



## Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 04:01 AM UTC

PDB ID : 7YED / pdb\_00007yed  
EMDB ID : EMD-33770  
Title : In situ structure of polymerase complex of mammalian reovirus in the elongation state  
Authors : Bao, K.Y.; Zhang, X.L.; Li, D.Y.; Zhu, P.  
Deposited on : 2022-07-05  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

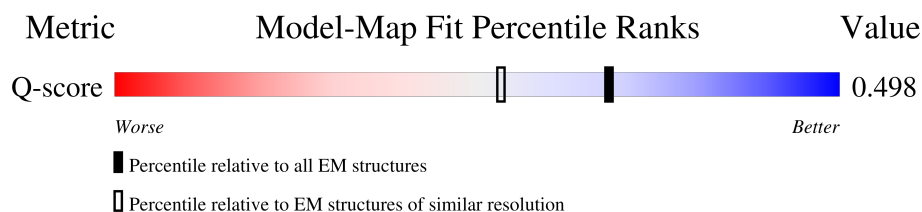
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 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  | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|---------|-----------------------------|----------------------------------------------------------|
| Q-score | 25397                       | 14081 ( 2.50 - 3.50 )                                    |

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

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 158907 atoms, of which 291 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called RNA helicase.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1   | 1     | 139      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 1035  | 616  | 197  | 219  | 3  |         |       |
| 1   | 2     | 139      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 1035  | 616  | 197  | 219  | 3  |         |       |
| 1   | 3     | 138      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 1030  | 613  | 196  | 218  | 3  |         |       |
| 1   | 4     | 131      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 969   | 577  | 183  | 206  | 3  |         |       |
| 1   | 5     | 139      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 1035  | 616  | 197  | 219  | 3  |         |       |
| 1   | A     | 1129     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 8875  | 5659 | 1511 | 1652 | 53 |         |       |
| 1   | B     | 1075     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 8455  | 5397 | 1433 | 1574 | 51 |         |       |
| 1   | C     | 1086     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 8563  | 5469 | 1450 | 1592 | 52 |         |       |
| 1   | D     | 1051     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 8306  | 5309 | 1404 | 1544 | 49 |         |       |
| 1   | E     | 1058     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 8361  | 5342 | 1416 | 1554 | 49 |         |       |
| 1   | a     | 1080     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 8525  | 5448 | 1448 | 1578 | 51 |         |       |
| 1   | b     | 1078     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 8511  | 5439 | 1446 | 1575 | 51 |         |       |
| 1   | c     | 1080     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 8527  | 5448 | 1449 | 1579 | 51 |         |       |
| 1   | d     | 1087     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 8576  | 5476 | 1456 | 1593 | 51 |         |       |
| 1   | e     | 1087     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 8576  | 5476 | 1456 | 1593 | 51 |         |       |

- Molecule 2 is a protein called Lambda-2 protein.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 2   | H     | 1288     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10143 | 6483 | 1699 | 1922 | 39 |         |       |
| 2   | I     | 1288     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10143 | 6483 | 1699 | 1922 | 39 |         |       |
| 2   | J     | 1288     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10143 | 6483 | 1699 | 1922 | 39 |         |       |
| 2   | K     | 1288     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10143 | 6483 | 1699 | 1922 | 39 |         |       |
| 2   | L     | 1288     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10143 | 6483 | 1699 | 1922 | 39 |         |       |

- Molecule 3 is a RNA chain called RNA (5'-R(P\*UP\*UP\*UP\*AP\*AP\*AP\*AP\*UP\*UP\*UP\*UP\*AP\*AP\*AP\*AP\*UP\*AP\*AP\*UP\*U)-3').

| Mol | Chain | Residues | Atoms |     |    |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 3   | M     | 21       | Total | C   | N  | O   | P  | 0       | 0     |
|     |       |          | 442   | 200 | 75 | 146 | 21 |         |       |

- Molecule 4 is a RNA chain called RNA (36-MER).

| Mol | Chain | Residues | Atoms |     |    |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 4   | N     | 26       | Total | C   | N  | O   | P  | 0       | 0     |
|     |       |          | 540   | 247 | 91 | 178 | 24 |         |       |

- Molecule 5 is a protein called RNA-directed RNA polymerase.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 5   | R     | 1254     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 9919  | 6332 | 1699 | 1824 | 64 |         |       |

- Molecule 6 is a RNA chain called RNA (36-MER).

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 6   | T     | 36       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 753   | 342 | 126 | 250 | 35 |         |       |

- Molecule 7 is a protein called Mu-2 protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7   | U     | 679      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5399  | 3460 | 917 | 991 | 31 |         |       |

- | Mol | Chain | Residues | Atoms           | AltConf |
|-----|-------|----------|-----------------|---------|
| 8   | A     | 1        | Total Zn<br>1 1 | 0       |
| 8   | B     | 1        | Total Zn<br>1 1 | 0       |
| 8   | C     | 1        | Total Zn<br>1 1 | 0       |
| 8   | a     | 1        | Total Zn<br>1 1 | 0       |
| 8   | b     | 1        | Total Zn<br>1 1 | 0       |
| 8   | c     | 1        | Total Zn<br>1 1 | 0       |
| 8   | d     | 1        | Total Zn<br>1 1 | 0       |
| 8   | e     | 1        | Total Zn<br>1 1 | 0       |

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- The chemical structure of S-adenosylmethionine (SAM) is shown with the following atom labels: N6, N7, N9, N1, N3, C6, C5, C8, C2, C4, C3, C1, C2, C3, C4, C5, C6, C7, C8, C9, C10, C11, C12, C13, C14, C15, C16, C17, C18, C19, C20, C21, C22, C23, C24, C25, C26, C27, C28, C29, C30, C31, C32, C33, C34, C35, C36, C37, C38, C39, C40, C41, C42, C43, C44, C45, C46, C47, C48, C49, C50, C51, C52, C53, C54, C55, C56, C57, C58, C59, C60, C61, C62, C63, C64, C65, C66, C67, C68, C69, C70, C71, C72, C73, C74, C75, C76, C77, C78, C79, C80, C81, C82, C83, C84, C85, C86, C87, C88, C89, C90, C91, C92, C93, C94, C95, C96, C97, C98, C99, C100, C101, C102, C103, C104, C105, C106, C107, C108, C109, C110, C111, C112, C113, C114, C115, C116, C117, C118, C119, C120, C121, C122, C123, C124, C125, C126, C127, C128, C129, C130, C131, C132, C133, C134, C135, C136, C137, C138, C139, C140, C141, C142, C143, C144, C145, C146, C147, C148, C149, C150, C151, C152, C153, C154, C155, C156, C157, C158, C159, C160, C161, C162, C163, C164, C165, C166, C167, C168, C169, C170, C171, C172, C173, C174, C175, C176, C177, C178, C179, C180, C181, C182, C183, C184, C185, C186, C187, C188, C189, C190, C191, C192, C193, C194, C195, C196, C197, C198, C199, C200, C201, C202, C203, C204, C205, C206, C207, C208, C209, C210, C211, C212, C213, C214, C215, C216, C217, C218, C219, C220, C221, C222, C223, C224, C225, C226, C227, C228, C229, C230, C231, C232, C233, C234, C235, C236, C237, C238, C239, C240, C241, C242, C243, C244, C245, C246, C247, C248, C249, C250, C251, C252, C253, C254, C255, C256, C257, C258, C259, C260, C261, C262, C263, C264, C265, C266, C267, C268, C269, C270, C271, C272, C273, C274, C275, C276, C277, C278, C279, C280, C281, C282, C283, C284, C285, C286, C287, C288, C289, C290, C291, C292, C293, C294, C295, C296, C297, C298, C299, C300, C301, C302, C303, C304, C305, C306, C307, C308, C309, C310, C311, C312, C313, C314, C315, C316, C317, C318, C319, C320, C321, C322, C323, C324, C325, C326, C327, C328, C329, C330, C331, C332, C333, C334, C335, C336, C337, C338, C339, C340, C341, C342, C343, C344, C345, C346, C347, C348, C349, C350, C351, C352, C353, C354, C355, C356, C357, C358, C359, C360, C361, C362, C363, C364, C365, C366, C367, C368, C369, C370, C371, C372, C373, C374, C375, C376, C377, C378, C379, C380, C381, C382, C383, C384, C385, C386, C387, C388, C389, C390, C391, C392, C393, C394, C395, C396, C397, C398, C399, C400, C401, C402, C403, C404, C405, C406, C407, C408, C409, C410, C411, C412, C413, C414, C415, C416, C417, C418, C419, C420, C421, C422, C423, C424, C425, C426, C427, C428, C429, C430, C431, C432, C433, C434, C435, C436, C437, C438, C439, C440, C441, C442, C443, C444, C445, C446, C447, C448, C449, C450, C451, C452, C453, C454, C455, C456, C457, C458, C459, C460, C461, C462, C463, C464, C465, C466, C467, C468, C469, C470, C471, C472, C473, C474, C475, C476, C477, C478, C479, C480, C481, C482, C483, C484, C485, C486, C487, C488, C489, C490, C491, C492, C493, C494, C495, C496, C497, C498, C499, C500, C501, C502, C503, C504, C505, C506, C507, C508, C509, C510, C511, C512, C513, C514, C515, C516, C517, C518, C519, C520, C521, C522, C523, C524, C525, C526, C527, C528, C529, C530, C531, C532, C533, C534, C535, C536, C537, C538, C539, C540, C541, C542, C543, C544, C545, C546, C547, C548, C549, C550, C551, C552, C553, C554, C555, C556, C557, C558, C559, C560, C561, C562, C563, C564, C565, C566, C567, C568, C569, C570, C571, C572, C573, C574, C575, C576, C577, C578, C579, C580, C581, C582, C583, C584, C585, C586, C587, C588, C589, C590, C591, C592, C593, C594, C595, C596, C597, C598, C599, C600, C601, C602, C603, C604, C605, C606, C607, C608, C609, C610, C611, C612, C613, C614, C615, C616, C617, C618, C619, C620, C621, C622, C623, C624, C625, C626, C627, C628, C629, C630, C631, C632, C633, C634, C635, C636, C637, C638, C639, C640, C641, C642, C643, C644, C645, C646, C647, C648, C649, C650, C651, C652, C653, C654, C655, C656, C657, C658, C659, C660, C661, C662, C663, C664, C665, C666, C667, C668, C669, C670, C671, C672, C673, C674, C675, C676, C677, C678, C679, C680, C681, C682, C683, C684, C685, C686, C687, C688, C689, C690, C691, C692, C693, C694, C695, C696, C697, C698, C699, C700, C701, C702, C703, C704, C705, C706, C707, C708, C709, C710, C711, C712, C713, C714, C715, C716, C717, C718, C719, C720, C721, C722, C723, C724, C725, C726, C727, C728, C729, C730, C731, C732, C733, C734, C735, C736, C737, C738, C739, C740, C741, C742, C743, C744, C745, C746, C747, C748, C749, C750, C751, C752, C753, C754, C755, C756, C757, C758, C759, C760, C761, C762, C763, C764, C765, C766, C767, C768, C769, C770, C771, C772, C773, C774, C775, C776, C777, C778, C779, C780, C781, C782, C783, C784, C785, C786, C787, C788, C789, C790, C791, C792, C793, C794, C795, C796, C797, C798, C799, C800, C801, C802, C803, C804, C805, C806, C807, C808, C809, C810, C811, C812, C813, C814, C815, C816, C817, C818, C819, C820, C821, C822, C823, C824, C82

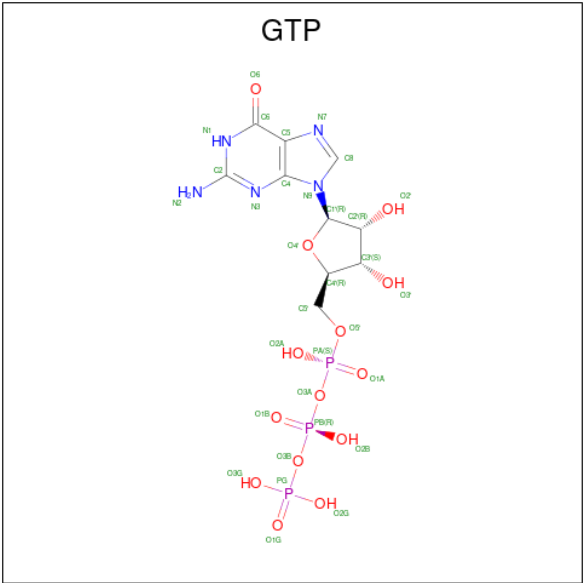
| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |   |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---|
| 9   | H     | 1        | Total<br>49 | C<br>15 | H<br>22 | N<br>6 | O<br>5 | S<br>1  | 0 |
| 9   | H     | 1        | Total<br>49 | C<br>15 | H<br>22 | N<br>6 | O<br>5 | S<br>1  | 0 |



Continued from previous page...

| Mol | Chain | Residues | Atoms |    |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---|---------|
| 9   | I     | 1        | Total | C  | H  | N | O | S | 0       |
|     |       |          | 49    | 15 | 22 | 6 | 5 | 1 |         |
| 9   | I     | 1        | Total | C  | H  | N | O | S | 0       |
|     |       |          | 49    | 15 | 22 | 6 | 5 | 1 |         |
| 9   | J     | 1        | Total | C  | H  | N | O | S | 0       |
|     |       |          | 49    | 15 | 22 | 6 | 5 | 1 |         |
| 9   | J     | 1        | Total | C  | H  | N | O | S | 0       |
|     |       |          | 49    | 15 | 22 | 6 | 5 | 1 |         |
| 9   | K     | 1        | Total | C  | H  | N | O | S | 0       |
|     |       |          | 49    | 15 | 22 | 6 | 5 | 1 |         |
| 9   | K     | 1        | Total | C  | H  | N | O | S | 0       |
|     |       |          | 49    | 15 | 22 | 6 | 5 | 1 |         |
| 9   | L     | 1        | Total | C  | H  | N | O | S | 0       |
|     |       |          | 49    | 15 | 22 | 6 | 5 | 1 |         |
| 9   | L     | 1        | Total | C  | H  | N | O | S | 0       |
|     |       |          | 49    | 15 | 22 | 6 | 5 | 1 |         |

- Molecule 10 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



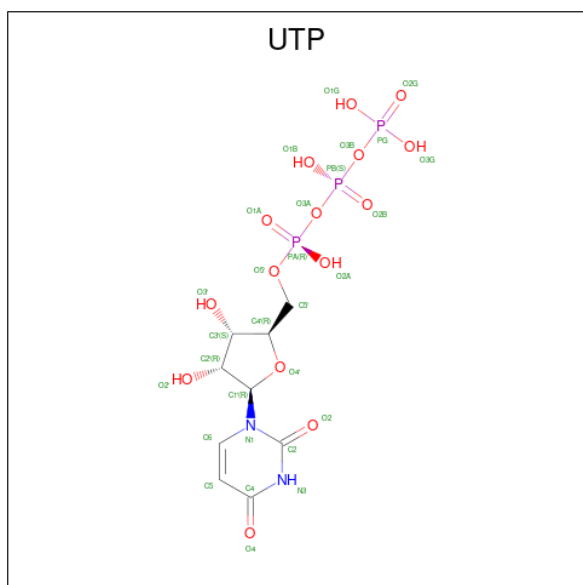
| Mol | Chain | Residues | Atoms |    |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|----|---|---------|
| 10  | H     | 1        | Total | C  | H  | N | O  | P | 0       |
|     |       |          | 44    | 10 | 12 | 5 | 14 | 3 |         |
| 10  | I     | 1        | Total | C  | H  | N | O  | P | 0       |
|     |       |          | 44    | 10 | 12 | 5 | 14 | 3 |         |
| 10  | J     | 1        | Total | C  | H  | N | O  | P | 0       |
|     |       |          | 44    | 10 | 12 | 5 | 14 | 3 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|----|---|---------|
| 10  | K     | 1        | Total | C  | H  | N | O  | P | 0       |
|     |       |          | 44    | 10 | 12 | 5 | 14 | 3 |         |
| 10  | L     | 1        | Total | C  | H  | N | O  | P | 0       |
|     |       |          | 44    | 10 | 12 | 5 | 14 | 3 |         |

- Molecule 11 is URIDINE 5'-TRIPHOSPHATE (CCD ID: UTP) (formula:  $C_9H_{15}N_2O_{15}P_3$ ).



| Mol | Chain | Residues | Atoms |   |    |   |    |   | AltConf |
|-----|-------|----------|-------|---|----|---|----|---|---------|
| 11  | R     | 1        | Total | C | H  | N | O  | P | 0       |
|     |       |          | 40    | 9 | 11 | 2 | 15 | 3 |         |

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 12  | R     | 2        | Total | Mg | 0       |
|     |       |          | 2     | 2  |         |

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

### 3 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 100968                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 30                                      | Depositor |
| Minimum defocus (nm)                 | 1500                                    | Depositor |
| Maximum defocus (nm)                 | 1800                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 3.336                                   | Depositor |
| Minimum map value                    | -1.852                                  | Depositor |
| Average map value                    | 0.032                                   | Depositor |
| Map value standard deviation         | 0.205                                   | Depositor |
| Recommended contour level            | 0.5                                     | Depositor |
| Map size (Å)                         | 435.2, 435.2, 435.2                     | wwPDB     |
| Map dimensions                       | 320, 320, 320                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.36, 1.36, 1.36                        | Depositor |

## 4 Model quality [i](#)

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

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

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

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

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

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

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

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

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

### 4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

Of 26 ligands modelled in this entry, 10 are monoatomic - leaving 16 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 |
| 9   | SAM  | H     | 1302 | -    | 27,29,29     | 4.11 | 11 (40%) | 34,42,42    | 4.52 | 16 (47%) |
| 9   | SAM  | K     | 1302 | -    | 27,29,29     | 1.42 | 4 (14%)  | 34,42,42    | 2.34 | 11 (32%) |
| 9   | SAM  | L     | 1303 | -    | 27,29,29     | 4.10 | 11 (40%) | 34,42,42    | 4.52 | 16 (47%) |
| 9   | SAM  | J     | 1301 | -    | 27,29,29     | 4.10 | 11 (40%) | 34,42,42    | 4.51 | 16 (47%) |
| 9   | SAM  | I     | 1301 | -    | 27,29,29     | 1.46 | 7 (25%)  | 34,42,42    | 2.24 | 13 (38%) |
| 9   | SAM  | L     | 1302 | -    | 27,29,29     | 1.46 | 7 (25%)  | 34,42,42    | 2.07 | 11 (32%) |
| 10  | GTP  | I     | 1302 | -    | 33,34,34     | 3.29 | 12 (36%) | 50,54,54    | 3.88 | 18 (36%) |
| 10  | GTP  | K     | 1303 | -    | 33,34,34     | 3.28 | 12 (36%) | 50,54,54    | 3.87 | 18 (36%) |
| 11  | UTP  | R     | 1301 | 12   | 29,30,30     | 3.78 | 8 (27%)  | 43,47,47    | 4.28 | 14 (32%) |
| 10  | GTP  | J     | 1303 | -    | 33,34,34     | 3.28 | 12 (36%) | 50,54,54    | 3.87 | 18 (36%) |
| 9   | SAM  | I     | 1303 | -    | 27,29,29     | 4.10 | 11 (40%) | 34,42,42    | 4.51 | 16 (47%) |
| 9   | SAM  | J     | 1302 | -    | 27,29,29     | 1.44 | 6 (22%)  | 34,42,42    | 2.25 | 11 (32%) |
| 9   | SAM  | K     | 1301 | -    | 27,29,29     | 4.10 | 11 (40%) | 34,42,42    | 4.51 | 16 (47%) |
| 10  | GTP  | L     | 1301 | -    | 33,34,34     | 3.28 | 12 (36%) | 50,54,54    | 3.87 | 18 (36%) |
| 10  | GTP  | H     | 1303 | -    | 33,34,34     | 3.27 | 12 (36%) | 50,54,54    | 3.87 | 18 (36%) |
| 9   | SAM  | H     | 1301 | -    | 27,29,29     | 1.46 | 7 (25%)  | 34,42,42    | 2.08 | 10 (29%) |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 9   | SAM  | H     | 1302 | -    | -       | 5/17/33/33 | 0/3/3/3 |
| 9   | SAM  | K     | 1302 | -    | -       | 4/17/33/33 | 0/3/3/3 |
| 9   | SAM  | L     | 1303 | -    | -       | 5/17/33/33 | 0/3/3/3 |
| 9   | SAM  | J     | 1301 | -    | -       | 5/17/33/33 | 0/3/3/3 |
| 9   | SAM  | I     | 1301 | -    | -       | 5/17/33/33 | 0/3/3/3 |
| 9   | SAM  | L     | 1302 | -    | -       | 4/17/33/33 | 0/3/3/3 |
| 10  | GTP  | I     | 1302 | -    | -       | 1/22/38/38 | 0/3/3/3 |
| 10  | GTP  | K     | 1303 | -    | -       | 1/22/38/38 | 0/3/3/3 |
| 11  | UTP  | R     | 1301 | 12   | -       | 1/22/38/38 | 0/2/2/2 |
| 10  | GTP  | J     | 1303 | -    | -       | 1/22/38/38 | 0/3/3/3 |
| 9   | SAM  | I     | 1303 | -    | -       | 5/17/33/33 | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 9   | SAM  | J     | 1302 | -    | -       | 4/17/33/33 | 0/3/3/3 |
| 9   | SAM  | K     | 1301 | -    | -       | 5/17/33/33 | 0/3/3/3 |
| 10  | GTP  | L     | 1301 | -    | -       | 1/22/38/38 | 0/3/3/3 |
| 10  | GTP  | H     | 1303 | -    | -       | 1/22/38/38 | 0/3/3/3 |
| 9   | SAM  | H     | 1301 | -    | -       | 5/17/33/33 | 0/3/3/3 |

All (154) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 11  | R     | 1301 | UTP  | O2-C2 | 11.55 | 1.43        | 1.23     |
| 10  | K     | 1303 | GTP  | O6-C6 | 10.49 | 1.43        | 1.23     |
| 10  | I     | 1302 | GTP  | O6-C6 | 10.47 | 1.43        | 1.23     |
| 10  | L     | 1301 | GTP  | O6-C6 | 10.46 | 1.43        | 1.23     |
| 10  | H     | 1303 | GTP  | O6-C6 | 10.44 | 1.43        | 1.23     |
| 10  | J     | 1303 | GTP  | O6-C6 | 10.43 | 1.43        | 1.23     |
| 11  | R     | 1301 | UTP  | O4-C4 | 9.43  | 1.42        | 1.24     |
| 9   | H     | 1302 | SAM  | C8-N7 | 8.67  | 1.48        | 1.31     |
| 9   | J     | 1301 | SAM  | C8-N7 | 8.65  | 1.48        | 1.31     |
| 9   | I     | 1303 | SAM  | C8-N7 | 8.65  | 1.48        | 1.31     |
| 9   | L     | 1303 | SAM  | C8-N7 | 8.64  | 1.48        | 1.31     |
| 9   | K     | 1301 | SAM  | C8-N7 | 8.59  | 1.48        | 1.31     |
| 9   | J     | 1301 | SAM  | C2-N1 | 8.39  | 1.48        | 1.33     |
| 9   | K     | 1301 | SAM  | C2-N1 | 8.37  | 1.48        | 1.33     |
| 9   | L     | 1303 | SAM  | C2-N1 | 8.37  | 1.48        | 1.33     |
| 9   | H     | 1302 | SAM  | C2-N1 | 8.35  | 1.48        | 1.33     |
| 9   | I     | 1303 | SAM  | C2-N1 | 8.28  | 1.48        | 1.33     |
| 9   | I     | 1303 | SAM  | C2-N3 | 8.09  | 1.48        | 1.33     |
| 9   | L     | 1303 | SAM  | C2-N3 | 8.07  | 1.48        | 1.33     |
| 9   | J     | 1301 | SAM  | C2-N3 | 8.06  | 1.48        | 1.33     |
| 9   | H     | 1302 | SAM  | C2-N3 | 8.06  | 1.48        | 1.33     |
| 9   | K     | 1301 | SAM  | C2-N3 | 8.04  | 1.48        | 1.33     |
| 11  | R     | 1301 | UTP  | C6-C5 | 7.54  | 1.52        | 1.35     |
| 9   | H     | 1302 | SAM  | C4-N3 | 6.72  | 1.47        | 1.34     |
| 9   | K     | 1301 | SAM  | C4-N3 | 6.71  | 1.47        | 1.34     |
| 9   | L     | 1303 | SAM  | C4-N3 | 6.71  | 1.47        | 1.34     |
| 9   | I     | 1303 | SAM  | C4-N3 | 6.70  | 1.46        | 1.34     |
| 9   | J     | 1301 | SAM  | C4-N3 | 6.67  | 1.46        | 1.34     |
| 9   | L     | 1303 | SAM  | C8-N9 | 6.43  | 1.48        | 1.37     |
| 9   | K     | 1301 | SAM  | C8-N9 | 6.41  | 1.48        | 1.37     |
| 9   | H     | 1302 | SAM  | C8-N9 | 6.41  | 1.48        | 1.37     |
| 9   | J     | 1301 | SAM  | C8-N9 | 6.40  | 1.48        | 1.37     |
| 9   | K     | 1301 | SAM  | C5-C4 | 6.39  | 1.50        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 9   | H     | 1302 | SAM  | C5-C4 | 6.37 | 1.50        | 1.39     |
| 9   | I     | 1303 | SAM  | C8-N9 | 6.37 | 1.48        | 1.37     |
| 9   | I     | 1303 | SAM  | C5-C4 | 6.36 | 1.50        | 1.39     |
| 9   | L     | 1303 | SAM  | C5-C4 | 6.33 | 1.50        | 1.39     |
| 9   | J     | 1301 | SAM  | C5-C4 | 6.32 | 1.50        | 1.39     |
| 11  | R     | 1301 | UTP  | C2-N1 | 6.20 | 1.48        | 1.38     |
| 10  | I     | 1302 | GTP  | C2-N3 | 5.83 | 1.47        | 1.33     |
| 10  | H     | 1303 | GTP  | C2-N3 | 5.83 | 1.47        | 1.33     |
| 10  | K     | 1303 | GTP  | C2-N3 | 5.82 | 1.47        | 1.33     |
| 10  | J     | 1303 | GTP  | C2-N3 | 5.78 | 1.47        | 1.33     |
| 10  | L     | 1301 | GTP  | C2-N3 | 5.78 | 1.47        | 1.33     |
| 10  | I     | 1302 | GTP  | C4-N3 | 5.65 | 1.47        | 1.34     |
| 10  | J     | 1303 | GTP  | C4-N3 | 5.61 | 1.47        | 1.34     |
| 10  | L     | 1301 | GTP  | C4-N3 | 5.61 | 1.47        | 1.34     |
| 10  | L     | 1301 | GTP  | C2-N2 | 5.58 | 1.47        | 1.34     |
| 10  | K     | 1303 | GTP  | C4-N3 | 5.58 | 1.47        | 1.34     |
| 10  | I     | 1302 | GTP  | C2-N2 | 5.57 | 1.47        | 1.34     |
| 10  | H     | 1303 | GTP  | C2-N2 | 5.57 | 1.47        | 1.34     |
| 10  | K     | 1303 | GTP  | C2-N2 | 5.57 | 1.47        | 1.34     |
| 10  | J     | 1303 | GTP  | C2-N2 | 5.57 | 1.47        | 1.34     |
| 10  | H     | 1303 | GTP  | C4-N3 | 5.49 | 1.46        | 1.34     |
| 10  | K     | 1303 | GTP  | C8-N7 | 5.39 | 1.47        | 1.32     |
| 10  | I     | 1302 | GTP  | C8-N7 | 5.38 | 1.47        | 1.32     |
| 10  | J     | 1303 | GTP  | C8-N7 | 5.37 | 1.47        | 1.32     |
| 9   | I     | 1303 | SAM  | C6-N6 | 5.35 | 1.47        | 1.34     |
| 10  | L     | 1301 | GTP  | C8-N7 | 5.35 | 1.47        | 1.32     |
| 10  | H     | 1303 | GTP  | C8-N7 | 5.35 | 1.47        | 1.32     |
| 9   | K     | 1301 | SAM  | C6-N6 | 5.32 | 1.47        | 1.34     |
| 9   | L     | 1303 | SAM  | C6-N6 | 5.31 | 1.47        | 1.34     |
| 9   | J     | 1301 | SAM  | C6-N6 | 5.31 | 1.47        | 1.34     |
| 11  | R     | 1301 | UTP  | C2-N3 | 5.28 | 1.47        | 1.38     |
| 9   | H     | 1302 | SAM  | C6-N6 | 5.27 | 1.47        | 1.34     |
| 9   | J     | 1301 | SAM  | C4-N9 | 4.90 | 1.47        | 1.37     |
| 9   | I     | 1303 | SAM  | C4-N9 | 4.90 | 1.47        | 1.37     |
| 9   | H     | 1302 | SAM  | C4-N9 | 4.87 | 1.47        | 1.37     |
| 9   | L     | 1303 | SAM  | C4-N9 | 4.85 | 1.47        | 1.37     |
| 9   | K     | 1301 | SAM  | C4-N9 | 4.83 | 1.47        | 1.37     |
| 11  | R     | 1301 | UTP  | C4-N3 | 4.75 | 1.46        | 1.38     |
| 10  | I     | 1302 | GTP  | C6-N1 | 4.73 | 1.47        | 1.38     |
| 10  | J     | 1303 | GTP  | C6-N1 | 4.72 | 1.47        | 1.38     |
| 10  | H     | 1303 | GTP  | C6-N1 | 4.71 | 1.47        | 1.38     |
| 10  | K     | 1303 | GTP  | C6-N1 | 4.71 | 1.47        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 10  | J     | 1303 | GTP  | C5-C4 | 4.70 | 1.51        | 1.38     |
| 10  | L     | 1301 | GTP  | C6-N1 | 4.69 | 1.47        | 1.38     |
| 10  | L     | 1301 | GTP  | C5-C4 | 4.67 | 1.51        | 1.38     |
| 10  | H     | 1303 | GTP  | C5-C4 | 4.67 | 1.51        | 1.38     |
| 10  | I     | 1302 | GTP  | C5-C4 | 4.66 | 1.51        | 1.38     |
| 10  | K     | 1303 | GTP  | C5-C4 | 4.64 | 1.51        | 1.38     |
| 9   | L     | 1303 | SAM  | C5-N7 | 4.54 | 1.47        | 1.39     |
| 9   | I     | 1303 | SAM  | C5-N7 | 4.52 | 1.47        | 1.39     |
| 9   | H     | 1302 | SAM  | C5-N7 | 4.52 | 1.47        | 1.39     |
| 9   | J     | 1301 | SAM  | C6-N1 | 4.52 | 1.48        | 1.35     |
| 9   | K     | 1301 | SAM  | C6-N1 | 4.51 | 1.48        | 1.35     |
| 9   | H     | 1302 | SAM  | C6-N1 | 4.51 | 1.48        | 1.35     |
| 9   | I     | 1303 | SAM  | C6-N1 | 4.49 | 1.48        | 1.35     |
| 9   | J     | 1301 | SAM  | C5-N7 | 4.49 | 1.47        | 1.39     |
| 9   | K     | 1301 | SAM  | C5-N7 | 4.47 | 1.47        | 1.39     |
| 9   | L     | 1303 | SAM  | C6-N1 | 4.44 | 1.48        | 1.35     |
| 11  | R     | 1301 | UTP  | C6-N1 | 4.27 | 1.48        | 1.38     |
| 10  | H     | 1303 | GTP  | C5-N7 | 4.23 | 1.47        | 1.39     |
| 10  | L     | 1301 | GTP  | C5-N7 | 4.20 | 1.47        | 1.39     |
| 10  | I     | 1302 | GTP  | C5-N7 | 4.20 | 1.47        | 1.39     |
| 10  | K     | 1303 | GTP  | C5-N7 | 4.20 | 1.47        | 1.39     |
| 10  | J     | 1303 | GTP  | C5-N7 | 4.19 | 1.47        | 1.39     |
| 10  | L     | 1301 | GTP  | C2-N1 | 4.19 | 1.47        | 1.37     |
| 9   | H     | 1301 | SAM  | C5-C4 | 4.18 | 1.46        | 1.39     |
| 10  | J     | 1303 | GTP  | C2-N1 | 4.18 | 1.47        | 1.37     |
| 10  | K     | 1303 | GTP  | C8-N9 | 4.17 | 1.46        | 1.37     |
| 10  | L     | 1301 | GTP  | C8-N9 | 4.17 | 1.46        | 1.37     |
| 9   | K     | 1302 | SAM  | C5-C4 | 4.16 | 1.46        | 1.39     |
| 10  | I     | 1302 | GTP  | C8-N9 | 4.16 | 1.46        | 1.37     |
| 10  | J     | 1303 | GTP  | C8-N9 | 4.15 | 1.46        | 1.37     |
| 10  | K     | 1303 | GTP  | C2-N1 | 4.15 | 1.47        | 1.37     |
| 10  | H     | 1303 | GTP  | C8-N9 | 4.15 | 1.46        | 1.37     |
| 10  | I     | 1302 | GTP  | C2-N1 | 4.15 | 1.47        | 1.37     |
| 9   | J     | 1302 | SAM  | C5-C4 | 4.15 | 1.46        | 1.39     |
| 10  | H     | 1303 | GTP  | C2-N1 | 4.14 | 1.47        | 1.37     |
| 9   | I     | 1301 | SAM  | C5-C4 | 4.13 | 1.46        | 1.39     |
| 9   | L     | 1302 | SAM  | C5-C4 | 4.11 | 1.46        | 1.39     |
| 9   | K     | 1301 | SAM  | C5-C6 | 3.87 | 1.51        | 1.41     |
| 9   | I     | 1303 | SAM  | C5-C6 | 3.87 | 1.51        | 1.41     |
| 9   | J     | 1301 | SAM  | C5-C6 | 3.86 | 1.51        | 1.41     |
| 9   | H     | 1302 | SAM  | C5-C6 | 3.86 | 1.51        | 1.41     |
| 9   | L     | 1303 | SAM  | C5-C6 | 3.86 | 1.51        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 11  | R     | 1301 | UTP  | C5-C4 | 3.60  | 1.51        | 1.43     |
| 10  | I     | 1302 | GTP  | C4-N9 | 3.19  | 1.46        | 1.38     |
| 10  | H     | 1303 | GTP  | C4-N9 | 3.16  | 1.46        | 1.38     |
| 10  | J     | 1303 | GTP  | C4-N9 | 3.15  | 1.46        | 1.38     |
| 10  | K     | 1303 | GTP  | C4-N9 | 3.14  | 1.46        | 1.38     |
| 10  | L     | 1301 | GTP  | C4-N9 | 3.14  | 1.46        | 1.38     |
| 9   | K     | 1302 | SAM  | C5-N7 | -2.80 | 1.34        | 1.39     |
| 9   | H     | 1301 | SAM  | C5-N7 | -2.72 | 1.34        | 1.39     |
| 9   | I     | 1301 | SAM  | C5-N7 | -2.68 | 1.34        | 1.39     |
| 9   | J     | 1302 | SAM  | C5-N7 | -2.67 | 1.34        | 1.39     |
| 9   | L     | 1302 | SAM  | C5-N7 | -2.65 | 1.34        | 1.39     |
| 9   | I     | 1301 | SAM  | OXT-C | -2.53 | 1.22        | 1.30     |
| 9   | J     | 1302 | SAM  | C5-C6 | 2.47  | 1.47        | 1.41     |
| 9   | L     | 1302 | SAM  | C5-C6 | 2.44  | 1.47        | 1.41     |
| 9   | K     | 1302 | SAM  | C5-C6 | 2.37  | 1.47        | 1.41     |
| 9   | I     | 1301 | SAM  | C5-C6 | 2.35  | 1.47        | 1.41     |
| 9   | H     | 1301 | SAM  | C5-C6 | 2.35  | 1.47        | 1.41     |
| 9   | J     | 1302 | SAM  | C8-N7 | 2.27  | 1.36        | 1.31     |
| 9   | L     | 1302 | SAM  | C4-N9 | -2.22 | 1.33        | 1.37     |
| 9   | L     | 1302 | SAM  | OXT-C | -2.21 | 1.23        | 1.30     |
| 9   | H     | 1301 | SAM  | C4-N9 | -2.20 | 1.33        | 1.37     |
| 9   | K     | 1302 | SAM  | C8-N7 | 2.19  | 1.35        | 1.31     |
| 9   | I     | 1301 | SAM  | C8-N7 | 2.17  | 1.35        | 1.31     |
| 9   | H     | 1301 | SAM  | C8-N7 | 2.17  | 1.35        | 1.31     |
| 9   | L     | 1302 | SAM  | C8-N7 | 2.11  | 1.35        | 1.31     |
| 9   | H     | 1301 | SAM  | OXT-C | -2.11 | 1.23        | 1.30     |
| 9   | J     | 1302 | SAM  | OXT-C | -2.10 | 1.23        | 1.30     |
| 9   | I     | 1301 | SAM  | C4-N9 | -2.10 | 1.33        | 1.37     |
| 10  | L     | 1301 | GTP  | C5-C6 | 2.07  | 1.52        | 1.44     |
| 10  | H     | 1303 | GTP  | C5-C6 | 2.07  | 1.52        | 1.44     |
| 10  | J     | 1303 | GTP  | C5-C6 | 2.07  | 1.52        | 1.44     |
| 10  | K     | 1303 | GTP  | C5-C6 | 2.06  | 1.52        | 1.44     |
| 9   | J     | 1302 | SAM  | C4-N9 | -2.04 | 1.33        | 1.37     |
| 10  | I     | 1302 | GTP  | C5-C6 | 2.04  | 1.52        | 1.44     |
| 9   | L     | 1302 | SAM  | CE-SD | -2.03 | 1.66        | 1.78     |
| 9   | I     | 1301 | SAM  | CE-SD | -2.01 | 1.66        | 1.78     |
| 9   | H     | 1301 | SAM  | CE-SD | -2.00 | 1.66        | 1.78     |

All (240) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 11  | R     | 1301 | UTP  | C4-N3-C2 | -16.70 | 105.88      | 126.61   |

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| Mol | Chain | Res  | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 9   | H     | 1302 | SAM  | C5-C4-N3 | -15.68 | 105.14      | 126.72   |
| 9   | I     | 1303 | SAM  | C5-C4-N3 | -15.66 | 105.15      | 126.72   |
| 9   | L     | 1303 | SAM  | C5-C4-N3 | -15.63 | 105.19      | 126.72   |
| 9   | K     | 1301 | SAM  | C5-C4-N3 | -15.63 | 105.20      | 126.72   |
| 9   | J     | 1301 | SAM  | C5-C4-N3 | -15.59 | 105.26      | 126.72   |
| 10  | I     | 1302 | GTP  | C5-C4-N3 | -12.81 | 108.00      | 128.39   |
| 10  | J     | 1303 | GTP  | C5-C4-N3 | -12.81 | 108.00      | 128.39   |
| 10  | K     | 1303 | GTP  | C5-C4-N3 | -12.78 | 108.06      | 128.39   |
| 10  | L     | 1301 | GTP  | C5-C4-N3 | -12.78 | 108.06      | 128.39   |
| 10  | H     | 1303 | GTP  | C5-C4-N3 | -12.75 | 108.10      | 128.39   |
| 10  | K     | 1303 | GTP  | C6-C5-N7 | -10.35 | 111.46      | 130.29   |
| 10  | H     | 1303 | GTP  | C6-C5-N7 | -10.33 | 111.49      | 130.29   |
| 10  | L     | 1301 | GTP  | C6-C5-N7 | -10.30 | 111.53      | 130.29   |
| 10  | I     | 1302 | GTP  | C6-C5-N7 | -10.29 | 111.56      | 130.29   |
| 10  | J     | 1303 | GTP  | C6-C5-N7 | -10.29 | 111.57      | 130.29   |
| 11  | R     | 1301 | UTP  | O2-C2-N1 | -9.99  | 109.80      | 122.80   |
| 9   | I     | 1303 | SAM  | C6-C5-C4 | -9.86  | 103.72      | 117.18   |
| 9   | J     | 1301 | SAM  | C6-C5-C4 | -9.84  | 103.74      | 117.18   |
| 9   | K     | 1301 | SAM  | C6-C5-C4 | -9.84  | 103.74      | 117.18   |
| 9   | L     | 1303 | SAM  | C6-C5-C4 | -9.84  | 103.74      | 117.18   |
| 9   | H     | 1302 | SAM  | C6-C5-C4 | -9.84  | 103.75      | 117.18   |
| 9   | L     | 1303 | SAM  | N3-C2-N1 | -9.29  | 114.53      | 128.58   |
| 9   | J     | 1301 | SAM  | N3-C2-N1 | -9.28  | 114.53      | 128.58   |
| 9   | H     | 1302 | SAM  | N3-C2-N1 | -9.27  | 114.55      | 128.58   |
| 9   | I     | 1303 | SAM  | N3-C2-N1 | -9.25  | 114.58      | 128.58   |
| 9   | K     | 1301 | SAM  | N3-C2-N1 | -9.24  | 114.60      | 128.58   |
| 11  | R     | 1301 | UTP  | C6-C5-C4 | -8.79  | 108.30      | 119.53   |
| 10  | L     | 1301 | GTP  | C2-N1-C6 | -8.71  | 109.32      | 125.11   |
| 10  | I     | 1302 | GTP  | C2-N1-C6 | -8.70  | 109.32      | 125.11   |
| 10  | K     | 1303 | GTP  | C2-N1-C6 | -8.70  | 109.33      | 125.11   |
| 10  | J     | 1303 | GTP  | C2-N1-C6 | -8.69  | 109.34      | 125.11   |
| 10  | H     | 1303 | GTP  | C2-N1-C6 | -8.69  | 109.34      | 125.11   |
| 11  | R     | 1301 | UTP  | O4-C4-C5 | -8.33  | 110.79      | 125.16   |
| 10  | I     | 1302 | GTP  | N9-C4-N3 | -7.94  | 110.08      | 125.95   |
| 10  | J     | 1303 | GTP  | N9-C4-N3 | -7.91  | 110.14      | 125.95   |
| 10  | L     | 1301 | GTP  | N9-C4-N3 | -7.90  | 110.16      | 125.95   |
| 10  | H     | 1303 | GTP  | N9-C4-N3 | -7.90  | 110.16      | 125.95   |
| 10  | K     | 1303 | GTP  | N9-C4-N3 | -7.89  | 110.18      | 125.95   |
| 9   | H     | 1302 | SAM  | C6-C5-N7 | -7.86  | 116.94      | 132.09   |
| 9   | J     | 1301 | SAM  | C6-C5-N7 | -7.85  | 116.95      | 132.09   |
| 9   | K     | 1301 | SAM  | C6-C5-N7 | -7.85  | 116.96      | 132.09   |
| 9   | I     | 1303 | SAM  | C6-C5-N7 | -7.84  | 116.98      | 132.09   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 9   | L     | 1303 | SAM  | C6-C5-N7  | -7.83 | 117.00      | 132.09   |
| 10  | K     | 1303 | GTP  | N1-C2-N3  | -7.55 | 109.51      | 123.32   |
| 10  | H     | 1303 | GTP  | N1-C2-N3  | -7.54 | 109.52      | 123.32   |
| 10  | I     | 1302 | GTP  | N1-C2-N3  | -7.54 | 109.52      | 123.32   |
| 10  | J     | 1303 | GTP  | N1-C2-N3  | -7.54 | 109.53      | 123.32   |
| 10  | L     | 1301 | GTP  | N1-C2-N3  | -7.54 | 109.53      | 123.32   |
| 11  | R     | 1301 | UTP  | C5-C4-N3  | -7.02 | 104.95      | 114.80   |
| 11  | R     | 1301 | UTP  | O2-C2-N3  | -6.67 | 109.19      | 121.49   |
| 10  | H     | 1303 | GTP  | C6-C5-C4  | -6.59 | 108.92      | 118.83   |
| 10  | L     | 1301 | GTP  | C6-C5-C4  | -6.58 | 108.93      | 118.83   |
| 10  | K     | 1303 | GTP  | C6-C5-C4  | -6.57 | 108.94      | 118.83   |
| 10  | J     | 1303 | GTP  | C1'-N9-C4 | -6.57 | 107.08      | 126.49   |
| 10  | I     | 1302 | GTP  | C1'-N9-C4 | -6.56 | 107.11      | 126.49   |
| 10  | J     | 1303 | GTP  | C6-C5-C4  | -6.55 | 108.97      | 118.83   |
| 10  | K     | 1303 | GTP  | C1'-N9-C4 | -6.55 | 107.15      | 126.49   |
| 10  | L     | 1301 | GTP  | C1'-N9-C4 | -6.54 | 107.16      | 126.49   |
| 10  | I     | 1302 | GTP  | C6-C5-C4  | -6.53 | 109.00      | 118.83   |
| 10  | H     | 1303 | GTP  | C1'-N9-C4 | -6.52 | 107.22      | 126.49   |
| 9   | K     | 1302 | SAM  | C5-C4-N3  | -6.30 | 118.04      | 126.72   |
| 10  | J     | 1303 | GTP  | O6-C6-C5  | -6.16 | 110.27      | 126.53   |
| 11  | R     | 1301 | UTP  | O4-C4-N3  | -6.15 | 110.35      | 119.27   |
| 10  | K     | 1303 | GTP  | O6-C6-C5  | -6.15 | 110.30      | 126.53   |
| 10  | I     | 1302 | GTP  | O6-C6-C5  | -6.15 | 110.31      | 126.53   |
| 10  | H     | 1303 | GTP  | O6-C6-C5  | -6.14 | 110.31      | 126.53   |
| 10  | L     | 1301 | GTP  | O6-C6-C5  | -6.14 | 110.32      | 126.53   |
| 9   | K     | 1302 | SAM  | CG-SD-C5' | 6.07  | 118.26      | 103.43   |
| 9   | J     | 1302 | SAM  | C5-C4-N3  | -6.01 | 118.44      | 126.72   |
| 9   | I     | 1301 | SAM  | C5-C4-N3  | -5.94 | 118.53      | 126.72   |
| 9   | H     | 1301 | SAM  | C5-C4-N3  | -5.93 | 118.56      | 126.72   |
| 9   | L     | 1302 | SAM  | C5-C4-N3  | -5.80 | 118.73      | 126.72   |
| 10  | I     | 1302 | GTP  | N2-C2-N3  | -5.64 | 108.66      | 119.67   |
| 10  | L     | 1301 | GTP  | N2-C2-N3  | -5.63 | 108.69      | 119.67   |
| 10  | J     | 1303 | GTP  | N2-C2-N3  | -5.60 | 108.74      | 119.67   |
| 10  | H     | 1303 | GTP  | N2-C2-N3  | -5.59 | 108.77      | 119.67   |
| 10  | K     | 1303 | GTP  | N2-C2-N3  | -5.59 | 108.77      | 119.67   |
| 11  | R     | 1301 | UTP  | C6-N1-C2  | -5.55 | 114.25      | 121.00   |
| 11  | R     | 1301 | UTP  | C1'-N1-C6 | -5.49 | 109.06      | 120.78   |
| 10  | K     | 1303 | GTP  | O6-C6-N1  | -5.41 | 109.94      | 120.11   |
| 10  | I     | 1302 | GTP  | O6-C6-N1  | -5.40 | 109.96      | 120.11   |
| 10  | L     | 1301 | GTP  | O6-C6-N1  | -5.39 | 109.98      | 120.11   |
| 10  | H     | 1303 | GTP  | O6-C6-N1  | -5.39 | 109.98      | 120.11   |
| 10  | J     | 1303 | GTP  | O6-C6-N1  | -5.37 | 110.01      | 120.11   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 9   | H     | 1302 | SAM  | C4-C5-N7  | -5.31 | 104.52      | 110.58   |
| 9   | L     | 1303 | SAM  | C4-C5-N7  | -5.29 | 104.53      | 110.58   |
| 9   | K     | 1301 | SAM  | C4-C5-N7  | -5.28 | 104.54      | 110.58   |
| 9   | I     | 1303 | SAM  | C4-C5-N7  | -5.26 | 104.57      | 110.58   |
| 9   | J     | 1301 | SAM  | C4-C5-N7  | -5.24 | 104.59      | 110.58   |
| 9   | J     | 1302 | SAM  | CG-SD-C5' | 5.22  | 116.20      | 103.43   |
| 10  | L     | 1301 | GTP  | C1'-N9-C8 | -5.12 | 112.19      | 126.73   |
| 10  | H     | 1303 | GTP  | C1'-N9-C8 | -5.11 | 112.20      | 126.73   |
| 10  | J     | 1303 | GTP  | C1'-N9-C8 | -5.11 | 112.22      | 126.73   |
| 10  | K     | 1303 | GTP  | C1'-N9-C8 | -5.10 | 112.25      | 126.73   |
| 10  | I     | 1302 | GTP  | C1'-N9-C8 | -5.10 | 112.25      | 126.73   |
| 9   | J     | 1301 | SAM  | C1'-N9-C8 | -4.92 | 116.18      | 127.09   |
| 9   | L     | 1303 | SAM  | C1'-N9-C8 | -4.91 | 116.19      | 127.09   |
| 9   | K     | 1301 | SAM  | C1'-N9-C8 | -4.90 | 116.21      | 127.09   |
| 9   | I     | 1303 | SAM  | C1'-N9-C8 | -4.90 | 116.22      | 127.09   |
| 9   | H     | 1302 | SAM  | C1'-N9-C8 | -4.90 | 116.23      | 127.09   |
| 11  | R     | 1301 | UTP  | C5-C6-N1  | -4.87 | 113.93      | 121.84   |
| 9   | L     | 1303 | SAM  | C5-C6-N6  | -4.74 | 111.54      | 123.29   |
| 9   | I     | 1303 | SAM  | C5-C6-N6  | -4.73 | 111.57      | 123.29   |
| 9   | H     | 1302 | SAM  | C5-C6-N6  | -4.73 | 111.58      | 123.29   |
| 9   | J     | 1301 | SAM  | C5-C6-N6  | -4.72 | 111.59      | 123.29   |
| 9   | K     | 1301 | SAM  | C5-C6-N6  | -4.72 | 111.59      | 123.29   |
| 9   | L     | 1303 | SAM  | C5-C6-N1  | -4.60 | 105.84      | 117.51   |
| 9   | H     | 1302 | SAM  | C5-C6-N1  | -4.60 | 105.84      | 117.51   |
| 9   | J     | 1301 | SAM  | C5-C6-N1  | -4.60 | 105.85      | 117.51   |
| 9   | K     | 1301 | SAM  | C5-C6-N1  | -4.59 | 105.85      | 117.51   |
| 9   | I     | 1303 | SAM  | C5-C6-N1  | -4.59 | 105.85      | 117.51   |
| 9   | K     | 1302 | SAM  | N3-C4-N9  | 4.58  | 134.96      | 127.17   |
| 9   | H     | 1301 | SAM  | N3-C4-N9  | 4.58  | 134.96      | 127.17   |
| 9   | J     | 1302 | SAM  | N3-C4-N9  | 4.57  | 134.93      | 127.17   |
| 9   | L     | 1302 | SAM  | N3-C4-N9  | 4.54  | 134.89      | 127.17   |
| 9   | I     | 1303 | SAM  | C4-N9-C1' | -4.44 | 116.25      | 126.63   |
| 9   | J     | 1301 | SAM  | C4-N9-C1' | -4.43 | 116.28      | 126.63   |
| 9   | K     | 1301 | SAM  | C4-N9-C1' | -4.41 | 116.31      | 126.63   |
| 9   | L     | 1303 | SAM  | C4-N9-C1' | -4.41 | 116.32      | 126.63   |
| 9   | I     | 1301 | SAM  | N3-C4-N9  | 4.40  | 134.66      | 127.17   |
| 9   | H     | 1302 | SAM  | C4-N9-C1' | -4.40 | 116.34      | 126.63   |
| 9   | J     | 1301 | SAM  | N9-C8-N7  | -4.31 | 107.83      | 113.94   |
| 9   | L     | 1303 | SAM  | N9-C8-N7  | -4.30 | 107.84      | 113.94   |
| 9   | K     | 1301 | SAM  | N9-C8-N7  | -4.28 | 107.86      | 113.94   |
| 9   | I     | 1303 | SAM  | N9-C8-N7  | -4.27 | 107.88      | 113.94   |
| 9   | H     | 1302 | SAM  | N9-C8-N7  | -4.26 | 107.89      | 113.94   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 9   | I     | 1301 | SAM  | CB-CA-N   | 4.20  | 121.07      | 110.12   |
| 11  | R     | 1301 | UTP  | C1'-N1-C2 | -4.15 | 110.14      | 117.59   |
| 9   | H     | 1302 | SAM  | N3-C4-N9  | -4.13 | 120.15      | 127.17   |
| 9   | L     | 1303 | SAM  | N3-C4-N9  | -4.12 | 120.17      | 127.17   |
| 9   | I     | 1303 | SAM  | N3-C4-N9  | -4.11 | 120.18      | 127.17   |
| 9   | K     | 1301 | SAM  | N3-C4-N9  | -4.11 | 120.18      | 127.17   |
| 9   | J     | 1301 | SAM  | N3-C4-N9  | -4.11 | 120.19      | 127.17   |
| 9   | K     | 1302 | SAM  | C2-N3-C4  | 4.08  | 121.80      | 111.83   |
| 9   | J     | 1302 | SAM  | C2-N3-C4  | 3.99  | 121.57      | 111.83   |
| 9   | L     | 1302 | SAM  | C2-N3-C4  | 3.97  | 121.53      | 111.83   |
| 9   | H     | 1301 | SAM  | C2-N3-C4  | 3.93  | 121.44      | 111.83   |
| 9   | I     | 1301 | SAM  | C2-N3-C4  | 3.90  | 121.35      | 111.83   |
| 9   | L     | 1302 | SAM  | N3-C2-N1  | -3.89 | 122.70      | 128.58   |
| 9   | H     | 1301 | SAM  | N3-C2-N1  | -3.86 | 122.73      | 128.58   |
| 9   | K     | 1302 | SAM  | N3-C2-N1  | -3.81 | 122.81      | 128.58   |
| 9   | J     | 1301 | SAM  | N6-C6-N1  | -3.79 | 109.93      | 118.38   |
| 9   | L     | 1303 | SAM  | N6-C6-N1  | -3.78 | 109.95      | 118.38   |
| 9   | I     | 1303 | SAM  | N6-C6-N1  | -3.77 | 109.97      | 118.38   |
| 9   | H     | 1302 | SAM  | N6-C6-N1  | -3.77 | 109.97      | 118.38   |
| 9   | K     | 1301 | SAM  | N6-C6-N1  | -3.77 | 109.97      | 118.38   |
| 9   | J     | 1302 | SAM  | N3-C2-N1  | -3.76 | 122.89      | 128.58   |
| 9   | K     | 1302 | SAM  | C4-C5-N7  | -3.69 | 106.36      | 110.58   |
| 9   | I     | 1301 | SAM  | N3-C2-N1  | -3.69 | 123.00      | 128.58   |
| 9   | I     | 1301 | SAM  | C4-C5-N7  | -3.53 | 106.55      | 110.58   |
| 9   | J     | 1302 | SAM  | C4-C5-N7  | -3.51 | 106.57      | 110.58   |
| 9   | L     | 1302 | SAM  | C4-C5-N7  | -3.43 | 106.66      | 110.58   |
| 10  | K     | 1303 | GTP  | N9-C8-N7  | -3.41 | 107.07      | 113.40   |
| 10  | L     | 1301 | GTP  | N9-C8-N7  | -3.41 | 107.08      | 113.40   |
| 9   | I     | 1301 | SAM  | CB-CA-C   | 3.41  | 119.47      | 110.45   |
| 10  | H     | 1303 | GTP  | N9-C8-N7  | -3.40 | 107.09      | 113.40   |
| 10  | I     | 1302 | GTP  | N9-C8-N7  | -3.40 | 107.10      | 113.40   |
| 10  | J     | 1303 | GTP  | N9-C8-N7  | -3.40 | 107.10      | 113.40   |
| 9   | H     | 1301 | SAM  | C4-C5-N7  | -3.37 | 106.73      | 110.58   |
| 10  | I     | 1302 | GTP  | C2-N3-C4  | -3.34 | 106.55      | 112.30   |
| 10  | H     | 1303 | GTP  | C2-N3-C4  | -3.29 | 106.62      | 112.30   |
| 10  | J     | 1303 | GTP  | C2-N3-C4  | -3.29 | 106.62      | 112.30   |
| 10  | L     | 1301 | GTP  | C2-N3-C4  | -3.29 | 106.63      | 112.30   |
| 10  | J     | 1303 | GTP  | N2-C2-N1  | -3.28 | 109.84      | 116.76   |
| 10  | L     | 1301 | GTP  | N2-C2-N1  | -3.25 | 109.90      | 116.76   |
| 10  | K     | 1303 | GTP  | C2-N3-C4  | -3.25 | 106.70      | 112.30   |
| 10  | H     | 1303 | GTP  | N2-C2-N1  | -3.25 | 109.91      | 116.76   |
| 10  | I     | 1302 | GTP  | N2-C2-N1  | -3.23 | 109.94      | 116.76   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 10  | K     | 1303 | GTP  | N2-C2-N1    | -3.22 | 109.95      | 116.76   |
| 9   | H     | 1302 | SAM  | C2-N1-C6    | -3.04 | 113.73      | 118.73   |
| 9   | J     | 1301 | SAM  | C2-N1-C6    | -3.04 | 113.73      | 118.73   |
| 9   | I     | 1303 | SAM  | C2-N1-C6    | -3.04 | 113.74      | 118.73   |
| 9   | K     | 1301 | SAM  | C2-N1-C6    | -3.04 | 113.74      | 118.73   |
| 9   | L     | 1303 | SAM  | C2-N1-C6    | -3.03 | 113.75      | 118.73   |
| 11  | R     | 1301 | UTP  | N3-C2-N1    | -3.00 | 110.99      | 114.89   |
| 9   | I     | 1303 | SAM  | C2-N3-C4    | -2.89 | 104.77      | 111.83   |
| 9   | L     | 1303 | SAM  | C2-N3-C4    | -2.89 | 104.78      | 111.83   |
| 9   | H     | 1302 | SAM  | C2-N3-C4    | -2.88 | 104.79      | 111.83   |
| 9   | J     | 1301 | SAM  | C2-N3-C4    | -2.88 | 104.79      | 111.83   |
| 9   | K     | 1301 | SAM  | C2-N3-C4    | -2.88 | 104.79      | 111.83   |
| 9   | L     | 1303 | SAM  | CG-SD-C5'   | 2.84  | 110.36      | 103.43   |
| 9   | J     | 1301 | SAM  | CG-SD-C5'   | 2.83  | 110.34      | 103.43   |
| 9   | H     | 1302 | SAM  | CG-SD-C5'   | 2.82  | 110.33      | 103.43   |
| 9   | K     | 1302 | SAM  | C5-N7-C8    | 2.81  | 107.87      | 103.45   |
| 9   | L     | 1302 | SAM  | C4-N9-C8    | 2.80  | 108.68      | 105.74   |
| 9   | I     | 1303 | SAM  | CG-SD-C5'   | 2.80  | 110.27      | 103.43   |
| 9   | K     | 1301 | SAM  | CG-SD-C5'   | 2.79  | 110.26      | 103.43   |
| 9   | J     | 1302 | SAM  | C5-N7-C8    | 2.72  | 107.72      | 103.45   |
| 9   | I     | 1301 | SAM  | C5-N7-C8    | 2.70  | 107.70      | 103.45   |
| 9   | L     | 1302 | SAM  | C5-N7-C8    | 2.67  | 107.65      | 103.45   |
| 9   | H     | 1301 | SAM  | C5-N7-C8    | 2.61  | 107.56      | 103.45   |
| 9   | H     | 1301 | SAM  | C4-N9-C8    | 2.58  | 108.44      | 105.74   |
| 9   | H     | 1301 | SAM  | CG-SD-C5'   | 2.56  | 109.69      | 103.43   |
| 9   | J     | 1302 | SAM  | C4-N9-C8    | 2.51  | 108.38      | 105.74   |
| 9   | L     | 1302 | SAM  | CG-SD-C5'   | 2.46  | 109.44      | 103.43   |
| 10  | K     | 1303 | GTP  | O4'-C1'-N9  | 2.46  | 113.92      | 108.36   |
| 10  | H     | 1303 | GTP  | O4'-C1'-N9  | 2.45  | 113.92      | 108.36   |
| 10  | I     | 1302 | GTP  | O4'-C1'-N9  | 2.45  | 113.91      | 108.36   |
| 10  | L     | 1301 | GTP  | C4-C5-N7    | -2.44 | 106.80      | 110.67   |
| 10  | L     | 1301 | GTP  | O4'-C1'-N9  | 2.44  | 113.88      | 108.36   |
| 11  | R     | 1301 | UTP  | C3'-C2'-C1' | 2.43  | 106.06      | 101.46   |
| 10  | J     | 1303 | GTP  | O4'-C1'-N9  | 2.43  | 113.86      | 108.36   |
| 9   | I     | 1301 | SAM  | CG-SD-C5'   | 2.42  | 109.35      | 103.43   |
| 10  | I     | 1302 | GTP  | C4-C5-N7    | -2.42 | 106.84      | 110.67   |
| 10  | J     | 1303 | GTP  | C4-C5-N7    | -2.41 | 106.85      | 110.67   |
| 10  | K     | 1303 | GTP  | C4-C5-N7    | -2.40 | 106.86      | 110.67   |
| 10  | H     | 1303 | GTP  | C4-C5-N7    | -2.40 | 106.87      | 110.67   |
| 10  | H     | 1303 | GTP  | C5-C6-N1    | -2.35 | 107.29      | 113.25   |
| 10  | J     | 1303 | GTP  | C5-C6-N1    | -2.34 | 107.30      | 113.25   |
| 10  | I     | 1302 | GTP  | C5-C6-N1    | -2.34 | 107.30      | 113.25   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 9   | L     | 1302 | SAM  | N9-C8-N7    | -2.33 | 110.63      | 113.94   |
| 10  | L     | 1301 | GTP  | C5-C6-N1    | -2.33 | 107.33      | 113.25   |
| 10  | K     | 1303 | GTP  | C5-C6-N1    | -2.32 | 107.34      | 113.25   |
| 9   | J     | 1302 | SAM  | N9-C8-N7    | -2.28 | 110.70      | 113.94   |
| 9   | I     | 1301 | SAM  | C4-N9-C8    | 2.26  | 108.11      | 105.74   |
| 9   | H     | 1301 | SAM  | N9-C8-N7    | -2.23 | 110.78      | 113.94   |
| 9   | J     | 1302 | SAM  | CE-SD-C5'   | 2.22  | 117.99      | 100.54   |
| 9   | I     | 1301 | SAM  | N9-C8-N7    | -2.19 | 110.83      | 113.94   |
| 9   | L     | 1302 | SAM  | C6-C5-N7    | 2.13  | 136.20      | 132.09   |
| 9   | H     | 1301 | SAM  | C2-N1-C6    | 2.12  | 122.21      | 118.73   |
| 9   | K     | 1302 | SAM  | N9-C8-N7    | -2.09 | 110.97      | 113.94   |
| 9   | J     | 1302 | SAM  | C6-C5-N7    | 2.09  | 136.12      | 132.09   |
| 9   | L     | 1302 | SAM  | C2-N1-C6    | 2.08  | 122.14      | 118.73   |
| 9   | J     | 1301 | SAM  | C2'-C1'-N9  | 2.07  | 118.44      | 113.30   |
| 9   | I     | 1301 | SAM  | C6-C5-N7    | 2.07  | 136.07      | 132.09   |
| 10  | H     | 1303 | GTP  | O2'-C2'-C1' | 2.06  | 117.21      | 110.10   |
| 9   | K     | 1301 | SAM  | C2'-C1'-N9  | 2.06  | 118.42      | 113.30   |
| 11  | R     | 1301 | UTP  | C2'-C3'-C4' | 2.06  | 106.58      | 102.61   |
| 10  | I     | 1302 | GTP  | O2'-C2'-C1' | 2.05  | 117.18      | 110.10   |
| 9   | I     | 1303 | SAM  | C2'-C1'-N9  | 2.05  | 118.39      | 113.30   |
| 10  | K     | 1303 | GTP  | O2'-C2'-C1' | 2.04  | 117.13      | 110.10   |
| 9   | K     | 1302 | SAM  | C2-N1-C6    | 2.04  | 122.08      | 118.73   |
| 10  | J     | 1303 | GTP  | O2'-C2'-C1' | 2.04  | 117.12      | 110.10   |
| 9   | L     | 1303 | SAM  | C2'-C1'-N9  | 2.04  | 118.36      | 113.30   |
| 10  | L     | 1301 | GTP  | O2'-C2'-C1' | 2.03  | 117.11      | 110.10   |
| 9   | H     | 1302 | SAM  | C2'-C1'-N9  | 2.03  | 118.36      | 113.30   |
| 9   | I     | 1301 | SAM  | C2-N1-C6    | 2.03  | 122.06      | 118.73   |
| 9   | K     | 1302 | SAM  | CE-SD-C5'   | 2.02  | 116.43      | 100.54   |
| 9   | K     | 1302 | SAM  | C6-C5-N7    | 2.02  | 135.98      | 132.09   |

There are no chirality outliers.

All (53) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms         |
|-----|-------|------|------|---------------|
| 9   | H     | 1302 | SAM  | O-C-CA-N      |
| 9   | H     | 1302 | SAM  | C4'-C5'-SD-CE |
| 9   | I     | 1301 | SAM  | N-CA-CB-CG    |
| 9   | I     | 1303 | SAM  | O-C-CA-N      |
| 9   | I     | 1303 | SAM  | C4'-C5'-SD-CE |
| 9   | J     | 1301 | SAM  | O-C-CA-N      |
| 9   | J     | 1301 | SAM  | C4'-C5'-SD-CE |
| 9   | J     | 1302 | SAM  | CA-CB-CG-SD   |

*Continued on next page...*

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 9   | K     | 1301 | SAM  | O-C-CA-N        |
| 9   | K     | 1301 | SAM  | C4'-C5'-SD-CE   |
| 9   | K     | 1302 | SAM  | CB-CG-SD-C5'    |
| 9   | L     | 1302 | SAM  | CB-CG-SD-CE     |
| 9   | L     | 1302 | SAM  | CB-CG-SD-C5'    |
| 9   | L     | 1303 | SAM  | O-C-CA-N        |
| 9   | L     | 1303 | SAM  | C4'-C5'-SD-CE   |
| 9   | H     | 1302 | SAM  | OXT-C-CA-N      |
| 9   | I     | 1303 | SAM  | OXT-C-CA-N      |
| 9   | J     | 1301 | SAM  | OXT-C-CA-N      |
| 9   | K     | 1301 | SAM  | OXT-C-CA-N      |
| 9   | L     | 1303 | SAM  | OXT-C-CA-N      |
| 9   | H     | 1301 | SAM  | CB-CG-SD-CE     |
| 9   | I     | 1301 | SAM  | CB-CG-SD-CE     |
| 9   | H     | 1301 | SAM  | OXT-C-CA-CB     |
| 9   | J     | 1302 | SAM  | O-C-CA-CB       |
| 9   | H     | 1302 | SAM  | O4'-C4'-C5'-SD  |
| 9   | I     | 1303 | SAM  | O4'-C4'-C5'-SD  |
| 9   | J     | 1301 | SAM  | O4'-C4'-C5'-SD  |
| 9   | K     | 1301 | SAM  | O4'-C4'-C5'-SD  |
| 9   | L     | 1303 | SAM  | O4'-C4'-C5'-SD  |
| 9   | H     | 1301 | SAM  | CB-CG-SD-C5'    |
| 9   | I     | 1301 | SAM  | CB-CG-SD-C5'    |
| 9   | J     | 1302 | SAM  | CB-CG-SD-C5'    |
| 10  | H     | 1303 | GTP  | C5'-O5'-PA-O2A  |
| 10  | I     | 1302 | GTP  | C5'-O5'-PA-O2A  |
| 10  | J     | 1303 | GTP  | C5'-O5'-PA-O2A  |
| 10  | K     | 1303 | GTP  | C5'-O5'-PA-O2A  |
| 10  | L     | 1301 | GTP  | C5'-O5'-PA-O2A  |
| 9   | H     | 1301 | SAM  | O-C-CA-CB       |
| 9   | L     | 1302 | SAM  | OXT-C-CA-N      |
| 9   | H     | 1302 | SAM  | C-CA-CB-CG      |
| 9   | I     | 1303 | SAM  | C-CA-CB-CG      |
| 9   | J     | 1301 | SAM  | C-CA-CB-CG      |
| 9   | K     | 1301 | SAM  | C-CA-CB-CG      |
| 9   | L     | 1303 | SAM  | C-CA-CB-CG      |
| 9   | J     | 1302 | SAM  | OXT-C-CA-CB     |
| 11  | R     | 1301 | UTP  | O4'-C4'-C5'-O5' |
| 9   | K     | 1302 | SAM  | C-CA-CB-CG      |
| 9   | K     | 1302 | SAM  | N-CA-CB-CG      |
| 9   | I     | 1301 | SAM  | O-C-CA-CB       |
| 9   | I     | 1301 | SAM  | OXT-C-CA-CB     |

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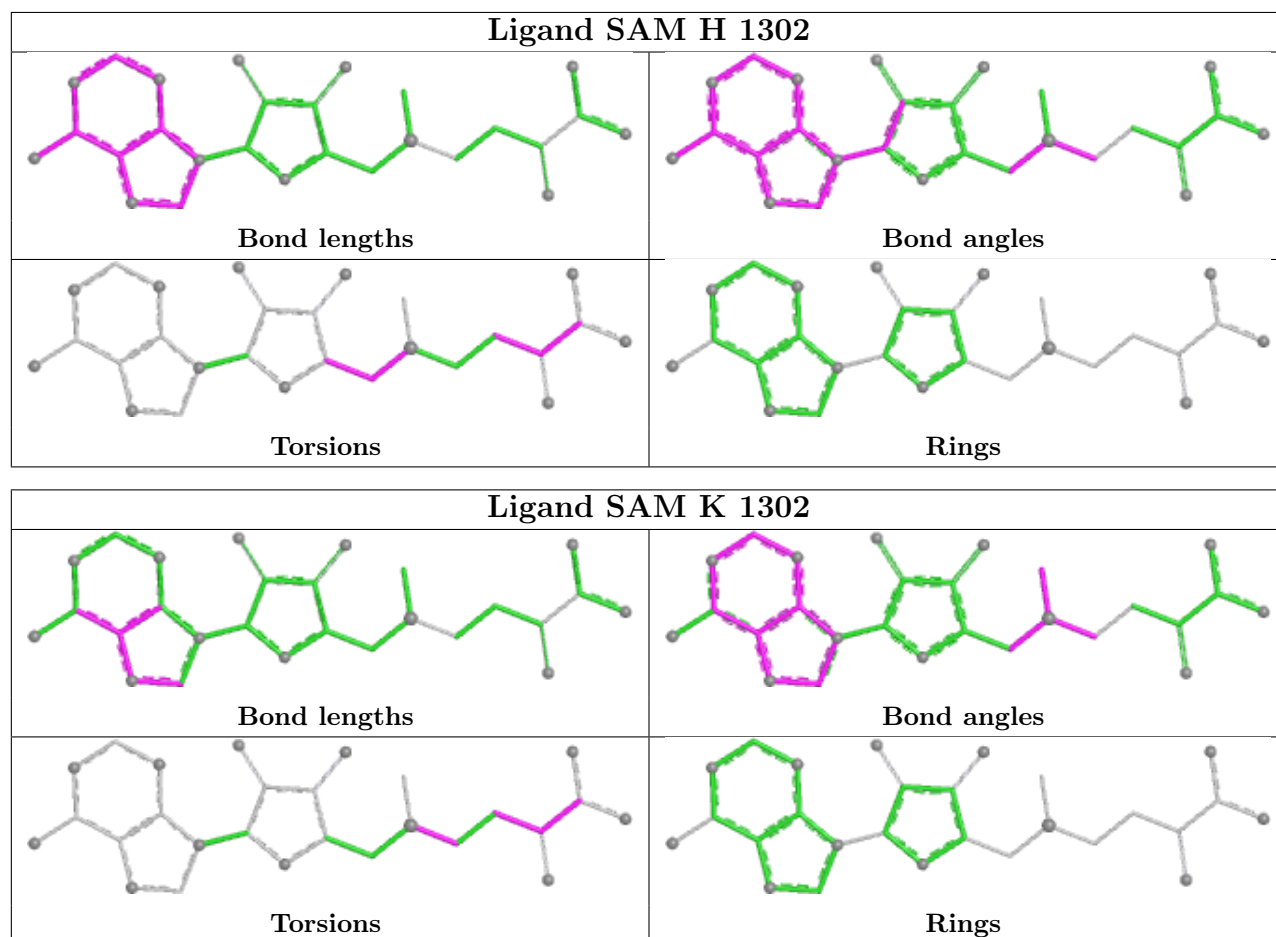
*Continued from previous page...*

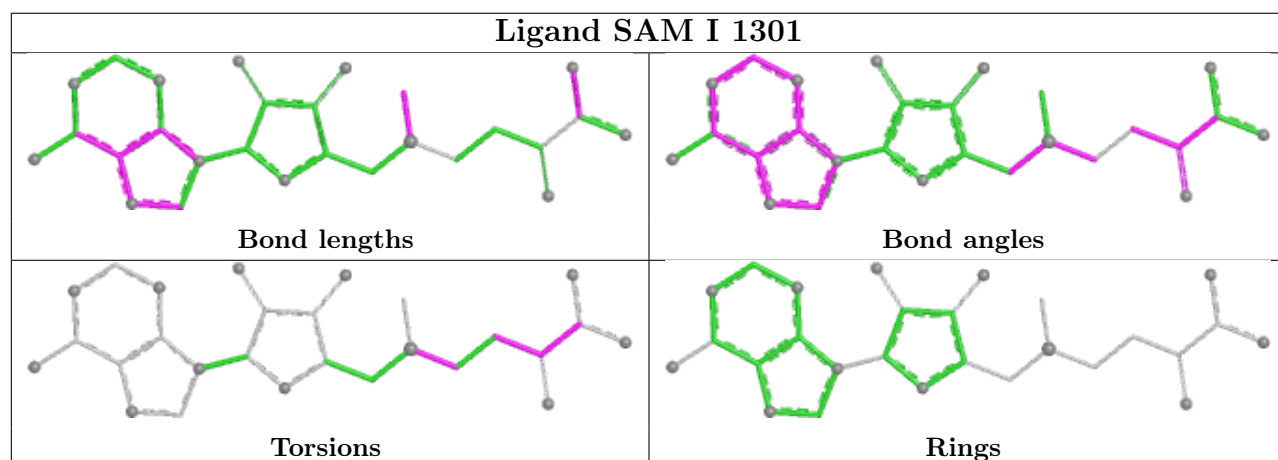
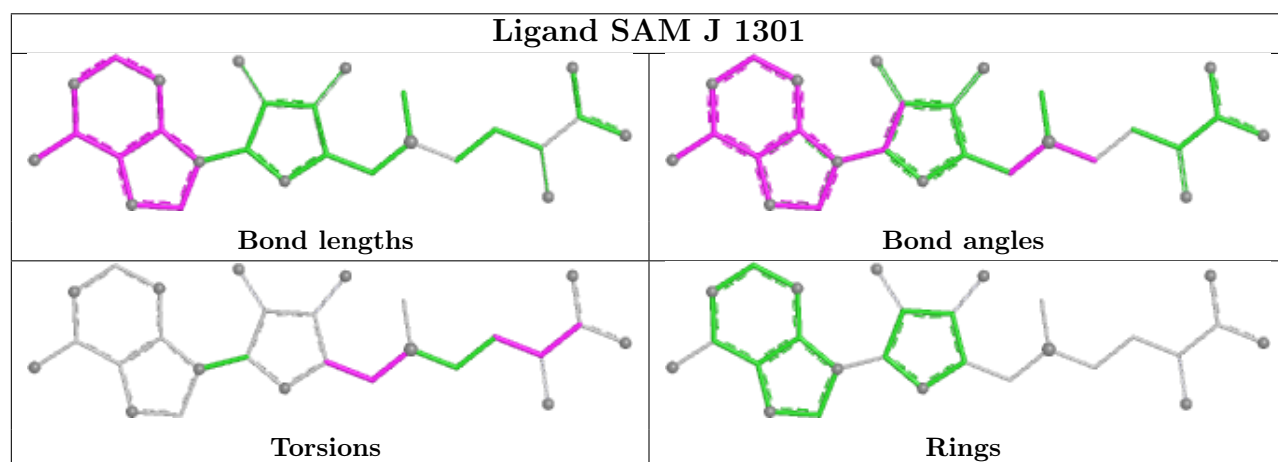
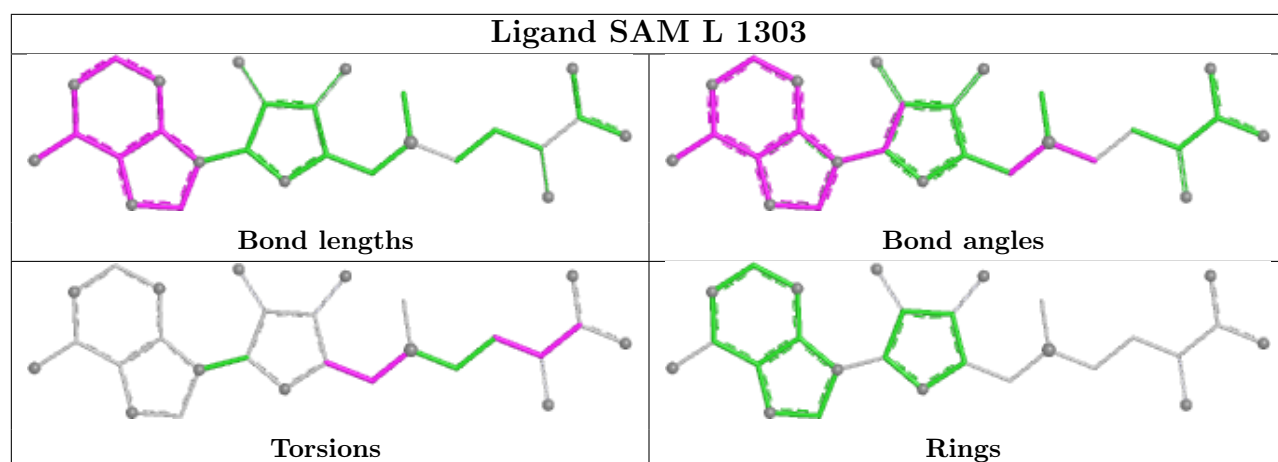
| Mol | Chain | Res  | Type | Atoms      |
|-----|-------|------|------|------------|
| 9   | K     | 1302 | SAM  | OXT-C-CA-N |
| 9   | L     | 1302 | SAM  | O-C-CA-N   |
| 9   | H     | 1301 | SAM  | OXT-C-CA-N |

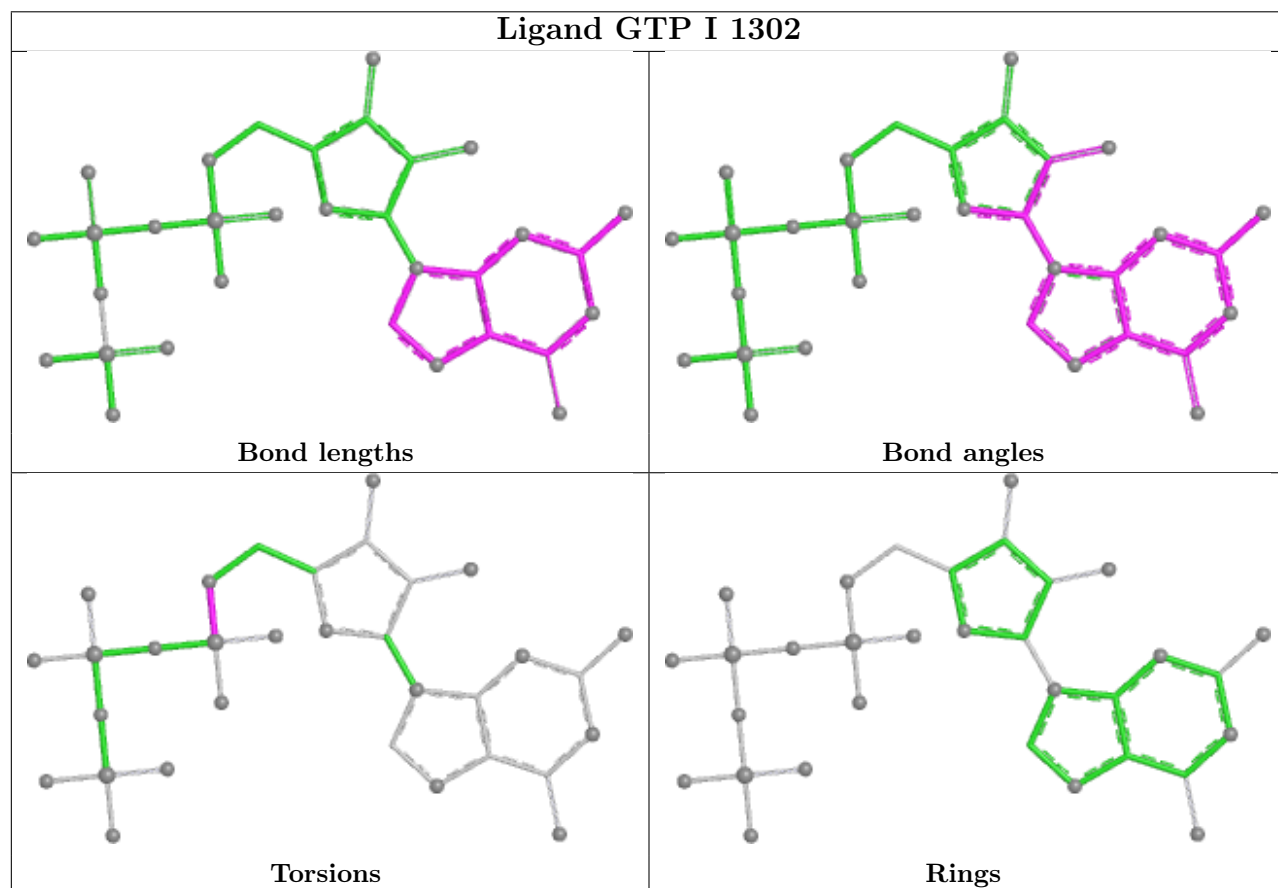
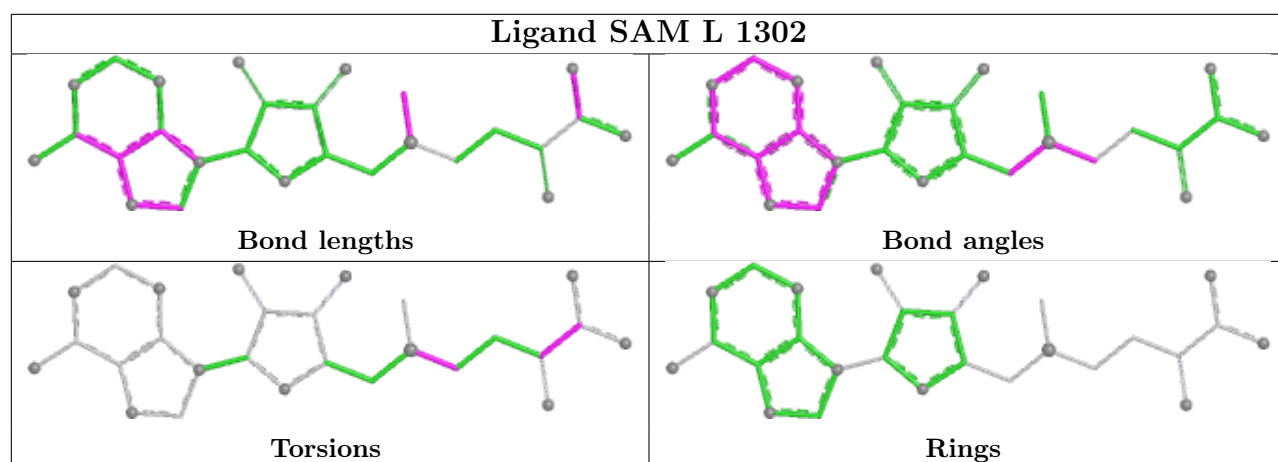
There are no ring outliers.

No monomer is involved in short contacts.

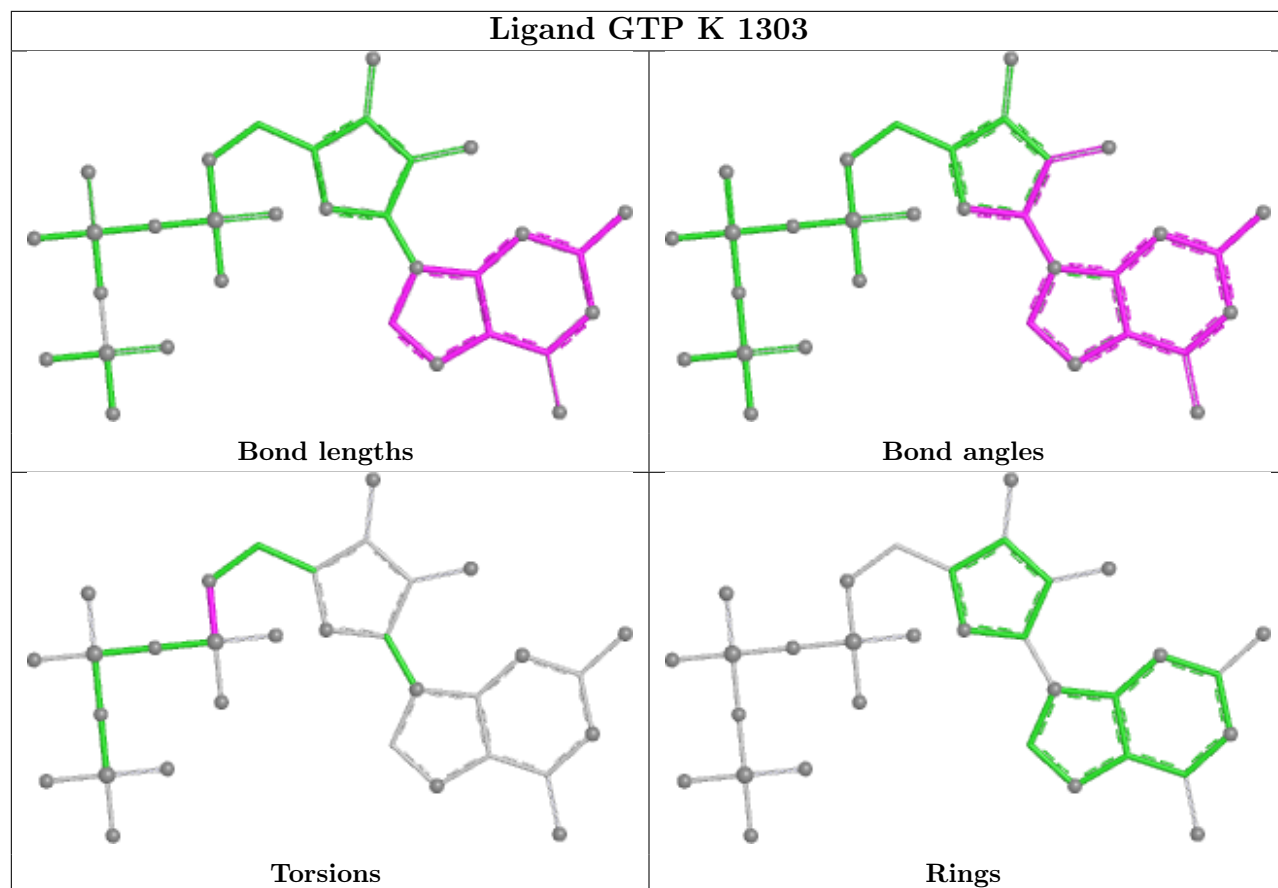
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



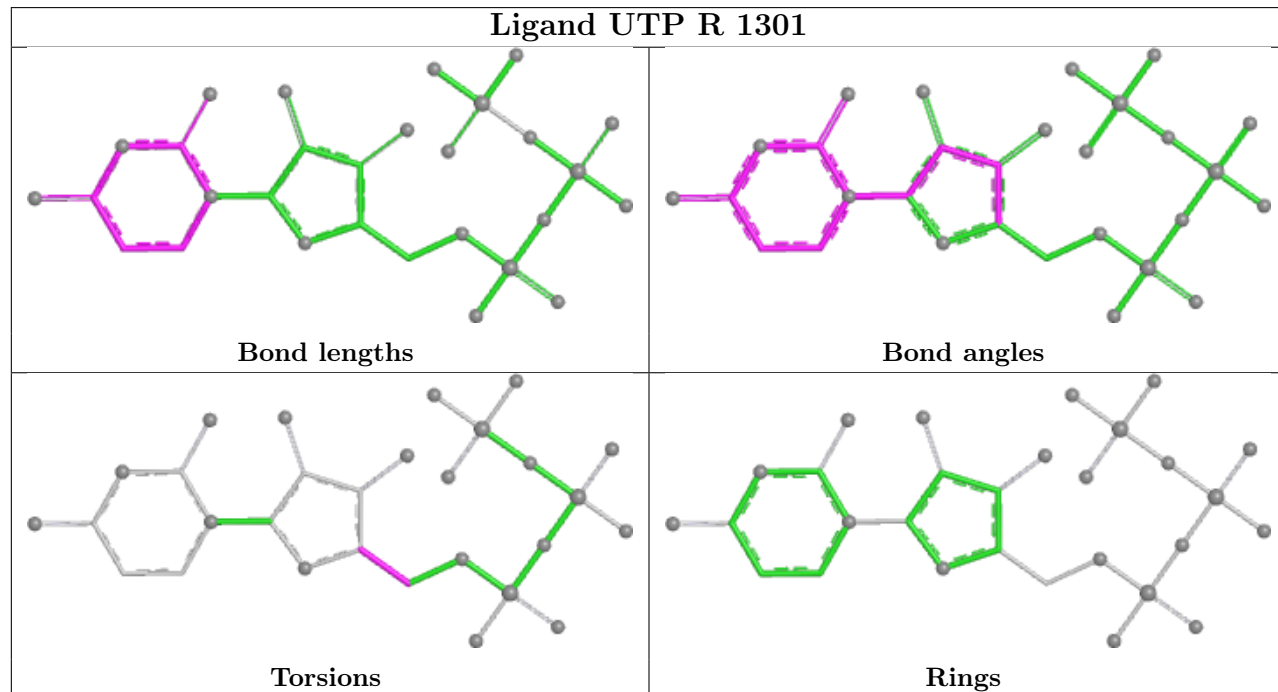


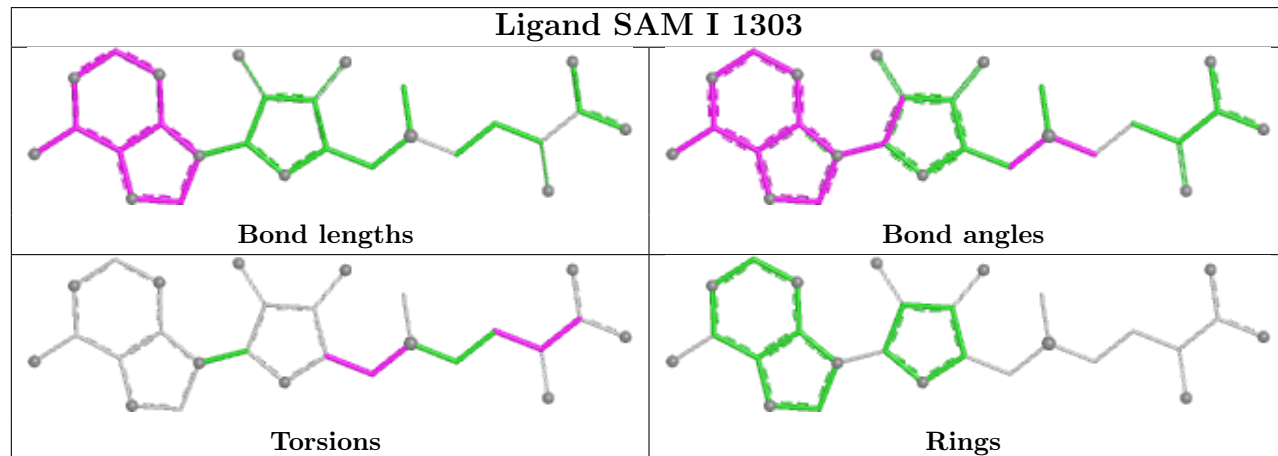
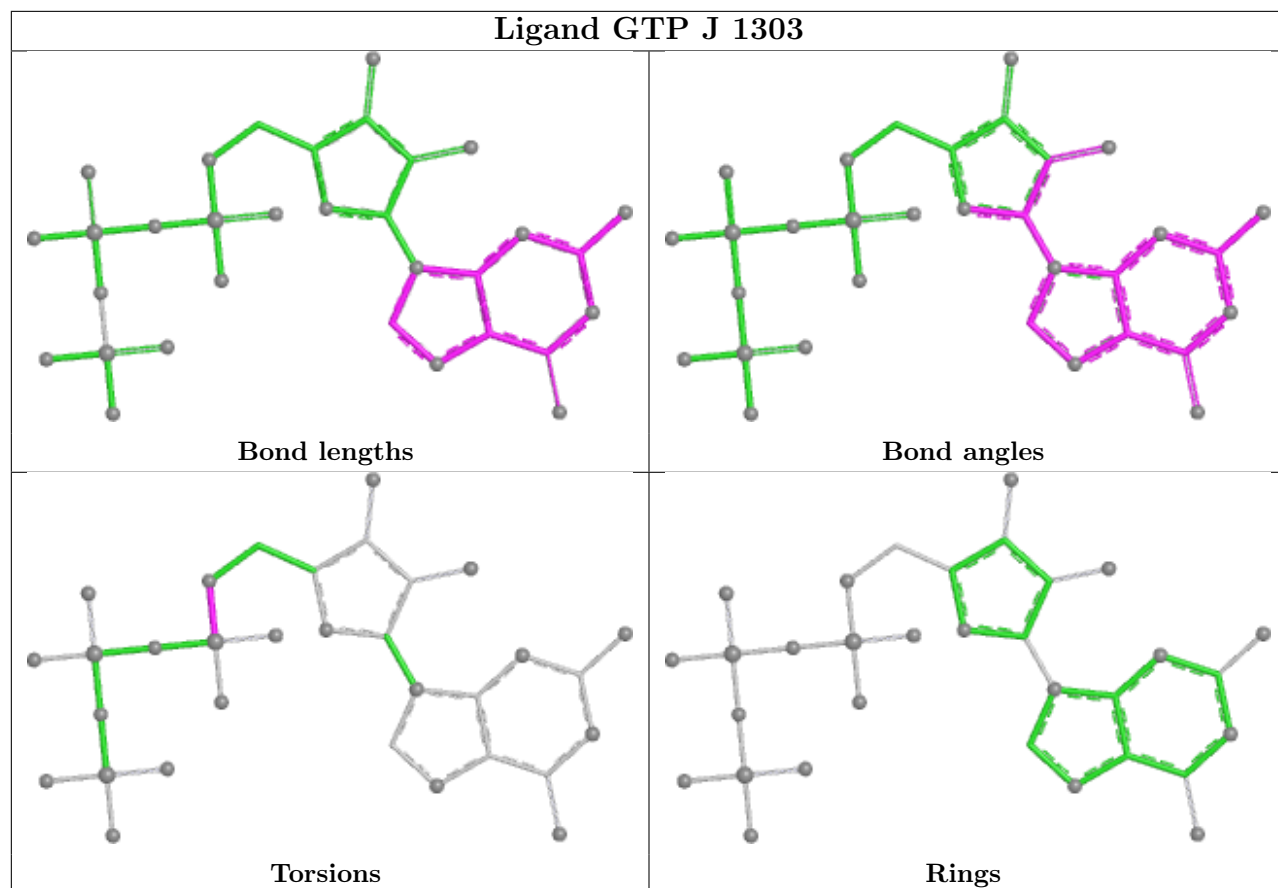


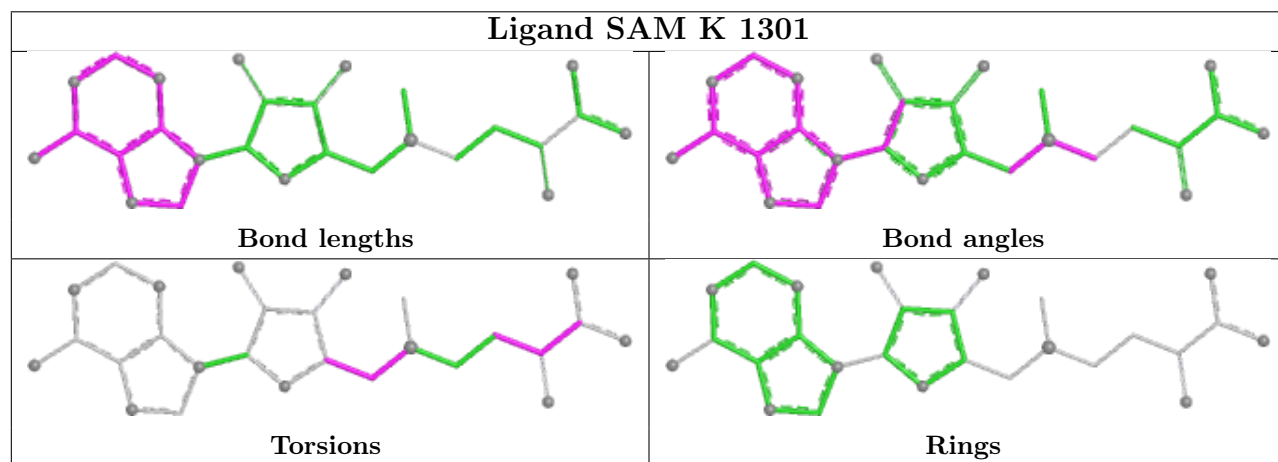
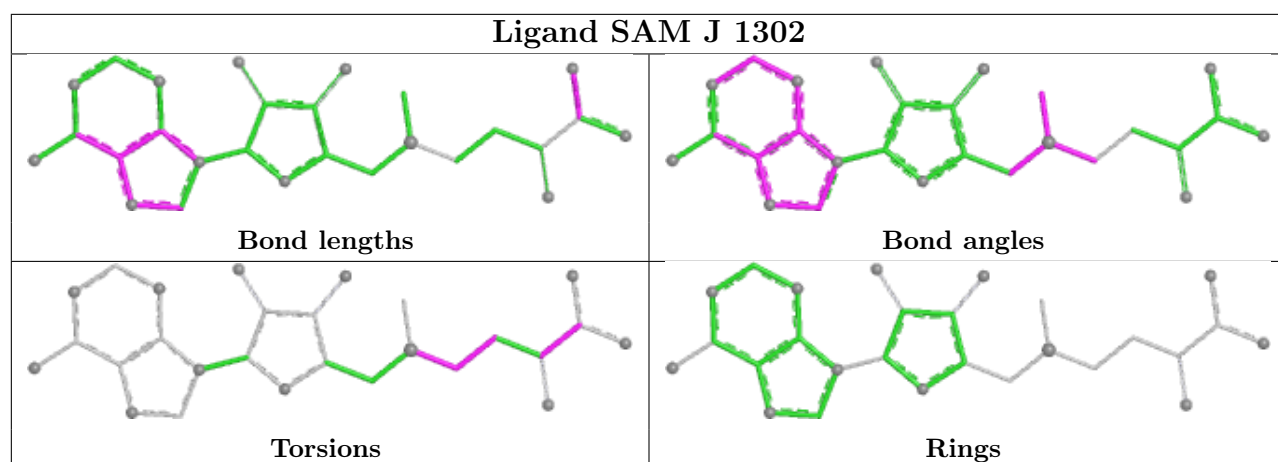
## Ligand GTP K 1303



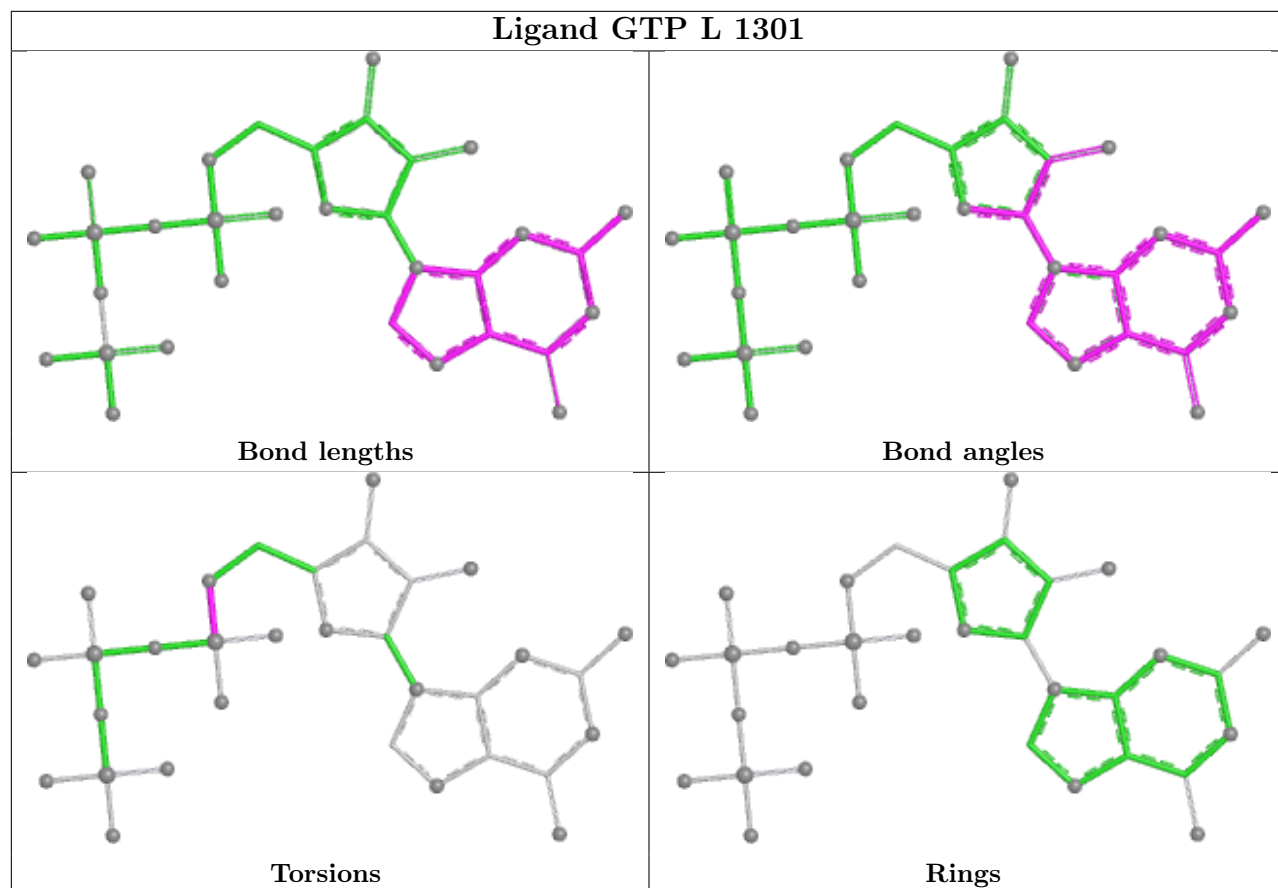
## Ligand UTP R 1301



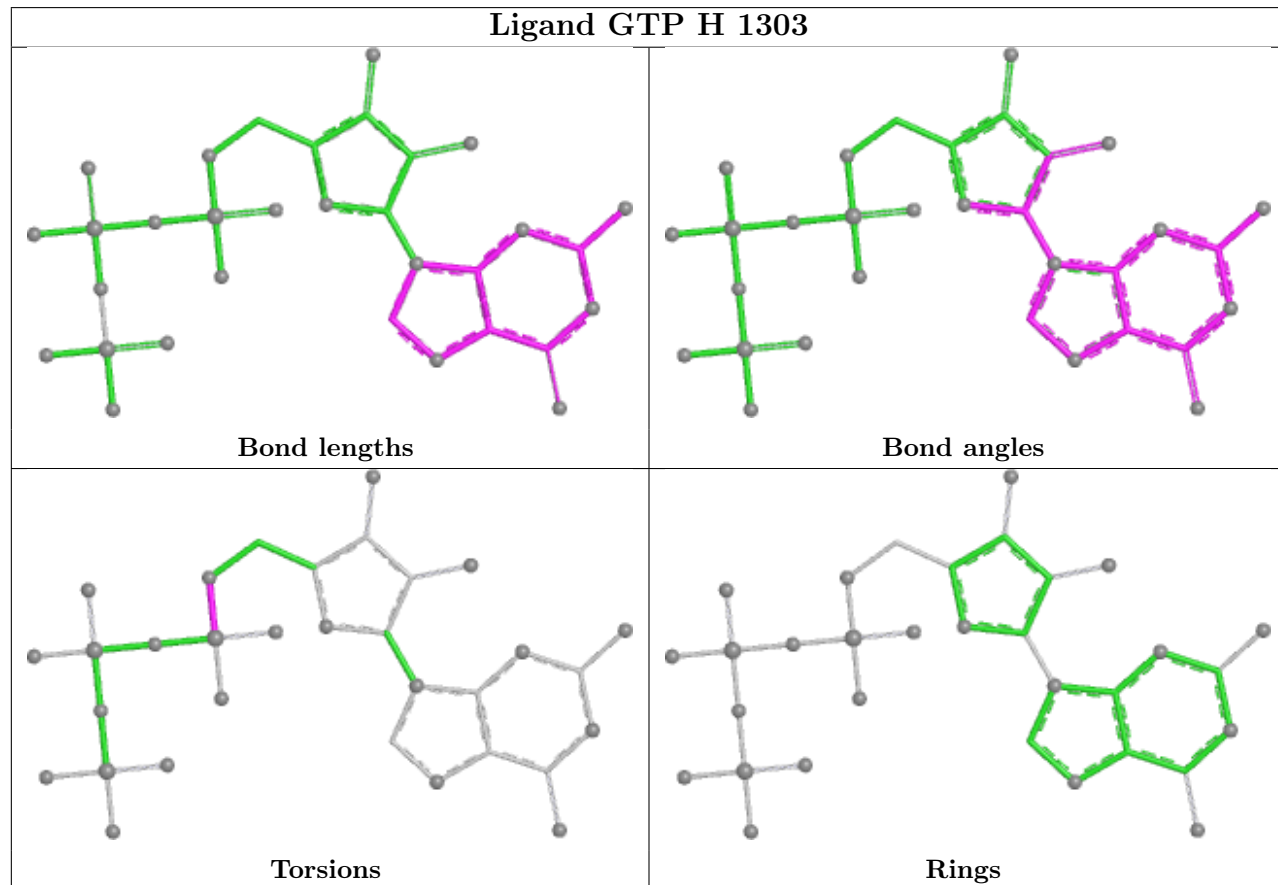


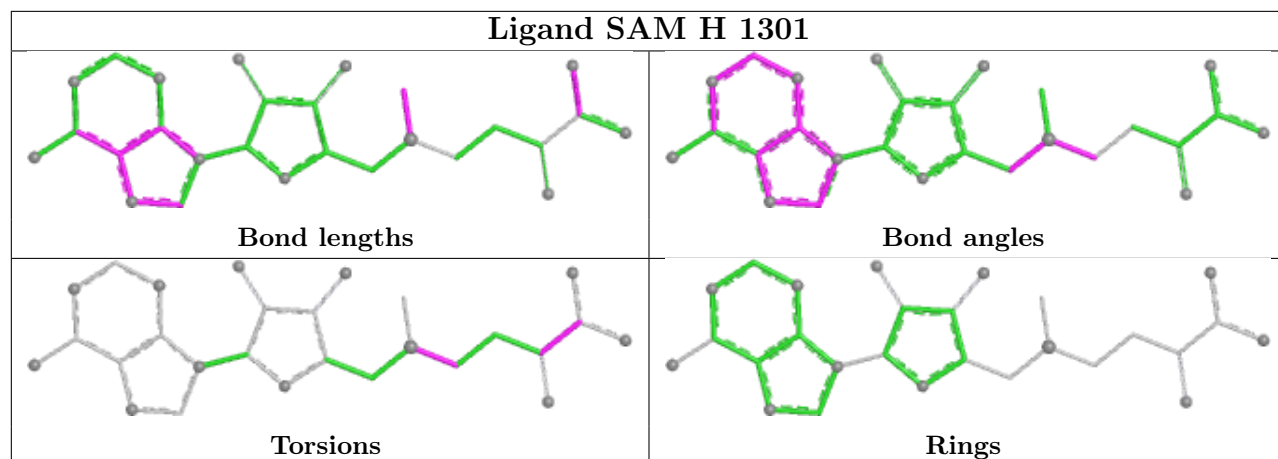


## Ligand GTP L 1301



## Ligand GTP H 1303





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

There are no such residues in this entry.

#### 4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

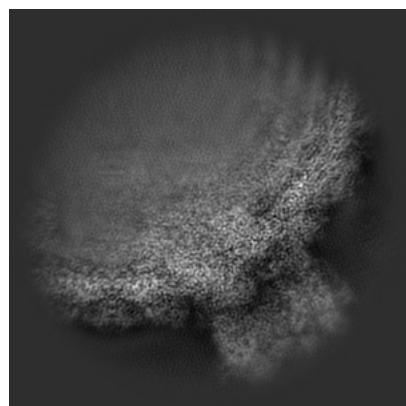
## 5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33770. These allow visual inspection of the internal detail of the map and identification of artifacts.

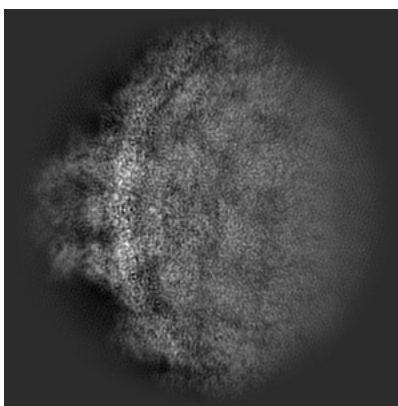
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

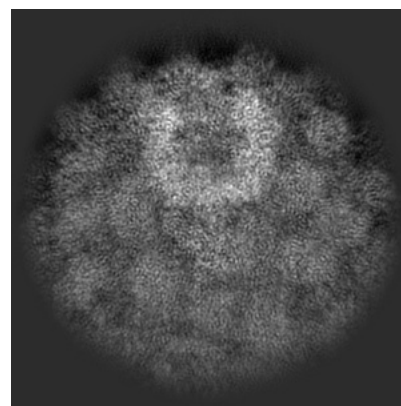
#### 5.1.1 Primary map



X

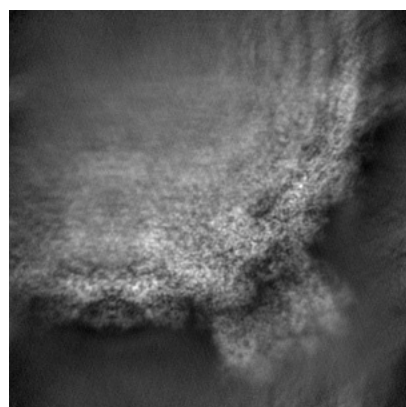


Y

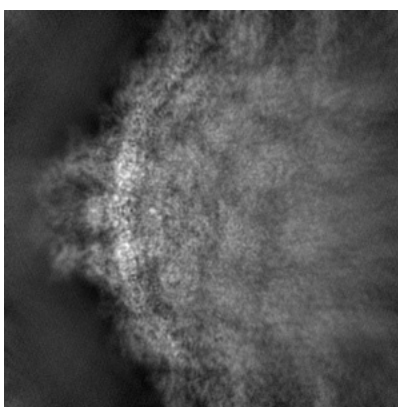


Z

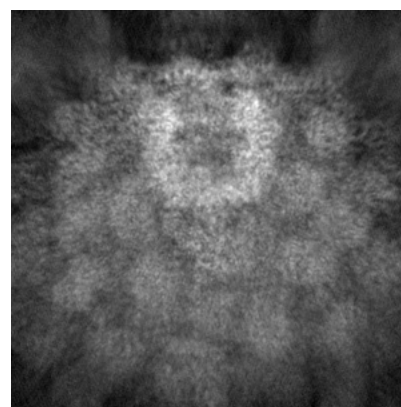
#### 5.1.2 Raw map



X



Y

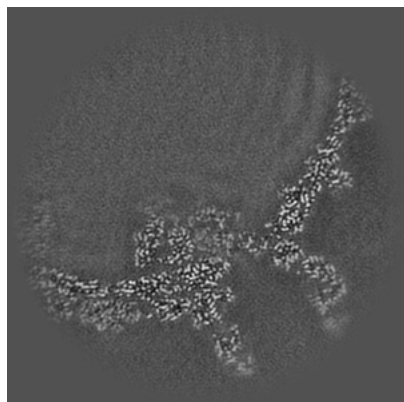


Z

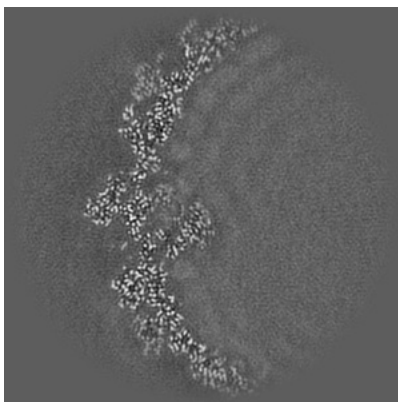
The images above show the map projected in three orthogonal directions.

## 5.2 Central slices [i](#)

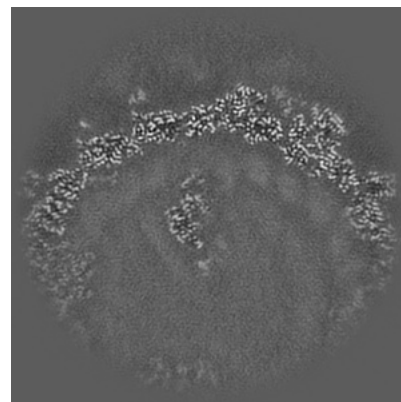
### 5.2.1 Primary map



X Index: 160

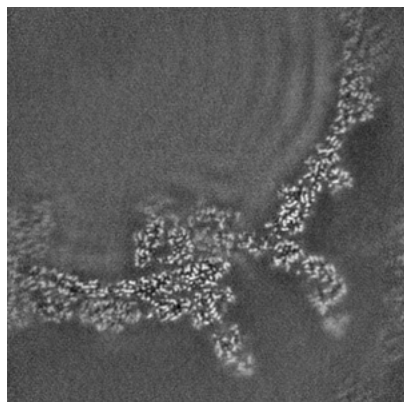


Y Index: 160

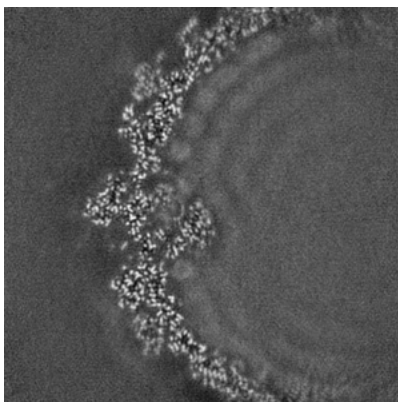


Z Index: 160

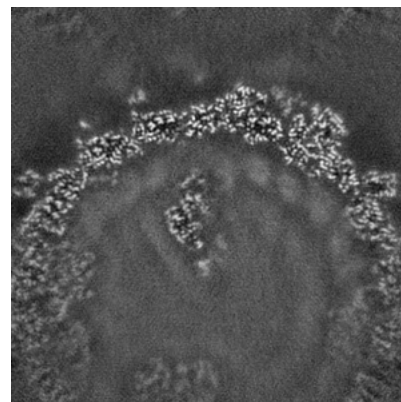
### 5.2.2 Raw map



X Index: 160



Y Index: 160

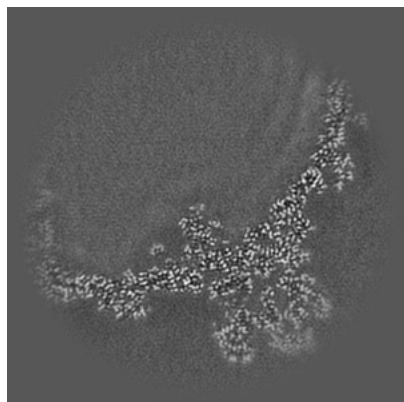


Z Index: 160

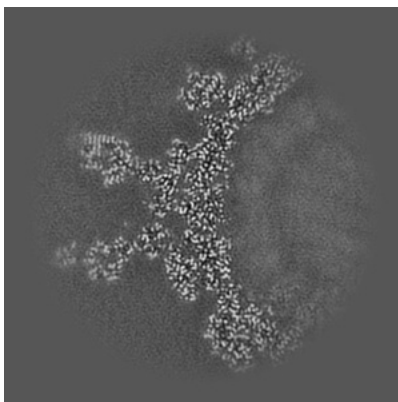
The images above show central slices of the map in three orthogonal directions.

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

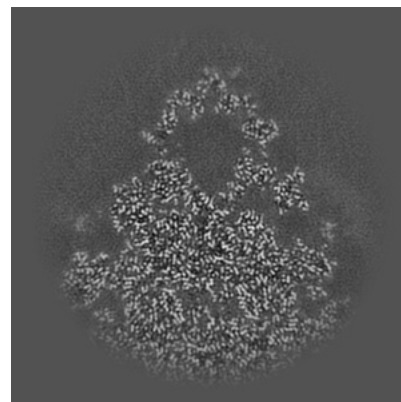
### 5.3.1 Primary map



X Index: 125

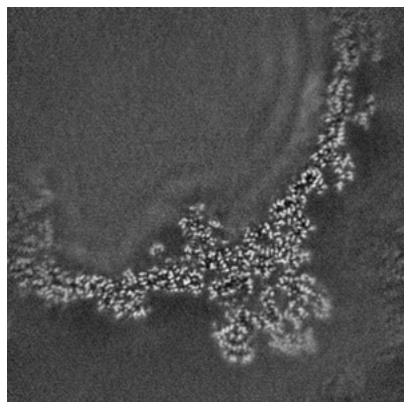


Y Index: 227

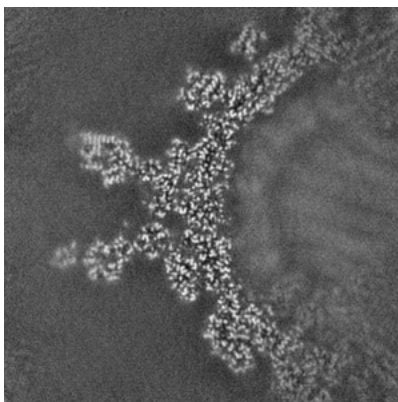


Z Index: 99

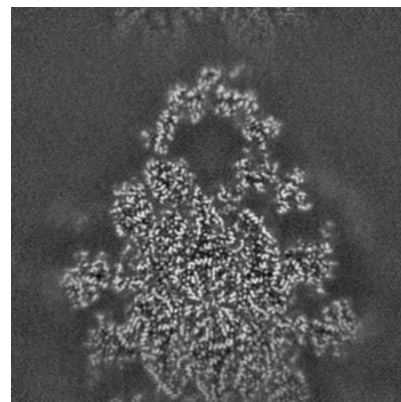
### 5.3.2 Raw map



X Index: 125



Y Index: 227

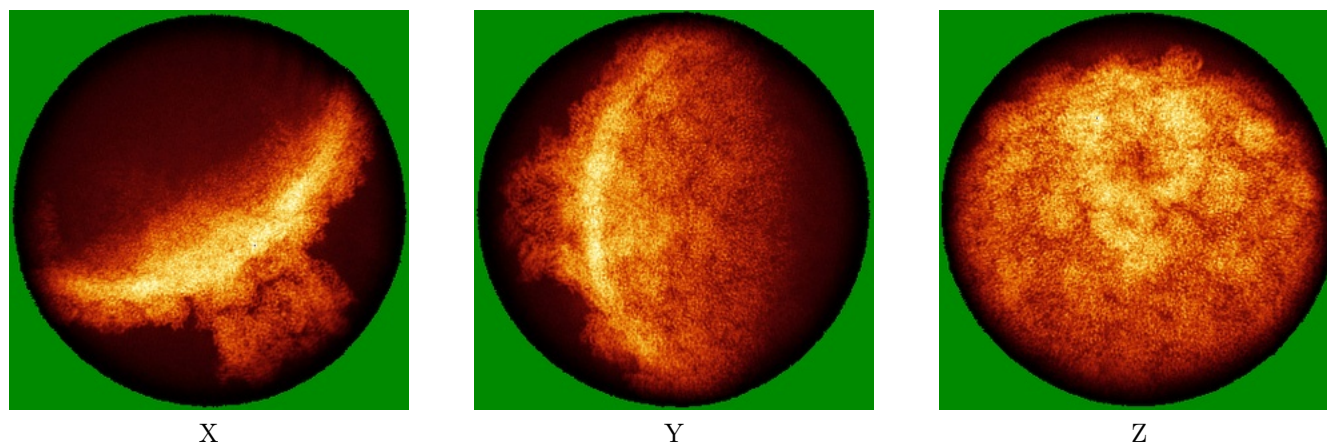


Z Index: 97

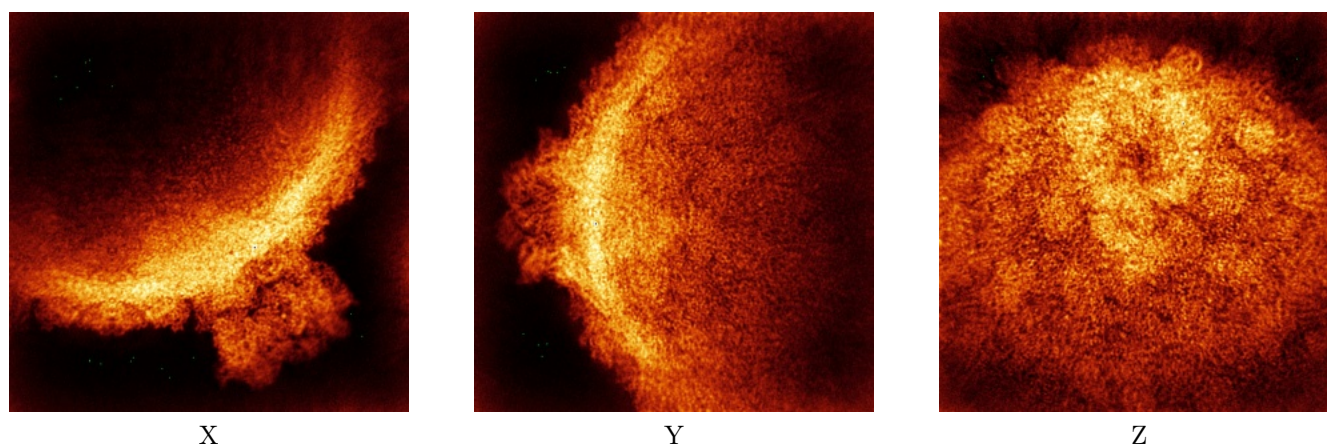
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 5.4.1 Primary map



### 5.4.2 Raw map



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

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

This section was not generated.

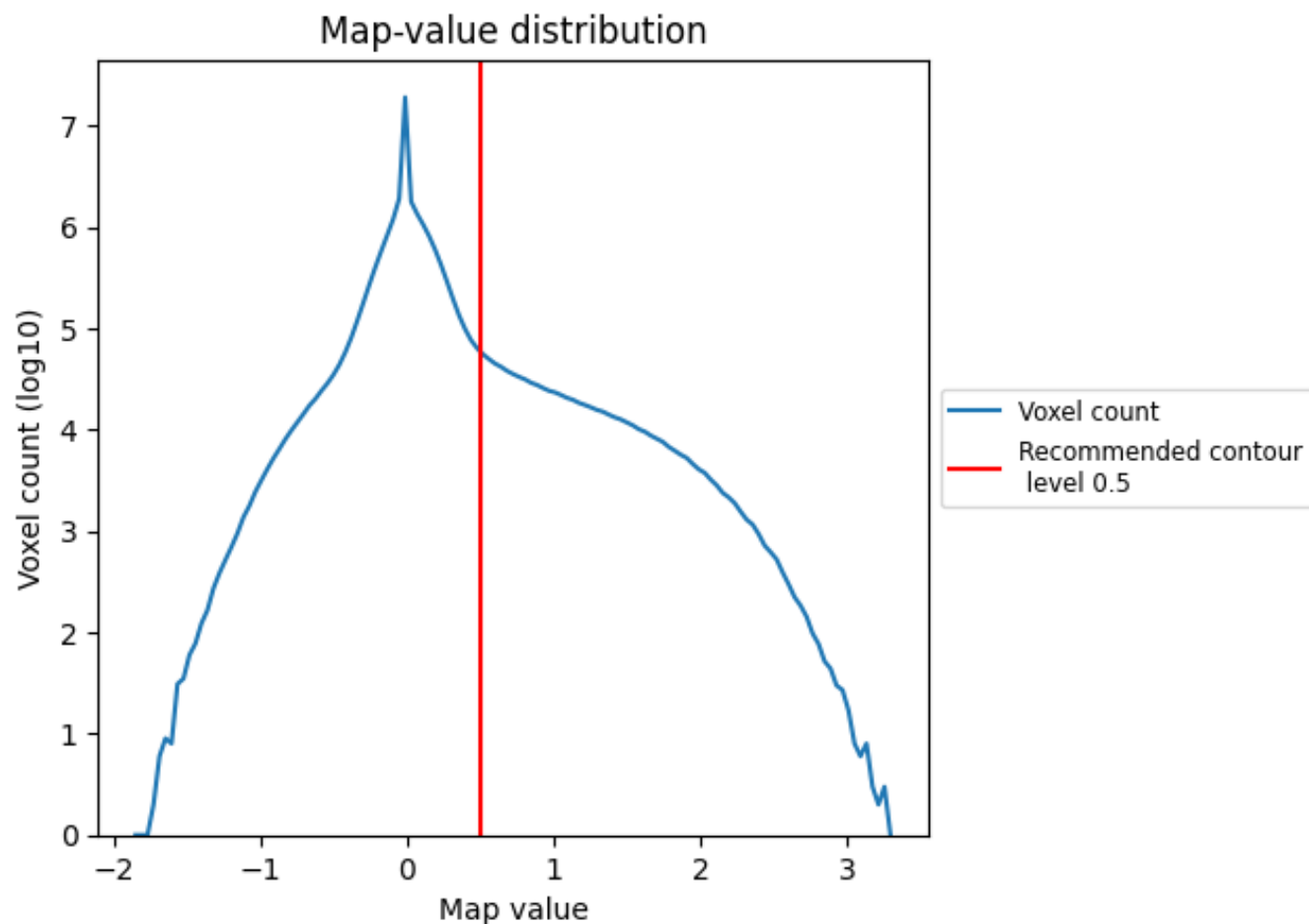
## 5.6 Mask visualisation [i](#)

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

## 6 Map analysis [i](#)

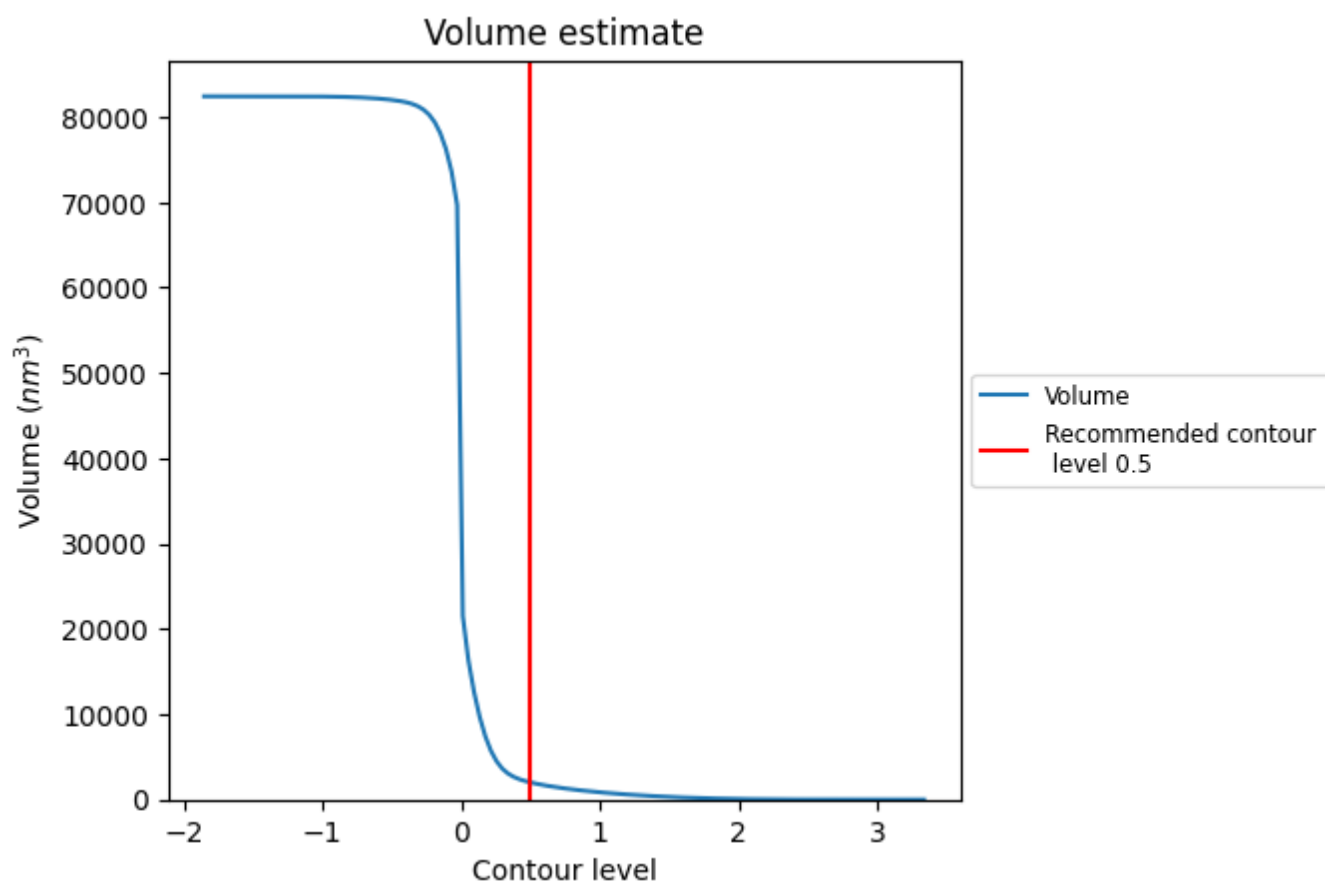
This section contains the results of statistical analysis of the map.

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



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

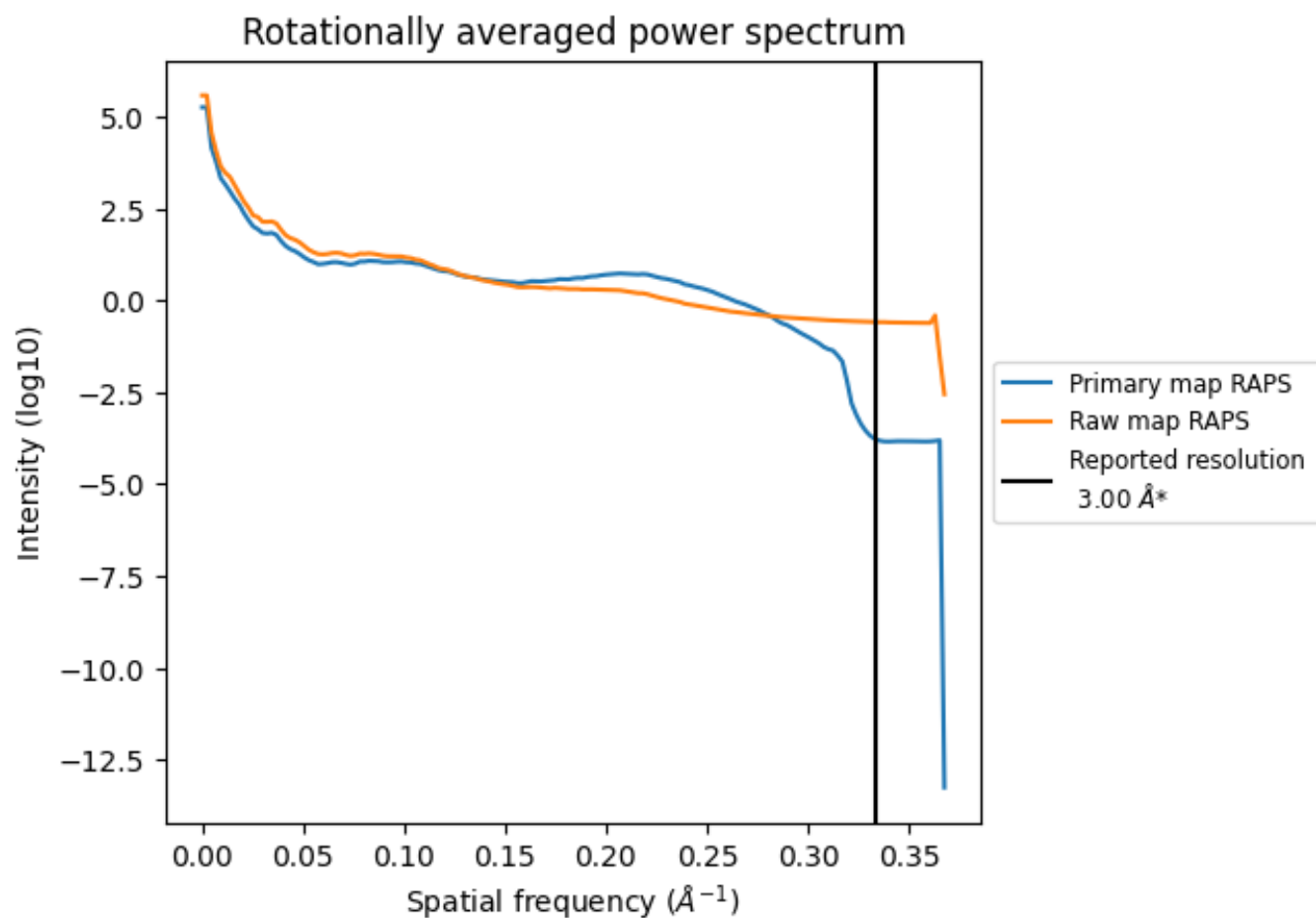
## 6.2 Volume estimate [i](#)



The volume at the recommended contour level is 2009 nm<sup>3</sup>; this corresponds to an approximate mass of 1815 kDa.

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

### 6.3 Rotationally averaged power spectrum ⓘ

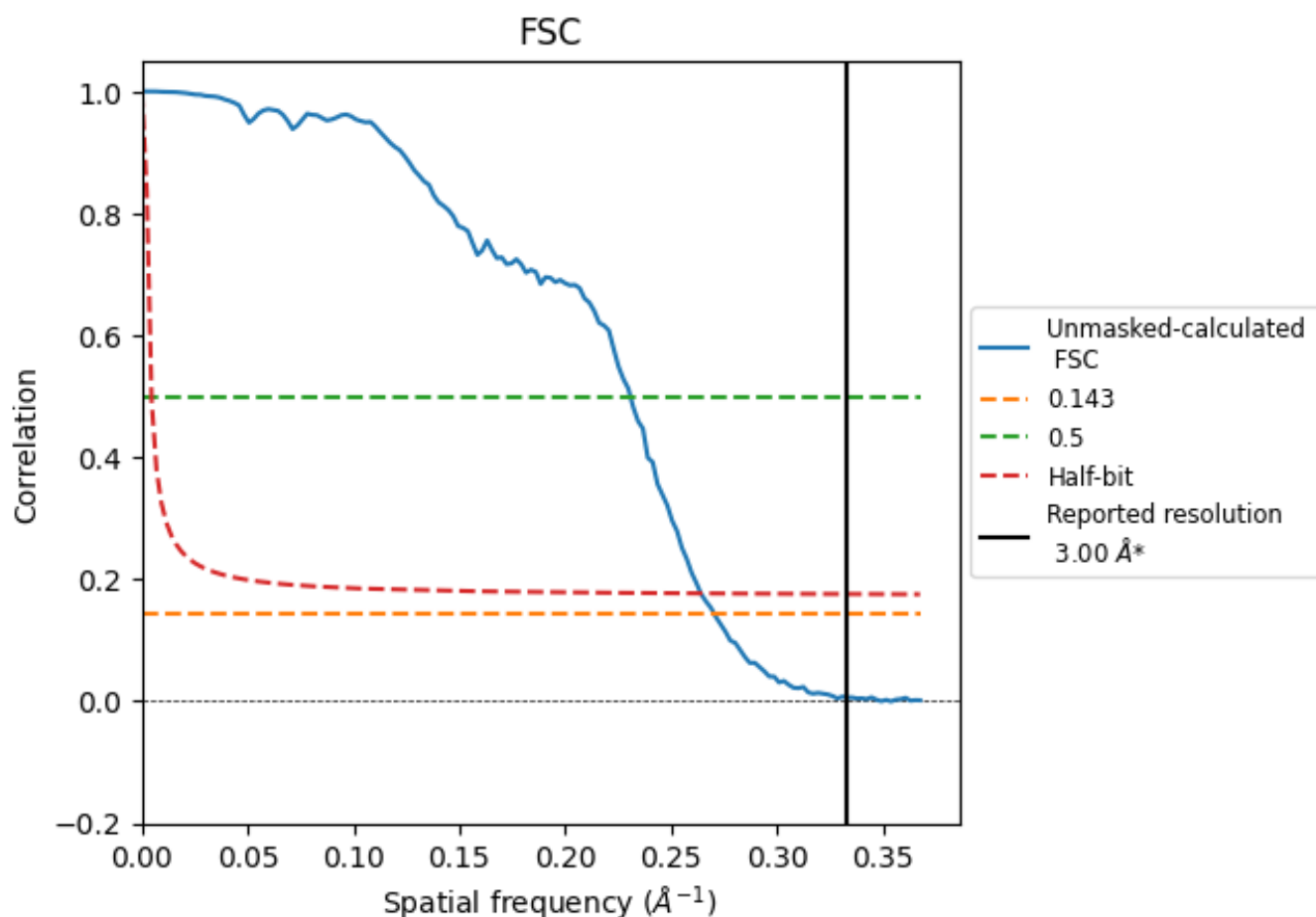


\*Reported resolution corresponds to spatial frequency of 0.333 Å<sup>-1</sup>

## 7 Fourier-Shell correlation [i](#)

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

### 7.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.333  $\text{\AA}^{-1}$

## 7.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.00                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 3.70                               | 4.33 | 3.79     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.70 differs from the reported value 3.0 by more than 10 %

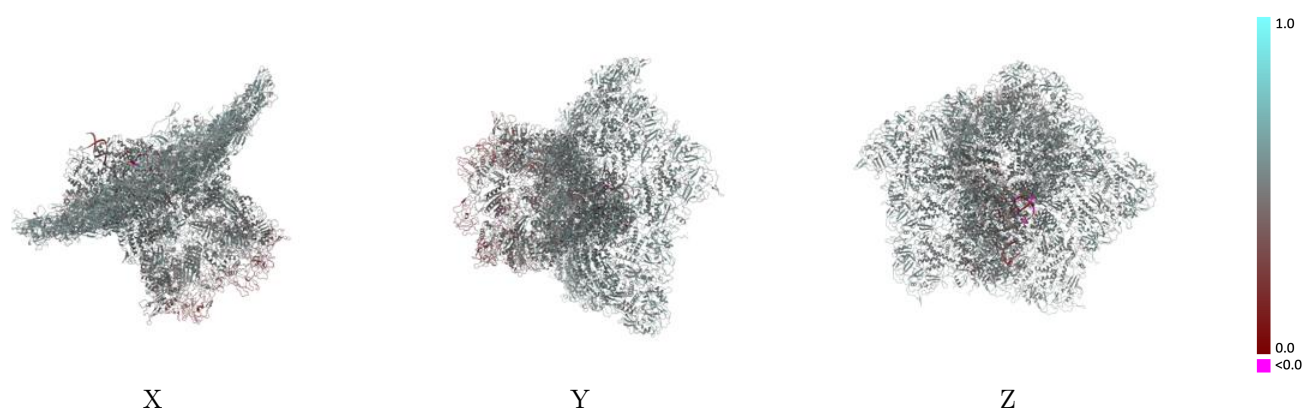
## 8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33770 and PDB model 7YED. Per-residue inclusion information can be found in section ?? on page ??.

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

This section was not generated.

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

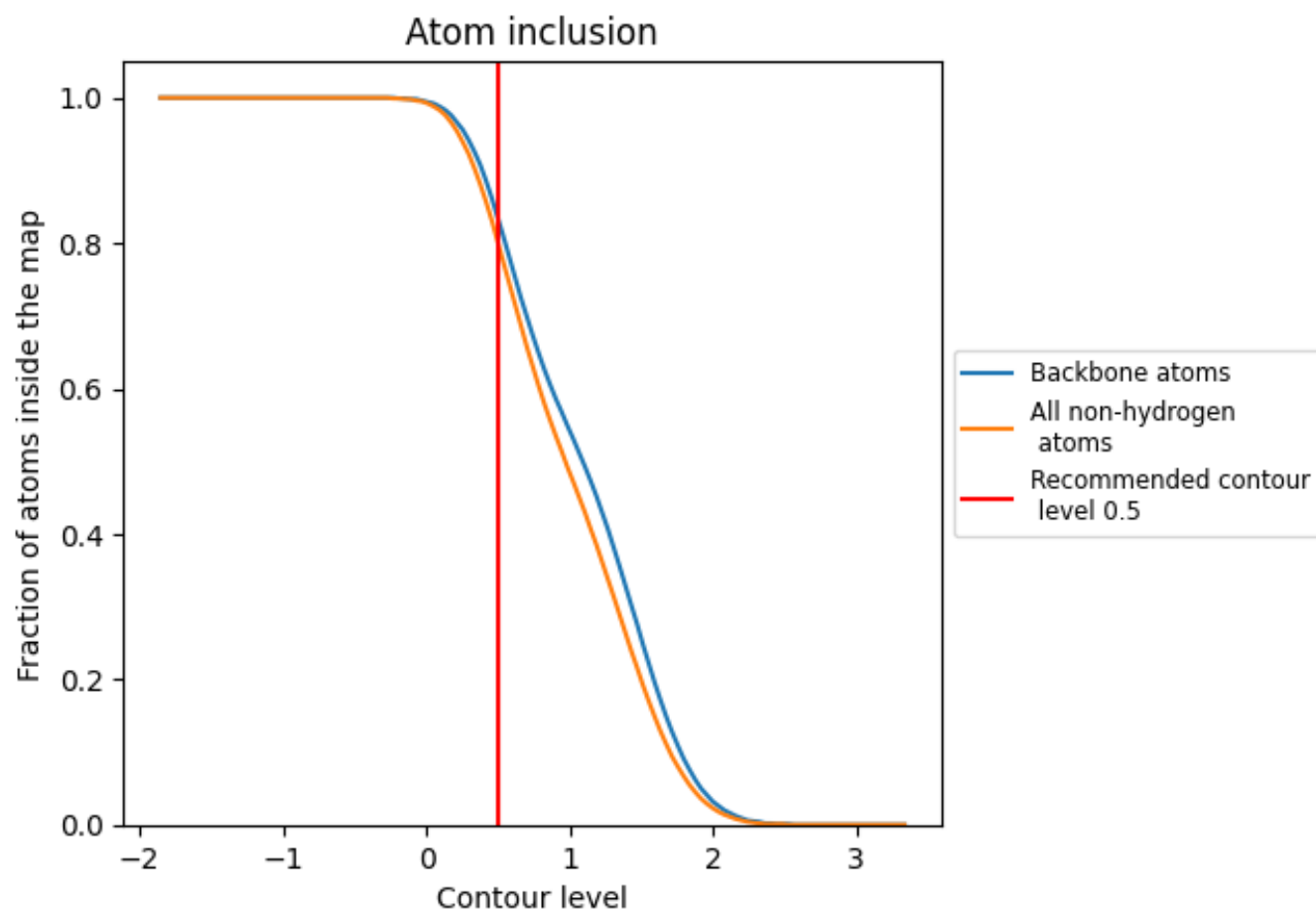


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

## 8.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

## 8.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8010   |  0.4980   |
| 1     |  0.7350   |  0.5050   |
| 2     |  0.7810   |  0.5090   |
| 3     |  0.7760   |  0.5090   |
| 4     |  0.6680   |  0.4840   |
| 5     |  0.6390   |  0.4930   |
| A     |  0.8410   |  0.5210   |
| B     |  0.8490   |  0.5250   |
| C     |  0.8550   |  0.5250   |
| D     |  0.8570   |  0.5260   |
| E     |  0.8430   |  0.5220   |
| H     |  0.7800   |  0.4650   |
| I     |  0.7790   |  0.4640   |
| J     |  0.7790   |  0.4650   |
| K     |  0.7750  |  0.4640  |
| L     |  0.7760 |  0.4630 |
| M     |  0.3350 |  0.3100 |
| N     |  0.0700 |  0.2090 |
| R     |  0.7560 |  0.5000 |
| T     |  0.2710 |  0.3060 |
| U     |  0.7550 |  0.4910 |
| a     |  0.8520 |  0.5240 |
| b     |  0.8580 |  0.5230 |
| c     |  0.8500 |  0.5250 |
| d     |  0.8540 |  0.5230 |
| e     |  0.8500 |  0.5220 |

