



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2022 – 06:38 PM EDT

PDB ID : 4TNZ  
Title : Structure basis of cellular dNTP regulation, SAMHD1-GTP-dATP-dTTP complex  
Authors : Ji, X.; Tang, C.; Zhao, Q.; Wang, W.; Xiong, Y.  
Deposited on : 2014-06-05  
Resolution : 2.38 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

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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) : 1.13  
EDS : 2.27  
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) : 2.27

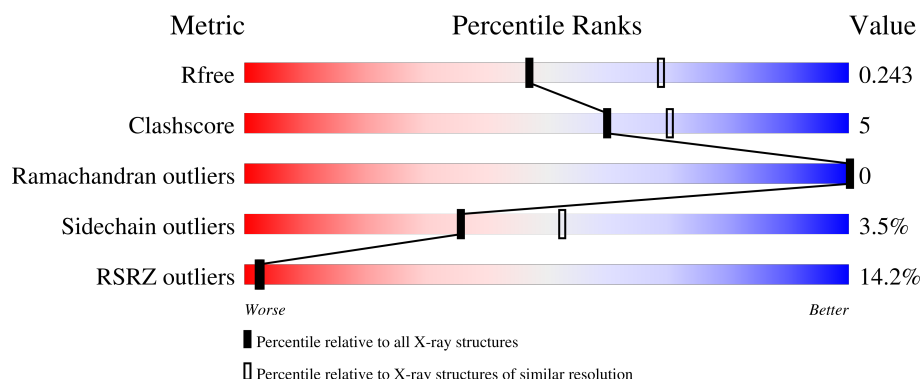
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.38 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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  $\geq 3$ , 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	514	<div> <div>12%</div> <div>83% 10% 7%</div> </div>
1	B	514	<div> <div>22%</div> <div>82% 11% 6%</div> </div>
1	C	514	<div> <div>5%</div> <div>82% 11% 6%</div> </div>
1	D	514	<div> <div>13%</div> <div>82% 10% 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
2	TTP	B	702	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16280 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.

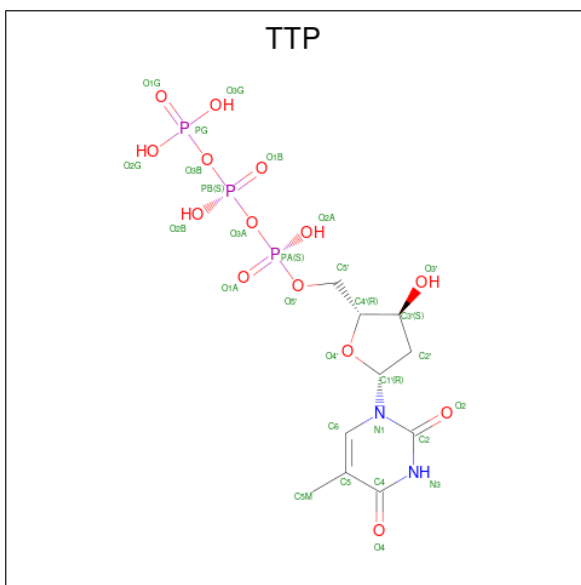
- Molecule 1 is a protein called Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	481	Total	C	N	O	S	0	2	0
			3948	2525	687	715	21			
1	A	480	Total	C	N	O	S	0	2	0
			3940	2521	686	712	21			
1	D	480	Total	C	N	O	S	0	1	0
			3934	2518	684	712	20			
1	B	481	Total	C	N	O	S	0	1	0
			3939	2520	686	712	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
C	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
A	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
A	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
D	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
D	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
B	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
B	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3

- Molecule 2 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula:  $C_{10}H_{17}N_2O_{14}P_3$ ).

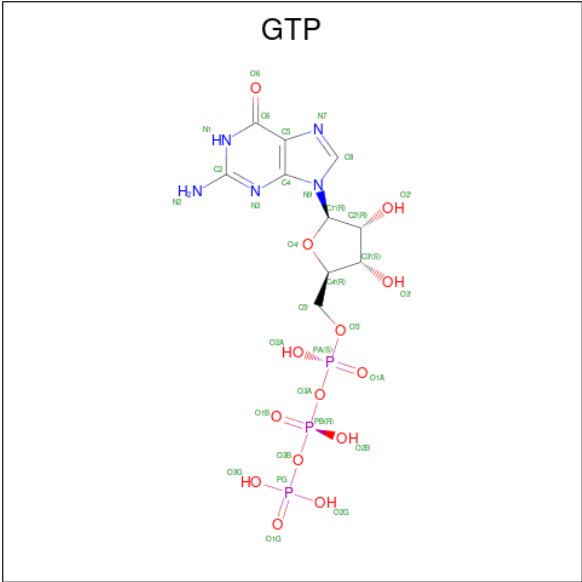


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total 29	C 10	N 2	O 14	P 3	0	0
2	A	1	Total 29	C 10	N 2	O 14	P 3	0	0
2	D	1	Total 29	C 10	N 2	O 14	P 3	0	0
2	B	1	Total 29	C 10	N 2	O 14	P 3	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

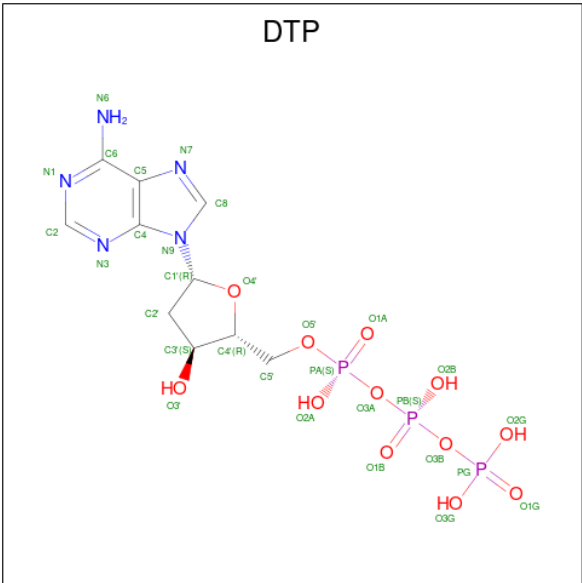
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	2	Total Mg 2 2	0	0
3	A	3	Total Mg 3 3	0	0
3	D	2	Total Mg 2 2	0	0
3	B	1	Total Mg 1 1	0	0

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{14}\text{P}_3$ ).



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

- Molecule 5 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
5	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
5	D	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
5	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

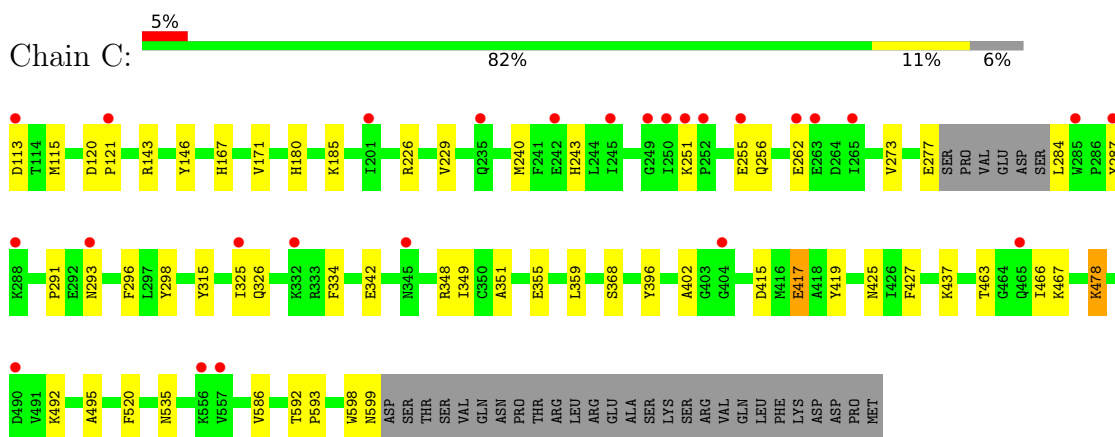
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	53	Total	O	0	0
			53	53		
6	A	47	Total	O	0	0
			47	47		
6	D	32	Total	O	0	0
			32	32		
6	B	15	Total	O	0	0
			15	15		

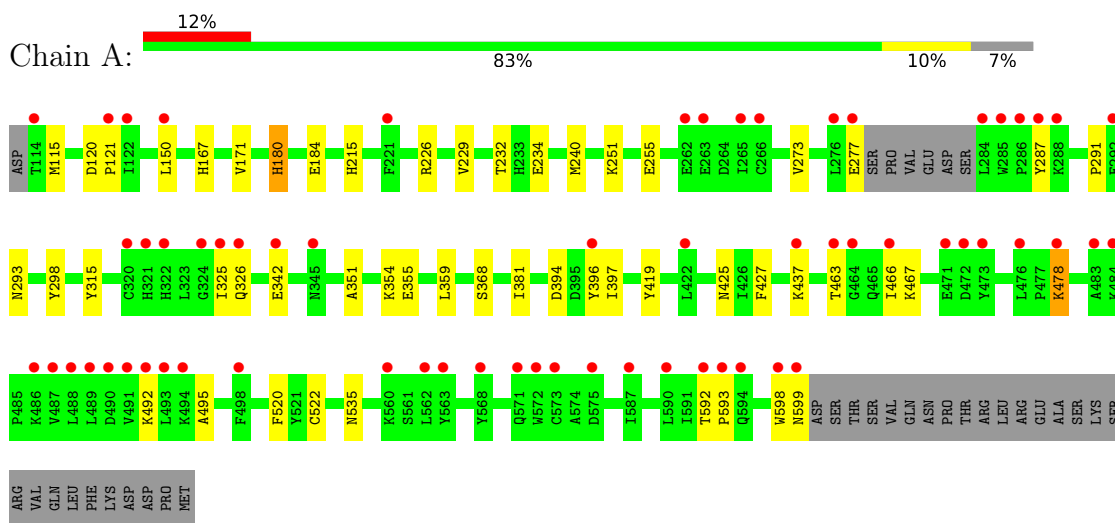
### 3 Residue-property plots

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

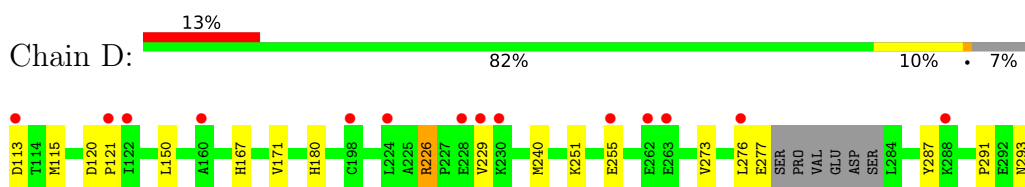
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

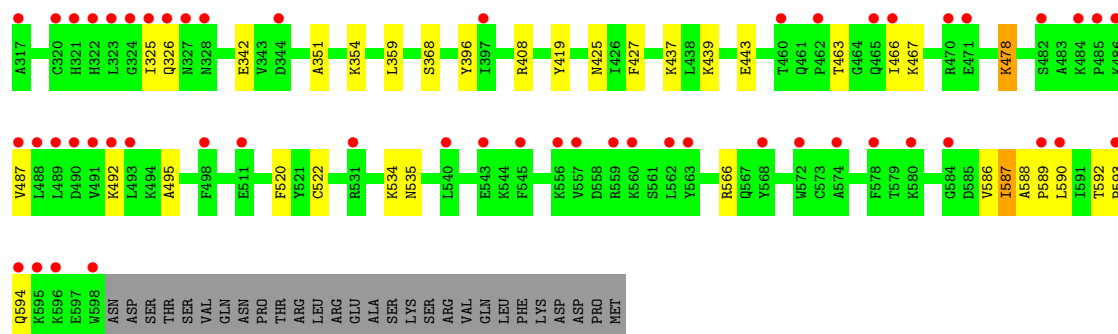


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

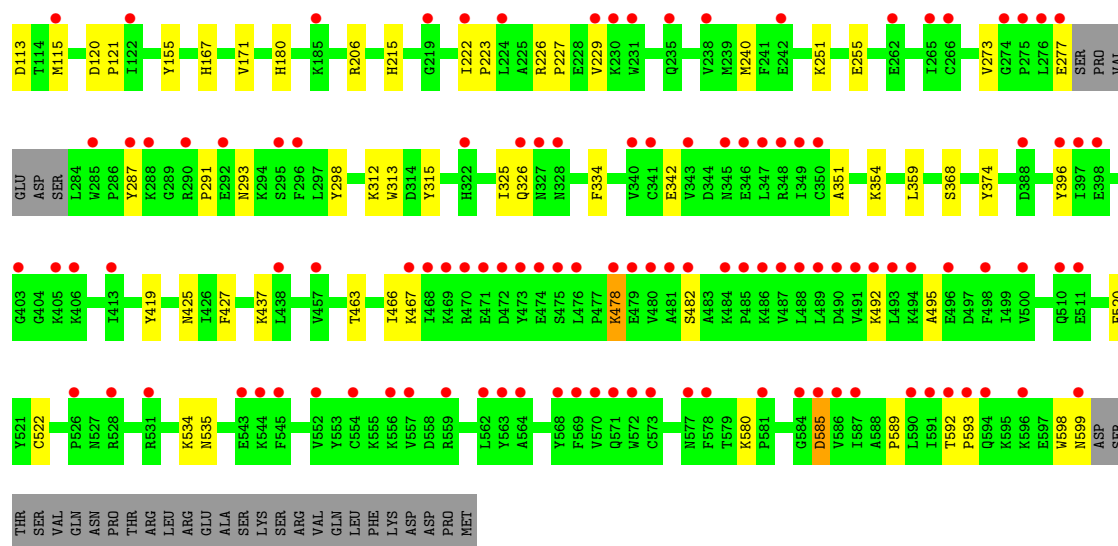
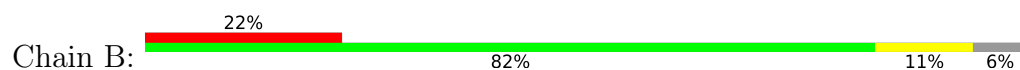


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





● Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.13Å 141.75Å 98.47Å 90.00° 116.29° 90.00°	Depositor
Resolution (Å)	88.29 – 2.38 48.74 – 2.38	Depositor EDS
% Data completeness (in resolution range)	98.4 (88.29-2.38) 98.4 (48.74-2.38)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.212 , 0.243 0.212 , 0.243	Depositor DCC
$R_{free}$ test set	4158 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.9	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 58.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16280	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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: MG, GTP, DTP, TTP

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	0.59	0/4032	0.69	0/5442
1	B	0.54	0/4031	0.68	1/5441 (0.0%)
1	C	0.62	0/4040	0.70	0/5453
1	D	0.58	0/4026	0.68	1/5434 (0.0%)
All	All	0.58	0/16129	0.69	2/21770 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	585	ASP	CB-CG-OD1	7.34	124.91	118.30
1	D	226	ARG	NE-CZ-NH2	5.10	122.85	120.30

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	3940	0	3926	31	0
1	B	3939	0	3925	37	0
1	C	3948	0	3930	40	0
1	D	3934	0	3920	44	0
2	A	29	0	13	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	29	0	13	9	0
2	C	29	0	13	1	0
2	D	29	0	13	3	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	32	0	12	0	0
4	B	32	0	12	0	0
4	C	32	0	12	1	0
4	D	32	0	12	0	0
5	A	30	0	12	1	0
5	B	30	0	12	1	0
5	C	30	0	12	0	0
5	D	30	0	12	1	0
6	A	47	0	0	3	0
6	B	15	0	0	1	0
6	C	53	0	0	7	0
6	D	32	0	0	2	0
All	All	16280	0	15849	148	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 5.

All (148) 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:D:566:ARG:CG	1:D:587:ILE:HD11	1.71	1.20
1:D:566:ARG:HG2	1:D:587:ILE:HD11	1.25	1.12
1:D:566:ARG:CB	1:D:587:ILE:HD11	1.82	1.10
1:D:566:ARG:HB3	1:D:587:ILE:CD1	1.88	1.04
1:D:566:ARG:HB3	1:D:587:ILE:HD11	1.45	0.95
1:D:588:ALA:O	1:D:592:THR:HG23	1.66	0.95
1:C:415:ASP:OD2	1:C:417:GLU:HG2	1.73	0.89
1:B:312:LYS:NZ	2:B:702:TTP:O1G	2.06	0.88
1:C:415:ASP:CG	1:C:417:GLU:HG2	1.97	0.84
1:D:408:ARG:HD2	6:D:831:HOH:O	1.86	0.75
1:D:566:ARG:HG2	1:D:587:ILE:CD1	2.11	0.74
1:D:589:PRO:O	1:D:593:PRO:HD3	1.88	0.73
1:C:415:ASP:OD1	1:C:417:GLU:HG2	1.90	0.70
1:A:355:GLU:OE1	6:A:822:HOH:O	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402:ALA:HB2	1:C:417:GLU:HG3	1.72	0.70
1:A:226:ARG:O	1:A:229:VAL:HG12	1.93	0.69
1:D:226:ARG:O	1:D:229:VAL:HG12	1.93	0.68
1:B:226:ARG:O	1:B:229:VAL:HG12	1.93	0.68
1:B:291:PRO:HG2	1:B:293:ASN:OD1	1.94	0.68
1:C:326:GLN:HG2	1:A:326:GLN:HG2	1.76	0.68
1:A:150:LEU:CD2	2:A:703:TTP:H2'1	2.23	0.68
1:C:226:ARG:O	1:C:229:VAL:HG12	1.94	0.67
1:C:417:GLU:H	1:C:417:GLU:CD	1.97	0.67
1:D:326:GLN:HG2	1:B:326:GLN:HG2	1.76	0.67
1:C:291:PRO:HG2	1:C:293:ASN:OD1	1.94	0.66
1:A:291:PRO:HG2	1:A:293:ASN:OD1	1.96	0.66
1:D:291:PRO:HG2	1:D:293:ASN:OD1	1.96	0.66
1:C:120:ASP:OD1	1:C:121:PRO:HD2	1.96	0.65
1:D:590:LEU:O	1:D:593:PRO:HD2	1.95	0.65
1:D:592:THR:N	1:D:593:PRO:CD	2.61	0.64
1:C:415:ASP:OD1	1:C:417:GLU:CG	2.46	0.64
1:B:120:ASP:OD1	1:B:121:PRO:HD2	1.98	0.64
1:D:120:ASP:OD1	1:D:121:PRO:HD2	1.98	0.64
1:B:589:PRO:O	1:B:593:PRO:HD3	1.98	0.64
1:D:566:ARG:CG	1:D:587:ILE:CD1	2.63	0.63
1:A:120:ASP:OD1	1:A:121:PRO:HD2	1.99	0.63
1:C:417:GLU:N	1:C:417:GLU:OE2	2.31	0.62
1:C:586:VAL:HG11	1:A:522[A]:CYS:SG	2.39	0.62
1:B:312:LYS:CE	2:B:702:TTP:O1G	2.48	0.61
1:C:348:ARG:HD3	6:C:835:HOH:O	2.00	0.61
1:C:262:GLU:HG3	6:C:843:HOH:O	2.01	0.60
1:D:566:ARG:HD3	1:D:587:ILE:CG1	2.31	0.60
1:C:425:ASN:OD1	1:B:425:ASN:OD1	2.19	0.59
1:D:566:ARG:HB3	1:D:587:ILE:HD13	1.80	0.59
1:C:355:GLU:OE1	6:C:849:HOH:O	2.17	0.58
1:A:287:TYR:CD1	1:A:298:TYR:CE1	2.93	0.57
1:B:287:TYR:CD1	1:B:298:TYR:CE1	2.93	0.57
1:B:206:ARG:NH2	2:B:702:TTP:O2B	2.38	0.56
1:C:287:TYR:CD1	1:C:298:TYR:CE1	2.95	0.55
1:B:215:HIS:CE1	2:B:702:TTP:O2A	2.59	0.55
1:D:240:MET:CE	1:D:419:TYR:HD2	2.21	0.53
1:B:313:TRP:CZ2	1:B:334:PHE:HD1	2.27	0.53
1:D:589:PRO:O	1:D:593:PRO:CD	2.55	0.53
1:C:240:MET:CE	1:C:419:TYR:HD2	2.23	0.52
1:A:240:MET:CE	1:A:419:TYR:HD2	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:ASP:OD1	1:C:417:GLU:OE1	2.27	0.52
1:D:287:TYR:CD1	1:D:298:TYR:CE1	2.98	0.52
1:B:374:TYR:O	2:B:702:TTP:HM52	2.10	0.52
1:C:592:THR:N	1:C:593:PRO:CD	2.73	0.51
1:A:167:HIS:O	1:A:171:VAL:HG23	2.10	0.51
1:D:167:HIS:O	1:D:171:VAL:HG23	2.10	0.51
1:C:167:HIS:O	1:C:171:VAL:HG23	2.10	0.51
1:A:592:THR:N	1:A:593:PRO:CD	2.73	0.51
1:B:592:THR:N	1:B:593:PRO:CD	2.73	0.51
1:B:240:MET:CE	1:B:419:TYR:HD2	2.24	0.51
1:B:167:HIS:O	1:B:171:VAL:HG23	2.11	0.51
1:A:397:ILE:HB	6:A:832:HOH:O	2.10	0.51
1:B:312:LYS:HE3	2:B:702:TTP:O1G	2.11	0.50
1:C:185:LYS:HD2	6:C:839:HOH:O	2.11	0.50
1:D:586:VAL:HG11	1:B:522[A]:CYS:SG	2.51	0.50
1:B:215:HIS:NE2	2:B:702:TTP:O5'	2.40	0.50
1:C:334:PHE:HA	6:C:849:HOH:O	2.12	0.50
1:C:256:GLN:HG3	6:C:801:HOH:O	2.12	0.49
1:A:598:TRP:O	1:A:599:ASN:HB2	2.12	0.49
2:B:702:TTP:O3G	2:B:702:TTP:O1B	2.29	0.49
1:B:589:PRO:O	1:B:593:PRO:CD	2.61	0.48
1:A:354:LYS:NZ	5:A:701:DTP:O1A	2.45	0.48
1:B:580:LYS:CE	1:B:585:ASP:OD2	2.62	0.48
1:C:415:ASP:OD1	1:C:417:GLU:CD	2.52	0.48
1:A:425:ASN:OD1	1:D:425:ASN:OD1	2.30	0.48
1:D:315:TYR:CE2	2:D:702:TTP:H5'1	2.49	0.47
1:C:417:GLU:CD	1:C:417:GLU:N	2.67	0.47
2:D:702:TTP:O2G	2:D:702:TTP:O2B	2.32	0.47
1:B:313:TRP:CZ2	1:B:334:PHE:CD1	3.02	0.47
1:A:396:TYR:CD1	1:A:437:LYS:HD2	2.50	0.47
1:D:354:LYS:NZ	5:D:705:DTP:O1A	2.48	0.47
1:B:478:LYS:HE2	1:B:495:ALA:HB1	1.98	0.46
1:B:463:THR:O	1:B:466:ILE:HG12	2.15	0.46
1:B:396:TYR:CD1	1:B:437:LYS:HD2	2.50	0.46
1:A:215:HIS:NE2	2:A:703:TTP:O5'	2.49	0.46
1:A:463:THR:O	1:A:466:ILE:HG12	2.16	0.46
1:D:478:LYS:HE2	1:D:495:ALA:HB1	1.98	0.46
1:D:592:THR:N	1:D:593:PRO:HD3	2.30	0.46
1:A:478:LYS:HE2	1:A:495:ALA:HB1	1.98	0.46
1:D:463:THR:O	1:D:466:ILE:HG12	2.16	0.46
1:C:251:LYS:O	1:C:255:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:396:TYR:CD1	1:D:437:LYS:HD2	2.51	0.45
1:C:478:LYS:HE2	1:C:495:ALA:HB1	1.98	0.45
4:C:703:GTP:O1B	4:C:703:GTP:O1A	2.33	0.45
1:A:287:TYR:HB3	1:A:298:TYR:OH	2.17	0.45
1:D:251:LYS:O	1:D:255:GLU:HG3	2.16	0.45
1:B:598:TRP:O	1:B:599:ASN:HB2	2.17	0.45
1:C:396:TYR:CD1	1:C:437:LYS:HD2	2.52	0.45
1:D:566:ARG:HD3	1:D:587:ILE:HG13	1.97	0.45
1:A:251:LYS:O	1:A:255:GLU:HG3	2.17	0.44
1:C:463:THR:O	1:C:466:ILE:HG12	2.17	0.44
1:B:580:LYS:NZ	1:B:585:ASP:OD2	2.50	0.44
1:D:487:VAL:HG22	1:D:590:LEU:CD1	2.48	0.44
1:B:251:LYS:O	1:B:255:GLU:HG3	2.17	0.44
1:D:276:LEU:C	6:D:830:HOH:O	2.56	0.44
1:B:215:HIS:HE1	2:B:702:TTP:O2A	2.01	0.44
1:D:287:TYR:HB3	1:D:298:TYR:OH	2.18	0.43
1:B:427:PHE:CD1	1:B:427:PHE:C	2.92	0.43
1:C:243:HIS:CE1	1:C:417:GLU:OE2	2.71	0.43
1:C:325:ILE:CG2	1:C:326:GLN:N	2.81	0.43
1:D:566:ARG:CB	1:D:587:ILE:CD1	2.57	0.43
1:B:287:TYR:HB3	1:B:298:TYR:OH	2.17	0.43
1:C:287:TYR:HB3	1:C:298:TYR:OH	2.18	0.43
1:A:215:HIS:HE2	2:A:703:TTP:PA	2.42	0.43
1:C:598:TRP:O	1:C:599:ASN:HB2	2.18	0.43
1:D:351:ALA:O	1:D:520:PHE:HA	2.18	0.43
1:D:487:VAL:HG22	1:D:590:LEU:HD12	2.01	0.43
1:A:351:ALA:O	1:A:520:PHE:HA	2.19	0.42
2:C:701:TTP:O2G	2:C:701:TTP:O1B	2.36	0.42
1:D:150:LEU:CD2	2:D:702:TTP:H2'1	2.50	0.42
1:B:351:ALA:O	1:B:520:PHE:HA	2.19	0.42
1:C:143:ARG:HD3	6:C:833:HOH:O	2.20	0.42
1:A:150:LEU:HD22	2:A:703:TTP:H2'1	1.99	0.42
1:B:354:LYS:NZ	5:B:701:DTP:O2A	2.53	0.42
1:A:232:THR:HB	1:A:234:GLU:OE1	2.19	0.42
1:A:381:ILE:HD12	1:A:381:ILE:HA	1.94	0.42
1:D:427:PHE:CD1	1:D:427:PHE:C	2.93	0.42
1:D:566:ARG:HD3	1:D:587:ILE:HG12	2.00	0.42
1:B:325:ILE:CG2	1:B:326:GLN:N	2.82	0.41
1:C:326:GLN:CG	1:A:326:GLN:HG2	2.48	0.41
1:C:351:ALA:O	1:C:520:PHE:HA	2.20	0.41
1:A:325:ILE:CG2	1:A:326:GLN:N	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:439:LYS:O	1:D:443:GLU:HG2	2.20	0.41
1:B:222:ILE:HB	1:B:223:PRO:HD3	2.02	0.41
1:D:325:ILE:CG2	1:D:326:GLN:N	2.83	0.41
1:A:427:PHE:CD1	1:A:427:PHE:C	2.94	0.41
1:A:394:ASP:HA	6:A:832:HOH:O	2.21	0.41
1:B:482:SER:C	6:B:814:HOH:O	2.59	0.41
1:C:146:TYR:HH	1:B:155:TYR:HH	1.69	0.41
1:C:427:PHE:CD1	1:C:427:PHE:C	2.94	0.41
1:A:180:HIS:O	1:A:184:GLU:HG2	2.20	0.40
1:D:592:THR:OG1	1:D:593:PRO:HD3	2.22	0.40
1:C:296:PHE:HB2	1:C:349:ILE:HG13	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	478/514 (93%)	470 (98%)	8 (2%)	0	100	100
1	B	478/514 (93%)	469 (98%)	9 (2%)	0	100	100
1	C	479/514 (93%)	471 (98%)	8 (2%)	0	100	100
1	D	477/514 (93%)	468 (98%)	9 (2%)	0	100	100
All	All	1912/2056 (93%)	1878 (98%)	34 (2%)	0	100	100

There are no Ramachandran outliers to report.

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

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	428/459 (93%)	416 (97%)	12 (3%)	43	61
1	B	428/459 (93%)	413 (96%)	15 (4%)	36	52
1	C	429/459 (94%)	414 (96%)	15 (4%)	36	52
1	D	427/459 (93%)	410 (96%)	17 (4%)	31	47
All	All	1712/1836 (93%)	1653 (97%)	59 (3%)	36	53

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	113	ASP
1	C	115	MET
1	C	180	HIS
1	C	273	VAL
1	C	277	GLU
1	C	284	LEU
1	C	315	TYR
1	C	342	GLU
1	C	359	LEU
1	C	368	SER
1	C	417	GLU
1	C	467	LYS
1	C	478	LYS
1	C	492	LYS
1	C	535	ASN
1	A	115	MET
1	A	180	HIS
1	A	273	VAL
1	A	277	GLU
1	A	315	TYR
1	A	342	GLU
1	A	359	LEU
1	A	368	SER
1	A	467	LYS
1	A	478	LYS
1	A	492	LYS
1	A	535	ASN
1	D	113	ASP
1	D	115	MET
1	D	180	HIS

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Mol	Chain	Res	Type
1	D	273	VAL
1	D	277	GLU
1	D	315	TYR
1	D	342	GLU
1	D	359	LEU
1	D	368	SER
1	D	467	LYS
1	D	478	LYS
1	D	492	LYS
1	D	522	CYS
1	D	534	LYS
1	D	535	ASN
1	D	587	ILE
1	D	594	GLN
1	B	113	ASP
1	B	115	MET
1	B	180	HIS
1	B	227	PRO
1	B	273	VAL
1	B	277	GLU
1	B	315	TYR
1	B	342	GLU
1	B	359	LEU
1	B	368	SER
1	B	467	LYS
1	B	478	LYS
1	B	492	LYS
1	B	534	LYS
1	B	535	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	235	GLN
1	C	243	HIS
1	C	364	HIS
1	A	235	GLN
1	A	364	HIS
1	D	235	GLN
1	D	364	HIS
1	D	571	GLN
1	D	594	GLN

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Mol	Chain	Res	Type
1	B	235	GLN
1	B	243	HIS
1	B	364	HIS

### 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 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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
4	GTP	A	705	3	26,34,34	1.01	1 (3%)	33,54,54	2.32	17 (51%)
4	GTP	B	704	3	26,34,34	1.23	2 (7%)	33,54,54	2.14	12 (36%)
5	DTP	A	701	3	26,32,32	1.30	5 (19%)	30,50,50	1.35	5 (16%)
5	DTP	D	705	3	26,32,32	0.95	1 (3%)	30,50,50	1.52	7 (23%)
2	TTP	A	703	3	23,30,30	1.25	3 (13%)	29,47,47	1.89	4 (13%)
4	GTP	D	704	3	26,34,34	1.36	3 (11%)	33,54,54	2.50	14 (42%)
2	TTP	C	701	3	23,30,30	1.14	1 (4%)	29,47,47	1.83	5 (17%)
5	DTP	B	701	3	26,32,32	1.21	3 (11%)	30,50,50	1.19	3 (10%)
5	DTP	C	704	3	26,32,32	0.94	1 (3%)	30,50,50	1.33	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GTP	C	703	3	26,34,34	1.28	2 (7%)	33,54,54	2.26	10 (30%)
2	TTP	B	702	3	23,30,30	1.12	1 (4%)	29,47,47	2.24	5 (17%)
2	TTP	D	702	3	23,30,30	0.90	1 (4%)	29,47,47	1.86	5 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	A	705	3	-	6/18/38/38	0/3/3/3
4	GTP	B	704	3	-	3/18/38/38	0/3/3/3
5	DTP	A	701	3	-	5/18/34/34	0/3/3/3
5	DTP	D	705	3	-	6/18/34/34	0/3/3/3
2	TTP	A	703	3	-	5/19/34/34	0/2/2/2
4	GTP	D	704	3	-	6/18/38/38	0/3/3/3
2	TTP	C	701	3	-	5/19/34/34	0/2/2/2
5	DTP	B	701	3	-	2/18/34/34	0/3/3/3
5	DTP	C	704	3	-	2/18/34/34	0/3/3/3
4	GTP	C	703	3	-	5/18/38/38	0/3/3/3
2	TTP	B	702	3	-	4/19/34/34	0/2/2/2
2	TTP	D	702	3	-	7/19/34/34	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	702	TTP	C5-C4	4.45	1.51	1.41
2	A	703	TTP	C5-C4	3.89	1.49	1.41
4	D	704	GTP	C5-C6	3.86	1.48	1.41
2	C	701	TTP	C5-C4	3.57	1.49	1.41
4	B	704	GTP	C5-C6	3.33	1.47	1.41
4	C	703	GTP	C5-C6	3.22	1.46	1.41
4	D	704	GTP	C2'-C1'	-3.05	1.49	1.53
5	A	701	DTP	O4'-C4'	-3.02	1.38	1.45
5	B	701	DTP	C5-C4	2.93	1.48	1.40
5	A	701	DTP	O4'-C1'	2.81	1.48	1.42
4	A	705	GTP	O4'-C1'	2.80	1.45	1.41
2	D	702	TTP	C5-C4	2.75	1.47	1.41
4	C	703	GTP	O4'-C1'	2.68	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	705	DTP	C5-C4	2.43	1.47	1.40
4	B	704	GTP	C5-C4	2.28	1.47	1.40
4	D	704	GTP	C5-C4	2.17	1.46	1.40
5	A	701	DTP	C2-N1	2.15	1.37	1.33
5	A	701	DTP	PA-O2A	-2.14	1.45	1.55
2	A	703	TTP	C2-N3	-2.12	1.34	1.38
2	A	703	TTP	PG-O2G	-2.11	1.46	1.54
5	B	701	DTP	PG-O2G	-2.09	1.46	1.54
5	A	701	DTP	C2-N3	2.07	1.35	1.32
5	C	704	DTP	C4-N3	-2.06	1.32	1.35
5	B	701	DTP	PG-O3G	-2.02	1.47	1.54

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	702	TTP	PB-O3B-PG	-6.99	108.83	132.83
4	D	704	GTP	C5-C6-N1	-6.11	115.08	123.43
2	D	702	TTP	C2-N3-C4	6.08	120.28	115.14
2	B	702	TTP	C2-N3-C4	5.75	120.00	115.14
2	B	702	TTP	PB-O3A-PA	-5.41	114.26	132.83
4	B	704	GTP	C5-C6-N1	-5.31	116.17	123.43
4	D	704	GTP	C2-N1-C6	5.22	124.22	115.93
2	A	703	TTP	PB-O3B-PG	-5.13	115.21	132.83
2	C	701	TTP	C2-N3-C4	5.04	119.40	115.14
4	A	705	GTP	C5-C6-N1	-4.89	116.74	123.43
4	C	703	GTP	C2-N3-C4	4.86	120.91	115.36
4	D	704	GTP	C3'-C2'-C1'	4.78	108.18	100.98
4	C	703	GTP	PA-O3A-PB	-4.74	116.57	132.83
2	A	703	TTP	C2-N3-C4	4.67	119.08	115.14
4	C	703	GTP	C4-C5-C6	-4.47	116.53	120.80
2	C	701	TTP	PB-O3A-PA	-4.43	117.62	132.83
4	B	704	GTP	C2-N1-C6	4.41	122.94	115.93
4	B	704	GTP	PA-O3A-PB	-4.37	117.84	132.83
4	A	705	GTP	PA-O3A-PB	-4.26	118.19	132.83
2	D	702	TTP	PB-O3B-PG	-4.21	118.37	132.83
2	D	702	TTP	PB-O3A-PA	-4.11	118.71	132.83
2	A	703	TTP	PB-O3A-PA	-4.09	118.80	132.83
2	C	701	TTP	PB-O3B-PG	-4.00	119.10	132.83
4	A	705	GTP	C2-N1-C6	3.98	122.25	115.93
4	C	703	GTP	C2-N1-C6	3.81	121.98	115.93
4	D	704	GTP	C2-N3-C4	3.66	119.54	115.36
4	C	703	GTP	O3G-PG-O2G	3.60	121.41	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	705	GTP	N2-C2-N1	3.57	122.80	117.25
5	C	704	DTP	N3-C2-N1	-3.54	123.15	128.68
4	D	704	GTP	PA-O3A-PB	-3.52	120.75	132.83
2	A	703	TTP	C5-C6-N1	-3.46	118.47	122.19
4	A	705	GTP	O2G-PG-O3B	3.45	116.19	104.64
4	D	704	GTP	O2G-PG-O3B	3.41	116.06	104.64
4	C	703	GTP	N3-C2-N1	-3.35	122.75	127.22
4	D	704	GTP	O4'-C1'-C2'	-3.35	102.03	106.93
4	C	703	GTP	C5-C6-N1	-3.33	118.88	123.43
2	B	702	TTP	C5-C6-N1	-3.31	118.62	122.19
4	B	704	GTP	C4-C5-C6	-3.30	117.64	120.80
4	C	703	GTP	C3'-C2'-C1'	3.25	105.87	100.98
5	D	705	DTP	PB-O3B-PG	-3.18	121.90	132.83
4	D	704	GTP	C4-C5-N7	-3.16	106.11	109.40
4	D	704	GTP	N3-C2-N1	-3.15	123.02	127.22
5	D	705	DTP	O3G-PG-O2G	3.12	119.58	107.64
4	B	704	GTP	C3'-C2'-C1'	3.09	105.63	100.98
4	B	704	GTP	C2-N3-C4	3.05	118.84	115.36
4	B	704	GTP	PB-O3B-PG	-3.03	122.43	132.83
4	A	705	GTP	C3'-C2'-C1'	2.98	105.46	100.98
2	D	702	TTP	C5-C6-N1	-2.95	119.01	122.19
4	A	705	GTP	O3B-PG-O1G	-2.94	94.89	111.19
2	C	701	TTP	C5-C6-N1	-2.92	119.05	122.19
4	B	704	GTP	O3G-PG-O2G	2.91	118.76	107.64
4	D	704	GTP	O5'-PA-O1A	-2.91	97.71	109.07
4	B	704	GTP	C4-C5-N7	-2.90	106.37	109.40
4	D	704	GTP	O3B-PG-O1G	-2.86	95.34	111.19
4	C	703	GTP	PB-O3B-PG	-2.84	123.08	132.83
5	A	701	DTP	PB-O3B-PG	-2.75	123.39	132.83
4	A	705	GTP	N3-C2-N1	-2.74	123.56	127.22
4	A	705	GTP	C4-C5-N7	-2.73	106.55	109.40
4	B	704	GTP	N3-C2-N1	-2.73	123.58	127.22
5	B	701	DTP	O3G-PG-O1G	2.70	121.24	110.68
4	A	705	GTP	O2B-PB-O1B	2.70	125.58	112.24
5	A	701	DTP	N6-C6-N1	2.68	124.14	118.57
5	A	701	DTP	O3B-PG-O1G	-2.64	96.57	111.19
5	A	701	DTP	O3G-PG-O2G	2.63	117.68	107.64
4	A	705	GTP	O2'-C2'-C1'	-2.60	101.24	110.85
4	D	704	GTP	C4-C5-C6	-2.60	118.31	120.80
4	D	704	GTP	PB-O3B-PG	-2.56	124.05	132.83
4	A	705	GTP	N2-C2-N3	-2.55	113.63	117.79
5	D	705	DTP	C4-C5-N7	-2.53	106.76	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	705	DTP	N3-C2-N1	-2.50	124.77	128.68
4	A	705	GTP	C2-N3-C4	2.47	118.18	115.36
4	A	705	GTP	C4-C5-C6	-2.44	118.47	120.80
5	A	701	DTP	C2'-C3'-C4'	2.43	107.82	102.76
5	D	705	DTP	PA-O3A-PB	-2.39	124.63	132.83
2	B	702	TTP	O3G-PG-O2G	2.35	116.62	107.64
5	C	704	DTP	O3G-PG-O1G	2.34	119.85	110.68
5	B	701	DTP	PB-O3B-PG	-2.31	124.90	132.83
4	A	705	GTP	O3G-PG-O1G	2.29	119.64	110.68
4	A	705	GTP	O5'-PA-O1A	-2.28	100.17	109.07
4	D	704	GTP	O4'-C4'-C3'	-2.23	100.70	105.11
4	C	703	GTP	O2'-C2'-C1'	-2.23	102.63	110.85
5	B	701	DTP	C2'-C3'-C4'	2.23	107.40	102.76
2	D	702	TTP	O3G-PG-O2G	2.20	116.03	107.64
4	B	704	GTP	O2'-C2'-C1'	-2.18	102.79	110.85
5	D	705	DTP	O2B-PB-O1B	2.11	122.65	112.24
5	D	705	DTP	C2-N1-C6	2.08	122.32	118.75
4	B	704	GTP	O2A-PA-O1A	2.07	122.49	112.24
5	C	704	DTP	C2-N1-C6	2.06	122.27	118.75
2	C	701	TTP	O3G-PG-O2G	2.04	115.41	107.64
4	A	705	GTP	O2A-PA-O1A	2.02	122.20	112.24

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	701	TTP	C5'-O5'-PA-O2A
2	C	701	TTP	C5'-O5'-PA-O3A
2	A	703	TTP	C5'-O5'-PA-O1A
2	A	703	TTP	C5'-O5'-PA-O2A
2	D	702	TTP	PB-O3A-PA-O5'
2	D	702	TTP	C5'-O5'-PA-O2A
4	C	703	GTP	PB-O3B-PG-O3G
4	A	705	GTP	PB-O3B-PG-O2G
4	D	704	GTP	PB-O3B-PG-O2G
4	B	704	GTP	PB-O3B-PG-O3G
5	A	701	DTP	PB-O3B-PG-O3G
5	D	705	DTP	PB-O3B-PG-O2G
5	D	705	DTP	PB-O3B-PG-O3G
2	C	701	TTP	O4'-C4'-C5'-O5'
2	C	701	TTP	C3'-C4'-C5'-O5'
2	D	702	TTP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
2	A	703	TTP	PB-O3A-PA-O1A
2	C	701	TTP	C4'-C5'-O5'-PA
2	D	702	TTP	C5'-O5'-PA-O3A
2	D	702	TTP	PG-O3B-PB-O2B
4	C	703	GTP	PG-O3B-PB-O1B
4	A	705	GTP	PG-O3B-PB-O2B
4	B	704	GTP	PG-O3B-PB-O1B
5	C	704	DTP	PG-O3B-PB-O2B
5	A	701	DTP	PG-O3B-PB-O1B
5	B	701	DTP	PG-O3B-PB-O1B
5	B	701	DTP	PB-O3A-PA-O1A
2	B	702	TTP	C3'-C4'-C5'-O5'
2	B	702	TTP	O4'-C4'-C5'-O5'
4	D	704	GTP	PB-O3B-PG-O1G
2	A	703	TTP	PB-O3A-PA-O2A
2	B	702	TTP	PA-O3A-PB-O2B
4	C	703	GTP	PB-O3A-PA-O1A
4	A	705	GTP	PG-O3B-PB-O1B
4	A	705	GTP	PB-O3A-PA-O2A
4	D	704	GTP	PG-O3B-PB-O2B
4	D	704	GTP	PB-O3A-PA-O2A
5	A	701	DTP	PB-O3A-PA-O2A
5	D	705	DTP	PG-O3B-PB-O2B
4	C	703	GTP	C4'-C5'-O5'-PA
4	A	705	GTP	C4'-C5'-O5'-PA
4	B	704	GTP	C4'-C5'-O5'-PA
4	D	704	GTP	C4'-C5'-O5'-PA
5	C	704	DTP	PG-O3B-PB-O1B
5	D	705	DTP	PB-O3B-PG-O1G
5	A	701	DTP	PB-O3B-PG-O2G
2	A	703	TTP	C5'-O5'-PA-O3A
2	B	702	TTP	PA-O3A-PB-O1B
4	C	703	GTP	PG-O3B-PB-O2B
4	D	704	GTP	PB-O3A-PA-O1A
5	A	701	DTP	PB-O3A-PA-O1A
5	D	705	DTP	PG-O3B-PB-O1B
5	D	705	DTP	PB-O3A-PA-O1A
2	D	702	TTP	C5'-O5'-PA-O1A
2	D	702	TTP	C3'-C4'-C5'-O5'
4	A	705	GTP	PB-O3B-PG-O1G

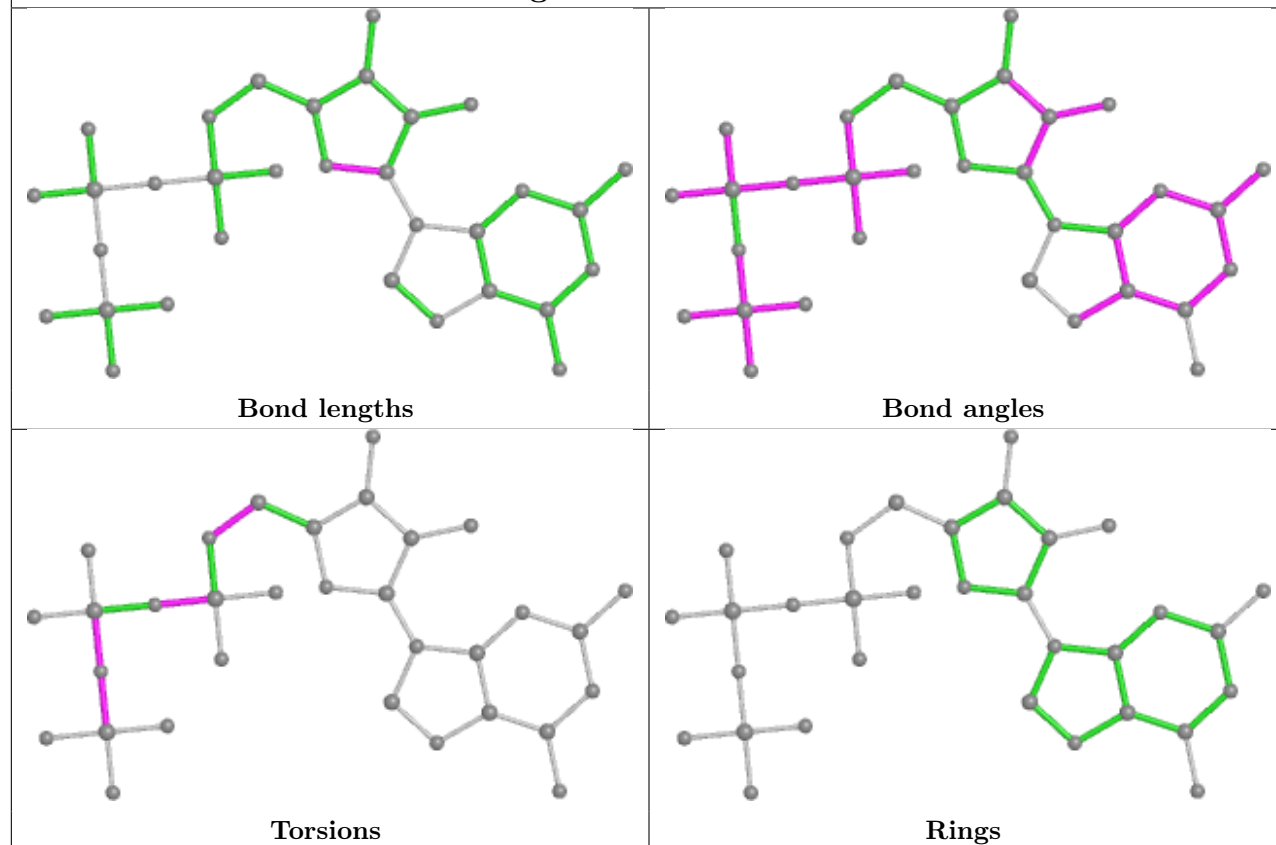
There are no ring outliers.

8 monomers are involved in 21 short contacts:

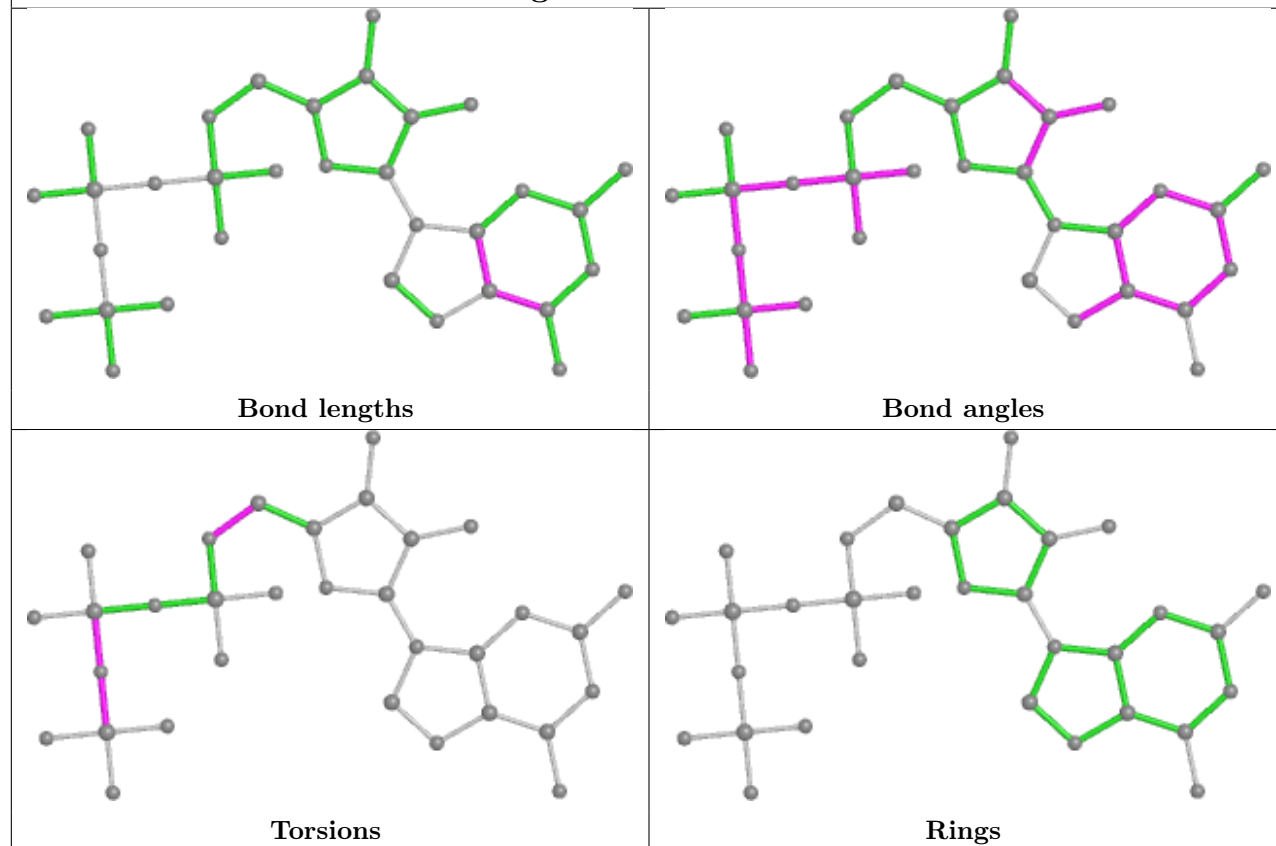
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	701	DTP	1	0
5	D	705	DTP	1	0
2	A	703	TTP	4	0
2	C	701	TTP	1	0
5	B	701	DTP	1	0
4	C	703	GTP	1	0
2	B	702	TTP	9	0
2	D	702	TTP	3	0

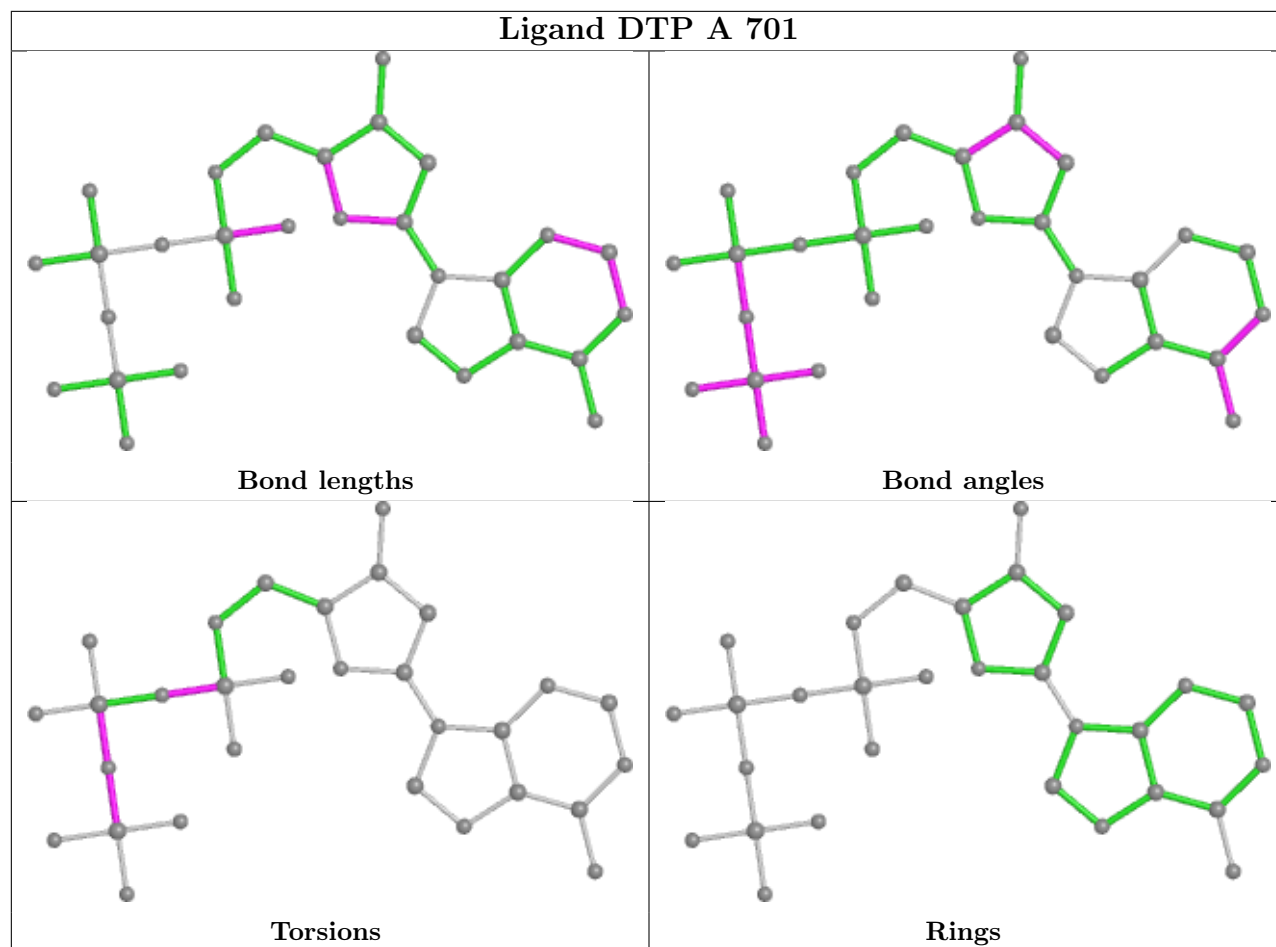
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 GTP A 705

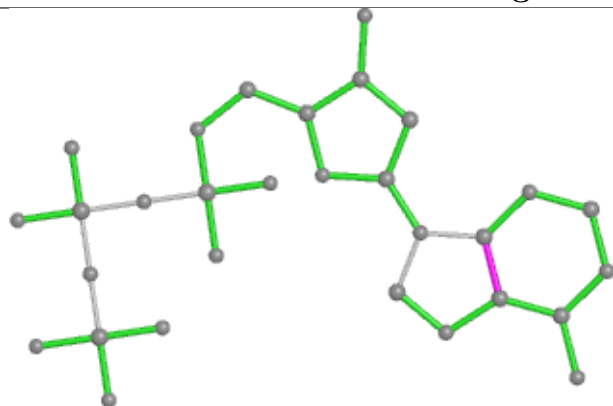


## Ligand GTP B 704

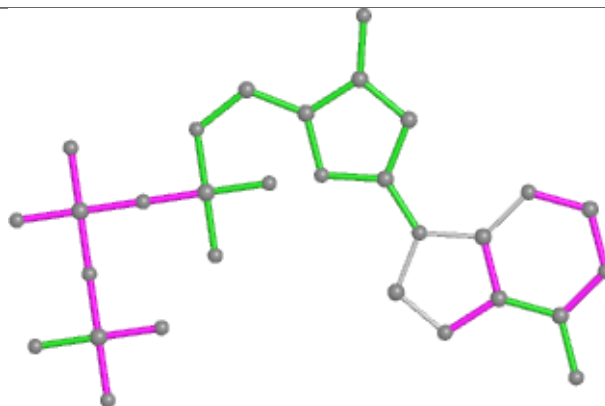




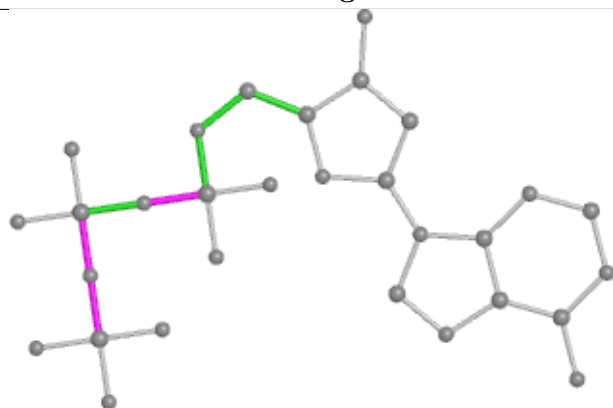
## Ligand DTP D 705



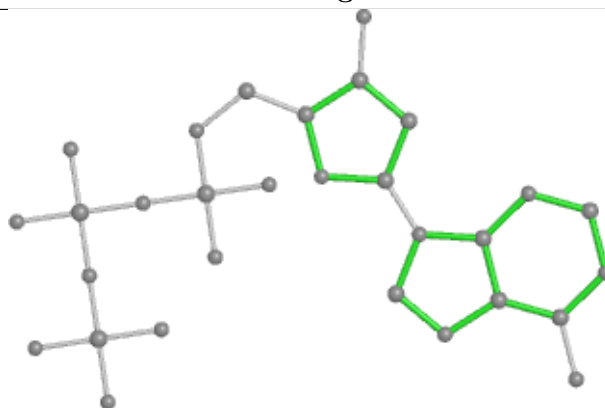
Bond lengths



Bond angles

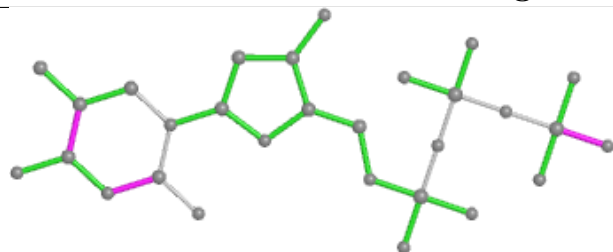


Torsions

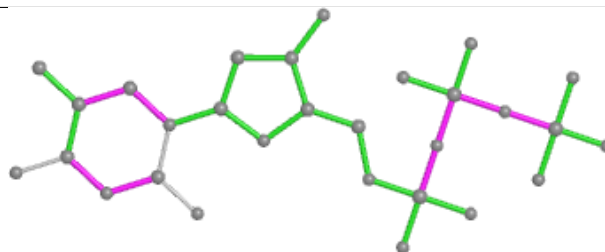


Rings

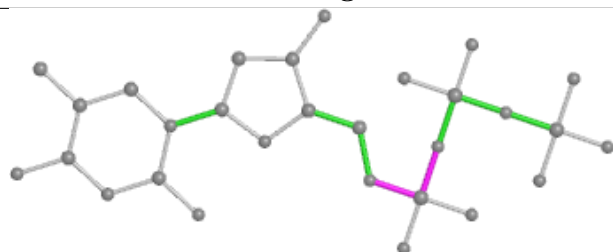
## Ligand TTP A 703



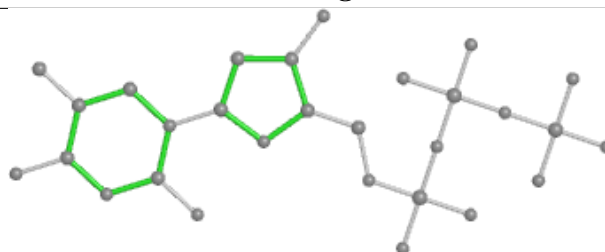
Bond lengths



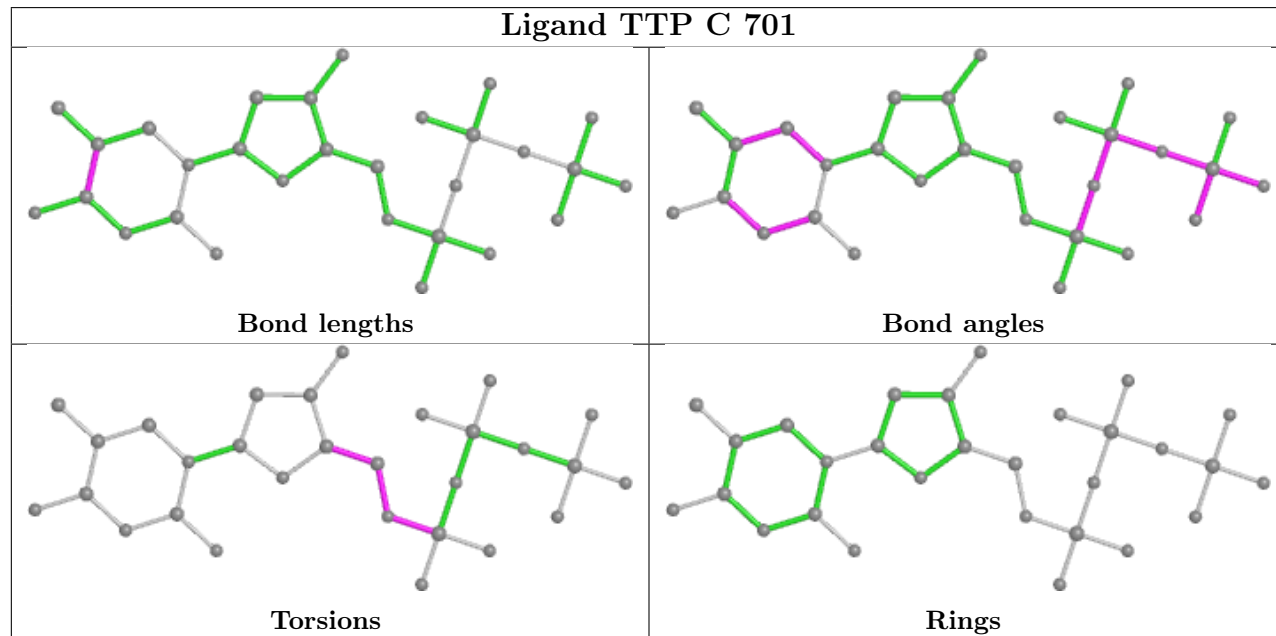
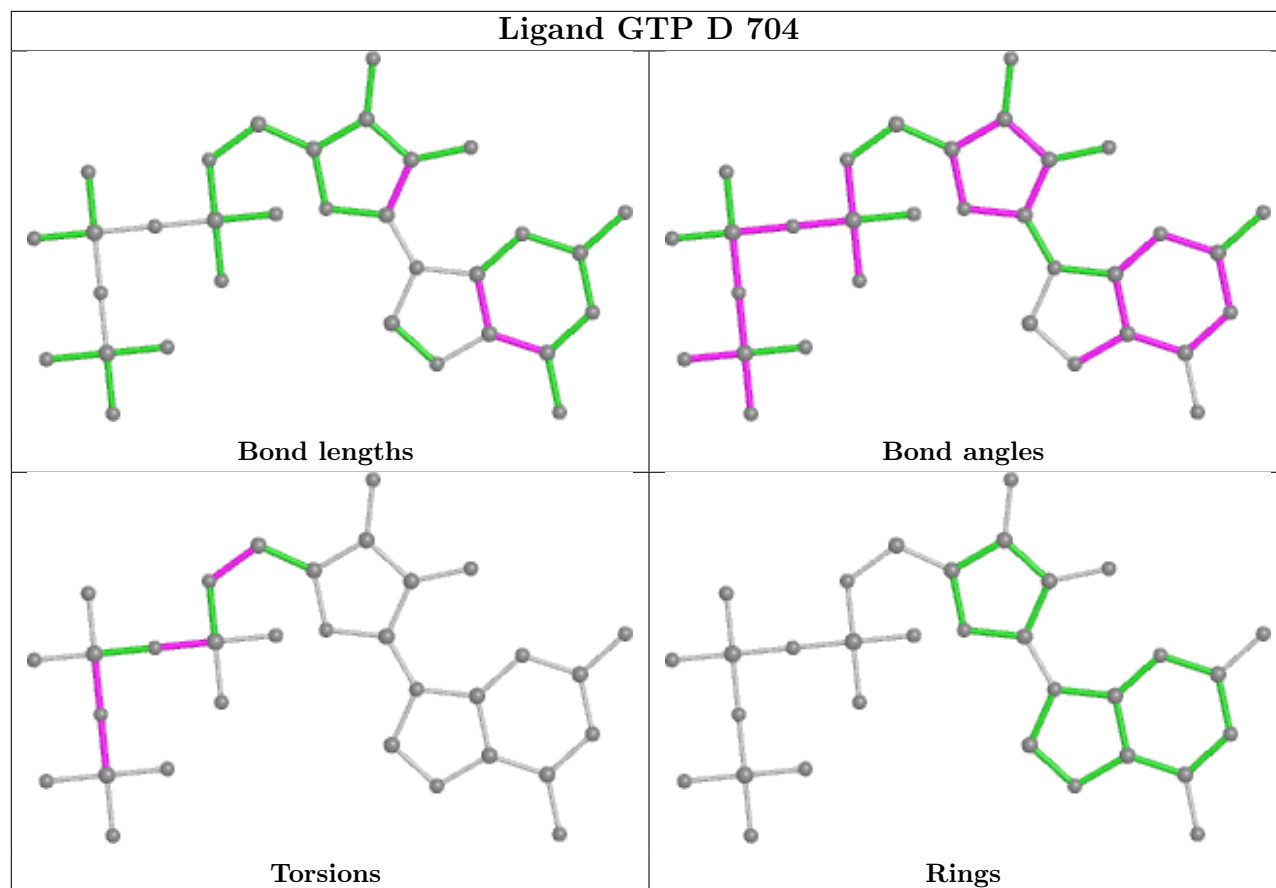
Bond angles

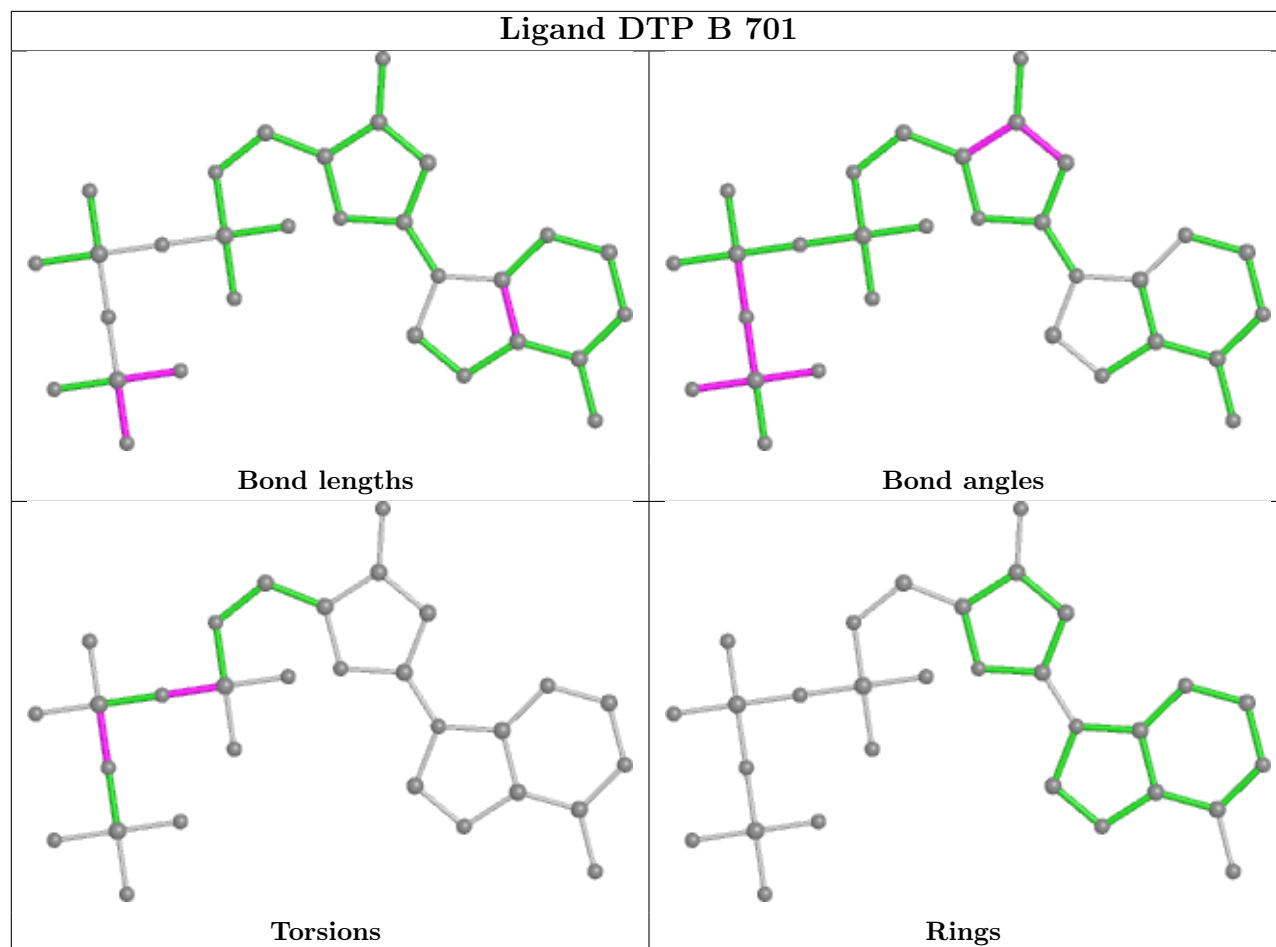


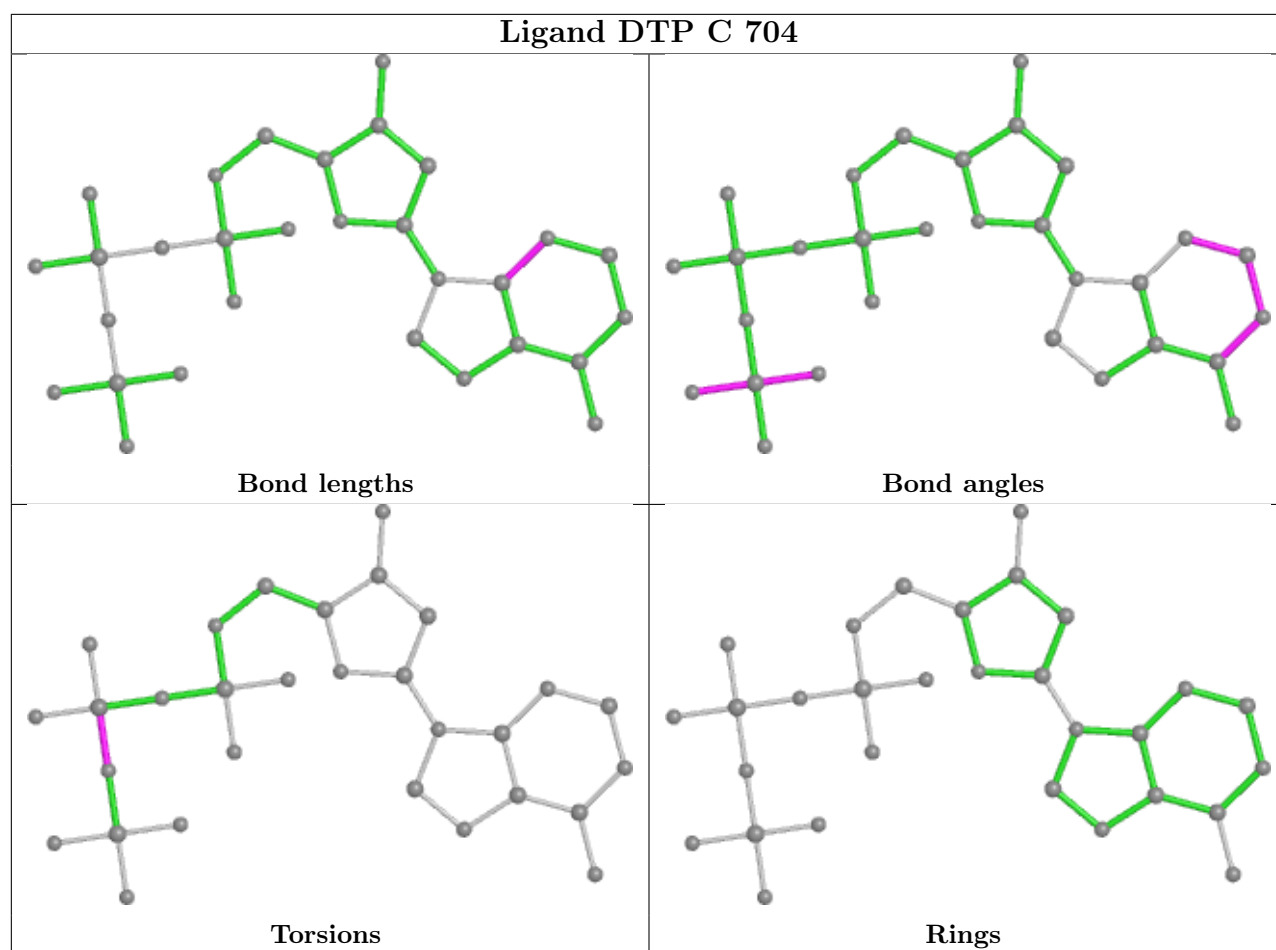
Torsions



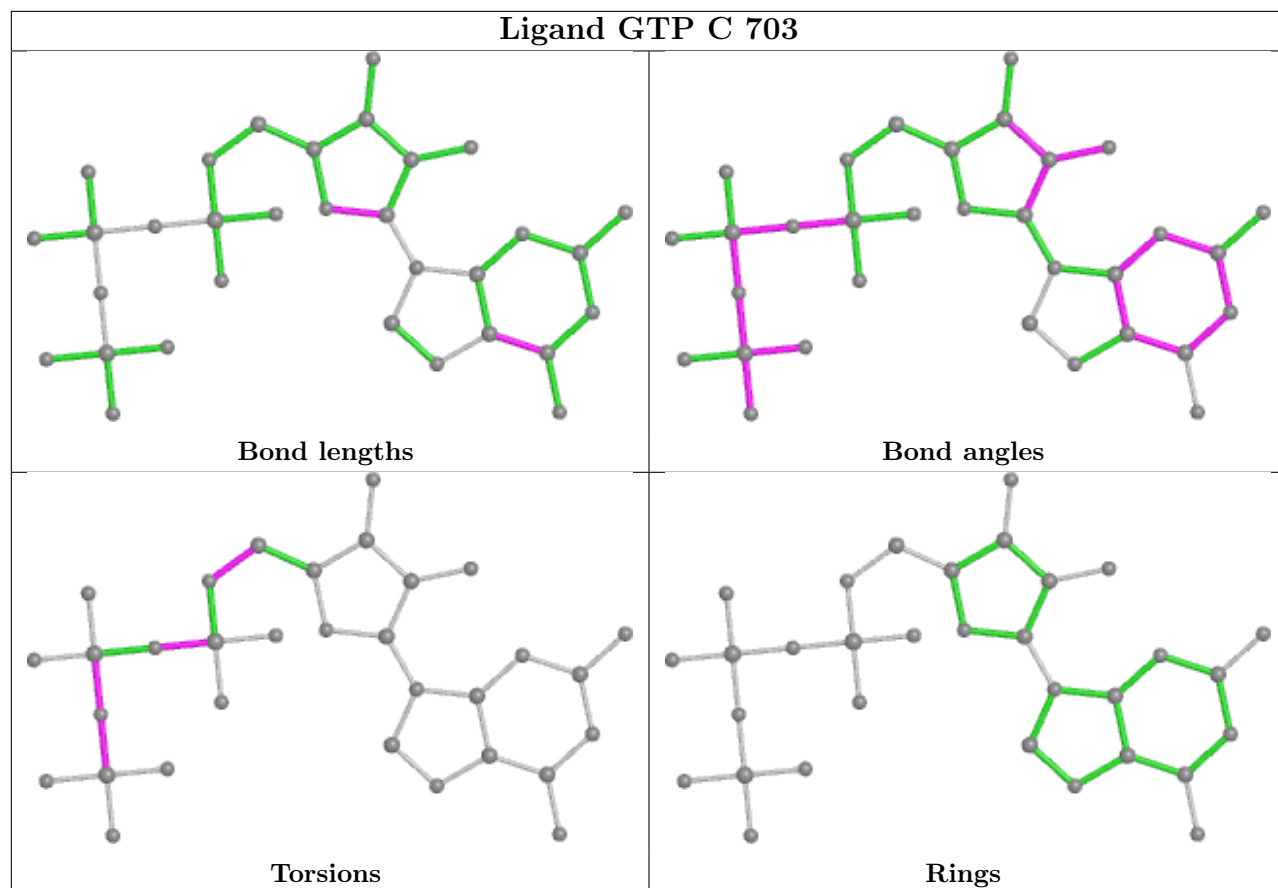
Rings



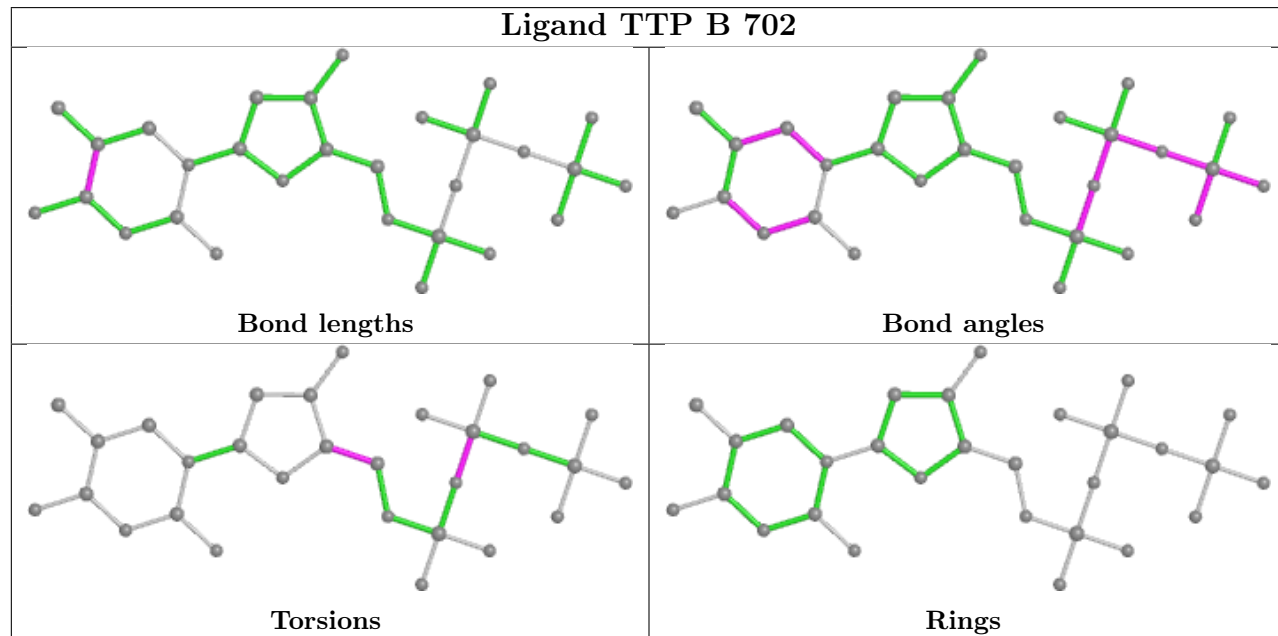


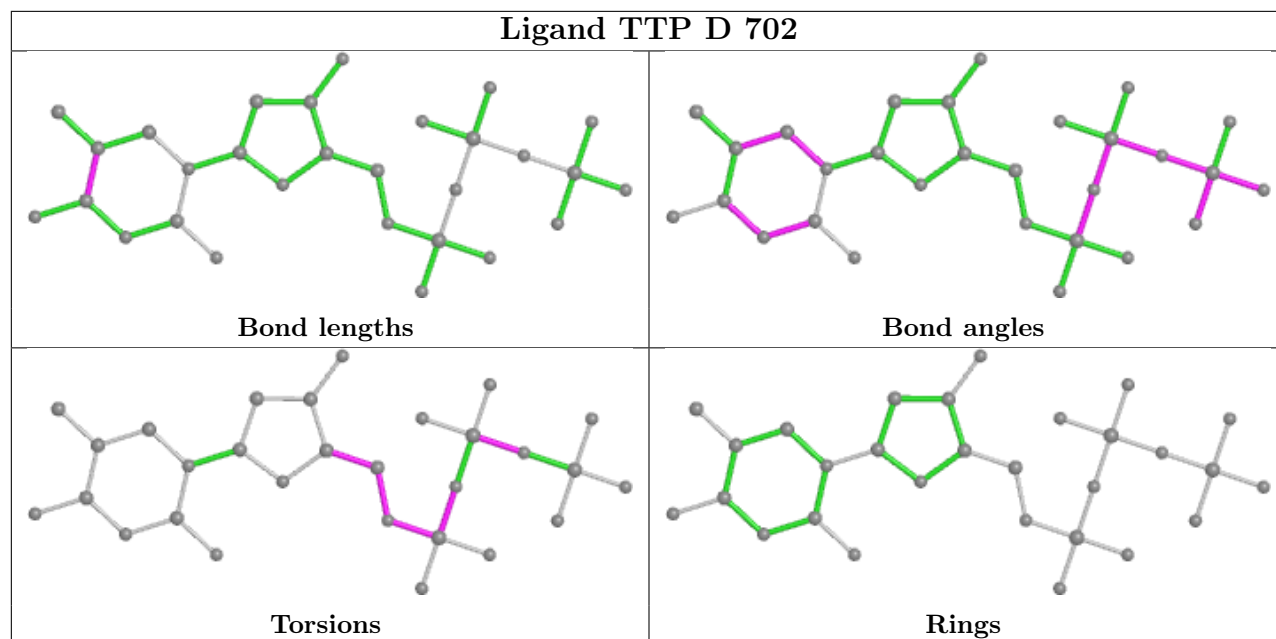


## Ligand GTP C 703



## Ligand TTP B 702





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	480/514 (93%)	0.78	63 (13%) <b>3</b> <b>3</b>	31, 73, 120, 159	0
1	B	481/514 (93%)	1.46	114 (23%) <b>0</b> <b>0</b>	40, 94, 159, 200	0
1	C	481/514 (93%)	0.47	26 (5%) <b>25</b> <b>28</b>	33, 63, 106, 136	0
1	D	480/514 (93%)	0.81	69 (14%) <b>2</b> <b>2</b>	34, 74, 119, 155	0
All	All	1922/2056 (93%)	0.88	272 (14%) <b>2</b> <b>3</b>	31, 75, 134, 200	0

All (272) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	480	VAL	9.9
1	B	573	CYS	9.4
1	B	485	PRO	9.2
1	B	493	LEU	8.4
1	B	481	ALA	8.3
1	B	488	LEU	7.9
1	B	347	LEU	7.8
1	B	592	THR	7.7
1	B	478	LYS	7.7
1	A	491	VAL	7.6
1	B	345	ASN	7.4
1	D	488	LEU	7.4
1	A	488	LEU	7.1
1	A	286	PRO	7.1
1	B	484	LYS	7.0
1	A	487	VAL	6.8
1	B	563	TYR	6.8
1	D	490	ASP	6.6
1	D	540	LEU	6.6
1	B	476	LEU	6.6
1	B	562	LEU	6.5

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Mol	Chain	Res	Type	RSRZ
1	A	489	LEU	6.4
1	B	498	PHE	6.4
1	B	276	LEU	6.2
1	D	466	ILE	6.1
1	B	578	PHE	6.0
1	B	489	LEU	6.0
1	A	490	ASP	5.8
1	B	230	LYS	5.7
1	D	590	LEU	5.5
1	B	341	CYS	5.4
1	A	284	LEU	5.4
1	A	493	LEU	5.3
1	D	491	VAL	5.3
1	A	568	TYR	5.0
1	B	469	LYS	5.0
1	B	569	PHE	5.0
1	A	492	LYS	4.9
1	B	596	LYS	4.9
1	B	285	TRP	4.8
1	B	570	VAL	4.8
1	D	493	LEU	4.7
1	B	492	LYS	4.6
1	B	572	TRP	4.6
1	A	484	LYS	4.5
1	B	557	VAL	4.5
1	B	591	ILE	4.5
1	D	543	GLU	4.5
1	B	288	LYS	4.5
1	B	568	TYR	4.5
1	A	486	LYS	4.5
1	B	511	GLU	4.5
1	B	554	CYS	4.4
1	B	467	LYS	4.4
1	A	285	TRP	4.3
1	D	492	LYS	4.3
1	B	348	ARG	4.3
1	B	590	LEU	4.2
1	B	457	VAL	4.2
1	D	589	PRO	4.2
1	D	559	ARG	4.2
1	B	266	CYS	4.2
1	B	584	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	563	TYR	4.1
1	B	396	TYR	4.1
1	B	491	VAL	4.0
1	D	489	LEU	4.0
1	B	486	LYS	3.9
1	B	350	CYS	3.9
1	B	475	SER	3.9
1	B	487	VAL	3.9
1	B	343	VAL	3.8
1	A	593	PRO	3.7
1	A	575	ASP	3.7
1	B	292	GLU	3.7
1	D	288	LYS	3.7
1	B	470	ARG	3.7
1	A	563	TYR	3.7
1	A	287	TYR	3.6
1	A	466	ILE	3.6
1	A	571	GLN	3.6
1	B	397	ILE	3.5
1	A	562	LEU	3.5
1	B	242	GLU	3.5
1	D	556	LYS	3.5
1	B	274	GLY	3.5
1	B	413	ILE	3.5
1	B	275	PRO	3.5
1	B	496	GLU	3.5
1	A	473	TYR	3.4
1	A	263	GLU	3.4
1	B	545	PHE	3.4
1	B	328	ASN	3.4
1	B	277	GLU	3.3
1	A	345	ASN	3.3
1	A	494	LYS	3.3
1	B	577	ASN	3.3
1	C	113	ASP	3.3
1	D	325	ILE	3.3
1	D	596	LYS	3.3
1	B	599	ASN	3.3
1	B	500	VAL	3.3
1	D	557	VAL	3.2
1	C	265	ILE	3.2
1	A	265	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	598	TRP	3.2
1	A	322	HIS	3.2
1	D	320	CYS	3.2
1	A	594	GLN	3.2
1	A	464	GLY	3.2
1	B	473	TYR	3.1
1	A	483	ALA	3.1
1	D	578	PHE	3.1
1	B	406	LYS	3.1
1	B	472	ASP	3.1
1	C	201	ILE	3.1
1	D	322	HIS	3.1
1	D	113	ASP	3.1
1	A	288	LYS	3.1
1	D	462	PRO	3.1
1	D	498	PHE	3.1
1	D	229	VAL	3.0
1	B	326	GLN	3.0
1	A	599	ASN	3.0
1	D	572	TRP	3.0
1	B	531	ARG	3.0
1	A	573	CYS	3.0
1	D	465	GLN	3.0
1	A	320	CYS	3.0
1	B	586	VAL	2.9
1	D	317	ALA	2.9
1	A	325	ILE	2.9
1	C	262	GLU	2.9
1	A	276	LEU	2.9
1	D	486	LYS	2.9
1	D	584	GLY	2.9
1	D	594	GLN	2.8
1	B	528	ARG	2.8
1	B	543	GLU	2.8
1	B	346	GLU	2.8
1	B	287	TYR	2.8
1	C	556	LYS	2.8
1	D	327	ASN	2.8
1	A	221	PHE	2.7
1	C	465	GLN	2.7
1	D	321	HIS	2.7
1	D	593	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	476	LEU	2.7
1	B	185	LYS	2.7
1	C	263	GLU	2.7
1	A	437	LYS	2.7
1	A	560	LYS	2.7
1	D	263	GLU	2.7
1	B	490	ASP	2.7
1	C	287	TYR	2.7
1	D	323	LEU	2.7
1	D	121	PRO	2.7
1	D	262	GLU	2.7
1	C	404	GLY	2.7
1	C	293	ASN	2.6
1	A	592	THR	2.6
1	D	324	GLY	2.6
1	D	595	LYS	2.6
1	A	463	THR	2.6
1	D	485	PRO	2.6
1	B	405	LYS	2.6
1	B	295	SER	2.6
1	D	545	PHE	2.5
1	C	325	ILE	2.5
1	A	122	ILE	2.5
1	B	398	GLU	2.5
1	B	122	ILE	2.5
1	A	121	PRO	2.5
1	B	552	VAL	2.5
1	B	231	TRP	2.5
1	B	564	ALA	2.5
1	B	327	ASN	2.5
1	D	562	LEU	2.5
1	B	238	VAL	2.5
1	D	560	LYS	2.5
1	D	471	GLU	2.4
1	D	328	ASN	2.4
1	D	460	THR	2.4
1	D	568	TYR	2.4
1	B	224	LEU	2.4
1	B	229	VAL	2.4
1	A	324	GLY	2.4
1	D	484	LYS	2.4
1	B	559	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	321	HIS	2.4
1	B	544	LYS	2.4
1	C	255	GLU	2.4
1	D	482	SER	2.4
1	D	122	ILE	2.4
1	B	526	PRO	2.4
1	C	235	GLN	2.4
1	D	230	LYS	2.3
1	A	471	GLU	2.3
1	A	598	TRP	2.3
1	D	224	LEU	2.3
1	D	511[A]	GLU	2.3
1	B	587	ILE	2.3
1	C	121	PRO	2.3
1	C	288	LYS	2.3
1	D	470	ARG	2.3
1	B	594	GLN	2.3
1	B	581	PRO	2.3
1	A	572	TRP	2.3
1	D	487	VAL	2.3
1	B	322	HIS	2.3
1	C	245	ILE	2.3
1	D	228	GLU	2.3
1	B	479	GLU	2.3
1	B	403	GLY	2.3
1	C	242	GLU	2.3
1	B	262	GLU	2.3
1	B	471	GLU	2.3
1	B	340	VAL	2.3
1	D	397	ILE	2.3
1	B	388	ASP	2.2
1	A	277	GLU	2.2
1	A	114	THR	2.2
1	A	498	PHE	2.2
1	B	593	PRO	2.2
1	C	251	LYS	2.2
1	C	250	ILE	2.2
1	A	262	GLU	2.2
1	A	150	LEU	2.2
1	D	326	GLN	2.2
1	B	510	GLN	2.2
1	C	249	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	472	ASP	2.2
1	C	285	TRP	2.2
1	B	494	LYS	2.2
1	A	422	LEU	2.2
1	A	590	LEU	2.2
1	B	571	GLN	2.2
1	D	160	ALA	2.2
1	A	587	ILE	2.2
1	B	482	SER	2.2
1	C	332	LYS	2.1
1	D	255	GLU	2.1
1	D	344	ASP	2.1
1	B	438	LEU	2.1
1	C	252	PRO	2.1
1	A	326	GLN	2.1
1	D	580	LYS	2.1
1	D	531	ARG	2.1
1	D	316	PHE	2.1
1	C	345	ASN	2.1
1	B	349	ILE	2.1
1	B	290	ARG	2.1
1	B	222	ILE	2.1
1	C	490	ASP	2.1
1	B	235	GLN	2.1
1	B	585	ASP	2.1
1	D	198	CYS	2.1
1	B	265	ILE	2.1
1	B	468	ILE	2.1
1	A	266	CYS	2.1
1	B	296	PHE	2.1
1	B	556	LYS	2.0
1	D	574	ALA	2.0
1	A	292	GLU	2.0
1	B	474	GLU	2.0
1	C	557	VAL	2.0
1	A	478	LYS	2.0
1	B	115	MET	2.0
1	A	396	TYR	2.0
1	A	342	GLU	2.0
1	D	276	LEU	2.0
1	B	219	GLY	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

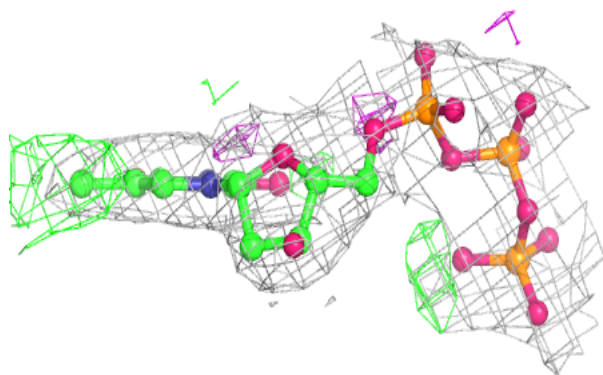
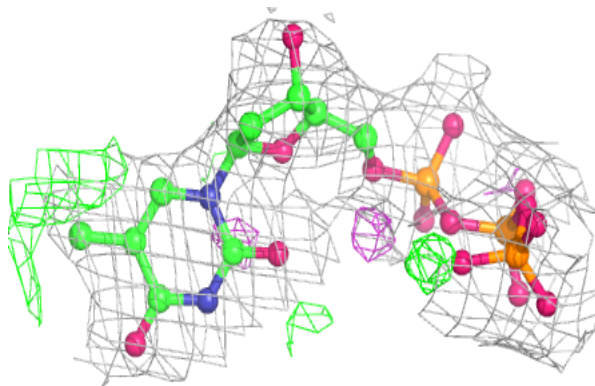
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	MG	C	702	1/1	0.54	0.27	77,77,77,77	0
3	MG	A	704	1/1	0.81	0.17	85,85,85,85	0
3	MG	B	703	1/1	0.81	0.27	92,92,92,92	0
2	TTP	B	702	29/29	0.87	0.17	77,86,112,129	0
3	MG	D	703	1/1	0.89	0.34	85,85,85,85	0
3	MG	C	705	1/1	0.91	0.12	77,77,77,77	0
2	TTP	C	701	29/29	0.93	0.15	40,56,96,101	0
2	TTP	A	703	29/29	0.93	0.14	50,66,100,108	0
2	TTP	D	702	29/29	0.93	0.15	48,65,100,100	0
3	MG	A	706	1/1	0.95	0.08	76,76,76,76	0
3	MG	D	701	1/1	0.95	0.12	52,52,52,52	0
3	MG	A	702	1/1	0.96	0.08	54,54,54,54	0
4	GTP	B	704	32/32	0.96	0.16	54,64,80,83	0
4	GTP	D	704	32/32	0.97	0.12	44,54,68,71	0
5	DTP	D	705	30/30	0.97	0.17	49,57,69,74	0
5	DTP	A	701	30/30	0.98	0.17	31,35,41,44	0
4	GTP	A	705	32/32	0.98	0.13	38,45,53,54	0
5	DTP	B	701	30/30	0.98	0.16	43,49,60,61	0
5	DTP	C	704	30/30	0.99	0.15	31,42,52,53	0
4	GTP	C	703	32/32	0.99	0.13	36,41,47,50	0

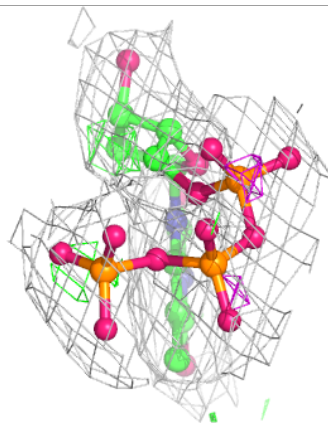
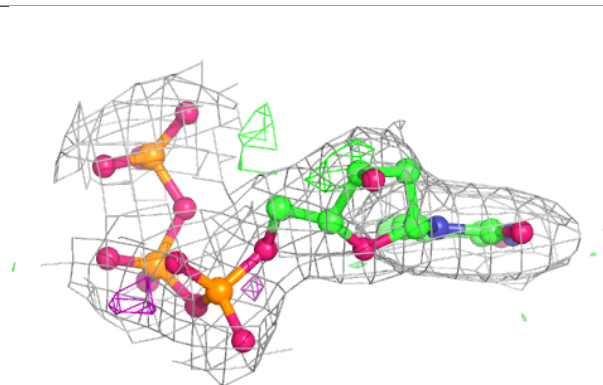
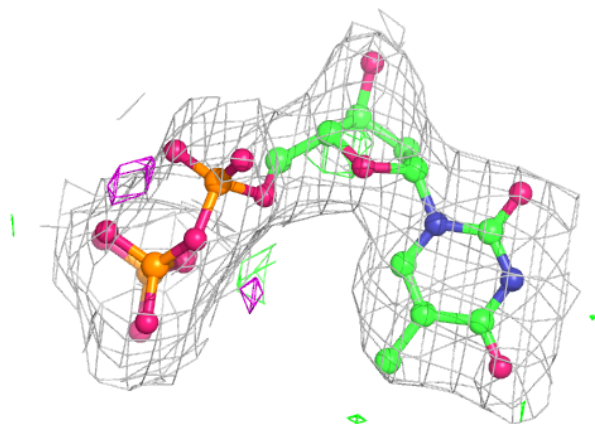
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around TTP B 702:**

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

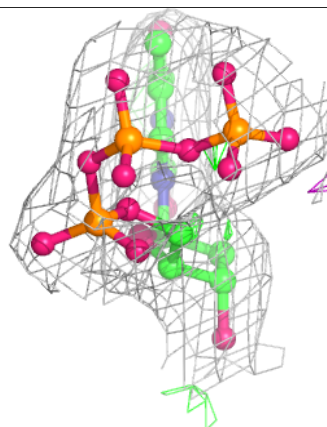
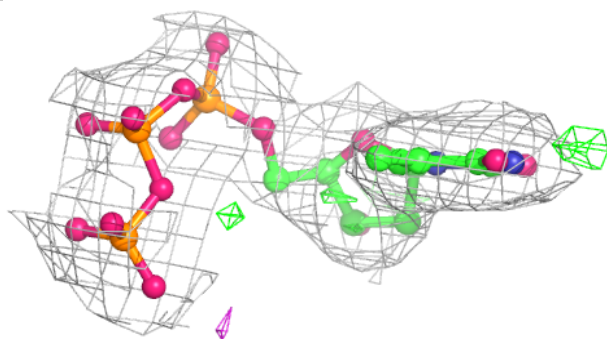
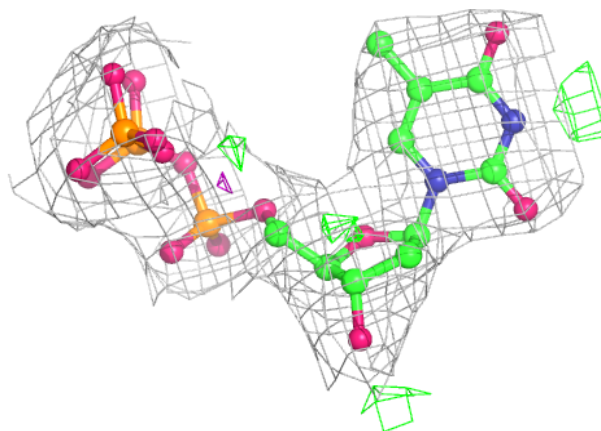
**Electron density around TTP C 701:**

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

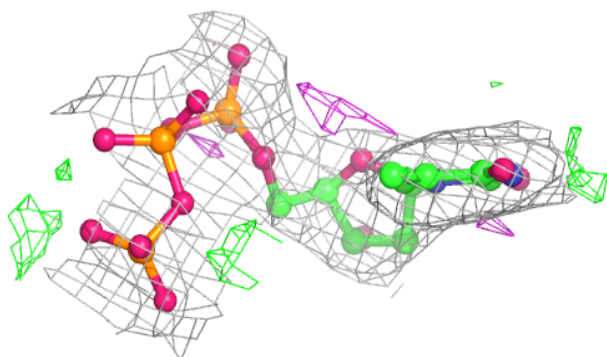
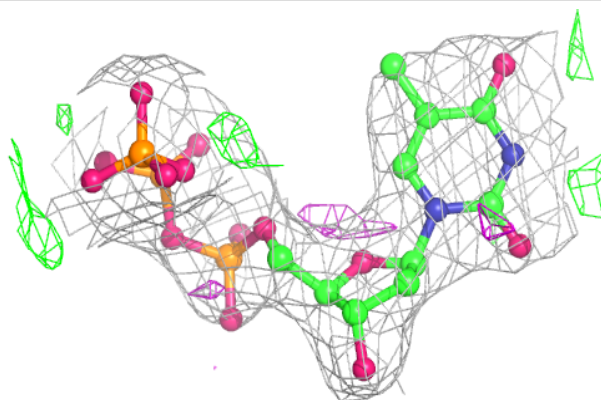


**Electron density around TTP A 703:**

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

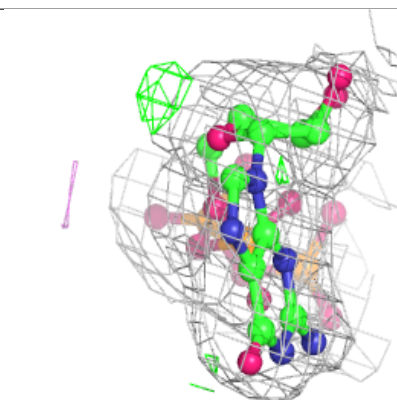
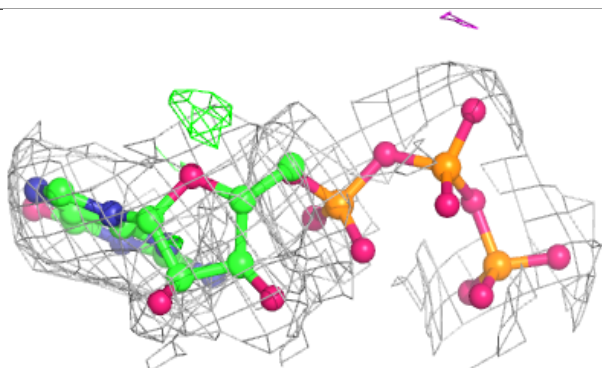
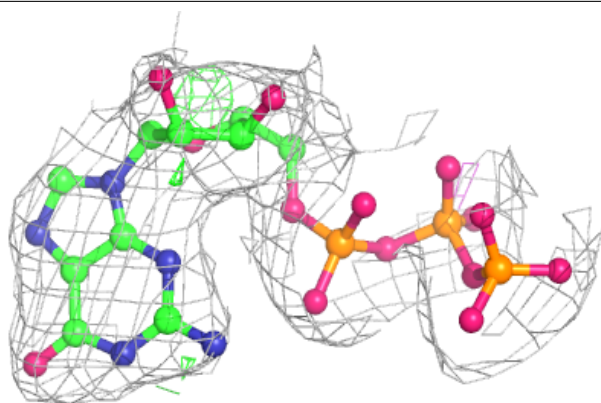
**Electron density around TTP D 702:**

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

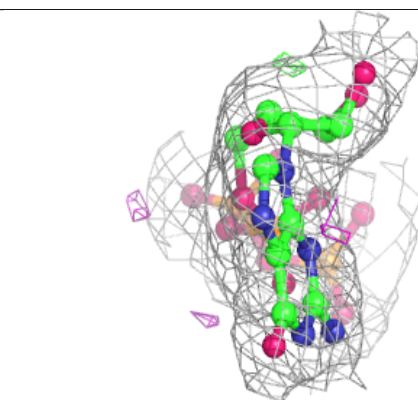
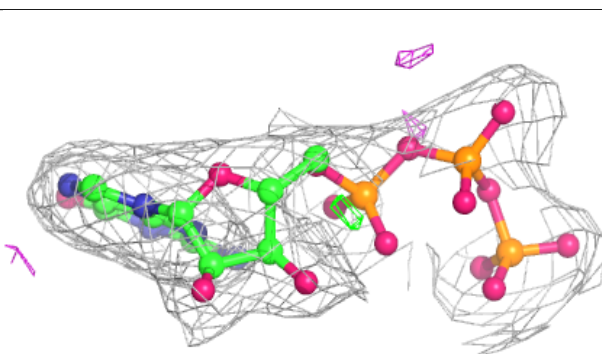
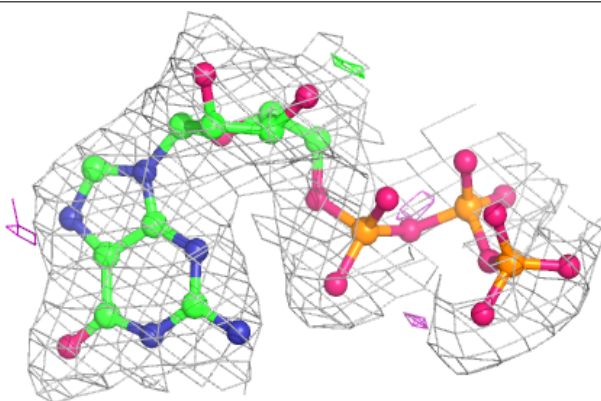


**Electron density around GTP B 704:**

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

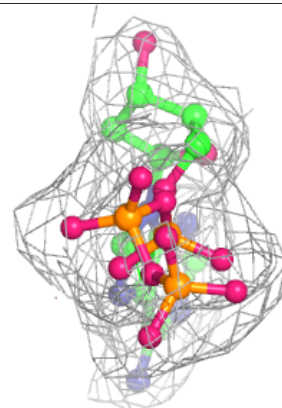
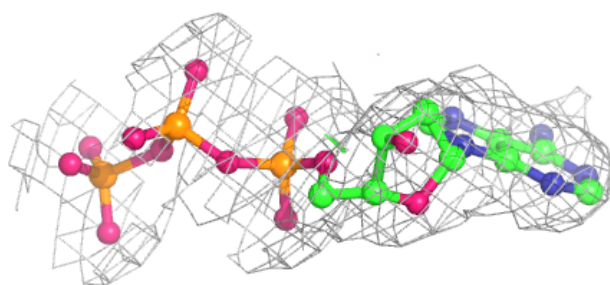
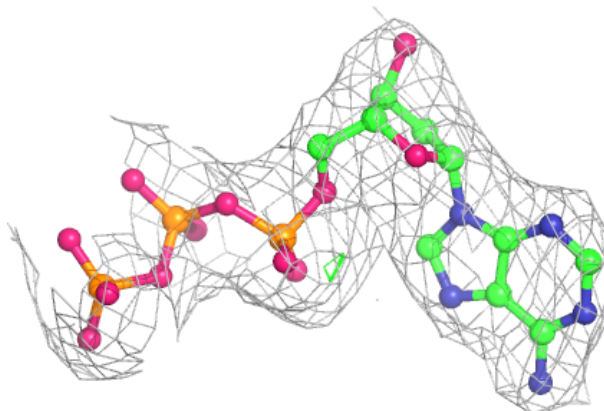
**Electron density around GTP D 704:**

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

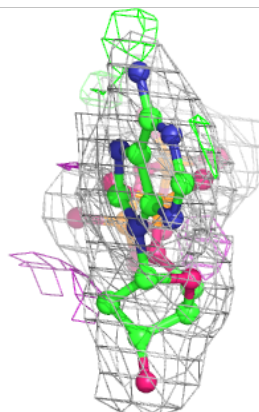
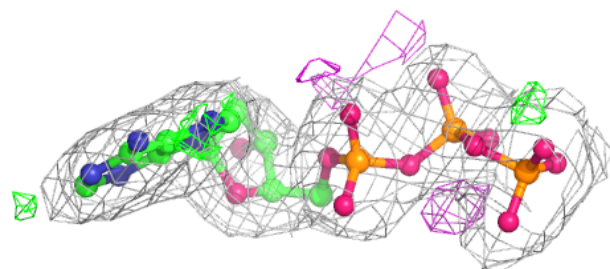
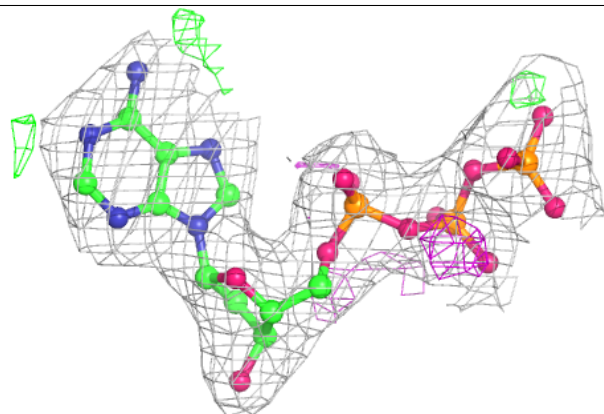


**Electron density around DTP D 705:**

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

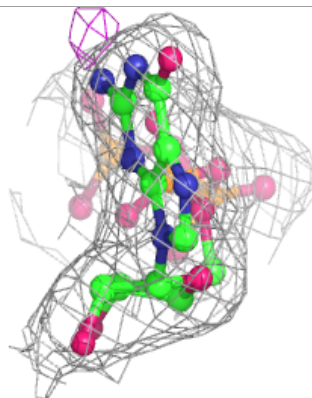
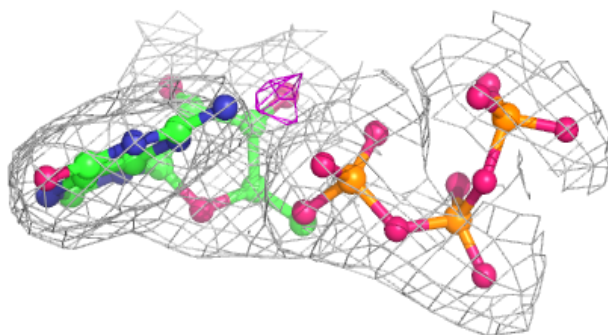
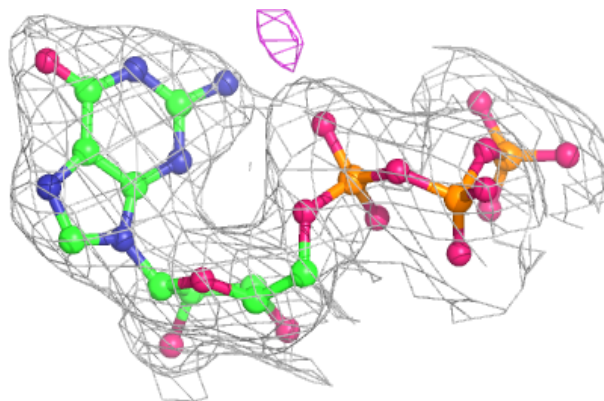
**Electron density around DTP A 701:**

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

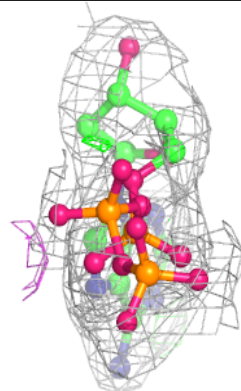
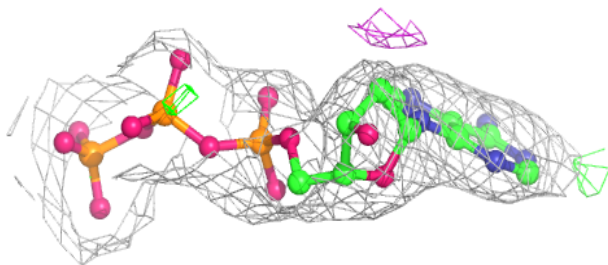
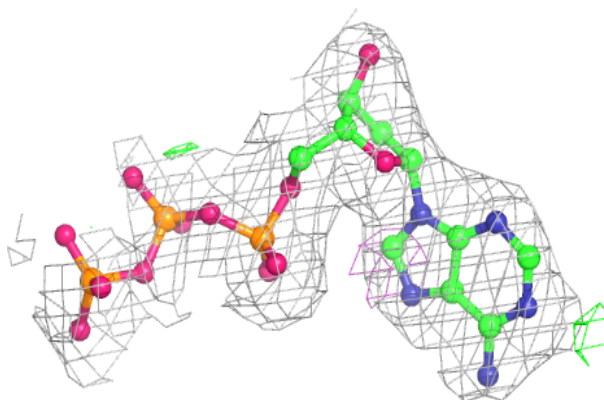


**Electron density around GTP A 705:**

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

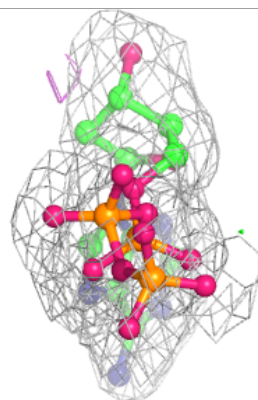
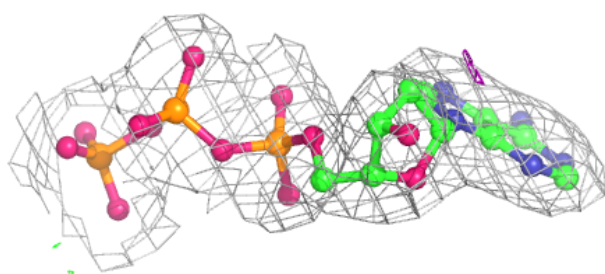
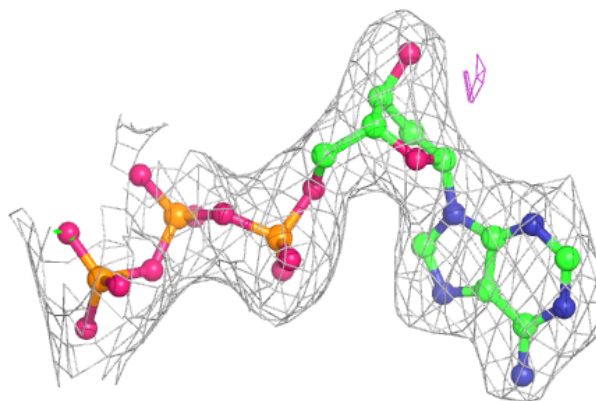
**Electron density around DTP B 701:**

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

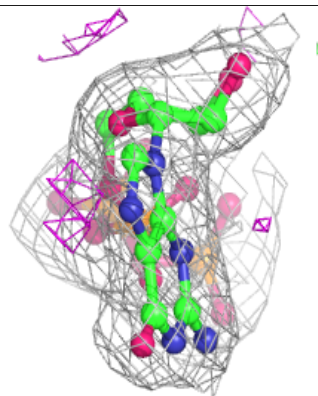
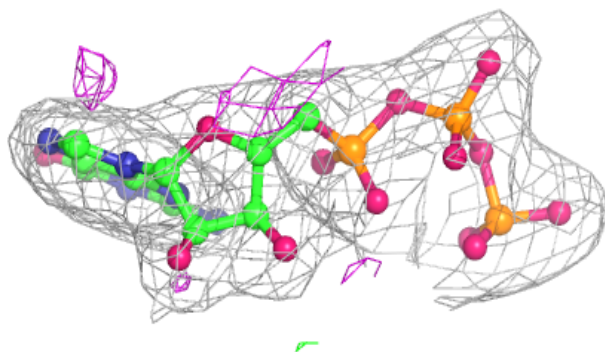
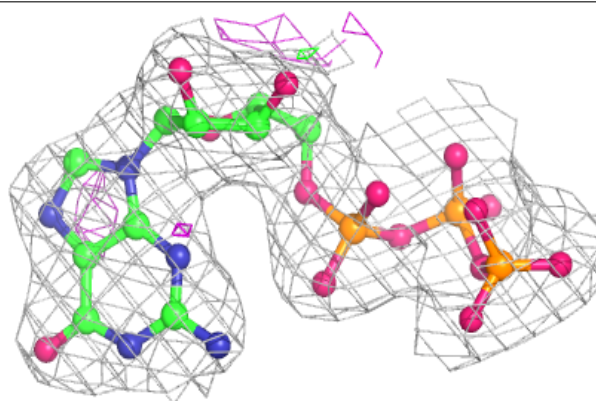


**Electron density around DTP C 704:**

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

**Electron density around GTP C 703:**

$2mF_o-DF_c$  (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.