



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 21, 2021 – 02:13 PM EDT

PDB ID : 5S4S
Title : Tubulin-Z240297434-complex
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Deposited on : 2020-11-08
Resolution : 2.35 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.20
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.20

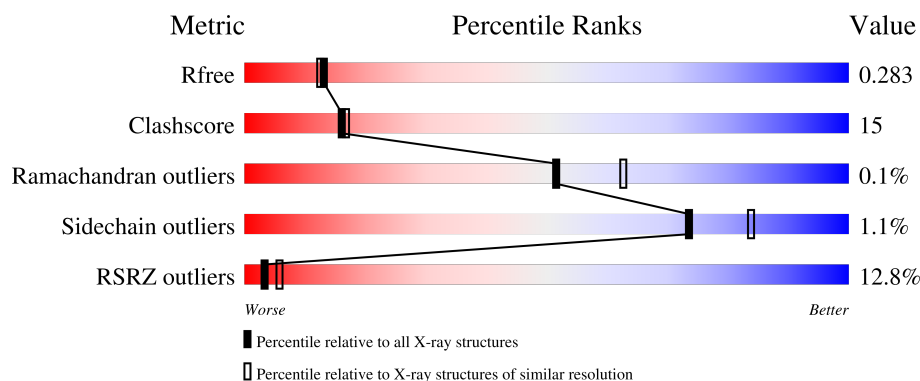
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	451	<div> <div>8%</div> <div>69%</div> <div>28%</div> <div>.</div> </div>
1	C	451	<div> <div>7%</div> <div>74%</div> <div>24%</div> <div>.</div> </div>
2	B	445	<div> <div>11%</div> <div>61%</div> <div>33%</div> <div>5%</div> </div>
2	D	445	<div> <div>13%</div> <div>67%</div> <div>29%</div> <div>.</div> </div>
3	E	143	<div> <div>23%</div> <div>67%</div> <div>15%</div> <div>.</div> <div>16%</div> </div>

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Mol	Chain	Length	Quality of chain
4	F	384	

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
7	CA	A	503	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17863 atoms, of which 40 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 protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	0	0
			3424	2167	582	653	22			
1	C	440	Total	C	N	O	S	0	1	0
			3443	2178	585	657	23			

- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	421	Total	C	N	O	S	4	1	0
			3326	2091	569	639	27			
2	D	431	Total	C	N	O	S	7	0	0
			3368	2113	575	653	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	120	Total	C	N	O	S	0	0	0
			993	613	180	195	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	350	Total	C	N	O	S	0	0	0
			2865	1835	493	523	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		

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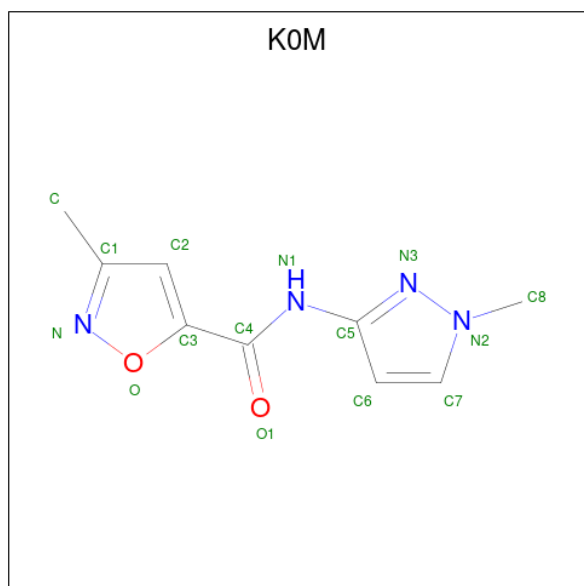
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is 3-methyl-N-(1-methyl-1H-pyrazol-3-yl)-1,2-oxazole-5-carboxamide (three-letter code: KOM) (formula: C₉H₁₀N₄O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	H	N	O	0	0
			25	9	10	4	2		
8	B	1	Total	C	H	N	O	0	0
			25	9	10	4	2		
8	D	1	Total	C	H	N	O	0	0
			25	9	10	4	2		
8	D	1	Total	C	H	N	O	0	0
			25	9	10	4	2		

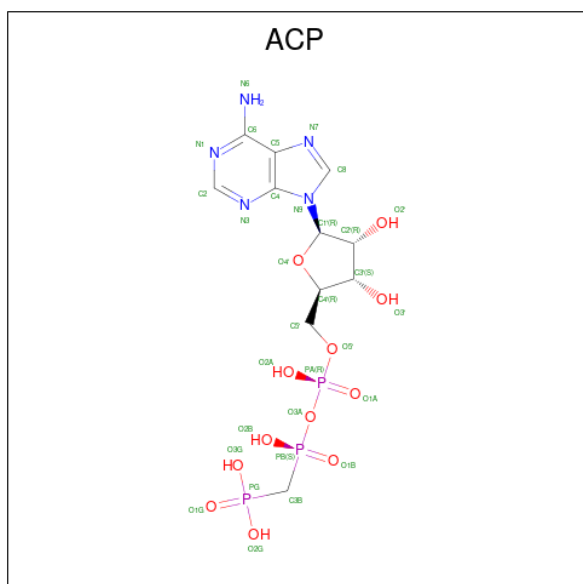
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- The diagram illustrates the chemical structure of Guanosine Diphosphate (GDP). It features a guanine base (N1-N9), a ribose sugar (C1' to C5'), and two phosphate groups (P(A/S) and P(B)). The guanine base is connected to the ribose sugar at the N9 position. The ribose sugar is connected to the first phosphate group at the C5' position. The first phosphate group is connected to the second phosphate group at the O3' position. The second phosphate group is shown with its own set of atoms (O1B, O2B, O3B, O4B).

MES

The chemical structure of MES (3-(Trimethylsilyl)urea) is shown. It consists of a central urea group (C=O, N-H) where the nitrogen atom is substituted with a trimethylsilyl group (Si(CH₃)₃). The silicon atom is bonded to three methyl groups and the nitrogen atom. The oxygen atom of the carbonyl group is double-bonded to the carbon atom. The nitrogen atom is single-bonded to the carbon atom and the silicon atom. The silicon atom is single-bonded to three methyl groups. The structure is labeled with atom names: O1, C2, C3, C4, C5, C6, C7, C8, S, O2S, O1S, O3S, and N4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $\text{C}_{11}\text{H}_{18}\text{N}_5\text{O}_{12}\text{P}_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	F	1	Total 31	C 11	N 5	O 12	P 3	0	0

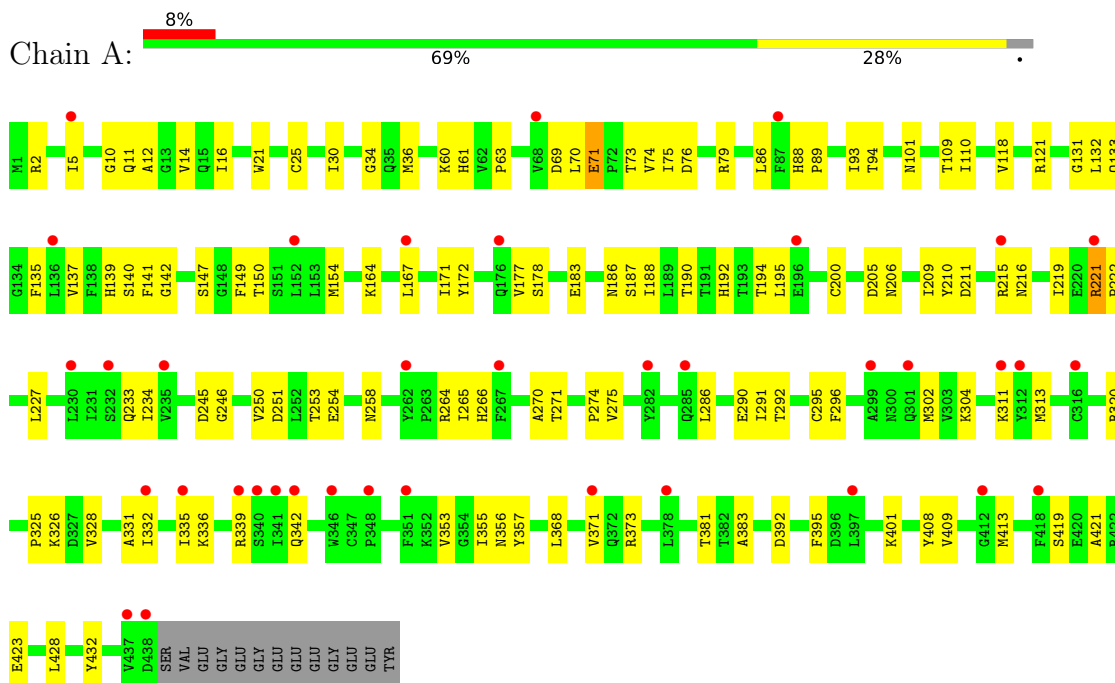
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	9	Total O 9 9	0	0
12	B	32	Total O 32 32	0	0
12	C	113	Total O 113 113	0	0
12	D	17	Total O 17 17	0	0
12	E	2	Total O 2 2	0	0

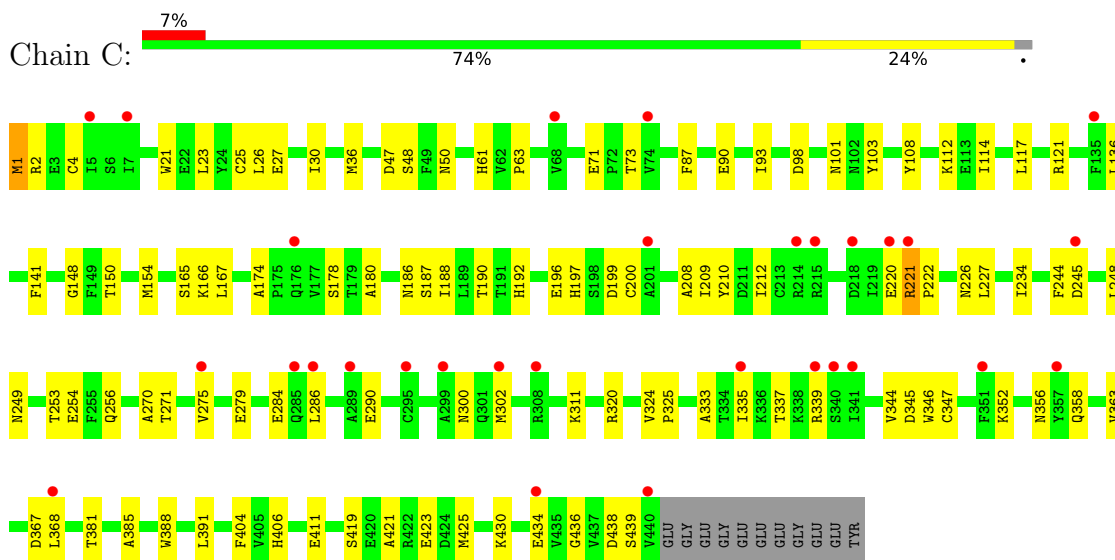
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

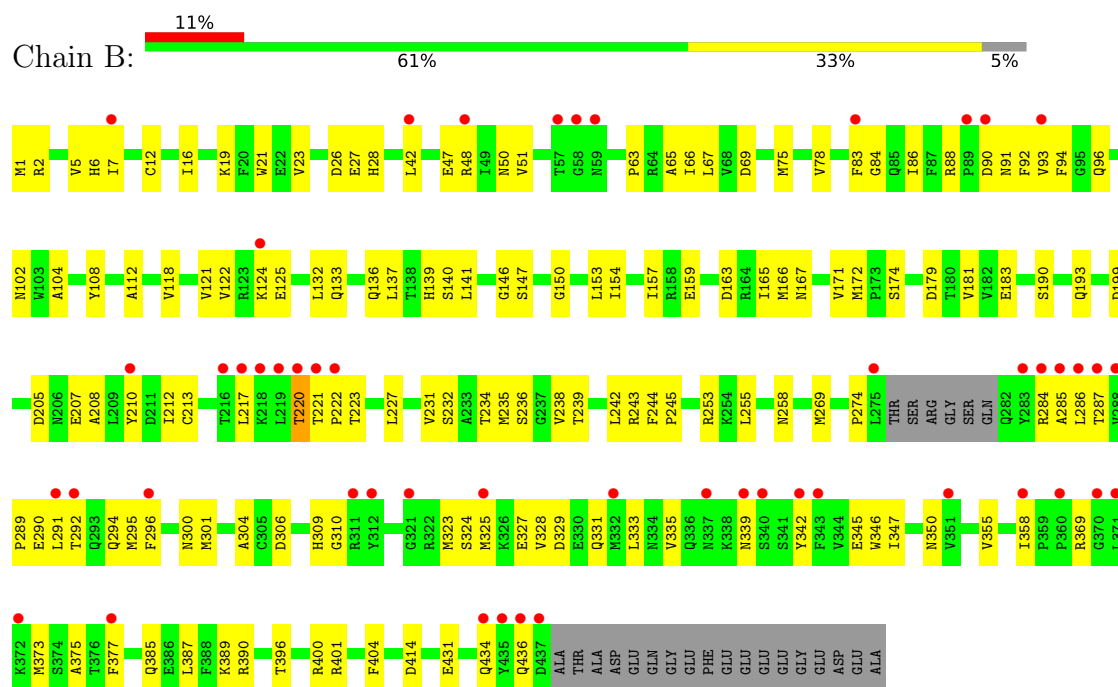
- Molecule 1: Tubulin alpha-1B chain



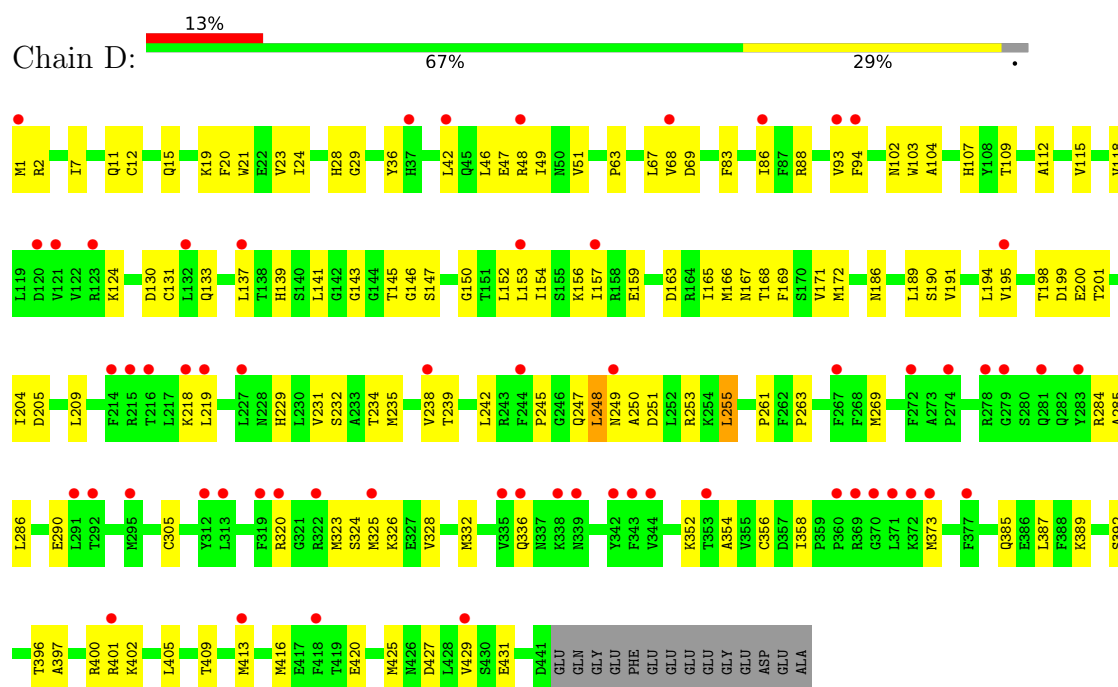
- Molecule 1: Tubulin alpha-1B chain



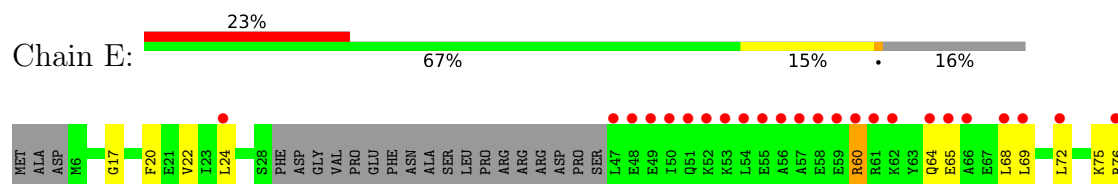
• Molecule 2: Tubulin beta-2B chain

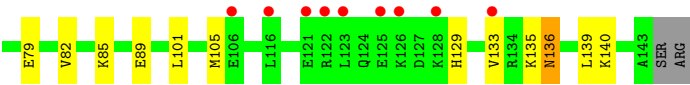


• Molecule 2: Tubulin beta-2B chain

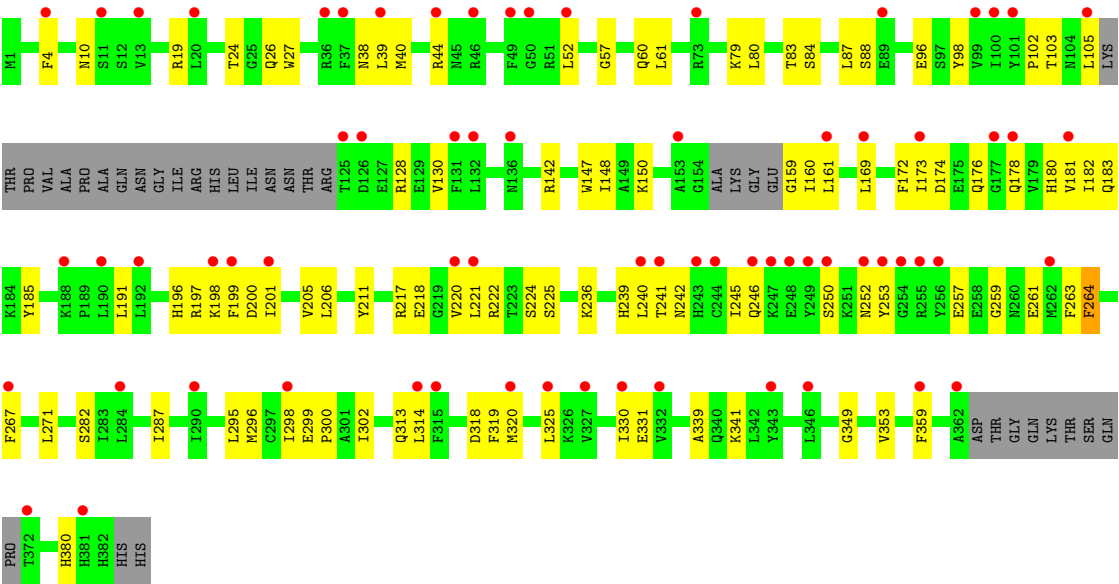


• Molecule 3: Stathmin-4





● Molecule 4: Tubulin-Tyrosine Ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.55Å 164.17Å 173.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.68 – 2.35 90.15 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.0 (86.68-2.35) 99.0 (90.15-2.35)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.244 , 0.284 0.244 , 0.283	Depositor DCC
R_{free} test set	6075 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	59.6	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17863	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: ACP, GTP, CA, MG, GDP, MES, KOM

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	0.26	0/3502	0.42	0/4754
1	C	0.26	0/3521	0.42	0/4780
2	B	0.26	0/3400	0.42	0/4603
2	D	0.25	0/3442	0.41	0/4664
3	E	0.24	0/1000	0.34	0/1325
4	F	0.24	0/2931	0.40	0/3960
All	All	0.25	0/17796	0.41	0/24086

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3424	0	3335	100	0
1	C	3443	0	3352	84	1
2	B	3326	0	3202	133	0
2	D	3368	0	3236	108	0
3	E	993	0	1013	21	0
4	F	2865	0	2826	80	0
5	A	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	15	10	0	0	0
8	B	15	10	0	0	0
8	D	30	20	0	3	0
9	B	28	0	12	1	0
9	D	28	0	12	3	0
10	B	12	0	12	3	0
11	F	31	0	14	5	0
12	A	9	0	0	1	0
12	B	32	0	0	3	1
12	C	113	0	0	4	0
12	D	17	0	0	1	0
12	E	2	0	0	0	0
All	All	17823	40	17038	503	1

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 15.

The worst 5 of 503 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:C:93:ILE:HD11	1:C:121:ARG:HG3	1.49	0.94
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.47	0.94
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.52	0.91
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.55	0.88
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.56	0.86

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:GLU:OE2	12:B:628:HOH:O[4_455]	1.99	0.21

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	
1	A	436/451 (97%)	417 (96%)	18 (4%)	1 (0%)	47	56
1	C	439/451 (97%)	427 (97%)	12 (3%)	0	100	100
2	B	418/445 (94%)	401 (96%)	16 (4%)	1 (0%)	47	56
2	D	429/445 (96%)	409 (95%)	19 (4%)	1 (0%)	47	56
3	E	116/143 (81%)	115 (99%)	1 (1%)	0	100	100
4	F	342/384 (89%)	322 (94%)	20 (6%)	0	100	100
All	All	2180/2319 (94%)	2091 (96%)	86 (4%)	3 (0%)	51	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	220	THR
1	A	109	THR
2	D	109	THR

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	
1	A	369/379 (97%)	365 (99%)	4 (1%)	73	84
1	C	372/379 (98%)	368 (99%)	4 (1%)	73	84
2	B	364/383 (95%)	362 (100%)	2 (0%)	88	94
2	D	368/383 (96%)	362 (98%)	6 (2%)	62	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	107/127 (84%)	105 (98%)	2 (2%)	57	68
4	F	314/342 (92%)	312 (99%)	2 (1%)	86	93
All	All	1894/1993 (95%)	1874 (99%)	20 (1%)	73	84

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	248	LEU
3	E	136	ASN
4	F	264	PHE
4	F	142	ARG
1	C	1	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	249	ASN
4	F	180	HIS
4	F	333	ASN
4	F	229	ASN
4	F	178	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 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	GDP	D	501	6	24,30,30	1.19	2 (8%)	31,47,47	1.91	8 (25%)
5	GTP	A	501	6	26,34,34	1.00	1 (3%)	33,54,54	1.73	7 (21%)
5	GTP	C	501	6	26,34,34	1.00	1 (3%)	33,54,54	1.75	6 (18%)
10	MES	B	504	-	12,12,12	2.24	1 (8%)	14,16,16	1.94	5 (35%)
8	K0M	D	503	-	10,16,16	0.74	0	12,22,22	0.74	0
8	K0M	D	504	-	10,16,16	0.75	0	12,22,22	0.71	0
9	GDP	B	501	6	24,30,30	1.20	2 (8%)	31,47,47	1.92	8 (25%)
8	K0M	B	505	-	10,16,16	0.75	0	12,22,22	0.74	0
8	K0M	A	504	-	10,16,16	0.74	0	12,22,22	0.71	0
11	ACP	F	401	6	27,33,33	1.39	5 (18%)	32,52,52	1.51	4 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GDP	D	501	6	-	6/12/32/32	0/3/3/3
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3
10	MES	B	504	-	-	4/6/14/14	0/1/1/1
8	K0M	D	503	-	-	0/3/8/8	0/2/2/2
8	K0M	D	504	-	-	0/3/8/8	0/2/2/2
9	GDP	B	501	6	-	3/12/32/32	0/3/3/3
8	K0M	B	505	-	-	0/3/8/8	0/2/2/2
8	K0M	A	504	-	-	0/3/8/8	0/2/2/2
11	ACP	F	401	6	-	11/15/38/38	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	504	MES	C8-S	-7.48	1.66	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	501	GDP	C6-C5	4.20	1.48	1.41
9	B	501	GDP	C6-C5	4.15	1.48	1.41
5	A	501	GTP	C6-N1	3.25	1.38	1.33
5	C	501	GTP	C6-N1	3.20	1.38	1.33

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	N3-C2-N1	-5.31	120.14	127.22
5	A	501	GTP	N3-C2-N1	-5.16	120.34	127.22
9	D	501	GDP	C2-N3-C4	4.98	121.05	115.36
9	B	501	GDP	C2-N3-C4	4.92	120.98	115.36
5	C	501	GTP	C2-N3-C4	4.36	120.33	115.36

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A

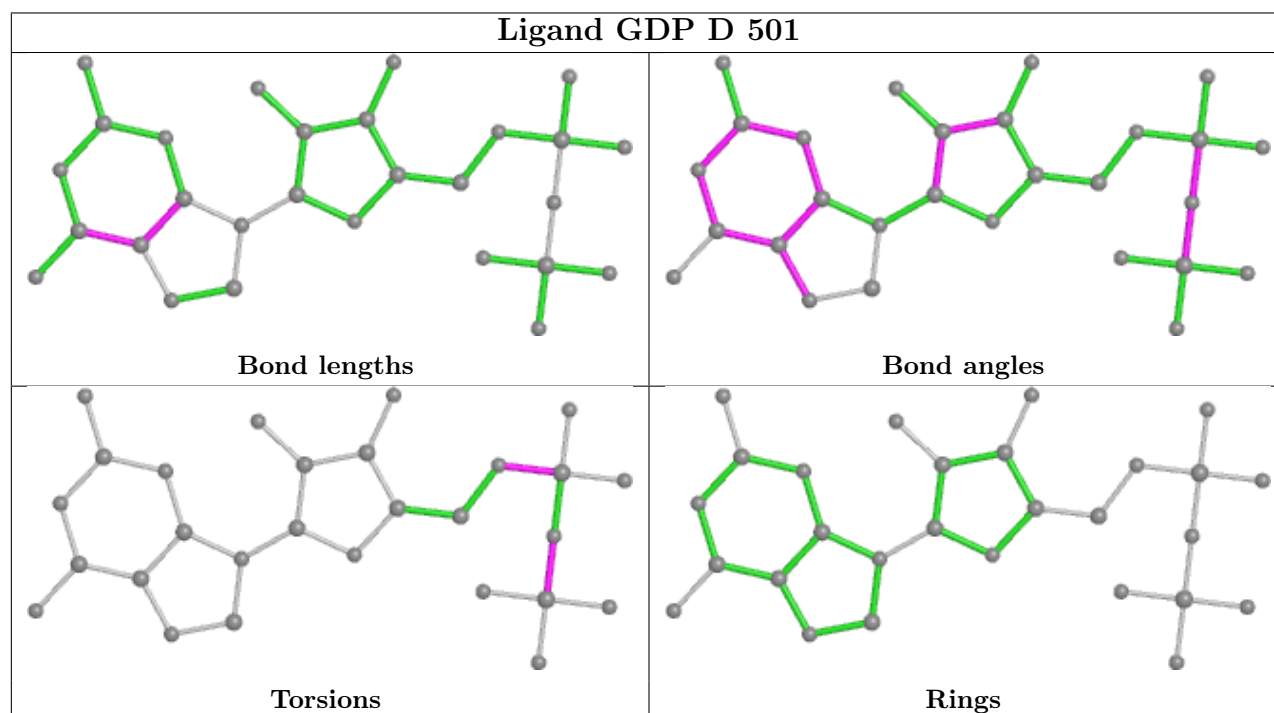
There are no ring outliers.

6 monomers are involved in 16 short contacts:

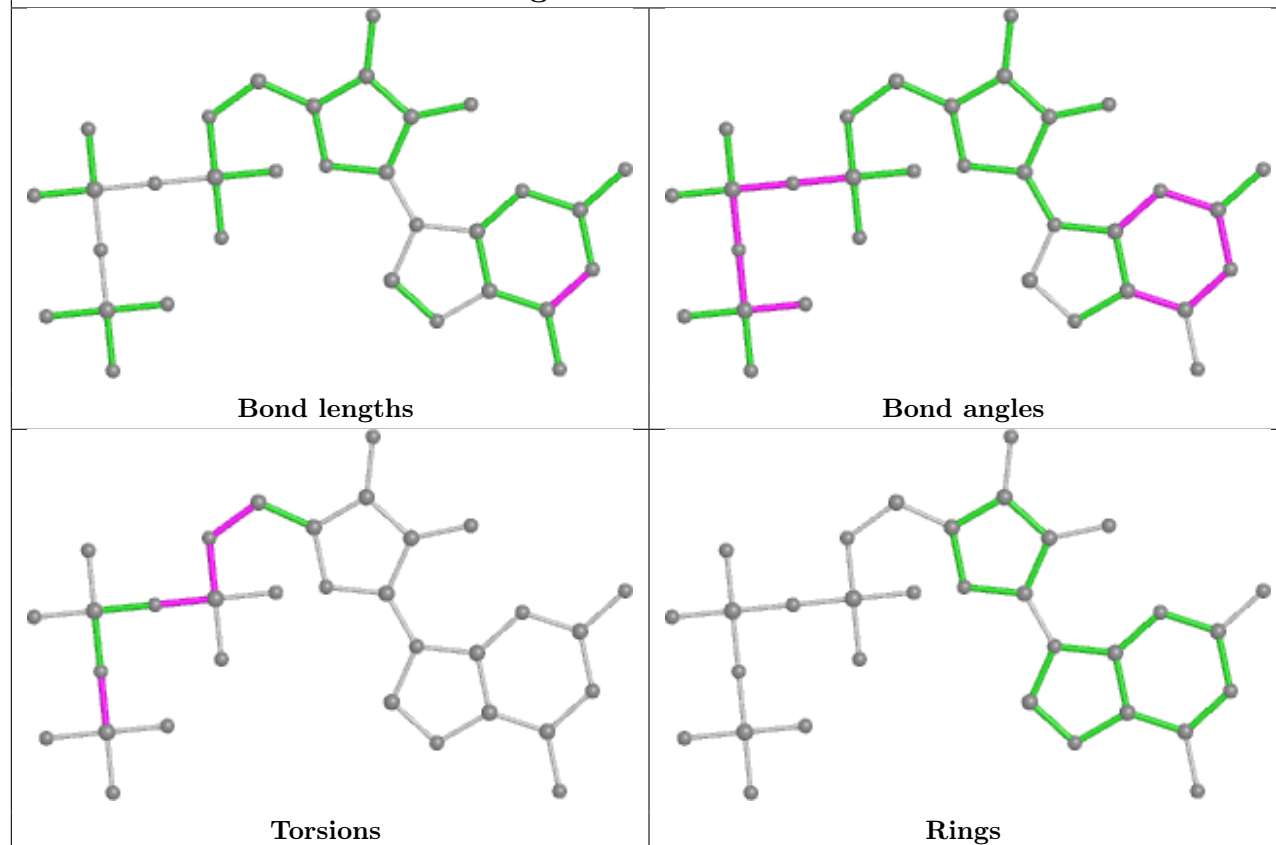
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	501	GDP	3	0
5	C	501	GTP	1	0
10	B	504	MES	3	0
8	D	503	K0M	3	0
9	B	501	GDP	1	0
11	F	401	ACP	5	0

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

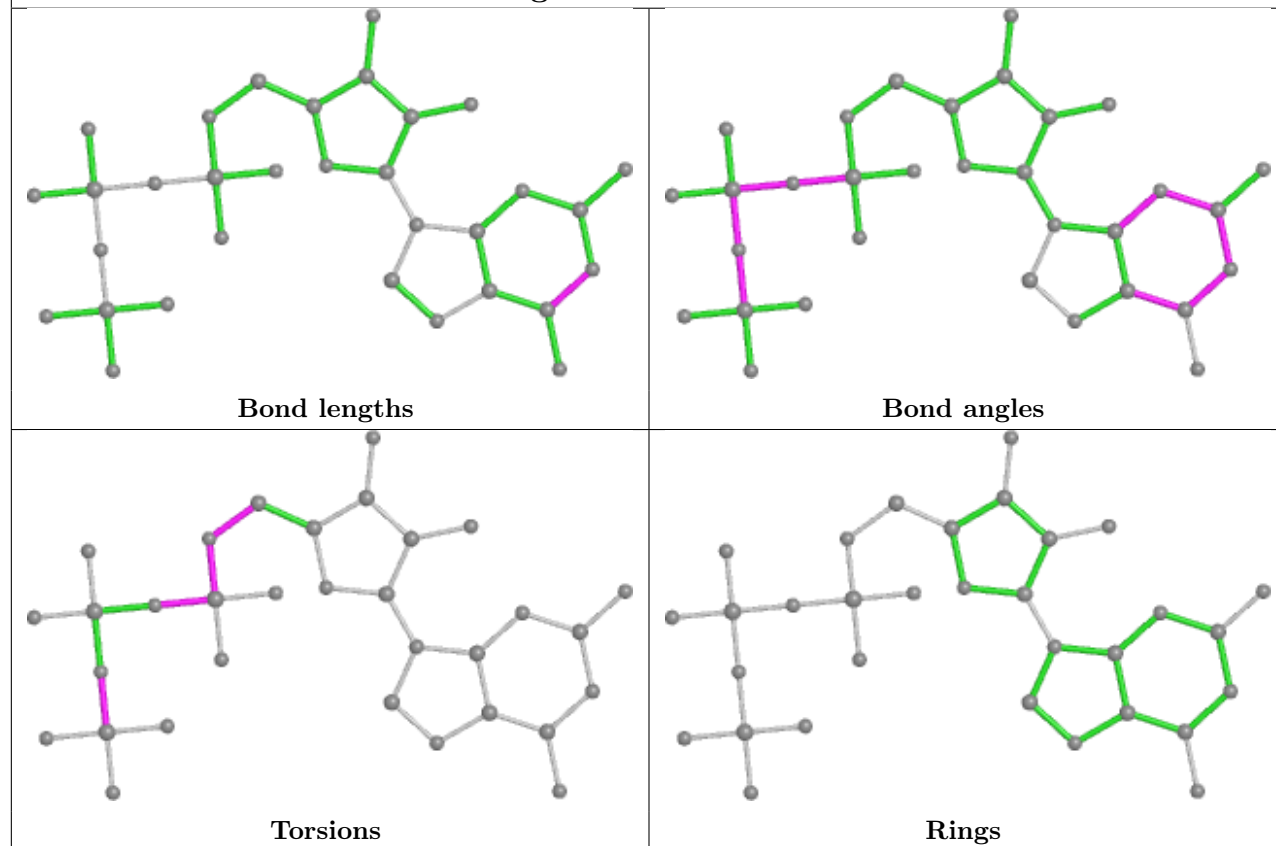
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

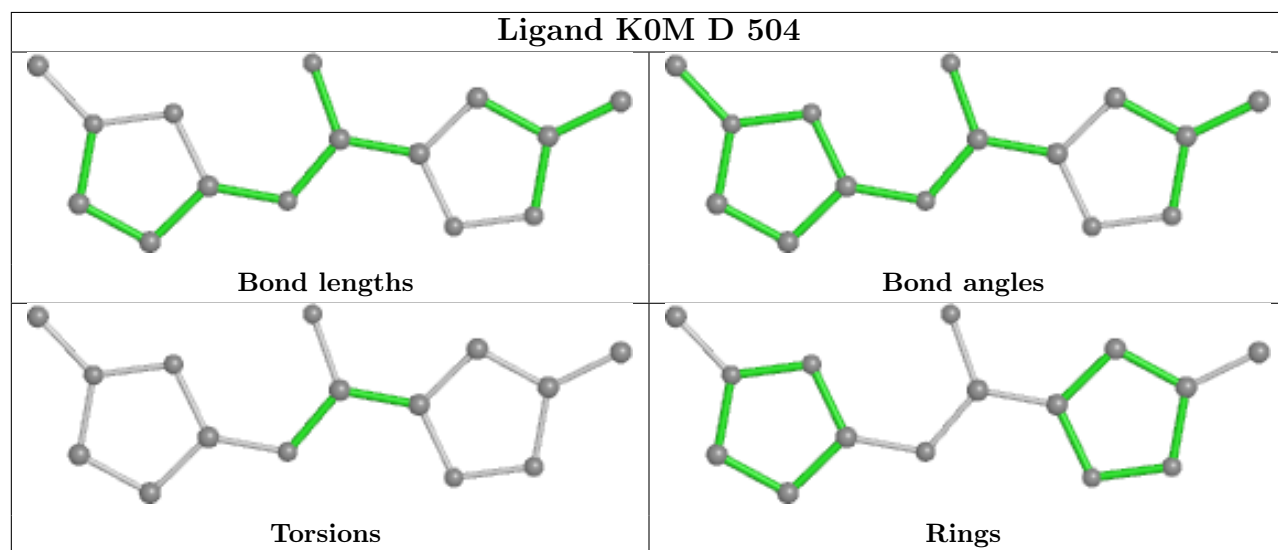
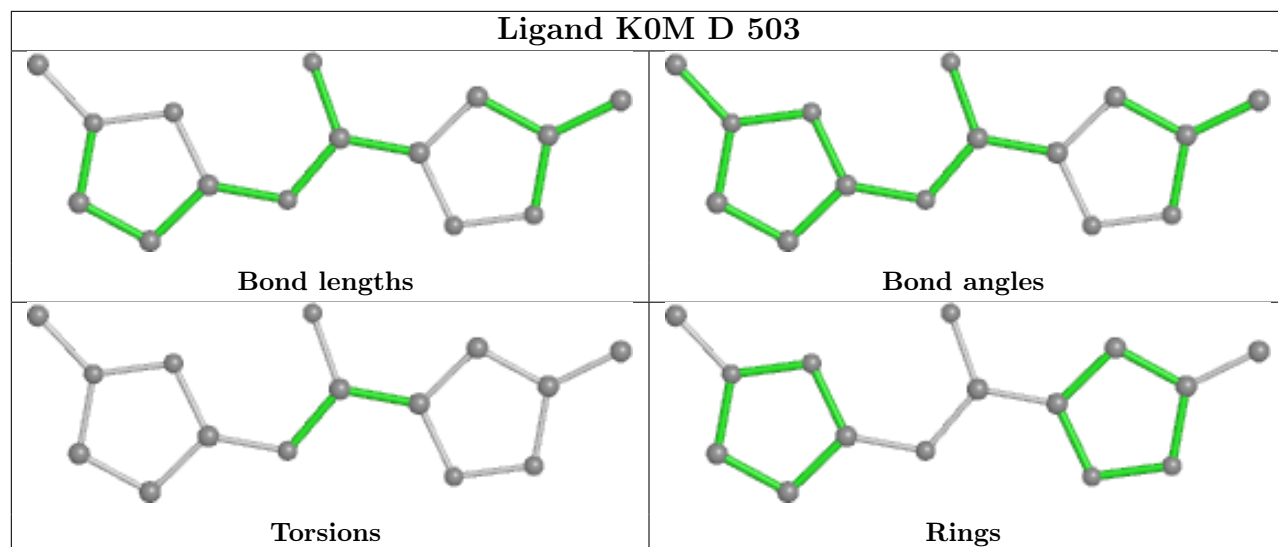


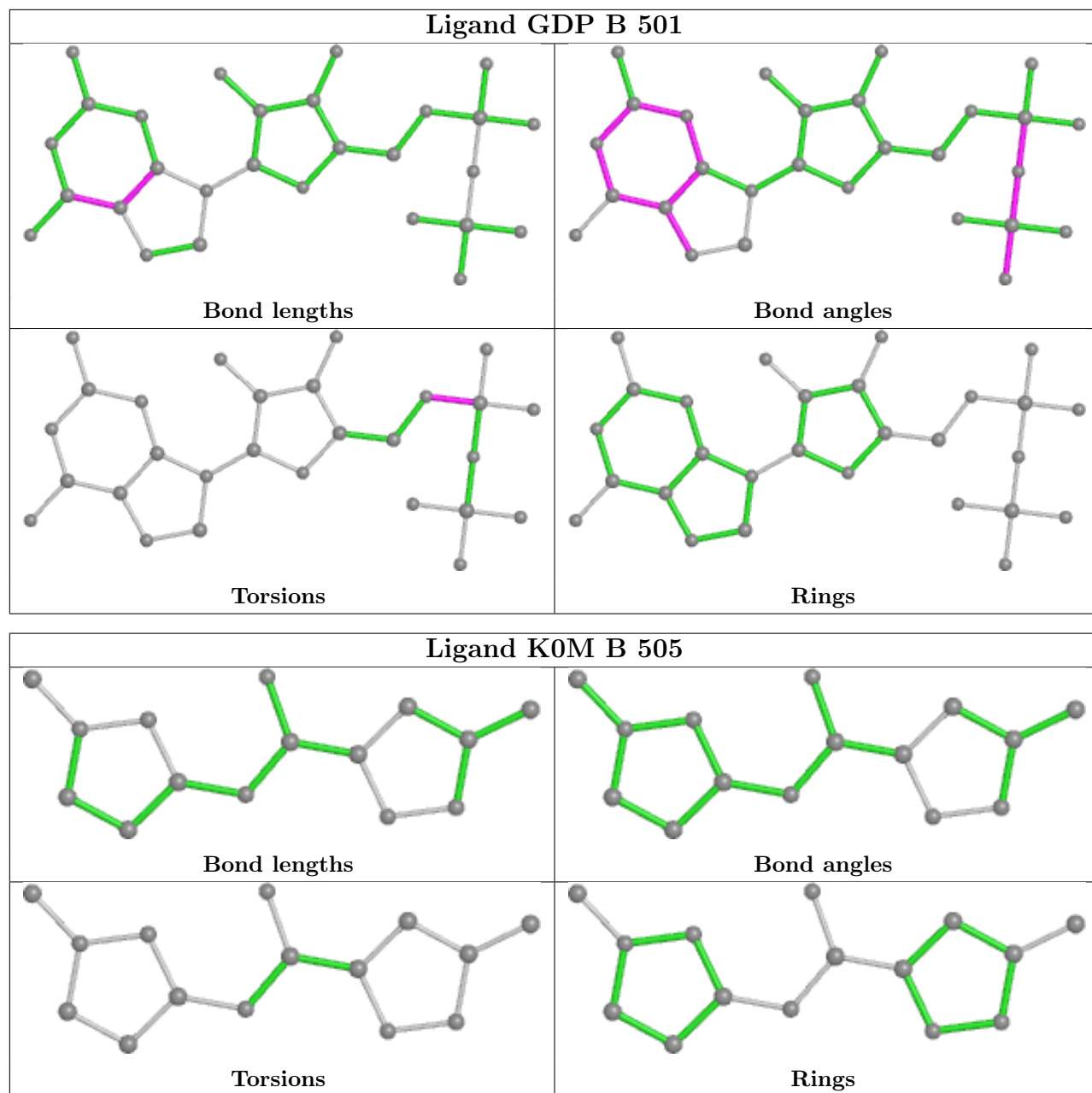
Ligand GTP A 501

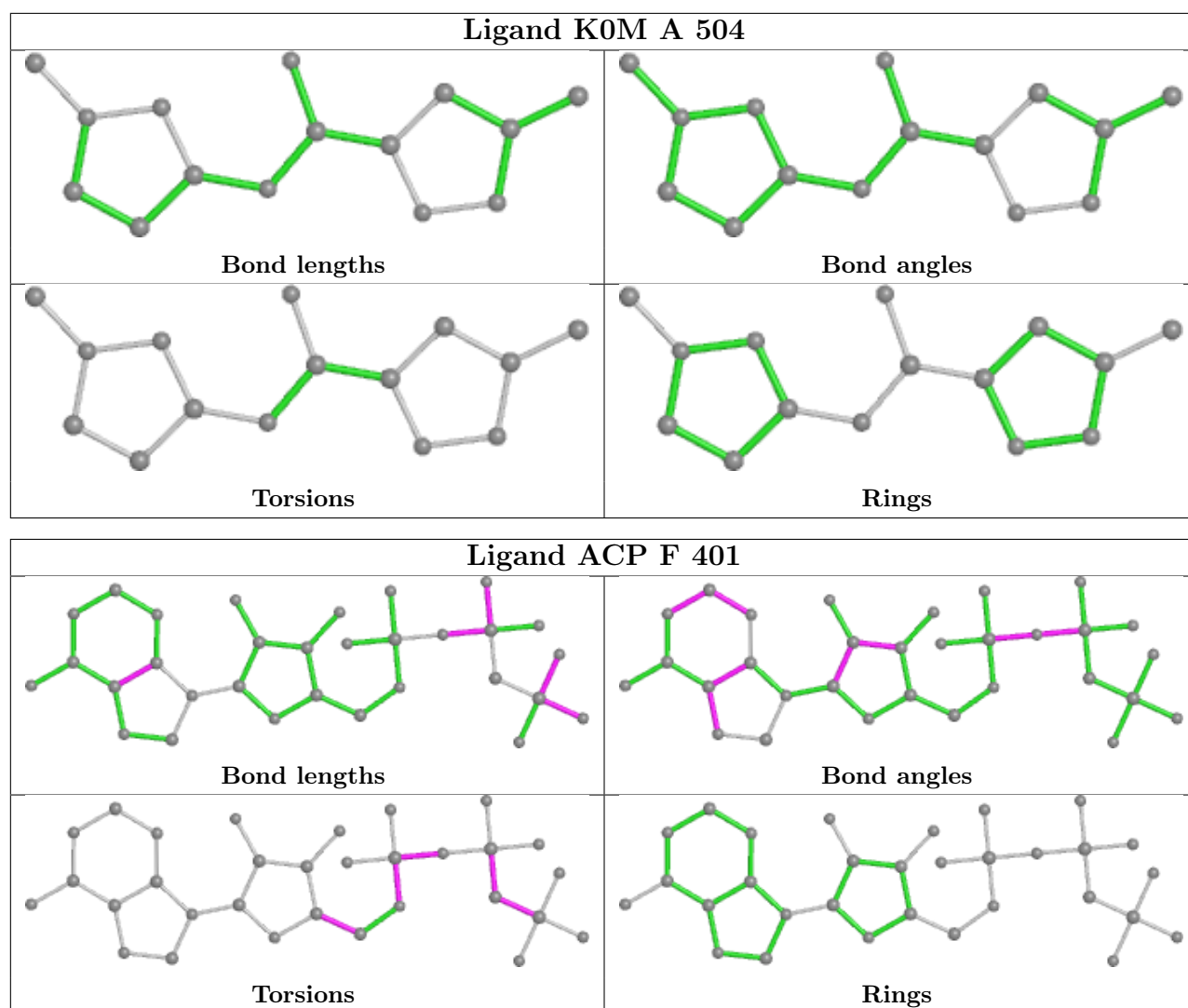


Ligand GTP C 501









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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	438/451 (97%)	0.70	38 (8%)	10 15	55, 70, 103, 143	0
1	C	440/451 (97%)	0.92	30 (6%)	17 25	53, 64, 90, 152	0
2	B	421/445 (94%)	0.94	50 (11%)	4 7	52, 68, 118, 193	5 (1%)
2	D	431/445 (96%)	0.91	60 (13%)	2 4	63, 87, 126, 168	6 (1%)
3	E	120/143 (83%)	1.73	33 (27%)	0 0	59, 89, 142, 189	0
4	F	350/384 (91%)	1.23	70 (20%)	1 2	68, 91, 143, 184	0
All	All	2200/2319 (94%)	0.97	281 (12%)	3 6	52, 76, 124, 193	11 (0%)

The worst 5 of 281 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	50	ILE	11.3
3	E	57	ALA	11.3
3	E	53	LYS	10.0
2	B	57	THR	8.0
2	B	283	TYR	8.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

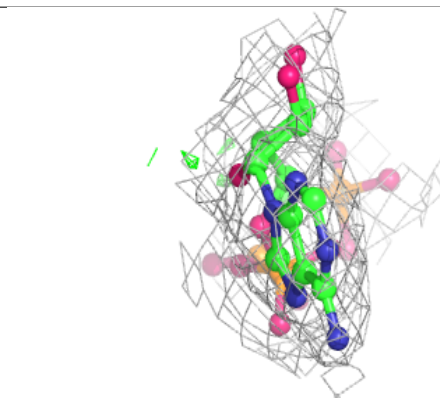
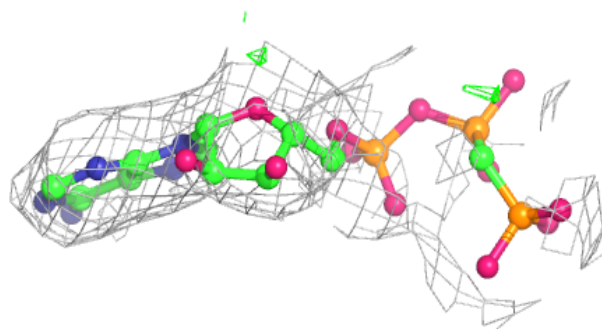
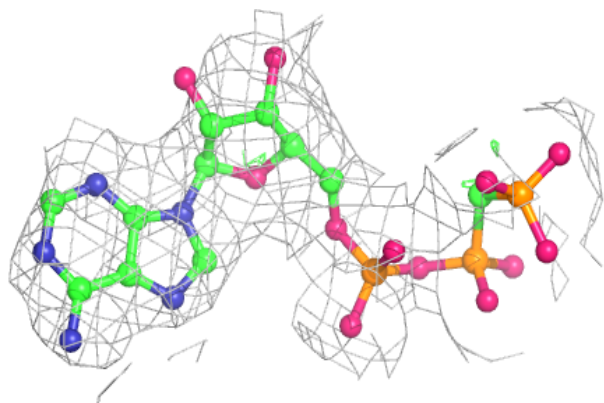
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	F	402	1/1	0.03	0.17	114,114,114,114	0
7	CA	A	503	1/1	0.46	0.64	138,138,138,138	0
6	MG	C	502	1/1	0.81	0.20	69,69,69,69	0
11	ACP	F	401	31/31	0.88	0.12	86,108,118,125	0
10	MES	B	504	12/12	0.89	0.15	85,91,100,100	0
6	MG	D	502	1/1	0.89	0.14	80,80,80,80	0
8	K0M	D	503	15/15	0.92	0.24	67,74,89,89	25
8	K0M	D	504	15/15	0.92	0.18	68,82,108,108	0
6	MG	B	502	1/1	0.92	0.23	51,51,51,51	0
8	K0M	B	505	15/15	0.92	0.17	60,69,86,86	0
7	CA	C	503	1/1	0.93	0.16	73,73,73,73	0
7	CA	B	503	1/1	0.94	0.34	110,110,110,110	0
9	GDP	D	501	28/28	0.94	0.14	73,82,88,90	0
5	GTP	A	501	32/32	0.95	0.15	53,57,61,62	0
5	GTP	C	501	32/32	0.96	0.19	57,59,66,72	0
8	K0M	A	504	15/15	0.96	0.18	60,69,88,89	0
9	GDP	B	501	28/28	0.97	0.19	50,54,57,62	0
6	MG	A	502	1/1	0.97	0.12	56,56,56,56	0

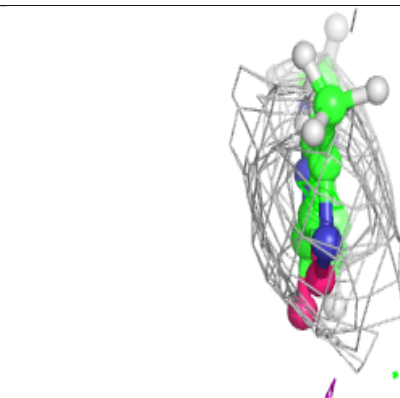
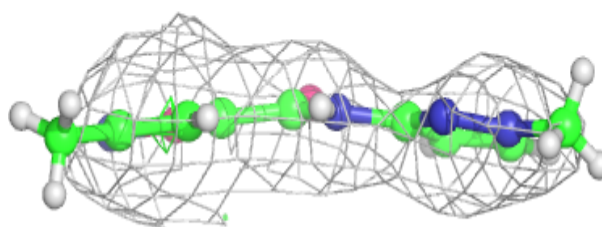
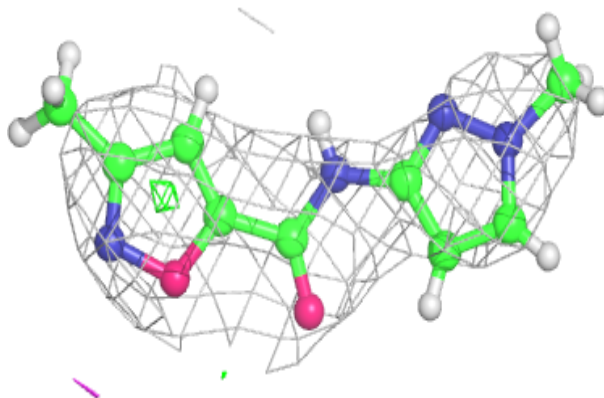
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP F 401:

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

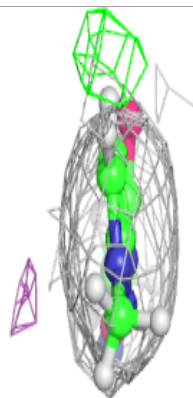
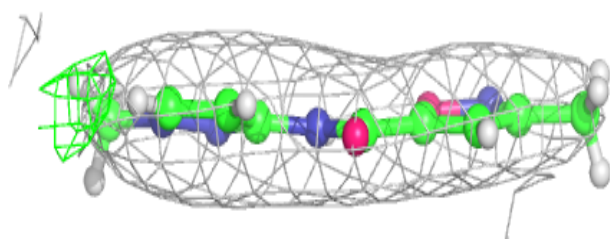
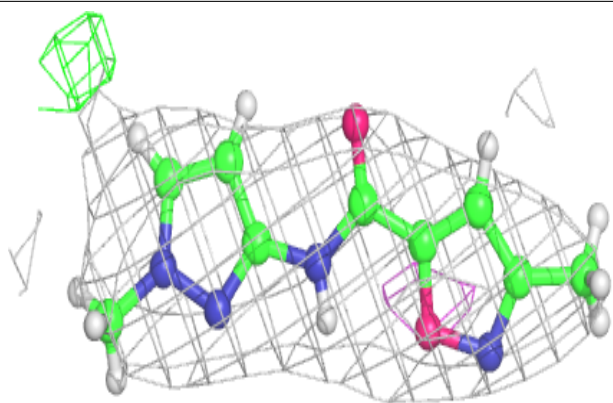
**Electron density around K0M D 503:**

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

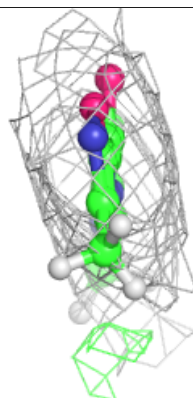
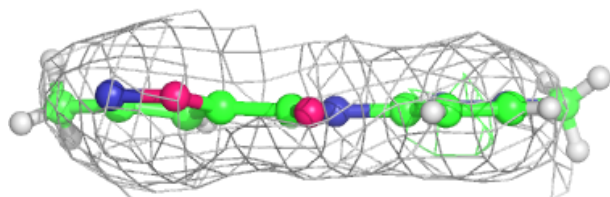
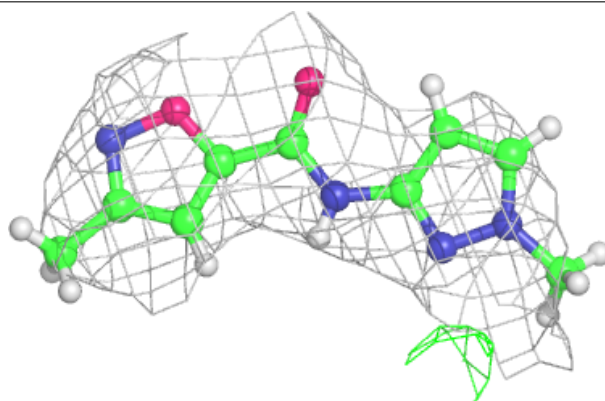


Electron density around K0M D 504:

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

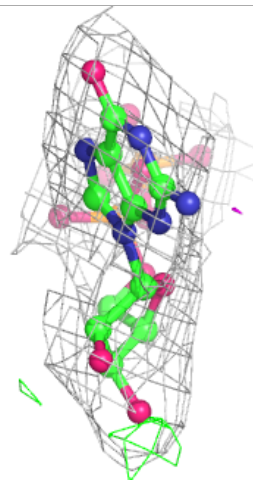
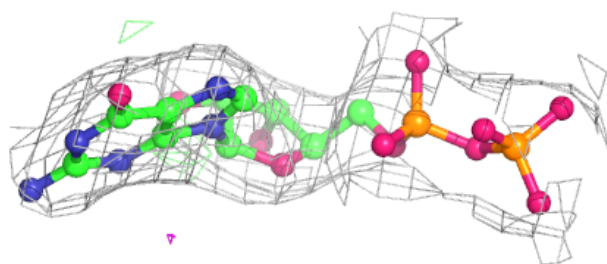
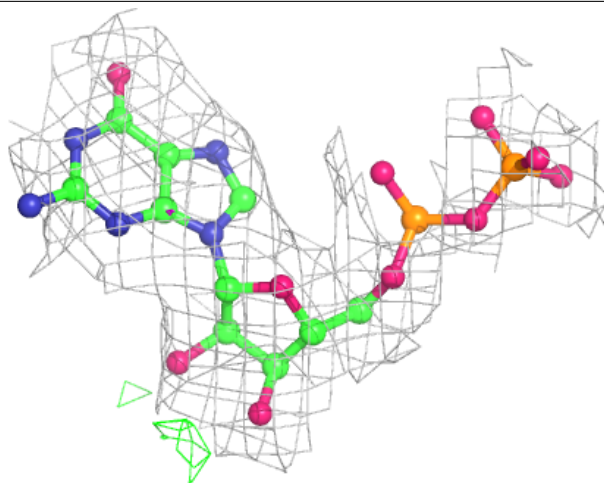
**Electron density around K0M B 505:**

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



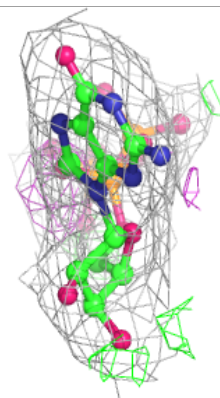
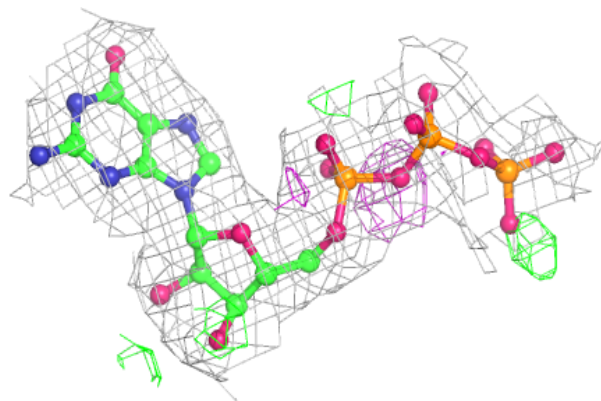
Electron density around GDP D 501:

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

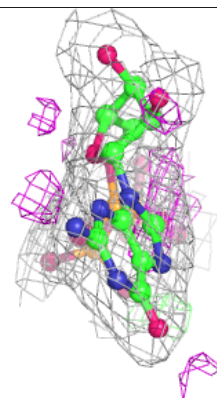
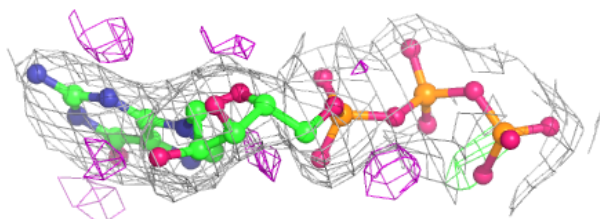
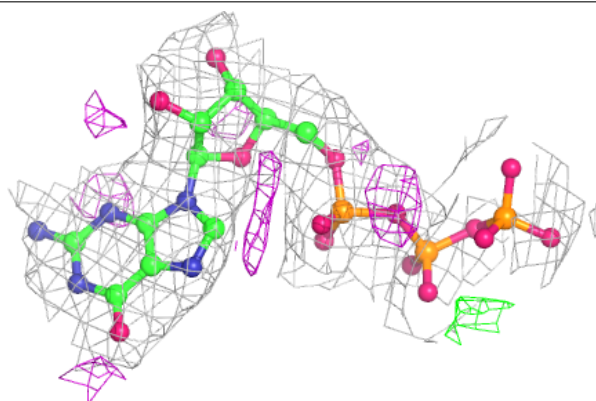


Electron density around GTP A 501:

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

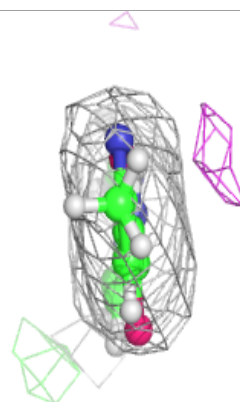
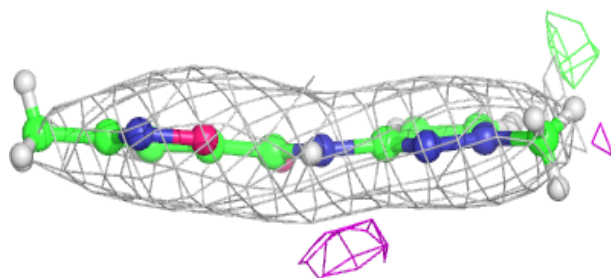
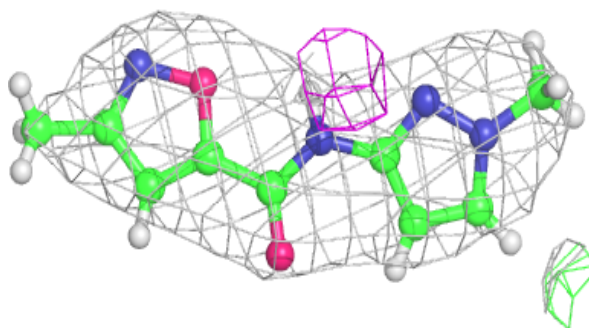
**Electron density around GTP C 501:**

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

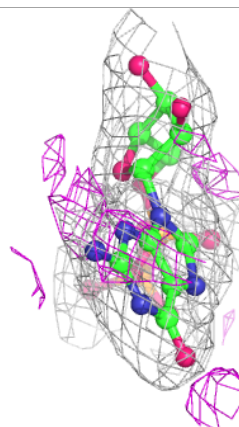
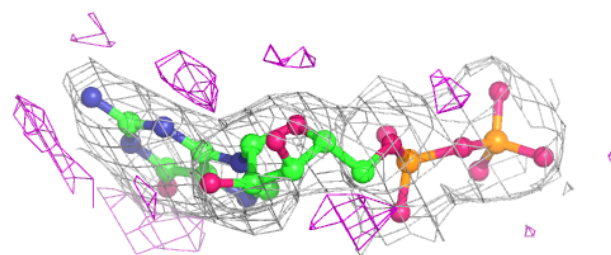
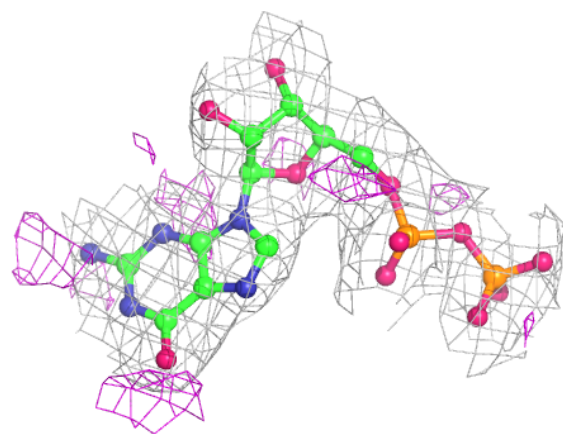


Electron density around K0M A 504:

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

**Electron density around GDP B 501:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.