 | 0.41 |
| 12:L:27:LEU:O | 12:L:29:GLY:N | 2.53 | 0.41 |
| 16:P:28:ARG:HG3 | 16:P:29:ASP:OD1 | 2.21 | 0.41 |
| 1:A:410:G:OP1 | 4:D:30:LYS:NZ | 2.33 | 0.41 |
| 1:A:664:G:OP1 | 18:R:64:ARG:HD2 | 2.21 | 0.41 |
| 1:A:994:A:OP1 | 1:A:994:A:C8 | 2.74 | 0.41 |
| 1:A:1225:A:H5'' | 1:A:1226:C:OP2 | 2.20 | 0.41 |
| 1:A:1281:U:O2' | 1:A:1282:C:OP1 | 2.33 | 0.41 |
| 2:B:127:ILE:H | 2:B:127:ILE:HG13 | 1.67 | 0.41 |
| 2:B:178:ARG:HH22 | 8:H:74:PRO:HB3 | 1.85 | 0.41 |
| 16:P:9:PHE:CE1 | 16:P:18:ARG:HD2 | 2.54 | 0.41 |
| 16:P:28:ARG:NH1 | 16:P:29:ASP:OD1 | 2.54 | 0.41 |
| 1:A:22:G:H2' | 1:A:23:C:H6 | 1.84 | 0.41 |
| 1:A:416:G:H2' | 1:A:417:C:H6 | 1.86 | 0.41 |
| 1:A:560:U:H5' | 1:A:566:G:N2 | 2.35 | 0.41 |
| 1:A:564:C:O2' | 8:H:91:ARG:NH2 | 2.54 | 0.41 |
| 1:A:642:A:N7 | 8:H:115:SER:HA | 2.36 | 0.41 |
| 1:A:1326:C:H2' | 1:A:1327:C:H6 | 1.85 | 0.41 |
| 2:B:74:LYS:C | 2:B:76:GLN:H | 2.24 | 0.41 |
| 6:F:11:ASN:HA | 6:F:12:PRO:HD2 | 1.94 | 0.41 |
| 19:S:31:ILE:HD13 | 19:S:32:LYS:H | 1.85 | 0.41 |
| 1:A:105:G:H2' | 1:A:106:C:H6 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:960:U:H4' | 1:A:961:U:C5' | 2.50 | 0.41 |
| 1:A:1073:U:H2' | 1:A:1074:G:H8 | 1.86 | 0.41 |
| 1:A:1116:C:O2' | 9:I:108:VAL:HG21 | 2.21 | 0.41 |
| 1:A:1241:G:H2' | 1:A:1242:C:H6 | 1.86 | 0.41 |
| 1:A:1309:G:C6 | 1:A:1329:A:C2 | 3.09 | 0.41 |
| 2:B:130:ARG:HD3 | 2:B:130:ARG:HA | 1.75 | 0.41 |
| 15:O:74:ASP:HA | 15:O:75:PRO:HD2 | 1.91 | 0.41 |
| 1:A:75:G:C6 | 1:A:96:G:C6 | 3.08 | 0.41 |
| 1:A:537:G:H2' | 1:A:538:G:H8 | 1.86 | 0.41 |
| 1:A:701:C:H5'' | 1:A:703:G:O4' | 2.21 | 0.41 |
| 2:B:43:ASP:O | 2:B:47:THR:OG1 | 2.38 | 0.41 |
| 1:A:106:C:H2' | 1:A:107:G:O4' | 2.21 | 0.40 |
| 1:A:222:U:H2' | 1:A:223:U:C6 | 2.56 | 0.40 |
| 1:A:409:G:H1 | 1:A:433:C:N4 | 2.14 | 0.40 |
| 1:A:689:C:H2' | 1:A:690:G:O4' | 2.21 | 0.40 |
| 1:A:922:G:H2' | 1:A:923:A:C8 | 2.56 | 0.40 |
| 1:A:985:C:H2' | 1:A:986:A:H8 | 1.86 | 0.40 |
| 19:S:5:LEU:HD21 | 19:S:70:LYS:NZ | 2.36 | 0.40 |
| 1:A:1468:A:H2' | 1:A:1469:G:O4' | 2.21 | 0.40 |
| 2:B:30:ARG:HG3 | 2:B:31:TYR:CD1 | 2.56 | 0.40 |
| 9:I:97:LYS:HB3 | 9:I:98:PRO:HD3 | 2.03 | 0.40 |
| 10:J:38:ILE:H | 10:J:71:LEU:CB | 2.33 | 0.40 |
| 1:A:614:A:H2' | 1:A:615:C:H6 | 1.86 | 0.40 |
| 1:A:1022:G:C2 | 1:A:1023:G:C8 | 3.08 | 0.40 |
| 1:A:1107:C:C4 | 1:A:1108:G:C8 | 3.09 | 0.40 |
| 1:A:1117:G:H5' | 1:A:1118:C:OP2 | 2.22 | 0.40 |
| 1:A:1163:C:C2 | 1:A:1164:G:C8 | 3.08 | 0.40 |
| 1:A:1232:U:P | 9:I:124:GLN:HE21 | 2.44 | 0.40 |
| 6:F:4:TYR:CE2 | 6:F:92:LYS:HG2 | 2.57 | 0.40 |
| 6:F:30:LEU:HA | 6:F:30:LEU:HD23 | 1.87 | 0.40 |
| 1:A:814:A:H2' | 1:A:816:A:H5'' | 2.04 | 0.40 |
| 1:A:892:A:H2' | 1:A:893:C:H6 | 1.87 | 0.40 |
| 8:H:33:GLU:HG3 | 8:H:48:TYR:CE2 | 2.57 | 0.40 |
| 20:T:81:LYS:O | 20:T:85:MET:HG3 | 2.22 | 0.40 |
| 1:A:157:G:C2 | 1:A:158:G:C8 | 3.09 | 0.40 |
| 1:A:500:G:H2' | 1:A:501:C:C6 | 2.56 | 0.40 |
| 1:A:865:A:H5' | 1:A:1078:U:O4 | 2.22 | 0.40 |
| 1:A:1308:U:OP2 | 13:M:99:ARG:HG3 | 2.21 | 0.40 |
| 1:A:1464:G:H2' | 1:A:1465:C:H6 | 1.85 | 0.40 |
| 2:B:112:VAL:O | 2:B:116:GLU:HG2 | 2.21 | 0.40 |
| 8:H:112:LEU:HD23 | 8:H:133:LEU:HA | 2.04 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 10:J:14:LYS:HE2 | 10:J:14:LYS:HB3 | 1.84 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 2 | B | 234/236 (99%) | 205 (88%) | 28 (12%) | 1 (0%) | 30 | 63 |
| 3 | C | 205/207 (99%) | 190 (93%) | 15 (7%) | 0 | 100 | 100 |
| 4 | D | 206/208 (99%) | 200 (97%) | 5 (2%) | 1 (0%) | 25 | 58 |
| 5 | E | 149/151 (99%) | 145 (97%) | 4 (3%) | 0 | 100 | 100 |
| 6 | F | 99/101 (98%) | 96 (97%) | 3 (3%) | 0 | 100 | 100 |
| 7 | G | 153/155 (99%) | 144 (94%) | 9 (6%) | 0 | 100 | 100 |
| 8 | H | 136/138 (99%) | 133 (98%) | 3 (2%) | 0 | 100 | 100 |
| 9 | I | 125/127 (98%) | 114 (91%) | 10 (8%) | 1 (1%) | 16 | 49 |
| 10 | J | 97/99 (98%) | 78 (80%) | 17 (18%) | 2 (2%) | 5 | 29 |
| 11 | K | 117/119 (98%) | 105 (90%) | 12 (10%) | 0 | 100 | 100 |
| 12 | L | 122/125 (98%) | 111 (91%) | 10 (8%) | 1 (1%) | 16 | 49 |
| 13 | M | 116/118 (98%) | 109 (94%) | 7 (6%) | 0 | 100 | 100 |
| 14 | N | 58/60 (97%) | 54 (93%) | 4 (7%) | 0 | 100 | 100 |
| 15 | O | 86/88 (98%) | 83 (96%) | 3 (4%) | 0 | 100 | 100 |
| 16 | P | 82/84 (98%) | 78 (95%) | 4 (5%) | 0 | 100 | 100 |
| 17 | Q | 97/99 (98%) | 94 (97%) | 3 (3%) | 0 | 100 | 100 |
| 18 | R | 71/73 (97%) | 67 (94%) | 4 (6%) | 0 | 100 | 100 |
| 19 | S | 79/81 (98%) | 71 (90%) | 7 (9%) | 1 (1%) | 10 | 38 |
| 20 | T | 97/99 (98%) | 85 (88%) | 12 (12%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 21 | U | 23/25 (92%) | 22 (96%) | 1 (4%) | 0 | 100 | 100 |
| All | All | 2352/2393 (98%) | 2184 (93%) | 161 (7%) | 7 (0%) | 37 | 68 |

All (7) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | L | 28 | LYS |
| 19 | S | 31 | ILE |
| 10 | J | 72 | VAL |
| 9 | I | 119 | ALA |
| 10 | J | 34 | VAL |
| 4 | D | 5 | ILE |
| 2 | B | 229 | VAL |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2 | B | 194/204 (95%) | 180 (93%) | 14 (7%) | 12 | 38 |
| 3 | C | 160/161 (99%) | 151 (94%) | 9 (6%) | 17 | 45 |
| 4 | D | 180/180 (100%) | 171 (95%) | 9 (5%) | 20 | 48 |
| 5 | E | 115/116 (99%) | 102 (89%) | 13 (11%) | 4 | 21 |
| 6 | F | 90/90 (100%) | 83 (92%) | 7 (8%) | 10 | 34 |
| 7 | G | 126/126 (100%) | 119 (94%) | 7 (6%) | 17 | 45 |
| 8 | H | 119/119 (100%) | 110 (92%) | 9 (8%) | 11 | 35 |
| 9 | I | 98/98 (100%) | 90 (92%) | 8 (8%) | 9 | 33 |
| 10 | J | 87/89 (98%) | 81 (93%) | 6 (7%) | 13 | 39 |
| 11 | K | 90/90 (100%) | 84 (93%) | 6 (7%) | 13 | 40 |
| 12 | L | 103/103 (100%) | 97 (94%) | 6 (6%) | 17 | 44 |
| 13 | M | 94/94 (100%) | 85 (90%) | 9 (10%) | 7 | 27 |
| 14 | N | 49/49 (100%) | 47 (96%) | 2 (4%) | 26 | 54 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 15 | O | 79/79 (100%) | 71 (90%) | 8 (10%) | 6 | 25 |
| 16 | P | 72/72 (100%) | 68 (94%) | 4 (6%) | 17 | 45 |
| 17 | Q | 94/94 (100%) | 88 (94%) | 6 (6%) | 14 | 41 |
| 18 | R | 64/64 (100%) | 61 (95%) | 3 (5%) | 22 | 51 |
| 19 | S | 71/71 (100%) | 62 (87%) | 9 (13%) | 3 | 17 |
| 20 | T | 76/76 (100%) | 67 (88%) | 9 (12%) | 4 | 19 |
| 21 | U | 19/20 (95%) | 18 (95%) | 1 (5%) | 19 | 46 |
| All | All | 1980/1995 (99%) | 1835 (93%) | 145 (7%) | 11 | 37 |

All (145) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 24 | TRP |
| 2 | B | 46 | LYS |
| 2 | B | 82 | ARG |
| 2 | B | 114 | ARG |
| 2 | B | 139 | LYS |
| 2 | B | 142 | LEU |
| 2 | B | 144 | ARG |
| 2 | B | 150 | SER |
| 2 | B | 157 | ARG |
| 2 | B | 187 | LEU |
| 2 | B | 190 | THR |
| 2 | B | 208 | ILE |
| 2 | B | 221 | LEU |
| 2 | B | 236 | TYR |
| 3 | C | 3 | ASN |
| 3 | C | 27 | LYS |
| 3 | C | 43 | LEU |
| 3 | C | 82 | GLU |
| 3 | C | 91 | LEU |
| 3 | C | 95 | THR |
| 3 | C | 126 | ARG |
| 3 | C | 167 | TRP |
| 3 | C | 204 | LEU |
| 4 | D | 3 | ARG |
| 4 | D | 4 | TYR |
| 4 | D | 8 | VAL |
| 4 | D | 15 | GLU |
| 4 | D | 64 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | D | 70 | ILE |
| 4 | D | 122 | ARG |
| 4 | D | 127 | THR |
| 4 | D | 135 | LEU |
| 5 | E | 6 | PHE |
| 5 | E | 10 | MET |
| 5 | E | 12 | LEU |
| 5 | E | 16 | THR |
| 5 | E | 24 | ARG |
| 5 | E | 31 | LEU |
| 5 | E | 41 | VAL |
| 5 | E | 64 | ARG |
| 5 | E | 76 | ILE |
| 5 | E | 79 | GLU |
| 5 | E | 80 | ILE |
| 5 | E | 89 | ILE |
| 5 | E | 150 | ARG |
| 6 | F | 10 | LEU |
| 6 | F | 24 | GLU |
| 6 | F | 43 | LEU |
| 6 | F | 69 | GLU |
| 6 | F | 73 | ASN |
| 6 | F | 86 | ARG |
| 6 | F | 100 | ASN |
| 7 | G | 8 | GLU |
| 7 | G | 11 | GLN |
| 7 | G | 48 | LYS |
| 7 | G | 114 | ARG |
| 7 | G | 124 | LEU |
| 7 | G | 149 | ARG |
| 7 | G | 156 | TRP |
| 8 | H | 25 | ASP |
| 8 | H | 26 | VAL |
| 8 | H | 39 | LEU |
| 8 | H | 85 | ARG |
| 8 | H | 91 | ARG |
| 8 | H | 92 | ARG |
| 8 | H | 102 | ARG |
| 8 | H | 105 | ARG |
| 8 | H | 133 | LEU |
| 9 | I | 12 | GLU |
| 9 | I | 35 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | I | 79 | LEU |
| 9 | I | 102 | LEU |
| 9 | I | 104 | ARG |
| 9 | I | 112 | LYS |
| 9 | I | 118 | LYS |
| 9 | I | 121 | ARG |
| 10 | J | 59 | SER |
| 10 | J | 62 | HIS |
| 10 | J | 71 | LEU |
| 10 | J | 74 | ILE |
| 10 | J | 80 | LYS |
| 10 | J | 83 | GLU |
| 11 | K | 11 | LYS |
| 11 | K | 29 | ILE |
| 11 | K | 48 | ILE |
| 11 | K | 91 | ARG |
| 11 | K | 92 | GLU |
| 11 | K | 117 | ASN |
| 12 | L | 20 | LYS |
| 12 | L | 33 | ARG |
| 12 | L | 53 | ARG |
| 12 | L | 93 | LEU |
| 12 | L | 100 | ILE |
| 12 | L | 111 | LYS |
| 13 | M | 44 | ARG |
| 13 | M | 56 | LEU |
| 13 | M | 58 | GLU |
| 13 | M | 62 | ASN |
| 13 | M | 63 | THR |
| 13 | M | 64 | TRP |
| 13 | M | 94 | ARG |
| 13 | M | 110 | ARG |
| 13 | M | 115 | LYS |
| 14 | N | 9 | LYS |
| 14 | N | 22 | THR |
| 15 | O | 5 | LYS |
| 15 | O | 6 | GLU |
| 15 | O | 21 | ASP |
| 15 | O | 34 | LEU |
| 15 | O | 39 | LEU |
| 15 | O | 57 | LEU |
| 15 | O | 70 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15 | O | 81 | LEU |
| 16 | P | 1 | MET |
| 16 | P | 2 | VAL |
| 16 | P | 20 | VAL |
| 16 | P | 53 | VAL |
| 17 | Q | 38 | ARG |
| 17 | Q | 52 | LYS |
| 17 | Q | 68 | ARG |
| 17 | Q | 74 | LEU |
| 17 | Q | 78 | GLU |
| 17 | Q | 98 | LEU |
| 18 | R | 39 | VAL |
| 18 | R | 47 | THR |
| 18 | R | 66 | LEU |
| 19 | S | 3 | ARG |
| 19 | S | 7 | LYS |
| 19 | S | 12 | ASP |
| 19 | S | 15 | LEU |
| 19 | S | 31 | ILE |
| 19 | S | 36 | ARG |
| 19 | S | 62 | ILE |
| 19 | S | 65 | ASN |
| 19 | S | 81 | ARG |
| 20 | T | 8 | ARG |
| 20 | T | 48 | LYS |
| 20 | T | 54 | LYS |
| 20 | T | 56 | MET |
| 20 | T | 57 | ARG |
| 20 | T | 73 | HIS |
| 20 | T | 74 | LYS |
| 20 | T | 75 | ASN |
| 20 | T | 84 | LEU |
| 21 | U | 9 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 6 | HIS |
| 4 | D | 119 | GLN |
| 9 | I | 73 | GLN |
| 13 | M | 106 | ASN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | A | 1507/1522 (99%) | 223 (14%) | 42 (2%) |
| 22 | a | 4/6 (66%) | 1 (25%) | 0 |
| 23 | b | 8/11 (72%) | 2 (25%) | 0 |
| All | All | 1519/1539 (98%) | 226 (14%) | 42 (2%) |

All (226) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | A | 7 | G |
| 1 | A | 9 | G |
| 1 | A | 32 | A |
| 1 | A | 39 | G |
| 1 | A | 47 | C |
| 1 | A | 48 | C |
| 1 | A | 51 | A |
| 1 | A | 59 | A |
| 1 | A | 61 | G |
| 1 | A | 63 | C |
| 1 | A | 101 | A |
| 1 | A | 116 | A |
| 1 | A | 117 | G |
| 1 | A | 121 | C |
| 1 | A | 129(A) | G |
| 1 | A | 130 | A |
| 1 | A | 131 | C |
| 1 | A | 163 | C |
| 1 | A | 182 | U |
| 1 | A | 190(E) | U |
| 1 | A | 195 | A |
| 1 | A | 197 | A |
| 1 | A | 201 | C |
| 1 | A | 202 | U |
| 1 | A | 204 | U |
| 1 | A | 216 | G |
| 1 | A | 220 | G |
| 1 | A | 244 | U |
| 1 | A | 245 | C |
| 1 | A | 247 | G |
| 1 | A | 251 | G |
| 1 | A | 267 | C |
| 1 | A | 289 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 298 | A |
| 1 | A | 301 | G |
| 1 | A | 321 | A |
| 1 | A | 328 | C |
| 1 | A | 329 | A |
| 1 | A | 332 | G |
| 1 | A | 344 | A |
| 1 | A | 347 | G |
| 1 | A | 351 | G |
| 1 | A | 352 | C |
| 1 | A | 353 | A |
| 1 | A | 354 | G |
| 1 | A | 367 | U |
| 1 | A | 373 | A |
| 1 | A | 384 | G |
| 1 | A | 390 | C |
| 1 | A | 397 | A |
| 1 | A | 398 | C |
| 1 | A | 406 | G |
| 1 | A | 412 | A |
| 1 | A | 413 | G |
| 1 | A | 414 | A |
| 1 | A | 421 | U |
| 1 | A | 424 | G |
| 1 | A | 429 | U |
| 1 | A | 433 | C |
| 1 | A | 439 | A |
| 1 | A | 442 | C |
| 1 | A | 452 | A |
| 1 | A | 460 | A |
| 1 | A | 461 | C |
| 1 | A | 485 | G |
| 1 | A | 497 | A |
| 1 | A | 498 | U |
| 1 | A | 509 | A |
| 1 | A | 510 | A |
| 1 | A | 511 | C |
| 1 | A | 518 | C |
| 1 | A | 521 | G |
| 1 | A | 527 | 7MG |
| 1 | A | 531 | U |
| 1 | A | 532 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 533 | A |
| 1 | A | 545 | C |
| 1 | A | 547 | A |
| 1 | A | 559 | A |
| 1 | A | 560 | U |
| 1 | A | 562 | C |
| 1 | A | 563 | A |
| 1 | A | 564 | C |
| 1 | A | 572 | A |
| 1 | A | 573 | A |
| 1 | A | 576 | G |
| 1 | A | 577 | G |
| 1 | A | 579 | G |
| 1 | A | 588 | G |
| 1 | A | 607 | A |
| 1 | A | 630 | G |
| 1 | A | 631 | G |
| 1 | A | 632 | A |
| 1 | A | 653 | A |
| 1 | A | 665 | A |
| 1 | A | 687 | A |
| 1 | A | 688 | G |
| 1 | A | 702 | A |
| 1 | A | 703 | G |
| 1 | A | 721 | G |
| 1 | A | 723 | U |
| 1 | A | 731 | G |
| 1 | A | 748 | C |
| 1 | A | 749 | C |
| 1 | A | 755 | G |
| 1 | A | 777 | A |
| 1 | A | 781 | A |
| 1 | A | 782 | A |
| 1 | A | 793 | U |
| 1 | A | 794 | A |
| 1 | A | 813 | U |
| 1 | A | 817 | C |
| 1 | A | 819 | A |
| 1 | A | 828 | A |
| 1 | A | 839 | U |
| 1 | A | 840 | C |
| 1 | A | 841 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 848 | C |
| 1 | A | 902 | G |
| 1 | A | 914 | A |
| 1 | A | 926 | G |
| 1 | A | 927 | G |
| 1 | A | 934 | C |
| 1 | A | 935 | A |
| 1 | A | 960 | U |
| 1 | A | 961 | U |
| 1 | A | 965 | A |
| 1 | A | 966 | M2G |
| 1 | A | 967 | 5MC |
| 1 | A | 968 | A |
| 1 | A | 969 | A |
| 1 | A | 971 | G |
| 1 | A | 974 | A |
| 1 | A | 975 | A |
| 1 | A | 976 | G |
| 1 | A | 977 | A |
| 1 | A | 989 | C |
| 1 | A | 991 | U |
| 1 | A | 992 | U |
| 1 | A | 993 | G |
| 1 | A | 994 | A |
| 1 | A | 1005 | A |
| 1 | A | 1025 | U |
| 1 | A | 1026 | G |
| 1 | A | 1027 | C |
| 1 | A | 1028 | C |
| 1 | A | 1031 | G |
| 1 | A | 1050 | G |
| 1 | A | 1054 | C |
| 1 | A | 1055 | A |
| 1 | A | 1065 | U |
| 1 | A | 1066 | C |
| 1 | A | 1068 | G |
| 1 | A | 1094 | G |
| 1 | A | 1095 | U |
| 1 | A | 1101 | A |
| 1 | A | 1108 | G |
| 1 | A | 1125 | U |
| 1 | A | 1126 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1127 | G |
| 1 | A | 1129 | C |
| 1 | A | 1130 | A |
| 1 | A | 1131 | G |
| 1 | A | 1137 | C |
| 1 | A | 1138 | G |
| 1 | A | 1139 | G |
| 1 | A | 1152 | A |
| 1 | A | 1158 | C |
| 1 | A | 1159 | U |
| 1 | A | 1171 | G |
| 1 | A | 1180 | A |
| 1 | A | 1181 | G |
| 1 | A | 1183 | A |
| 1 | A | 1196 | U |
| 1 | A | 1197 | G |
| 1 | A | 1201 | A |
| 1 | A | 1202 | G |
| 1 | A | 1212 | U |
| 1 | A | 1213 | A |
| 1 | A | 1214 | C |
| 1 | A | 1227 | A |
| 1 | A | 1238 | A |
| 1 | A | 1257 | U |
| 1 | A | 1258 | G |
| 1 | A | 1270 | C |
| 1 | A | 1280 | A |
| 1 | A | 1281 | U |
| 1 | A | 1282 | C |
| 1 | A | 1286 | A |
| 1 | A | 1287 | A |
| 1 | A | 1300 | G |
| 1 | A | 1301 | U |
| 1 | A | 1302 | U |
| 1 | A | 1312 | G |
| 1 | A | 1320 | C |
| 1 | A | 1322 | C |
| 1 | A | 1332 | A |
| 1 | A | 1338 | G |
| 1 | A | 1348 | U |
| 1 | A | 1353 | G |
| 1 | A | 1362 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1363 | A |
| 1 | A | 1370 | G |
| 1 | A | 1381 | U |
| 1 | A | 1397 | C |
| 1 | A | 1398 | A |
| 1 | A | 1421 | G |
| 1 | A | 1442 | G |
| 1 | A | 1443 | G |
| 1 | A | 1446 | A |
| 1 | A | 1487 | G |
| 1 | A | 1492 | A |
| 1 | A | 1497 | G |
| 1 | A | 1499 | A |
| 1 | A | 1502 | A |
| 1 | A | 1503 | A |
| 1 | A | 1504 | G |
| 1 | A | 1505 | G |
| 1 | A | 1506 | U |
| 1 | A | 1517 | G |
| 1 | A | 1520 | G |
| 1 | A | 1529 | G |
| 1 | A | 1530 | G |
| 22 | a | 6 | U |
| 23 | b | 32 | C |
| 23 | b | 33 | U |

All (42) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | A | 60 | A |
| 1 | A | 115 | G |
| 1 | A | 129(A) | G |
| 1 | A | 181 | G |
| 1 | A | 250 | A |
| 1 | A | 266 | G |
| 1 | A | 328 | C |
| 1 | A | 329 | A |
| 1 | A | 372 | C |
| 1 | A | 428 | G |
| 1 | A | 432 | A |
| 1 | A | 484 | G |
| 1 | A | 496 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 509 | A |
| 1 | A | 530 | G |
| 1 | A | 532 | A |
| 1 | A | 559 | A |
| 1 | A | 687 | A |
| 1 | A | 701 | C |
| 1 | A | 748 | C |
| 1 | A | 812 | C |
| 1 | A | 913 | A |
| 1 | A | 960 | U |
| 1 | A | 965 | A |
| 1 | A | 1049 | U |
| 1 | A | 1065 | U |
| 1 | A | 1067 | A |
| 1 | A | 1129 | C |
| 1 | A | 1179 | A |
| 1 | A | 1182 | G |
| 1 | A | 1201 | A |
| 1 | A | 1212 | U |
| 1 | A | 1256 | A |
| 1 | A | 1281 | U |
| 1 | A | 1285 | A |
| 1 | A | 1300 | G |
| 1 | A | 1301 | U |
| 1 | A | 1331 | G |
| 1 | A | 1347 | G |
| 1 | A | 1443 | G |
| 1 | A | 1505 | G |
| 1 | A | 1528 | U |

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

19 non-standard protein/DNA/RNA residues are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 23 | PSU | b | 39 | 23 | 18,21,22 | 1.97 | 7 (38%) | 21,30,33 | 1.62 | 3 (14%) |
| 1 | 2MG | A | 1207 | 1 | 18,26,27 | 1.34 | 4 (22%) | 16,38,41 | 1.45 | 2 (12%) |
| 1 | MA6 | A | 1518 | 1 | 19,26,27 | 0.84 | 1 (5%) | 18,38,41 | 0.83 | 0 |
| 1 | 4OC | A | 1402 | 1 | 20,23,24 | 0.96 | 2 (10%) | 25,32,35 | 0.77 | 0 |
| 23 | 70U | b | 34 | 23 | 22,26,27 | 3.55 | 10 (45%) | 27,37,40 | 1.43 | 5 (18%) |
| 12 | 0TD | L | 92 | 12 | 8,9,10 | 2.49 | 1 (12%) | 6,11,13 | 2.12 | 4 (66%) |
| 1 | 5MC | A | 1400 | 1 | 19,22,23 | 1.06 | 2 (10%) | 26,32,35 | 1.02 | 2 (7%) |
| 1 | UR3 | A | 1498 | 1 | 19,22,23 | 0.71 | 1 (5%) | 26,32,35 | 1.06 | 1 (3%) |
| 1 | MA6 | A | 1519 | 26,1 | 19,26,27 | 0.97 | 1 (5%) | 18,38,41 | 0.69 | 0 |
| 1 | PSU | A | 1541 | 25,1 | 18,21,22 | 1.93 | 7 (38%) | 21,30,33 | 1.63 | 4 (19%) |
| 1 | M2G | A | 966 | 1 | 20,27,28 | 1.43 | 4 (20%) | 19,40,43 | 1.21 | 2 (10%) |
| 1 | 5MC | A | 1407 | 1 | 19,22,23 | 1.05 | 0 | 26,32,35 | 1.06 | 2 (7%) |
| 23 | 12A | b | 37 | 25,23 | 28,36,37 | 2.54 | 3 (10%) | 30,52,55 | 2.43 | 6 (20%) |
| 1 | 5MC | A | 967 | 1 | 19,22,23 | 1.03 | 2 (10%) | 26,32,35 | 0.96 | 2 (7%) |
| 1 | PSU | A | 516 | 25,1 | 18,21,22 | 2.04 | 7 (38%) | 21,30,33 | 1.55 | 4 (19%) |
| 1 | 5MC | A | 1404 | 1 | 19,22,23 | 1.41 | 1 (5%) | 26,32,35 | 0.89 | 2 (7%) |
| 22 | 6MZ | a | 3 | 22 | 17,25,26 | 0.98 | 1 (5%) | 15,36,39 | 0.52 | 0 |
| 1 | 7MG | A | 527 | 1 | 23,26,27 | 4.30 | 4 (17%) | 27,39,42 | 2.22 | 9 (33%) |
| 1 | PSU | A | 1540 | 1 | 18,21,22 | 1.93 | 7 (38%) | 21,30,33 | 1.62 | 4 (19%) |

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 |
|-----|------|-------|------|------|---------|------------|---------|
| 23 | PSU | b | 39 | 23 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 2MG | A | 1207 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | MA6 | A | 1518 | 1 | - | 2/7/29/30 | 0/3/3/3 |
| 1 | 4OC | A | 1402 | 1 | - | 2/9/29/30 | 0/2/2/2 |
| 23 | 70U | b | 34 | 23 | - | 5/13/31/32 | 0/2/2/2 |
| 12 | 0TD | L | 92 | 12 | - | 3/7/12/14 | - |
| 1 | 5MC | A | 1400 | 1 | - | 2/7/25/26 | 0/2/2/2 |
| 1 | UR3 | A | 1498 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | MA6 | A | 1519 | 26,1 | - | 4/7/29/30 | 0/3/3/3 |
| 1 | PSU | A | 1541 | 25,1 | - | 1/7/25/26 | 0/2/2/2 |
| 1 | M2G | A | 966 | 1 | - | 3/7/29/30 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|-------|---------|------------|---------|
| 1 | 5MC | A | 1407 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 23 | 12A | b | 37 | 25,23 | - | 7/21/43/44 | 0/3/3/3 |
| 1 | 5MC | A | 967 | 1 | - | 2/7/25/26 | 0/2/2/2 |
| 1 | PSU | A | 516 | 25,1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MC | A | 1404 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | 6MZ | a | 3 | 22 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | 7MG | A | 527 | 1 | - | 2/7/37/38 | 0/3/3/3 |
| 1 | PSU | A | 1540 | 1 | - | 0/7/25/26 | 0/2/2/2 |

All (65) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 1 | A | 527 | 7MG | C8-N9 | -19.62 | 1.33 | 1.45 |
| 23 | b | 37 | 12A | C2-S2 | 11.11 | 1.84 | 1.75 |
| 23 | b | 34 | 70U | O4-C4 | 8.70 | 1.40 | 1.23 |
| 23 | b | 34 | 70U | C2-S2 | 8.33 | 1.81 | 1.67 |
| 12 | L | 92 | 0TD | CB-CA | -6.49 | 1.52 | 1.54 |
| 23 | b | 34 | 70U | C6-N1 | -5.88 | 1.28 | 1.38 |
| 1 | A | 1404 | 5MC | C5-C4 | -5.07 | 1.40 | 1.44 |
| 23 | b | 34 | 70U | C4-N3 | -5.02 | 1.29 | 1.38 |
| 23 | b | 37 | 12A | CC-N | 4.86 | 1.48 | 1.35 |
| 23 | b | 37 | 12A | CC-N6 | 4.17 | 1.46 | 1.37 |
| 23 | b | 34 | 70U | C5M-C5 | 4.10 | 1.57 | 1.51 |
| 1 | A | 527 | 7MG | C2-N2 | 3.94 | 1.43 | 1.34 |
| 1 | A | 516 | PSU | C2-N1 | -3.71 | 1.31 | 1.36 |
| 23 | b | 34 | 70U | O9-C8 | 3.70 | 1.44 | 1.33 |
| 1 | A | 516 | PSU | C6-C5 | 3.64 | 1.39 | 1.35 |
| 1 | A | 1540 | PSU | C6-C5 | 3.58 | 1.39 | 1.35 |
| 23 | b | 39 | PSU | C6-C5 | 3.56 | 1.39 | 1.35 |
| 1 | A | 1541 | PSU | C6-C5 | 3.55 | 1.39 | 1.35 |
| 23 | b | 39 | PSU | C2-N1 | -3.50 | 1.32 | 1.36 |
| 23 | b | 34 | 70U | O9-C9 | -3.46 | 1.37 | 1.45 |
| 23 | b | 39 | PSU | C4-N3 | -3.36 | 1.32 | 1.38 |
| 1 | A | 516 | PSU | C4-N3 | -3.35 | 1.32 | 1.38 |
| 1 | A | 1540 | PSU | C4-N3 | -3.33 | 1.32 | 1.38 |
| 23 | b | 34 | 70U | C4-C5 | -3.32 | 1.37 | 1.45 |
| 1 | A | 1541 | PSU | C2-N1 | -3.32 | 1.32 | 1.36 |
| 1 | A | 1540 | PSU | C2-N1 | -3.27 | 1.32 | 1.36 |
| 1 | A | 516 | PSU | C2-N3 | -3.26 | 1.32 | 1.37 |
| 1 | A | 1541 | PSU | C4-N3 | -3.26 | 1.32 | 1.38 |
| 1 | A | 966 | M2G | C6-N1 | 3.20 | 1.42 | 1.37 |
| 23 | b | 39 | PSU | C2-N3 | -3.16 | 1.32 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | A | 1540 | PSU | C2-N3 | -3.15 | 1.32 | 1.37 |
| 1 | A | 1541 | PSU | C2-N3 | -3.12 | 1.32 | 1.37 |
| 23 | b | 34 | 70U | C6-C5 | 2.98 | 1.43 | 1.35 |
| 1 | A | 1207 | 2MG | C2-N2 | 2.95 | 1.39 | 1.33 |
| 1 | A | 966 | M2G | C2-N2 | 2.90 | 1.40 | 1.35 |
| 1 | A | 966 | M2G | C2-N3 | 2.75 | 1.34 | 1.30 |
| 1 | A | 1207 | 2MG | C5-C6 | -2.73 | 1.42 | 1.47 |
| 1 | A | 1207 | 2MG | C6-N1 | 2.72 | 1.42 | 1.37 |
| 1 | A | 516 | PSU | O4-C4 | -2.69 | 1.18 | 1.23 |
| 1 | A | 1400 | 5MC | C2-N1 | 2.67 | 1.45 | 1.40 |
| 1 | A | 966 | M2G | C5-C6 | -2.64 | 1.42 | 1.47 |
| 1 | A | 1519 | MA6 | C6-N1 | 2.54 | 1.36 | 1.32 |
| 23 | b | 34 | 70U | C2-N3 | -2.51 | 1.31 | 1.38 |
| 23 | b | 39 | PSU | O4-C4 | -2.49 | 1.18 | 1.23 |
| 1 | A | 1402 | 4OC | C2-N3 | 2.47 | 1.41 | 1.36 |
| 1 | A | 967 | 5MC | C2-N1 | 2.47 | 1.45 | 1.40 |
| 1 | A | 527 | 7MG | C5-N7 | 2.46 | 1.38 | 1.35 |
| 1 | A | 1540 | PSU | O4-C4 | -2.45 | 1.18 | 1.23 |
| 1 | A | 1541 | PSU | O4-C4 | -2.42 | 1.19 | 1.23 |
| 1 | A | 1207 | 2MG | C2-N1 | 2.38 | 1.40 | 1.36 |
| 1 | A | 527 | 7MG | C4-N3 | 2.36 | 1.39 | 1.34 |
| 1 | A | 967 | 5MC | C2-N3 | 2.36 | 1.41 | 1.36 |
| 1 | A | 1541 | PSU | C6-N1 | -2.30 | 1.32 | 1.36 |
| 23 | b | 39 | PSU | C6-N1 | -2.29 | 1.32 | 1.36 |
| 1 | A | 1518 | MA6 | C6-N1 | 2.22 | 1.35 | 1.32 |
| 1 | A | 1540 | PSU | C6-N1 | -2.22 | 1.32 | 1.36 |
| 1 | A | 1498 | UR3 | C2-N1 | 2.21 | 1.41 | 1.38 |
| 22 | a | 3 | 6MZ | C6-N1 | 2.20 | 1.36 | 1.34 |
| 1 | A | 516 | PSU | O2-C2 | -2.15 | 1.18 | 1.23 |
| 23 | b | 39 | PSU | O2-C2 | -2.15 | 1.18 | 1.23 |
| 1 | A | 516 | PSU | C6-N1 | -2.12 | 1.32 | 1.36 |
| 1 | A | 1400 | 5MC | C2-N3 | 2.12 | 1.40 | 1.36 |
| 1 | A | 1540 | PSU | O2-C2 | -2.10 | 1.18 | 1.23 |
| 1 | A | 1541 | PSU | O2-C2 | -2.10 | 1.18 | 1.23 |
| 1 | A | 1402 | 4OC | O2-C2 | -2.01 | 1.20 | 1.23 |

All (52) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 23 | b | 37 | 12A | C2M-S2-C2 | 10.14 | 109.86 | 102.25 |
| 1 | A | 527 | 7MG | C5-C6-N1 | 4.95 | 119.66 | 110.94 |
| 1 | A | 527 | 7MG | C2-N3-C4 | 4.75 | 120.48 | 112.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | b | 37 | 12A | N6-CC-N | 4.57 | 120.06 | 113.77 |
| 1 | A | 1540 | PSU | N1-C2-N3 | 4.52 | 119.93 | 115.17 |
| 1 | A | 1541 | PSU | N1-C2-N3 | 4.49 | 119.91 | 115.17 |
| 23 | b | 39 | PSU | N1-C2-N3 | 4.46 | 119.87 | 115.17 |
| 1 | A | 527 | 7MG | N9-C4-N3 | 4.45 | 131.97 | 125.46 |
| 23 | b | 34 | 70U | O9-C8-C5M | 4.36 | 120.08 | 111.28 |
| 1 | A | 1207 | 2MG | O6-C6-N1 | -4.16 | 115.68 | 120.62 |
| 1 | A | 527 | 7MG | C5-C4-N3 | -4.12 | 120.40 | 128.13 |
| 1 | A | 516 | PSU | N1-C2-N3 | 4.05 | 119.44 | 115.17 |
| 1 | A | 527 | 7MG | N9-C8-N7 | 3.57 | 108.42 | 103.37 |
| 1 | A | 1207 | 2MG | O6-C6-C5 | 3.41 | 131.07 | 124.32 |
| 1 | A | 1541 | PSU | C4-N3-C2 | -3.27 | 121.87 | 126.37 |
| 1 | A | 1540 | PSU | C4-N3-C2 | -3.23 | 121.92 | 126.37 |
| 1 | A | 966 | M2G | O6-C6-C5 | 3.17 | 130.61 | 124.32 |
| 23 | b | 39 | PSU | C4-N3-C2 | -3.14 | 122.04 | 126.37 |
| 23 | b | 37 | 12A | OO-CC-N6 | -2.96 | 118.39 | 123.64 |
| 1 | A | 1498 | UR3 | C6-N1-C2 | -2.95 | 119.39 | 121.80 |
| 23 | b | 37 | 12A | N3-C2-N1 | -2.92 | 121.69 | 127.03 |
| 12 | L | 92 | 0TD | CSB-SB-CB | -2.92 | 97.12 | 102.36 |
| 23 | b | 39 | PSU | O2-C2-N1 | -2.89 | 119.81 | 122.79 |
| 23 | b | 34 | 70U | C5-C6-N1 | -2.82 | 119.14 | 122.94 |
| 1 | A | 527 | 7MG | C2-N1-C6 | -2.78 | 120.08 | 125.11 |
| 1 | A | 1541 | PSU | O2-C2-N1 | -2.77 | 119.93 | 122.79 |
| 1 | A | 516 | PSU | C4-N3-C2 | -2.77 | 122.56 | 126.37 |
| 1 | A | 527 | 7MG | O6-C6-C5 | -2.76 | 120.84 | 127.62 |
| 23 | b | 34 | 70U | C5-C4-N3 | 2.75 | 119.40 | 115.21 |
| 1 | A | 527 | 7MG | C6-C5-C4 | -2.74 | 117.58 | 122.40 |
| 1 | A | 966 | M2G | O6-C6-N1 | -2.65 | 117.47 | 120.62 |
| 1 | A | 1540 | PSU | O2-C2-N1 | -2.65 | 120.05 | 122.79 |
| 23 | b | 37 | 12A | CA-N-CC | 2.64 | 126.38 | 121.99 |
| 12 | L | 92 | 0TD | OD1-CG-CB | -2.62 | 116.95 | 122.44 |
| 1 | A | 516 | PSU | C6-C5-C4 | -2.52 | 116.47 | 118.17 |
| 1 | A | 1407 | 5MC | N4-C4-N3 | -2.43 | 114.11 | 118.51 |
| 1 | A | 527 | 7MG | C6-C5-N7 | 2.38 | 135.63 | 131.93 |
| 1 | A | 967 | 5MC | N4-C4-N3 | -2.37 | 114.22 | 118.51 |
| 1 | A | 516 | PSU | O2-C2-N1 | -2.35 | 120.36 | 122.79 |
| 23 | b | 37 | 12A | C4-C5-N7 | -2.34 | 106.87 | 109.34 |
| 1 | A | 1400 | 5MC | N4-C4-N3 | -2.31 | 114.33 | 118.51 |
| 1 | A | 1404 | 5MC | C5-C4-N3 | 2.22 | 124.03 | 121.75 |
| 1 | A | 1400 | 5MC | C5-C4-N3 | 2.20 | 124.01 | 121.75 |
| 1 | A | 1407 | 5MC | C5-C4-N3 | 2.16 | 123.97 | 121.75 |
| 12 | L | 92 | 0TD | CB-CA-N | -2.15 | 104.75 | 109.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | b | 34 | 70U | O4-C4-C5 | -2.13 | 121.13 | 124.71 |
| 23 | b | 34 | 70U | C5M-C5-C4 | 2.11 | 120.86 | 118.00 |
| 1 | A | 1540 | PSU | C5-C6-N1 | -2.09 | 119.24 | 122.14 |
| 1 | A | 967 | 5MC | C5-C4-N3 | 2.05 | 123.86 | 121.75 |
| 1 | A | 1404 | 5MC | N4-C4-N3 | -2.03 | 114.84 | 118.51 |
| 12 | L | 92 | 0TD | OD2-CG-CB | 2.02 | 117.51 | 113.15 |
| 1 | A | 1541 | PSU | C5-C6-N1 | -2.01 | 119.36 | 122.14 |

There are no chirality outliers.

All (33) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 1 | A | 966 | M2G | C4'-C5'-O5'-P |
| 1 | A | 967 | 5MC | O4'-C4'-C5'-O5' |
| 1 | A | 1402 | 4OC | O4'-C4'-C5'-O5' |
| 23 | b | 37 | 12A | N1-C2-S2-C2M |
| 23 | b | 37 | 12A | N3-C2-S2-C2M |
| 23 | b | 37 | 12A | CB-CA-N-CC |
| 23 | b | 37 | 12A | C-CA-CB-OG1 |
| 23 | b | 37 | 12A | C-CA-CB-CG2 |
| 23 | b | 34 | 70U | C5M-C8-O9-C9 |
| 1 | A | 527 | 7MG | C3'-C4'-C5'-O5' |
| 1 | A | 1519 | MA6 | C3'-C4'-C5'-O5' |
| 1 | A | 527 | 7MG | O4'-C4'-C5'-O5' |
| 1 | A | 1519 | MA6 | O4'-C4'-C5'-O5' |
| 23 | b | 34 | 70U | O8-C8-O9-C9 |
| 1 | A | 967 | 5MC | C3'-C4'-C5'-O5' |
| 1 | A | 1402 | 4OC | C3'-C4'-C5'-O5' |
| 1 | A | 1400 | 5MC | O4'-C4'-C5'-O5' |
| 1 | A | 966 | M2G | O4'-C4'-C5'-O5' |
| 1 | A | 1518 | MA6 | O4'-C4'-C5'-O5' |
| 1 | A | 1518 | MA6 | C3'-C4'-C5'-O5' |
| 1 | A | 966 | M2G | C3'-C4'-C5'-O5' |
| 23 | b | 37 | 12A | N-CA-CB-CG2 |
| 23 | b | 34 | 70U | C3'-C4'-C5'-O5' |
| 12 | L | 92 | 0TD | CG-CB-SB-CSB |
| 1 | A | 1400 | 5MC | C3'-C4'-C5'-O5' |
| 1 | A | 1519 | MA6 | C5-C6-N6-C10 |
| 12 | L | 92 | 0TD | SB-CB-CG-OD1 |
| 23 | b | 34 | 70U | O4'-C4'-C5'-O5' |
| 1 | A | 1541 | PSU | O4'-C1'-C5-C4 |
| 23 | b | 37 | 12A | C5-C6-N6-CC |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|--------------|
| 1 | A | 1519 | MA6 | N1-C6-N6-C9 |
| 23 | b | 34 | 70U | C5-C5M-C8-O9 |
| 12 | L | 92 | 0TD | SB-CB-CG-OD2 |

There are no ring outliers.

7 monomers are involved in 13 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1 | A | 1207 | 2MG | 2 | 0 |
| 1 | A | 1402 | 4OC | 1 | 0 |
| 12 | L | 92 | 0TD | 5 | 0 |
| 1 | A | 1400 | 5MC | 1 | 0 |
| 1 | A | 1498 | UR3 | 2 | 0 |
| 1 | A | 1519 | MA6 | 1 | 0 |
| 1 | A | 966 | M2G | 2 | 0 |

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 355 ligands modelled in this entry, 349 are monoatomic - leaving 6 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 | $\# Z > 2$ |
| 24 | PAR | A | 1601 | - | 44,45,45 | 1.20 | 4 (9%) | 63,67,67 | 1.64 | 12 (19%) |
| 24 | PAR | A | 1605 | - | 44,45,45 | 1.25 | 5 (11%) | 63,67,67 | 1.64 | 11 (17%) |
| 24 | PAR | A | 1606 | - | 44,45,45 | 1.27 | 4 (9%) | 63,67,67 | 1.66 | 11 (17%) |
| 24 | PAR | A | 1603 | - | 44,45,45 | 1.39 | 5 (11%) | 63,67,67 | 1.68 | 12 (19%) |
| 24 | PAR | A | 1604 | - | 44,45,45 | 1.26 | 6 (13%) | 63,67,67 | 1.64 | 12 (19%) |
| 24 | PAR | A | 1602 | - | 44,45,45 | 1.29 | 7 (15%) | 63,67,67 | 1.66 | 11 (17%) |

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 |
|-----|------|-------|------|------|---------|------------|---------|
| 24 | PAR | A | 1601 | - | - | 6/18/94/94 | 0/4/4/4 |
| 24 | PAR | A | 1605 | - | - | 4/18/94/94 | 1/4/4/4 |
| 24 | PAR | A | 1606 | - | - | 5/18/94/94 | 1/4/4/4 |
| 24 | PAR | A | 1603 | - | - | 6/18/94/94 | 1/4/4/4 |
| 24 | PAR | A | 1604 | - | - | 5/18/94/94 | 1/4/4/4 |
| 24 | PAR | A | 1602 | - | - | 4/18/94/94 | 0/4/4/4 |

All (31) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 24 | A | 1603 | PAR | C13-C23 | 4.74 | 1.59 | 1.52 |
| 24 | A | 1601 | PAR | C52-C42 | 3.90 | 1.60 | 1.52 |
| 24 | A | 1602 | PAR | C13-C23 | 3.56 | 1.57 | 1.52 |
| 24 | A | 1603 | PAR | C52-C42 | 3.54 | 1.59 | 1.52 |
| 24 | A | 1606 | PAR | C13-C23 | 3.53 | 1.57 | 1.52 |
| 24 | A | 1604 | PAR | C52-C42 | 3.21 | 1.58 | 1.52 |
| 24 | A | 1605 | PAR | C13-C23 | 3.14 | 1.56 | 1.52 |
| 24 | A | 1605 | PAR | C52-C42 | 2.88 | 1.58 | 1.52 |
| 24 | A | 1606 | PAR | C31-C21 | 2.87 | 1.57 | 1.53 |
| 24 | A | 1606 | PAR | C52-C42 | 2.84 | 1.58 | 1.52 |
| 24 | A | 1605 | PAR | C34-C24 | 2.79 | 1.57 | 1.53 |
| 24 | A | 1604 | PAR | C13-C23 | 2.66 | 1.56 | 1.52 |
| 24 | A | 1603 | PAR | O43-C13 | 2.66 | 1.46 | 1.41 |
| 24 | A | 1604 | PAR | C34-C24 | 2.56 | 1.56 | 1.53 |
| 24 | A | 1606 | PAR | C34-C24 | 2.55 | 1.56 | 1.53 |
| 24 | A | 1602 | PAR | C31-C21 | 2.45 | 1.56 | 1.53 |
| 24 | A | 1602 | PAR | C34-C24 | 2.45 | 1.56 | 1.53 |
| 24 | A | 1603 | PAR | C34-C24 | 2.40 | 1.56 | 1.53 |
| 24 | A | 1604 | PAR | C31-C21 | 2.39 | 1.56 | 1.53 |
| 24 | A | 1602 | PAR | C52-C42 | 2.38 | 1.57 | 1.52 |
| 24 | A | 1603 | PAR | C14-C24 | 2.34 | 1.56 | 1.52 |
| 24 | A | 1604 | PAR | C33-C43 | 2.29 | 1.58 | 1.52 |
| 24 | A | 1602 | PAR | C14-C24 | 2.24 | 1.56 | 1.52 |
| 24 | A | 1601 | PAR | C62-C52 | 2.24 | 1.58 | 1.52 |
| 24 | A | 1601 | PAR | C13-C23 | 2.20 | 1.55 | 1.52 |
| 24 | A | 1605 | PAR | C33-C43 | 2.20 | 1.58 | 1.52 |
| 24 | A | 1605 | PAR | C14-C24 | 2.19 | 1.56 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 24 | A | 1604 | PAR | C14-C24 | 2.15 | 1.56 | 1.52 |
| 24 | A | 1602 | PAR | C11-C21 | 2.14 | 1.56 | 1.52 |
| 24 | A | 1601 | PAR | C33-C43 | 2.11 | 1.58 | 1.52 |
| 24 | A | 1602 | PAR | C33-C43 | 2.05 | 1.58 | 1.52 |

All (69) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24 | A | 1603 | PAR | O33-C14-C24 | 6.55 | 118.80 | 108.08 |
| 24 | A | 1606 | PAR | O33-C14-C24 | 6.51 | 118.73 | 108.08 |
| 24 | A | 1604 | PAR | O33-C14-C24 | 6.50 | 118.72 | 108.08 |
| 24 | A | 1602 | PAR | O33-C14-C24 | 6.49 | 118.70 | 108.08 |
| 24 | A | 1605 | PAR | O33-C14-C24 | 6.47 | 118.66 | 108.08 |
| 24 | A | 1601 | PAR | O33-C14-C24 | 6.44 | 118.61 | 108.08 |
| 24 | A | 1603 | PAR | C13-C23-C33 | 3.87 | 106.75 | 102.10 |
| 24 | A | 1606 | PAR | C13-C23-C33 | 3.65 | 106.49 | 102.10 |
| 24 | A | 1602 | PAR | C13-C23-C33 | 3.49 | 106.30 | 102.10 |
| 24 | A | 1605 | PAR | C13-C23-C33 | 3.22 | 105.97 | 102.10 |
| 24 | A | 1601 | PAR | C34-C24-N24 | -3.17 | 104.55 | 111.05 |
| 24 | A | 1603 | PAR | C34-C24-N24 | -3.13 | 104.63 | 111.05 |
| 24 | A | 1605 | PAR | C34-C24-N24 | -3.13 | 104.64 | 111.05 |
| 24 | A | 1602 | PAR | O11-C11-O51 | 3.10 | 118.84 | 110.69 |
| 24 | A | 1606 | PAR | C34-C24-N24 | -3.08 | 104.75 | 111.05 |
| 24 | A | 1601 | PAR | O11-C11-O51 | 3.07 | 118.76 | 110.69 |
| 24 | A | 1604 | PAR | C34-C24-N24 | -3.05 | 104.81 | 111.05 |
| 24 | A | 1602 | PAR | C34-C24-N24 | -3.05 | 104.81 | 111.05 |
| 24 | A | 1603 | PAR | O34-C34-C44 | -3.02 | 103.26 | 110.38 |
| 24 | A | 1601 | PAR | C13-C23-C33 | 3.01 | 105.72 | 102.10 |
| 24 | A | 1604 | PAR | C13-C23-C33 | 3.01 | 105.72 | 102.10 |
| 24 | A | 1603 | PAR | C14-O33-C33 | -3.01 | 110.85 | 117.98 |
| 24 | A | 1601 | PAR | O34-C34-C44 | -3.00 | 103.30 | 110.38 |
| 24 | A | 1606 | PAR | O52-C13-O43 | -2.98 | 108.33 | 111.37 |
| 24 | A | 1605 | PAR | O11-C11-O51 | 2.96 | 118.49 | 110.69 |
| 24 | A | 1602 | PAR | O34-C34-C44 | -2.92 | 103.48 | 110.38 |
| 24 | A | 1603 | PAR | O11-C11-O51 | 2.92 | 118.37 | 110.69 |
| 24 | A | 1604 | PAR | O34-C34-C44 | -2.92 | 103.50 | 110.38 |
| 24 | A | 1606 | PAR | O34-C34-C44 | -2.91 | 103.52 | 110.38 |
| 24 | A | 1604 | PAR | C13-O52-C52 | -2.88 | 111.16 | 117.98 |
| 24 | A | 1605 | PAR | O34-C34-C44 | -2.86 | 103.63 | 110.38 |
| 24 | A | 1606 | PAR | C14-O33-C33 | -2.85 | 111.21 | 117.98 |
| 24 | A | 1605 | PAR | C14-O33-C33 | -2.85 | 111.23 | 117.98 |
| 24 | A | 1604 | PAR | C14-O33-C33 | -2.83 | 111.26 | 117.98 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24 | A | 1604 | PAR | O11-C11-O51 | 2.79 | 118.04 | 110.69 |
| 24 | A | 1606 | PAR | C13-O52-C52 | -2.77 | 111.41 | 117.98 |
| 24 | A | 1602 | PAR | C14-O33-C33 | -2.76 | 111.45 | 117.98 |
| 24 | A | 1601 | PAR | C14-O33-C33 | -2.75 | 111.45 | 117.98 |
| 24 | A | 1606 | PAR | O11-C11-O51 | 2.74 | 117.90 | 110.69 |
| 24 | A | 1601 | PAR | O52-C13-O43 | -2.72 | 108.59 | 111.37 |
| 24 | A | 1605 | PAR | C13-O52-C52 | -2.64 | 111.72 | 117.98 |
| 24 | A | 1603 | PAR | C13-O52-C52 | -2.60 | 111.80 | 117.98 |
| 24 | A | 1602 | PAR | C13-O52-C52 | -2.58 | 111.85 | 117.98 |
| 24 | A | 1604 | PAR | O52-C13-O43 | -2.57 | 108.75 | 111.37 |
| 24 | A | 1603 | PAR | O52-C13-O43 | -2.51 | 108.81 | 111.37 |
| 24 | A | 1605 | PAR | O52-C13-O43 | -2.48 | 108.83 | 111.37 |
| 24 | A | 1602 | PAR | C22-C12-C62 | 2.43 | 113.72 | 110.08 |
| 24 | A | 1605 | PAR | O51-C51-C61 | 2.41 | 112.42 | 106.44 |
| 24 | A | 1603 | PAR | O51-C51-C61 | 2.39 | 112.37 | 106.44 |
| 24 | A | 1601 | PAR | C13-O52-C52 | -2.38 | 112.33 | 117.98 |
| 24 | A | 1601 | PAR | C11-O51-C51 | 2.35 | 118.31 | 113.72 |
| 24 | A | 1602 | PAR | O52-C13-O43 | -2.32 | 109.00 | 111.37 |
| 24 | A | 1602 | PAR | O51-C51-C61 | 2.29 | 112.13 | 106.44 |
| 24 | A | 1602 | PAR | C11-O51-C51 | 2.26 | 118.13 | 113.72 |
| 24 | A | 1606 | PAR | O51-C51-C61 | 2.25 | 112.02 | 106.44 |
| 24 | A | 1604 | PAR | O51-C51-C61 | 2.25 | 112.02 | 106.44 |
| 24 | A | 1601 | PAR | O51-C51-C61 | 2.19 | 111.87 | 106.44 |
| 24 | A | 1604 | PAR | O54-C54-C44 | 2.19 | 113.64 | 109.70 |
| 24 | A | 1606 | PAR | O54-C54-C44 | 2.17 | 113.62 | 109.70 |
| 24 | A | 1604 | PAR | C22-C12-C62 | 2.12 | 113.25 | 110.08 |
| 24 | A | 1603 | PAR | C22-C32-C42 | 2.11 | 114.68 | 109.50 |
| 24 | A | 1606 | PAR | C22-C12-C62 | 2.11 | 113.23 | 110.08 |
| 24 | A | 1605 | PAR | O54-C54-C44 | 2.08 | 113.45 | 109.70 |
| 24 | A | 1603 | PAR | C11-O51-C51 | 2.06 | 117.74 | 113.72 |
| 24 | A | 1601 | PAR | O33-C14-O54 | -2.05 | 105.31 | 110.69 |
| 24 | A | 1601 | PAR | O54-C54-C44 | 2.04 | 113.38 | 109.70 |
| 24 | A | 1604 | PAR | O52-C52-C42 | 2.04 | 112.59 | 107.42 |
| 24 | A | 1603 | PAR | O52-C52-C42 | 2.03 | 112.57 | 107.42 |
| 24 | A | 1605 | PAR | O33-C14-O54 | -2.02 | 105.38 | 110.69 |

There are no chirality outliers.

All (30) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 24 | A | 1601 | PAR | C43-C33-O33-C14 |
| 24 | A | 1602 | PAR | C23-C13-O52-C52 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 24 | A | 1602 | PAR | O43-C13-O52-C52 |
| 24 | A | 1603 | PAR | C44-C54-C64-N64 |
| 24 | A | 1603 | PAR | O54-C54-C64-N64 |
| 24 | A | 1604 | PAR | C21-C11-O11-C42 |
| 24 | A | 1605 | PAR | C21-C11-O11-C42 |
| 24 | A | 1605 | PAR | C44-C54-C64-N64 |
| 24 | A | 1605 | PAR | O54-C54-C64-N64 |
| 24 | A | 1606 | PAR | C23-C13-O52-C52 |
| 24 | A | 1606 | PAR | O51-C11-O11-C42 |
| 24 | A | 1602 | PAR | O54-C14-O33-C33 |
| 24 | A | 1605 | PAR | O51-C11-O11-C42 |
| 24 | A | 1606 | PAR | O54-C14-O33-C33 |
| 24 | A | 1603 | PAR | O51-C11-O11-C42 |
| 24 | A | 1601 | PAR | C33-C43-C53-O53 |
| 24 | A | 1601 | PAR | O43-C43-C53-O53 |
| 24 | A | 1606 | PAR | O43-C43-C53-O53 |
| 24 | A | 1606 | PAR | C33-C43-C53-O53 |
| 24 | A | 1603 | PAR | C41-C51-C61-O61 |
| 24 | A | 1604 | PAR | O54-C14-O33-C33 |
| 24 | A | 1601 | PAR | C44-C54-C64-N64 |
| 24 | A | 1601 | PAR | C52-C42-O11-C11 |
| 24 | A | 1604 | PAR | O43-C13-O52-C52 |
| 24 | A | 1604 | PAR | O54-C54-C64-N64 |
| 24 | A | 1601 | PAR | C24-C14-O33-C33 |
| 24 | A | 1602 | PAR | C43-C33-O33-C14 |
| 24 | A | 1603 | PAR | C23-C33-O33-C14 |
| 24 | A | 1604 | PAR | C23-C33-O33-C14 |
| 24 | A | 1603 | PAR | O51-C51-C61-O61 |

All (4) ring outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-------------------------|
| 24 | A | 1603 | PAR | C12-C22-C32-C42-C52-C62 |
| 24 | A | 1605 | PAR | C12-C22-C32-C42-C52-C62 |
| 24 | A | 1606 | PAR | C12-C22-C32-C42-C52-C62 |
| 24 | A | 1604 | PAR | C12-C22-C32-C42-C52-C62 |

5 monomers are involved in 13 short contacts:

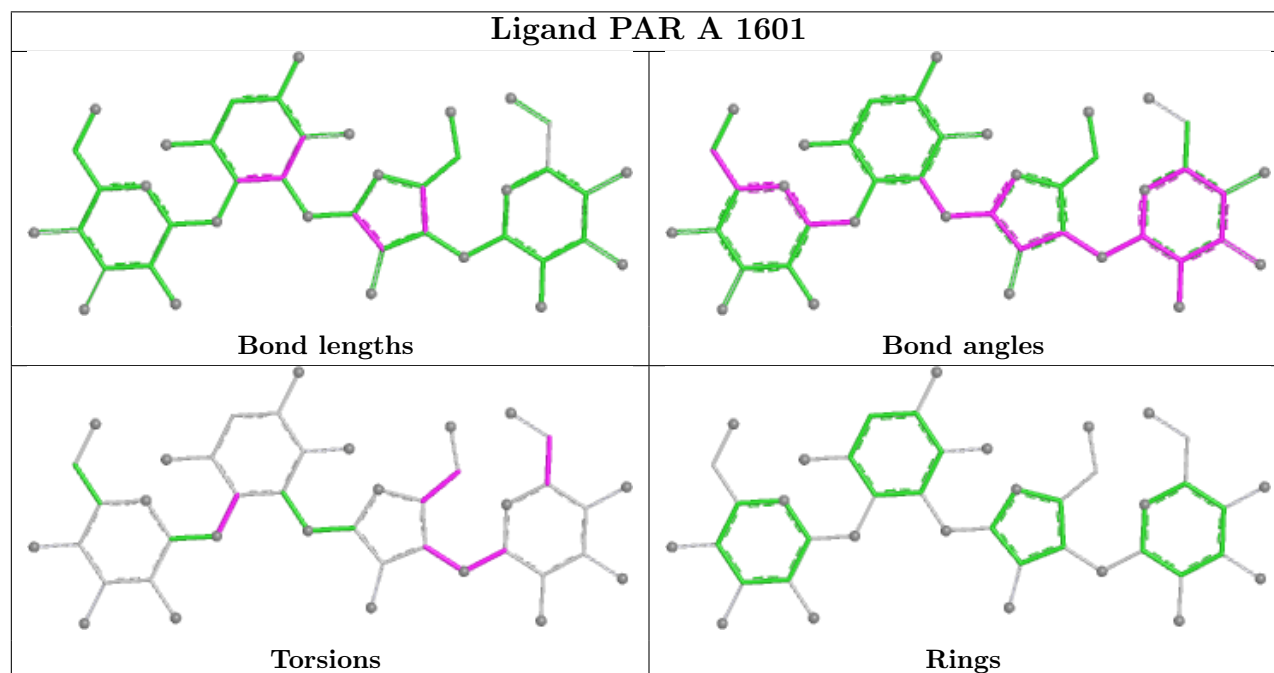
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 24 | A | 1601 | PAR | 2 | 0 |
| 24 | A | 1605 | PAR | 1 | 0 |

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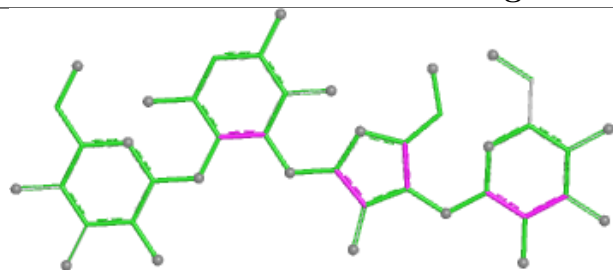
Continued from previous page...

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 24 | A | 1603 | PAR | 5 | 0 |
| 24 | A | 1604 | PAR | 3 | 0 |
| 24 | A | 1602 | PAR | 2 | 0 |

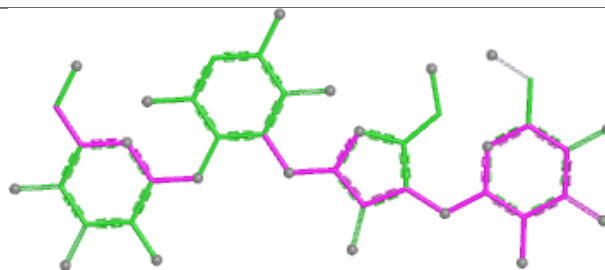
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



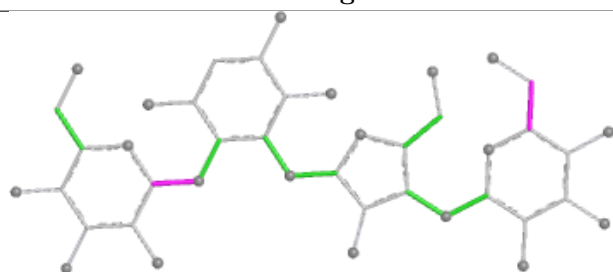
Ligand PAR A 1605



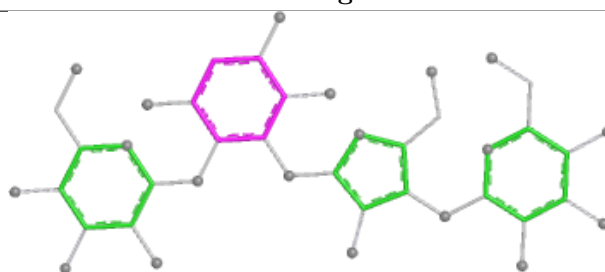
Bond lengths



Bond angles

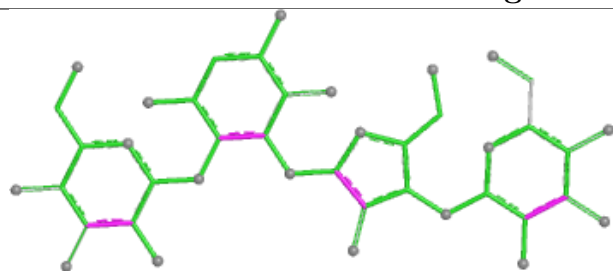


Torsions

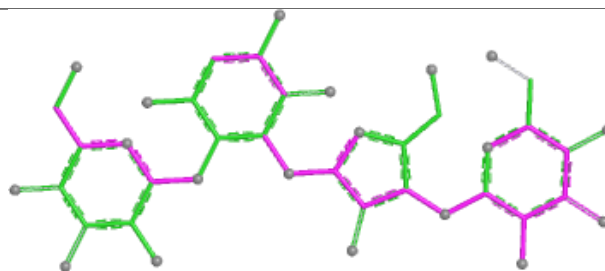


Rings

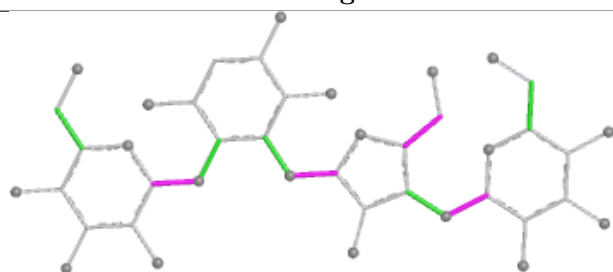
Ligand PAR A 1606



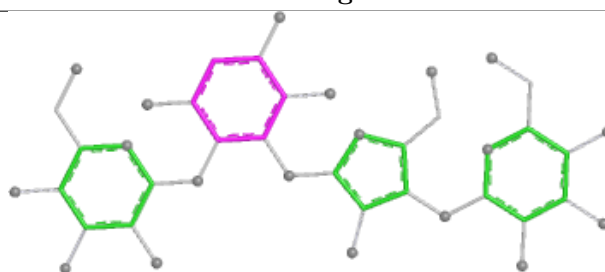
Bond lengths



Bond angles

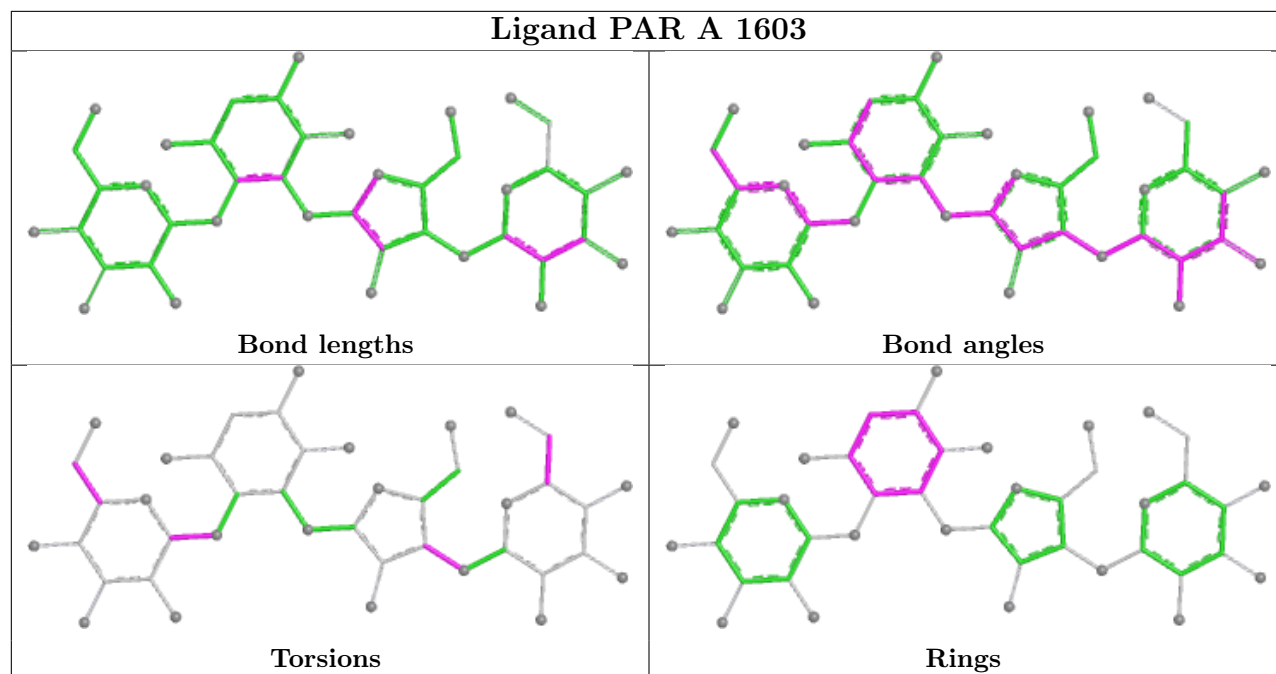


Torsions

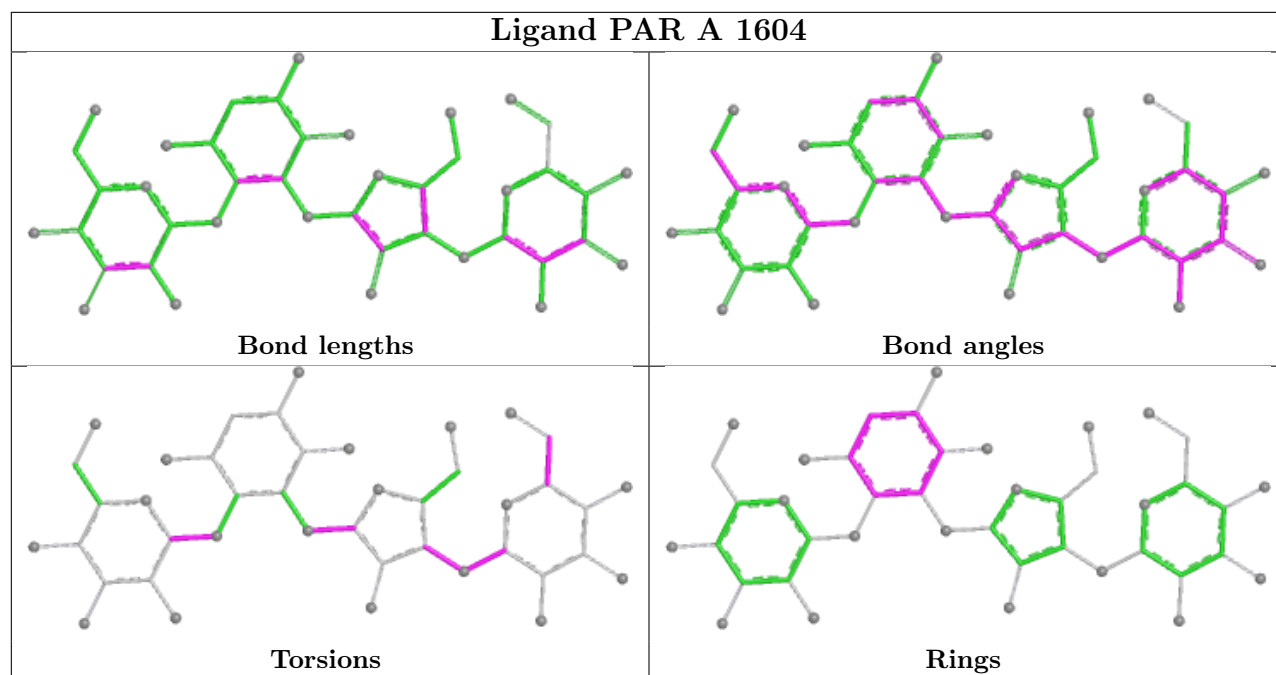


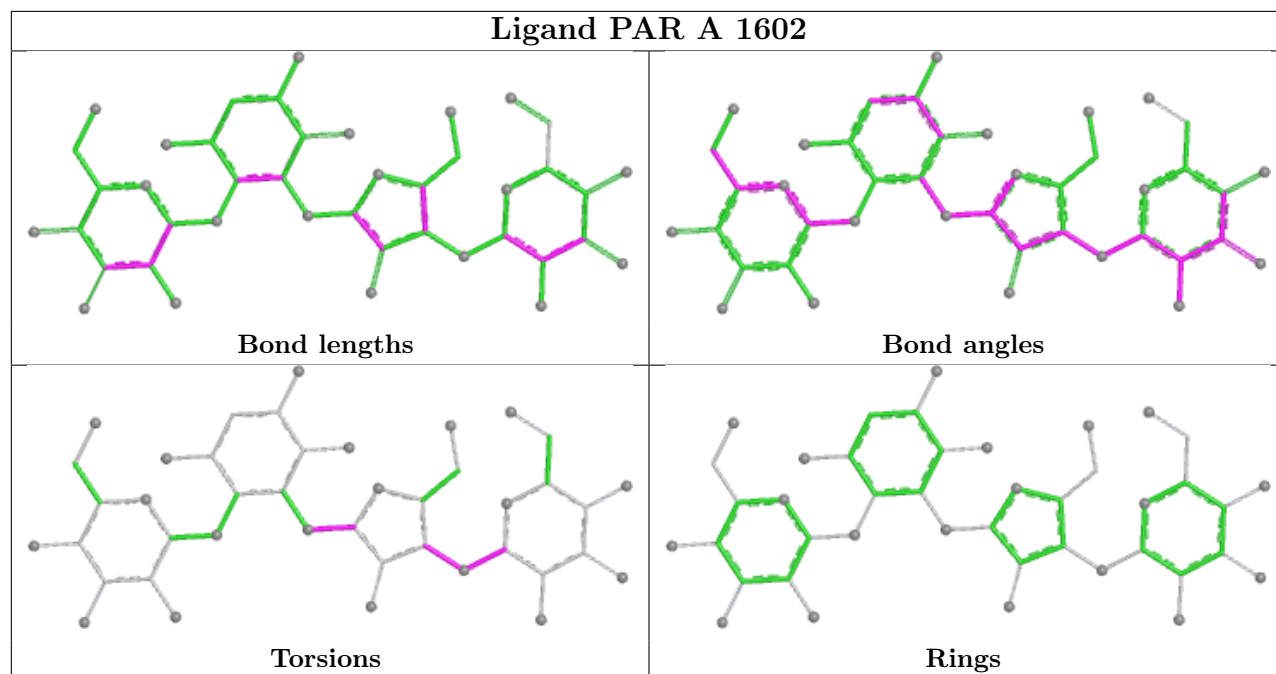
Rings

Ligand PAR A 1603



Ligand PAR A 1604





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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 | A | 1498/1522 (98%) | 0.15 | 25 (1%) 69 53 | 48, 77, 149, 270 | 0 |
| 2 | B | 236/236 (100%) | 0.55 | 18 (7%) 21 18 | 71, 114, 202, 338 | 0 |
| 3 | C | 207/207 (100%) | 0.55 | 17 (8%) 19 17 | 42, 110, 165, 224 | 0 |
| 4 | D | 208/208 (100%) | 0.58 | 18 (8%) 17 16 | 59, 83, 129, 173 | 0 |
| 5 | E | 151/151 (100%) | 0.13 | 2 (1%) 74 59 | 48, 73, 104, 190 | 0 |
| 6 | F | 101/101 (100%) | 0.23 | 3 (2%) 52 40 | 73, 110, 149, 183 | 0 |
| 7 | G | 155/155 (100%) | 0.55 | 14 (9%) 17 15 | 60, 92, 158, 228 | 0 |
| 8 | H | 138/138 (100%) | 0.14 | 4 (2%) 54 40 | 50, 70, 95, 132 | 0 |
| 9 | I | 127/127 (100%) | 0.79 | 15 (11%) 10 11 | 78, 111, 157, 196 | 0 |
| 10 | J | 99/99 (100%) | 1.64 | 33 (33%) 1 2 | 64, 140, 237, 311 | 0 |
| 11 | K | 119/119 (100%) | 0.66 | 9 (7%) 21 18 | 57, 76, 120, 171 | 0 |
| 12 | L | 124/125 (99%) | 0.79 | 17 (13%) 8 9 | 44, 77, 115, 245 | 0 |
| 13 | M | 118/118 (100%) | 0.68 | 12 (10%) 13 13 | 65, 96, 137, 217 | 0 |
| 14 | N | 60/60 (100%) | 1.35 | 14 (23%) 2 4 | 80, 96, 154, 229 | 0 |
| 15 | O | 88/88 (100%) | 0.52 | 5 (5%) 30 25 | 62, 86, 127, 184 | 0 |
| 16 | P | 84/84 (100%) | 0.48 | 1 (1%) 76 61 | 56, 69, 102, 156 | 0 |
| 17 | Q | 99/99 (100%) | 0.50 | 5 (5%) 34 27 | 53, 71, 119, 156 | 0 |
| 18 | R | 73/73 (100%) | 0.35 | 3 (4%) 42 32 | 55, 89, 147, 202 | 0 |
| 19 | S | 81/81 (100%) | 0.99 | 12 (14%) 7 7 | 39, 112, 196, 229 | 0 |
| 20 | T | 99/99 (100%) | 0.80 | 10 (10%) 14 13 | 60, 74, 129, 193 | 0 |
| 21 | U | 25/25 (100%) | 1.30 | 4 (16%) 6 7 | 48, 95, 133, 172 | 0 |
| 22 | a | 5/6 (83%) | 1.39 | 2 (40%) 1 1 | 89, 95, 127, 140 | 0 |
| 23 | b | 8/11 (72%) | 1.32 | 3 (37%) 1 1 | 91, 127, 166, 178 | 0 |
| All | All | 3903/3932 (99%) | 0.44 | 246 (6%) 27 23 | 39, 87, 159, 338 | 0 |

All (246) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 11 | K | 129 | SER | 9.2 |
| 11 | K | 128 | ALA | 8.7 |
| 15 | O | 89 | GLY | 7.9 |
| 14 | N | 12 | ARG | 7.6 |
| 4 | D | 2 | GLY | 7.0 |
| 14 | N | 13 | THR | 6.7 |
| 19 | S | 2 | PRO | 6.7 |
| 11 | K | 127 | LYS | 6.4 |
| 4 | D | 9 | CYS | 6.2 |
| 7 | G | 82 | GLY | 6.0 |
| 7 | G | 84 | ASN | 5.9 |
| 4 | D | 31 | CYS | 5.7 |
| 21 | U | 25 | LYS | 5.5 |
| 19 | S | 3 | ARG | 5.4 |
| 20 | T | 9 | ASN | 5.4 |
| 14 | N | 8 | GLU | 5.2 |
| 4 | D | 26 | CYS | 5.1 |
| 7 | G | 33 | ASP | 5.1 |
| 12 | L | 29 | GLY | 5.0 |
| 2 | B | 136 | VAL | 5.0 |
| 12 | L | 28 | LYS | 4.8 |
| 10 | J | 3 | LYS | 4.6 |
| 11 | K | 126 | ARG | 4.6 |
| 1 | A | 81 | U | 4.5 |
| 10 | J | 64 | GLU | 4.5 |
| 12 | L | 47 | LYS | 4.5 |
| 1 | A | 202 | U | 4.3 |
| 13 | M | 8 | GLU | 4.3 |
| 10 | J | 73 | ASP | 4.1 |
| 10 | J | 6 | ILE | 4.1 |
| 12 | L | 20 | LYS | 4.1 |
| 7 | G | 81 | GLY | 4.0 |
| 10 | J | 5 | ARG | 4.0 |
| 11 | K | 123 | LYS | 4.0 |
| 10 | J | 34 | VAL | 4.0 |
| 19 | S | 4 | SER | 4.0 |
| 1 | A | 1539 | C | 4.0 |
| 20 | T | 73 | HIS | 3.9 |
| 4 | D | 23 | GLY | 3.9 |
| 21 | U | 6 | ARG | 3.9 |
| 9 | I | 125 | TYR | 3.9 |
| 3 | C | 161 | GLU | 3.9 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 7 | G | 13 | GLN | 3.8 |
| 20 | T | 100 | ILE | 3.7 |
| 11 | K | 111 | ASP | 3.7 |
| 10 | J | 46 | ARG | 3.7 |
| 12 | L | 19 | ARG | 3.7 |
| 14 | N | 3 | ARG | 3.7 |
| 4 | D | 19 | LEU | 3.6 |
| 2 | B | 134 | GLU | 3.6 |
| 17 | Q | 100 | LYS | 3.5 |
| 10 | J | 21 | GLN | 3.5 |
| 2 | B | 12 | GLU | 3.5 |
| 10 | J | 90 | LEU | 3.5 |
| 7 | G | 83 | ALA | 3.4 |
| 14 | N | 2 | ALA | 3.4 |
| 2 | B | 227 | GLY | 3.3 |
| 10 | J | 35 | SER | 3.3 |
| 9 | I | 127 | LYS | 3.3 |
| 2 | B | 13 | ALA | 3.3 |
| 7 | G | 5 | ARG | 3.3 |
| 21 | U | 23 | PRO | 3.3 |
| 1 | A | 82 | U | 3.3 |
| 4 | D | 49 | ARG | 3.2 |
| 10 | J | 58 | ASP | 3.2 |
| 19 | S | 5 | LEU | 3.2 |
| 9 | I | 128 | ARG | 3.2 |
| 9 | I | 75 | ASP | 3.1 |
| 8 | H | 1 | MET | 3.1 |
| 12 | L | 115 | LYS | 3.1 |
| 9 | I | 126 | SER | 3.1 |
| 13 | M | 32 | GLU | 3.1 |
| 14 | N | 55 | GLY | 3.1 |
| 10 | J | 4 | ILE | 3.1 |
| 3 | C | 190 | ARG | 3.1 |
| 7 | G | 8 | GLU | 3.0 |
| 10 | J | 88 | LEU | 3.0 |
| 10 | J | 59 | SER | 3.0 |
| 20 | T | 8 | ARG | 3.0 |
| 2 | B | 88 | ALA | 3.0 |
| 19 | S | 6 | LYS | 3.0 |
| 7 | G | 85 | TYR | 3.0 |
| 9 | I | 105 | ASP | 3.0 |
| 14 | N | 9 | LYS | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 19 | S | 33 | THR | 2.9 |
| 12 | L | 17 | LYS | 2.9 |
| 1 | A | 723 | U | 2.9 |
| 15 | O | 2 | PRO | 2.9 |
| 10 | J | 7 | LYS | 2.9 |
| 1 | A | 1125 | U | 2.9 |
| 12 | L | 48 | PRO | 2.9 |
| 22 | a | 6 | U | 2.9 |
| 15 | O | 88 | ARG | 2.8 |
| 23 | b | 40 | C | 2.8 |
| 11 | K | 117 | ASN | 2.8 |
| 2 | B | 133 | LYS | 2.8 |
| 1 | A | 994 | A | 2.8 |
| 7 | G | 11 | GLN | 2.8 |
| 4 | D | 179 | GLU | 2.8 |
| 13 | M | 10 | PRO | 2.7 |
| 11 | K | 118 | GLY | 2.7 |
| 10 | J | 91 | PRO | 2.7 |
| 20 | T | 21 | LYS | 2.7 |
| 2 | B | 230 | VAL | 2.7 |
| 5 | E | 81 | GLU | 2.7 |
| 4 | D | 86 | LYS | 2.7 |
| 10 | J | 80 | LYS | 2.7 |
| 7 | G | 12 | LEU | 2.7 |
| 5 | E | 5 | ASP | 2.7 |
| 8 | H | 55 | GLY | 2.7 |
| 19 | S | 14 | HIS | 2.7 |
| 4 | D | 141 | ARG | 2.7 |
| 13 | M | 13 | LYS | 2.7 |
| 9 | I | 15 | ALA | 2.7 |
| 3 | C | 188 | LEU | 2.6 |
| 20 | T | 13 | LEU | 2.6 |
| 4 | D | 22 | LYS | 2.6 |
| 7 | G | 9 | VAL | 2.6 |
| 3 | C | 206 | GLU | 2.6 |
| 10 | J | 83 | GLU | 2.6 |
| 21 | U | 9 | ARG | 2.6 |
| 12 | L | 25 | PRO | 2.6 |
| 17 | Q | 68 | ARG | 2.6 |
| 20 | T | 22 | ARG | 2.5 |
| 1 | A | 1224 | G | 2.5 |
| 1 | A | 1257 | U | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 4 | D | 12 | CYS | 2.5 |
| 10 | J | 69 | ASN | 2.5 |
| 10 | J | 75 | ILE | 2.5 |
| 10 | J | 40 | LEU | 2.5 |
| 20 | T | 58 | LYS | 2.5 |
| 10 | J | 47 | PHE | 2.5 |
| 10 | J | 89 | ASP | 2.5 |
| 14 | N | 4 | LYS | 2.5 |
| 13 | M | 7 | VAL | 2.5 |
| 17 | Q | 97 | SER | 2.5 |
| 1 | A | 326 | G | 2.5 |
| 23 | b | 31 | A | 2.5 |
| 17 | Q | 99 | SER | 2.5 |
| 10 | J | 66 | ARG | 2.4 |
| 17 | Q | 91 | ARG | 2.4 |
| 9 | I | 38 | GLN | 2.4 |
| 13 | M | 100 | GLY | 2.4 |
| 13 | M | 5 | ALA | 2.4 |
| 14 | N | 10 | ALA | 2.4 |
| 1 | A | 440 | A | 2.4 |
| 7 | G | 146 | GLU | 2.4 |
| 10 | J | 36 | GLY | 2.4 |
| 2 | B | 7 | VAL | 2.4 |
| 19 | S | 7 | LYS | 2.4 |
| 4 | D | 48 | ALA | 2.4 |
| 22 | a | 5 | U | 2.4 |
| 3 | C | 173 | VAL | 2.4 |
| 2 | B | 156 | LYS | 2.4 |
| 1 | A | 1531 | A | 2.4 |
| 7 | G | 151 | TYR | 2.3 |
| 10 | J | 8 | LEU | 2.3 |
| 2 | B | 160 | ASP | 2.3 |
| 2 | B | 89 | GLY | 2.3 |
| 10 | J | 100 | THR | 2.3 |
| 14 | N | 32 | SER | 2.3 |
| 12 | L | 73 | GLU | 2.3 |
| 2 | B | 140 | HIS | 2.3 |
| 12 | L | 119 | LYS | 2.3 |
| 20 | T | 75 | ASN | 2.3 |
| 12 | L | 26 | ALA | 2.3 |
| 1 | A | 1347 | G | 2.3 |
| 1 | A | 1054 | C | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 3 | C | 168 | ALA | 2.3 |
| 2 | B | 148 | TYR | 2.3 |
| 10 | J | 22 | LYS | 2.3 |
| 12 | L | 18 | VAL | 2.3 |
| 12 | L | 128 | ALA | 2.3 |
| 12 | L | 16 | GLU | 2.3 |
| 9 | I | 90 | PRO | 2.2 |
| 11 | K | 54 | ARG | 2.2 |
| 14 | N | 35 | ARG | 2.2 |
| 3 | C | 2 | GLY | 2.2 |
| 12 | L | 129 | ALA | 2.2 |
| 2 | B | 131 | PRO | 2.2 |
| 19 | S | 56 | GLN | 2.2 |
| 1 | A | 89 | C | 2.2 |
| 3 | C | 172 | ARG | 2.2 |
| 8 | H | 84 | ARG | 2.2 |
| 3 | C | 192 | THR | 2.2 |
| 4 | D | 4 | TYR | 2.2 |
| 3 | C | 178 | LEU | 2.2 |
| 9 | I | 8 | GLY | 2.2 |
| 3 | C | 44 | GLU | 2.2 |
| 3 | C | 167 | TRP | 2.2 |
| 13 | M | 102 | ARG | 2.2 |
| 13 | M | 104 | ARG | 2.2 |
| 14 | N | 15 | LYS | 2.2 |
| 2 | B | 95 | GLN | 2.2 |
| 8 | H | 102 | ARG | 2.2 |
| 3 | C | 207 | VAL | 2.2 |
| 4 | D | 21 | LEU | 2.2 |
| 10 | J | 48 | THR | 2.2 |
| 4 | D | 5 | ILE | 2.1 |
| 1 | A | 400 | C | 2.1 |
| 2 | B | 137 | ARG | 2.1 |
| 6 | F | 97 | PHE | 2.1 |
| 12 | L | 127 | GLU | 2.1 |
| 13 | M | 35 | GLU | 2.1 |
| 2 | B | 97 | TRP | 2.1 |
| 23 | b | 30 | G | 2.1 |
| 1 | A | 1280 | A | 2.1 |
| 1 | A | 1286 | A | 2.1 |
| 9 | I | 66 | ARG | 2.1 |
| 19 | S | 38 | SER | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 216 | G | 2.1 |
| 6 | F | 14 | LEU | 2.1 |
| 18 | R | 16 | PRO | 2.1 |
| 20 | T | 84 | LEU | 2.1 |
| 10 | J | 24 | VAL | 2.1 |
| 10 | J | 87 | THR | 2.1 |
| 13 | M | 109 | THR | 2.1 |
| 14 | N | 22 | THR | 2.1 |
| 1 | A | 5 | U | 2.1 |
| 3 | C | 196 | LEU | 2.1 |
| 6 | F | 98 | LEU | 2.1 |
| 19 | S | 34 | TRP | 2.1 |
| 3 | C | 126 | ARG | 2.1 |
| 18 | R | 85 | LEU | 2.1 |
| 15 | O | 50 | HIS | 2.1 |
| 18 | R | 83 | GLU | 2.1 |
| 9 | I | 104 | ARG | 2.0 |
| 13 | M | 9 | ILE | 2.0 |
| 1 | A | 263 | A | 2.0 |
| 1 | A | 108 | G | 2.0 |
| 1 | A | 1182 | G | 2.0 |
| 9 | I | 39 | GLY | 2.0 |
| 14 | N | 60 | SER | 2.0 |
| 19 | S | 35 | SER | 2.0 |
| 16 | P | 23 | ASP | 2.0 |
| 4 | D | 37 | PRO | 2.0 |
| 10 | J | 50 | ILE | 2.0 |
| 9 | I | 67 | GLY | 2.0 |
| 3 | C | 15 | THR | 2.0 |
| 9 | I | 37 | PHE | 2.0 |
| 1 | A | 532 | A | 2.0 |
| 3 | C | 154 | SER | 2.0 |
| 4 | D | 3 | ARG | 2.0 |
| 15 | O | 54 | ARG | 2.0 |
| 1 | A | 1528 | U | 2.0 |
| 10 | J | 96 | ILE | 2.0 |

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 1 | PSU | A | 1540 | 20/21 | 0.85 | 0.21 | 165,171,179,181 | 0 |
| 12 | 0TD | L | 92 | 10/11 | 0.86 | 0.25 | 70,79,96,100 | 0 |
| 23 | PSU | b | 39 | 20/21 | 0.86 | 0.11 | 114,128,144,147 | 0 |
| 1 | PSU | A | 1541 | 20/21 | 0.87 | 0.21 | 164,174,180,214 | 0 |
| 1 | PSU | A | 516 | 20/21 | 0.90 | 0.11 | 78,81,85,86 | 0 |
| 23 | 70U | b | 34 | 25/26 | 0.90 | 0.15 | 84,105,118,130 | 0 |
| 1 | 5MC | A | 967 | 21/22 | 0.90 | 0.16 | 68,73,80,84 | 0 |
| 23 | 12A | b | 37 | 34/35 | 0.91 | 0.13 | 82,96,119,122 | 0 |
| 1 | 2MG | A | 1207 | 24/25 | 0.93 | 0.12 | 95,100,106,108 | 0 |
| 1 | UR3 | A | 1498 | 21/22 | 0.94 | 0.12 | 57,59,62,63 | 0 |
| 1 | M2G | A | 966 | 25/26 | 0.94 | 0.12 | 67,68,87,95 | 0 |
| 22 | 6MZ | a | 3 | 23/24 | 0.94 | 0.12 | 86,98,109,113 | 0 |
| 1 | MA6 | A | 1518 | 24/25 | 0.95 | 0.11 | 59,62,64,64 | 0 |
| 1 | 5MC | A | 1400 | 21/22 | 0.95 | 0.13 | 64,65,69,74 | 0 |
| 1 | 5MC | A | 1404 | 21/22 | 0.95 | 0.12 | 62,63,64,65 | 0 |
| 1 | 7MG | A | 527 | 24/25 | 0.95 | 0.12 | 63,66,67,67 | 0 |
| 1 | MA6 | A | 1519 | 24/25 | 0.96 | 0.11 | 58,60,62,62 | 0 |
| 1 | 5MC | A | 1407 | 21/22 | 0.96 | 0.09 | 68,69,71,72 | 0 |
| 1 | 4OC | A | 1402 | 22/23 | 0.97 | 0.09 | 62,65,68,71 | 0 |

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 25 | MG | A | 1709 | 1/1 | 0.03 | 0.37 | 162,162,162,162 | 0 |
| 25 | MG | A | 1775 | 1/1 | 0.36 | 0.88 | 99,99,99,99 | 0 |
| 26 | K | A | 1904 | 1/1 | 0.44 | 0.52 | 138,138,138,138 | 0 |
| 25 | MG | A | 1727 | 1/1 | 0.46 | 0.62 | 126,126,126,126 | 0 |
| 25 | MG | A | 1778 | 1/1 | 0.49 | 0.18 | 82,82,82,82 | 0 |
| 25 | MG | H | 201 | 1/1 | 0.51 | 0.15 | 61,61,61,61 | 0 |
| 26 | K | A | 1923 | 1/1 | 0.51 | 0.22 | 113,113,113,113 | 0 |
| 26 | K | A | 1902 | 1/1 | 0.53 | 0.12 | 129,129,129,129 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 26 | K | A | 1929 | 1/1 | 0.53 | 0.32 | 127,127,127,127 | 0 |
| 26 | K | A | 1893 | 1/1 | 0.54 | 0.26 | 131,131,131,131 | 0 |
| 25 | MG | A | 1689 | 1/1 | 0.55 | 0.25 | 135,135,135,135 | 0 |
| 25 | MG | A | 1681 | 1/1 | 0.57 | 0.20 | 198,198,198,198 | 0 |
| 25 | MG | H | 202 | 1/1 | 0.58 | 0.13 | 84,84,84,84 | 0 |
| 26 | K | A | 1899 | 1/1 | 0.58 | 0.18 | 117,117,117,117 | 0 |
| 25 | MG | A | 1770 | 1/1 | 0.62 | 0.24 | 71,71,71,71 | 0 |
| 26 | K | A | 1910 | 1/1 | 0.63 | 0.18 | 126,126,126,126 | 0 |
| 25 | MG | A | 1717 | 1/1 | 0.63 | 0.18 | 61,61,61,61 | 0 |
| 25 | MG | A | 1803 | 1/1 | 0.63 | 0.25 | 38,38,38,38 | 0 |
| 25 | MG | A | 1648 | 1/1 | 0.64 | 0.26 | 61,61,61,61 | 0 |
| 25 | MG | A | 1715 | 1/1 | 0.64 | 0.34 | 102,102,102,102 | 0 |
| 26 | K | A | 1905 | 1/1 | 0.64 | 0.34 | 117,117,117,117 | 0 |
| 25 | MG | A | 1885 | 1/1 | 0.65 | 0.17 | 63,63,63,63 | 0 |
| 25 | MG | A | 1616 | 1/1 | 0.67 | 0.33 | 78,78,78,78 | 0 |
| 25 | MG | A | 1852 | 1/1 | 0.68 | 0.33 | 73,73,73,73 | 0 |
| 25 | MG | A | 1748 | 1/1 | 0.68 | 0.15 | 85,85,85,85 | 0 |
| 25 | MG | A | 1876 | 1/1 | 0.69 | 0.14 | 80,80,80,80 | 0 |
| 25 | MG | A | 1686 | 1/1 | 0.69 | 0.21 | 33,33,33,33 | 0 |
| 25 | MG | A | 1871 | 1/1 | 0.69 | 0.21 | 58,58,58,58 | 0 |
| 26 | K | G | 202 | 1/1 | 0.69 | 0.46 | 143,143,143,143 | 0 |
| 25 | MG | A | 1765 | 1/1 | 0.70 | 0.30 | 66,66,66,66 | 0 |
| 25 | MG | A | 1819 | 1/1 | 0.70 | 0.48 | 74,74,74,74 | 0 |
| 26 | K | A | 1928 | 1/1 | 0.70 | 0.17 | 131,131,131,131 | 0 |
| 25 | MG | A | 1731 | 1/1 | 0.70 | 0.23 | 58,58,58,58 | 0 |
| 26 | K | A | 1896 | 1/1 | 0.70 | 0.17 | 132,132,132,132 | 0 |
| 26 | K | A | 1886 | 1/1 | 0.71 | 0.15 | 107,107,107,107 | 0 |
| 25 | MG | A | 1879 | 1/1 | 0.71 | 0.17 | 51,51,51,51 | 0 |
| 25 | MG | A | 1793 | 1/1 | 0.71 | 0.35 | 181,181,181,181 | 0 |
| 25 | MG | A | 1613 | 1/1 | 0.71 | 0.17 | 49,49,49,49 | 0 |
| 25 | MG | A | 1610 | 1/1 | 0.71 | 0.15 | 101,101,101,101 | 0 |
| 25 | MG | Q | 201 | 1/1 | 0.71 | 0.22 | 92,92,92,92 | 0 |
| 26 | K | A | 1903 | 1/1 | 0.72 | 0.13 | 118,118,118,118 | 0 |
| 26 | K | A | 1918 | 1/1 | 0.72 | 0.36 | 127,127,127,127 | 0 |
| 25 | MG | A | 1730 | 1/1 | 0.73 | 0.23 | 59,59,59,59 | 0 |
| 25 | MG | A | 1743 | 1/1 | 0.73 | 0.27 | 81,81,81,81 | 0 |
| 25 | MG | A | 1707 | 1/1 | 0.74 | 0.17 | 106,106,106,106 | 0 |
| 25 | MG | A | 1725 | 1/1 | 0.74 | 0.10 | 64,64,64,64 | 0 |
| 25 | MG | A | 1762 | 1/1 | 0.75 | 0.23 | 67,67,67,67 | 0 |
| 25 | MG | A | 1873 | 1/1 | 0.75 | 0.09 | 66,66,66,66 | 0 |
| 25 | MG | A | 1673 | 1/1 | 0.75 | 0.19 | 56,56,56,56 | 0 |
| 25 | MG | Q | 202 | 1/1 | 0.75 | 0.29 | 67,67,67,67 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 25 | MG | A | 1830 | 1/1 | 0.75 | 0.92 | 95,95,95,95 | 0 |
| 25 | MG | A | 1795 | 1/1 | 0.75 | 0.32 | 75,75,75,75 | 0 |
| 25 | MG | A | 1855 | 1/1 | 0.76 | 0.36 | 77,77,77,77 | 0 |
| 25 | MG | A | 1824 | 1/1 | 0.76 | 0.24 | 66,66,66,66 | 0 |
| 25 | MG | C | 301 | 1/1 | 0.76 | 0.22 | 82,82,82,82 | 0 |
| 25 | MG | A | 1684 | 1/1 | 0.76 | 0.10 | 73,73,73,73 | 0 |
| 25 | MG | A | 1609 | 1/1 | 0.76 | 0.15 | 96,96,96,96 | 0 |
| 26 | K | A | 1907 | 1/1 | 0.76 | 0.25 | 131,131,131,131 | 0 |
| 25 | MG | A | 1634 | 1/1 | 0.77 | 0.14 | 103,103,103,103 | 0 |
| 25 | MG | A | 1746 | 1/1 | 0.77 | 0.17 | 55,55,55,55 | 0 |
| 25 | MG | A | 1864 | 1/1 | 0.77 | 0.27 | 67,67,67,67 | 0 |
| 25 | MG | S | 103 | 1/1 | 0.77 | 0.12 | 71,71,71,71 | 0 |
| 25 | MG | A | 1825 | 1/1 | 0.77 | 0.29 | 78,78,78,78 | 0 |
| 25 | MG | A | 1791 | 1/1 | 0.77 | 0.10 | 104,104,104,104 | 0 |
| 26 | K | A | 1906 | 1/1 | 0.77 | 0.25 | 92,92,92,92 | 0 |
| 25 | MG | A | 1785 | 1/1 | 0.78 | 0.25 | 85,85,85,85 | 0 |
| 25 | MG | A | 1828 | 1/1 | 0.78 | 0.65 | 72,72,72,72 | 0 |
| 25 | MG | A | 1806 | 1/1 | 0.78 | 0.20 | 56,56,56,56 | 0 |
| 26 | K | A | 1891 | 1/1 | 0.78 | 0.23 | 142,142,142,142 | 0 |
| 25 | MG | A | 1818 | 1/1 | 0.78 | 0.27 | 72,72,72,72 | 0 |
| 26 | K | A | 1912 | 1/1 | 0.78 | 0.15 | 116,116,116,116 | 0 |
| 25 | MG | A | 1663 | 1/1 | 0.78 | 0.16 | 50,50,50,50 | 0 |
| 26 | K | A | 1897 | 1/1 | 0.78 | 0.51 | 98,98,98,98 | 0 |
| 25 | MG | A | 1820 | 1/1 | 0.78 | 0.38 | 74,74,74,74 | 0 |
| 25 | MG | A | 1868 | 1/1 | 0.78 | 0.17 | 71,71,71,71 | 0 |
| 25 | MG | A | 1797 | 1/1 | 0.78 | 0.28 | 69,69,69,69 | 0 |
| 25 | MG | A | 1724 | 1/1 | 0.79 | 0.16 | 60,60,60,60 | 0 |
| 26 | K | A | 1895 | 1/1 | 0.79 | 0.10 | 81,81,81,81 | 0 |
| 26 | K | A | 1920 | 1/1 | 0.79 | 0.16 | 100,100,100,100 | 0 |
| 26 | K | A | 1921 | 1/1 | 0.79 | 0.21 | 125,125,125,125 | 0 |
| 25 | MG | A | 1692 | 1/1 | 0.79 | 0.28 | 89,89,89,89 | 0 |
| 26 | K | A | 1888 | 1/1 | 0.79 | 0.36 | 113,113,113,113 | 0 |
| 25 | MG | A | 1753 | 1/1 | 0.79 | 0.35 | 84,84,84,84 | 0 |
| 26 | K | A | 1892 | 1/1 | 0.79 | 0.23 | 111,111,111,111 | 0 |
| 25 | MG | A | 1667 | 1/1 | 0.80 | 0.30 | 52,52,52,52 | 0 |
| 25 | MG | A | 1754 | 1/1 | 0.80 | 0.13 | 52,52,52,52 | 0 |
| 25 | MG | A | 1710 | 1/1 | 0.80 | 0.16 | 64,64,64,64 | 0 |
| 26 | K | A | 1922 | 1/1 | 0.80 | 0.12 | 99,99,99,99 | 0 |
| 25 | MG | A | 1776 | 1/1 | 0.80 | 0.23 | 47,47,47,47 | 0 |
| 25 | MG | A | 1763 | 1/1 | 0.80 | 0.34 | 74,74,74,74 | 0 |
| 25 | MG | A | 1822 | 1/1 | 0.80 | 0.26 | 56,56,56,56 | 0 |
| 26 | K | A | 1917 | 1/1 | 0.80 | 0.16 | 122,122,122,122 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 25 | MG | A | 1781 | 1/1 | 0.81 | 0.25 | 58,58,58,58 | 0 |
| 26 | K | A | 1915 | 1/1 | 0.81 | 0.28 | 146,146,146,146 | 0 |
| 25 | MG | A | 1866 | 1/1 | 0.81 | 0.17 | 46,46,46,46 | 0 |
| 25 | MG | A | 1650 | 1/1 | 0.81 | 0.13 | 41,41,41,41 | 0 |
| 25 | MG | A | 1721 | 1/1 | 0.81 | 0.42 | 204,204,204,204 | 0 |
| 25 | MG | A | 1678 | 1/1 | 0.81 | 0.30 | 69,69,69,69 | 0 |
| 25 | MG | A | 1747 | 1/1 | 0.81 | 0.13 | 59,59,59,59 | 0 |
| 25 | MG | A | 1772 | 1/1 | 0.81 | 0.16 | 62,62,62,62 | 0 |
| 25 | MG | A | 1661 | 1/1 | 0.81 | 0.18 | 57,57,57,57 | 0 |
| 25 | MG | A | 1714 | 1/1 | 0.81 | 0.17 | 159,159,159,159 | 0 |
| 25 | MG | A | 1682 | 1/1 | 0.81 | 0.14 | 66,66,66,66 | 0 |
| 25 | MG | A | 1878 | 1/1 | 0.82 | 0.21 | 56,56,56,56 | 0 |
| 25 | MG | A | 1834 | 1/1 | 0.82 | 0.17 | 44,44,44,44 | 0 |
| 25 | MG | A | 1841 | 1/1 | 0.82 | 0.40 | 103,103,103,103 | 0 |
| 25 | MG | A | 1794 | 1/1 | 0.82 | 0.14 | 131,131,131,131 | 0 |
| 25 | MG | A | 1665 | 1/1 | 0.82 | 0.24 | 86,86,86,86 | 0 |
| 25 | MG | A | 1788 | 1/1 | 0.82 | 0.48 | 68,68,68,68 | 0 |
| 25 | MG | A | 1801 | 1/1 | 0.82 | 0.17 | 70,70,70,70 | 0 |
| 25 | MG | A | 1802 | 1/1 | 0.82 | 0.24 | 63,63,63,63 | 0 |
| 25 | MG | A | 1744 | 1/1 | 0.82 | 0.15 | 51,51,51,51 | 0 |
| 26 | K | A | 1926 | 1/1 | 0.82 | 0.20 | 119,119,119,119 | 0 |
| 25 | MG | A | 1767 | 1/1 | 0.82 | 0.14 | 55,55,55,55 | 0 |
| 25 | MG | A | 1874 | 1/1 | 0.82 | 0.25 | 58,58,58,58 | 0 |
| 25 | MG | A | 1808 | 1/1 | 0.82 | 0.18 | 52,52,52,52 | 0 |
| 25 | MG | A | 1677 | 1/1 | 0.83 | 0.21 | 86,86,86,86 | 0 |
| 26 | K | A | 1919 | 1/1 | 0.83 | 0.08 | 102,102,102,102 | 0 |
| 25 | MG | A | 1774 | 1/1 | 0.83 | 0.12 | 59,59,59,59 | 0 |
| 25 | MG | A | 1716 | 1/1 | 0.83 | 0.24 | 79,79,79,79 | 0 |
| 25 | MG | A | 1817 | 1/1 | 0.83 | 0.25 | 52,52,52,52 | 0 |
| 25 | MG | A | 1827 | 1/1 | 0.83 | 0.25 | 65,65,65,65 | 0 |
| 25 | MG | A | 1865 | 1/1 | 0.83 | 0.24 | 67,67,67,67 | 0 |
| 26 | K | A | 1913 | 1/1 | 0.83 | 0.28 | 139,139,139,139 | 0 |
| 25 | MG | A | 1706 | 1/1 | 0.83 | 0.19 | 54,54,54,54 | 0 |
| 25 | MG | A | 1735 | 1/1 | 0.83 | 0.28 | 58,58,58,58 | 0 |
| 25 | MG | A | 1723 | 1/1 | 0.84 | 0.18 | 31,31,31,31 | 0 |
| 25 | MG | A | 1789 | 1/1 | 0.84 | 0.15 | 60,60,60,60 | 0 |
| 25 | MG | A | 1790 | 1/1 | 0.84 | 0.21 | 120,120,120,120 | 0 |
| 25 | MG | A | 1816 | 1/1 | 0.84 | 0.30 | 50,50,50,50 | 0 |
| 25 | MG | A | 1701 | 1/1 | 0.84 | 0.21 | 53,53,53,53 | 0 |
| 25 | MG | A | 1761 | 1/1 | 0.84 | 0.19 | 54,54,54,54 | 0 |
| 25 | MG | A | 1862 | 1/1 | 0.84 | 0.21 | 53,53,53,53 | 0 |
| 25 | MG | A | 1875 | 1/1 | 0.84 | 0.17 | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 25 | MG | L | 202 | 1/1 | 0.85 | 0.11 | 54,54,54,54 | 0 |
| 25 | MG | A | 1782 | 1/1 | 0.85 | 0.25 | 63,63,63,63 | 0 |
| 26 | K | A | 1908 | 1/1 | 0.85 | 0.09 | 77,77,77,77 | 0 |
| 25 | MG | A | 1800 | 1/1 | 0.85 | 0.34 | 68,68,68,68 | 0 |
| 25 | MG | A | 1670 | 1/1 | 0.85 | 0.31 | 55,55,55,55 | 0 |
| 25 | MG | A | 1636 | 1/1 | 0.85 | 0.10 | 44,44,44,44 | 0 |
| 25 | MG | A | 1736 | 1/1 | 0.85 | 0.21 | 55,55,55,55 | 0 |
| 25 | MG | A | 1740 | 1/1 | 0.85 | 0.19 | 70,70,70,70 | 0 |
| 25 | MG | A | 1641 | 1/1 | 0.85 | 0.13 | 66,66,66,66 | 0 |
| 25 | MG | A | 1831 | 1/1 | 0.85 | 0.14 | 58,58,58,58 | 0 |
| 25 | MG | A | 1833 | 1/1 | 0.85 | 0.15 | 45,45,45,45 | 0 |
| 25 | MG | A | 1814 | 1/1 | 0.85 | 0.31 | 56,56,56,56 | 0 |
| 25 | MG | A | 1792 | 1/1 | 0.85 | 0.15 | 173,173,173,173 | 0 |
| 25 | MG | A | 1851 | 1/1 | 0.85 | 0.18 | 60,60,60,60 | 0 |
| 24 | PAR | A | 1605 | 42/42 | 0.85 | 0.32 | 149,168,179,187 | 0 |
| 26 | K | A | 1927 | 1/1 | 0.85 | 0.14 | 115,115,115,115 | 0 |
| 25 | MG | G | 201 | 1/1 | 0.85 | 0.12 | 52,52,52,52 | 0 |
| 25 | MG | A | 1745 | 1/1 | 0.85 | 0.18 | 62,62,62,62 | 0 |
| 24 | PAR | A | 1603 | 42/42 | 0.85 | 0.33 | 92,128,169,179 | 0 |
| 25 | MG | A | 1798 | 1/1 | 0.86 | 0.17 | 46,46,46,46 | 0 |
| 25 | MG | A | 1726 | 1/1 | 0.86 | 0.26 | 58,58,58,58 | 0 |
| 25 | MG | A | 1861 | 1/1 | 0.86 | 0.18 | 73,73,73,73 | 0 |
| 25 | MG | A | 1640 | 1/1 | 0.86 | 0.13 | 128,128,128,128 | 0 |
| 25 | MG | P | 102 | 1/1 | 0.86 | 0.14 | 71,71,71,71 | 0 |
| 25 | MG | A | 1675 | 1/1 | 0.86 | 0.20 | 80,80,80,80 | 0 |
| 25 | MG | A | 1629 | 1/1 | 0.86 | 0.13 | 63,63,63,63 | 0 |
| 25 | MG | A | 1751 | 1/1 | 0.86 | 0.22 | 54,54,54,54 | 0 |
| 24 | PAR | A | 1602 | 42/42 | 0.86 | 0.44 | 120,192,236,255 | 0 |
| 26 | K | A | 1887 | 1/1 | 0.86 | 0.10 | 104,104,104,104 | 0 |
| 25 | MG | A | 1870 | 1/1 | 0.86 | 0.28 | 58,58,58,58 | 0 |
| 26 | K | A | 1889 | 1/1 | 0.86 | 0.17 | 124,124,124,124 | 0 |
| 25 | MG | A | 1810 | 1/1 | 0.86 | 0.12 | 195,195,195,195 | 0 |
| 25 | MG | A | 1813 | 1/1 | 0.86 | 0.26 | 64,64,64,64 | 0 |
| 25 | MG | A | 1666 | 1/1 | 0.86 | 0.10 | 75,75,75,75 | 0 |
| 25 | MG | A | 1611 | 1/1 | 0.86 | 0.10 | 37,37,37,37 | 0 |
| 26 | K | A | 1925 | 1/1 | 0.86 | 0.14 | 92,92,92,92 | 0 |
| 25 | MG | A | 1840 | 1/1 | 0.86 | 0.18 | 76,76,76,76 | 0 |
| 25 | MG | A | 1653 | 1/1 | 0.86 | 0.11 | 105,105,105,105 | 0 |
| 25 | MG | A | 1847 | 1/1 | 0.86 | 0.15 | 51,51,51,51 | 0 |
| 25 | MG | A | 1848 | 1/1 | 0.86 | 0.21 | 61,61,61,61 | 0 |
| 25 | MG | A | 1685 | 1/1 | 0.86 | 0.30 | 80,80,80,80 | 0 |
| 25 | MG | A | 1672 | 1/1 | 0.87 | 0.09 | 44,44,44,44 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 25 | MG | A | 1755 | 1/1 | 0.87 | 0.11 | 40,40,40,40 | 0 |
| 25 | MG | A | 1720 | 1/1 | 0.87 | 0.24 | 37,37,37,37 | 0 |
| 25 | MG | T | 201 | 1/1 | 0.87 | 0.17 | 38,38,38,38 | 0 |
| 25 | MG | a | 101 | 1/1 | 0.87 | 0.17 | 50,50,50,50 | 0 |
| 25 | MG | A | 1845 | 1/1 | 0.87 | 0.15 | 32,32,32,32 | 0 |
| 24 | PAR | A | 1606 | 42/42 | 0.87 | 0.21 | 100,122,134,139 | 0 |
| 25 | MG | P | 104 | 1/1 | 0.87 | 0.20 | 72,72,72,72 | 0 |
| 25 | MG | A | 1680 | 1/1 | 0.88 | 0.22 | 55,55,55,55 | 0 |
| 25 | MG | A | 1766 | 1/1 | 0.88 | 0.36 | 56,56,56,56 | 0 |
| 25 | MG | A | 1836 | 1/1 | 0.88 | 0.23 | 55,55,55,55 | 0 |
| 25 | MG | A | 1839 | 1/1 | 0.88 | 0.22 | 51,51,51,51 | 0 |
| 25 | MG | L | 201 | 1/1 | 0.88 | 0.15 | 64,64,64,64 | 0 |
| 25 | MG | A | 1623 | 1/1 | 0.88 | 0.17 | 46,46,46,46 | 0 |
| 25 | MG | A | 1668 | 1/1 | 0.88 | 0.15 | 30,30,30,30 | 0 |
| 25 | MG | A | 1796 | 1/1 | 0.88 | 0.15 | 71,71,71,71 | 0 |
| 25 | MG | A | 1756 | 1/1 | 0.88 | 0.25 | 61,61,61,61 | 0 |
| 25 | MG | A | 1656 | 1/1 | 0.88 | 0.21 | 85,85,85,85 | 0 |
| 25 | MG | A | 1815 | 1/1 | 0.88 | 0.09 | 29,29,29,29 | 0 |
| 25 | MG | A | 1607 | 1/1 | 0.88 | 0.25 | 87,87,87,87 | 0 |
| 25 | MG | A | 1679 | 1/1 | 0.88 | 0.21 | 78,78,78,78 | 0 |
| 25 | MG | A | 1857 | 1/1 | 0.88 | 0.19 | 45,45,45,45 | 0 |
| 25 | MG | A | 1881 | 1/1 | 0.88 | 0.36 | 79,79,79,79 | 0 |
| 25 | MG | A | 1832 | 1/1 | 0.88 | 0.18 | 57,57,57,57 | 0 |
| 25 | MG | A | 1637 | 1/1 | 0.89 | 0.18 | 52,52,52,52 | 0 |
| 25 | MG | A | 1867 | 1/1 | 0.89 | 0.21 | 43,43,43,43 | 0 |
| 25 | MG | A | 1804 | 1/1 | 0.89 | 0.09 | 61,61,61,61 | 0 |
| 25 | MG | A | 1823 | 1/1 | 0.89 | 0.22 | 63,63,63,63 | 0 |
| 25 | MG | A | 1842 | 1/1 | 0.89 | 0.18 | 57,57,57,57 | 0 |
| 25 | MG | A | 1844 | 1/1 | 0.89 | 0.19 | 65,65,65,65 | 0 |
| 25 | MG | A | 1759 | 1/1 | 0.89 | 0.13 | 47,47,47,47 | 0 |
| 25 | MG | A | 1625 | 1/1 | 0.89 | 0.25 | 61,61,61,61 | 0 |
| 25 | MG | b | 101 | 1/1 | 0.89 | 0.12 | 46,46,46,46 | 0 |
| 26 | K | A | 1914 | 1/1 | 0.89 | 0.09 | 124,124,124,124 | 0 |
| 25 | MG | A | 1777 | 1/1 | 0.89 | 0.09 | 72,72,72,72 | 0 |
| 26 | K | A | 1916 | 1/1 | 0.89 | 0.12 | 108,108,108,108 | 0 |
| 25 | MG | A | 1877 | 1/1 | 0.89 | 0.19 | 69,69,69,69 | 0 |
| 25 | MG | A | 1737 | 1/1 | 0.89 | 0.12 | 62,62,62,62 | 0 |
| 25 | MG | A | 1738 | 1/1 | 0.89 | 0.27 | 52,52,52,52 | 0 |
| 25 | MG | A | 1749 | 1/1 | 0.89 | 0.17 | 34,34,34,34 | 0 |
| 25 | MG | A | 1882 | 1/1 | 0.89 | 0.20 | 67,67,67,67 | 0 |
| 25 | MG | A | 1704 | 1/1 | 0.89 | 0.15 | 51,51,51,51 | 0 |
| 25 | MG | A | 1742 | 1/1 | 0.89 | 0.12 | 63,63,63,63 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 26 | K | A | 1924 | 1/1 | 0.89 | 0.17 | 113,113,113,113 | 0 |
| 25 | MG | A | 1671 | 1/1 | 0.89 | 0.14 | 30,30,30,30 | 0 |
| 25 | MG | A | 1863 | 1/1 | 0.89 | 0.30 | 60,60,60,60 | 0 |
| 26 | K | A | 1898 | 1/1 | 0.89 | 0.08 | 120,120,120,120 | 0 |
| 24 | PAR | A | 1604 | 42/42 | 0.89 | 0.24 | 83,126,184,192 | 0 |
| 26 | K | A | 1901 | 1/1 | 0.89 | 0.15 | 112,112,112,112 | 0 |
| 26 | K | E | 202 | 1/1 | 0.89 | 0.24 | 80,80,80,80 | 0 |
| 25 | MG | A | 1838 | 1/1 | 0.89 | 0.29 | 59,59,59,59 | 0 |
| 25 | MG | A | 1674 | 1/1 | 0.90 | 0.14 | 65,65,65,65 | 0 |
| 26 | K | A | 1911 | 1/1 | 0.90 | 0.07 | 70,70,70,70 | 0 |
| 26 | K | A | 1900 | 1/1 | 0.90 | 0.10 | 113,113,113,113 | 0 |
| 26 | K | A | 1890 | 1/1 | 0.90 | 0.17 | 89,89,89,89 | 0 |
| 25 | MG | A | 1694 | 1/1 | 0.90 | 0.22 | 122,122,122,122 | 0 |
| 25 | MG | A | 1858 | 1/1 | 0.90 | 0.16 | 64,64,64,64 | 0 |
| 25 | MG | A | 1769 | 1/1 | 0.90 | 0.26 | 70,70,70,70 | 0 |
| 25 | MG | A | 1811 | 1/1 | 0.90 | 0.18 | 41,41,41,41 | 0 |
| 25 | MG | A | 1688 | 1/1 | 0.90 | 0.11 | 68,68,68,68 | 0 |
| 25 | MG | A | 1639 | 1/1 | 0.90 | 0.27 | 52,52,52,52 | 0 |
| 25 | MG | A | 1773 | 1/1 | 0.90 | 0.11 | 30,30,30,30 | 0 |
| 25 | MG | A | 1812 | 1/1 | 0.91 | 0.25 | 59,59,59,59 | 0 |
| 25 | MG | A | 1860 | 1/1 | 0.91 | 0.08 | 56,56,56,56 | 0 |
| 25 | MG | A | 1799 | 1/1 | 0.91 | 0.09 | 73,73,73,73 | 0 |
| 24 | PAR | A | 1601 | 42/42 | 0.91 | 0.17 | 50,61,121,159 | 0 |
| 25 | MG | A | 1732 | 1/1 | 0.91 | 0.24 | 66,66,66,66 | 0 |
| 25 | MG | A | 1843 | 1/1 | 0.91 | 0.17 | 70,70,70,70 | 0 |
| 25 | MG | A | 1635 | 1/1 | 0.91 | 0.17 | 46,46,46,46 | 0 |
| 25 | MG | A | 1771 | 1/1 | 0.91 | 0.12 | 68,68,68,68 | 0 |
| 25 | MG | A | 1846 | 1/1 | 0.91 | 0.13 | 41,41,41,41 | 0 |
| 25 | MG | A | 1728 | 1/1 | 0.91 | 0.12 | 41,41,41,41 | 0 |
| 25 | MG | A | 1764 | 1/1 | 0.91 | 0.15 | 53,53,53,53 | 0 |
| 25 | MG | A | 1787 | 1/1 | 0.91 | 0.21 | 43,43,43,43 | 0 |
| 25 | MG | A | 1631 | 1/1 | 0.91 | 0.29 | 75,75,75,75 | 0 |
| 25 | MG | A | 1837 | 1/1 | 0.91 | 0.21 | 70,70,70,70 | 0 |
| 26 | K | A | 1894 | 1/1 | 0.91 | 0.11 | 100,100,100,100 | 0 |
| 25 | MG | P | 103 | 1/1 | 0.91 | 0.10 | 65,65,65,65 | 0 |
| 25 | MG | A | 1758 | 1/1 | 0.91 | 0.21 | 59,59,59,59 | 0 |
| 25 | MG | A | 1700 | 1/1 | 0.92 | 0.15 | 35,35,35,35 | 0 |
| 25 | MG | A | 1624 | 1/1 | 0.92 | 0.12 | 51,51,51,51 | 0 |
| 25 | MG | A | 1702 | 1/1 | 0.92 | 0.08 | 113,113,113,113 | 0 |
| 25 | MG | A | 1643 | 1/1 | 0.92 | 0.33 | 92,92,92,92 | 0 |
| 25 | MG | A | 1826 | 1/1 | 0.92 | 0.08 | 40,40,40,40 | 0 |
| 25 | MG | A | 1626 | 1/1 | 0.92 | 0.16 | 47,47,47,47 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 25 | MG | S | 102 | 1/1 | 0.92 | 0.09 | 43,43,43,43 | 0 |
| 25 | MG | A | 1869 | 1/1 | 0.92 | 0.14 | 58,58,58,58 | 0 |
| 25 | MG | A | 1693 | 1/1 | 0.92 | 0.17 | 67,67,67,67 | 0 |
| 25 | MG | D | 302 | 1/1 | 0.92 | 0.12 | 72,72,72,72 | 0 |
| 25 | MG | A | 1783 | 1/1 | 0.92 | 0.18 | 54,54,54,54 | 0 |
| 25 | MG | A | 1784 | 1/1 | 0.92 | 0.10 | 35,35,35,35 | 0 |
| 25 | MG | A | 1649 | 1/1 | 0.92 | 0.11 | 35,35,35,35 | 0 |
| 25 | MG | A | 1697 | 1/1 | 0.92 | 0.26 | 51,51,51,51 | 0 |
| 25 | MG | A | 1722 | 1/1 | 0.93 | 0.16 | 31,31,31,31 | 0 |
| 25 | MG | A | 1676 | 1/1 | 0.93 | 0.16 | 49,49,49,49 | 0 |
| 25 | MG | A | 1632 | 1/1 | 0.93 | 0.21 | 26,26,26,26 | 0 |
| 25 | MG | A | 1883 | 1/1 | 0.93 | 0.10 | 59,59,59,59 | 0 |
| 25 | MG | A | 1884 | 1/1 | 0.93 | 0.15 | 59,59,59,59 | 0 |
| 25 | MG | A | 1658 | 1/1 | 0.93 | 0.12 | 40,40,40,40 | 0 |
| 25 | MG | A | 1711 | 1/1 | 0.93 | 0.12 | 61,61,61,61 | 0 |
| 25 | MG | A | 1712 | 1/1 | 0.93 | 0.06 | 20,20,20,20 | 0 |
| 25 | MG | A | 1659 | 1/1 | 0.93 | 0.13 | 92,92,92,92 | 0 |
| 25 | MG | A | 1687 | 1/1 | 0.93 | 0.08 | 53,53,53,53 | 0 |
| 25 | MG | A | 1644 | 1/1 | 0.93 | 0.23 | 60,60,60,60 | 0 |
| 25 | MG | A | 1621 | 1/1 | 0.93 | 0.08 | 50,50,50,50 | 0 |
| 25 | MG | A | 1805 | 1/1 | 0.93 | 0.08 | 39,39,39,39 | 0 |
| 25 | MG | A | 1821 | 1/1 | 0.93 | 0.11 | 32,32,32,32 | 0 |
| 25 | MG | A | 1690 | 1/1 | 0.93 | 0.15 | 84,84,84,84 | 0 |
| 25 | MG | A | 1691 | 1/1 | 0.93 | 0.12 | 50,50,50,50 | 0 |
| 25 | MG | A | 1809 | 1/1 | 0.93 | 0.12 | 160,160,160,160 | 0 |
| 25 | MG | A | 1872 | 1/1 | 0.94 | 0.07 | 49,49,49,49 | 0 |
| 25 | MG | A | 1856 | 1/1 | 0.94 | 0.14 | 53,53,53,53 | 0 |
| 25 | MG | A | 1741 | 1/1 | 0.94 | 0.09 | 49,49,49,49 | 0 |
| 25 | MG | P | 101 | 1/1 | 0.94 | 0.21 | 38,38,38,38 | 0 |
| 25 | MG | A | 1695 | 1/1 | 0.94 | 0.10 | 51,51,51,51 | 0 |
| 25 | MG | A | 1859 | 1/1 | 0.94 | 0.24 | 61,61,61,61 | 0 |
| 25 | MG | A | 1696 | 1/1 | 0.94 | 0.25 | 269,269,269,269 | 0 |
| 25 | MG | A | 1645 | 1/1 | 0.94 | 0.10 | 128,128,128,128 | 0 |
| 25 | MG | A | 1780 | 1/1 | 0.94 | 0.18 | 42,42,42,42 | 0 |
| 25 | MG | S | 101 | 1/1 | 0.94 | 0.07 | 30,30,30,30 | 0 |
| 25 | MG | A | 1708 | 1/1 | 0.94 | 0.08 | 39,39,39,39 | 0 |
| 25 | MG | A | 1757 | 1/1 | 0.94 | 0.09 | 34,34,34,34 | 0 |
| 25 | MG | A | 1657 | 1/1 | 0.94 | 0.07 | 18,18,18,18 | 0 |
| 25 | MG | A | 1662 | 1/1 | 0.94 | 0.25 | 115,115,115,115 | 0 |
| 25 | MG | A | 1850 | 1/1 | 0.94 | 0.07 | 30,30,30,30 | 0 |
| 25 | MG | A | 1760 | 1/1 | 0.94 | 0.12 | 35,35,35,35 | 0 |
| 25 | MG | A | 1646 | 1/1 | 0.94 | 0.10 | 38,38,38,38 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 25 | MG | E | 201 | 1/1 | 0.94 | 0.08 | 80,80,80,80 | 0 |
| 25 | MG | A | 1854 | 1/1 | 0.94 | 0.17 | 48,48,48,48 | 0 |
| 25 | MG | A | 1729 | 1/1 | 0.94 | 0.09 | 51,51,51,51 | 0 |
| 25 | MG | A | 1829 | 1/1 | 0.95 | 0.18 | 62,62,62,62 | 0 |
| 25 | MG | A | 1752 | 1/1 | 0.95 | 0.07 | 38,38,38,38 | 0 |
| 25 | MG | A | 1880 | 1/1 | 0.95 | 0.12 | 48,48,48,48 | 0 |
| 25 | MG | A | 1664 | 1/1 | 0.95 | 0.07 | 68,68,68,68 | 0 |
| 25 | MG | A | 1614 | 1/1 | 0.95 | 0.07 | 72,72,72,72 | 0 |
| 25 | MG | A | 1734 | 1/1 | 0.95 | 0.08 | 45,45,45,45 | 0 |
| 25 | MG | A | 1849 | 1/1 | 0.95 | 0.19 | 57,57,57,57 | 0 |
| 25 | MG | A | 1642 | 1/1 | 0.95 | 0.19 | 75,75,75,75 | 0 |
| 25 | MG | A | 1835 | 1/1 | 0.95 | 0.11 | 55,55,55,55 | 0 |
| 25 | MG | A | 1768 | 1/1 | 0.95 | 0.09 | 46,46,46,46 | 0 |
| 25 | MG | A | 1853 | 1/1 | 0.95 | 0.20 | 49,49,49,49 | 0 |
| 25 | MG | A | 1655 | 1/1 | 0.95 | 0.13 | 52,52,52,52 | 0 |
| 25 | MG | A | 1718 | 1/1 | 0.95 | 0.18 | 32,32,32,32 | 0 |
| 25 | MG | A | 1619 | 1/1 | 0.95 | 0.11 | 69,69,69,69 | 0 |
| 25 | MG | A | 1633 | 1/1 | 0.95 | 0.18 | 50,50,50,50 | 0 |
| 26 | K | A | 1909 | 1/1 | 0.95 | 0.11 | 102,102,102,102 | 0 |
| 25 | MG | A | 1786 | 1/1 | 0.95 | 0.07 | 49,49,49,49 | 0 |
| 25 | MG | A | 1750 | 1/1 | 0.95 | 0.14 | 54,54,54,54 | 0 |
| 25 | MG | A | 1705 | 1/1 | 0.95 | 0.13 | 83,83,83,83 | 0 |
| 25 | MG | A | 1617 | 1/1 | 0.96 | 0.16 | 23,23,23,23 | 0 |
| 25 | MG | A | 1703 | 1/1 | 0.96 | 0.08 | 65,65,65,65 | 0 |
| 25 | MG | A | 1628 | 1/1 | 0.96 | 0.09 | 42,42,42,42 | 0 |
| 25 | MG | A | 1647 | 1/1 | 0.96 | 0.12 | 78,78,78,78 | 0 |
| 25 | MG | A | 1683 | 1/1 | 0.96 | 0.13 | 68,68,68,68 | 0 |
| 25 | MG | A | 1733 | 1/1 | 0.96 | 0.17 | 53,53,53,53 | 0 |
| 25 | MG | A | 1652 | 1/1 | 0.96 | 0.18 | 56,56,56,56 | 0 |
| 25 | MG | A | 1807 | 1/1 | 0.96 | 0.12 | 42,42,42,42 | 0 |
| 25 | MG | A | 1779 | 1/1 | 0.97 | 0.17 | 26,26,26,26 | 0 |
| 25 | MG | A | 1739 | 1/1 | 0.97 | 0.10 | 14,14,14,14 | 0 |
| 25 | MG | F | 201 | 1/1 | 0.97 | 0.04 | 52,52,52,52 | 0 |
| 25 | MG | A | 1627 | 1/1 | 0.97 | 0.06 | 48,48,48,48 | 0 |
| 25 | MG | A | 1698 | 1/1 | 0.97 | 0.11 | 48,48,48,48 | 0 |
| 25 | MG | A | 1651 | 1/1 | 0.97 | 0.07 | 32,32,32,32 | 0 |
| 25 | MG | A | 1713 | 1/1 | 0.97 | 0.19 | 242,242,242,242 | 0 |
| 25 | MG | A | 1620 | 1/1 | 0.97 | 0.10 | 66,66,66,66 | 0 |
| 25 | MG | A | 1608 | 1/1 | 0.97 | 0.09 | 67,67,67,67 | 0 |
| 25 | MG | A | 1930 | 1/1 | 0.97 | 0.05 | 57,57,57,57 | 0 |
| 25 | MG | A | 1654 | 1/1 | 0.97 | 0.06 | 57,57,57,57 | 0 |
| 25 | MG | A | 1630 | 1/1 | 0.98 | 0.24 | 10,10,10,10 | 0 |

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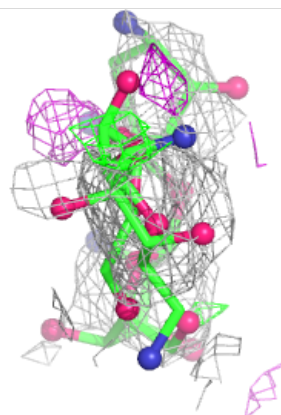
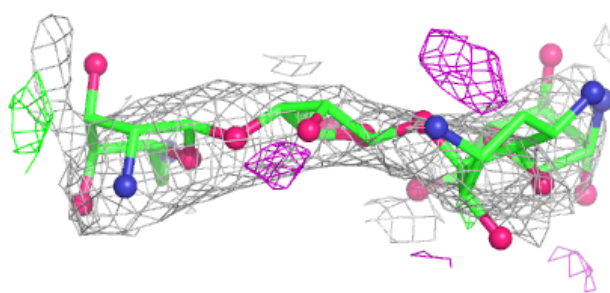
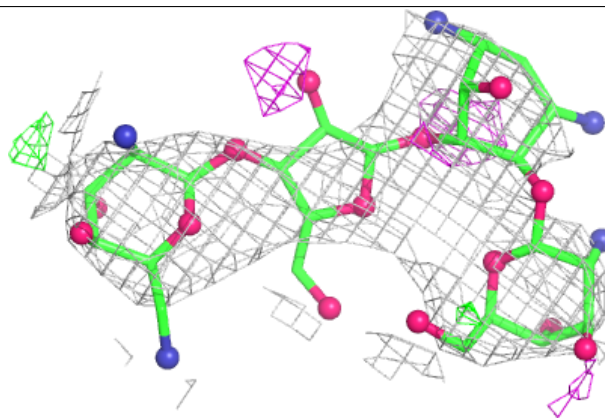
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 25 | MG | A | 1660 | 1/1 | 0.98 | 0.07 | 18,18,18,18 | 0 |
| 25 | MG | A | 1612 | 1/1 | 0.98 | 0.09 | 56,56,56,56 | 0 |
| 25 | MG | A | 1622 | 1/1 | 0.98 | 0.06 | 29,29,29,29 | 0 |
| 25 | MG | A | 1618 | 1/1 | 0.98 | 0.08 | 97,97,97,97 | 0 |
| 25 | MG | A | 1669 | 1/1 | 0.98 | 0.08 | 42,42,42,42 | 0 |
| 25 | MG | A | 1615 | 1/1 | 0.99 | 0.07 | 34,34,34,34 | 0 |
| 25 | MG | A | 1719 | 1/1 | 0.99 | 0.07 | 43,43,43,43 | 0 |
| 25 | MG | A | 1638 | 1/1 | 0.99 | 0.03 | 46,46,46,46 | 0 |
| 25 | MG | A | 1699 | 1/1 | 0.99 | 0.14 | 21,21,21,21 | 0 |
| 27 | ZN | D | 301 | 1/1 | 0.99 | 0.17 | 46,46,46,46 | 0 |
| 27 | ZN | N | 101 | 1/1 | 0.99 | 0.03 | 77,77,77,77 | 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.

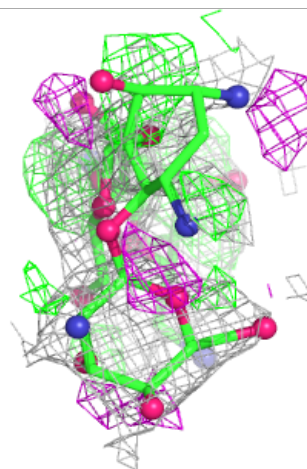
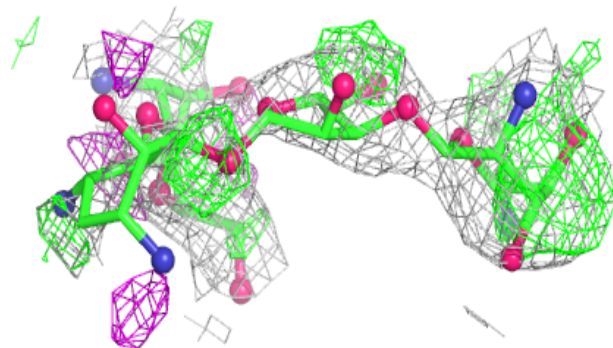
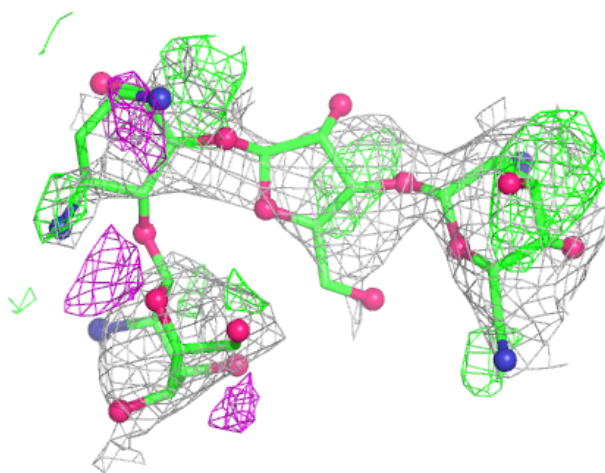
Electron density around PAR A 1605:

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



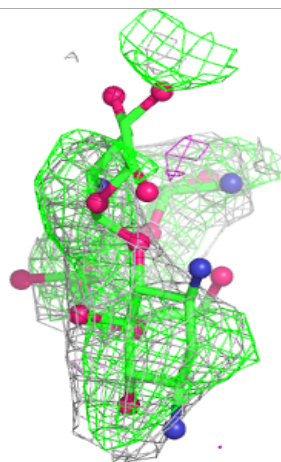
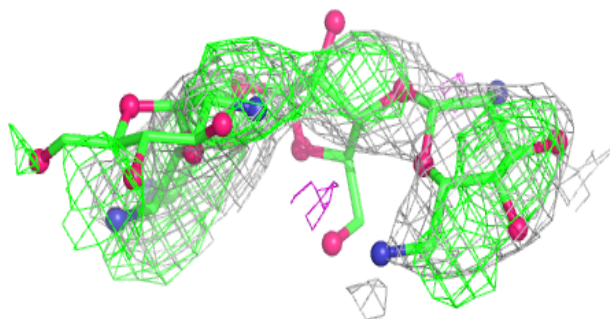
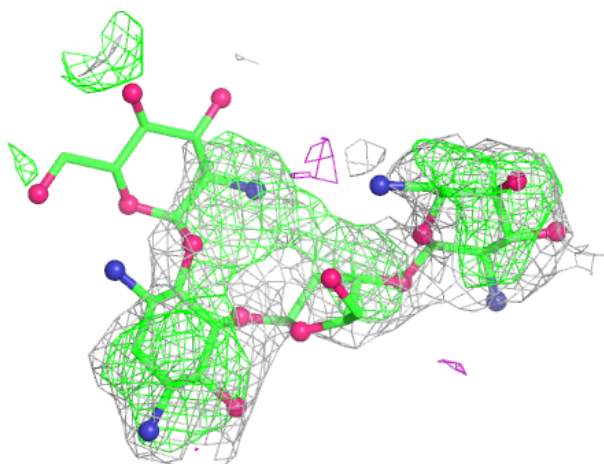
Electron density around PAR A 1603:

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



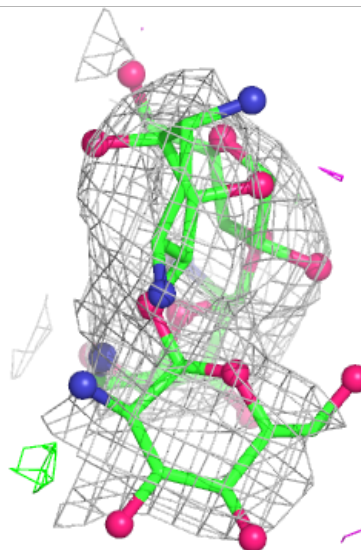
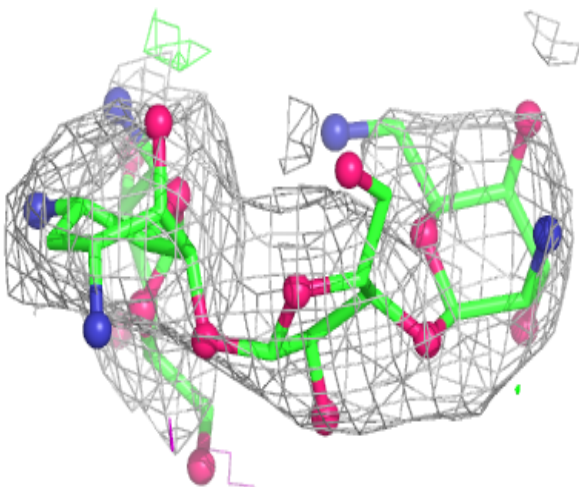
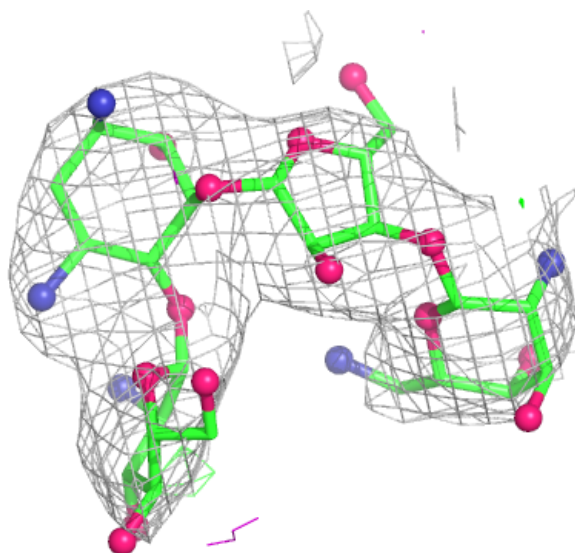
Electron density around PAR A 1602:

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



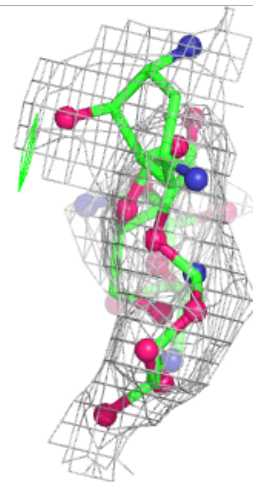
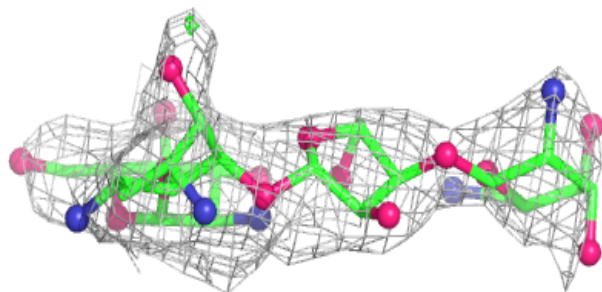
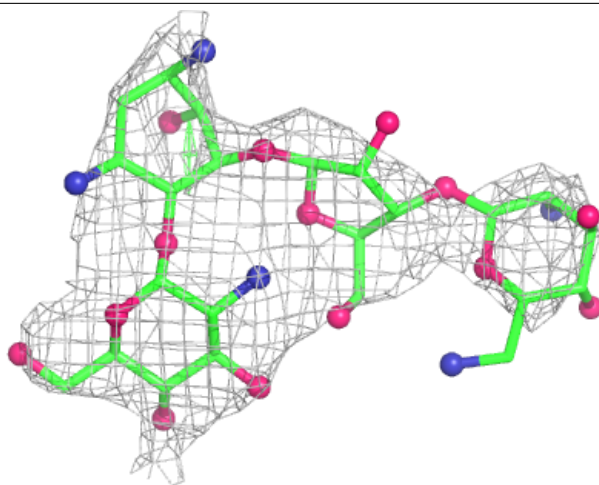
Electron density around PAR A 1606:

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



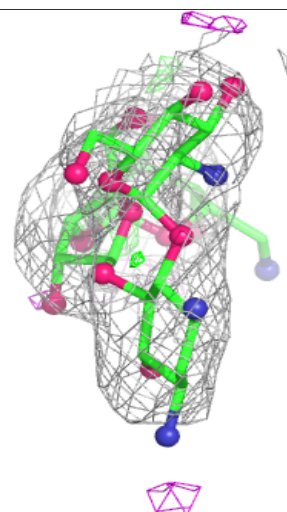
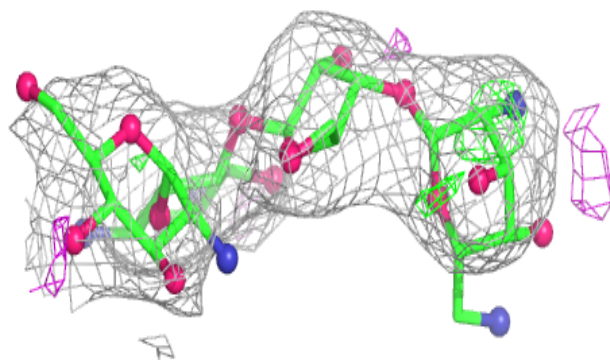
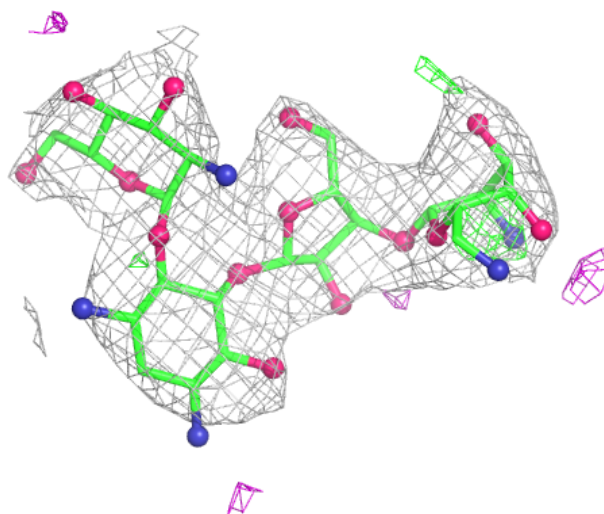
Electron density around PAR A 1604:

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



Electron density around PAR A 1601:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.