



wwPDB X-ray Structure Validation Summary Report ⓘ

May 18, 2020 – 03:15 pm BST

PDB ID : 6EG5
Title : The structure of SB-1-202-tubulin complex
Authors : Banerjee, A.K.; Wang, Y.; Chen, H.; Miller, D.; Li, W.
Deposited on : 2018-08-18
Resolution : 2.45 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	:	2.11
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)	:	2.11

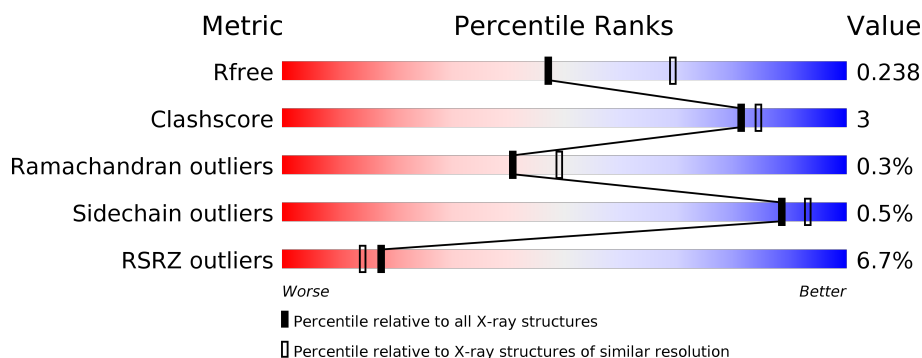
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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 on 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	450	<div> <div>2%</div> <div>94%</div> <div>• •</div> </div>
1	C	450	<div> <div>%</div> <div>93%</div> <div>• •</div> </div>
2	B	445	<div> <div>3%</div> <div>89%</div> <div>7%</div> <div>•</div> </div>
2	D	445	<div> <div>7%</div> <div>88%</div> <div>6%</div> <div>6%</div> </div>
3	E	143	<div> <div>9%</div> <div>84%</div> <div>•</div> <div>12%</div> </div>
4	F	384	<div> <div>21%</div> <div>85%</div> <div>7%</div> <div>7%</div> </div>

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
9	GOL	A	506	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 18509 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	2	0
			3436	2174	583	655	24			
1	C	441	Total	C	N	O	S	0	3	0
			3456	2187	585	661	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	428	Total	C	N	O	S	0	0	0
			3369	2115	577	650	27			
2	D	420	Total	C	N	O	S	0	1	0
			3301	2075	561	639	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	126	Total	C	N	O	S	0	1	0
			1052	649	189	208	6			

There are 2 discrepancies between the modelled and reference sequences:

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

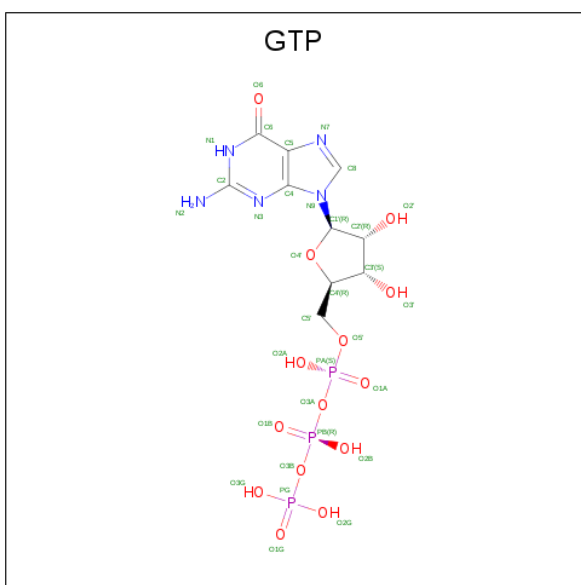
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	356	Total	C	N	O	S	0	0	0
			2913	1863	504	532	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		
5	D	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	B	1	Total	Mg	0	0
			1	1		
6	A	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total 1	Mg 1	0	0
6	F	2	Total 2	Mg 2	0	0

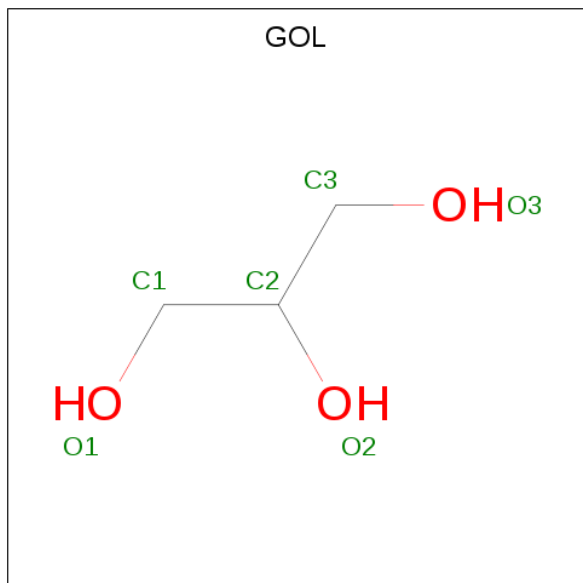
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

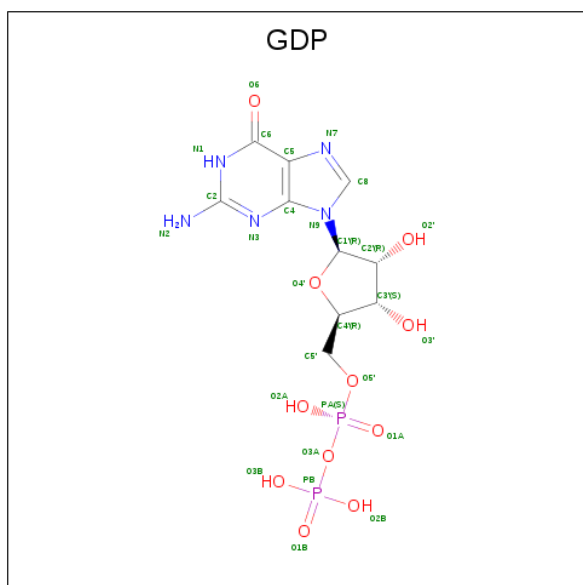
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total 1	Cl 1	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			6	3	3		
9	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 10 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



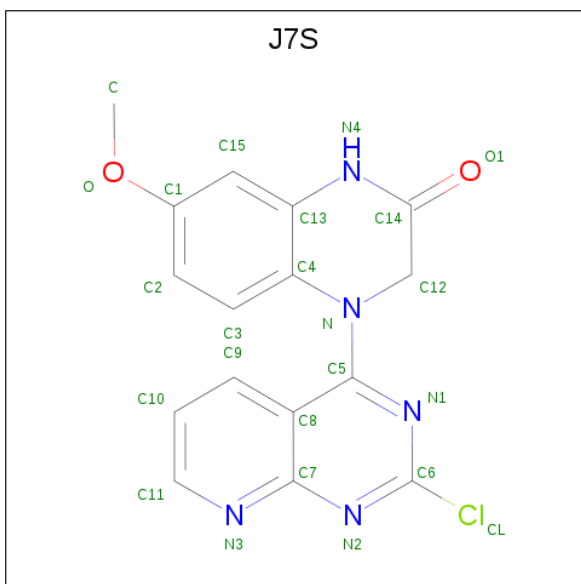
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 11 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 12 is 4-(2-chloropyrido[2,3-d]pyrimidin-4-yl)-7-methoxy-3,4-dihydroquinoxalin-2(1H)-one (three-letter code: J7S) (formula: C₁₆H₁₂ClN₅O₂).



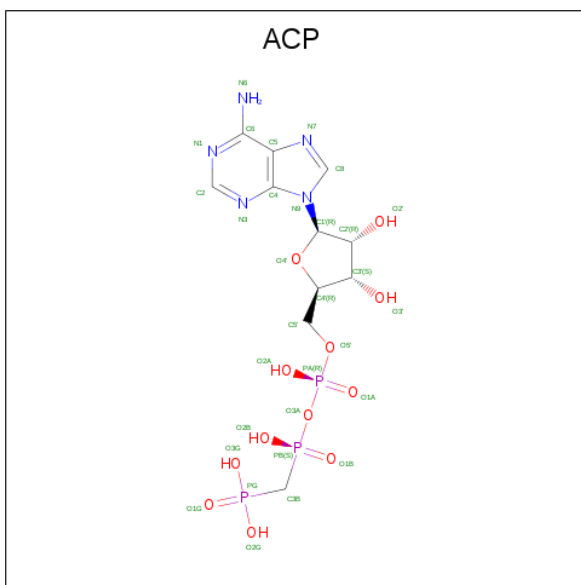
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	B	1	Total	C	Cl	N	O	0	0
			24	16	1	5	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	D	1	Total	C	Cl	N	O	
			24	16	1	5	2	
							0	0

- Molecule 13 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



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

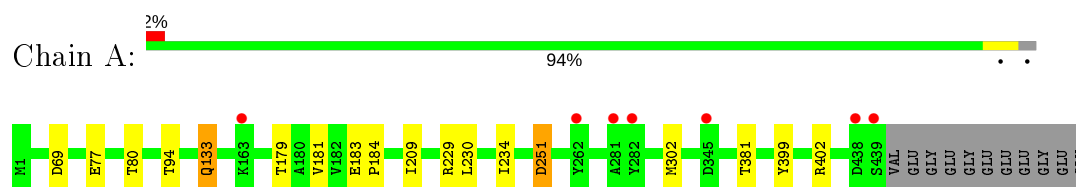
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	156	Total	O		
			156	156	0	0
14	B	144	Total	O		
			144	144	0	0
14	C	267	Total	O		
			267	267	0	0
14	D	65	Total	O		
			65	65	0	0
14	E	28	Total	O		
			28	28	0	0
14	F	72	Total	O		
			72	72	0	0

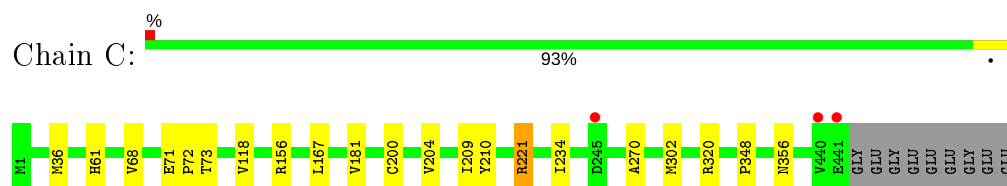
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

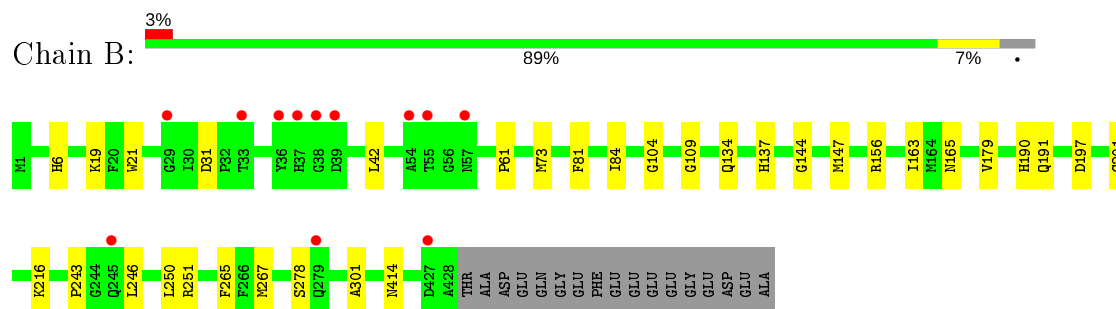
- Molecule 1: Tubulin alpha-1B chain



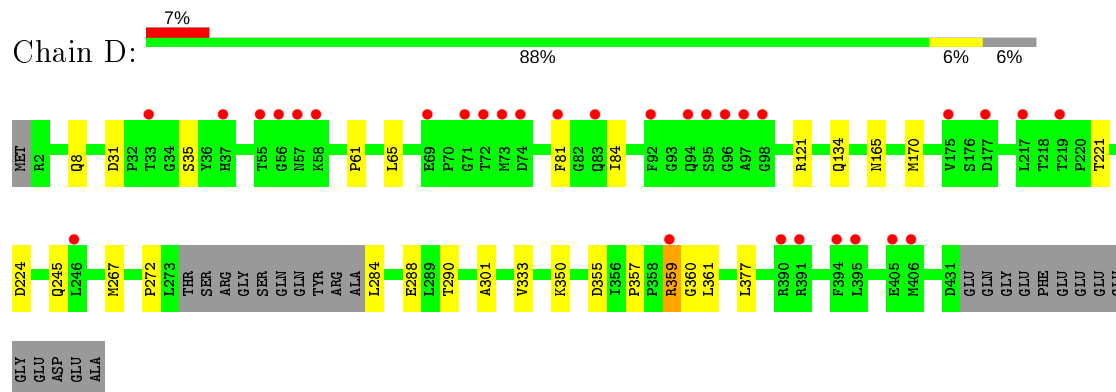
- Molecule 1: Tubulin alpha-1B chain




- Molecule 2: Tubulin beta-2B chain

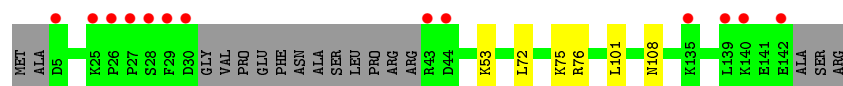


- Molecule 2: Tubulin beta-2B chain




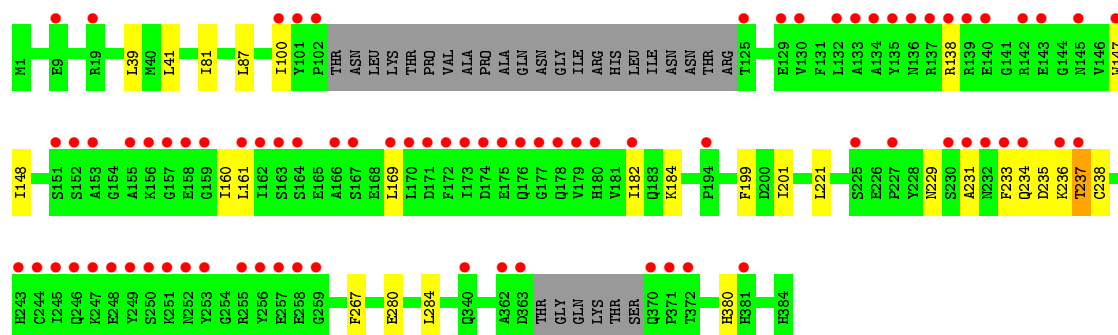
- Molecule 3: Stathmin-4

Chain E: 



- Molecule 4: Tubulin tyrosine ligase

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.54Å 158.03Å 181.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.45 49.88 – 2.45	Depositor EDS
% Data completeness (in resolution range)	97.5 (50.00-2.45) 97.6 (49.88-2.45)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.196 , 0.236 0.200 , 0.238	Depositor DCC
R_{free} test set	5580 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18509	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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: GDP, GOL, MG, CL, CA, J7S, GTP, ACP, MES

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	0.47	0/3520	0.68	0/4778
1	C	0.49	0/3540	0.70	0/4805
2	B	0.48	0/3444	0.66	0/4664
2	D	0.45	0/3374	0.65	0/4571
3	E	0.47	0/1064	0.63	0/1411
4	F	0.45	0/2983	0.65	0/4031
All	All	0.47	0/17925	0.67	0/24260

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	3436	0	3350	14	0
1	C	3456	0	3366	18	0
2	B	3369	0	3250	24	0
2	D	3301	0	3177	24	0
3	E	1052	0	1063	4	0
4	F	2913	0	2863	12	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	0	0
5	D	32	0	12	0	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	2	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
7	E	1	0	0	0	0
8	A	1	0	0	0	0
9	A	12	0	16	0	0
10	B	28	0	12	0	0
11	B	24	0	26	4	0
12	B	24	0	0	3	0
12	D	24	0	0	2	0
13	F	31	0	14	0	0
14	A	156	0	0	1	0
14	B	144	0	0	2	0
14	C	267	0	0	0	0
14	D	65	0	0	3	0
14	E	28	0	0	1	0
14	F	72	0	0	1	0
All	All	18509	0	17173	92	0

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

The worst 5 of 92 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)
2:D:359:ARG:NH1	2:D:359:ARG:HB3	1.89	0.86
1:C:234:ILE:HD13	1:C:302[A]:MET:SD	2.22	0.80
2:D:359:ARG:CZ	2:D:359:ARG:HB3	2.24	0.68
2:B:42:LEU:HD22	2:B:243:PRO:HG2	1.75	0.68
1:C:204:VAL:HG22	1:C:302[B]:MET:HE1	1.75	0.66

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	439/450 (98%)	429 (98%)	10 (2%)	0	100	100
1	C	441/450 (98%)	431 (98%)	10 (2%)	0	100	100
2	B	426/445 (96%)	415 (97%)	11 (3%)	0	100	100
2	D	416/445 (94%)	407 (98%)	9 (2%)	0	100	100
3	E	123/143 (86%)	120 (98%)	2 (2%)	1 (1%)	19	22
4	F	350/384 (91%)	329 (94%)	15 (4%)	6 (2%)	9	7
All	All	2195/2317 (95%)	2131 (97%)	57 (3%)	7 (0%)	41	49

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	234	GLN
4	F	380	HIS
3	E	53	LYS
4	F	231	ALA
4	F	237	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	372/378 (98%)	369 (99%)	3 (1%)	81	88
1	C	374/378 (99%)	373 (100%)	1 (0%)	92	95
2	B	370/383 (97%)	368 (100%)	2 (0%)	88	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	363/383 (95%)	361 (99%)	2 (1%)	86	91
3	E	115/127 (91%)	115 (100%)	0	100	100
4	F	318/342 (93%)	316 (99%)	2 (1%)	86	91
All	All	1912/1991 (96%)	1902 (100%)	10 (0%)	88	93

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	278	SER
1	C	221	ARG
2	D	359	ARG
2	B	19	LYS
2	D	35	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	190	HIS
3	E	108	ASN
2	D	99	ASN
2	B	137	HIS
3	E	18	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 11 are monoatomic - leaving 11 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$
11	MES	B	504	-	12,12,12	2.25	1 (8%)	14,16,16	1.91	4 (28%)
9	GOL	A	505	-	5,5,5	0.34	0	5,5,5	0.74	0
12	J7S	D	603	-	27,27,27	2.89	8 (29%)	34,39,39	2.63	9 (26%)
9	GOL	A	506	-	5,5,5	0.37	0	5,5,5	0.53	0
11	MES	B	505	-	12,12,12	2.13	1 (8%)	14,16,16	1.32	2 (14%)
5	GTP	A	501	6	26,34,34	1.09	2 (7%)	33,54,54	1.90	7 (21%)
10	GDP	B	501	6	24,30,30	1.18	3 (12%)	31,47,47	1.93	7 (22%)
5	GTP	C	501	6	26,34,34	1.02	2 (7%)	33,54,54	1.92	6 (18%)
12	J7S	B	506	-	27,27,27	2.89	8 (29%)	34,39,39	2.57	15 (44%)
13	ACP	F	703	6	27,33,33	2.12	9 (33%)	32,52,52	1.47	3 (9%)
5	GTP	D	601	6	26,34,34	1.25	2 (7%)	33,54,54	2.02	10 (30%)

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
11	MES	B	504	-	-	3/6/14/14	0/1/1/1
9	GOL	A	505	-	-	2/4/4/4	-
12	J7S	D	603	-	-	4/6/18/18	0/4/4/4
9	GOL	A	506	-	-	1/4/4/4	-
11	MES	B	505	-	-	2/6/14/14	0/1/1/1
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
10	GDP	B	501	6	-	3/12/32/32	0/3/3/3
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3
12	J7S	B	506	-	-	3/6/18/18	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	ACP	F	703	6	-	3/15/38/38	0/3/3/3
5	GTP	D	601	6	-	6/18/38/38	0/3/3/3

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	603	J7S	O1-C14	8.62	1.40	1.23
12	B	506	J7S	O1-C14	8.40	1.40	1.23
11	B	504	MES	C8-S	-7.43	1.66	1.77
11	B	505	MES	C8-S	-7.13	1.67	1.77
12	D	603	J7S	C14-N4	6.97	1.42	1.35

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	603	J7S	N2-C6-N1	-6.88	123.69	130.62
12	D	603	J7S	CL-C6-N2	6.34	121.11	115.70
12	B	506	J7S	C13-N4-C14	-5.85	117.25	124.49
12	B	506	J7S	N2-C6-N1	-5.77	124.80	130.62
12	D	603	J7S	C6-N2-C7	5.60	118.52	114.09

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	505	GOL	C1-C2-C3-O3
12	B	506	J7S	C8-C5-N-C12
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	601	GTP	C5'-O5'-PA-O2A

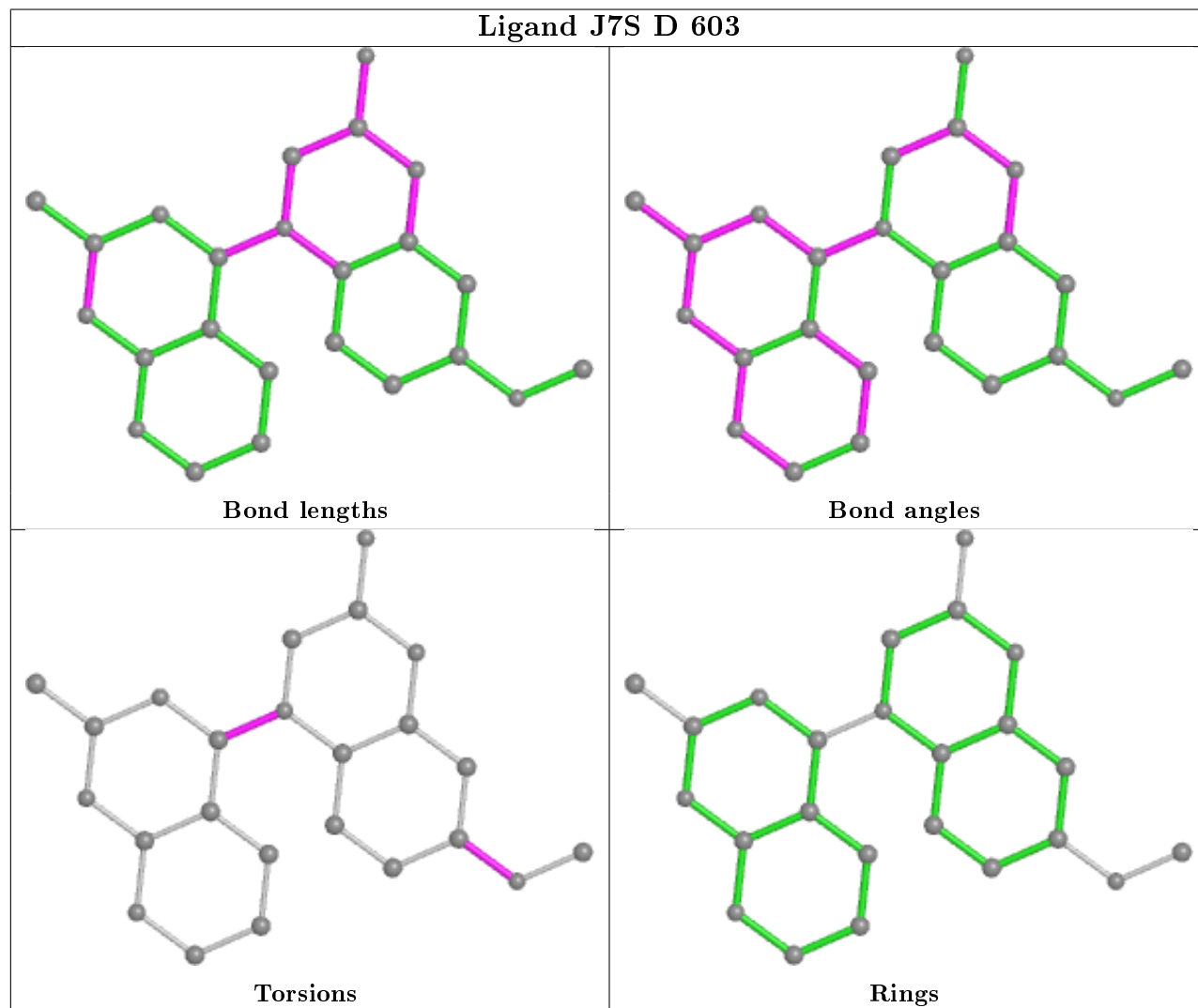
There are no ring outliers.

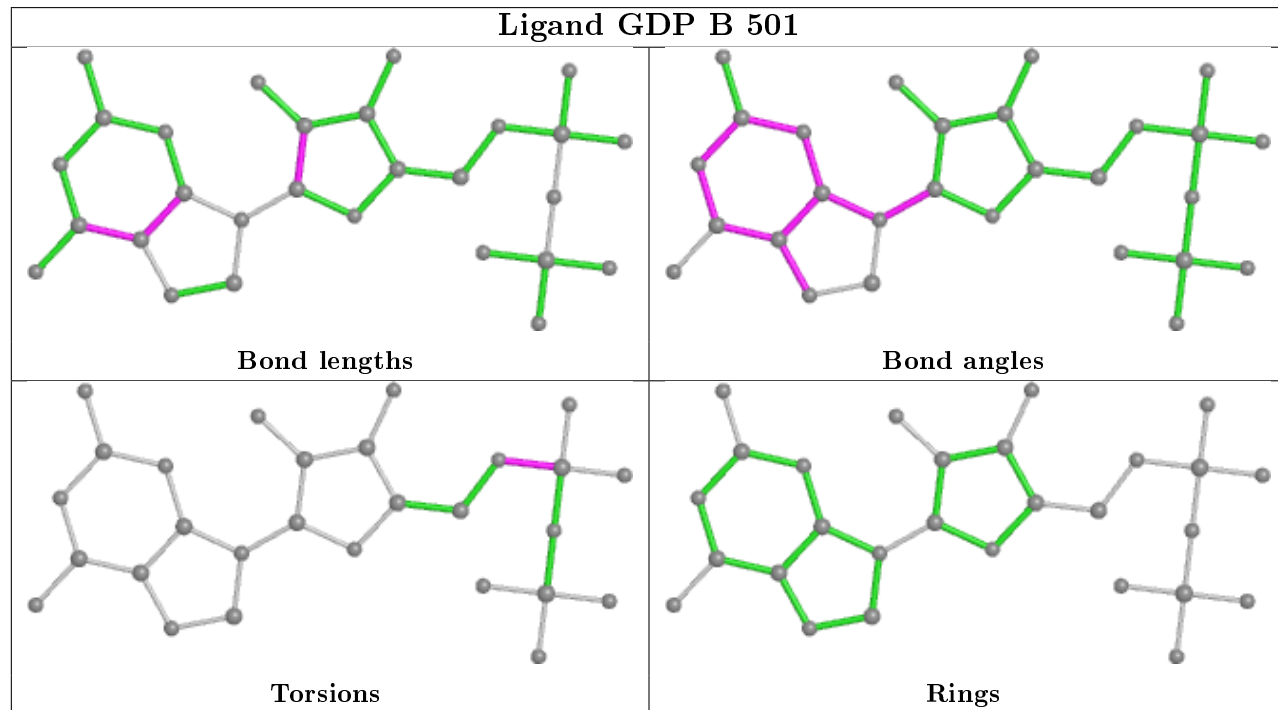
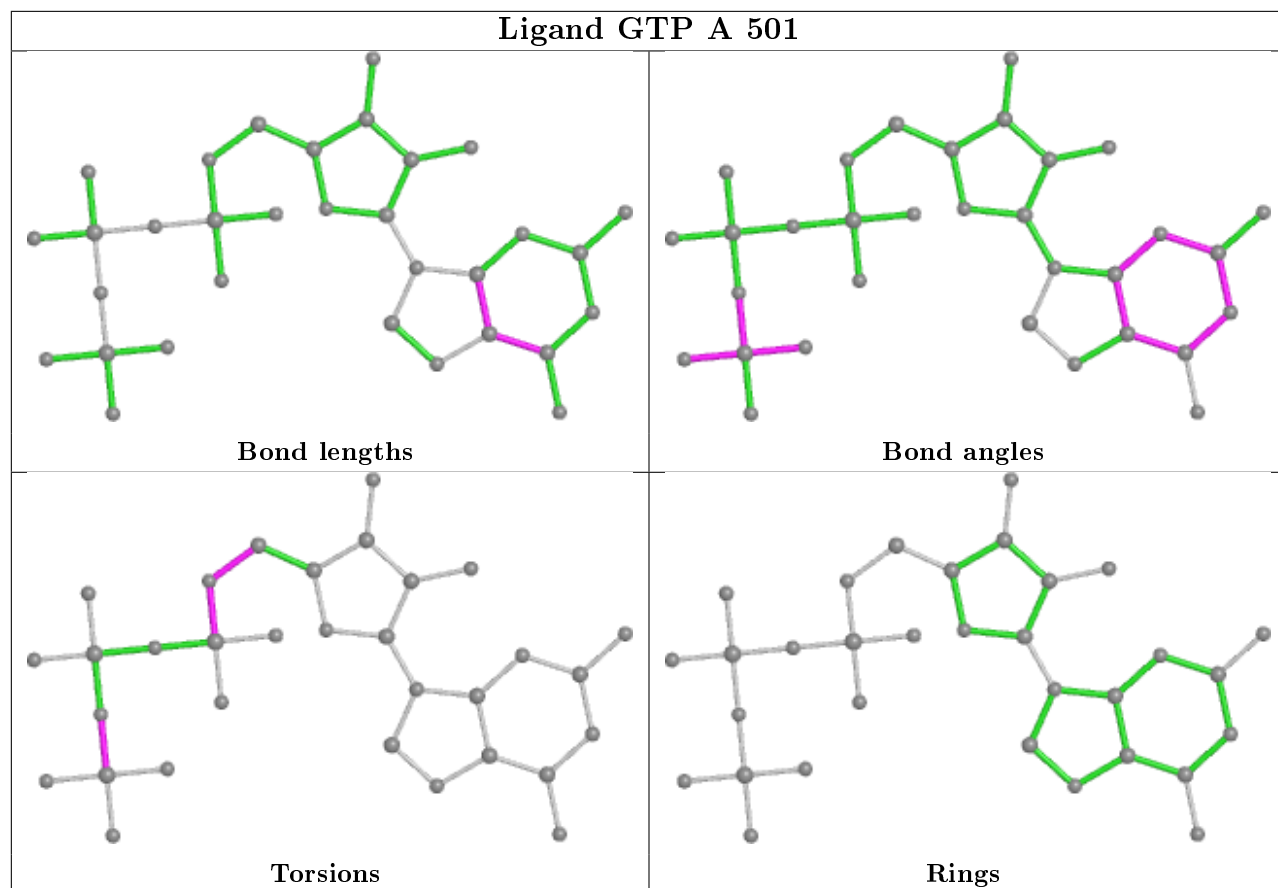
3 monomers are involved in 9 short contacts:

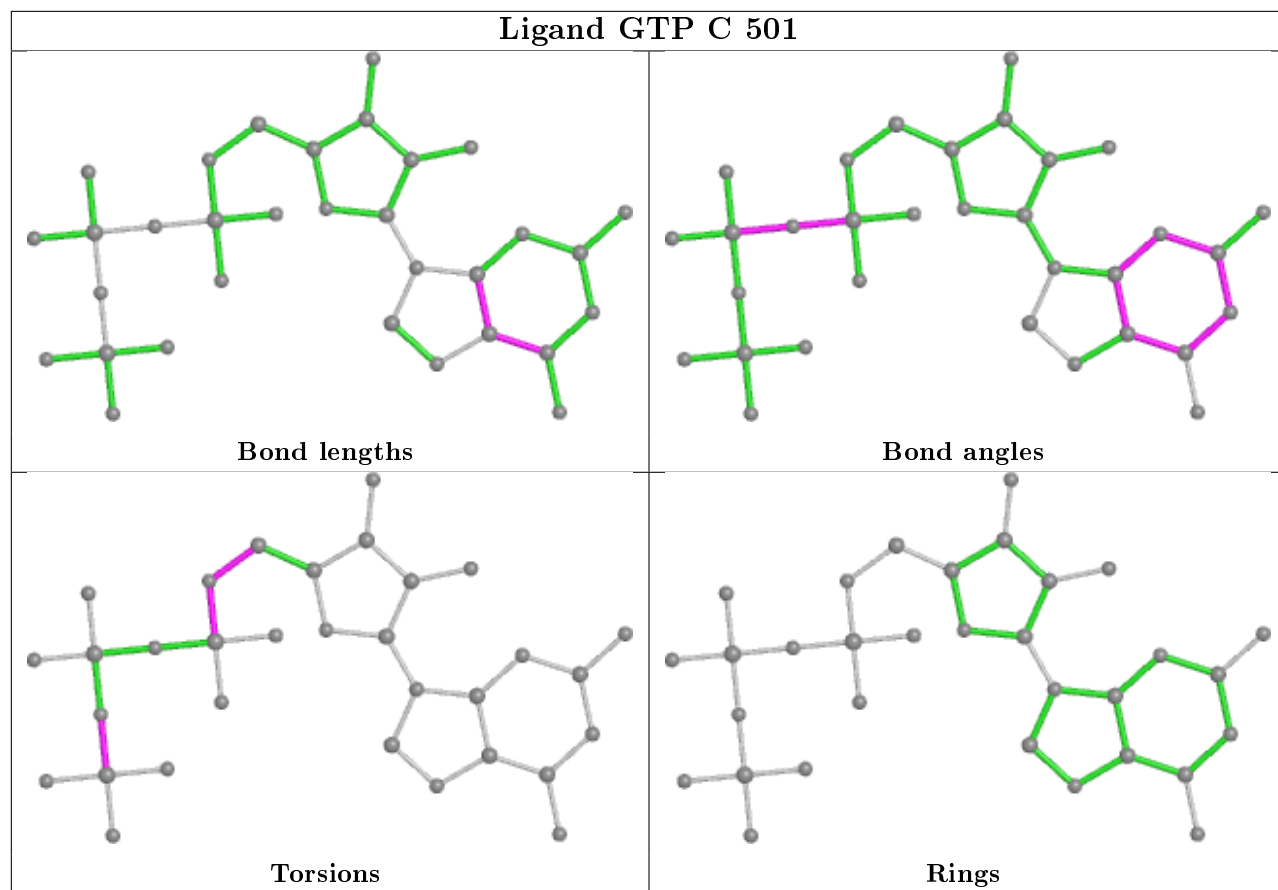
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	504	MES	4	0
12	D	603	J7S	2	0
12	B	506	J7S	3	0

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

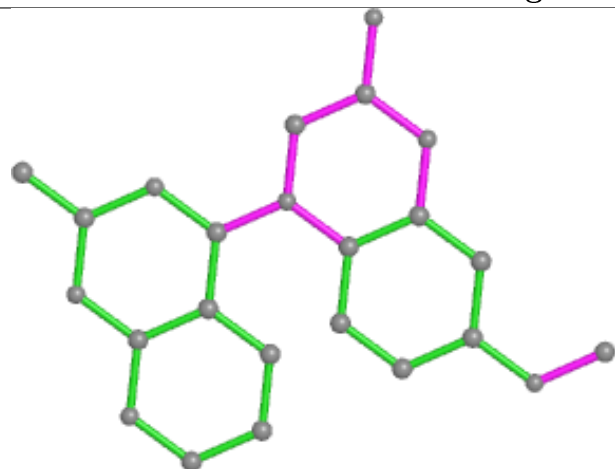
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.



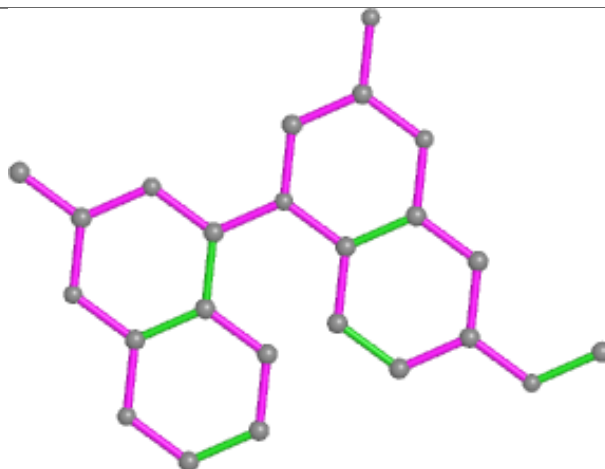




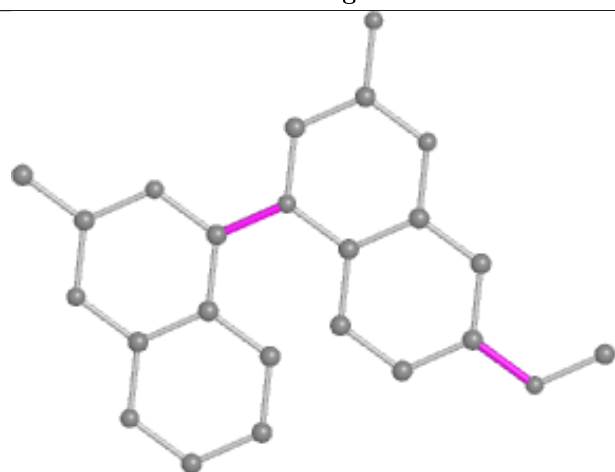
Ligand J7S B 506



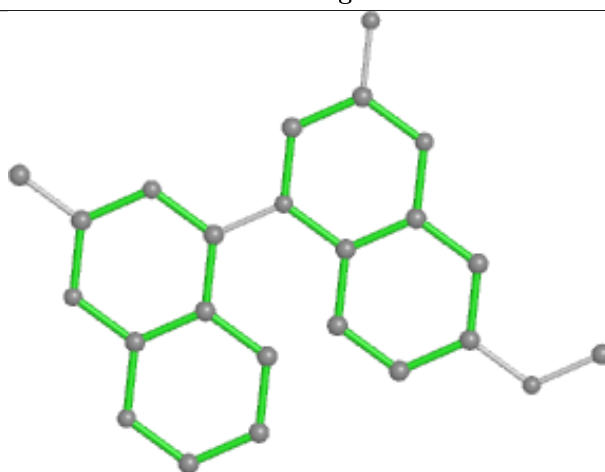
Bond lengths



Bond angles

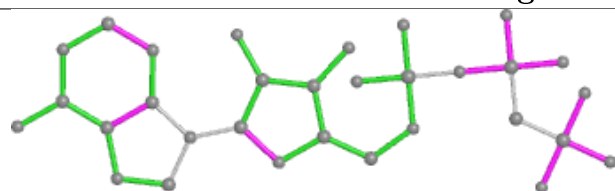


Torsions

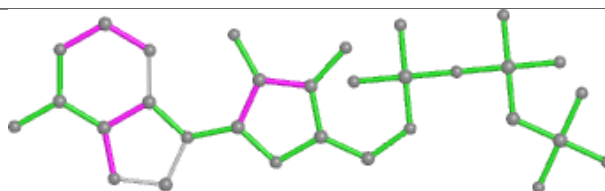


Rings

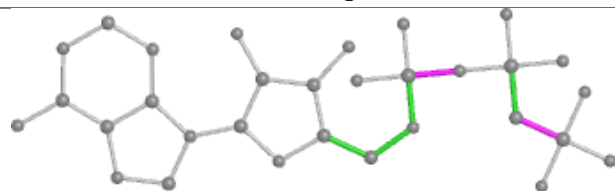
Ligand ACP F 703



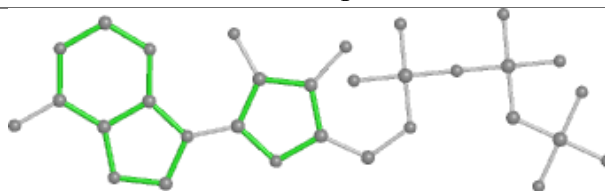
Bond lengths



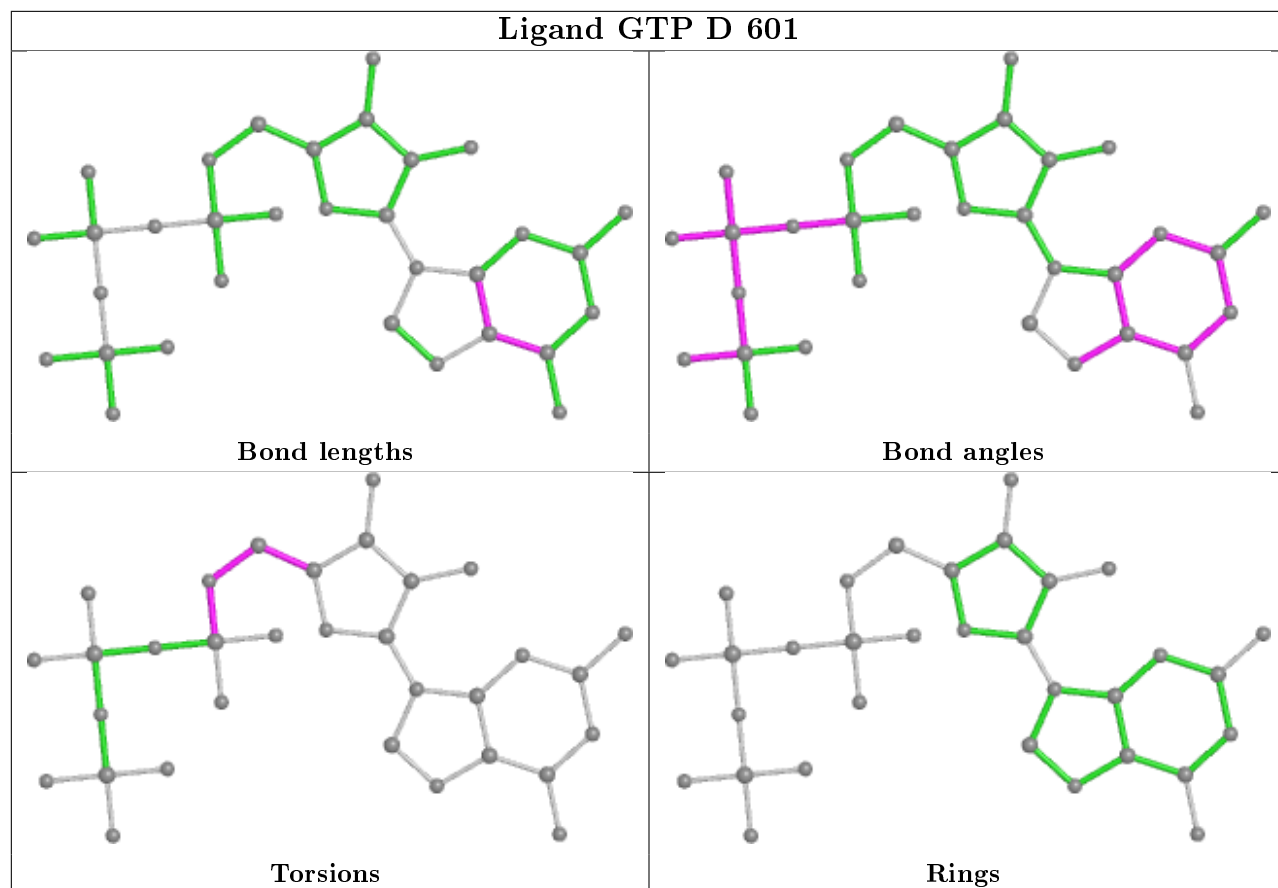
Bond angles



Torsions



Rings



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	439/450 (97%)	-0.10	7 (1%) 72 69	19, 37, 64, 92	0
1	C	441/450 (98%)	-0.35	3 (0%) 87 88	14, 27, 49, 104	0
2	B	428/445 (96%)	-0.16	12 (2%) 53 49	17, 34, 74, 110	2 (0%)
2	D	420/445 (94%)	0.42	31 (7%) 14 11	25, 53, 89, 112	3 (0%)
3	E	126/143 (88%)	0.59	13 (10%) 6 4	29, 51, 100, 123	0
4	F	356/384 (92%)	0.93	81 (22%) 0 0	27, 62, 129, 155	0
All	All	2210/2317 (95%)	0.14	147 (6%) 17 14	14, 41, 97, 155	5 (0%)

The worst 5 of 147 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	143	GLU	10.4
4	F	370	GLN	10.4
3	E	30	ASP	7.6
4	F	232	ASN	7.3
4	F	372	THR	6.7

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 carbohydrates in this entry.

6.4 Ligands ⓘ

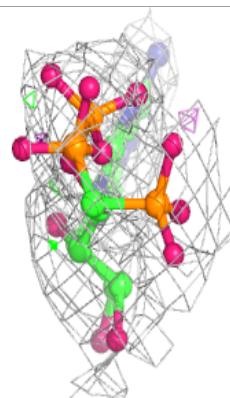
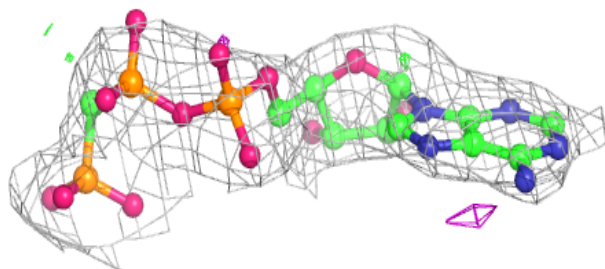
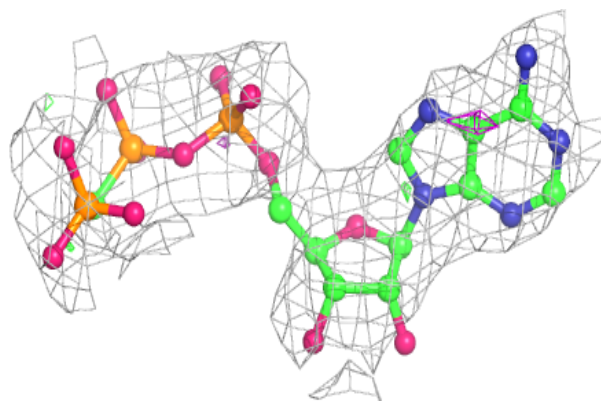
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	GOL	A	506	6/6	0.68	0.41	78,80,84,90	0
6	MG	F	702	1/1	0.75	0.25	76,76,76,76	0
7	CA	B	503	1/1	0.79	0.09	76,76,76,76	0
6	MG	D	602	1/1	0.80	0.14	63,63,63,63	0
13	ACP	F	703	31/31	0.88	0.18	75,90,107,112	0
9	GOL	A	505	6/6	0.88	0.18	53,59,61,65	0
7	CA	E	201	1/1	0.91	0.08	73,73,73,73	0
5	GTP	D	601	32/32	0.91	0.17	39,46,72,79	0
11	MES	B	504	12/12	0.92	0.16	40,45,58,63	0
8	CL	A	504	1/1	0.92	0.20	74,74,74,74	0
6	MG	F	701	1/1	0.92	0.22	72,72,72,72	0
6	MG	B	502	1/1	0.94	0.13	27,27,27,27	0
11	MES	B	505	12/12	0.94	0.18	60,66,68,68	0
6	MG	A	502	1/1	0.96	0.08	28,28,28,28	0
12	J7S	B	506	24/24	0.96	0.15	25,28,32,39	0
7	CA	A	503	1/1	0.96	0.05	52,52,52,52	0
12	J7S	D	603	24/24	0.97	0.17	26,33,44,48	0
6	MG	C	502	1/1	0.98	0.07	25,25,25,25	0
7	CA	C	503	1/1	0.99	0.04	35,35,35,35	0
5	GTP	A	501	32/32	0.99	0.14	19,21,22,23	0
10	GDP	B	501	28/28	0.99	0.14	18,21,23,24	0
5	GTP	C	501	32/32	0.99	0.11	18,19,20,21	0

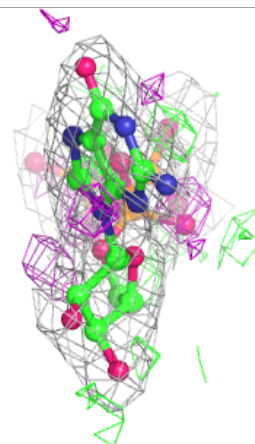
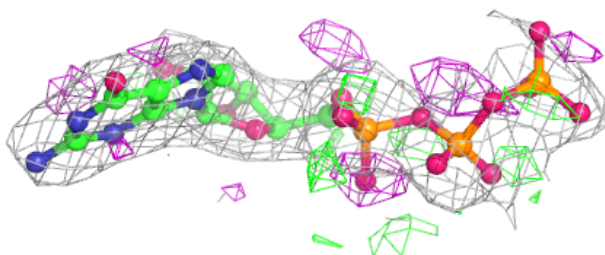
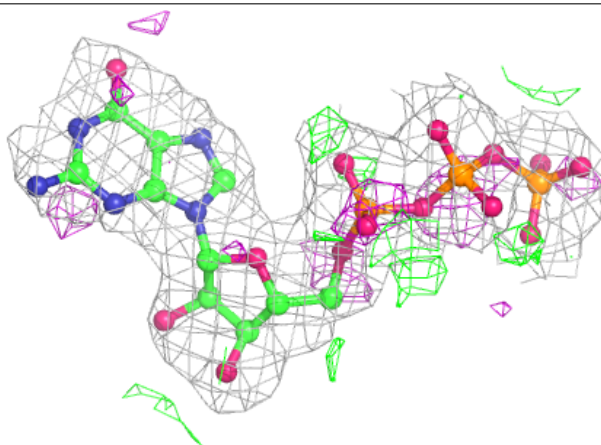
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP F 703:

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

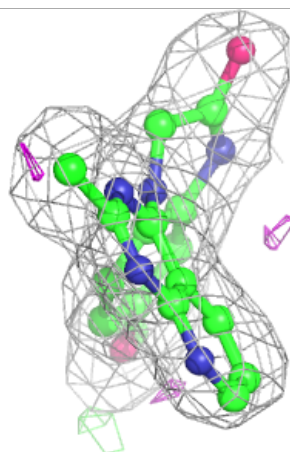
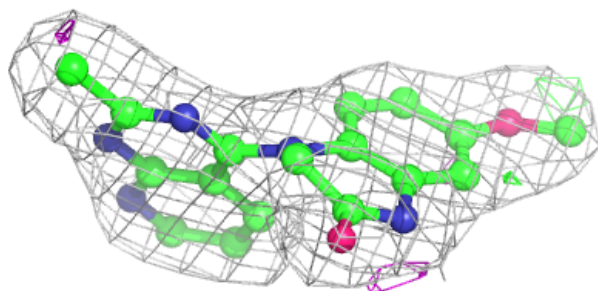
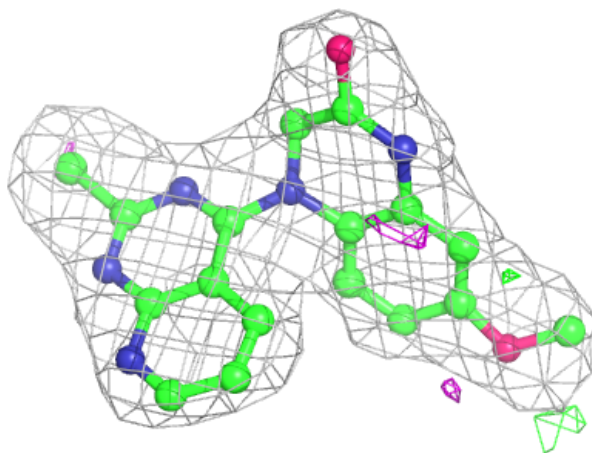
**Electron density around GTP D 601:**

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



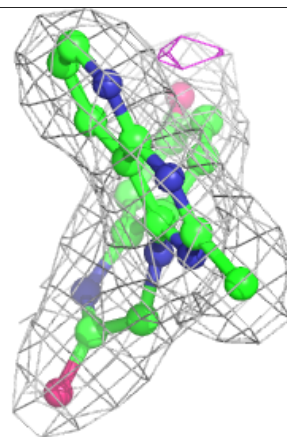
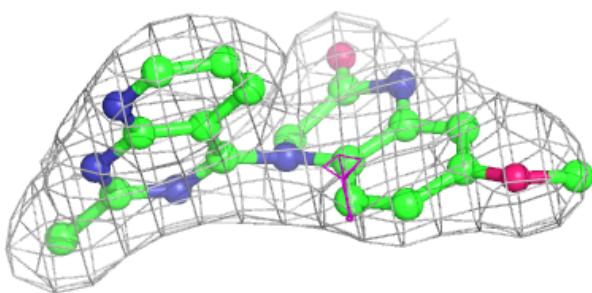
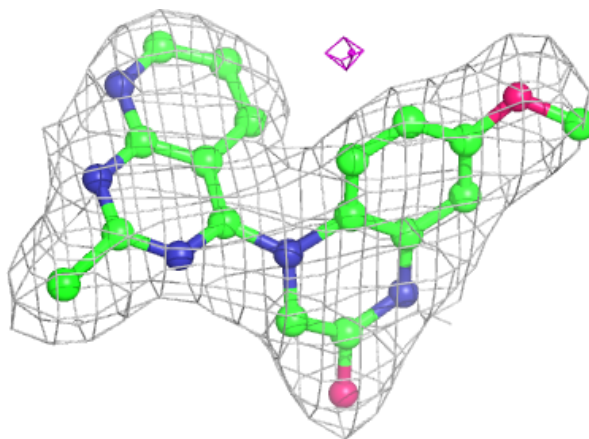
Electron density around J7S B 506:

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

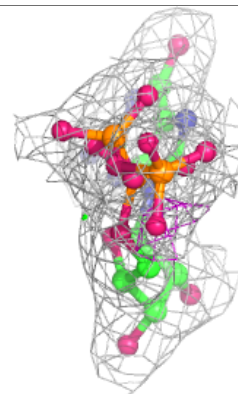
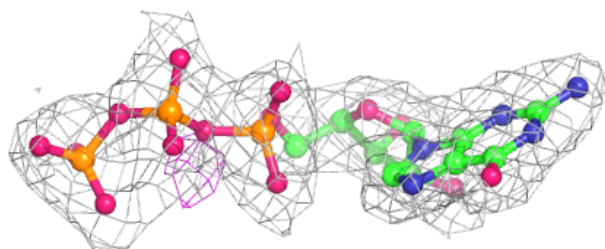
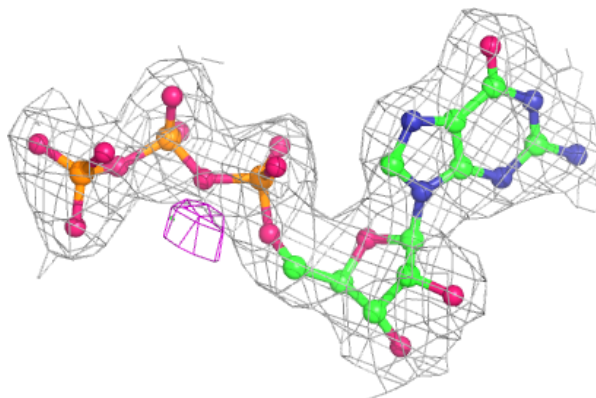


Electron density around J7S D 603:

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

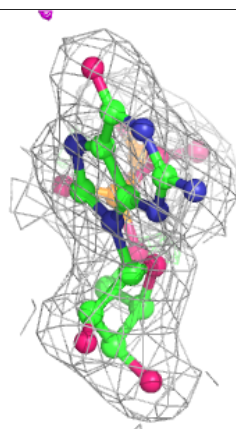
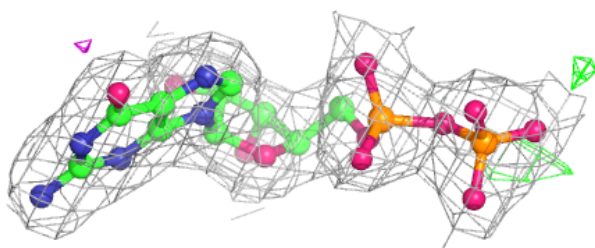
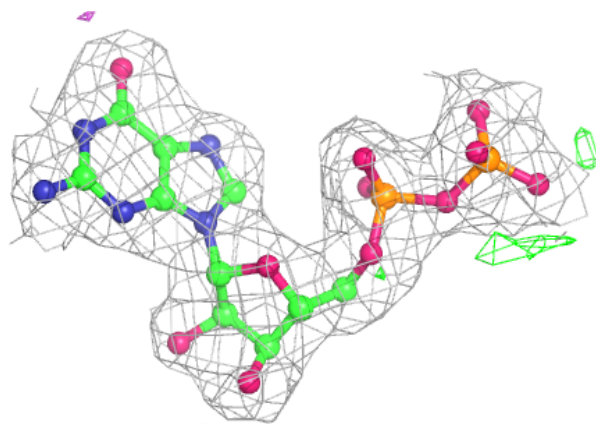
**Electron density around GTP A 501:**

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and green (positive)

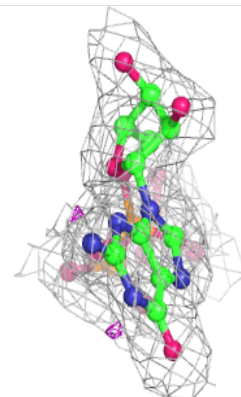
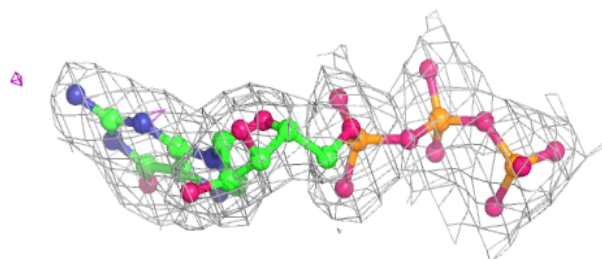
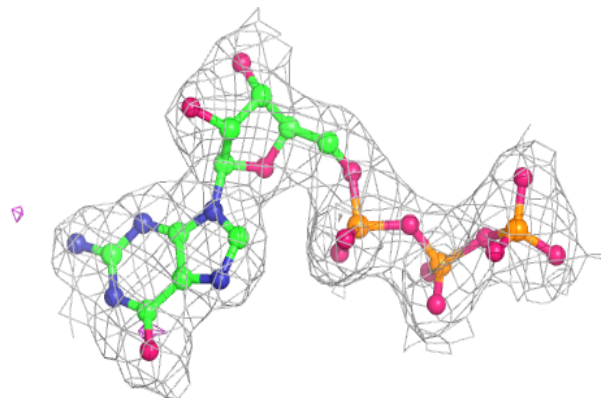


Electron density around GDP B 501:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.