



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 24, 2025 – 01:43 PM JST

PDB ID : 8YRK  
Title : Tubulin-Compound KY216: stathmin-like domain complex  
Authors : Xia, Y.Z.; He, X.Y.  
Deposited on : 2024-03-21  
Resolution : 2.74 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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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) : 1.21  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.004 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41.2

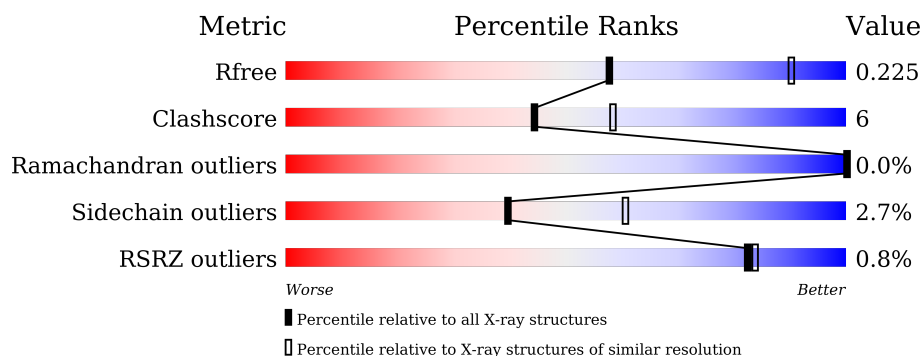
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.74 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1649 (2.76-2.72)
Clashscore	180529	1744 (2.76-2.72)
Ramachandran outliers	177936	1710 (2.76-2.72)
Sidechain outliers	177891	1711 (2.76-2.72)
RSRZ outliers	164620	1649 (2.76-2.72)

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  $\geq 3$ , 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 style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 0%, yellow 83%, green 14%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>83%</span> <span>14%</span> <span>•</span> </div> </div>
1	C	450	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, orange 0%, yellow 83%, green 15%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>83%</span> <span>15%</span> <span>•</span> </div> </div>
2	B	445	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, orange 0%, yellow 80%, green 15%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>80%</span> <span>15%</span> <span>5%</span> </div> </div>
2	D	445	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 0%, yellow 78%, green 16%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>78%</span> <span>16%</span> <span>• 5%</span> </div> </div>
3	E	143	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 0%, yellow 71%, green 14%, grey 14%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>71%</span> <span>14%</span> <span>• 14%</span> </div> </div>
4	F	384	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 0%, yellow 72%, green 18%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>72%</span> <span>18%</span> <span>• 10%</span> </div> </div>

## 2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 17720 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 Detyrosinated tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	4	0
			3431	2173	581	653	24			
1	C	440	Total	C	N	O	S	3	8	0
			3465	2193	585	663	24			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	2	0
			3350	2107	572	645	26			
2	D	421	Total	C	N	O	S	0	0	0
			3306	2078	562	640	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	2	0
			1026	633	186	202	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63042
E	4	ALA	-	expression tag	UNP P63042

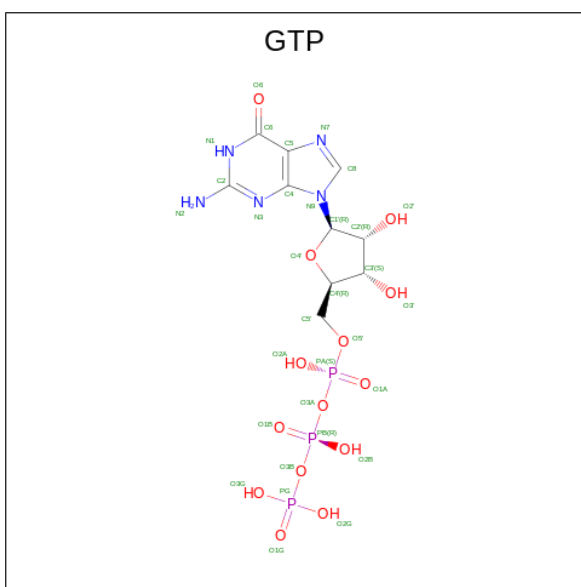
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	346	Total	C	N	O	S	0	4	0
			2859	1835	488	521	15			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	MET	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	PRO	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	LYS	deletion	UNP A0A8V0Z8P0
F	?	-	ASN	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	PHE	deletion	UNP A0A8V0Z8P0
F	379	HIS	-	expression tag	UNP A0A8V0Z8P0
F	380	HIS	-	expression tag	UNP A0A8V0Z8P0
F	381	HIS	-	expression tag	UNP A0A8V0Z8P0
F	382	HIS	-	expression tag	UNP A0A8V0Z8P0
F	383	HIS	-	expression tag	UNP A0A8V0Z8P0
F	384	HIS	-	expression tag	UNP A0A8V0Z8P0

- 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 32	C 10	N 5	O 14	P 3	0	0
5	C	1	Total 32	C 10	N 5	O 14	P 3	0	0

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

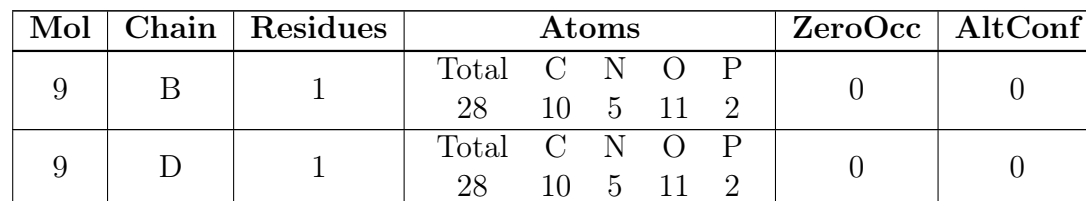
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Mg 1 1	0	0
6	B	1	Total Mg 1 1	0	0
6	D	2	Total Mg 2 2	0	0

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

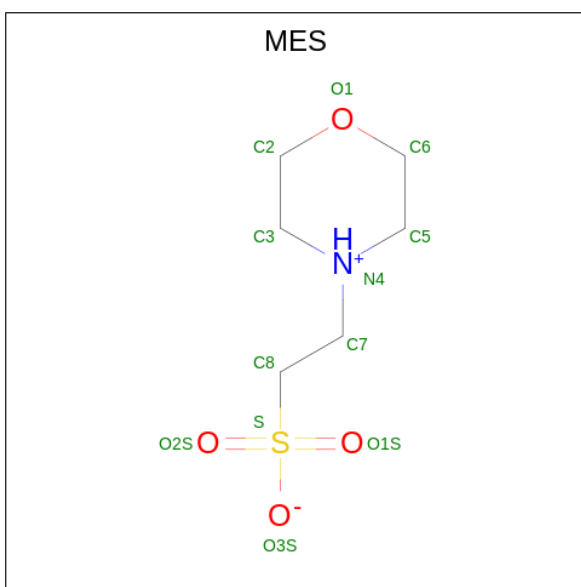
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0

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

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$ ).

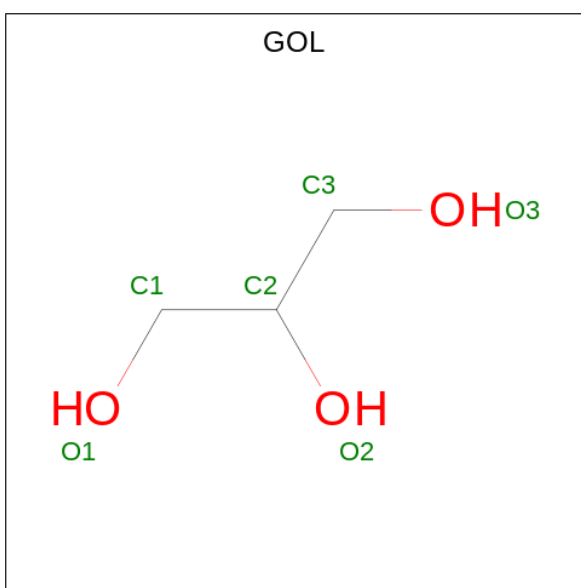


- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $\text{C}_6\text{H}_{13}\text{NO}_4\text{S}$ ).



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

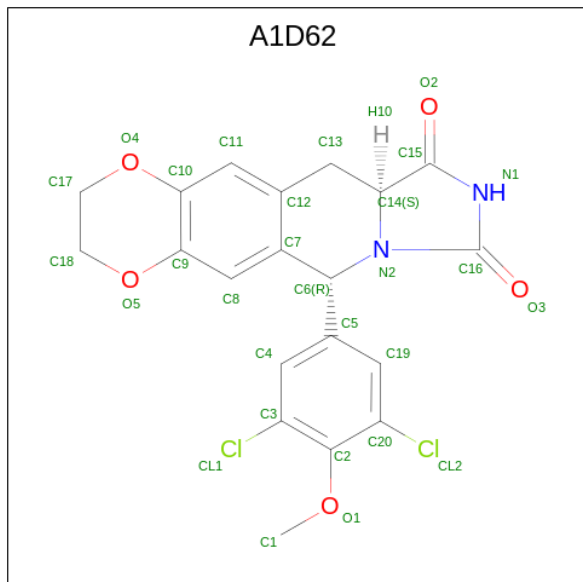
- Molecule 11 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			6	3	3		

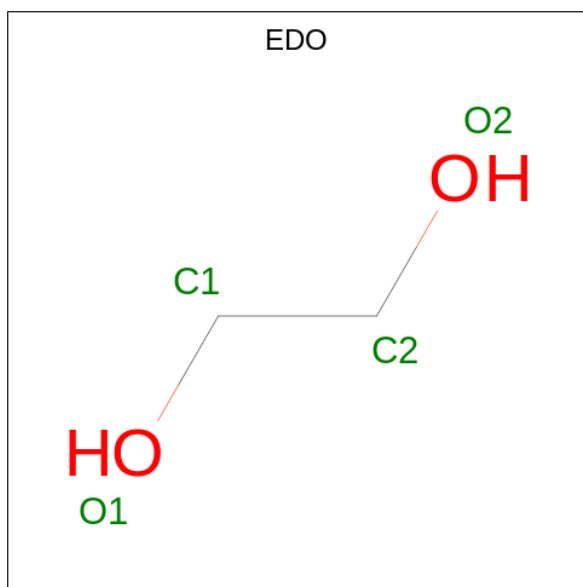
- Molecule 12 is (11R,16S)-11-(3,5-dichloro-4-methoxyphenyl)-4,7-dioxa-12,14-diazatetracyclo

[8.7.0.03,8.012,16]heptadeca-1,3(8),9-triene-13,15-dione (three-letter code: A1D62) (formula:  $C_{20}H_{16}Cl_2N_2O_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	B	1	Total	C	Cl	N	O	0	0
			29	20	2	2	5		
12	D	1	Total	C	Cl	N	O	0	0
			29	20	2	2	5		

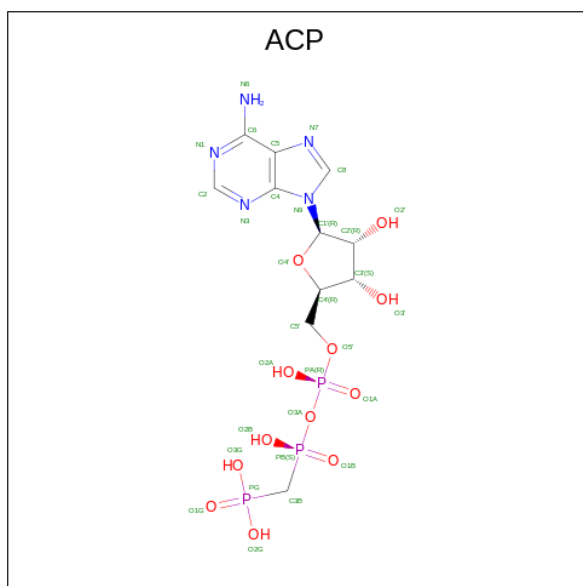
- Molecule 13 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 14 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula:  $C_{11}H_{18}N_5O_{12}P_3$ ).

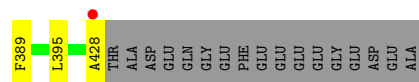


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

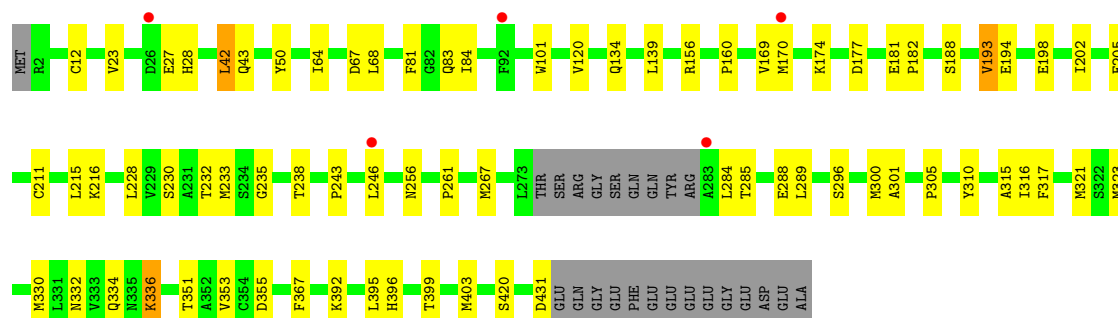
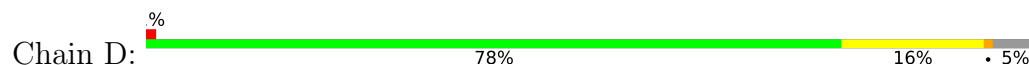
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	5	Total	O	0	0
			5	5		
15	B	9	Total	O	0	0
			9	9		
15	C	12	Total	O	0	0
			12	12		
15	D	6	Total	O	0	0
			6	6		
15	E	1	Total	O	0	0
			1	1		

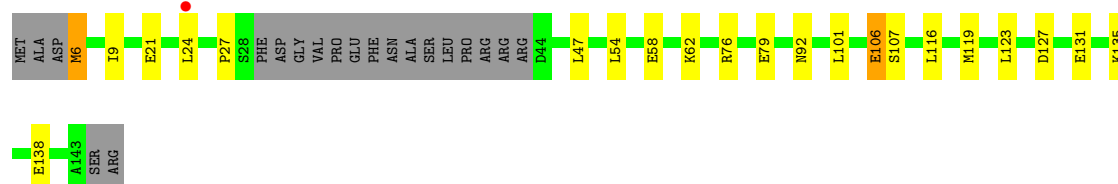




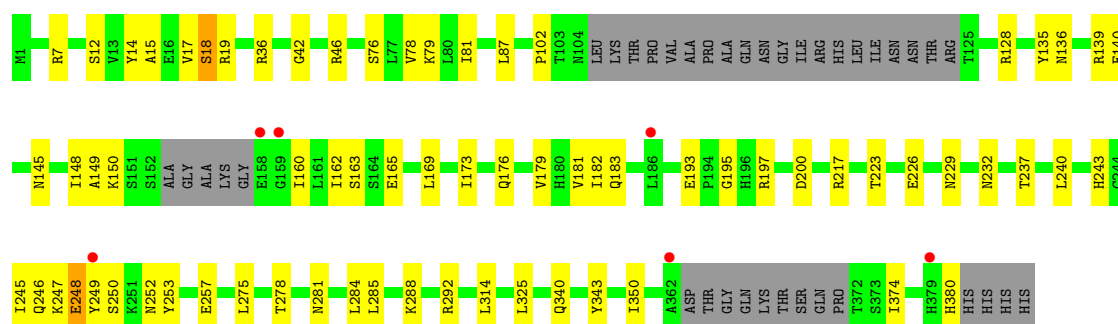
• Molecule 2: Tubulin beta chain



• 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, $\alpha$ , $\beta$ , $\gamma$	104.10Å 158.98Å 179.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.54 – 2.74 43.54 – 2.74	Depositor EDS
% Data completeness (in resolution range)	96.0 (43.54-2.74) 95.9 (43.54-2.74)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.03 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.173 , 0.226 0.173 , 0.225	Depositor DCC
$R_{free}$ test set	3866 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.8	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 52.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17720	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, CA, MES, MG, ACP, EDO, GTP, CL, A1D62

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	0.29	0/3521	0.49	0/4780
1	C	0.31	0/3564	0.52	0/4838
2	B	0.30	0/3430	0.52	0/4645
2	D	0.29	0/3379	0.49	0/4578
3	E	0.29	0/1041	0.45	0/1382
4	F	0.27	0/2935	0.50	0/3964
All	All	0.29	0/17870	0.50	0/24187

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	3431	0	3352	40	0
1	C	3465	0	3383	34	0
2	B	3350	0	3237	42	0
2	D	3306	0	3182	44	0
3	E	1026	0	1042	14	0
4	F	2859	0	2841	38	0
5	A	32	0	12	2	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	D	2	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	1	0	0	0	0
9	B	28	0	12	0	0
9	D	28	0	12	2	0
10	B	24	0	24	6	0
11	B	6	0	8	1	0
12	B	29	0	0	1	0
12	D	29	0	0	3	0
13	C	4	0	6	0	0
14	F	31	0	14	1	0
15	A	5	0	0	0	0
15	B	9	0	0	0	0
15	C	12	0	0	0	0
15	D	6	0	0	1	0
15	E	1	0	0	0	0
All	All	17720	0	17137	204	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 6.

The worst 5 of 204 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)
9:D:502:GDP:O3B	15:D:601:HOH:O	1.85	0.93
1:A:336:LYS:HD2	3:E:24:LEU:HD13	1.62	0.81
1:A:161:TYR:HB3	1:A:164:LYS:HG3	1.64	0.78
2:B:114:ASP:HB3	11:B:505:GOL:H32	1.66	0.75
2:D:330:MET:HG3	2:D:351:THR:HG21	1.68	0.75

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%)	428 (98%)	11 (2%)	0	100	100
1	C	445/450 (99%)	435 (98%)	9 (2%)	1 (0%)	44	63
2	B	422/445 (95%)	408 (97%)	14 (3%)	0	100	100
2	D	417/445 (94%)	413 (99%)	4 (1%)	0	100	100
3	E	121/143 (85%)	120 (99%)	1 (1%)	0	100	100
4	F	342/384 (89%)	328 (96%)	14 (4%)	0	100	100
All	All	2186/2317 (94%)	2132 (98%)	53 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	131	GLY

### 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%)	361 (97%)	11 (3%)	36	57
1	C	378/378 (100%)	369 (98%)	9 (2%)	44	64
2	B	369/383 (96%)	363 (98%)	6 (2%)	58	75
2	D	363/383 (95%)	353 (97%)	10 (3%)	38	59
3	E	112/127 (88%)	106 (95%)	6 (5%)	18	33
4	F	316/342 (92%)	305 (96%)	11 (4%)	31	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1910/1991 (96%)	1857 (97%)	53 (3%)	40 59

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	193	VAL
2	D	431	ASP
4	F	223	THR
2	D	198	GLU
2	D	355	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	165	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 7 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
9	GDP	B	501	6	24,30,30	0.95	1 (4%)	30,47,47	0.98	2 (6%)
12	A1D62	D	504	-	32,33,33	0.63	0	39,50,50	1.73	5 (12%)
9	GDP	D	502	6	24,30,30	0.98	1 (4%)	30,47,47	1.17	4 (13%)
10	MES	B	503	-	12,12,12	2.16	1 (8%)	14,16,16	1.93	4 (28%)
14	ACP	F	401	-	27,33,33	0.94	1 (3%)	32,52,52	1.15	2 (6%)
11	GOL	B	505	-	5,5,5	0.91	0	5,5,5	0.92	0
5	GTP	C	501	6	26,34,34	1.12	2 (7%)	32,54,54	1.46	6 (18%)
10	MES	B	504	-	12,12,12	2.31	1 (8%)	14,16,16	2.58	8 (57%)
13	EDO	C	503	-	3,3,3	0.51	0	2,2,2	0.19	0
12	A1D62	B	506	-	32,33,33	0.61	0	39,50,50	1.67	5 (12%)
5	GTP	A	501	6	26,34,34	1.13	1 (3%)	32,54,54	1.39	5 (15%)

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	B	501	6	-	3/12/32/32	0/3/3/3
12	A1D62	D	504	-	-	2/6/41/41	0/5/5/5
9	GDP	D	502	6	-	3/12/32/32	0/3/3/3
10	MES	B	503	-	-	3/6/14/14	0/1/1/1
14	ACP	F	401	-	-	7/15/38/38	0/3/3/3
11	GOL	B	505	-	-	2/4/4/4	-
5	GTP	C	501	6	-	5/18/38/38	0/3/3/3
10	MES	B	504	-	-	4/6/14/14	0/1/1/1
13	EDO	C	503	-	-	0/1/1/1	-
12	A1D62	B	506	-	-	2/6/41/41	0/5/5/5
5	GTP	A	501	6	-	8/18/38/38	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	504	MES	C8-S	-7.68	1.66	1.77
10	B	503	MES	C8-S	-7.24	1.67	1.77
5	C	501	GTP	C5-C6	-3.97	1.39	1.47
14	F	401	ACP	PB-O3A	3.95	1.62	1.58
5	A	501	GTP	C5-C6	-3.88	1.39	1.47

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	504	A1D62	O1-C2-C3	-6.24	109.40	121.26
12	B	506	A1D62	O1-C2-C3	-6.18	109.52	121.26
12	D	504	A1D62	O1-C2-C20	5.39	131.51	121.26
14	F	401	ACP	PB-O3A-PA	-5.35	115.60	132.56
12	B	506	A1D62	O1-C2-C20	5.32	131.37	121.26

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O1A
9	D	502	GDP	C5'-O5'-PA-O1A
10	B	503	MES	C8-C7-N4-C5

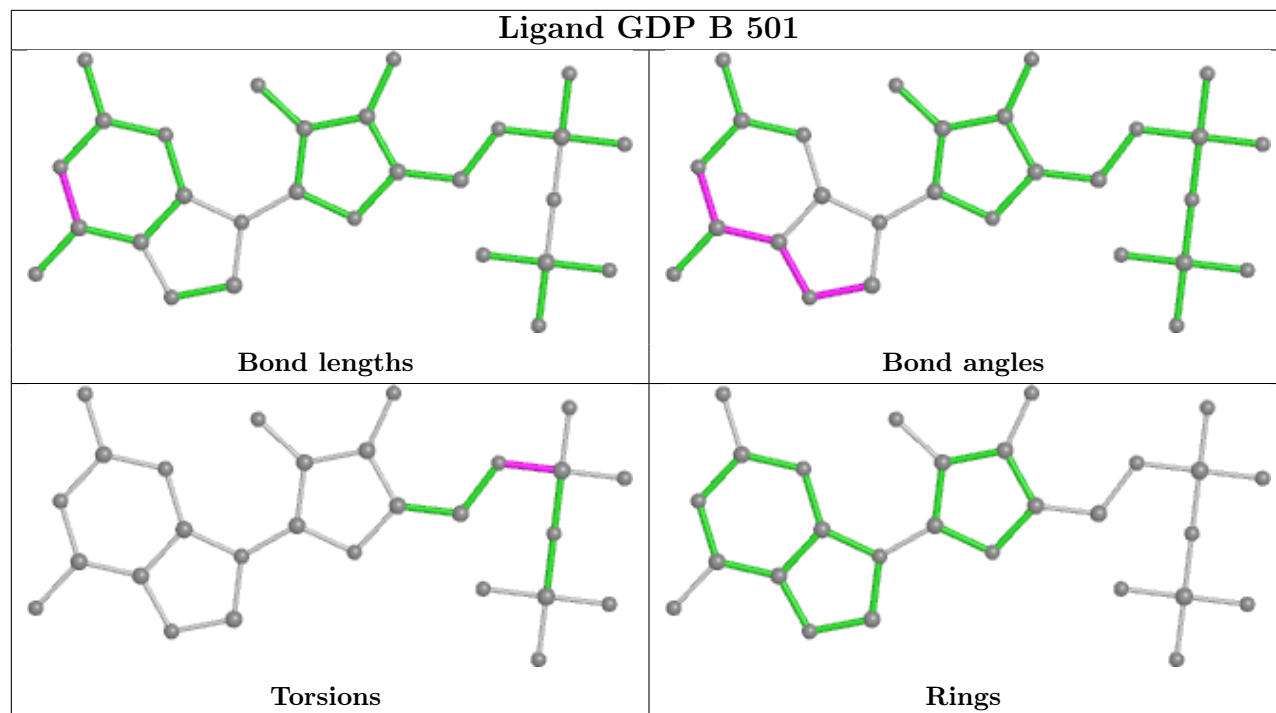
There are no ring outliers.

9 monomers are involved in 17 short contacts:

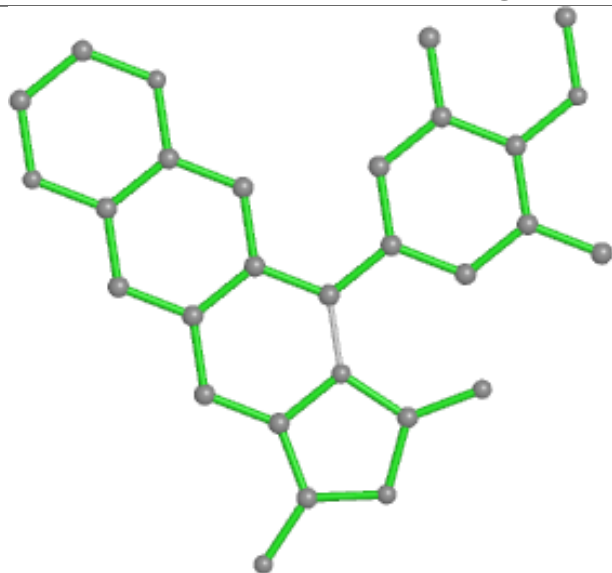
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	D	504	A1D62	3	0
9	D	502	GDP	2	0
10	B	503	MES	3	0
14	F	401	ACP	1	0
11	B	505	GOL	1	0
5	C	501	GTP	1	0
10	B	504	MES	3	0
12	B	506	A1D62	1	0
5	A	501	GTP	2	0

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

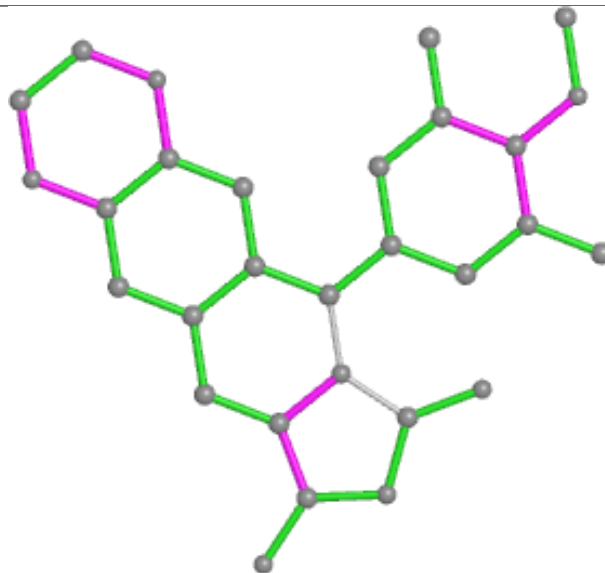
equivalents in the CSD to analyse the geometry.



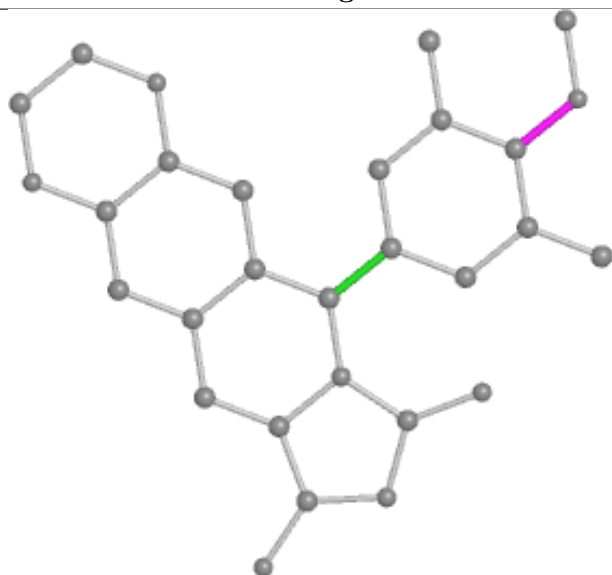
## Ligand A1D62 D 504



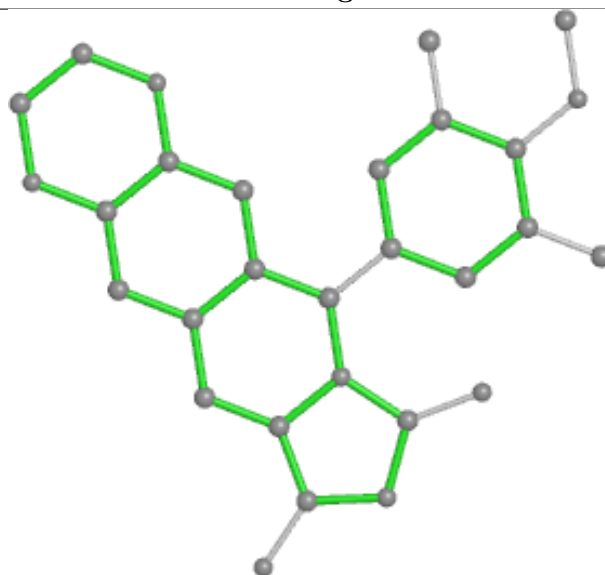
Bond lengths



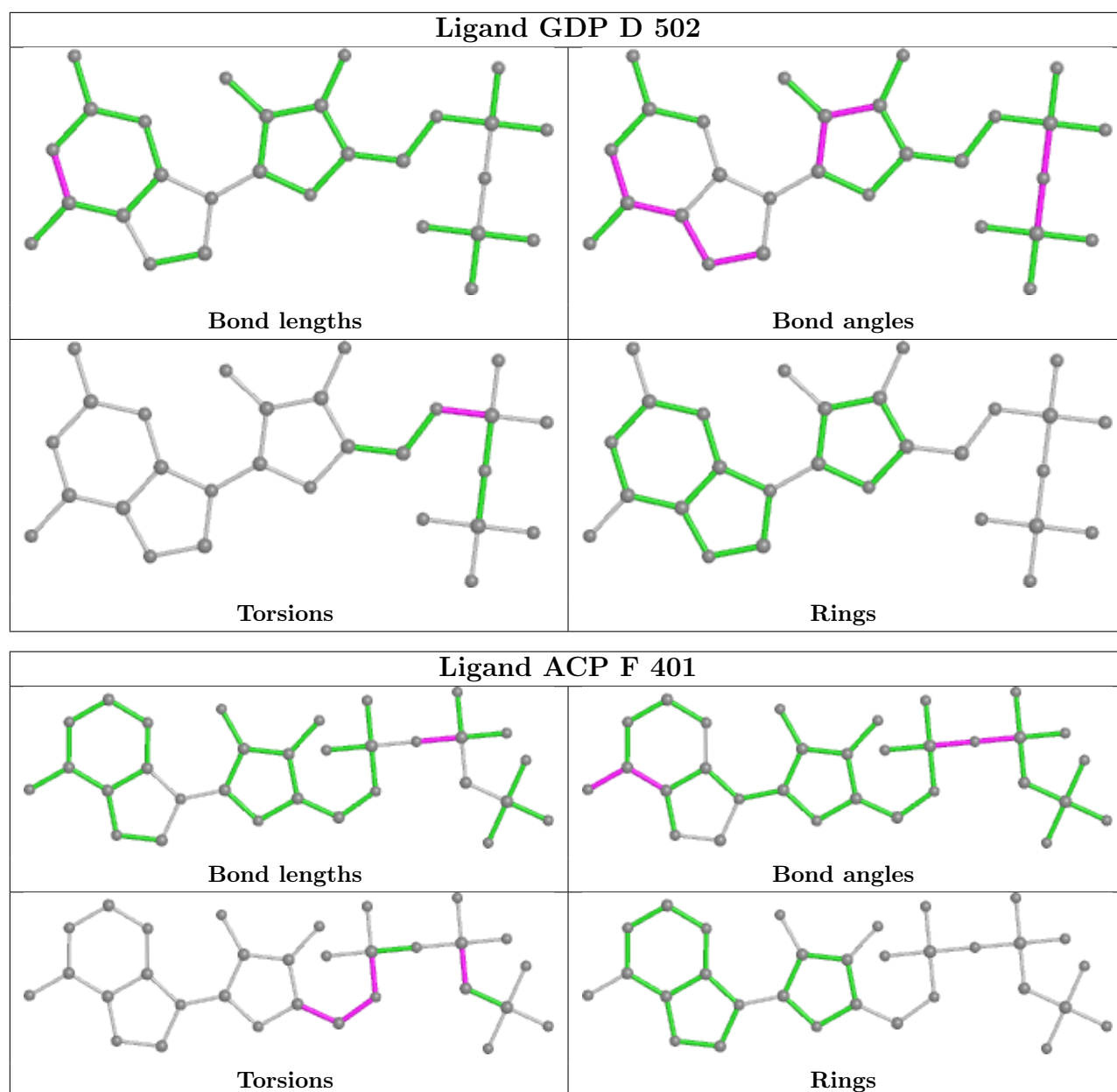
Bond angles

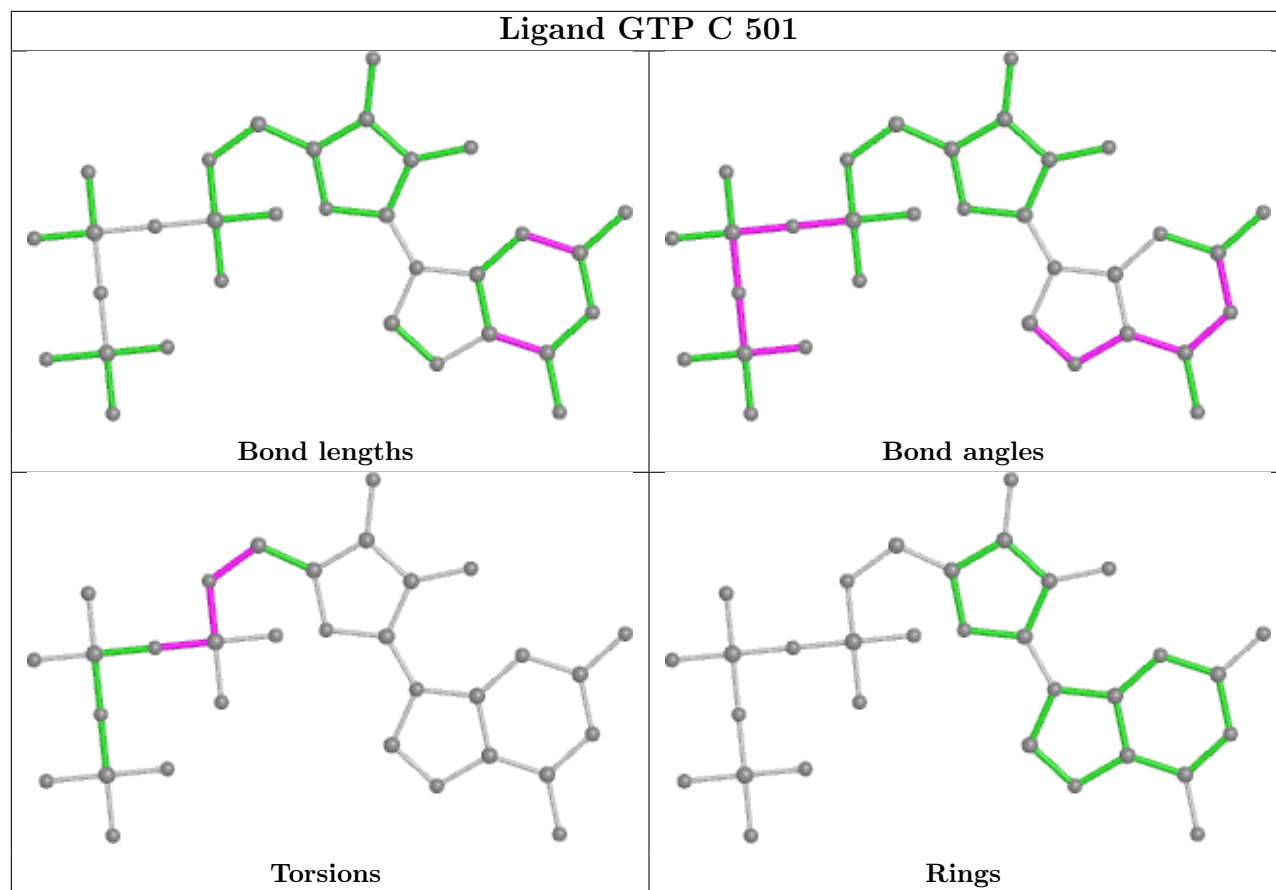


Torsions

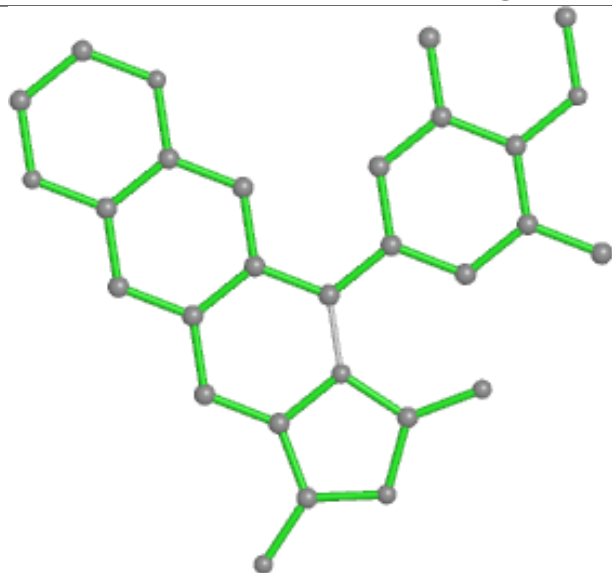


Rings

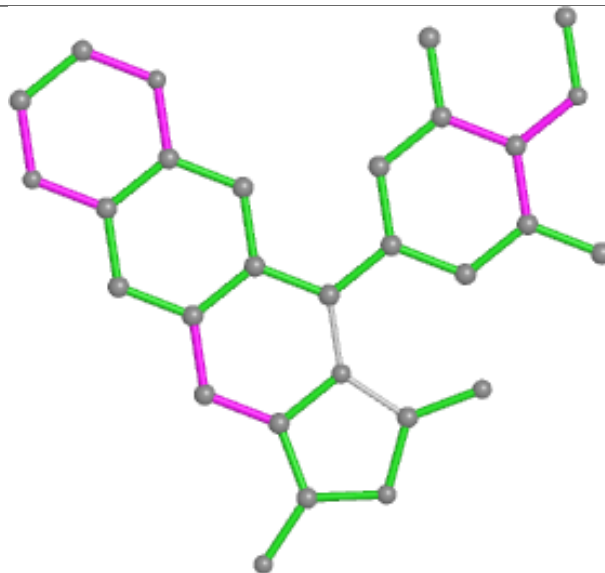




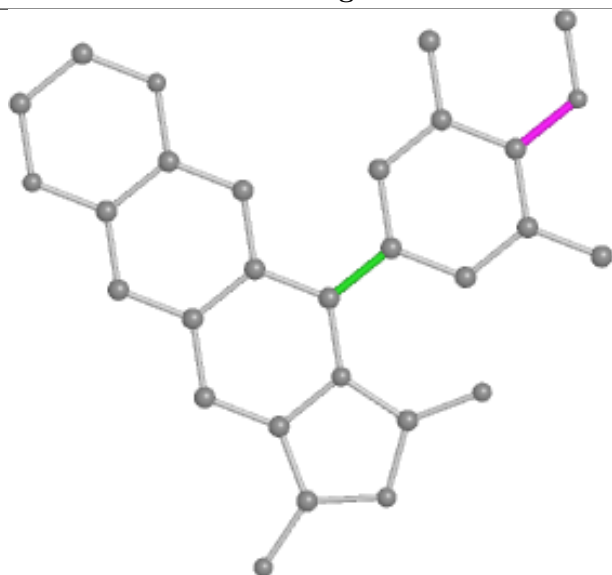
## Ligand A1D62 B 506



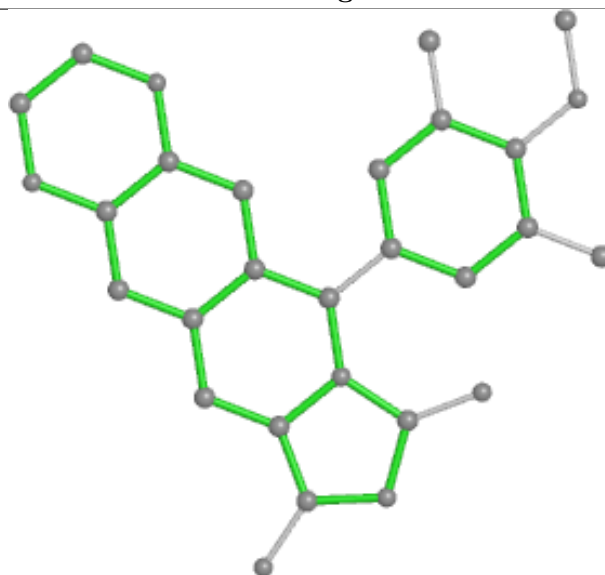
Bond lengths



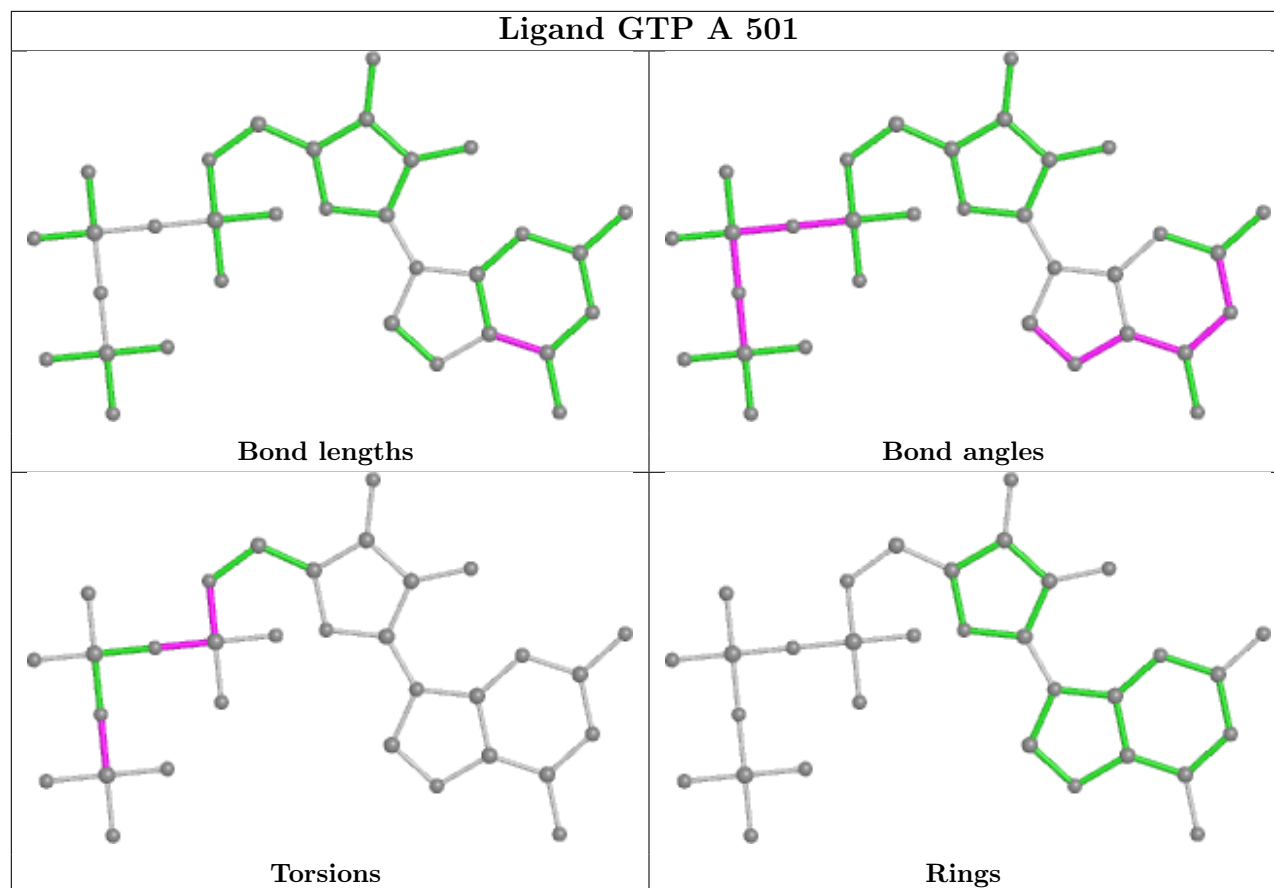
Bond angles



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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	437/450 (97%)	-0.38	3 (0%) 84 85	37, 61, 96, 134	4 (0%)
1	C	440/450 (97%)	-0.58	1 (0%) 92 92	28, 48, 75, 105	7 (1%)
2	B	424/445 (95%)	-0.38	2 (0%) 87 88	27, 57, 96, 136	2 (0%)
2	D	421/445 (94%)	-0.23	5 (1%) 76 78	42, 70, 110, 150	0
3	E	123/143 (86%)	-0.07	1 (0%) 82 84	34, 75, 116, 149	2 (1%)
4	F	346/384 (90%)	0.13	6 (1%) 69 69	37, 91, 154, 175	4 (1%)
All	All	2191/2317 (94%)	-0.29	18 (0%) 82 84	27, 64, 118, 175	19 (0%)

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	428	ALA	3.5
1	A	437	VAL	3.2
2	D	170	MET	2.7
4	F	379	HIS	2.6
1	A	349	THR	2.6

### 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

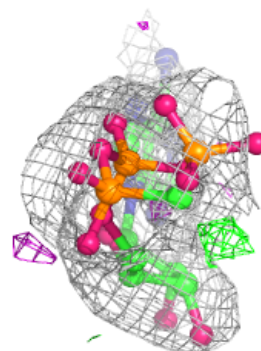
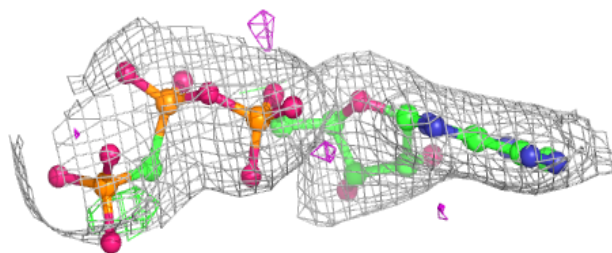
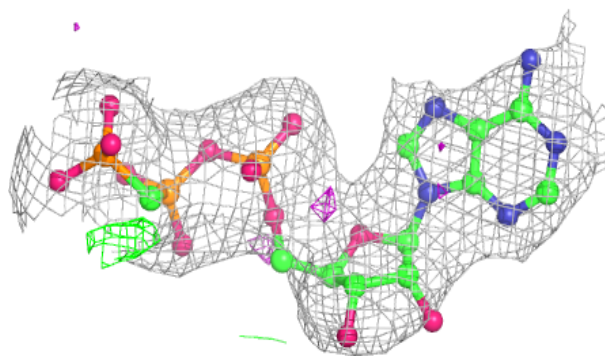
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
11	GOL	B	505	6/6	0.72	0.18	84,94,96,101	0
13	EDO	C	503	4/4	0.84	0.24	61,69,72,75	0
10	MES	B	504	12/12	0.87	0.12	98,102,126,129	0
8	CL	A	504	1/1	0.88	0.10	86,86,86,86	0
14	ACP	F	401	31/31	0.88	0.10	87,100,129,147	0
6	MG	D	503	1/1	0.91	0.12	63,63,63,63	0
12	A1D62	D	504	29/29	0.91	0.16	55,81,119,161	0
12	A1D62	B	506	29/29	0.95	0.12	49,64,96,159	0
9	GDP	D	502	28/28	0.95	0.09	51,64,77,78	0
10	MES	B	503	12/12	0.96	0.07	48,60,72,77	0
5	GTP	A	501	32/32	0.98	0.05	33,46,52,63	0
7	CA	A	503	1/1	0.98	0.03	94,94,94,94	0
5	GTP	C	501	32/32	0.98	0.06	31,38,49,55	0
9	GDP	B	501	28/28	0.98	0.06	31,44,51,55	0
6	MG	D	501	1/1	0.99	0.04	35,35,35,35	0
7	CA	C	502	1/1	0.99	0.03	58,58,58,58	0
6	MG	B	502	1/1	0.99	0.05	50,50,50,50	0
6	MG	A	502	1/1	1.00	0.04	46,46,46,46	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.

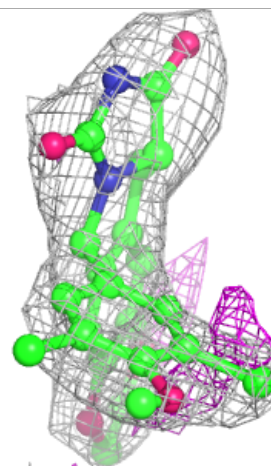
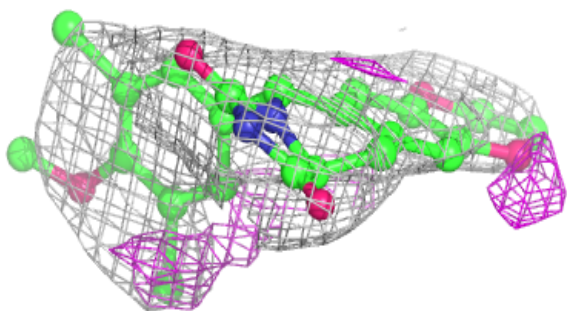
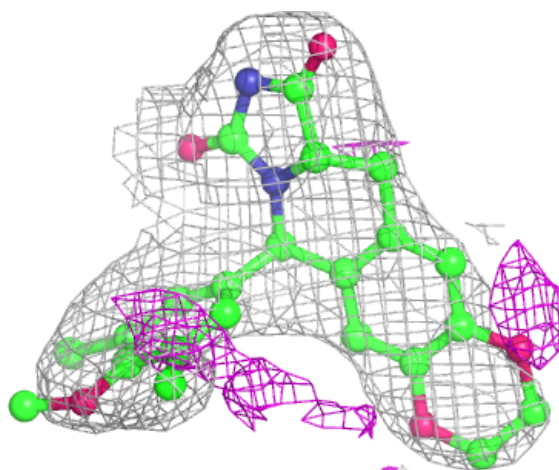
**Electron density around ACP F 401:**

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



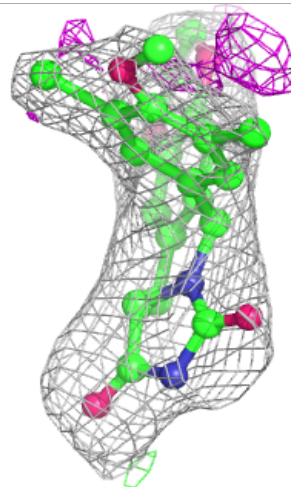
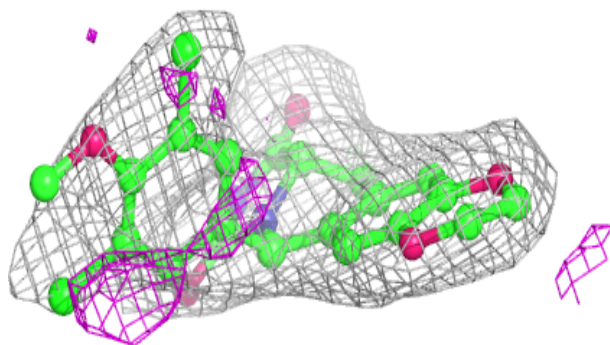
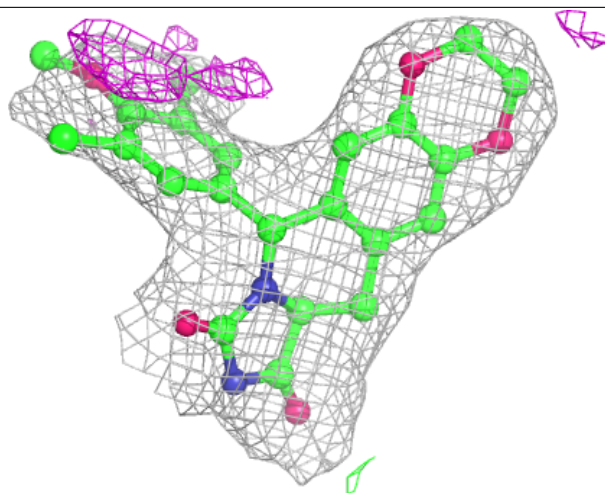
**Electron density around A1D62 D 504:**

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



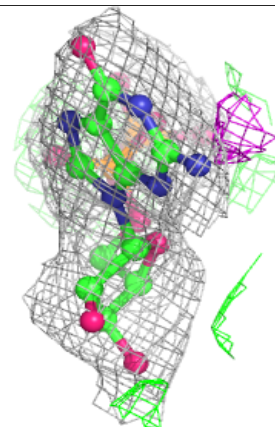
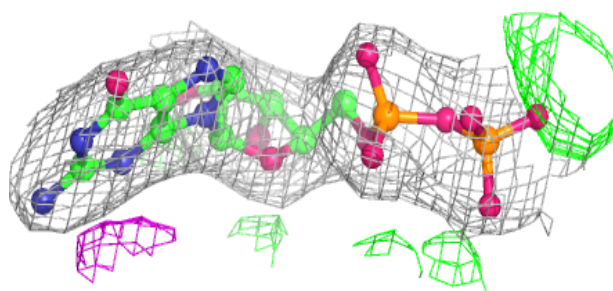
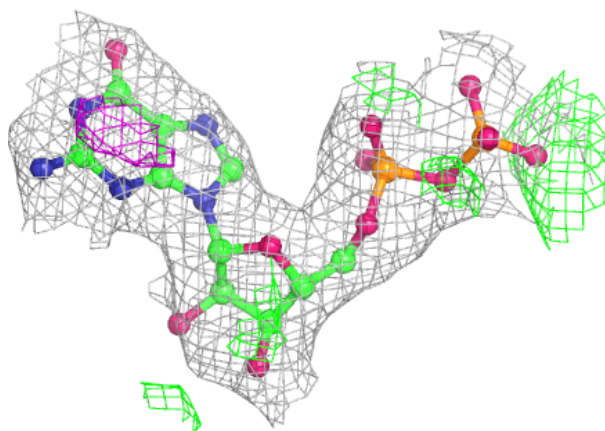
**Electron density around A1D62 B 506:**

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and green (positive)

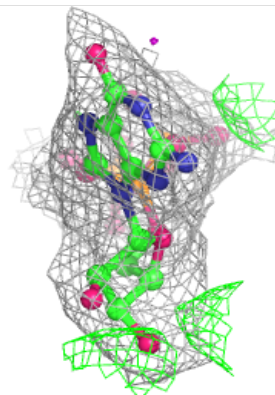
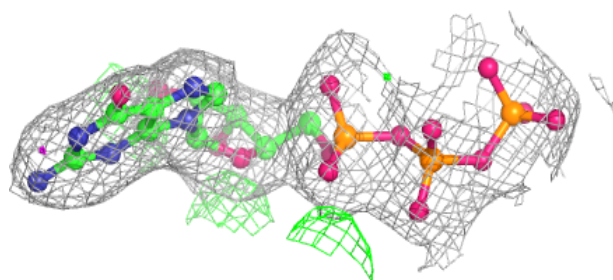
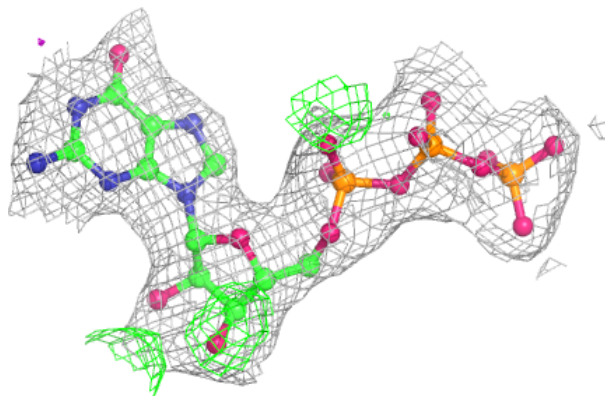


**Electron density around GDP D 502:**

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

**Electron density around GTP A 501:**

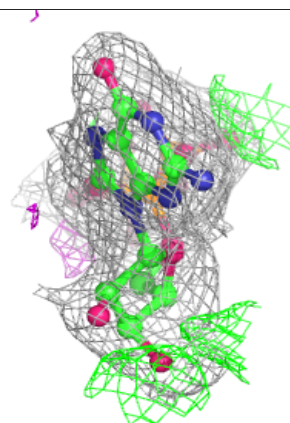
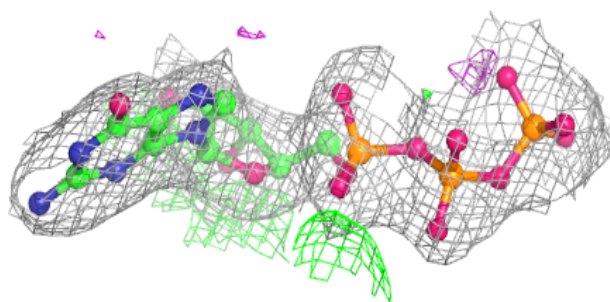
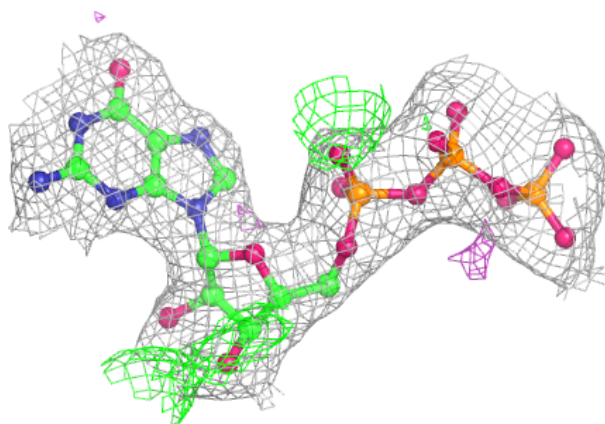
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





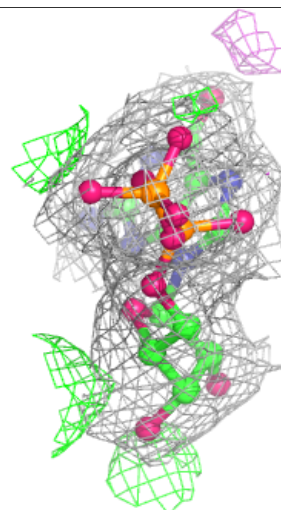
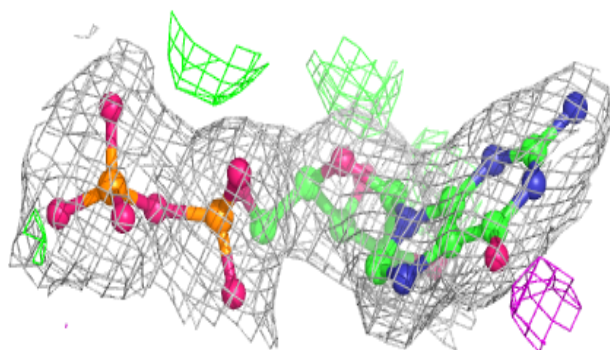
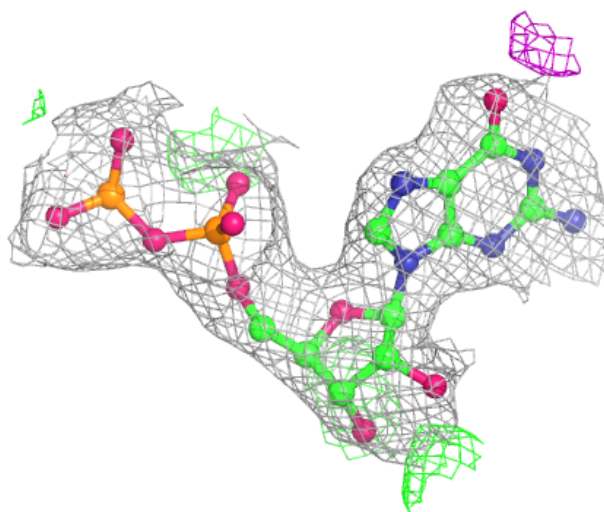
**Electron density around GTP C 501:**

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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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.