



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 14, 2020 – 12:42 AM BST

PDB ID : 6DWK  
Title : SAMHD1 Bound to Fludarabine-TP in the Catalytic Pocket  
Authors : Knecht, K.M.; Buzovetsky, O.; Schneider, C.; Thomas, D.; Srikanth, V.; Kaderali, L.; Tofoleanu, F.; Reiss, K.; Ferreira, N.; Geisslinger, G.; Batista, V.S.; Ji, X.; Cinatl, J.; Keppler, O.T.; Xiong, Y.  
Deposited on : 2018-06-26  
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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 : 2.14.4.dev1  
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) : 2.14.4.dev1

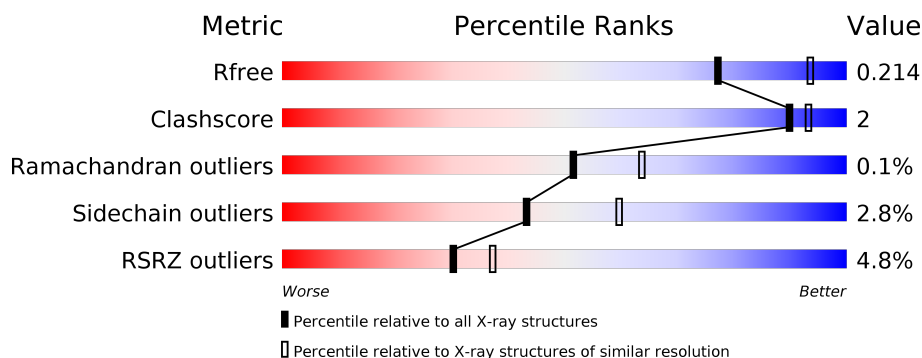
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	550	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>6%</div> <div>13%</div> </div> </div>
1	B	550	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>7%</div> <div>13%</div> </div> </div>
1	C	550	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>7%</div> <div>13%</div> </div> </div>
1	D	550	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>8%</div> <div>13%</div> </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MG	B	710	-	-	-	X
7	GLY	D	713	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 16439 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	A	480	Total	C	N	O	S	0	2	0
			3939	2523	687	709	20			
1	B	478	Total	C	N	O	S	0	0	0
			3908	2502	681	705	20			
1	C	478	Total	C	N	O	S	0	2	0
			3921	2511	683	707	20			
1	D	478	Total	C	N	O	S	0	0	0
			3908	2502	681	705	20			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	MET	-	initiating methionine	UNP Q9Y3Z3
A	78	GLY	-	expression tag	UNP Q9Y3Z3
A	79	SER	-	expression tag	UNP Q9Y3Z3
A	80	SER	-	expression tag	UNP Q9Y3Z3
A	81	HIS	-	expression tag	UNP Q9Y3Z3
A	82	HIS	-	expression tag	UNP Q9Y3Z3
A	83	HIS	-	expression tag	UNP Q9Y3Z3
A	84	HIS	-	expression tag	UNP Q9Y3Z3
A	85	HIS	-	expression tag	UNP Q9Y3Z3
A	86	HIS	-	expression tag	UNP Q9Y3Z3
A	87	SER	-	expression tag	UNP Q9Y3Z3
A	88	SER	-	expression tag	UNP Q9Y3Z3
A	89	GLY	-	expression tag	UNP Q9Y3Z3
A	90	LEU	-	expression tag	UNP Q9Y3Z3
A	91	VAL	-	expression tag	UNP Q9Y3Z3
A	92	PRO	-	expression tag	UNP Q9Y3Z3
A	93	ARG	-	expression tag	UNP Q9Y3Z3
A	94	GLY	-	expression tag	UNP Q9Y3Z3
A	95	SER	-	expression tag	UNP Q9Y3Z3
A	96	HIS	-	expression tag	UNP Q9Y3Z3
A	97	MET	-	expression tag	UNP Q9Y3Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	98	ALA	-	expression tag	UNP Q9Y3Z3
A	99	SER	-	expression tag	UNP Q9Y3Z3
A	100	MET	-	expression tag	UNP Q9Y3Z3
A	101	THR	-	expression tag	UNP Q9Y3Z3
A	102	GLY	-	expression tag	UNP Q9Y3Z3
A	103	GLY	-	expression tag	UNP Q9Y3Z3
A	104	GLN	-	expression tag	UNP Q9Y3Z3
A	105	GLN	-	expression tag	UNP Q9Y3Z3
A	106	MET	-	expression tag	UNP Q9Y3Z3
A	107	GLY	-	expression tag	UNP Q9Y3Z3
A	108	ARG	-	expression tag	UNP Q9Y3Z3
A	109	ASP	-	expression tag	UNP Q9Y3Z3
A	110	PRO	-	expression tag	UNP Q9Y3Z3
A	111	ASN	-	expression tag	UNP Q9Y3Z3
A	112	SER	-	expression tag	UNP Q9Y3Z3
A	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
A	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
B	77	MET	-	initiating methionine	UNP Q9Y3Z3
B	78	GLY	-	expression tag	UNP Q9Y3Z3
B	79	SER	-	expression tag	UNP Q9Y3Z3
B	80	SER	-	expression tag	UNP Q9Y3Z3
B	81	HIS	-	expression tag	UNP Q9Y3Z3
B	82	HIS	-	expression tag	UNP Q9Y3Z3
B	83	HIS	-	expression tag	UNP Q9Y3Z3
B	84	HIS	-	expression tag	UNP Q9Y3Z3
B	85	HIS	-	expression tag	UNP Q9Y3Z3
B	86	HIS	-	expression tag	UNP Q9Y3Z3
B	87	SER	-	expression tag	UNP Q9Y3Z3
B	88	SER	-	expression tag	UNP Q9Y3Z3
B	89	GLY	-	expression tag	UNP Q9Y3Z3
B	90	LEU	-	expression tag	UNP Q9Y3Z3
B	91	VAL	-	expression tag	UNP Q9Y3Z3
B	92	PRO	-	expression tag	UNP Q9Y3Z3
B	93	ARG	-	expression tag	UNP Q9Y3Z3
B	94	GLY	-	expression tag	UNP Q9Y3Z3
B	95	SER	-	expression tag	UNP Q9Y3Z3
B	96	HIS	-	expression tag	UNP Q9Y3Z3
B	97	MET	-	expression tag	UNP Q9Y3Z3
B	98	ALA	-	expression tag	UNP Q9Y3Z3
B	99	SER	-	expression tag	UNP Q9Y3Z3
B	100	MET	-	expression tag	UNP Q9Y3Z3
B	101	THR	-	expression tag	UNP Q9Y3Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	102	GLY	-	expression tag	UNP Q9Y3Z3
B	103	GLY	-	expression tag	UNP Q9Y3Z3
B	104	GLN	-	expression tag	UNP Q9Y3Z3
B	105	GLN	-	expression tag	UNP Q9Y3Z3
B	106	MET	-	expression tag	UNP Q9Y3Z3
B	107	GLY	-	expression tag	UNP Q9Y3Z3
B	108	ARG	-	expression tag	UNP Q9Y3Z3
B	109	ASP	-	expression tag	UNP Q9Y3Z3
B	110	PRO	-	expression tag	UNP Q9Y3Z3
B	111	ASN	-	expression tag	UNP Q9Y3Z3
B	112	SER	-	expression tag	UNP Q9Y3Z3
B	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
B	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
C	77	MET	-	initiating methionine	UNP Q9Y3Z3
C	78	GLY	-	expression tag	UNP Q9Y3Z3
C	79	SER	-	expression tag	UNP Q9Y3Z3
C	80	SER	-	expression tag	UNP Q9Y3Z3
C	81	HIS	-	expression tag	UNP Q9Y3Z3
C	82	HIS	-	expression tag	UNP Q9Y3Z3
C	83	HIS	-	expression tag	UNP Q9Y3Z3
C	84	HIS	-	expression tag	UNP Q9Y3Z3
C	85	HIS	-	expression tag	UNP Q9Y3Z3
C	86	HIS	-	expression tag	UNP Q9Y3Z3
C	87	SER	-	expression tag	UNP Q9Y3Z3
C	88	SER	-	expression tag	UNP Q9Y3Z3
C	89	GLY	-	expression tag	UNP Q9Y3Z3
C	90	LEU	-	expression tag	UNP Q9Y3Z3
C	91	VAL	-	expression tag	UNP Q9Y3Z3
C	92	PRO	-	expression tag	UNP Q9Y3Z3
C	93	ARG	-	expression tag	UNP Q9Y3Z3
C	94	GLY	-	expression tag	UNP Q9Y3Z3
C	95	SER	-	expression tag	UNP Q9Y3Z3
C	96	HIS	-	expression tag	UNP Q9Y3Z3
C	97	MET	-	expression tag	UNP Q9Y3Z3
C	98	ALA	-	expression tag	UNP Q9Y3Z3
C	99	SER	-	expression tag	UNP Q9Y3Z3
C	100	MET	-	expression tag	UNP Q9Y3Z3
C	101	THR	-	expression tag	UNP Q9Y3Z3
C	102	GLY	-	expression tag	UNP Q9Y3Z3
C	103	GLY	-	expression tag	UNP Q9Y3Z3
C	104	GLN	-	expression tag	UNP Q9Y3Z3
C	105	GLN	-	expression tag	UNP Q9Y3Z3

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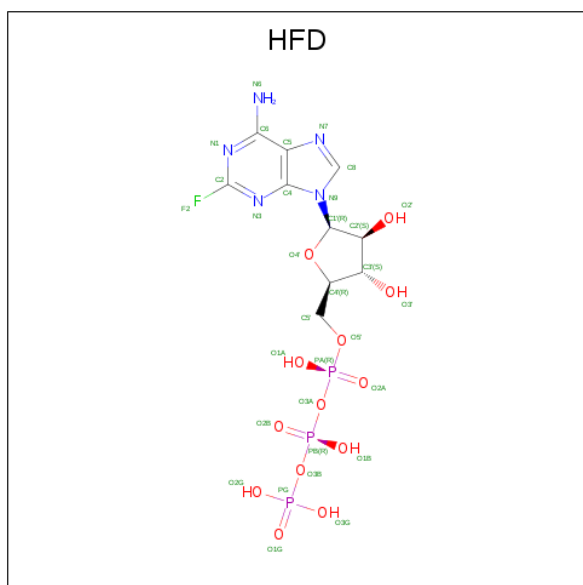
Chain	Residue	Modelled	Actual	Comment	Reference
C	106	MET	-	expression tag	UNP Q9Y3Z3
C	107	GLY	-	expression tag	UNP Q9Y3Z3
C	108	ARG	-	expression tag	UNP Q9Y3Z3
C	109	ASP	-	expression tag	UNP Q9Y3Z3
C	110	PRO	-	expression tag	UNP Q9Y3Z3
C	111	ASN	-	expression tag	UNP Q9Y3Z3
C	112	SER	-	expression tag	UNP Q9Y3Z3
C	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
C	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
D	77	MET	-	initiating methionine	UNP Q9Y3Z3
D	78	GLY	-	expression tag	UNP Q9Y3Z3
D	79	SER	-	expression tag	UNP Q9Y3Z3
D	80	SER	-	expression tag	UNP Q9Y3Z3
D	81	HIS	-	expression tag	UNP Q9Y3Z3
D	82	HIS	-	expression tag	UNP Q9Y3Z3
D	83	HIS	-	expression tag	UNP Q9Y3Z3
D	84	HIS	-	expression tag	UNP Q9Y3Z3
D	85	HIS	-	expression tag	UNP Q9Y3Z3
D	86	HIS	-	expression tag	UNP Q9Y3Z3
D	87	SER	-	expression tag	UNP Q9Y3Z3
D	88	SER	-	expression tag	UNP Q9Y3Z3
D	89	GLY	-	expression tag	UNP Q9Y3Z3
D	90	LEU	-	expression tag	UNP Q9Y3Z3
D	91	VAL	-	expression tag	UNP Q9Y3Z3
D	92	PRO	-	expression tag	UNP Q9Y3Z3
D	93	ARG	-	expression tag	UNP Q9Y3Z3
D	94	GLY	-	expression tag	UNP Q9Y3Z3
D	95	SER	-	expression tag	UNP Q9Y3Z3
D	96	HIS	-	expression tag	UNP Q9Y3Z3
D	97	MET	-	expression tag	UNP Q9Y3Z3
D	98	ALA	-	expression tag	UNP Q9Y3Z3
D	99	SER	-	expression tag	UNP Q9Y3Z3
D	100	MET	-	expression tag	UNP Q9Y3Z3
D	101	THR	-	expression tag	UNP Q9Y3Z3
D	102	GLY	-	expression tag	UNP Q9Y3Z3
D	103	GLY	-	expression tag	UNP Q9Y3Z3
D	104	GLN	-	expression tag	UNP Q9Y3Z3
D	105	GLN	-	expression tag	UNP Q9Y3Z3
D	106	MET	-	expression tag	UNP Q9Y3Z3
D	107	GLY	-	expression tag	UNP Q9Y3Z3
D	108	ARG	-	expression tag	UNP Q9Y3Z3
D	109	ASP	-	expression tag	UNP Q9Y3Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	110	PRO	-	expression tag	UNP Q9Y3Z3
D	111	ASN	-	expression tag	UNP Q9Y3Z3
D	112	SER	-	expression tag	UNP Q9Y3Z3
D	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
D	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3

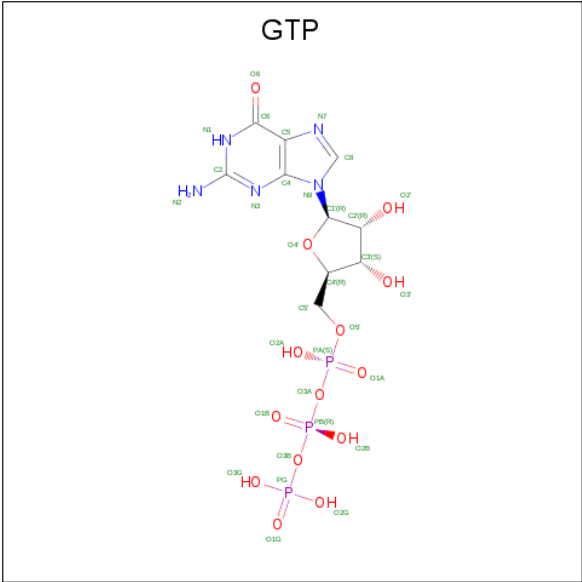
- Molecule 2 is 2-fluoro-9-{5-O-[(R)-hydroxy{[(R)-hydroxy(phosphonooxy)phosphoryl]oxy}phosphoryl]-beta-D-arabinofuranosyl}-9H-purin-6-amine (three-letter code: HFD) (formula:  $C_{10}H_{15}FN_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	P	0	0
			32	10	1	5	13	3		
2	B	1	Total	C	F	N	O	P	0	0
			32	10	1	5	13	3		
2	C	1	Total	C	F	N	O	P	0	0
			32	10	1	5	13	3		
2	D	1	Total	C	F	N	O	P	0	0
			32	10	1	5	13	3		

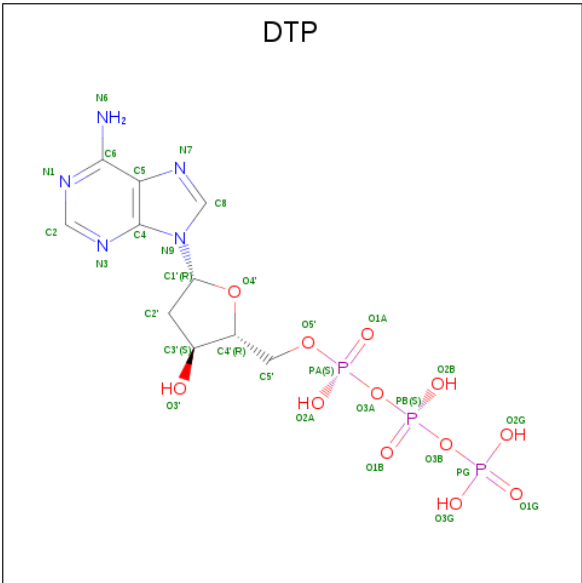
- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	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		
3	B	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		

- Molecule 4 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula:  $C_{10}H_{16}N_5O_{12}P_3$ ).



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

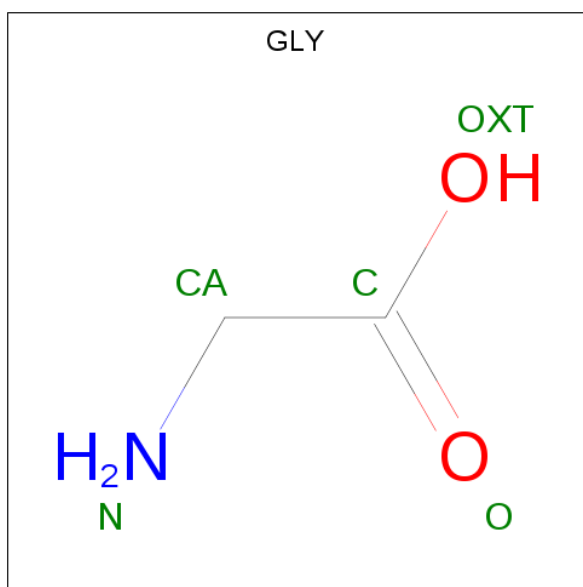
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	6	Total	Na	0	0
			6	6		
6	A	7	Total	Na	0	0
			7	7		
6	D	6	Total	Na	0	0
			6	6		
6	C	4	Total	Na	0	0
			4	4		

- Molecule 7 is GLYCINE (three-letter code: GLY) (formula: C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub>).



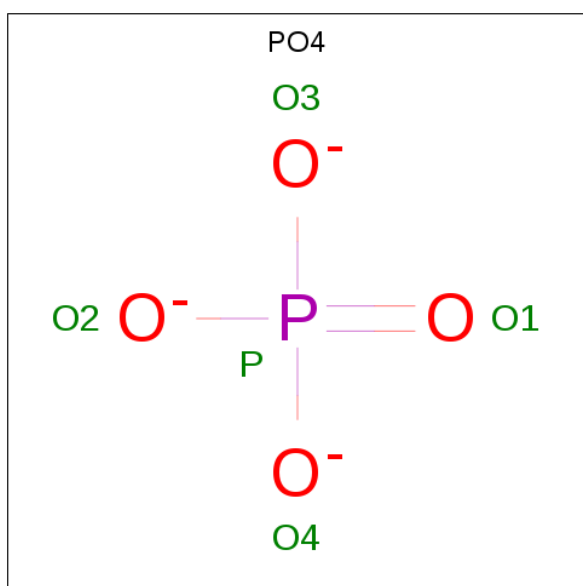
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			5	2	1	2		
7	B	1	Total	C	N	O	0	0
			5	2	1	2		
7	B	1	Total	C	N	O	0	0
			5	2	1	2		
7	C	1	Total	C	N	O	0	0
			5	2	1	2		
7	C	1	Total	C	N	O	0	0
			5	2	1	2		
7	C	1	Total	C	N	O	0	0
			5	2	1	2		
7	C	1	Total	C	N	O	0	0
			5	2	1	2		
7	D	1	Total	C	N	O	0	0
			5	2	1	2		
7	D	1	Total	C	N	O	0	0
			5	2	1	2		
7	D	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 8 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			8	4	1	3		
8	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	O	P	0	0
			5	4	1		

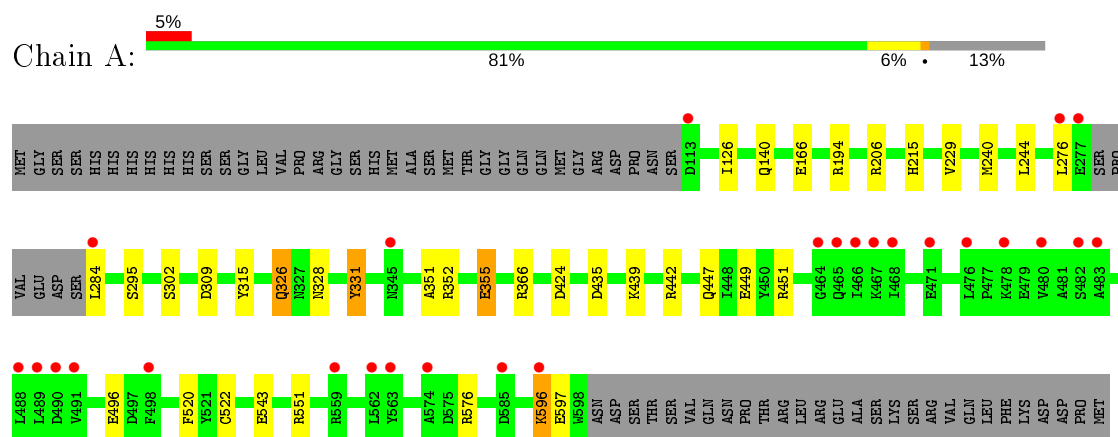
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	54	Total 54	O 54	0	0
10	B	81	Total 81	O 81	0	0
10	C	46	Total 46	O 46	0	0
10	D	93	Total 93	O 93	0	0

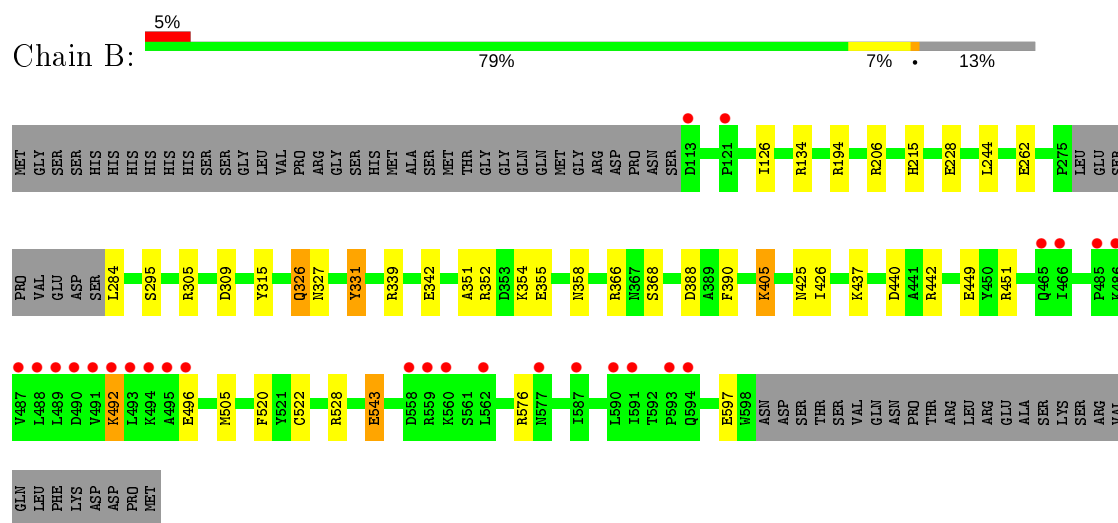
### 3 Residue-property plots [i](#)

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

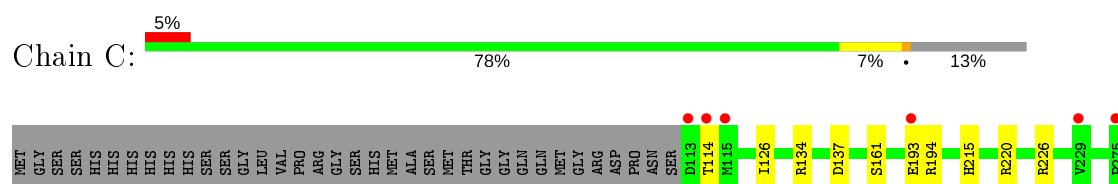
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

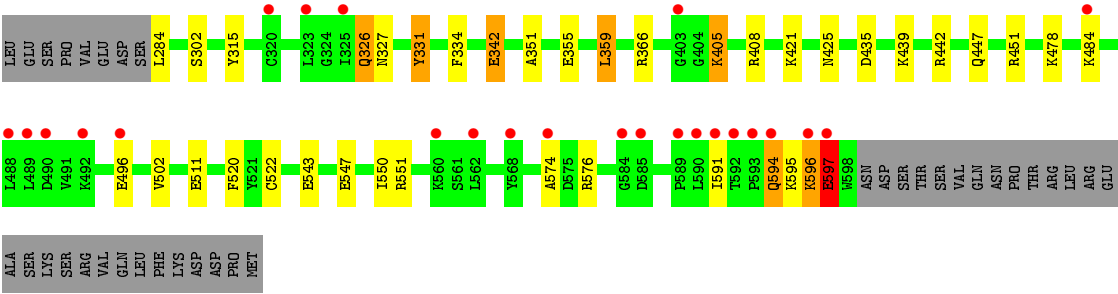


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

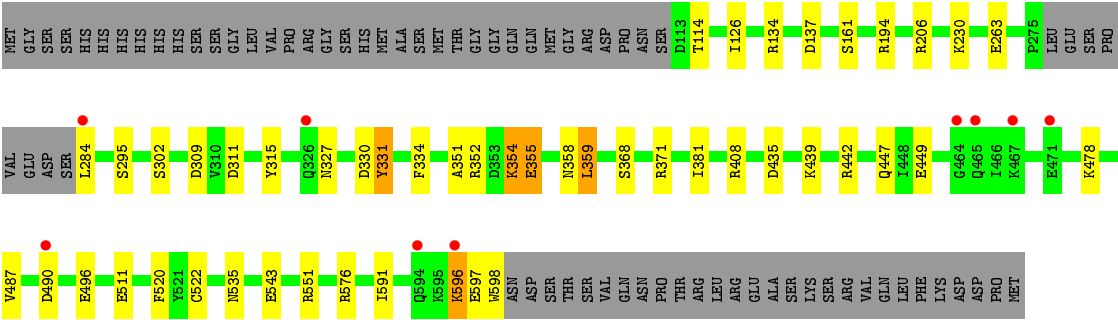
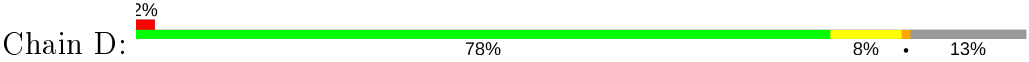


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





● 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, $\alpha$ , $\beta$ , $\gamma$	87.69Å 146.67Å 99.13Å 90.00° 114.53° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 48.90 – 2.28	Depositor EDS
% Data completeness (in resolution range)	96.3 (50.00-2.30) 96.3 (48.90-2.28)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.09 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, $R_{free}$	0.176 , 0.212 0.181 , 0.214	Depositor DCC
$R_{free}$ test set	5169 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.8	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 39.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16439	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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: MG, NA, PO4, GTP, TRS, DTP, HFD

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	1.01	7/4039 (0.2%)	1.01	14/5452 (0.3%)
1	B	1.03	11/4000 (0.3%)	1.04	21/5399 (0.4%)
1	C	0.99	7/4020 (0.2%)	1.04	17/5426 (0.3%)
1	D	1.07	13/4000 (0.3%)	1.04	17/5399 (0.3%)
All	All	1.02	38/16059 (0.2%)	1.03	69/21676 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	528	ARG	NE-CZ	13.97	1.51	1.33
1	C	355	GLU	CD-OE1	10.31	1.36	1.25
1	A	449	GLU	CD-OE1	10.29	1.36	1.25
1	A	449	GLU	CD-OE2	8.81	1.35	1.25
1	C	355	GLU	CD-OE2	7.87	1.34	1.25

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	339	ARG	NE-CZ-NH2	-10.94	114.83	120.30
1	C	551	ARG	NE-CZ-NH1	-9.29	115.66	120.30
1	A	435	ASP	CB-CG-OD2	-8.89	110.30	118.30
1	B	388	ASP	CB-CG-OD2	8.87	126.28	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	366	ARG	NE-CZ-NH2	-8.71	115.94	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	276	LEU	Peptide

## 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	3939	0	3928	16	0
1	B	3908	0	3898	13	0
1	C	3921	0	3909	16	0
1	D	3908	0	3898	14	0
2	A	32	0	0	1	0
2	B	32	0	0	3	0
2	C	32	0	0	2	0
2	D	32	0	0	1	0
3	A	64	0	24	2	0
3	B	32	0	12	2	0
3	C	32	0	12	2	0
4	A	30	0	12	0	0
4	B	30	0	12	0	0
4	C	30	0	12	0	0
4	D	30	0	12	0	0
5	A	3	0	0	0	0
5	B	1	0	0	0	0
5	C	2	0	0	0	0
5	D	3	0	0	0	0
6	A	7	0	0	0	0
6	B	6	0	0	0	0
6	C	4	0	0	0	0
6	D	6	0	0	0	0
7	A	5	0	2	0	0
7	B	10	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	25	0	10	0	0
7	D	20	0	8	0	0
8	B	16	0	24	0	0
9	D	5	0	0	0	0
10	A	54	0	0	1	0
10	B	81	0	0	2	0
10	C	46	0	0	0	0
10	D	93	0	0	3	0
All	All	16439	0	15777	58	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 2.

The worst 5 of 58 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:701:HFD:O2G	10:B:801:HOH:O	1.99	0.79
1:B:326:GLN:HG2	1:D:327:ASN:O	1.89	0.73
1:D:355:GLU:OE1	1:D:358:ASN:ND2	2.27	0.68
1:A:451:ARG:HH11	3:A:702:GTP:H5'	1.59	0.67
1:B:355:GLU:OE1	1:B:358:ASN:ND2	2.28	0.66

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	478/550 (87%)	470 (98%)	8 (2%)	0	100	100
1	B	474/550 (86%)	463 (98%)	11 (2%)	0	100	100
1	C	476/550 (86%)	463 (97%)	11 (2%)	2 (0%)	34	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	474/550 (86%)	464 (98%)	10 (2%)	0	100	100
All	All	1902/2200 (86%)	1860 (98%)	40 (2%)	2 (0%)	51	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	597	GLU
1	C	596	LYS

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	428/488 (88%)	417 (97%)	11 (3%)	46	63
1	B	424/488 (87%)	417 (98%)	7 (2%)	60	76
1	C	426/488 (87%)	408 (96%)	18 (4%)	30	42
1	D	424/488 (87%)	413 (97%)	11 (3%)	46	63
All	All	1702/1952 (87%)	1655 (97%)	47 (3%)	43	60

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	284	LEU
1	C	342	GLU
1	D	439	LYS
1	C	315	TYR
1	C	359	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	235	GLN
1	C	425	ASN

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Mol	Chain	Res	Type
1	D	345	ASN
1	C	215	HIS
1	D	215	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 59 ligands modelled in this entry, 32 are monoatomic - leaving 27 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	$\# Z  > 2$
7	GLY	B	711	-	1,4,4	0.12	0	0,4,4	0.00	-
2	HFD	B	701	5	27,34,34	3.07	12 (44%)	33,54,54	3.43	12 (36%)
7	GLY	A	715	-	1,4,4	0.14	0	0,4,4	0.00	-
7	GLY	C	712	-	1,4,4	0.10	0	0,4,4	0.00	-
2	HFD	D	703	5	27,34,34	3.08	9 (33%)	33,54,54	3.49	16 (48%)
8	TRS	B	713	-	7,7,7	0.51	0	9,9,9	0.72	0
7	GLY	C	710	-	1,4,4	0.08	0	0,4,4	0.00	-
8	TRS	B	714	-	7,7,7	0.74	0	9,9,9	1.08	0
2	HFD	C	704	5	27,34,34	3.08	11 (40%)	33,54,54	3.31	19 (57%)
3	GTP	A	706	5	26,34,34	1.25	2 (7%)	33,54,54	2.44	10 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	DTP	C	702	5	26,32,32	1.45	4 (15%)	30,50,50	1.18	3 (10%)
7	GLY	D	714	-	1,4,4	0.14	0	0,4,4	0.00	-
4	DTP	B	703	5	26,32,32	1.31	4 (15%)	30,50,50	1.23	4 (13%)
7	GLY	D	712	-	1,4,4	0.17	0	0,4,4	0.00	-
3	GTP	C	705	5	26,34,34	1.82	7 (26%)	33,54,54	2.60	13 (39%)
7	GLY	C	714	-	1,4,4	0.11	0	0,4,4	0.00	-
7	GLY	D	713	-	1,4,4	0.14	0	0,4,4	0.00	-
7	GLY	C	711	-	1,4,4	0.09	0	0,4,4	0.00	-
2	HFD	A	701	5	27,34,34	2.77	9 (33%)	33,54,54	3.61	14 (42%)
7	GLY	B	712	-	1,4,4	0.10	0	0,4,4	0.00	-
4	DTP	A	703	5	26,32,32	1.27	6 (23%)	30,50,50	1.43	3 (10%)
7	GLY	D	715	-	1,4,4	0.05	0	0,4,4	0.00	-
4	DTP	D	702	5	26,32,32	1.23	3 (11%)	30,50,50	1.20	3 (10%)
7	GLY	C	713	-	1,4,4	0.13	0	0,4,4	0.00	-
9	PO4	D	716	-	4,4,4	0.84	0	6,6,6	0.43	0
3	GTP	B	702	5	26,34,34	1.85	7 (26%)	33,54,54	2.33	10 (30%)
3	GTP	A	702	5	26,34,34	1.82	8 (30%)	33,54,54	1.96	9 (27%)

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
7	GLY	B	711	-	-	0/0/2/2	-
2	HFD	B	701	5	-	8/18/38/38	0/3/3/3
7	GLY	A	715	-	-	0/0/2/2	-
7	GLY	C	712	-	-	0/0/2/2	-
2	HFD	D	703	5	-	5/18/38/38	0/3/3/3
8	TRS	B	713	-	-	3/9/9/9	-
8	TRS	B	714	-	-	8/9/9/9	-
2	HFD	C	704	5	-	8/18/38/38	0/3/3/3
3	GTP	A	706	5	-	5/18/38/38	0/3/3/3
4	DTP	C	702	5	-	5/18/34/34	0/3/3/3
7	GLY	D	714	-	-	0/0/2/2	-
4	DTP	B	703	5	-	3/18/34/34	0/3/3/3
7	GLY	D	712	-	-	0/0/2/2	-
3	GTP	C	705	5	-	7/18/38/38	0/3/3/3
7	GLY	C	714	-	-	0/0/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GLY	D	713	-	-	0/0/2/2	-
7	GLY	C	711	-	-	0/0/2/2	-
2	HFD	A	701	5	-	4/18/38/38	0/3/3/3
7	GLY	B	712	-	-	0/0/2/2	-
4	DTP	A	703	5	-	2/18/34/34	0/3/3/3
7	GLY	D	715	-	-	0/0/2/2	-
4	DTP	D	702	5	-	4/18/34/34	0/3/3/3
7	GLY	C	713	-	-	0/0/2/2	-
7	GLY	C	710	-	-	0/0/2/2	-
3	GTP	B	702	5	-	8/18/38/38	0/3/3/3
3	GTP	A	702	5	-	8/18/38/38	0/3/3/3

The worst 5 of 82 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	703	HFD	O4'-C1'	11.43	1.57	1.41
2	C	704	HFD	O4'-C1'	9.79	1.54	1.41
2	B	701	HFD	C2-N3	7.63	1.38	1.31
2	B	701	HFD	O4'-C1'	7.00	1.50	1.41
2	A	701	HFD	C2-N3	6.76	1.38	1.31

The worst 5 of 116 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	703	HFD	F2-C2-N3	11.94	126.07	114.73
2	A	701	HFD	F2-C2-N3	11.73	125.87	114.73
2	B	701	HFD	F2-C2-N3	9.60	123.84	114.73
2	A	701	HFD	C5-C6-N1	-8.94	115.14	121.01
2	C	704	HFD	F2-C2-N3	8.88	123.16	114.73

There are no chirality outliers.

5 of 78 torsion outliers are listed below:

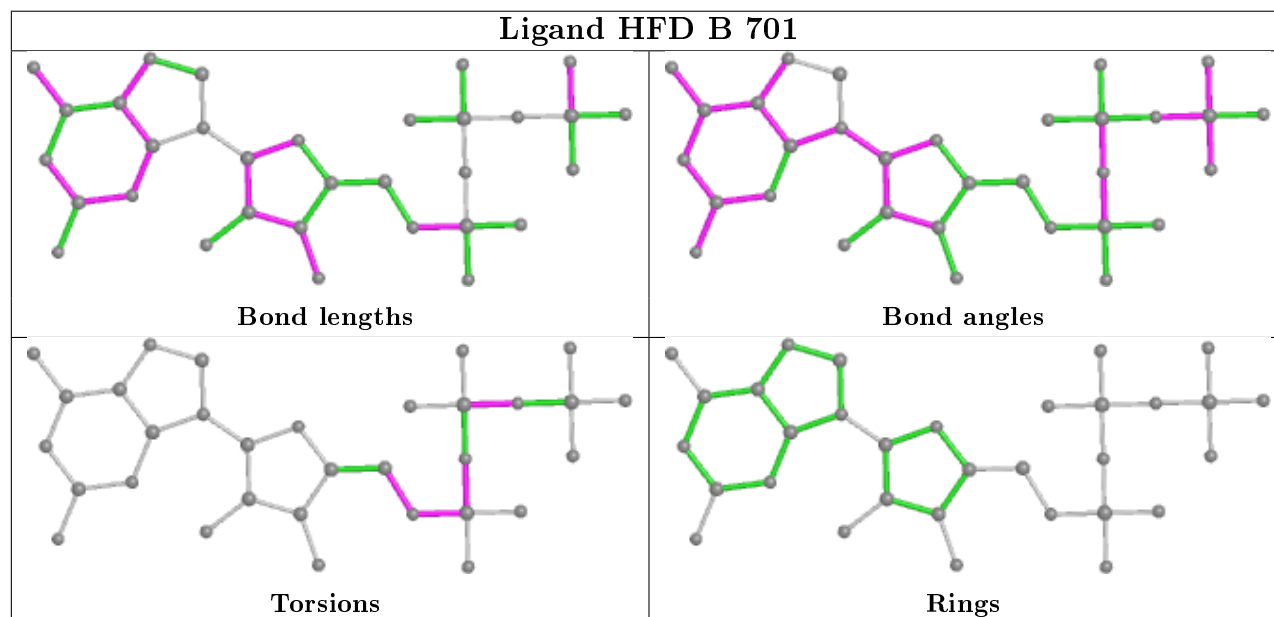
Mol	Chain	Res	Type	Atoms
3	B	702	GTP	PB-O3B-PG-O2G
3	B	702	GTP	C5'-O5'-PA-O1A
2	B	701	HFD	PB-O3A-PA-O5'
2	B	701	HFD	C5'-O5'-PA-O2A
2	B	701	HFD	C5'-O5'-PA-O1A

There are no ring outliers.

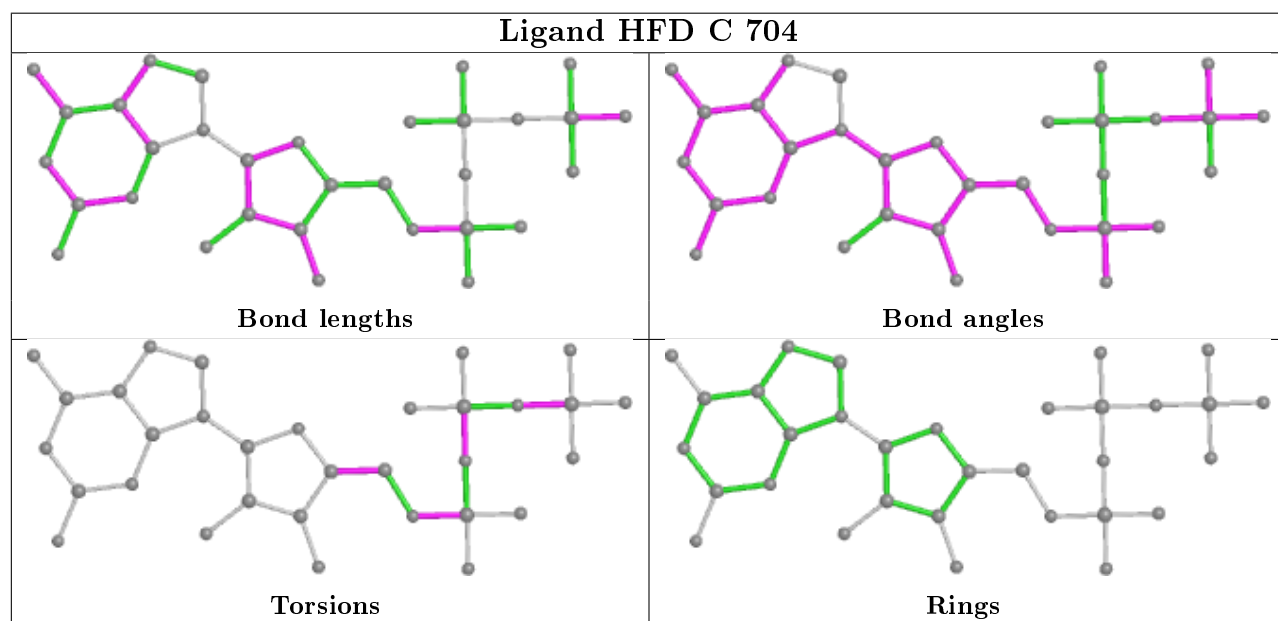
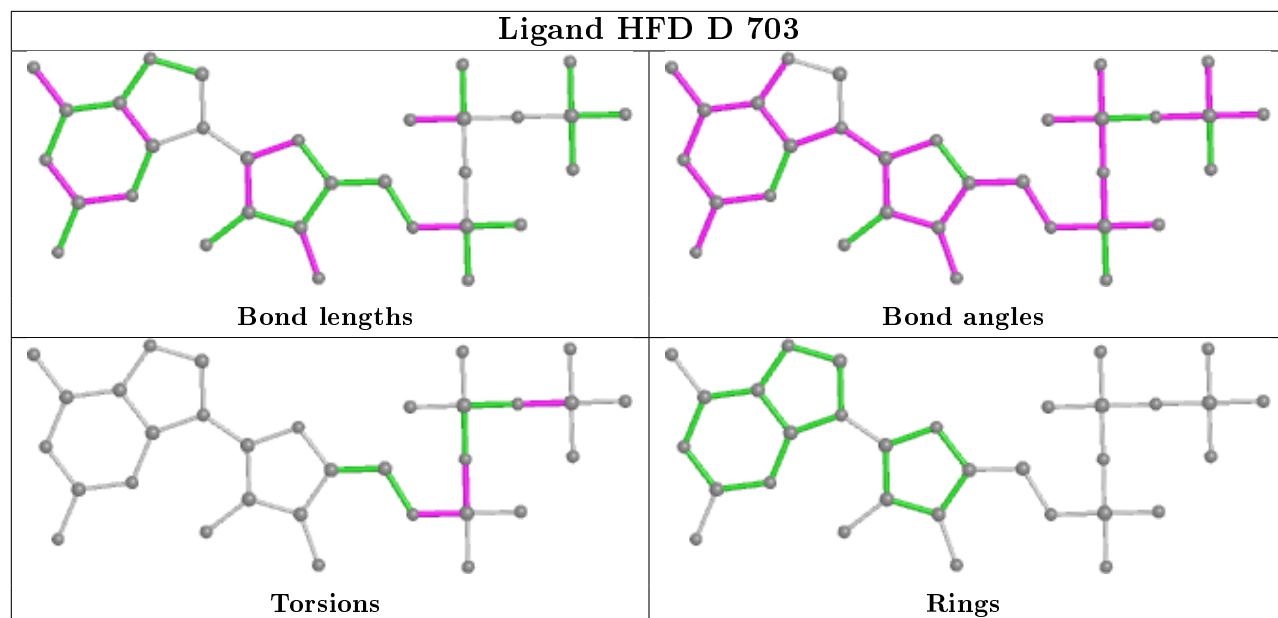
7 monomers are involved in 13 short contacts:

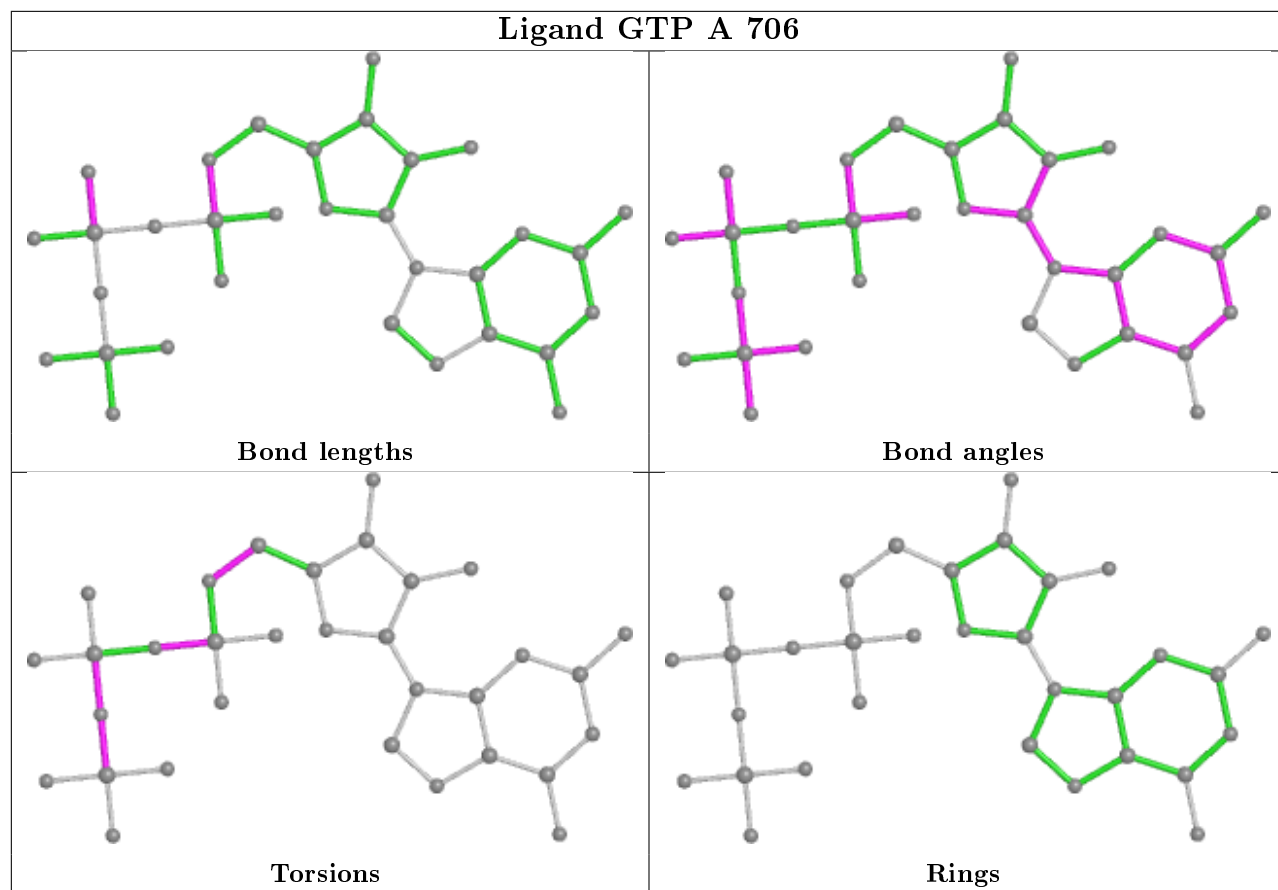
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	HFD	3	0
2	D	703	HFD	1	0
2	C	704	HFD	2	0
3	C	705	GTP	2	0
2	A	701	HFD	1	0
3	B	702	GTP	2	0
3	A	702	GTP	2	0

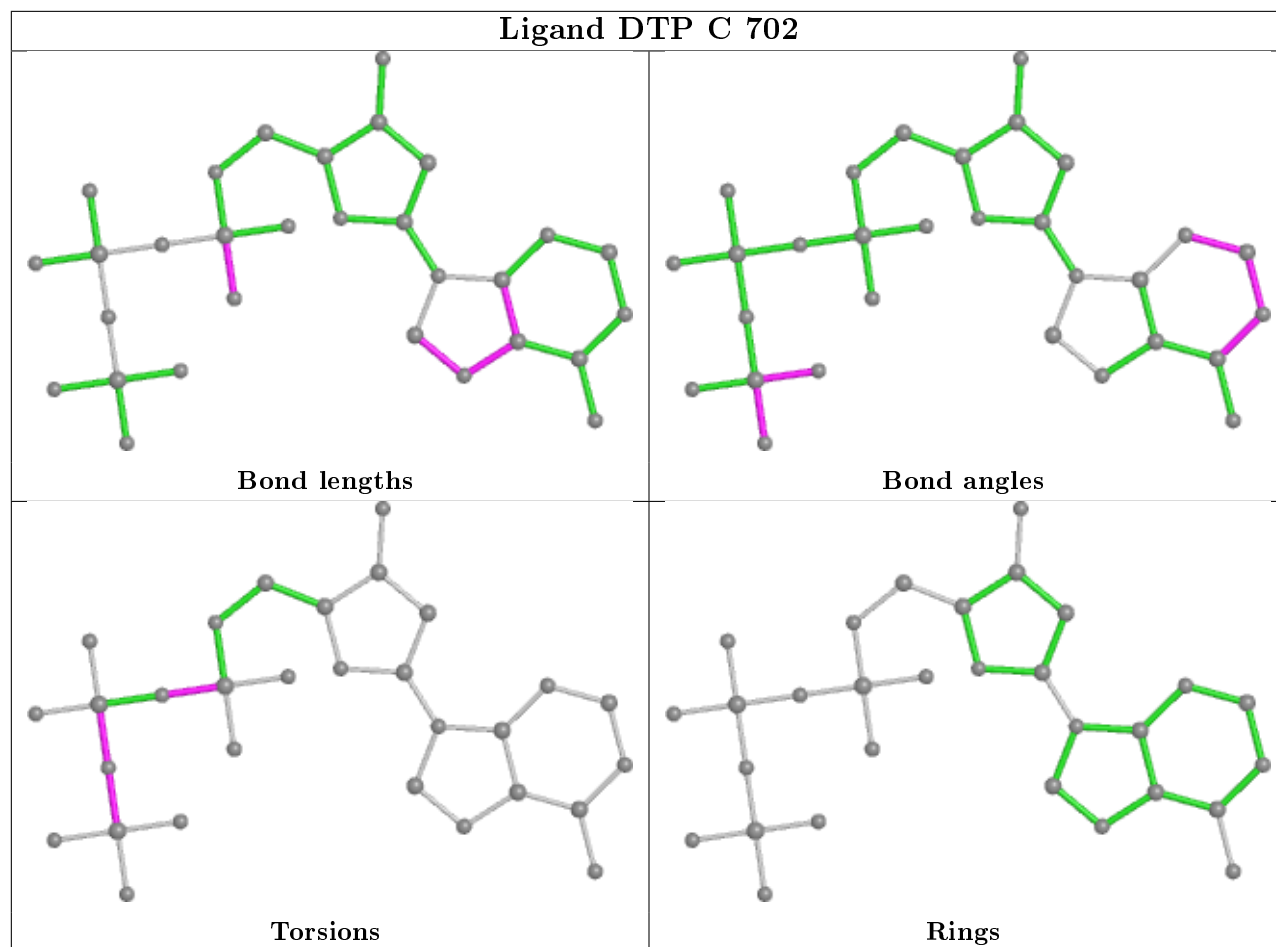
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

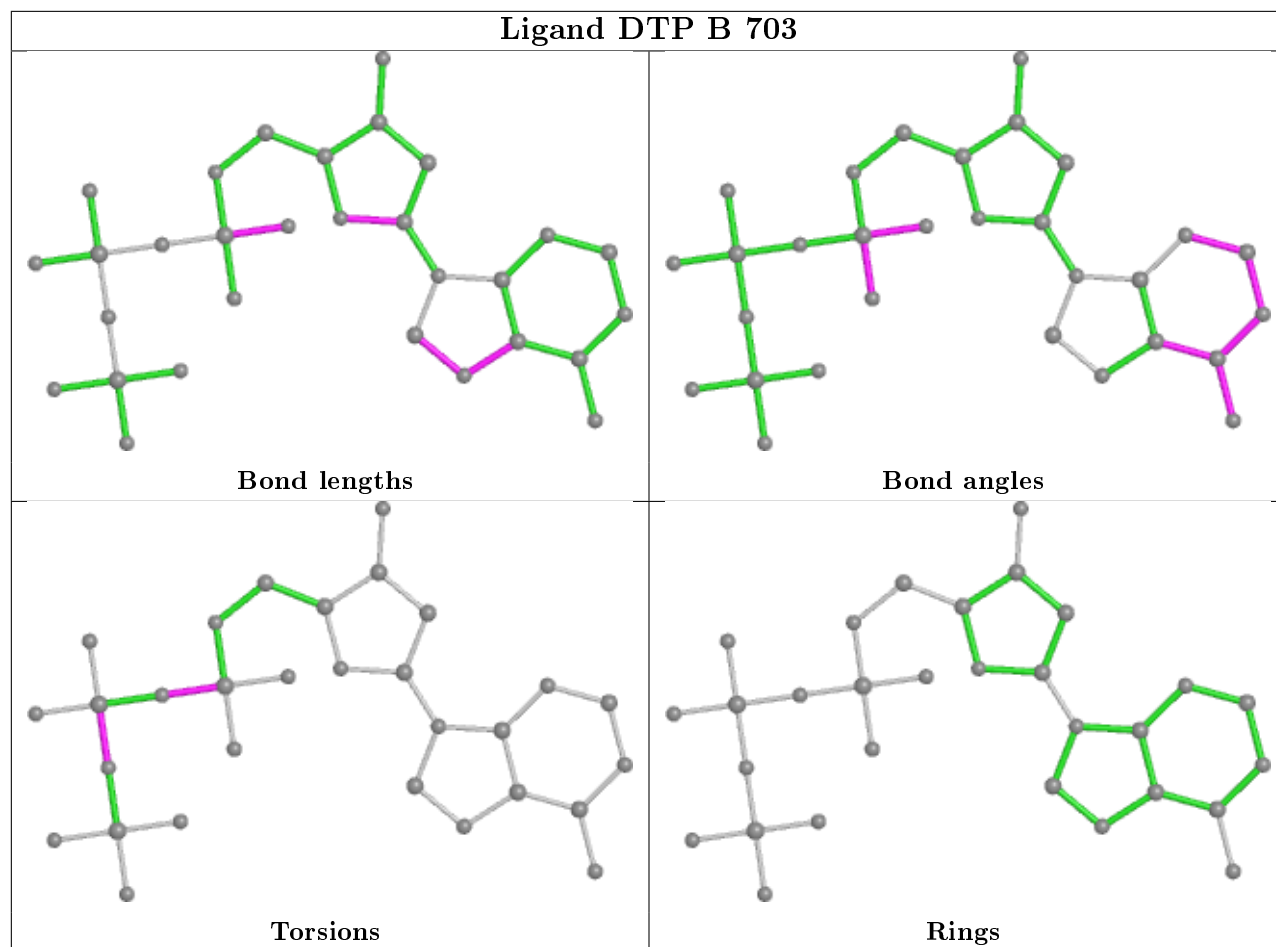


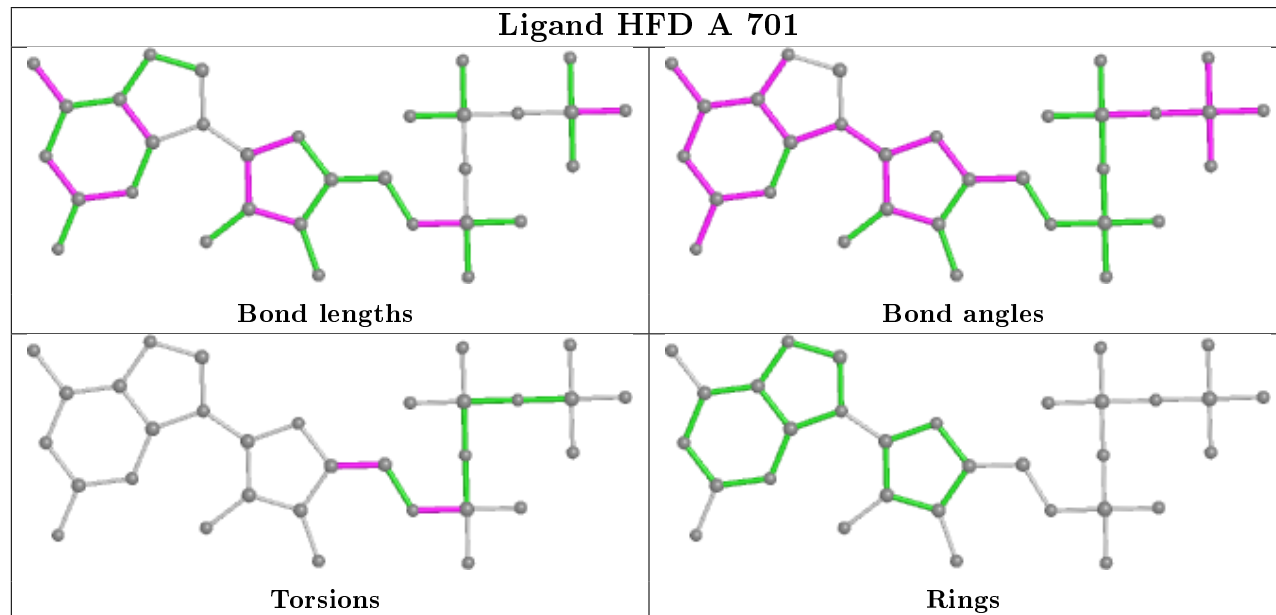
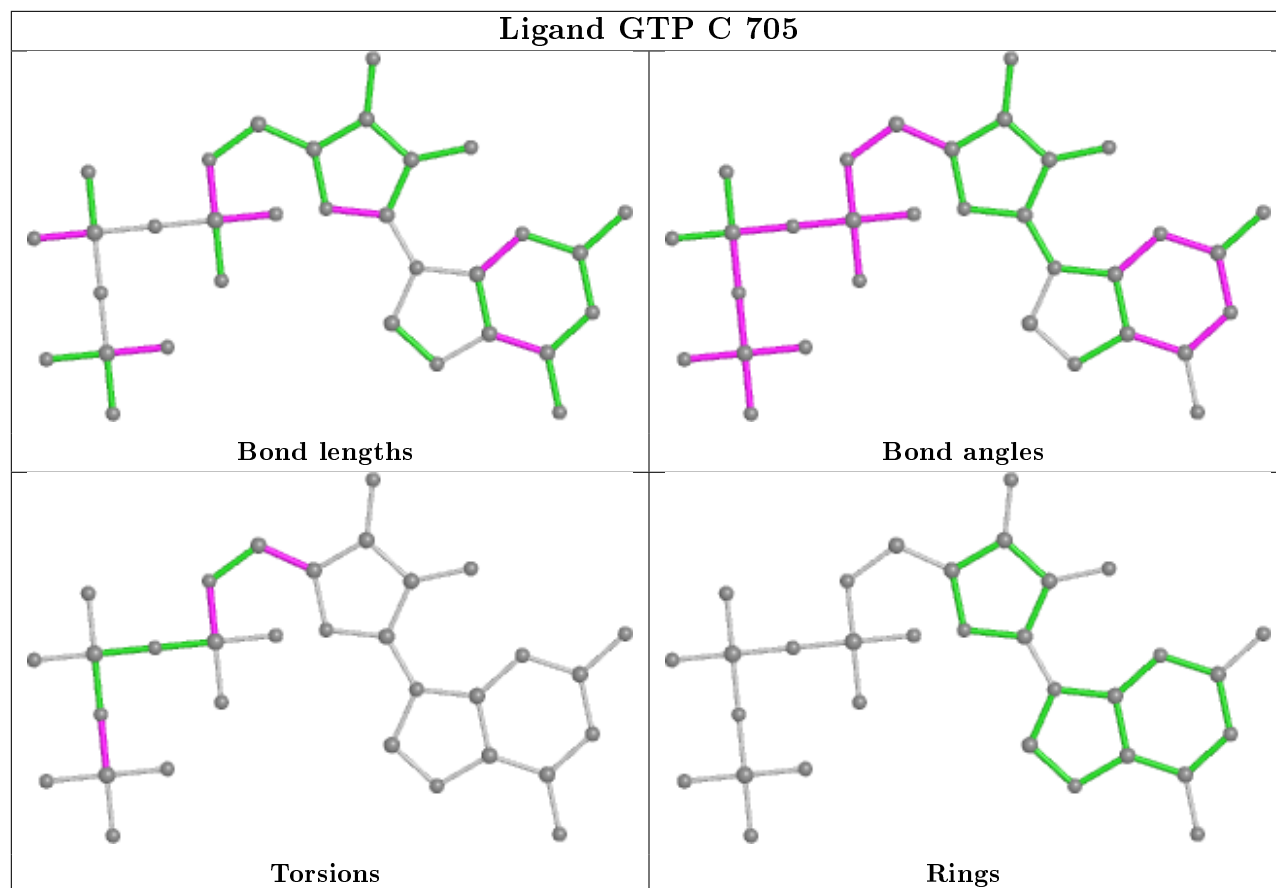


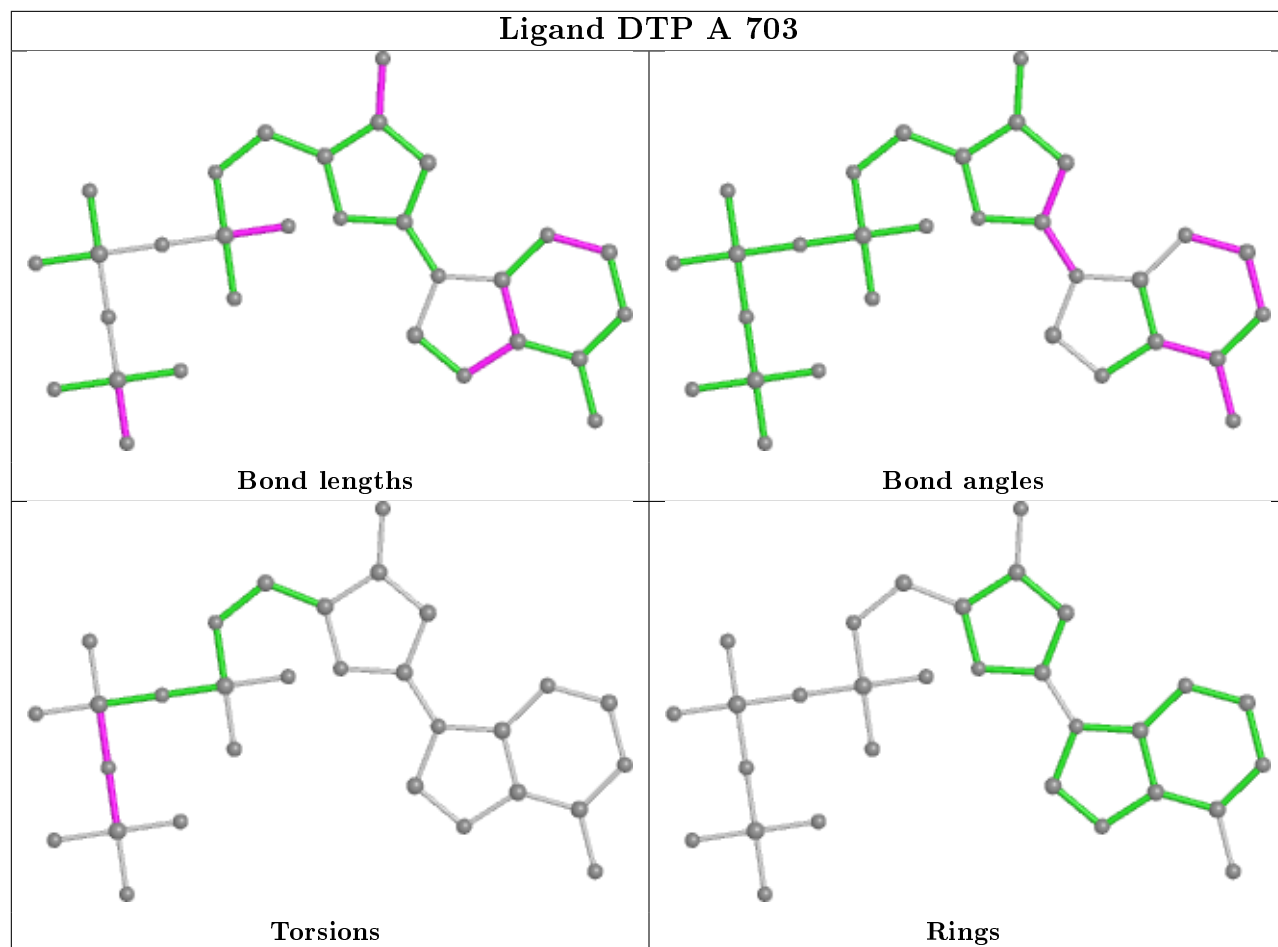


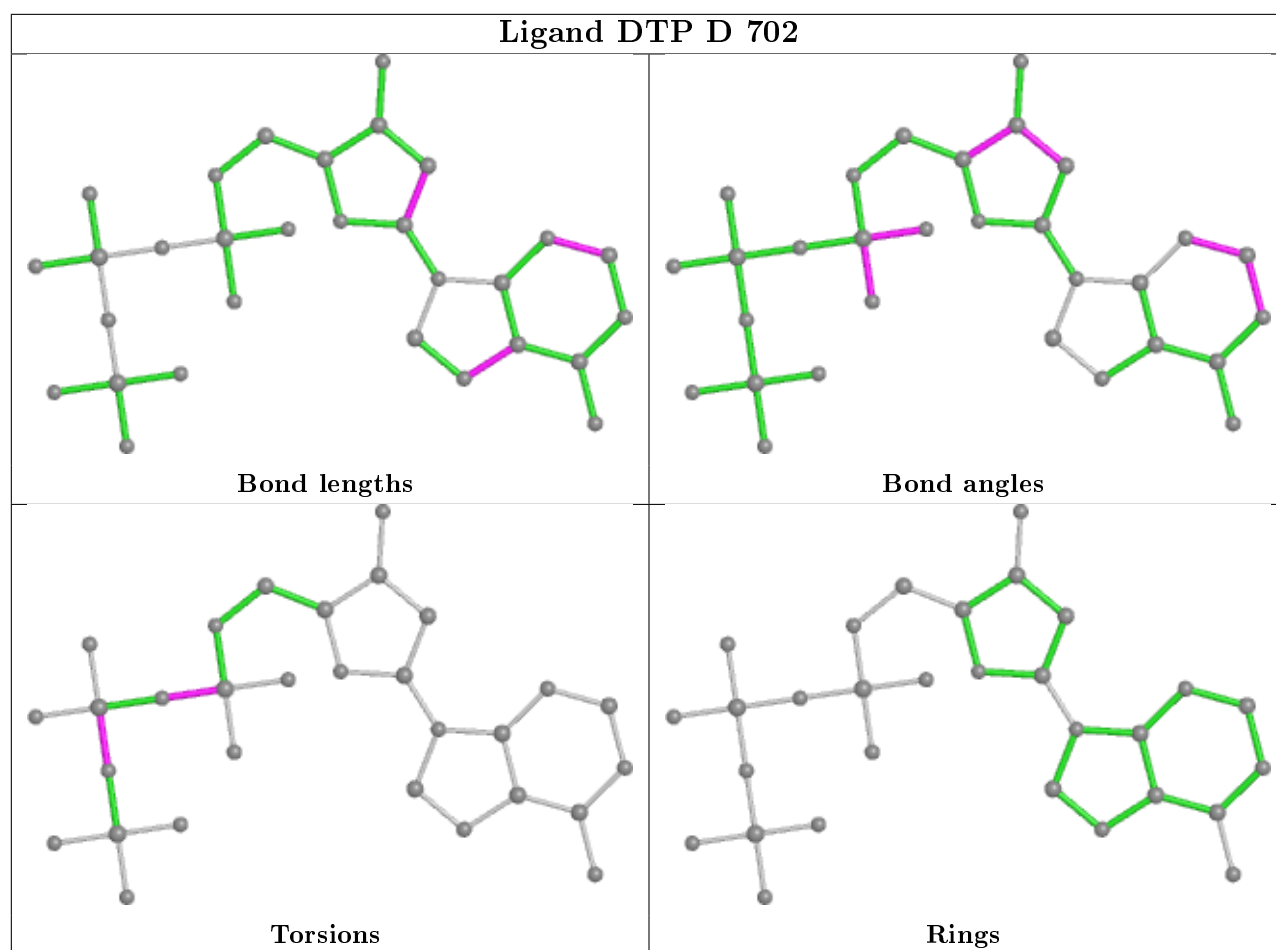




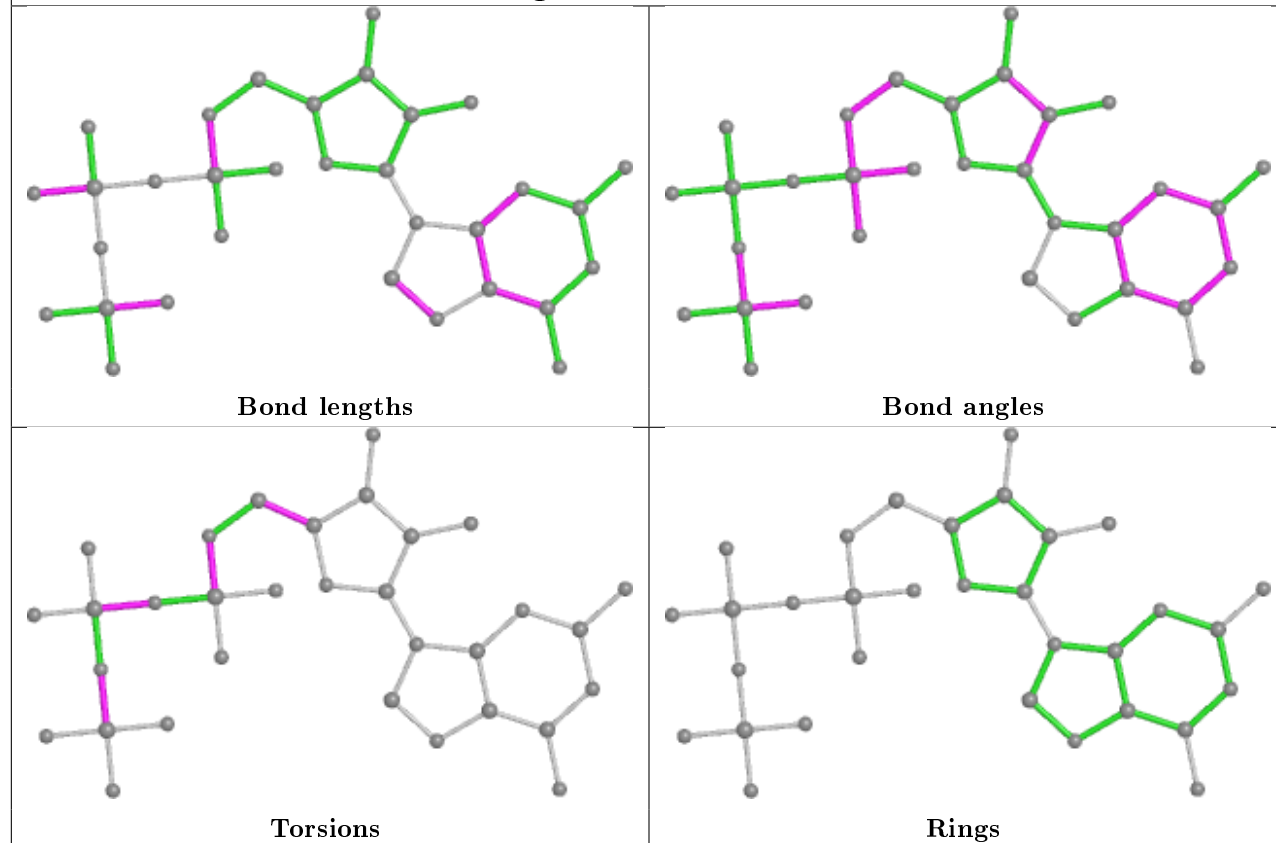




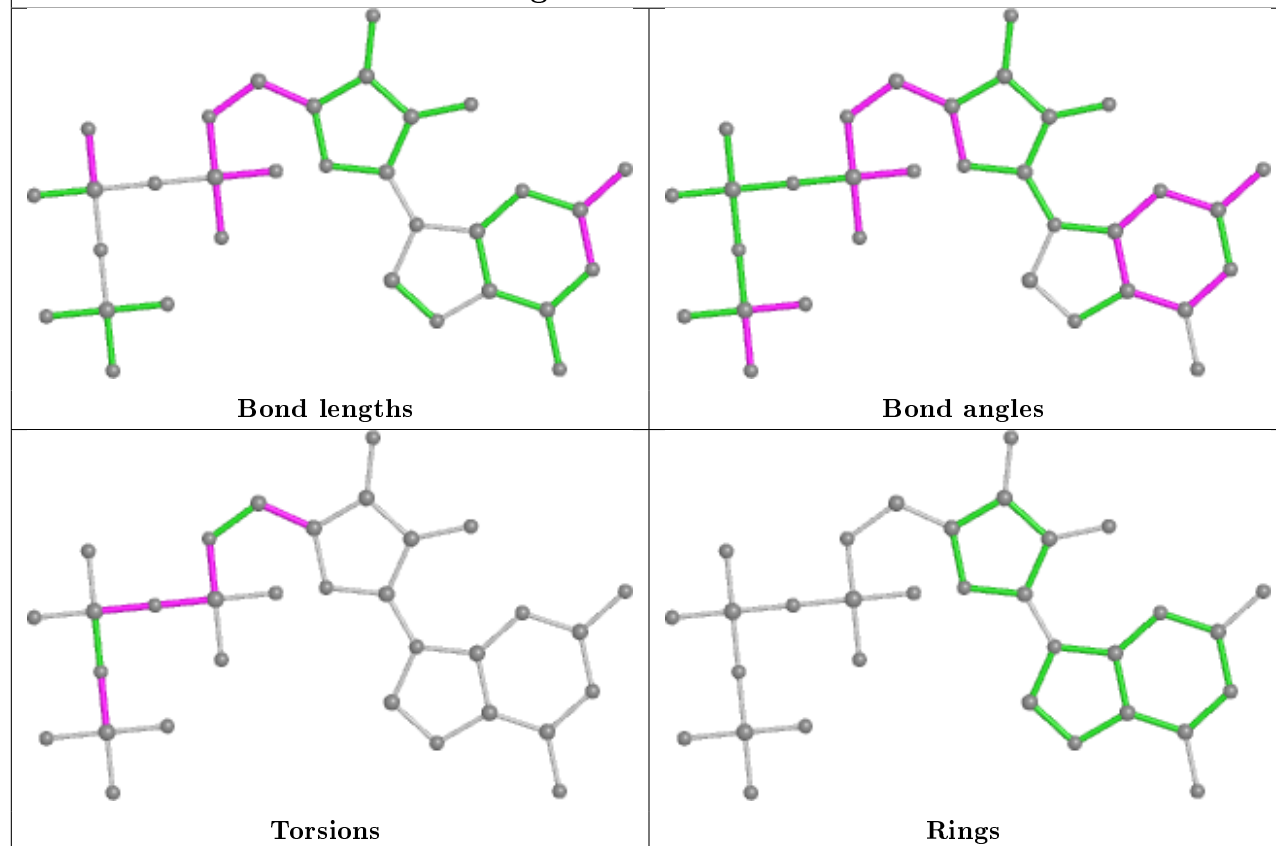




## Ligand GTP B 702



## Ligand GTP A 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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	480/550 (87%)	0.13	27 (5%) 24 30	20, 46, 86, 109	0
1	B	478/550 (86%)	0.04	26 (5%) 25 32	20, 41, 79, 107	0
1	C	478/550 (86%)	0.27	30 (6%) 20 25	23, 48, 85, 120	0
1	D	478/550 (86%)	-0.15	9 (1%) 66 73	17, 36, 68, 92	0
All	All	1914/2200 (87%)	0.07	92 (4%) 30 37	17, 42, 80, 120	0

The worst 5 of 92 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	488	LEU	8.2
1	C	113	ASP	7.3
1	C	488	LEU	7.2
1	B	487	VAL	6.4
1	B	113	ASP	6.4

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

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.

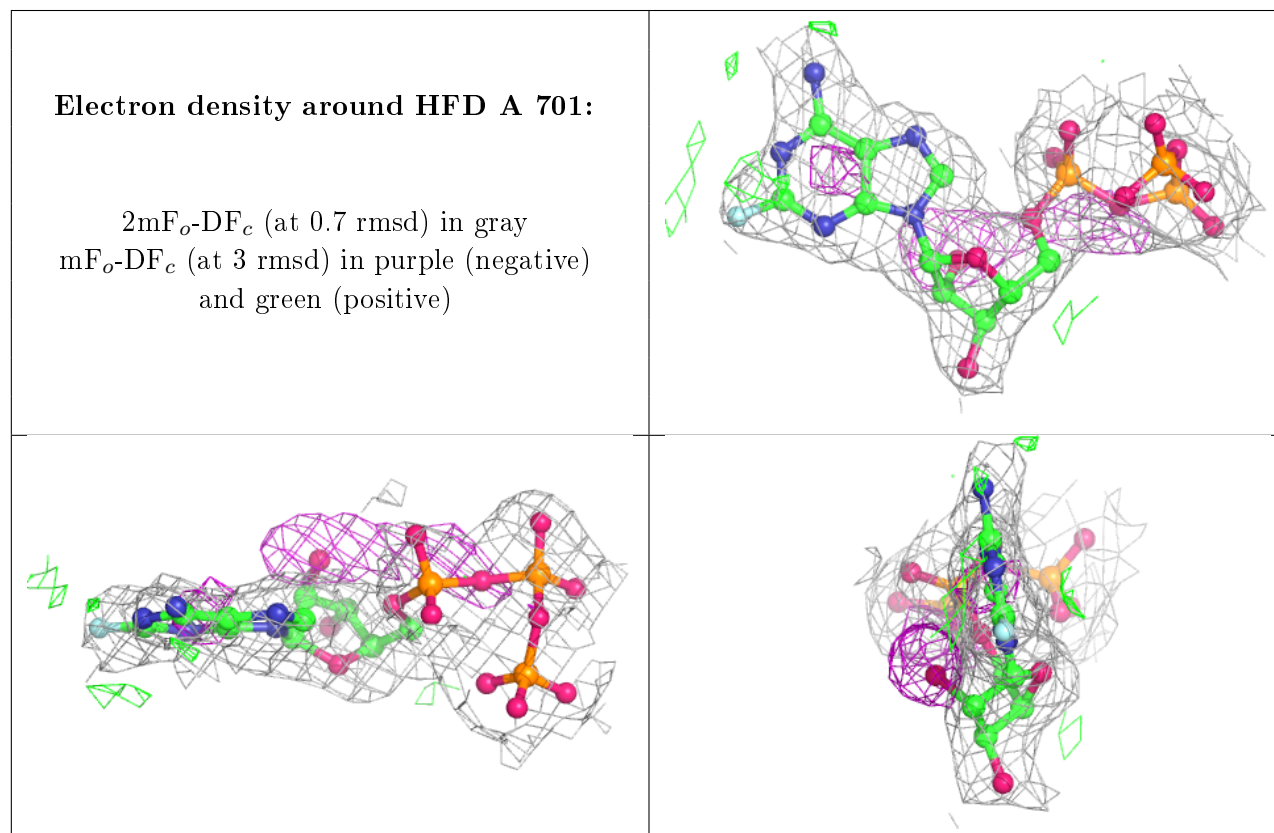
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	GLY	D	714	5/5	0.45	0.17	72,81,88,92	0
7	GLY	D	713	5/5	0.50	0.55	64,67,75,92	0
7	GLY	C	713	5/5	0.60	0.30	67,69,76,77	0
8	TRS	B	713	8/8	0.62	0.20	92,100,104,106	0
6	NA	D	708	1/1	0.63	0.32	73,73,73,73	0
9	PO4	D	716	5/5	0.67	0.39	104,121,137,137	0
7	GLY	B	712	5/5	0.68	0.27	78,80,86,90	0
8	TRS	B	714	8/8	0.69	0.35	57,73,79,83	0
7	GLY	C	711	5/5	0.71	0.24	72,78,80,81	0
7	GLY	D	712	5/5	0.72	0.17	57,63,68,69	0
5	MG	B	710	1/1	0.72	0.45	67,67,67,67	0
7	GLY	C	712	5/5	0.74	0.17	67,69,76,82	0
6	NA	A	711	1/1	0.75	0.14	66,66,66,66	0
7	GLY	A	715	5/5	0.76	0.20	72,76,80,84	0
7	GLY	C	714	5/5	0.82	0.27	65,69,76,76	0
7	GLY	D	715	5/5	0.83	0.24	62,65,67,68	0
7	GLY	C	710	5/5	0.84	0.29	79,79,84,91	0
7	GLY	B	711	5/5	0.84	0.27	58,62,67,72	0
2	HFD	A	701	32/32	0.85	0.16	45,63,96,98	0
6	NA	B	709	1/1	0.85	0.21	64,64,64,64	0
2	HFD	C	704	32/32	0.86	0.16	40,65,116,119	0
6	NA	C	701	1/1	0.87	0.13	62,62,62,62	0
2	HFD	B	701	32/32	0.88	0.16	33,59,73,82	0
6	NA	D	709	1/1	0.91	0.14	51,51,51,51	0
5	MG	C	703	1/1	0.91	0.11	30,30,30,30	0
6	NA	A	713	1/1	0.92	0.32	60,60,60,60	0
5	MG	D	710	1/1	0.92	0.10	78,78,78,78	0
6	NA	B	707	1/1	0.92	0.13	47,47,47,47	0
2	HFD	D	703	32/32	0.93	0.11	32,54,81,84	0
5	MG	D	701	1/1	0.94	0.07	29,29,29,29	0
6	NA	A	710	1/1	0.94	0.23	43,43,43,43	0
6	NA	C	707	1/1	0.95	0.10	60,60,60,60	0
5	MG	D	711	1/1	0.95	0.15	51,51,51,51	0
5	MG	C	709	1/1	0.95	0.12	69,69,69,69	0
6	NA	D	707	1/1	0.96	0.20	52,52,52,52	0
5	MG	A	704	1/1	0.96	0.09	31,31,31,31	0
6	NA	D	704	1/1	0.96	0.14	45,45,45,45	0
5	MG	A	714	1/1	0.96	0.07	61,61,61,61	0
6	NA	D	705	1/1	0.97	0.08	38,38,38,38	0
6	NA	C	706	1/1	0.97	0.13	41,41,41,41	0
6	NA	D	706	1/1	0.97	0.11	46,46,46,46	0
6	NA	A	709	1/1	0.97	0.10	51,51,51,51	0
3	GTP	C	705	32/32	0.97	0.11	26,30,37,39	0

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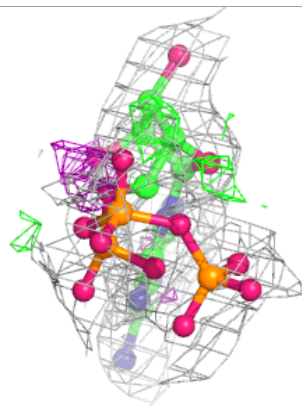
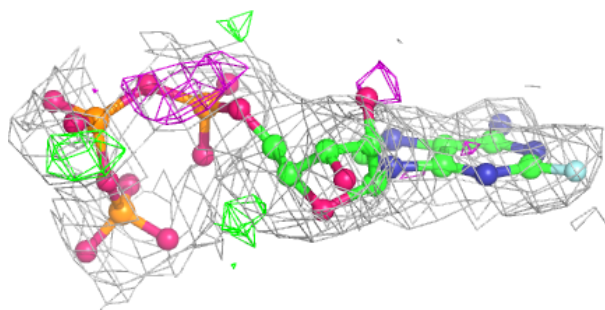
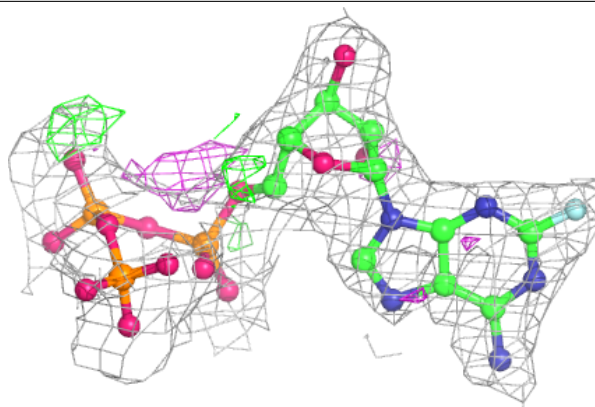
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NA	B	704	1/1	0.97	0.09	40,40,40,40	0
6	NA	B	705	1/1	0.97	0.39	47,47,47,47	0
6	NA	B	708	1/1	0.97	0.31	53,53,53,53	0
6	NA	B	706	1/1	0.98	0.11	42,42,42,42	0
3	GTP	B	702	32/32	0.98	0.10	20,23,35,38	0
6	NA	C	708	1/1	0.98	0.20	58,58,58,58	0
6	NA	A	707	1/1	0.98	0.13	39,39,39,39	0
3	GTP	A	702	32/32	0.98	0.11	20,24,36,41	0
6	NA	A	708	1/1	0.98	0.13	41,41,41,41	0
6	NA	A	712	1/1	0.98	0.17	56,56,56,56	0
3	GTP	A	706	32/32	0.99	0.11	18,21,29,30	0
4	DTP	C	702	30/30	0.99	0.11	19,23,30,33	0
4	DTP	D	702	30/30	0.99	0.12	20,22,28,31	0
4	DTP	B	703	30/30	0.99	0.11	17,19,23,25	0
4	DTP	A	703	30/30	0.99	0.12	23,25,34,38	0
5	MG	A	705	1/1	1.00	0.07	20,20,20,20	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.

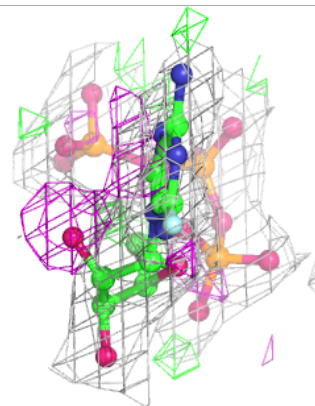
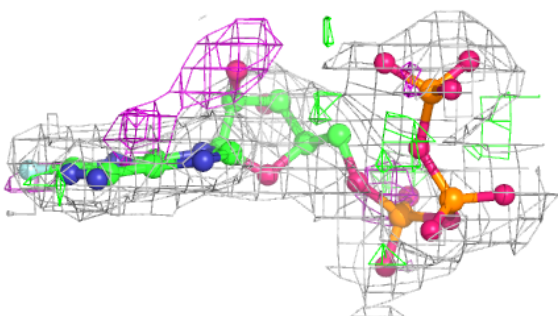
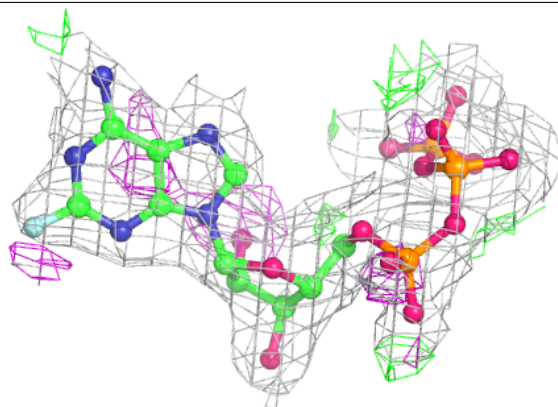


**Electron density around HFD C 704:**

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

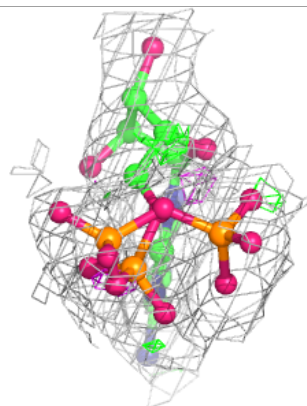
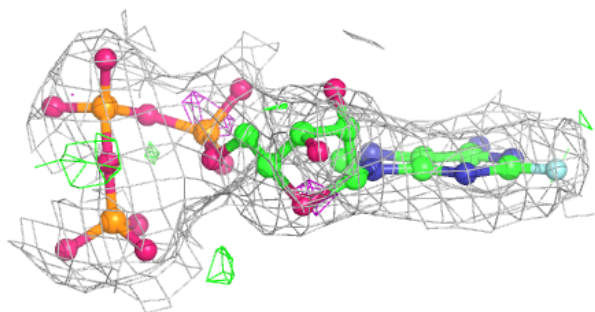
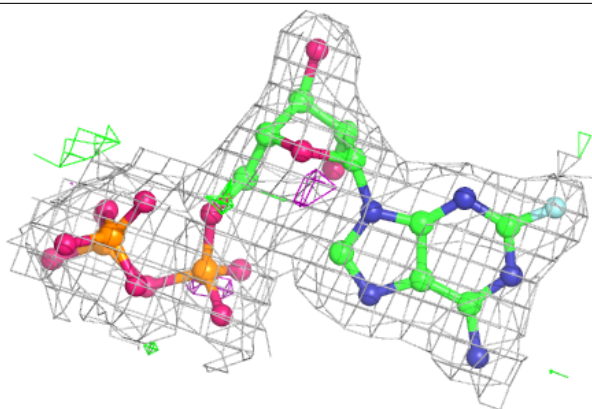
**Electron density around HFD B 701:**

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

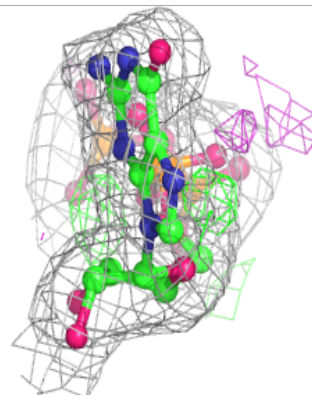
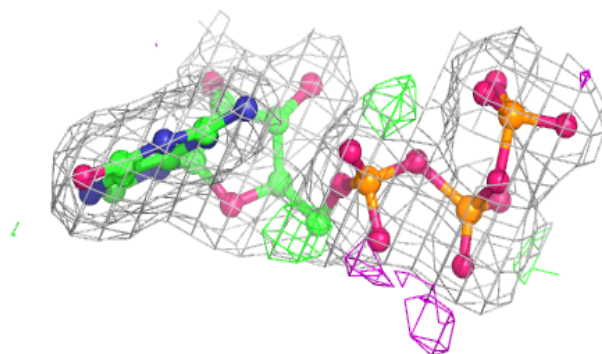
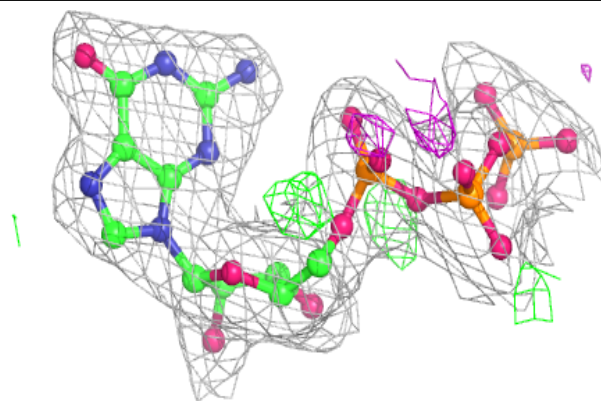


**Electron density around HFD D 703:**

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

**Electron density around GTP C 705:**

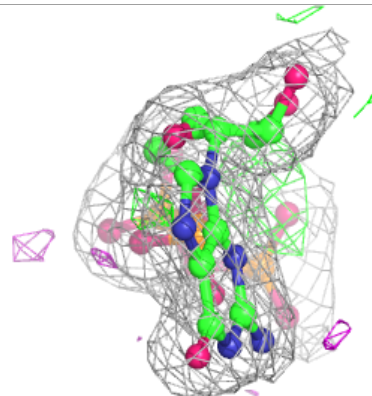
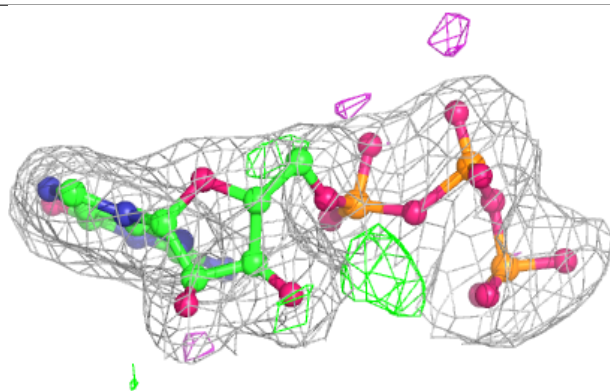
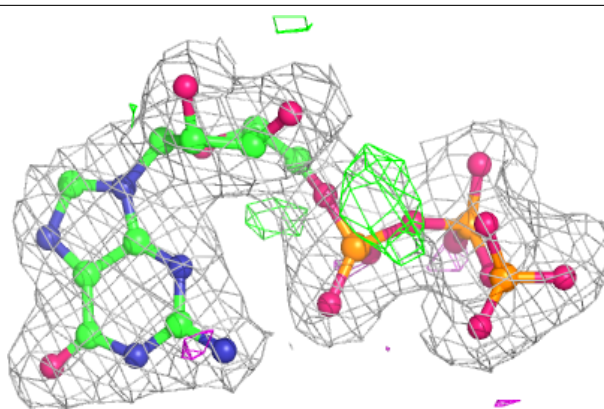
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



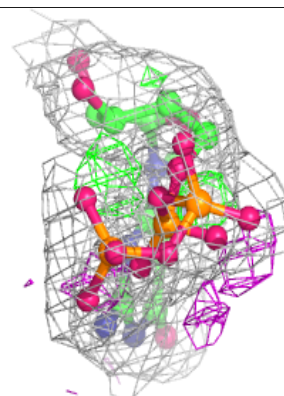
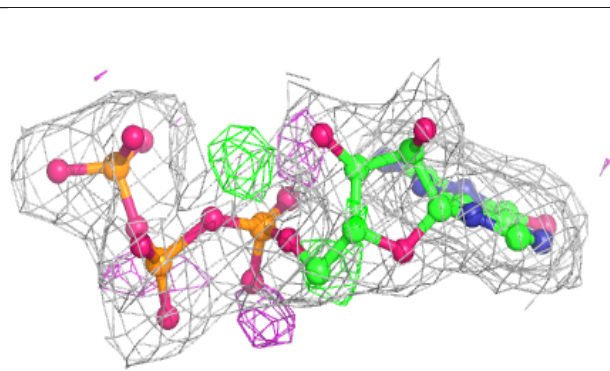
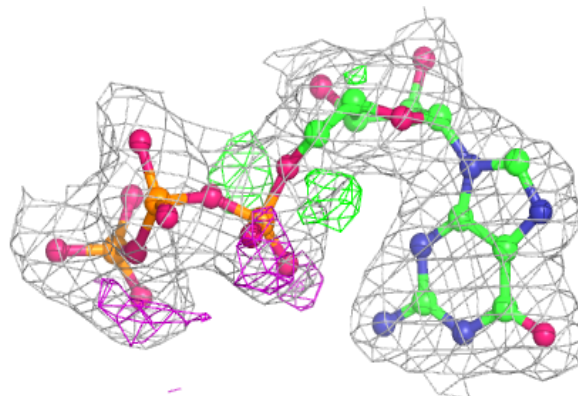


**Electron density around GTP B 702:**

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

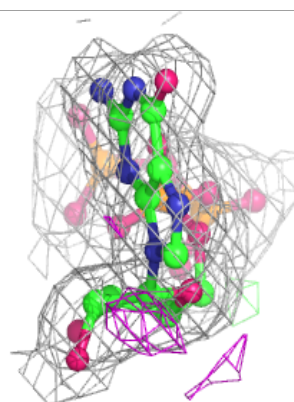
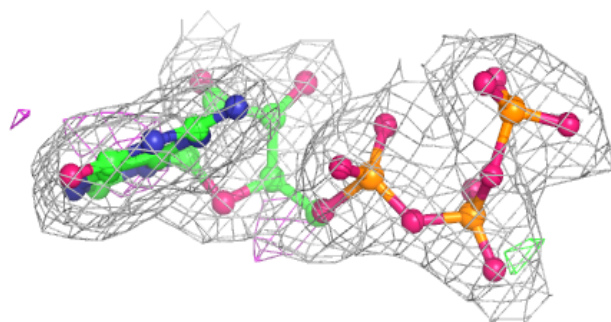
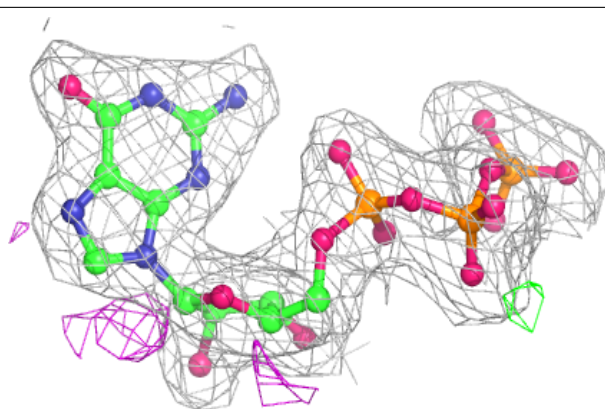
**Electron density around GTP A 702:**

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

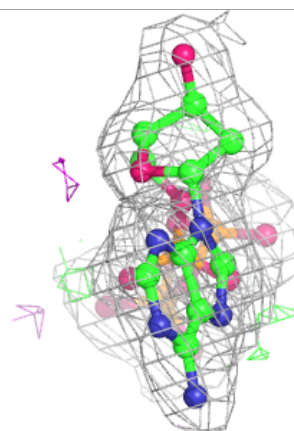
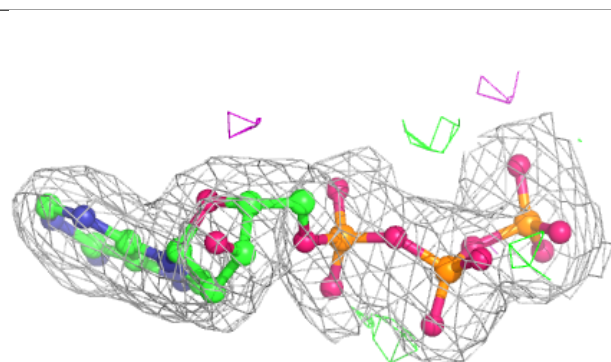
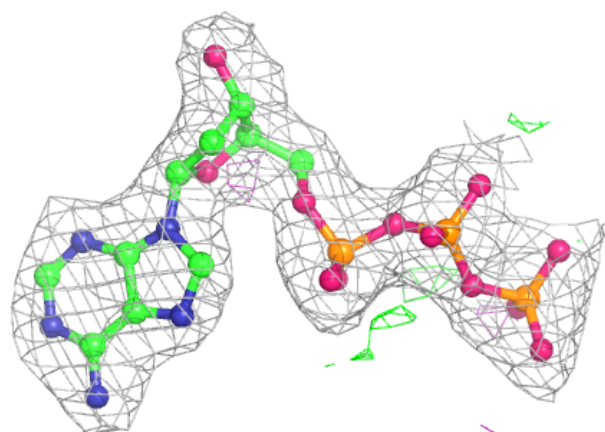


**Electron density around GTP A 706:**

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

**Electron density around DTP C 702:**

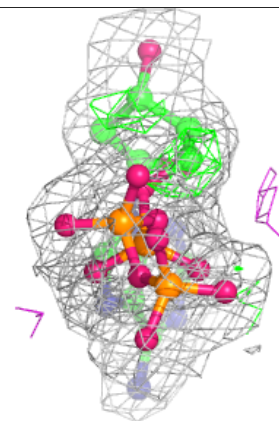
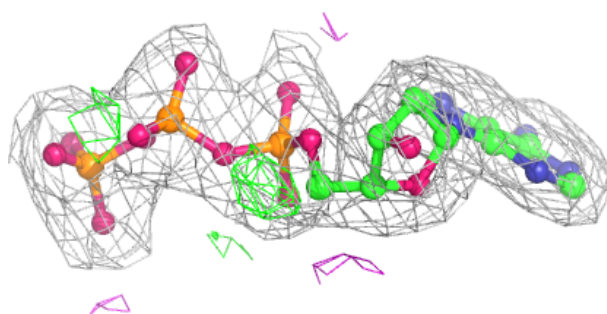
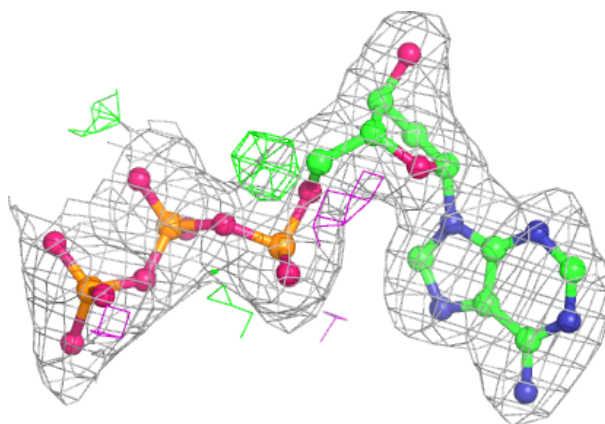
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



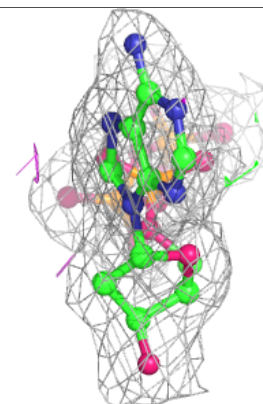
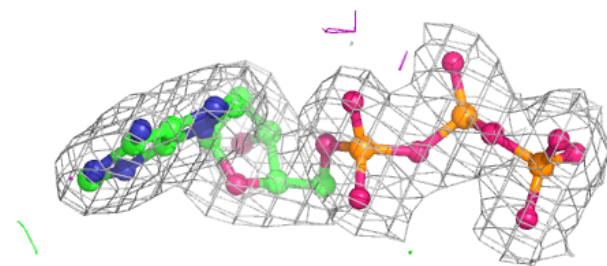
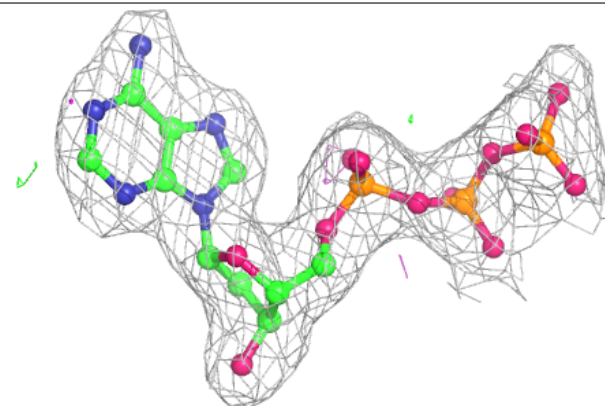


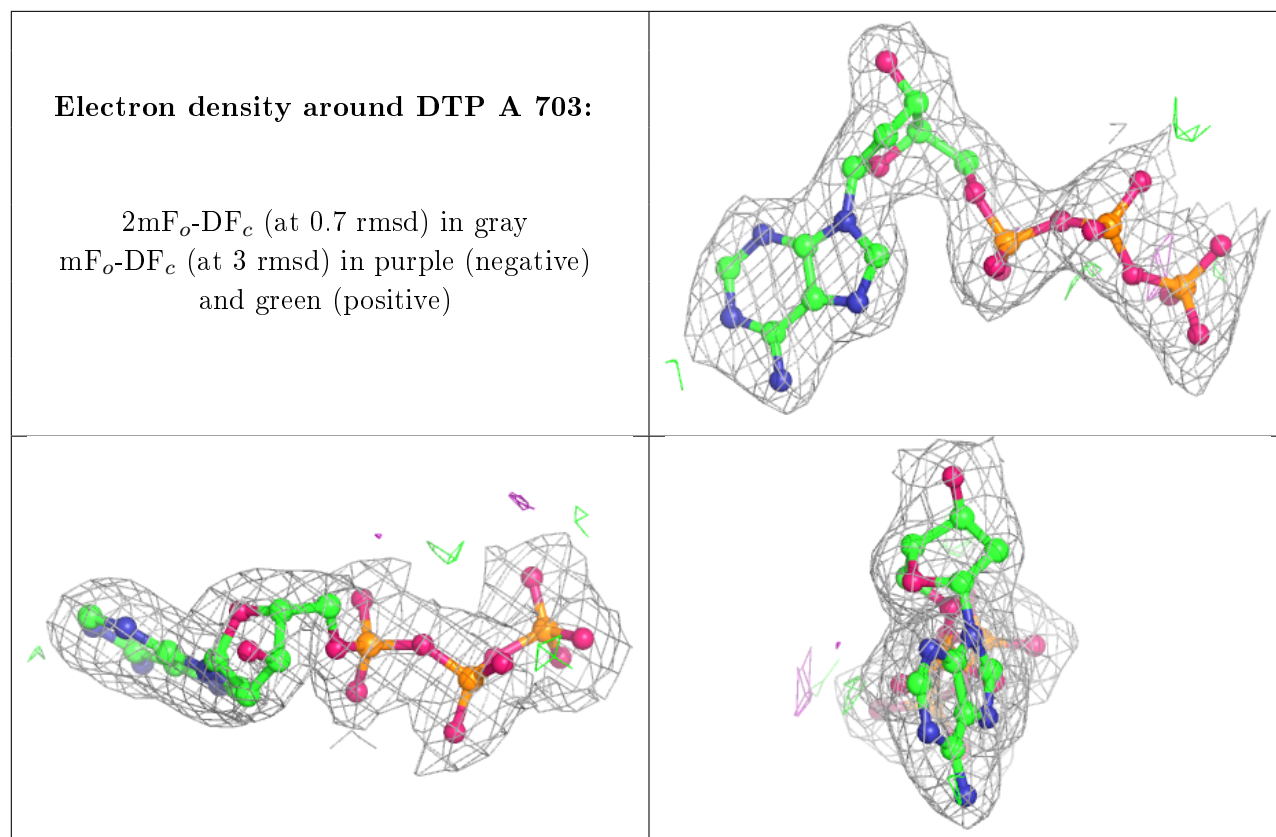
**Electron density around DTP D 702:**

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

**Electron density around DTP B 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.