



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2022 – 06:42 PM EDT

PDB ID : 4TNR  
Title : Structure basis of cellular dNTP regulation, SAMHD1-GTP-dATP-dATP complex  
Authors : Ji, X.; Tang, C.; Zhao, Q.; Wang, W.; Xiong, Y.  
Deposited on : 2014-06-04  
Resolution : 2.75 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.

---

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

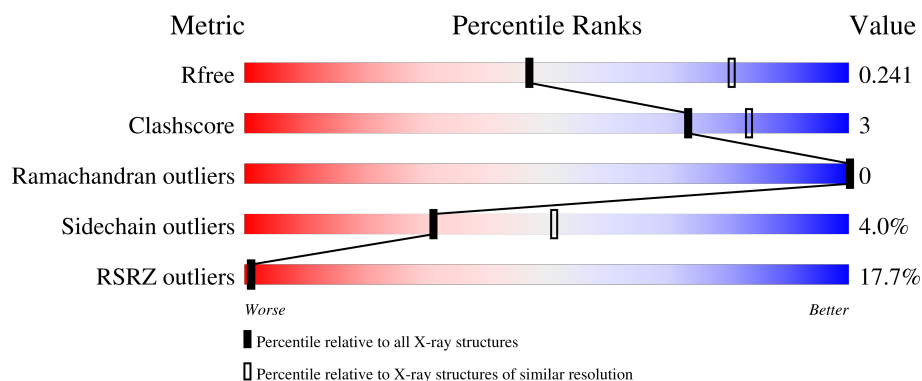
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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>26%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>6%</div> </div> </div>
1	B	514	<div> <div>17%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>6%</div> </div> </div>
1	C	514	<div> <div>17%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>6%</div> </div> </div>
1	D	514	<div> <div>6%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>6%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16156 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.

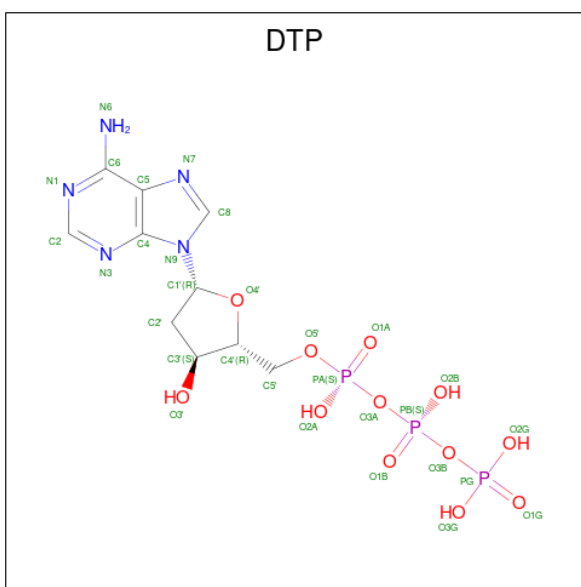
- Molecule 1 is a protein called Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	481	Total	C	N	O	S	0	2	0
			3948	2525	687	715	21			
1	C	481	Total	C	N	O	S	0	2	0
			3948	2525	687	715	21			
1	B	481	Total	C	N	O	S	0	2	0
			3948	2525	687	715	21			
1	A	481	Total	C	N	O	S	0	2	0
			3948	2525	687	715	21			

There are 8 discrepancies between the modelled and reference sequences:

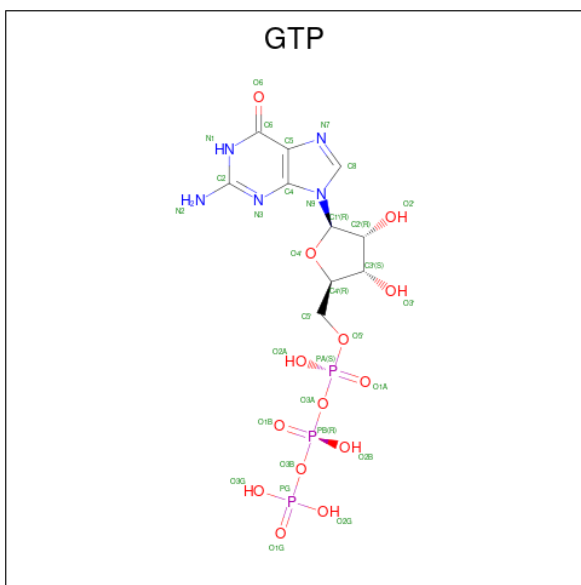
Chain	Residue	Modelled	Actual	Comment	Reference
D	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
D	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
C	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
C	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
B	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
B	207	ASN	ASP	engineered mutation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

- Molecule 2 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
2	D	1	Total 30	C 10	N 5	O 12	P 3	0	0
2	D	1	Total 30	C 10	N 5	O 12	P 3	0	0
2	C	1	Total 30	C 10	N 5	O 12	P 3	0	0
2	C	1	Total 30	C 10	N 5	O 12	P 3	0	0
2	B	1	Total 30	C 10	N 5	O 12	P 3	0	0
2	B	1	Total 30	C 10	N 5	O 12	P 3	0	0
2	A	1	Total 30	C 10	N 5	O 12	P 3	0	0

- Molecule 3 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
3	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	8	Total	O	0	0
			8	8		

*Continued on next page...*

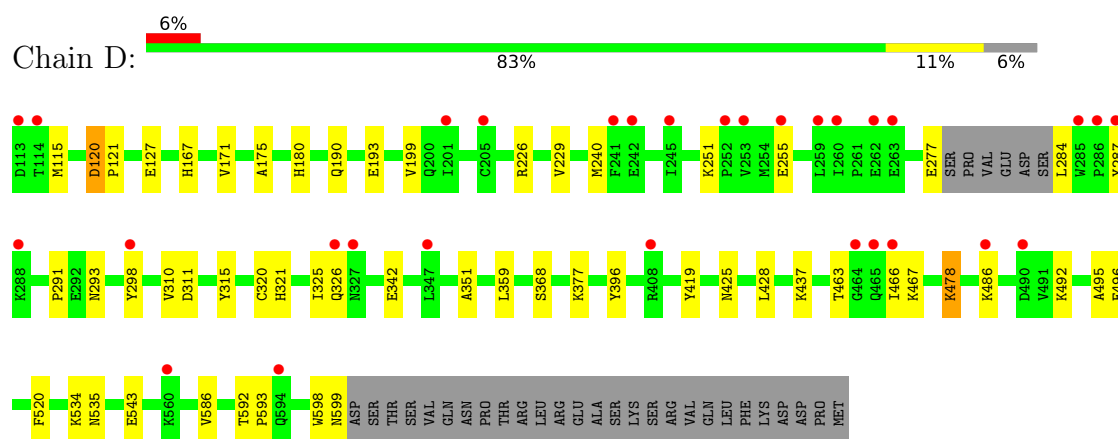
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	2	Total	O	0	0
			2	2		
5	B	9	Total	O	0	0
			9	9		
5	A	3	Total	O	0	0
			3	3		

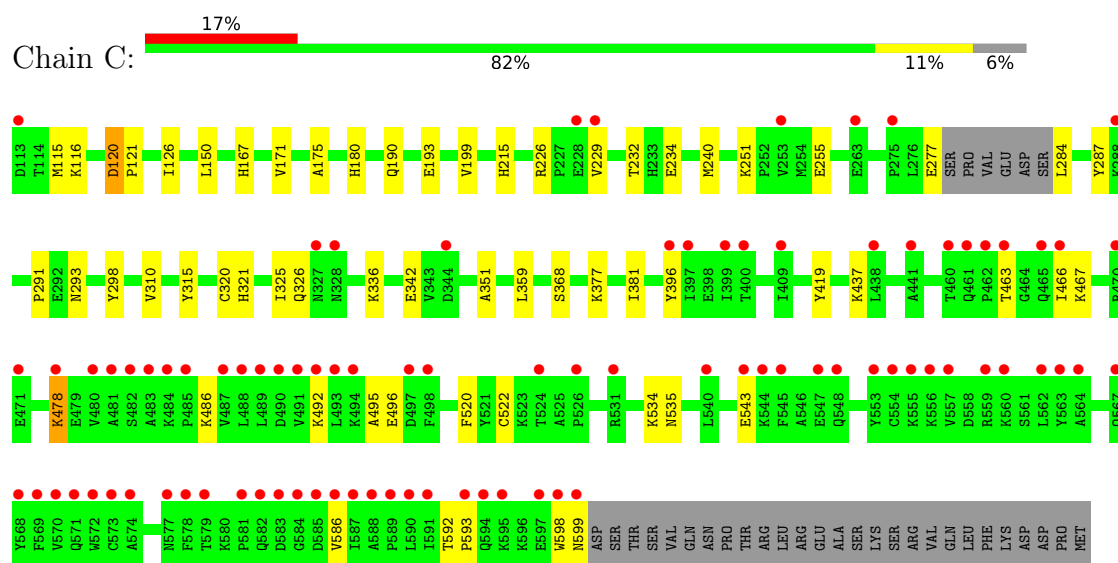
### 3 Residue-property plots [i](#)

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

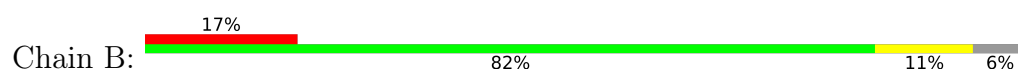
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

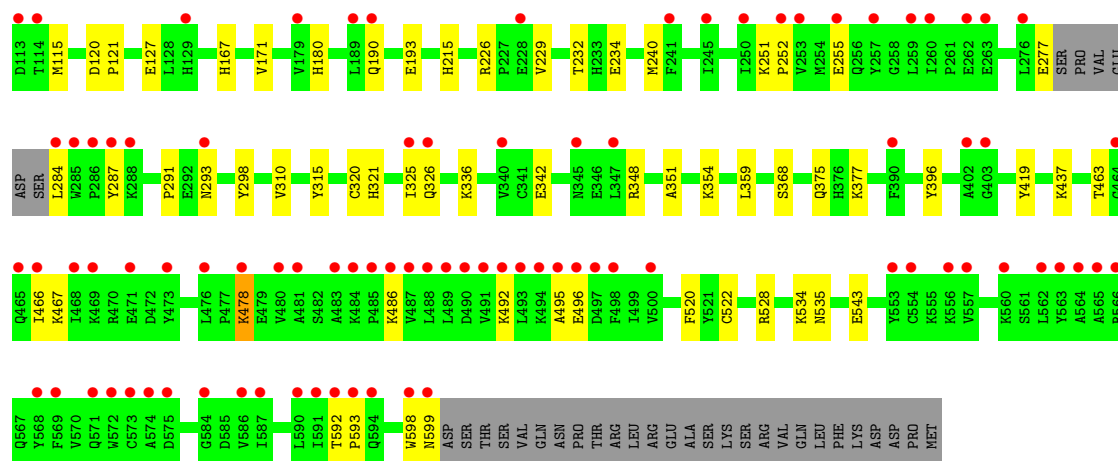


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

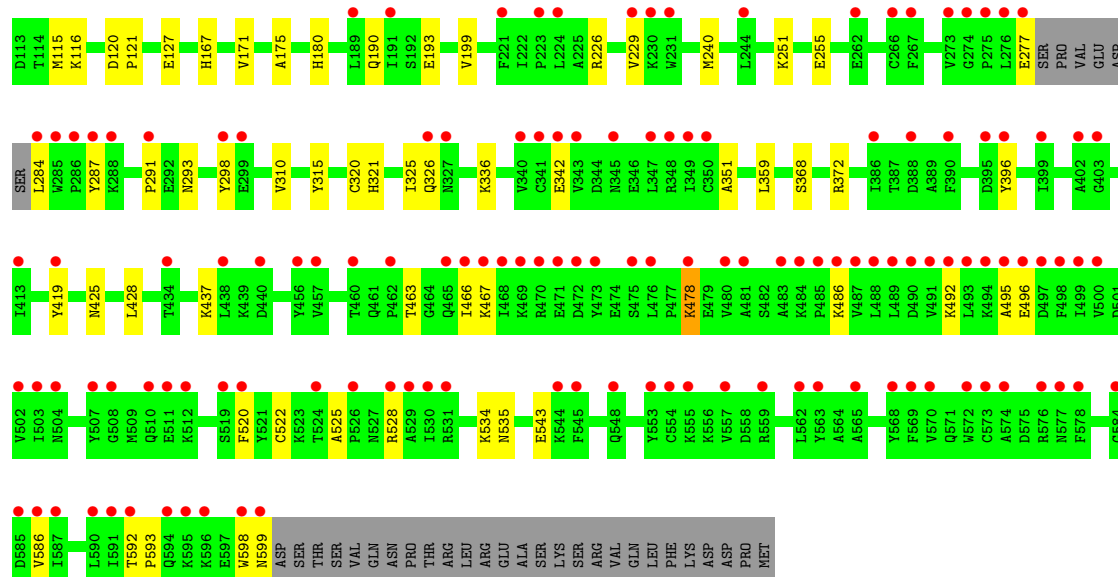
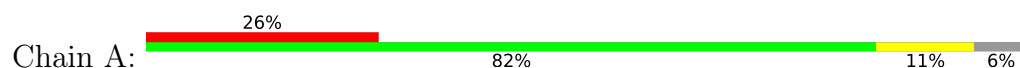


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





● 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, $\alpha$ , $\beta$ , $\gamma$	84.92Å 141.70Å 97.52Å 90.00° 115.40° 90.00°	Depositor
Resolution (Å)	50.00 – 2.75 48.46 – 2.72	Depositor EDS
% Data completeness (in resolution range)	96.3 (50.00-2.75) 96.3 (48.46-2.72)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, $R_{free}$	0.224 , 0.242 0.222 , 0.241	Depositor DCC
$R_{free}$ test set	2727 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.3	Xtriage
Anisotropy	1.250	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 58.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16156	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DTP, GTP, MG

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	0.57	0/4040	0.71	0/5453
1	B	0.63	2/4040 (0.0%)	0.73	1/5453 (0.0%)
1	C	0.59	0/4040	0.72	1/5453 (0.0%)
1	D	0.64	0/4040	0.73	1/5453 (0.0%)
All	All	0.61	2/16160 (0.0%)	0.72	3/21812 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	528	ARG	CZ-NH2	10.12	1.46	1.33
1	B	528	ARG	CD-NE	5.14	1.55	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	528	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	D	120	ASP	CB-CG-OD1	5.23	123.00	118.30
1	C	120	ASP	CB-CG-OD1	5.20	122.98	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts ⓘ

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	3948	0	3930	32	0
1	B	3948	0	3930	33	0
1	C	3948	0	3930	34	0
1	D	3948	0	3930	29	0
2	A	30	0	12	1	0
2	B	60	0	24	5	0
2	C	60	0	24	4	0
2	D	60	0	24	2	0
3	A	32	0	12	0	0
3	B	32	0	12	0	0
3	C	32	0	12	1	0
3	D	32	0	12	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	3	0	0	0	0
5	B	9	0	0	1	0
5	C	2	0	0	0	0
5	D	8	0	0	0	0
All	All	16156	0	15852	107	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.

All (107) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:LYS:NZ	2:A:702:DTP:O2B	1.97	0.96
1:C:326:GLN:HG2	1:A:326:GLN:HG2	1.62	0.81
1:D:326:GLN:HG2	1:B:326:GLN:HG2	1.66	0.76
1:C:215:HIS:CD2	2:C:701:DTP:C8	2.70	0.75
1:A:291:PRO:HG2	1:A:293:ASN:OD1	1.90	0.72
1:C:291:PRO:HG2	1:C:293:ASN:OD1	1.90	0.71
1:B:291:PRO:HG2	1:B:293:ASN:OD1	1.91	0.70
1:D:291:PRO:HG2	1:D:293:ASN:OD1	1.92	0.69
1:B:375:GLN:HE22	2:B:704:DTP:HN61	1.44	0.65
1:D:311:ASP:OD2	2:D:701:DTP:O1A	2.15	0.64
2:D:703:DTP:O2B	1:B:377:LYS:NZ	2.31	0.63
1:B:127:GLU:HG3	1:A:336:LYS:HE3	1.82	0.62
1:B:348:ARG:HD3	5:B:809:HOH:O	1.98	0.62
1:D:543:GLU:HG3	1:B:543:GLU:HG3	1.85	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:ASP:OD1	1:D:121:PRO:HD2	2.02	0.58
1:B:226:ARG:O	1:B:229:VAL:HG12	2.05	0.57
1:B:375:GLN:NE2	2:B:704:DTP:N6	2.49	0.57
1:D:586:VAL:HG11	1:B:522[A]:CYS:SG	2.45	0.56
1:B:287:TYR:CD1	1:B:298:TYR:CE1	2.93	0.56
1:A:287:TYR:CD1	1:A:298:TYR:CE1	2.93	0.56
1:D:287:TYR:CD1	1:D:298:TYR:CE1	2.94	0.56
1:A:226:ARG:O	1:A:229:VAL:HG12	2.05	0.56
1:D:226:ARG:O	1:D:229:VAL:HG12	2.06	0.55
1:C:226:ARG:O	1:C:229:VAL:HG12	2.05	0.55
1:B:120:ASP:OD1	1:B:121:PRO:HD2	2.05	0.55
1:A:120:ASP:OD1	1:A:121:PRO:HD2	2.07	0.55
1:C:120:ASP:OD1	1:C:121:PRO:HD2	2.06	0.54
1:D:321:HIS:CE1	1:A:321:HIS:CE1	2.96	0.54
1:C:586:VAL:HG22	1:A:528:ARG:HD3	1.91	0.52
1:C:287:TYR:CD1	1:C:298:TYR:CE1	2.96	0.52
1:D:377:LYS:NZ	2:B:701:DTP:O2B	2.43	0.52
2:C:704:DTP:N6	1:A:372:ARG:HG2	2.26	0.51
1:A:167:HIS:O	1:A:171:VAL:HG23	2.10	0.51
1:C:586:VAL:HG11	1:A:522[A]:CYS:SG	2.50	0.51
1:A:463:THR:O	1:A:466:ILE:HG12	2.11	0.51
1:D:127:GLU:HG3	1:C:336:LYS:HE3	1.93	0.50
1:B:167:HIS:O	1:B:171:VAL:HG23	2.11	0.50
1:C:167:HIS:O	1:C:171:VAL:HG23	2.10	0.50
1:C:543:GLU:HG3	1:A:543:GLU:HG3	1.93	0.50
1:C:326:GLN:HG2	1:A:326:GLN:CG	2.39	0.50
1:B:463:THR:O	1:B:466:ILE:HG12	2.12	0.50
1:D:463:THR:O	1:D:466:ILE:HG12	2.11	0.49
1:C:326:GLN:CG	1:A:326:GLN:HG2	2.39	0.49
1:C:463:THR:O	1:C:466:ILE:HG12	2.12	0.49
1:D:167:HIS:O	1:D:171:VAL:HG23	2.13	0.48
1:C:116:LYS:HE3	3:C:703:GTP:O1A	2.14	0.48
1:C:592:THR:N	1:C:593:PRO:CD	2.77	0.48
1:C:251:LYS:O	1:C:255:GLU:HG3	2.14	0.47
1:B:336:LYS:HE3	1:A:127:GLU:HG3	1.97	0.47
1:D:592:THR:N	1:D:593:PRO:CD	2.78	0.47
1:A:592:THR:N	1:A:593:PRO:CD	2.78	0.47
1:D:251:LYS:O	1:D:255:GLU:HG3	2.14	0.47
1:D:320:CYS:HB3	1:D:325:ILE:O	2.15	0.47
1:B:592:THR:N	1:B:593:PRO:CD	2.78	0.47
1:A:251:LYS:O	1:A:255:GLU:HG3	2.16	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:ALA:O	1:C:520:PHE:HA	2.16	0.46
1:B:232:THR:HB	1:B:234:GLU:OE1	2.16	0.46
1:D:326:GLN:HG2	1:B:326:GLN:CG	2.42	0.46
1:D:478:LYS:HE2	1:D:495:ALA:HB1	1.98	0.46
1:B:240:MET:CE	1:B:419:TYR:HD2	2.28	0.46
1:A:478:LYS:HE2	1:A:495:ALA:HB1	1.98	0.46
1:B:251:LYS:O	1:B:255:GLU:HG3	2.16	0.45
1:A:396:TYR:CD1	1:A:437:LYS:HD2	2.50	0.45
1:B:396:TYR:CD1	1:B:437:LYS:HD2	2.52	0.45
3:D:702:GTP:O2G	1:A:116:LYS:NZ	2.29	0.45
1:C:478:LYS:HE2	1:C:495:ALA:HB1	1.98	0.45
1:C:522[A]:CYS:SG	1:A:586:VAL:HG11	2.56	0.45
1:D:396:TYR:CD1	1:D:437:LYS:HD2	2.52	0.45
1:D:543:GLU:CG	1:B:543:GLU:CG	2.95	0.44
1:C:240:MET:CE	1:C:419:TYR:HD2	2.31	0.44
1:A:351:ALA:O	1:A:520:PHE:HA	2.17	0.44
1:C:320:CYS:HB3	1:C:325:ILE:O	2.17	0.44
1:D:171:VAL:HG13	1:D:310:VAL:HG23	2.00	0.44
1:B:478:LYS:HE2	1:B:495:ALA:HB1	1.98	0.44
1:D:543:GLU:HG2	1:B:543:GLU:HG2	2.00	0.44
1:D:240:MET:CE	1:D:419:TYR:HD2	2.30	0.44
1:C:396:TYR:CD1	1:C:437:LYS:HD2	2.53	0.44
1:D:351:ALA:O	1:D:520:PHE:HA	2.17	0.43
1:A:240:MET:CE	1:A:419:TYR:HD2	2.30	0.43
1:C:171:VAL:HG13	1:C:310:VAL:HG23	2.01	0.43
3:D:702:GTP:PA	3:D:702:GTP:H3'	2.58	0.43
1:B:351:ALA:O	1:B:520:PHE:HA	2.18	0.43
1:B:598:TRP:O	1:B:599:ASN:HB2	2.19	0.43
1:C:215:HIS:NE2	2:C:701:DTP:H8	2.34	0.43
1:A:171:VAL:HG13	1:A:310:VAL:HG23	2.01	0.43
1:D:598:TRP:O	1:D:599:ASN:HB2	2.19	0.43
1:C:598:TRP:O	1:C:599:ASN:HB2	2.18	0.42
1:A:598:TRP:O	1:A:599:ASN:HB2	2.18	0.42
1:C:381:ILE:HD12	1:C:381:ILE:HA	1.91	0.42
1:C:586:VAL:HG11	1:A:525:ALA:HB3	2.01	0.42
1:A:320:CYS:HB3	1:A:325:ILE:O	2.18	0.42
1:D:428:LEU:HD12	1:A:425:ASN:HB2	2.01	0.42
1:D:428:LEU:CD1	1:A:425:ASN:HB2	2.50	0.42
1:B:215:HIS:HE1	2:B:704:DTP:O2B	2.03	0.42
1:D:175:ALA:HB1	1:D:199:VAL:HG12	2.02	0.41
1:B:251:LYS:N	1:B:252:PRO:HD2	2.35	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ALA:HB1	1:A:199:VAL:HG12	2.02	0.41
1:D:425:ASN:HB2	1:A:428:LEU:CD1	2.51	0.41
1:C:321:HIS:CE1	1:B:321:HIS:CE1	3.09	0.41
1:C:175:ALA:HB1	1:C:199:VAL:HG12	2.03	0.41
1:B:320:CYS:HB3	1:B:325:ILE:O	2.20	0.41
1:B:354:LYS:NZ	2:B:701:DTP:O1A	2.54	0.41
1:C:150:LEU:CD2	2:C:701:DTP:H2'1	2.51	0.41
1:C:232:THR:HB	1:C:234:GLU:OE1	2.21	0.41
1:B:287:TYR:HB3	1:B:298:TYR:OH	2.21	0.40
1:B:171:VAL:HG13	1:B:310:VAL:HG23	2.02	0.40
1:C:126:ILE:HD13	1:C:126:ILE:HG21	1.89	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	479/514 (93%)	474 (99%)	5 (1%)	0	100	100
1	B	479/514 (93%)	475 (99%)	4 (1%)	0	100	100
1	C	479/514 (93%)	474 (99%)	5 (1%)	0	100	100
1	D	479/514 (93%)	473 (99%)	6 (1%)	0	100	100
All	All	1916/2056 (93%)	1896 (99%)	20 (1%)	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	429/459 (94%)	412 (96%)	17 (4%)	31	51
1	B	429/459 (94%)	412 (96%)	17 (4%)	31	51
1	C	429/459 (94%)	412 (96%)	17 (4%)	31	51
1	D	429/459 (94%)	412 (96%)	17 (4%)	31	51
All	All	1716/1836 (94%)	1648 (96%)	68 (4%)	31	51

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	115	MET
1	D	180	HIS
1	D	190	GLN
1	D	193	GLU
1	D	277	GLU
1	D	284	LEU
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	486	LYS
1	D	492	LYS
1	D	496	GLU
1	D	534	LYS
1	D	535	ASN
1	C	115	MET
1	C	180	HIS
1	C	190	GLN
1	C	193	GLU
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	467	LYS
1	C	478	LYS
1	C	486	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	492	LYS
1	C	496	GLU
1	C	534	LYS
1	C	535	ASN
1	B	115	MET
1	B	180	HIS
1	B	190	GLN
1	B	193	GLU
1	B	277	GLU
1	B	284	LEU
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	486	LYS
1	B	492	LYS
1	B	496	GLU
1	B	534	LYS
1	B	535	ASN
1	A	115	MET
1	A	180	HIS
1	A	190	GLN
1	A	193	GLU
1	A	277	GLU
1	A	284	LEU
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	486	LYS
1	A	492	LYS
1	A	496	GLU
1	A	534	LYS
1	A	535	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:



Mol	Chain	Res	Type
1	D	235	GLN
1	D	364	HIS
1	D	375	GLN
1	D	380	ASN
1	C	235	GLN
1	C	243	HIS
1	C	364	HIS
1	B	235	GLN
1	B	364	HIS
1	B	375	GLN
1	B	380	ASN
1	A	235	GLN
1	A	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 15 ligands modelled in this entry, 4 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	$\# Z  > 2$
2	DTP	D	701	-	26,32,32	1.22	3 (11%)	30,50,50	1.53	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	DTP	D	703	4	26,32,32	1.08	2 (7%)	30,50,50	1.93	10 (33%)
2	DTP	B	704	-	26,32,32	1.14	3 (11%)	30,50,50	1.45	6 (20%)
3	GTP	A	703	4	26,34,34	1.27	3 (11%)	33,54,54	2.11	9 (27%)
3	GTP	D	702	4	26,34,34	1.49	3 (11%)	33,54,54	2.40	12 (36%)
2	DTP	C	701	-	26,32,32	1.15	2 (7%)	30,50,50	1.55	6 (20%)
2	DTP	C	704	4	26,32,32	1.03	1 (3%)	30,50,50	1.53	8 (26%)
2	DTP	A	702	4	26,32,32	1.29	3 (11%)	30,50,50	1.88	7 (23%)
3	GTP	C	703	4	26,34,34	1.12	1 (3%)	33,54,54	2.20	12 (36%)
3	GTP	B	703	4	26,34,34	1.12	3 (11%)	33,54,54	2.10	9 (27%)
2	DTP	B	701	4	26,32,32	1.22	3 (11%)	30,50,50	1.53	6 (20%)

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
2	DTP	D	701	-	-	2/18/34/34	0/3/3/3
2	DTP	D	703	4	-	0/18/34/34	0/3/3/3
2	DTP	B	704	-	-	2/18/34/34	0/3/3/3
3	GTP	A	703	4	-	4/18/38/38	0/3/3/3
3	GTP	D	702	4	-	5/18/38/38	0/3/3/3
2	DTP	C	701	-	-	1/18/34/34	0/3/3/3
2	DTP	C	704	4	-	5/18/34/34	0/3/3/3
2	DTP	A	702	4	-	0/18/34/34	0/3/3/3
3	GTP	C	703	4	-	4/18/38/38	0/3/3/3
3	GTP	B	703	4	-	3/18/38/38	0/3/3/3
2	DTP	B	701	4	-	2/18/34/34	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	702	GTP	C5-C6	4.48	1.49	1.41
3	D	702	GTP	C2'-C1'	-3.64	1.48	1.53
3	C	703	GTP	C5-C6	3.43	1.47	1.41
2	D	701	DTP	C5-C4	3.26	1.49	1.40
3	A	703	GTP	C5-C6	3.21	1.46	1.41
2	B	704	DTP	C5-C4	3.17	1.49	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	DTP	C5-C4	2.80	1.48	1.40
2	C	701	DTP	C2-N3	2.74	1.36	1.32
3	A	703	GTP	C5-C4	2.70	1.48	1.40
3	B	703	GTP	C5-C6	2.65	1.45	1.41
2	A	702	DTP	C2-N3	2.64	1.36	1.32
3	D	702	GTP	C5-C4	2.64	1.47	1.40
2	D	701	DTP	C2-N3	2.63	1.36	1.32
2	A	702	DTP	C5-C4	2.62	1.47	1.40
2	D	703	DTP	O4'-C4'	-2.60	1.39	1.45
2	B	701	DTP	C2-N3	2.52	1.36	1.32
3	A	703	GTP	C6-N1	2.49	1.37	1.33
3	B	703	GTP	C2'-C1'	-2.45	1.50	1.53
2	B	704	DTP	C2-N3	2.42	1.36	1.32
2	B	701	DTP	O4'-C1'	2.27	1.47	1.42
2	C	704	DTP	C5-C4	2.19	1.46	1.40
2	B	701	DTP	C5-C4	2.14	1.46	1.40
2	D	701	DTP	C6-C5	2.14	1.51	1.43
3	B	703	GTP	C5-C4	2.12	1.46	1.40
2	D	703	DTP	C5-C4	2.08	1.46	1.40
2	A	702	DTP	PG-O2G	-2.05	1.47	1.54
2	B	704	DTP	C6-C5	2.02	1.50	1.43

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	702	GTP	C3'-C2'-C1'	5.57	109.37	100.98
3	D	702	GTP	PA-O3A-PB	-5.30	114.63	132.83
3	C	703	GTP	C2-N3-C4	5.19	121.28	115.36
3	B	703	GTP	C2-N1-C6	4.83	123.61	115.93
2	A	702	DTP	PA-O3A-PB	-4.72	116.64	132.83
2	D	703	DTP	N3-C2-N1	-4.71	121.32	128.68
3	A	703	GTP	C2-N3-C4	4.71	120.73	115.36
3	D	702	GTP	C2-N3-C4	4.67	120.69	115.36
3	B	703	GTP	C4-C5-C6	-4.66	116.35	120.80
3	B	703	GTP	C5-C6-N1	-4.56	117.19	123.43
3	A	703	GTP	N3-C2-N1	-4.48	121.25	127.22
3	C	703	GTP	C4-C5-C6	-4.47	116.53	120.80
2	A	702	DTP	C4-C5-N7	-4.39	104.82	109.40
3	D	702	GTP	C4-C5-C6	-4.34	116.65	120.80
3	A	703	GTP	C2-N1-C6	4.29	122.75	115.93
3	B	703	GTP	N3-C2-N1	-4.25	121.55	127.22
3	A	703	GTP	C4-C5-C6	-4.23	116.75	120.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	703	GTP	C2-N3-C4	4.22	120.17	115.36
3	D	702	GTP	C5-C6-N1	-4.14	117.77	123.43
3	A	703	GTP	C5-C6-N1	-4.12	117.80	123.43
3	D	702	GTP	C2-N1-C6	4.03	122.34	115.93
3	C	703	GTP	C3'-C2'-C1'	3.91	106.87	100.98
2	C	701	DTP	N3-C2-N1	-3.89	122.60	128.68
3	C	703	GTP	C2-N1-C6	3.76	121.91	115.93
2	D	703	DTP	C2-N1-C6	3.67	125.04	118.75
3	C	703	GTP	PA-O3A-PB	-3.65	120.30	132.83
2	B	704	DTP	N3-C2-N1	-3.62	123.01	128.68
2	C	704	DTP	C4-C5-N7	-3.62	105.63	109.40
3	C	703	GTP	N3-C2-N1	-3.59	122.44	127.22
2	B	701	DTP	PA-O3A-PB	-3.53	120.73	132.83
2	D	703	DTP	O2G-PG-O1G	3.46	124.23	110.68
3	C	703	GTP	C5-C6-N1	-3.28	118.94	123.43
2	D	701	DTP	N3-C2-N1	-3.27	123.57	128.68
2	A	702	DTP	C2'-C3'-C4'	3.26	109.54	102.76
3	A	703	GTP	PA-O3A-PB	-3.21	121.83	132.83
2	A	702	DTP	N3-C2-N1	-3.20	123.68	128.68
2	D	703	DTP	C2'-C3'-C4'	3.19	109.41	102.76
2	D	701	DTP	PB-O3B-PG	-3.12	122.12	132.83
3	D	702	GTP	N3-C2-N1	-3.11	123.08	127.22
2	D	701	DTP	C4-C5-N7	-3.00	106.27	109.40
2	C	704	DTP	PB-O3B-PG	-2.98	122.60	132.83
2	D	703	DTP	PB-O3B-PG	-2.97	122.63	132.83
3	B	703	GTP	PB-O3B-PG	-2.97	122.64	132.83
2	C	701	DTP	PB-O3B-PG	-2.96	122.67	132.83
2	A	702	DTP	PB-O3B-PG	-2.96	122.68	132.83
2	D	701	DTP	PA-O3A-PB	-2.91	122.85	132.83
3	A	703	GTP	N2-C2-N1	2.90	121.77	117.25
2	B	704	DTP	C4-C5-N7	-2.90	106.38	109.40
2	B	701	DTP	O2G-PG-O1G	2.88	121.96	110.68
3	D	702	GTP	O2G-PG-O1G	2.88	121.95	110.68
2	B	704	DTP	PB-O3B-PG	-2.86	123.01	132.83
2	D	703	DTP	O3G-PG-O3B	2.80	114.02	104.64
3	D	702	GTP	O4'-C1'-C2'	-2.77	102.87	106.93
2	B	701	DTP	C4-C5-N7	-2.74	106.54	109.40
2	B	704	DTP	PA-O3A-PB	-2.73	123.45	132.83
2	C	701	DTP	C4-C5-N7	-2.64	106.65	109.40
3	A	703	GTP	C3'-C2'-C1'	2.60	104.89	100.98
2	A	702	DTP	C5-C6-N6	2.59	124.30	120.35
2	A	702	DTP	C2-N1-C6	2.58	123.17	118.75

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	DTP	PA-O3A-PB	-2.58	123.98	132.83
3	B	703	GTP	C3'-C2'-C1'	2.51	104.75	100.98
2	C	704	DTP	C2'-C3'-C4'	2.50	107.98	102.76
3	C	703	GTP	C4-C5-N7	-2.48	106.81	109.40
2	D	703	DTP	C4-C5-N7	-2.45	106.85	109.40
3	B	703	GTP	N2-C2-N1	2.43	121.03	117.25
2	B	701	DTP	O2G-PG-O3B	-2.43	96.49	104.64
3	D	702	GTP	O2'-C2'-C1'	-2.41	101.95	110.85
3	C	703	GTP	O5'-PA-O1A	-2.40	99.68	109.07
2	C	704	DTP	PA-O3A-PB	-2.39	124.62	132.83
2	C	704	DTP	C5-C6-N6	2.39	123.98	120.35
2	D	703	DTP	O2G-PG-O3B	-2.37	96.68	104.64
2	D	703	DTP	PA-O3A-PB	-2.33	124.82	132.83
2	C	704	DTP	N3-C2-N1	-2.32	125.05	128.68
2	B	701	DTP	N3-C2-N1	-2.31	125.06	128.68
2	B	704	DTP	O3G-PG-O2G	2.30	116.42	107.64
2	C	701	DTP	C2'-C3'-C4'	2.28	107.51	102.76
3	D	702	GTP	O3B-PG-O1G	-2.28	98.55	111.19
3	B	703	GTP	PA-O3A-PB	-2.28	125.01	132.83
2	C	701	DTP	O2A-PA-O1A	2.23	123.26	112.24
3	A	703	GTP	O3B-PG-O1G	-2.23	98.83	111.19
2	D	703	DTP	C5-C6-N6	2.22	123.73	120.35
3	D	702	GTP	PB-O3B-PG	-2.22	125.22	132.83
3	C	703	GTP	PB-O3B-PG	-2.19	125.30	132.83
2	B	704	DTP	C2-N1-C6	2.19	122.50	118.75
3	C	703	GTP	O2'-C2'-C1'	-2.14	102.94	110.85
2	C	704	DTP	O2B-PB-O1B	2.14	122.80	112.24
3	C	703	GTP	O2G-PG-O1G	2.09	118.88	110.68
2	B	701	DTP	PB-O3B-PG	-2.06	125.75	132.83
2	C	704	DTP	C2-N1-C6	2.05	122.27	118.75

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	701	DTP	C5'-O5'-PA-O2A
2	D	701	DTP	C5'-O5'-PA-O3A
3	D	702	GTP	PB-O3B-PG-O3G
3	A	703	GTP	PB-O3B-PG-O1G
2	B	701	DTP	PB-O3B-PG-O2G
2	B	701	DTP	PB-O3B-PG-O3G
2	C	704	DTP	PG-O3B-PB-O1B

*Continued on next page...*

*Continued from previous page...*

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

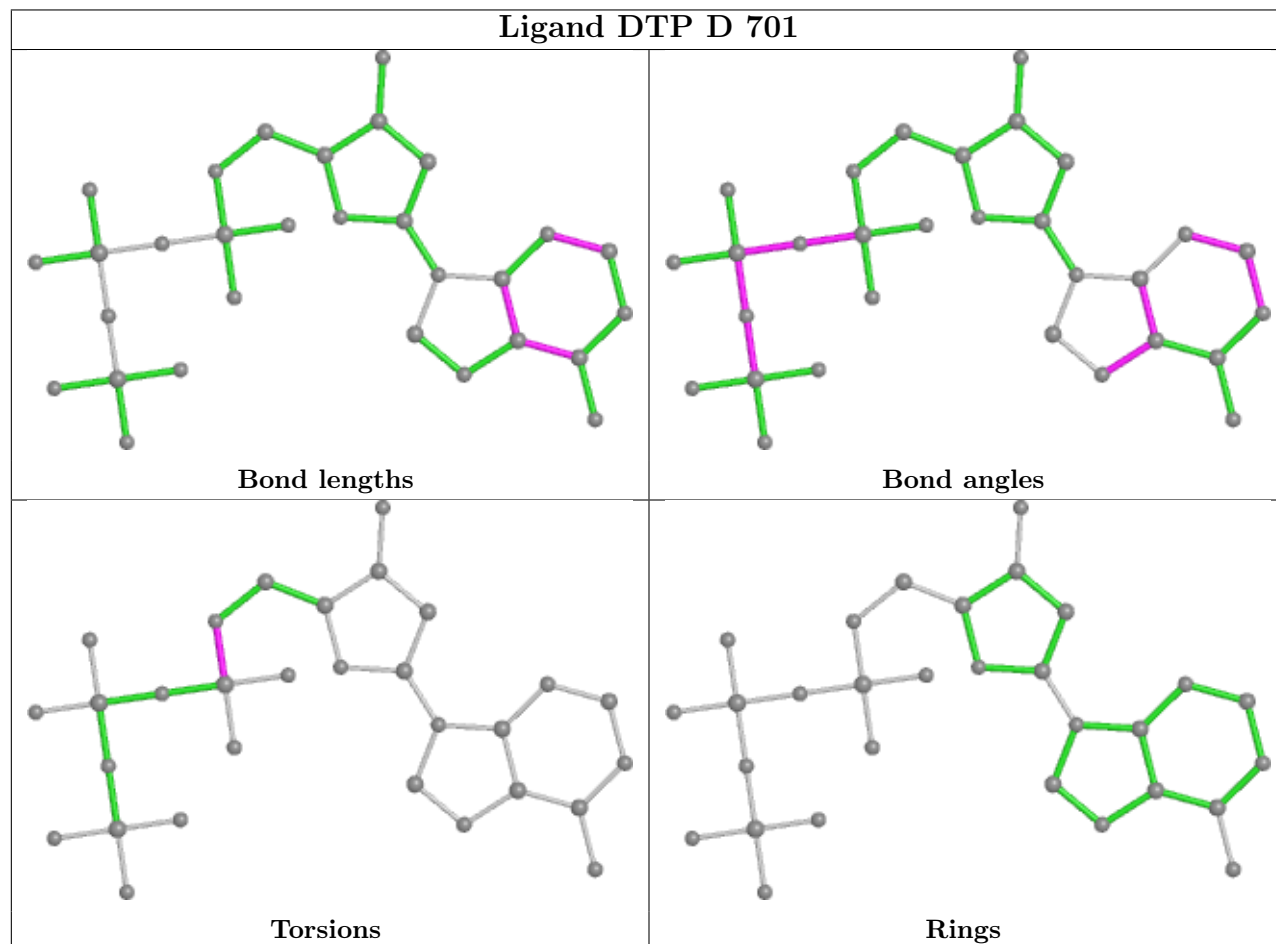
There are no ring outliers.

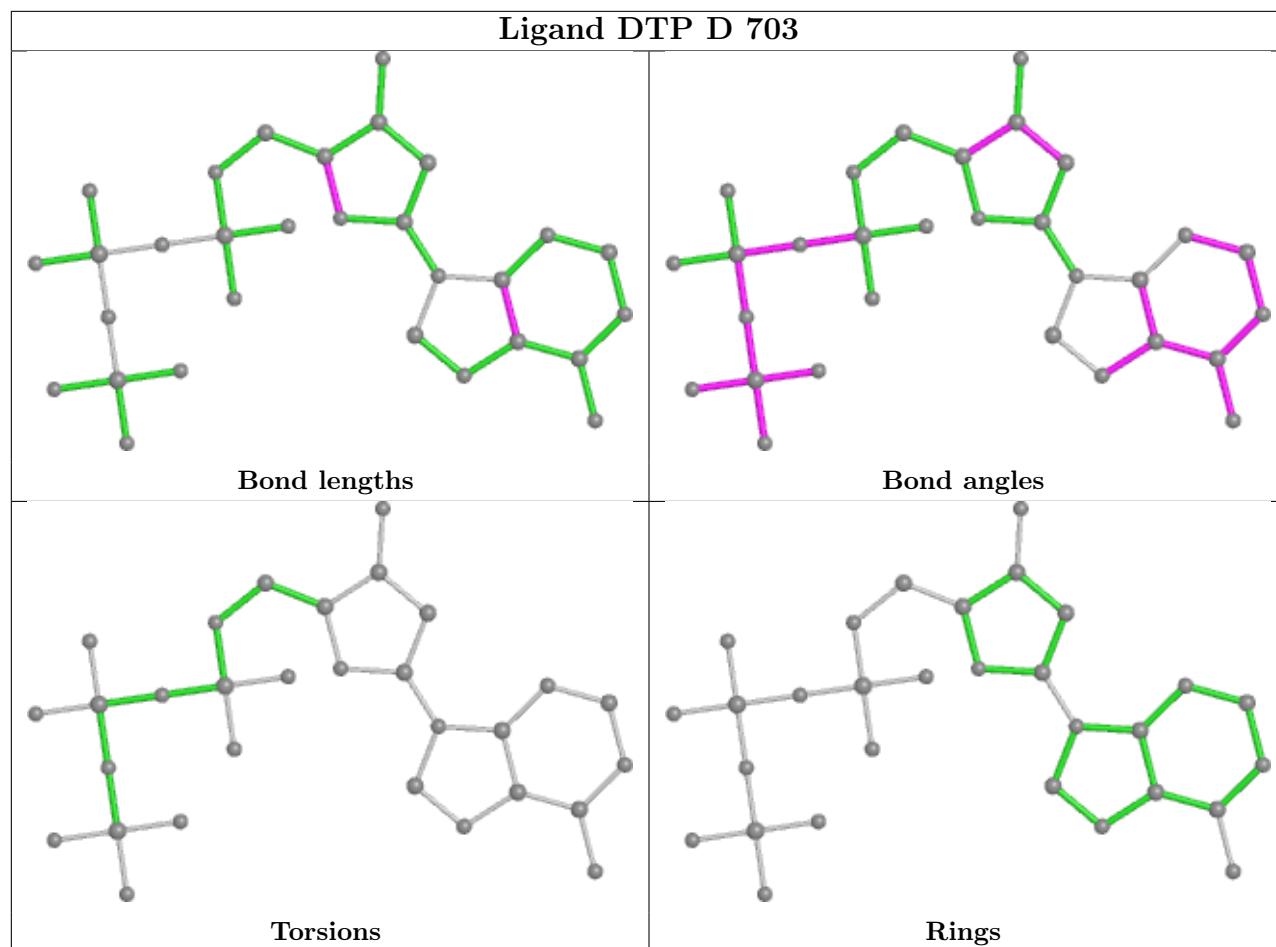
9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	701	DTP	1	0
2	D	703	DTP	1	0
2	B	704	DTP	3	0
3	D	702	GTP	2	0
2	C	701	DTP	3	0
2	C	704	DTP	1	0
2	A	702	DTP	1	0
3	C	703	GTP	1	0
2	B	701	DTP	2	0

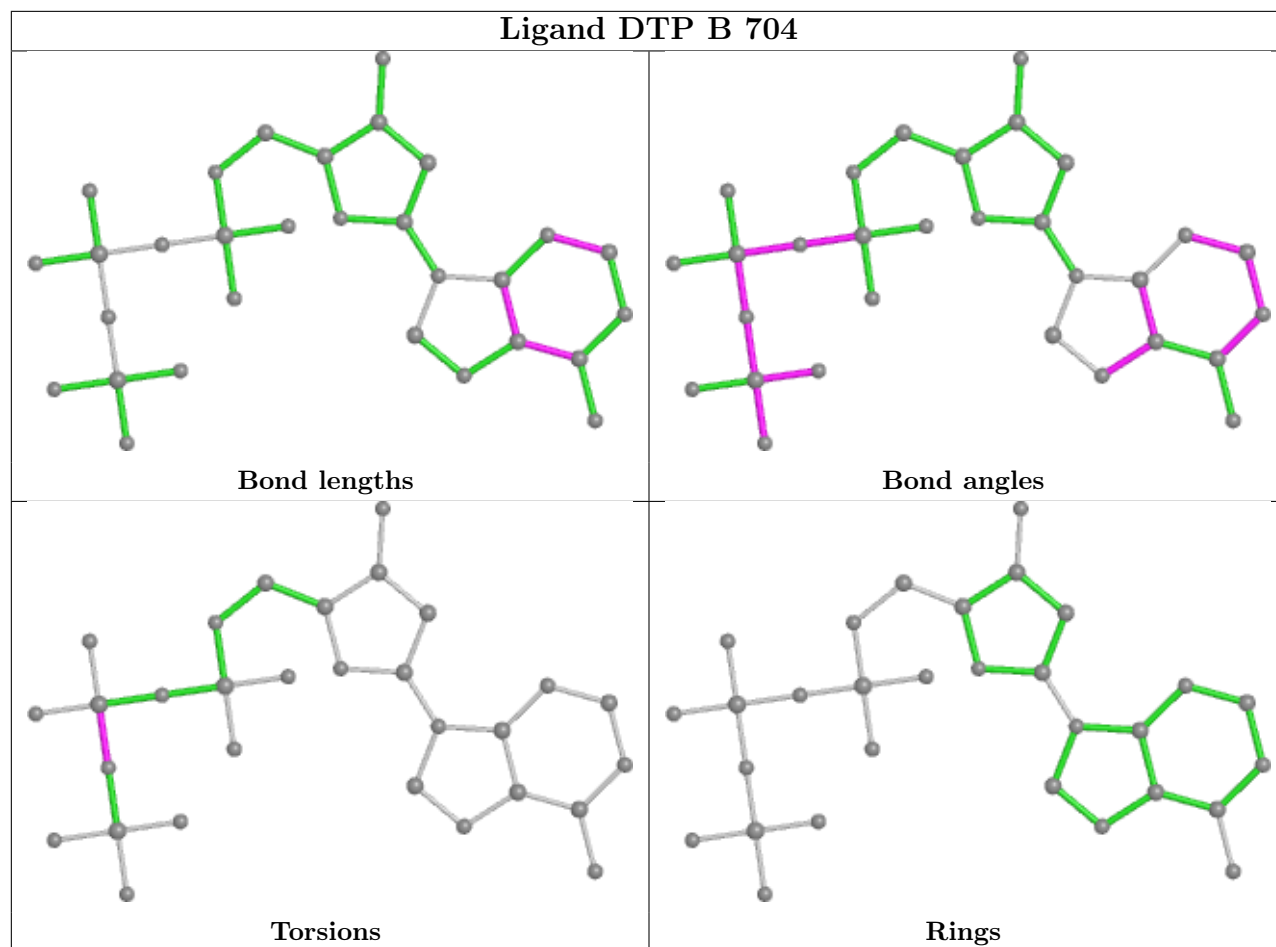
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

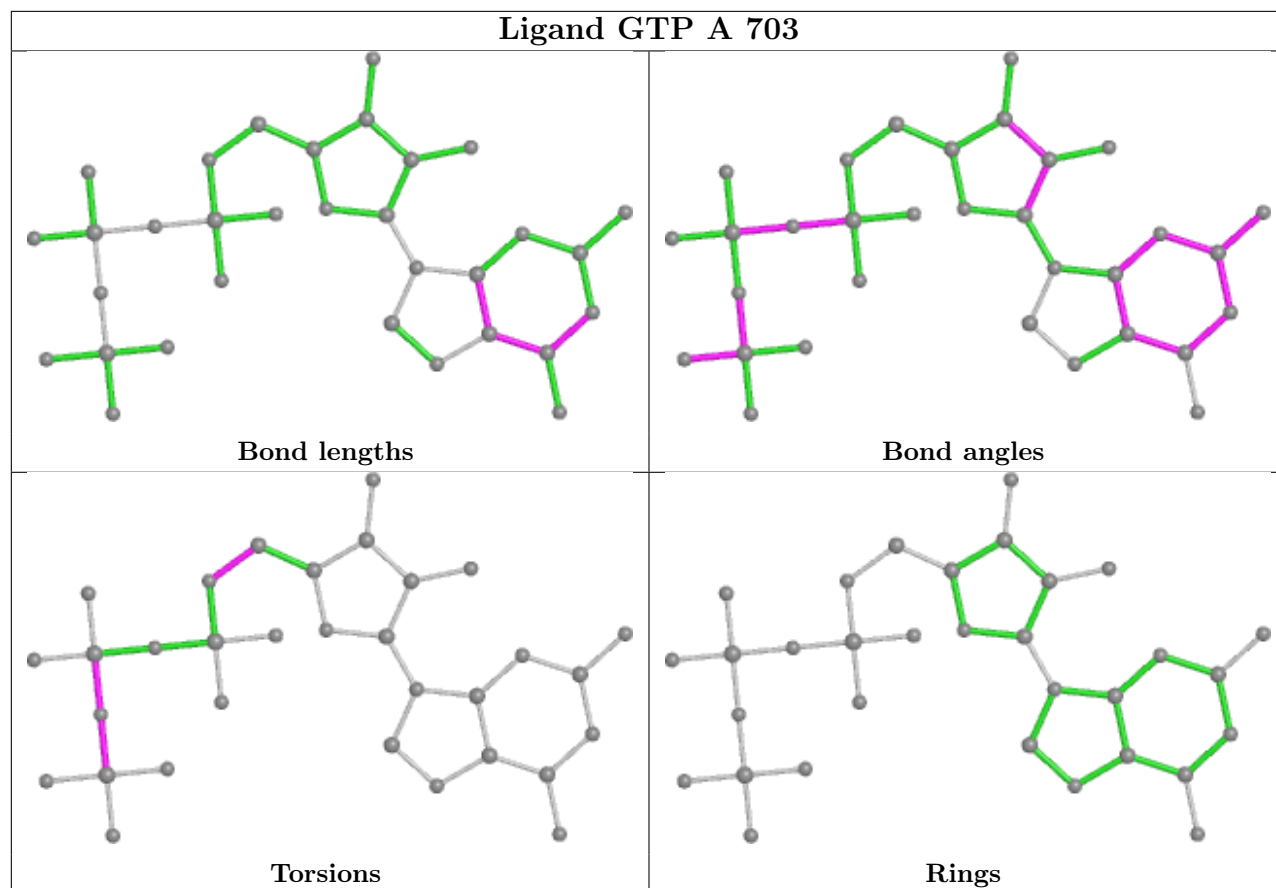




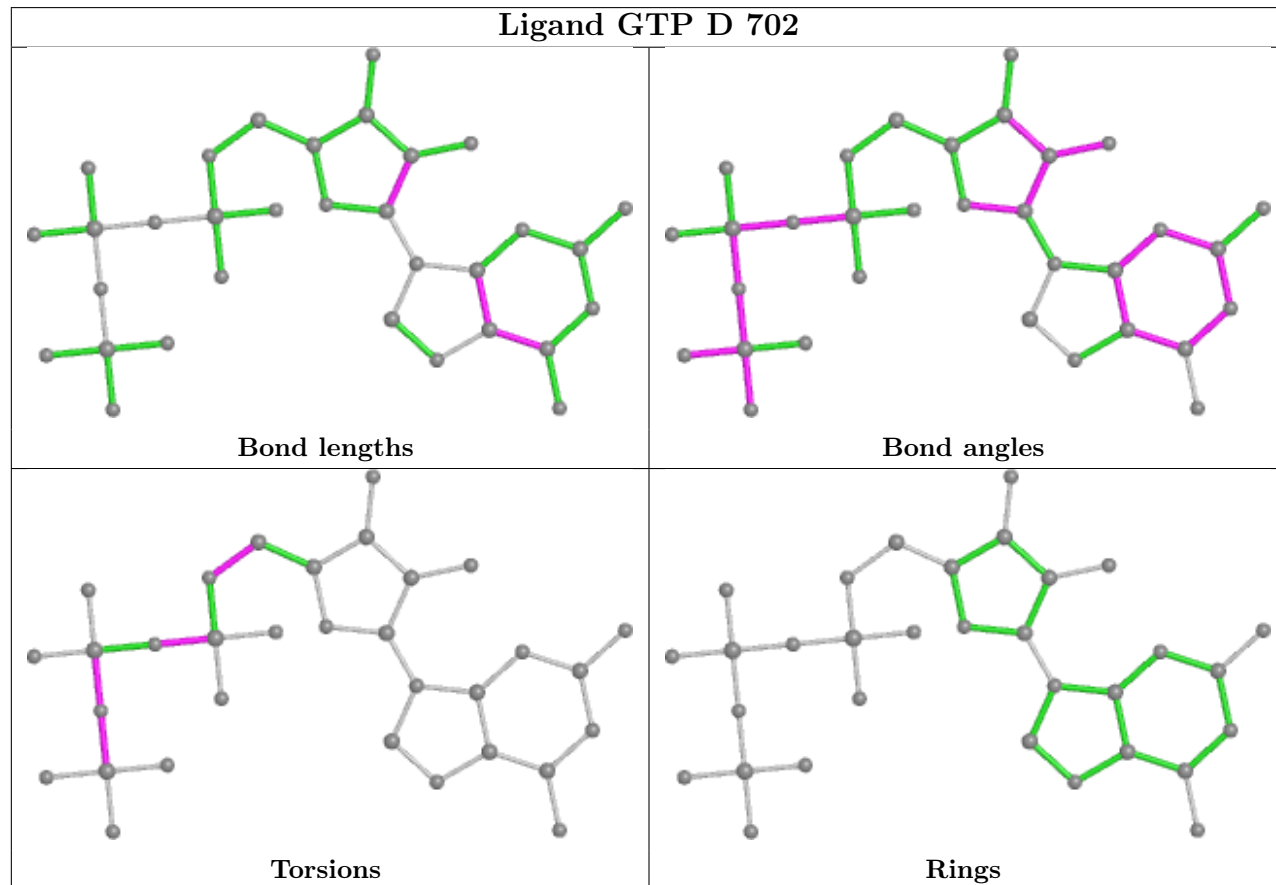


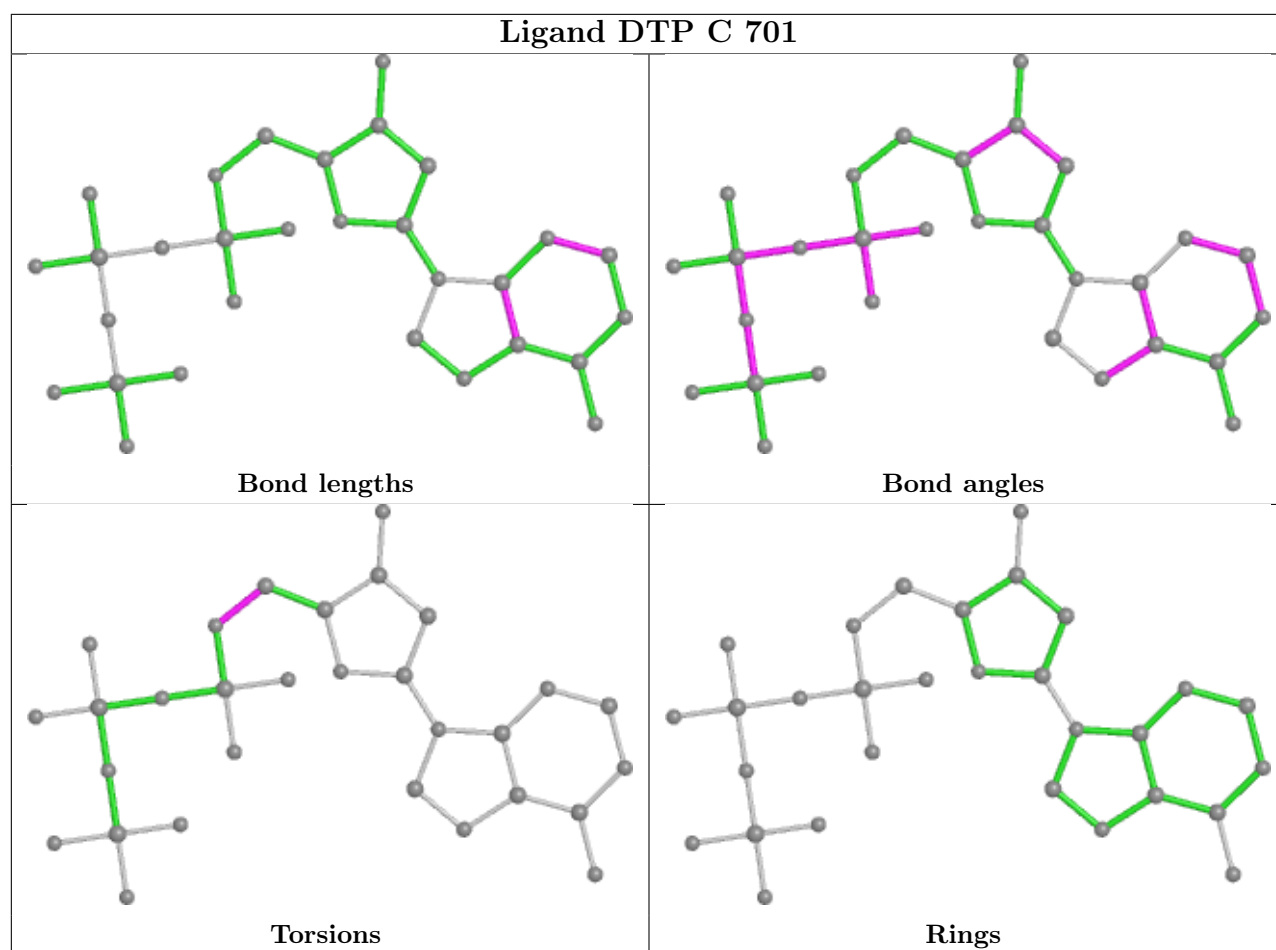


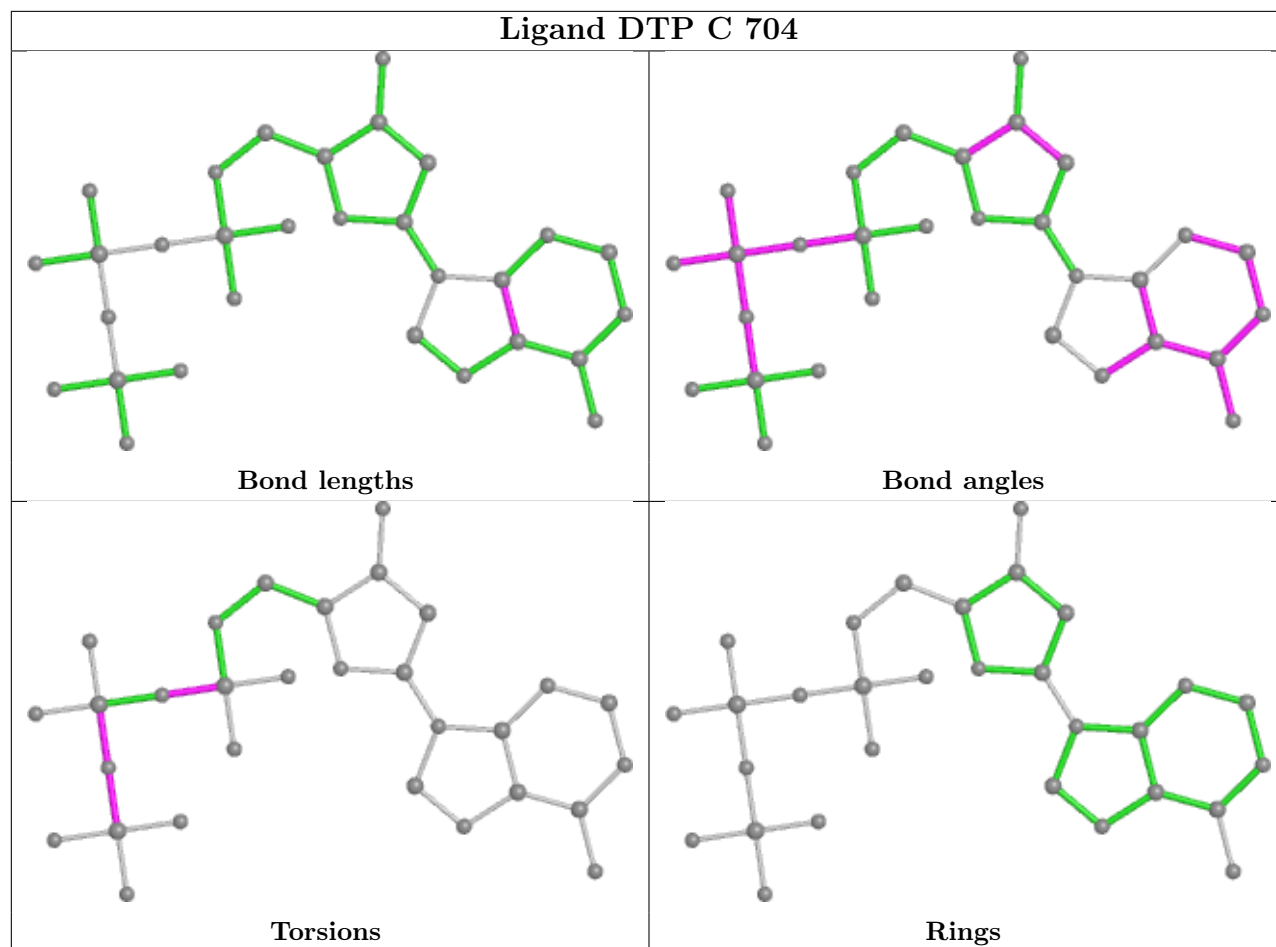
## Ligand GTP A 703

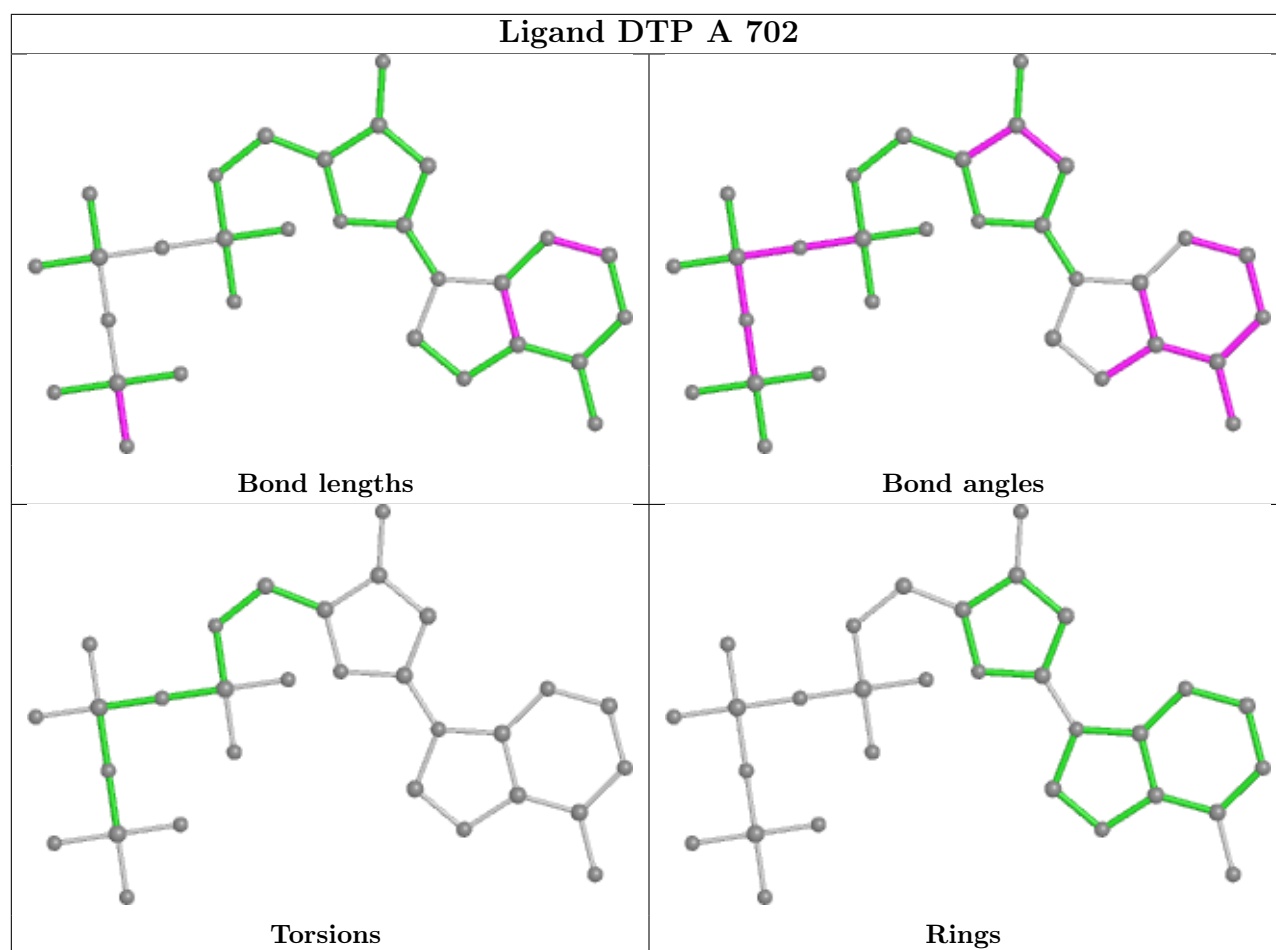


## Ligand GTP D 702

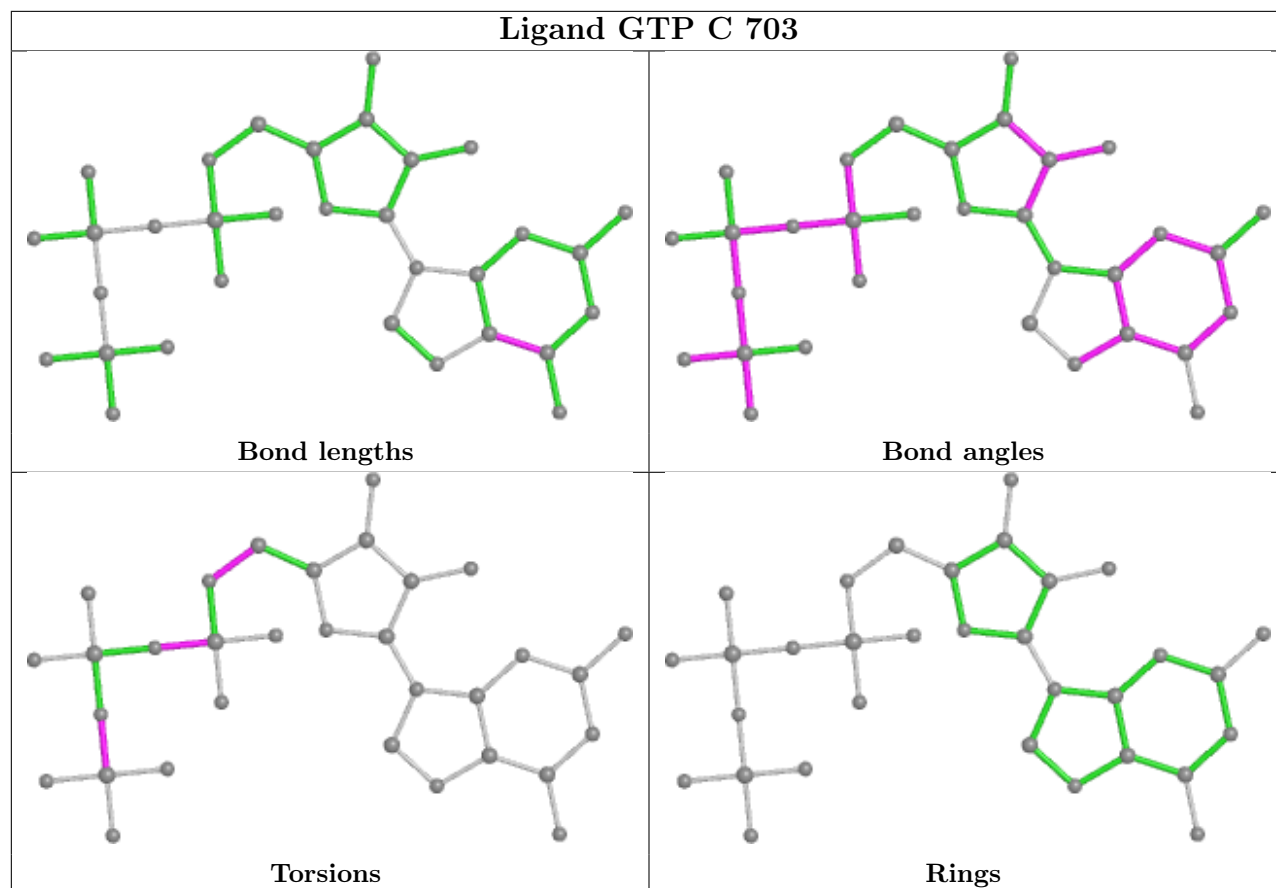




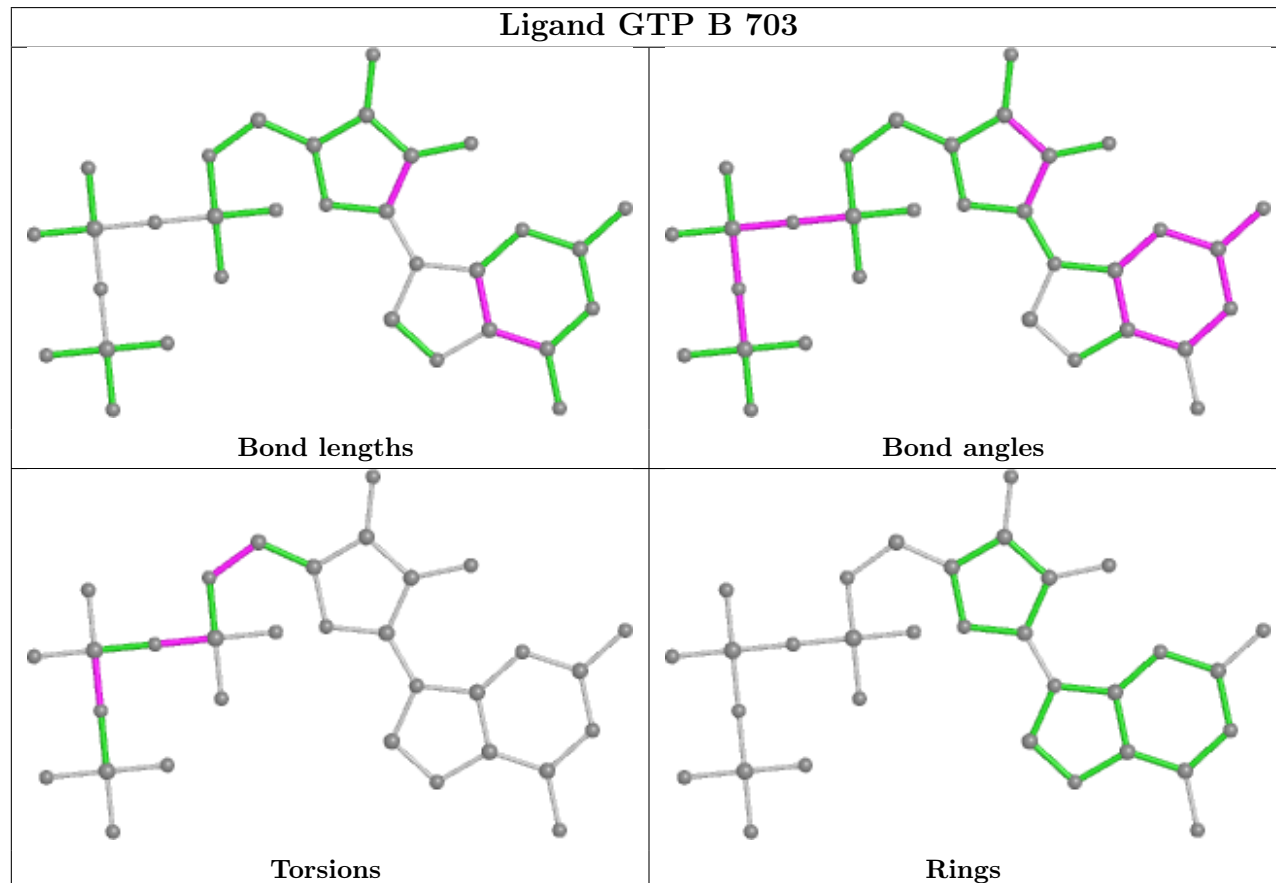


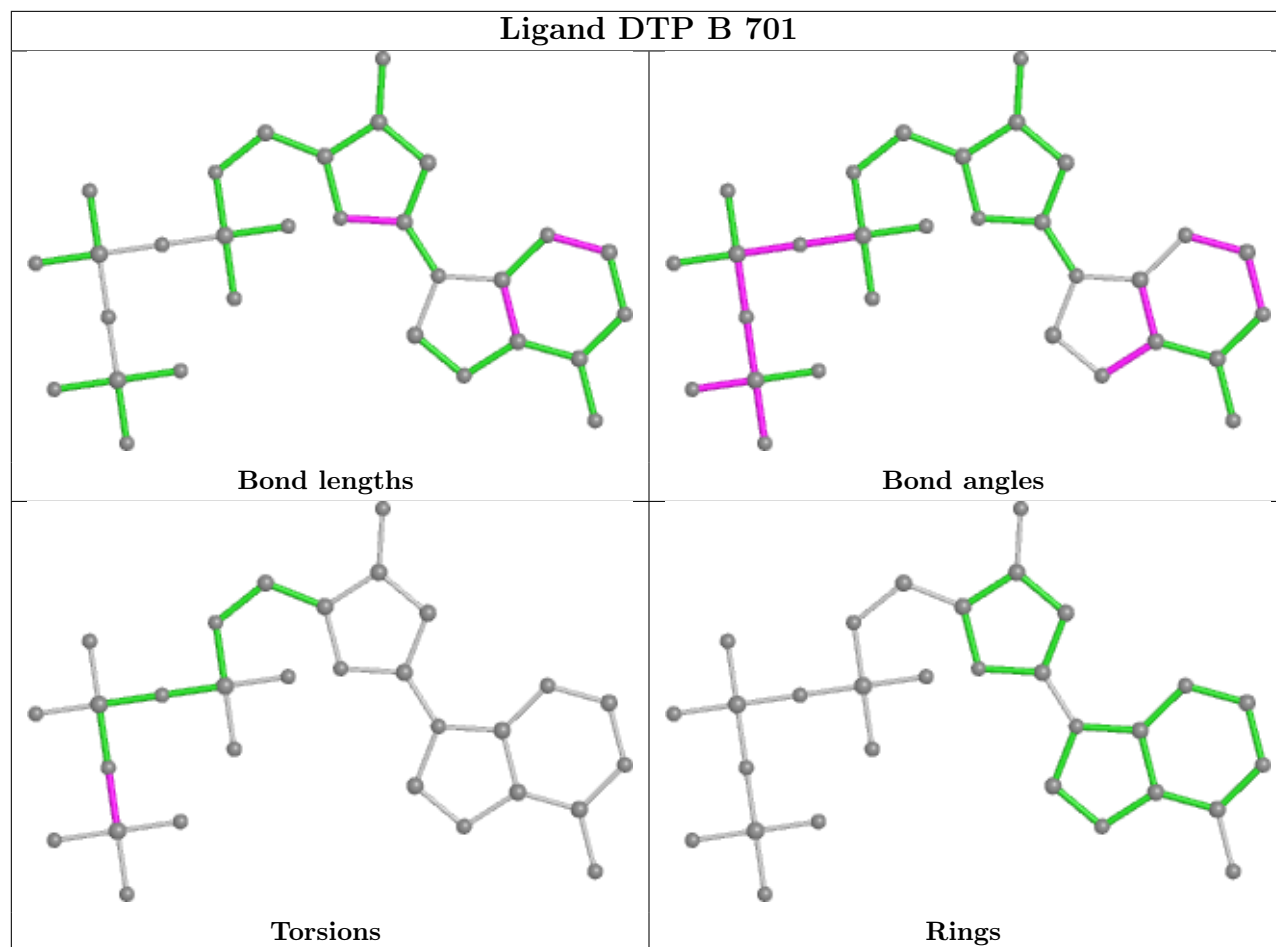


## Ligand GTP C 703



## Ligand GTP B 703





## 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	481/514 (93%)	1.47	133 (27%) <b>0</b> <b>0</b>	43, 114, 190, 223	0
1	B	481/514 (93%)	1.01	88 (18%) <b>1</b> <b>1</b>	42, 91, 150, 190	0
1	C	481/514 (93%)	1.05	89 (18%) <b>1</b> <b>1</b>	37, 87, 161, 200	0
1	D	481/514 (93%)	0.56	30 (6%) <b>20</b> <b>25</b>	37, 74, 115, 162	0
All	All	1924/2056 (93%)	1.02	340 (17%) <b>1</b> <b>1</b>	37, 89, 164, 223	0

All (340) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	489	LEU	10.5
1	C	493	LEU	9.4
1	A	573	CYS	8.4
1	C	488	LEU	7.7
1	C	598	TRP	7.7
1	C	590	LEU	7.7
1	B	490	ASP	7.6
1	A	485	PRO	7.5
1	A	569	PHE	7.2
1	C	584	GLY	7.0
1	A	275	PRO	7.0
1	A	478	LYS	6.9
1	A	473	TYR	6.9
1	A	345	ASN	6.9
1	C	490	ASP	6.9
1	A	493	LEU	6.9
1	A	341	CYS	6.8
1	C	498	PHE	6.7
1	C	543	GLU	6.5
1	A	578	PHE	6.4
1	C	572	TRP	6.3

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	488	LEU	6.2
1	B	493	LEU	6.2
1	C	485	PRO	6.2
1	B	498	PHE	6.2
1	A	476	LEU	6.1
1	A	489	LEU	6.1
1	A	480	VAL	6.1
1	A	498	PHE	6.1
1	A	599	ASN	6.0
1	A	230	LYS	6.0
1	A	572	TRP	5.9
1	C	587	ILE	5.9
1	B	464	GLY	5.9
1	A	457	VAL	5.8
1	B	471	GLU	5.8
1	A	481	ALA	5.8
1	A	488	LEU	5.7
1	D	408	ARG	5.7
1	B	487	VAL	5.7
1	C	484	LYS	5.6
1	C	487	VAL	5.5
1	C	489	LEU	5.5
1	C	492	LYS	5.5
1	C	557	VAL	5.5
1	B	473	TYR	5.4
1	A	554	CYS	5.3
1	C	589	PRO	5.3
1	A	468	ILE	5.2
1	B	486	LYS	5.1
1	A	350	CYS	4.9
1	A	563	TYR	4.9
1	B	113	ASP	4.9
1	B	575	ASP	4.9
1	B	484	LYS	4.8
1	C	491	VAL	4.7
1	B	590	LEU	4.7
1	B	263	GLU	4.6
1	C	483	ALA	4.6
1	B	255	GLU	4.6
1	A	511[A]	GLU	4.6
1	C	578	PHE	4.6
1	B	599	ASN	4.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	554	CYS	4.5
1	A	530	ILE	4.5
1	B	568	TYR	4.5
1	A	586	VAL	4.4
1	A	340	VAL	4.3
1	A	472	ASP	4.3
1	A	577	ASN	4.3
1	C	229	VAL	4.3
1	C	582	GLN	4.3
1	D	245	ILE	4.3
1	A	484	LYS	4.3
1	B	573	CYS	4.3
1	C	573	CYS	4.3
1	A	500	VAL	4.2
1	D	255	GLU	4.2
1	C	494	LYS	4.1
1	B	571	GLN	4.1
1	B	468	ILE	4.1
1	C	563	TYR	4.1
1	A	592	THR	4.0
1	A	343	VAL	4.0
1	B	572	TRP	4.0
1	B	592	THR	4.0
1	A	277	GLU	4.0
1	C	480	VAL	4.0
1	B	594	GLN	3.9
1	A	347	LEU	3.9
1	D	242	GLU	3.9
1	C	478	LYS	3.8
1	C	554	CYS	3.8
1	A	568	TYR	3.8
1	D	263	GLU	3.8
1	B	586	VAL	3.8
1	A	562	LEU	3.8
1	A	349	ILE	3.8
1	A	529	ALA	3.8
1	A	467	LYS	3.8
1	B	500	VAL	3.8
1	A	544	LYS	3.8
1	C	461	GLN	3.8
1	A	390	PHE	3.8
1	B	276	LEU	3.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	287	TYR	3.7
1	A	471	GLU	3.7
1	B	492	LYS	3.6
1	C	571	GLN	3.6
1	A	491	VAL	3.6
1	C	465	GLN	3.6
1	A	262	GLU	3.6
1	C	583	ASP	3.6
1	A	229	VAL	3.6
1	A	492	LYS	3.6
1	A	520	PHE	3.5
1	C	471	GLU	3.5
1	B	562	LEU	3.5
1	A	585	ASP	3.5
1	A	531	ARG	3.5
1	B	250	ILE	3.5
1	D	288	LYS	3.5
1	A	286	PRO	3.5
1	A	470	ARG	3.5
1	B	565	ALA	3.5
1	B	253	VAL	3.5
1	B	491	VAL	3.5
1	B	591	ILE	3.5
1	A	434	THR	3.4
1	B	403	GLY	3.4
1	A	487	VAL	3.4
1	A	494	LYS	3.4
1	B	483	ALA	3.4
1	A	504	ASN	3.4
1	A	590	LEU	3.4
1	D	466	ILE	3.4
1	C	228	GLU	3.4
1	C	569	PHE	3.4
1	C	599	ASN	3.4
1	B	497	ASP	3.3
1	B	262	GLU	3.3
1	A	490	ASP	3.3
1	A	403	GLY	3.3
1	B	556	LYS	3.3
1	A	469	LYS	3.2
1	D	287	TYR	3.2
1	C	556	LYS	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	557	VAL	3.2
1	A	502	VAL	3.2
1	B	257	TYR	3.2
1	B	485	PRO	3.2
1	A	284	LEU	3.2
1	C	113	ASP	3.2
1	B	553	TYR	3.2
1	A	483	ALA	3.2
1	B	560	LYS	3.2
1	A	291	PRO	3.2
1	A	465	GLN	3.2
1	A	496	GLU	3.1
1	D	252	PRO	3.1
1	C	594	GLN	3.1
1	B	593	PRO	3.1
1	B	478	LYS	3.1
1	B	480	VAL	3.1
1	D	465	GLN	3.1
1	A	499	ILE	3.1
1	D	113	ASP	3.1
1	C	497	ASP	3.1
1	C	562	LEU	3.1
1	C	586	VAL	3.1
1	A	574	ALA	3.1
1	A	497	ASP	3.1
1	B	285	TRP	3.0
1	A	557	VAL	3.0
1	A	528	ARG	3.0
1	C	482	SER	3.0
1	D	201	ILE	3.0
1	C	288	LYS	3.0
1	A	587	ILE	3.0
1	C	595	LYS	3.0
1	B	259	LEU	3.0
1	C	462	PRO	3.0
1	C	568	TYR	2.9
1	C	597	GLU	2.9
1	D	114	THR	2.9
1	A	548	GLN	2.9
1	A	507	TYR	2.9
1	A	595	LYS	2.9
1	D	262	GLU	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	347	LEU	2.9
1	B	286	PRO	2.9
1	D	486	LYS	2.9
1	C	555	LYS	2.9
1	A	189	LEU	2.9
1	C	397	ILE	2.8
1	C	544	LYS	2.8
1	B	129	HIS	2.8
1	A	288	LYS	2.8
1	A	395	ASP	2.8
1	A	399	ILE	2.8
1	C	328	ASN	2.8
1	B	345	ASN	2.8
1	B	287	TYR	2.8
1	D	464	GLY	2.8
1	A	508	GLY	2.8
1	A	413	ILE	2.8
1	A	524	THR	2.8
1	B	563	TYR	2.7
1	A	299	GLU	2.7
1	C	481	ALA	2.7
1	A	388	ASP	2.7
1	A	266	CYS	2.7
1	A	440	ASP	2.7
1	A	591	ILE	2.7
1	B	584	GLY	2.7
1	B	569	PHE	2.7
1	A	224	LEU	2.7
1	C	553	TYR	2.7
1	A	342	GLU	2.7
1	B	481	ALA	2.7
1	C	593	PRO	2.6
1	A	273	VAL	2.6
1	A	545	PHE	2.6
1	C	567	GLN	2.6
1	C	574	ALA	2.6
1	D	298	TYR	2.6
1	C	396	TYR	2.6
1	A	191	ILE	2.6
1	D	326	GLN	2.6
1	C	470	ARG	2.6
1	D	205	CYS	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	564	ALA	2.6
1	A	555	LYS	2.6
1	C	400	THR	2.5
1	B	245	ILE	2.5
1	C	263	GLU	2.5
1	A	348	ARG	2.5
1	A	244	LEU	2.5
1	A	276	LEU	2.5
1	C	524	THR	2.5
1	A	462	PRO	2.5
1	A	466	ILE	2.5
1	A	576	ARG	2.5
1	A	326	GLN	2.5
1	A	475	SER	2.5
1	C	526	PRO	2.5
1	A	526	PRO	2.5
1	C	570	VAL	2.5
1	C	564	ALA	2.5
1	A	510	GLN	2.5
1	D	259	LEU	2.5
1	B	252	PRO	2.4
1	B	241	PHE	2.4
1	B	293	ASN	2.4
1	B	190	GLN	2.4
1	A	519	SER	2.4
1	B	228	GLU	2.4
1	A	565	ALA	2.4
1	A	598	TRP	2.4
1	A	267	PHE	2.4
1	D	490	ASP	2.4
1	D	286	PRO	2.4
1	B	495	ALA	2.4
1	C	581	PRO	2.4
1	B	284	LEU	2.4
1	C	275	PRO	2.3
1	B	496	GLU	2.3
1	A	298	TYR	2.3
1	A	584	GLY	2.3
1	A	570	VAL	2.3
1	C	559	ARG	2.3
1	D	241	PHE	2.3
1	C	344	ASP	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	585	ASP	2.3
1	A	512	LYS	2.3
1	C	460	THR	2.3
1	B	390	PHE	2.3
1	B	466	ILE	2.3
1	A	596	LYS	2.3
1	B	469	LYS	2.2
1	C	409	ILE	2.2
1	A	223	PRO	2.2
1	A	438	LEU	2.2
1	A	495	ALA	2.2
1	C	548	GLN	2.2
1	B	326	GLN	2.2
1	A	594	GLN	2.2
1	B	288	LYS	2.2
1	C	579	THR	2.2
1	A	221	PHE	2.2
1	B	260	ILE	2.2
1	C	438	LEU	2.2
1	C	588	ALA	2.2
1	B	494	LYS	2.2
1	A	274	GLY	2.2
1	C	545	PHE	2.2
1	B	179	VAL	2.2
1	B	340	VAL	2.2
1	D	285	TRP	2.2
1	B	465	GLN	2.2
1	C	577	ASN	2.2
1	C	253	VAL	2.1
1	B	566	ARG	2.1
1	B	574	ALA	2.1
1	A	559	ARG	2.1
1	A	327	ASN	2.1
1	D	253	VAL	2.1
1	B	114	THR	2.1
1	A	285	TRP	2.1
1	A	460	THR	2.1
1	C	327	ASN	2.1
1	C	560	LYS	2.1
1	D	327	ASN	2.1
1	D	594	GLN	2.1
1	A	419	TYR	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	456	TYR	2.1
1	C	547	GLU	2.1
1	A	231	TRP	2.1
1	C	540	LEU	2.1
1	C	591	ILE	2.1
1	B	325	ILE	2.1
1	A	503	ILE	2.1
1	C	463	THR	2.1
1	A	402	ALA	2.1
1	A	486	LYS	2.1
1	B	476	LEU	2.1
1	D	260	ILE	2.1
1	C	441	ALA	2.1
1	C	531	ARG	2.1
1	B	587	ILE	2.0
1	A	553	TYR	2.0
1	B	402	ALA	2.0
1	B	598	TRP	2.0
1	C	399	ILE	2.0
1	C	466	ILE	2.0
1	A	386	ILE	2.0
1	D	560	LYS	2.0
1	A	396	TYR	2.0
1	B	189	LEU	2.0
1	B	347	LEU	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.

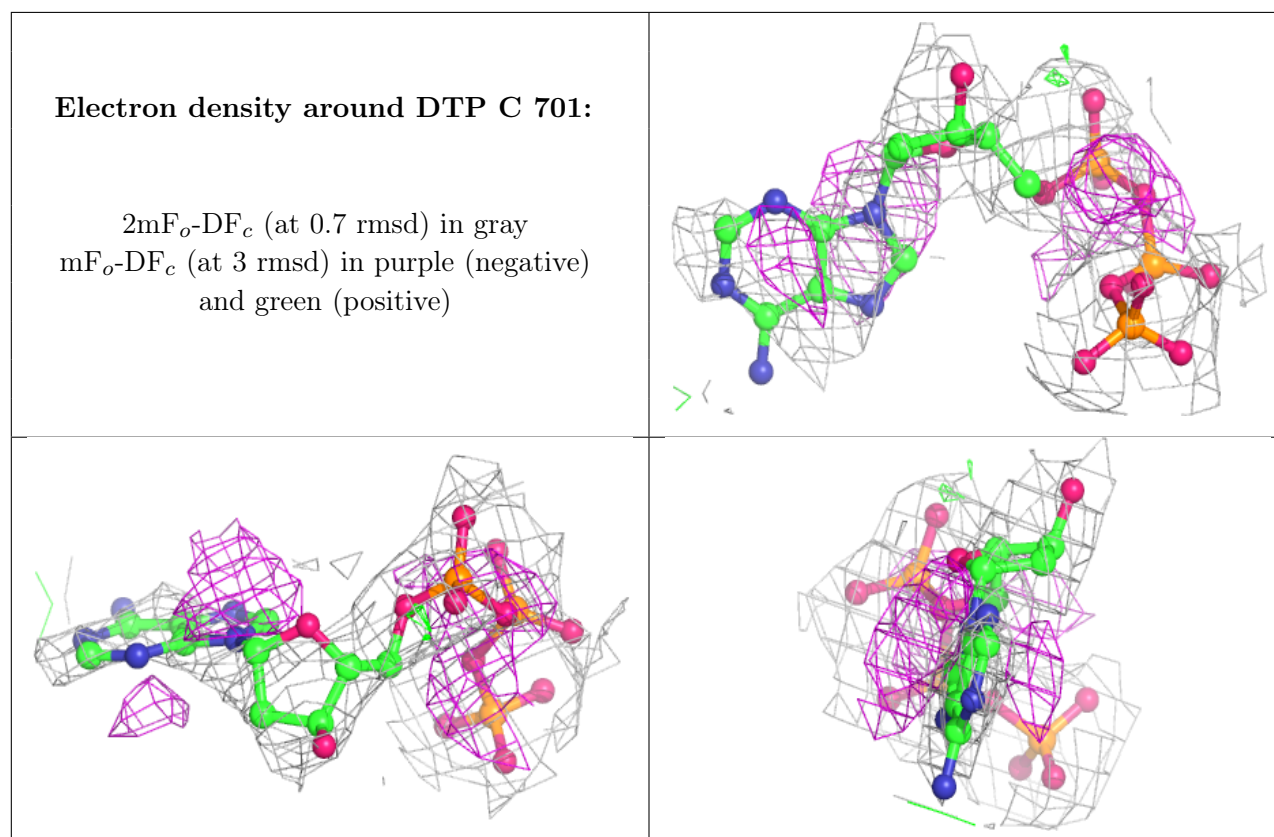
## 6.4 Ligands ⓘ

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.



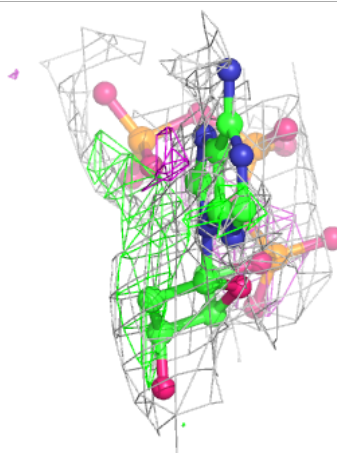
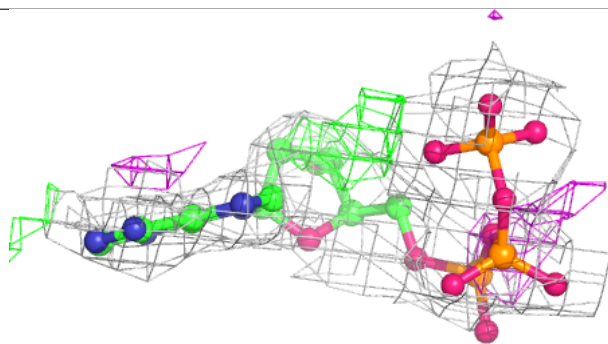
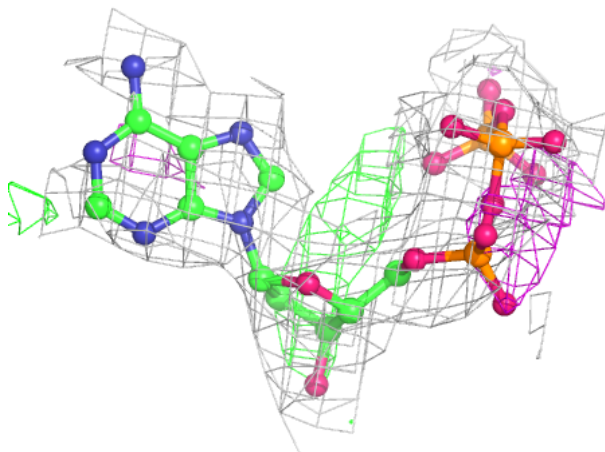
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	DTP	C	701	30/30	0.70	0.31	84,115,131,132	0
2	DTP	B	704	30/30	0.78	0.28	81,126,144,148	0
2	DTP	D	701	30/30	0.80	0.23	56,84,110,114	0
4	MG	D	704	1/1	0.90	0.08	72,72,72,72	0
4	MG	A	701	1/1	0.93	0.09	46,46,46,46	0
4	MG	B	702	1/1	0.94	0.12	88,88,88,88	0
4	MG	C	702	1/1	0.94	0.07	46,46,46,46	0
3	GTP	B	703	32/32	0.95	0.16	63,73,91,94	0
3	GTP	A	703	32/32	0.95	0.17	63,72,89,93	0
2	DTP	C	704	30/30	0.97	0.16	52,60,75,79	0
2	DTP	A	702	30/30	0.97	0.20	60,67,89,90	0
3	GTP	C	703	32/32	0.97	0.13	39,43,54,57	0
3	GTP	D	702	32/32	0.98	0.14	37,41,45,46	0
2	DTP	B	701	30/30	0.98	0.17	41,42,45,46	0
2	DTP	D	703	30/30	0.99	0.16	42,48,61,63	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.



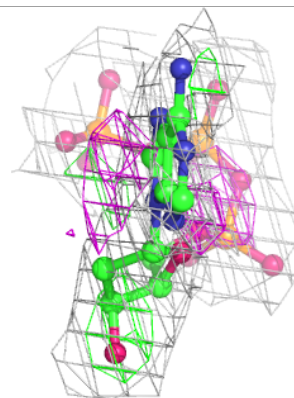
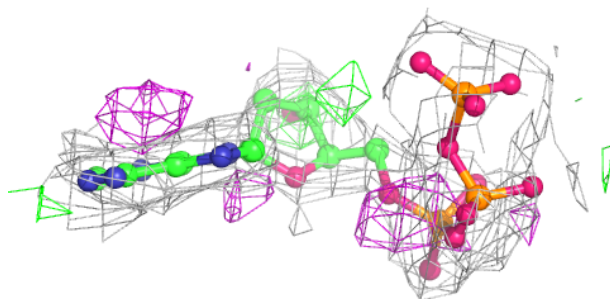
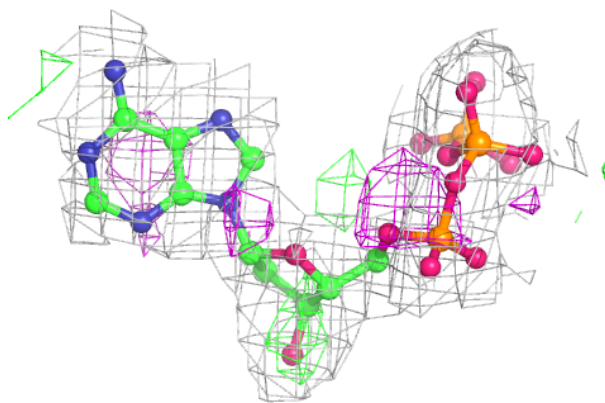
**Electron density around DTP B 704:**

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

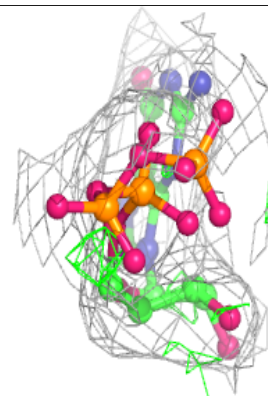
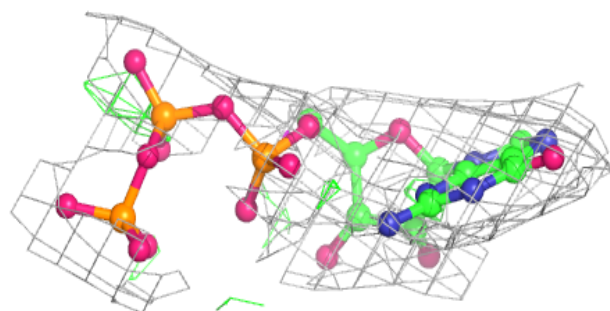
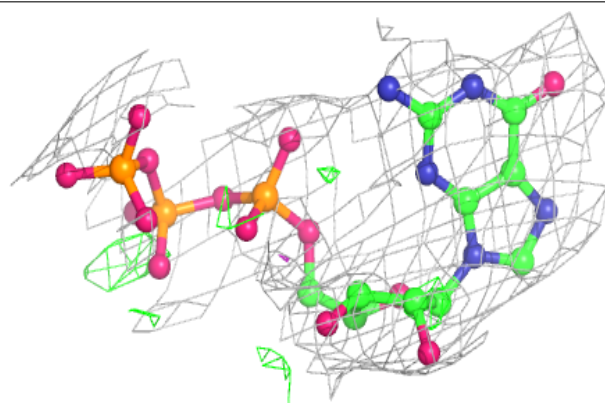


**Electron density around DTP D 701:**

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

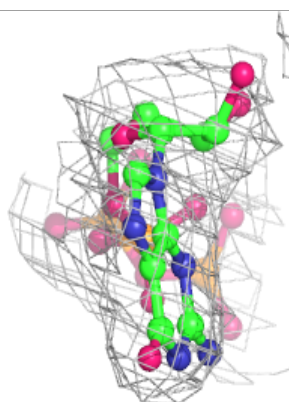
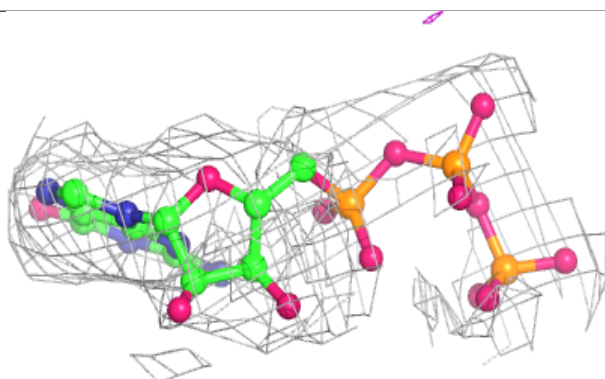
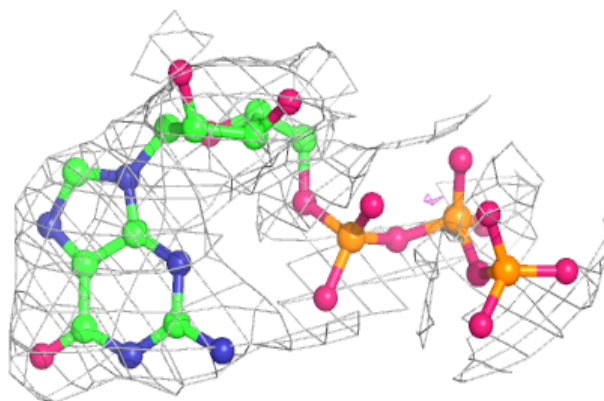
**Electron density around GTP B 703:**

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

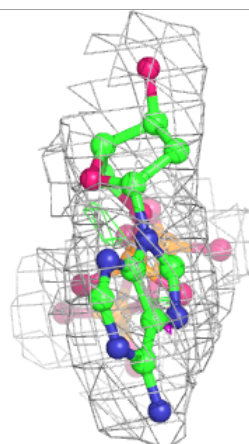
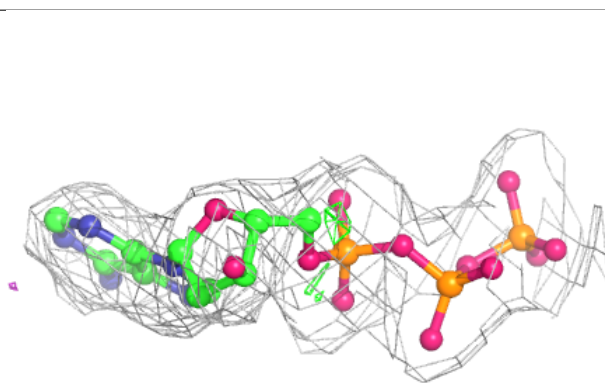
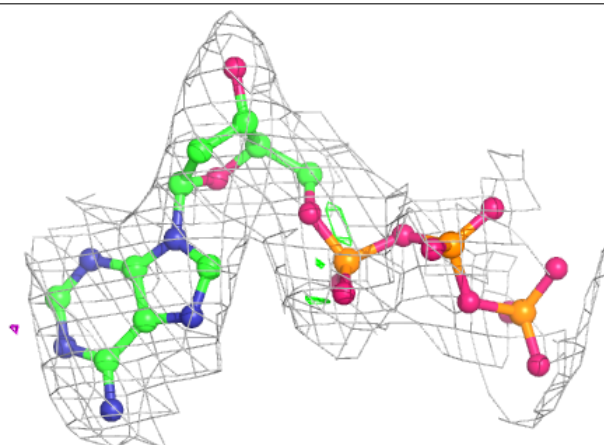


**Electron density around GTP A 703:**

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

**Electron density around DTP C 704:**

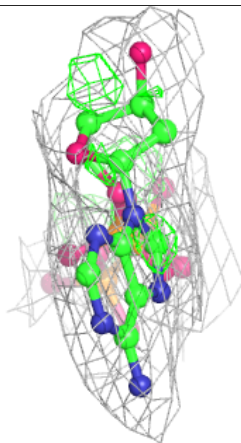
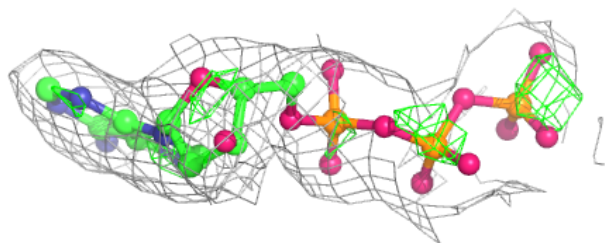
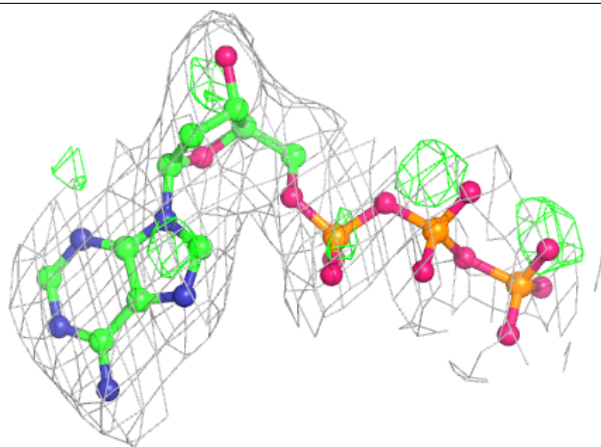
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



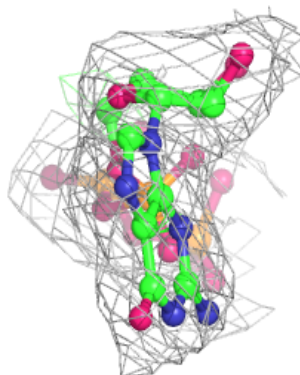
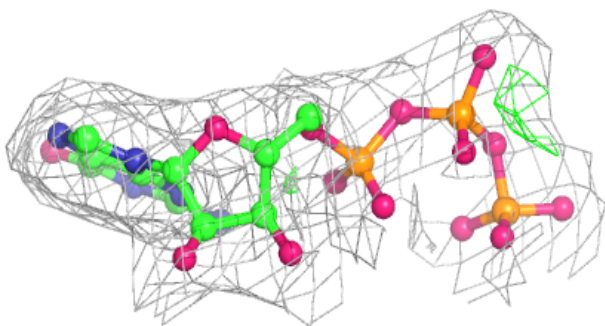
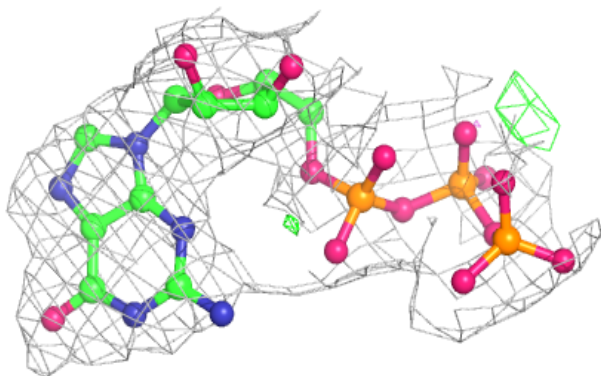


**Electron density around DTP A 702:**

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

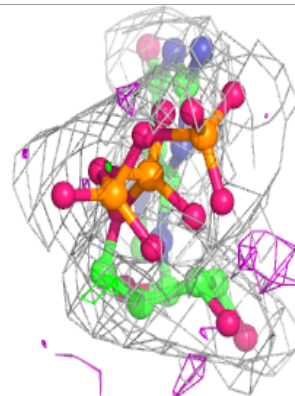
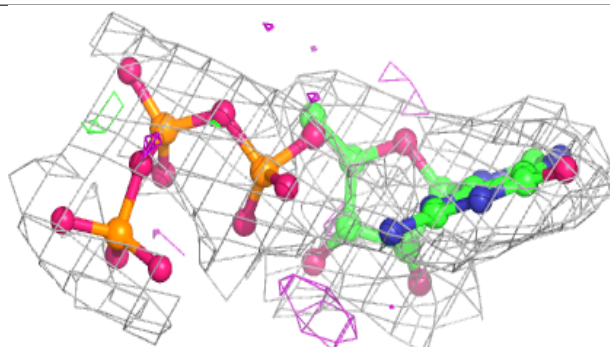
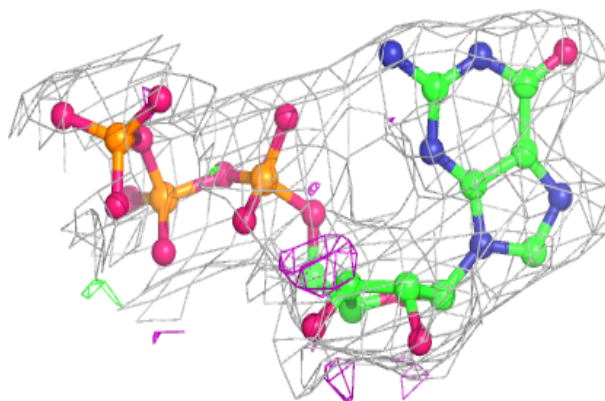
**Electron density around GTP C 703:**

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

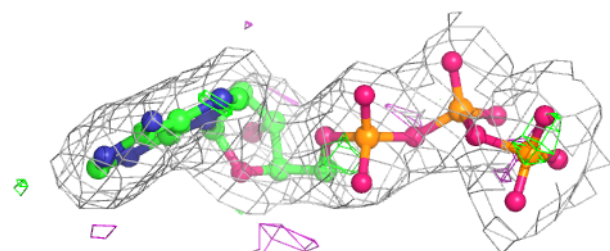
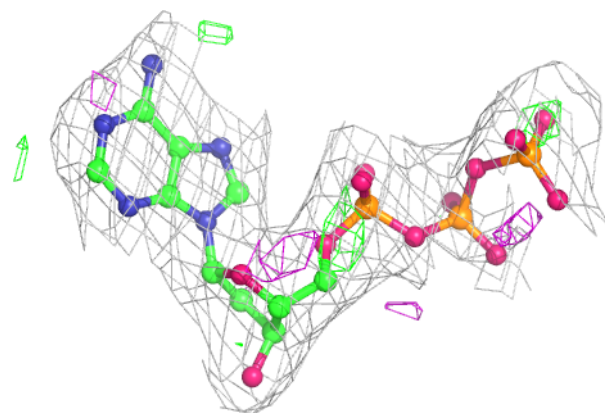


**Electron density around GTP D 702:**

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

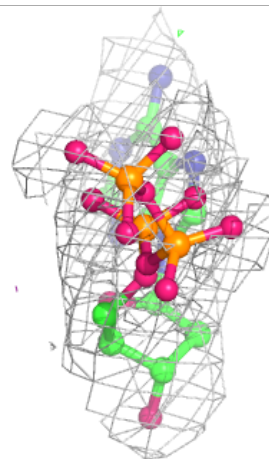
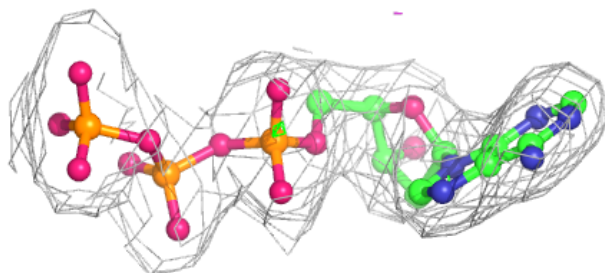
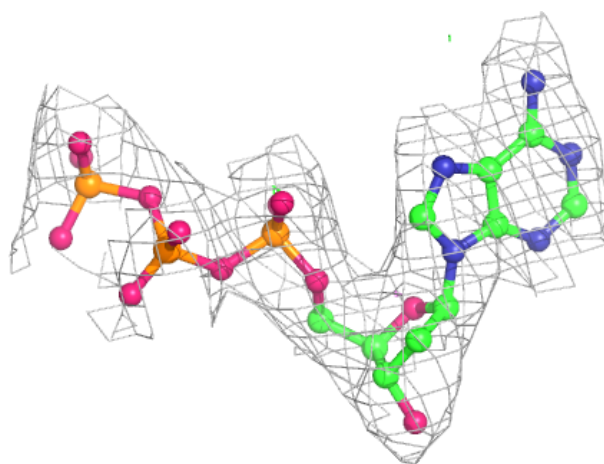
**Electron density around DTP B 701:**

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



**Electron density around DTP D 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.