Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2023 – 10:40 PM EDT

PDB ID	:	6DW3
Title	:	SAMHD1 Bound to Cytarabine-TP in the Catalytic Pocket
Authors	:	Knecht, K.M.; Buzovetsky, O.; Schneider, C.; Thomas, D.; Srikanth, V.; Kaderali, L.; Tofoleanu, F.; Reiss, K.; Ferreiros, N.; Geisslinger, G.; Batista, V.S.; Ji, X.; Cinatl, J.; Keppler, O.T.; Xiong, Y.
Deposited on	:	2018-06-26
Resolution	:	2.20 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

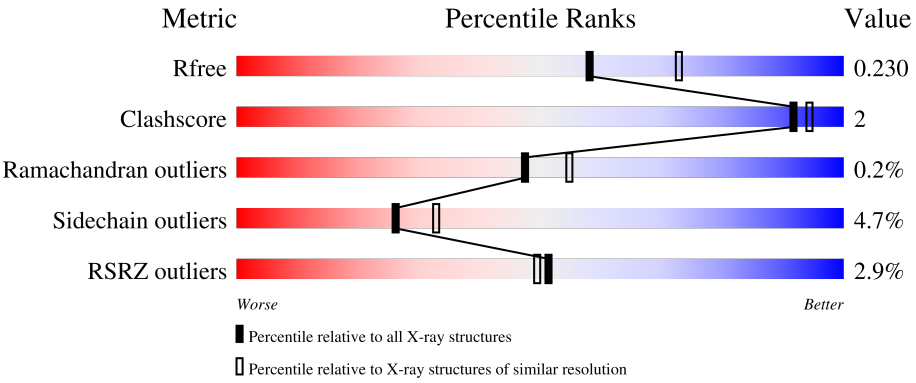
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 >=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 <=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	3% 76% 11% • 13%
1	B	550	4% 77% 9% • 13%
1	C	550	2% 79% 8% 13%
1	D	550	% 79% 7% • 13%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 16399 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	480	Total	C	N	O	S	0	1	0
			3930	2515	685	709	21			
1	C	479	Total	C	N	O	S	0	2	0
			3931	2516	685	709	21			
1	B	480	Total	C	N	O	S	0	2	0
			3940	2521	686	712	21			
1	A	480	Total	C	N	O	S	0	1	0
			3931	2516	685	709	21			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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

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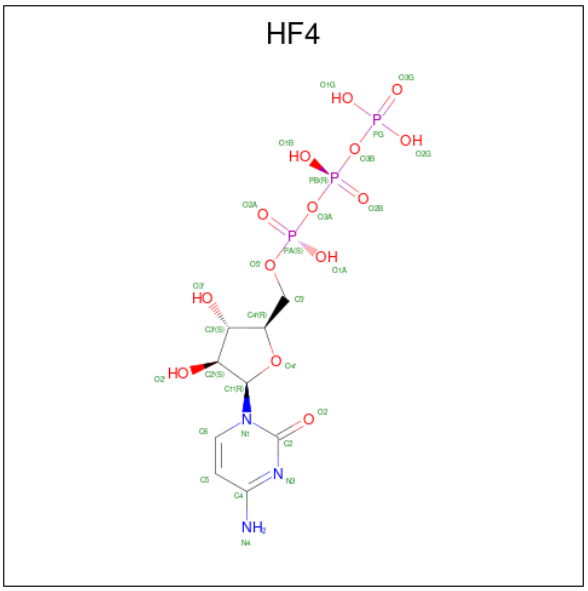
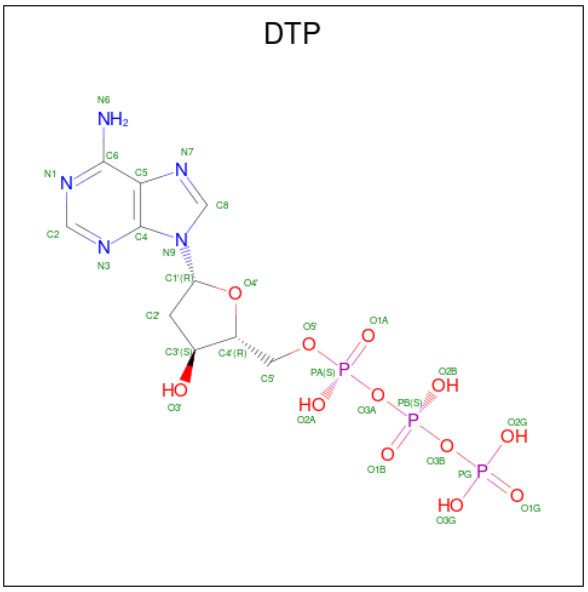
Chain	Residue	Modelled	Actual	Comment	Reference
A	110	PRO	-	expression tag	UNP Q9Y3Z3
A	111	ASN	-	expression tag	UNP Q9Y3Z3
A	112	SER	-	expression tag	UNP Q9Y3Z3
A	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
A	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3

- Molecule 2 is 4-amino-1-{5-O-[(S)-hydroxy{[(R)-hydroxy(phosphonooxy)phosphoryl]oxy}phosphoryl]-beta-D-arabinofuranosyl}pyrimidin-2(1H)-one (three-letter code: HF4) (formula: $C_9H_{16}N_3O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	0
			29	9	3	14	3		
2	C	1	Total	C	N	O	P	0	0
			29	9	3	14	3		
2	B	1	Total	C	N	O	P	0	0
			29	9	3	14	3		
2	A	1	Total	C	N	O	P	0	0
			29	9	3	14	3		

- Molecule 3 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$).

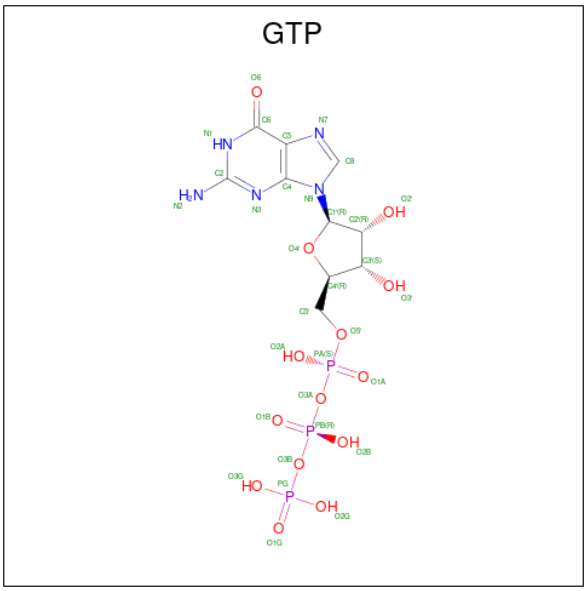


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C N O P 30 10 5 12 3	0	0
3	C	1	Total C N O P 30 10 5 12 3	0	0
3	B	1	Total C N O P 30 10 5 12 3	0	0
3	A	1	Total C N O P 30 10 5 12 3	0	0

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

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

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



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

- Molecule 6 is water.

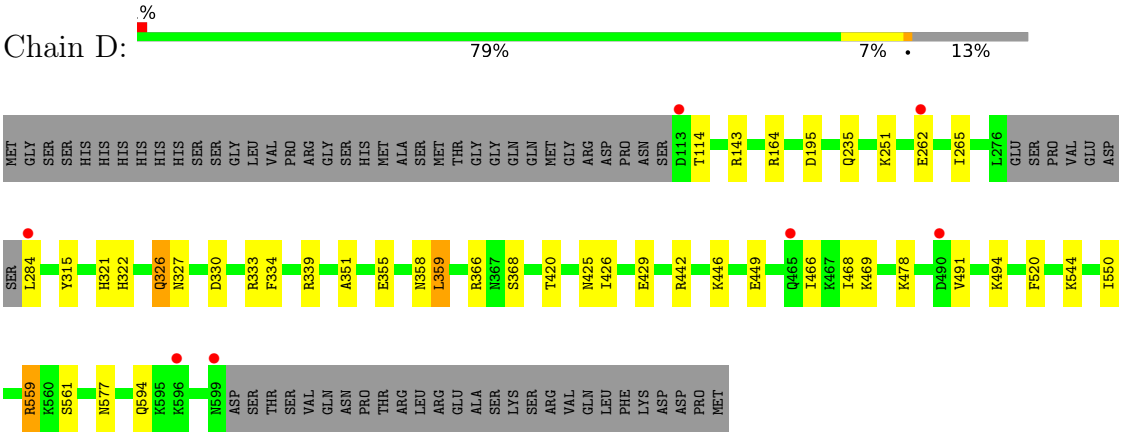
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	93	Total	O	0	0
			93	93		
6	C	53	Total	O	0	0
			53	53		
6	B	70	Total	O	0	0
			70	70		
6	A	79	Total	O	0	0
			79	79		

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.

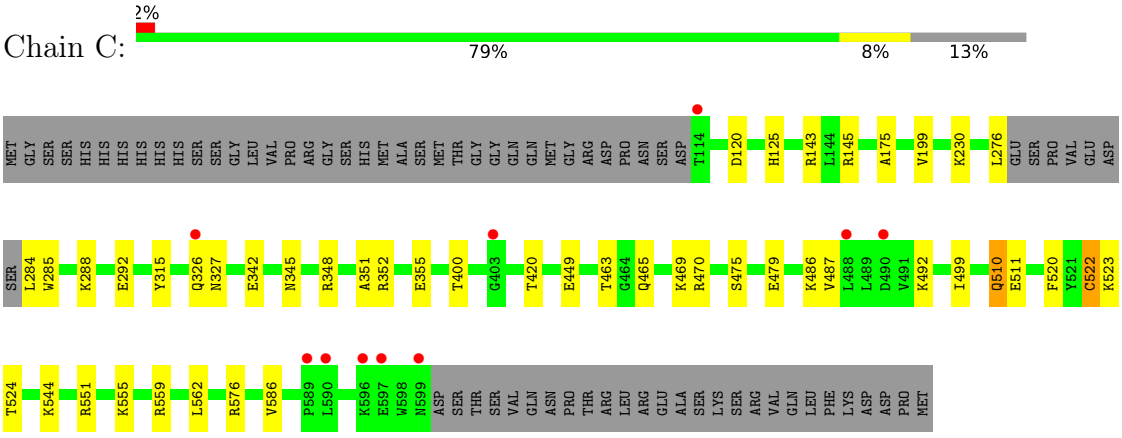
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain D:



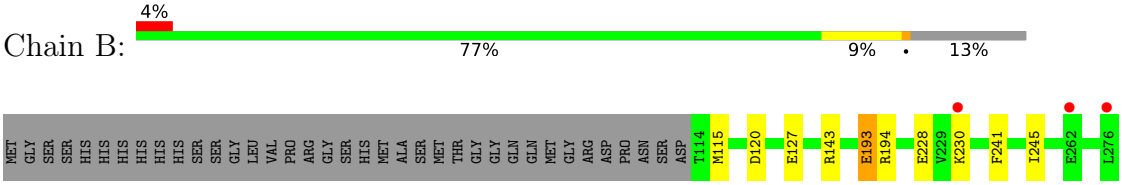
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

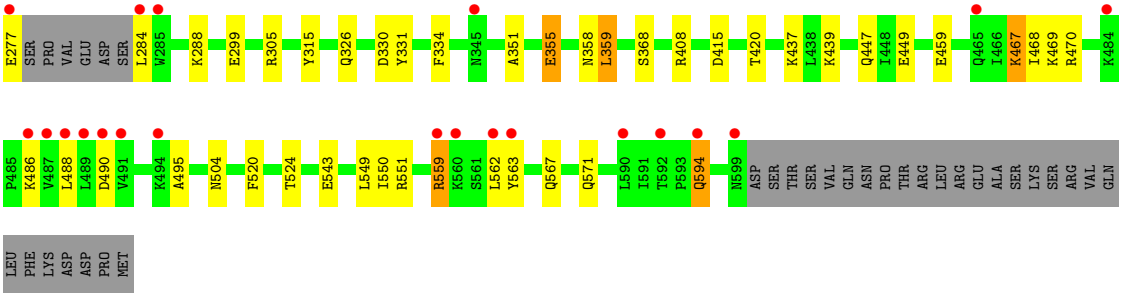
Chain C:



• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

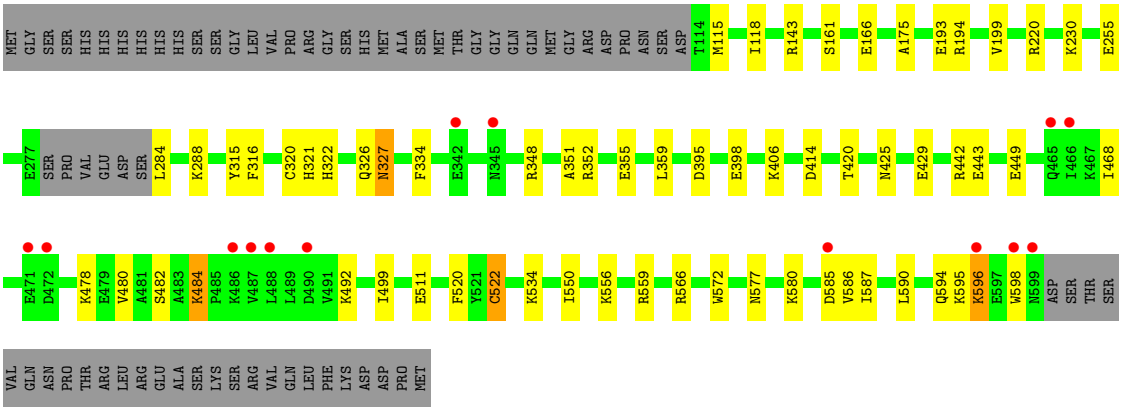
Chain B:





• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.34Å 147.32Å 98.54Å 90.00° 114.64° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 49.96 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.6 (50.00-2.20) 96.6 (49.96-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.190 , 0.228 0.196 , 0.230	Depositor DCC
R_{free} test set	5562 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	31.4	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 41.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16399	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GTP, MG, HF4, DTP

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	0.98	7/4023 (0.2%)	1.00	12/5430 (0.2%)
1	B	0.95	6/4032 (0.1%)	1.00	11/5442 (0.2%)
1	C	0.97	3/4023 (0.1%)	1.00	10/5430 (0.2%)
1	D	1.00	2/4022 (0.0%)	1.01	9/5429 (0.2%)
All	All	0.97	18/16100 (0.1%)	1.00	42/21731 (0.2%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	449	GLU	CD-OE1	9.06	1.35	1.25
1	C	355	GLU	CD-OE1	8.74	1.35	1.25
1	B	449	GLU	CD-OE1	6.91	1.33	1.25
1	C	449	GLU	CD-OE2	6.48	1.32	1.25
1	D	449	GLU	CD-OE1	6.42	1.32	1.25
1	A	449	GLU	CD-OE2	6.30	1.32	1.25
1	A	166	GLU	CG-CD	6.16	1.61	1.51
1	A	161	SER	CB-OG	6.05	1.50	1.42
1	C	449	GLU	CD-OE1	5.93	1.32	1.25
1	A	355	GLU	CD-OE2	5.77	1.32	1.25
1	B	368	SER	CB-OG	-5.72	1.34	1.42
1	B	543	GLU	CG-CD	5.63	1.60	1.51
1	B	193	GLU	CG-CD	5.46	1.60	1.51
1	B	355	GLU	CD-OE1	5.39	1.31	1.25
1	B	449	GLU	CD-OE2	5.37	1.31	1.25
1	D	262	GLU	CD-OE1	5.18	1.31	1.25
1	A	443	GLU	CG-CD	5.18	1.59	1.51
1	A	429	GLU	CD-OE2	5.04	1.31	1.25

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	120	ASP	CB-CG-OD1	11.95	129.06	118.30
1	C	559	ARG	NE-CZ-NH2	7.29	123.94	120.30
1	C	551	ARG	NE-CZ-NH1	-7.28	116.66	120.30
1	D	330	ASP	CB-CG-OD2	-7.01	111.99	118.30
1	D	559	ARG	NE-CZ-NH2	6.94	123.77	120.30
1	D	442	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	B	415	ASP	CB-CG-OD2	-6.45	112.50	118.30
1	C	145	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	B	305	ARG	NE-CZ-NH2	6.20	123.40	120.30
1	A	414	ASP	CB-CG-OD1	6.18	123.86	118.30
1	B	115	MET	CG-SD-CE	6.15	110.04	100.20
1	A	442	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	D	164	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	C	348	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	A	596	LYS	CB-CG-CD	5.98	127.15	111.60
1	A	559	ARG	NE-CZ-NH2	5.95	123.27	120.30
1	D	366	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	B	299	GLU	OE1-CD-OE2	-5.91	116.21	123.30
1	D	195	ASP	CB-CG-OD1	5.89	123.60	118.30
1	D	330	ASP	CB-CG-OD1	5.89	123.60	118.30
1	D	429	GLU	OE1-CD-OE2	5.83	130.29	123.30
1	B	415	ASP	CB-CG-OD1	5.82	123.54	118.30
1	B	559	ARG	NE-CZ-NH2	5.81	123.20	120.30
1	B	331	TYR	CB-CG-CD1	-5.70	117.58	121.00
1	A	585	ASP	CB-CG-OD1	5.70	123.42	118.30
1	A	194	ARG	NE-CZ-NH2	5.64	123.12	120.30
1	C	352	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	352	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	C	120	ASP	CB-CG-OD2	5.48	123.24	118.30
1	A	220	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	B	127	GLU	OE1-CD-OE2	-5.45	116.76	123.30
1	C	470	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	330	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	A	348	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	551	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	C	145	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	A	255	GLU	OE1-CD-OE2	-5.14	117.13	123.30
1	C	511[A]	GLU	OE1-CD-OE2	-5.12	117.16	123.30
1	C	511[B]	GLU	OE1-CD-OE2	-5.12	117.16	123.30
1	A	316	PHE	CB-CG-CD1	5.08	124.36	120.80
1	A	395	ASP	CB-CG-OD2	-5.03	113.77	118.30
1	D	339	ARG	NE-CZ-NH1	-5.03	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3931	0	3921	20	0
1	B	3940	0	3926	12	0
1	C	3931	0	3920	12	0
1	D	3930	0	3919	16	0
2	A	29	0	0	0	0
2	B	29	0	0	0	0
2	C	29	0	0	1	0
2	D	29	0	0	0	0
3	A	30	0	12	0	0
3	B	30	0	12	0	0
3	C	30	0	12	0	0
3	D	30	0	12	0	0
4	A	3	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	32	0	12	0	0
5	B	32	0	12	0	0
5	C	32	0	12	0	0
5	D	32	0	12	0	0
6	A	79	0	0	2	0
6	B	70	0	0	1	0
6	C	53	0	0	0	0
6	D	93	0	0	4	0
All	All	16399	0	15782	52	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.

All (52) 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:522[A]:CYS:SG	1:A:586:VAL:HG21	2.28	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:HIS:NE2	6:D:801:HOH:O	2.24	0.71
1:A:322:HIS:NE2	6:A:801:HOH:O	2.28	0.66
1:C:327:ASN:O	1:A:326:GLN:HG2	1.96	0.64
1:C:499:ILE:HD11	1:C:555:LYS:HE2	1.80	0.63
1:C:586:VAL:HG21	1:A:522[B]:CYS:SG	2.42	0.59
1:D:425:ASN:OD1	1:A:425:ASN:OD1	2.21	0.58
1:A:320:CYS:SG	1:A:327:ASN:HB3	2.44	0.58
1:D:327:ASN:HA	6:D:803:HOH:O	2.08	0.52
1:A:468:ILE:CD1	1:A:550:ILE:HD11	2.41	0.50
1:D:446:LYS:HE2	6:D:878:HOH:O	2.10	0.49
1:B:355:GLU:OE1	1:B:358:ASN:ND2	2.42	0.49
1:C:326:GLN:HB3	1:A:326:GLN:NE2	2.28	0.49
1:B:143:ARG:HD2	1:B:420:THR:HA	1.94	0.49
1:B:563:TYR:O	1:B:567:GLN:HG2	2.13	0.49
1:A:468:ILE:HD12	1:A:550:ILE:HD11	1.95	0.48
1:C:143:ARG:HD2	1:C:420:THR:HA	1.95	0.48
1:A:566:ARG:HD3	1:A:587:ILE:HB	1.96	0.47
1:D:326:GLN:OE1	1:B:326:GLN:CD	2.53	0.47
1:B:571:GLN:HE22	1:B:594:GLN:NE2	2.13	0.47
1:D:251:LYS:HE2	1:D:265:ILE:CD1	2.46	0.46
1:D:114:THR:HG22	6:D:889:HOH:O	2.15	0.45
1:A:334:PHE:CE2	1:A:359:LEU:HD11	2.52	0.45
1:A:580:LYS:HD2	1:A:598:TRP:HB3	1.98	0.45
1:D:355:GLU:OE1	1:D:358:ASN:ND2	2.50	0.45
1:B:468:ILE:CD1	1:B:550:ILE:HD11	2.47	0.44
1:D:143:ARG:HD2	1:D:420:THR:HA	1.99	0.44
1:C:479:GLU:OE1	1:C:576:ARG:HD2	2.18	0.44
1:B:241:PHE:O	1:B:245:ILE:HG12	2.17	0.44
1:B:351:ALA:O	1:B:520:PHE:HA	2.18	0.43
1:B:334:PHE:CE2	1:B:359:LEU:HD11	2.54	0.43
1:A:143:ARG:HD2	1:A:420:THR:HA	2.00	0.43
1:D:468:ILE:CD1	1:D:550:ILE:HD11	2.49	0.43
1:A:351:ALA:O	1:A:520:PHE:HA	2.19	0.43
1:D:334:PHE:CE2	1:D:359:LEU:HD11	2.54	0.43
1:A:322:HIS:CE1	6:A:801:HOH:O	2.70	0.43
1:C:175:ALA:HB1	1:C:199:VAL:HG12	2.01	0.42
1:B:459:GLU:OE2	1:B:549:LEU:HD22	2.20	0.42
1:D:491:VAL:HG21	1:D:561:SER:HA	2.01	0.42
1:C:285:TRP:CD2	1:C:292:GLU:HG3	2.54	0.42
1:C:326:GLN:HB3	1:A:326:GLN:HE21	1.84	0.42
1:D:333:ARG:HB2	1:C:125:HIS:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:351:ALA:O	1:D:520:PHE:HA	2.20	0.41
1:B:504:ASN:HD22	1:B:504:ASN:N	2.18	0.41
1:A:480:VAL:HG22	1:A:572:TRP:CD2	2.54	0.41
1:C:351:ALA:O	1:C:520:PHE:HA	2.20	0.41
1:D:426:ILE:HD13	1:D:426:ILE:HA	1.92	0.41
2:C:701:HF4:O1B	2:C:701:HF4:O2G	2.39	0.41
1:B:467:LYS:HE2	6:B:854:HOH:O	2.20	0.41
1:A:175:ALA:HB1	1:A:199:VAL:HG12	2.02	0.41
1:D:321:HIS:CE1	1:A:321:HIS:CE1	3.08	0.40
1:A:482:SER:O	1:A:484:LYS:HE2	2.21	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	477/550 (87%)	468 (98%)	9 (2%)	0	100	100
1	B	478/550 (87%)	465 (97%)	12 (2%)	1 (0%)	47	55
1	C	477/550 (87%)	464 (97%)	12 (2%)	1 (0%)	47	55
1	D	477/550 (87%)	466 (98%)	10 (2%)	1 (0%)	47	55
All	All	1909/2200 (87%)	1863 (98%)	43 (2%)	3 (0%)	47	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	466	ILE
1	C	510	GLN
1	B	495	ALA

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	427/488 (88%)	403 (94%)	24 (6%)	21	25
1	B	428/488 (88%)	405 (95%)	23 (5%)	22	26
1	C	427/488 (88%)	405 (95%)	22 (5%)	23	28
1	D	427/488 (88%)	414 (97%)	13 (3%)	41	53
All	All	1709/1952 (88%)	1627 (95%)	82 (5%)	26	32

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	235	GLN
1	D	284	LEU
1	D	315	TYR
1	D	326	GLN
1	D	359	LEU
1	D	368	SER
1	D	469	LYS
1	D	478	LYS
1	D	494	LYS
1	D	544	LYS
1	D	559	ARG
1	D	577	ASN
1	D	594	GLN
1	C	230	LYS
1	C	276	LEU
1	C	284	LEU
1	C	288	LYS
1	C	315	TYR
1	C	342	GLU
1	C	345	ASN
1	C	400	THR
1	C	463	THR
1	C	465	GLN
1	C	469	LYS

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Mol	Chain	Res	Type
1	C	475	SER
1	C	486	LYS
1	C	487	VAL
1	C	492	LYS
1	C	510	GLN
1	C	522[A]	CYS
1	C	522[B]	CYS
1	C	523	LYS
1	C	524	THR
1	C	544	LYS
1	C	562	LEU
1	B	193	GLU
1	B	194	ARG
1	B	228	GLU
1	B	230	LYS
1	B	277	GLU
1	B	284	LEU
1	B	288	LYS
1	B	315	TYR
1	B	359	LEU
1	B	408	ARG
1	B	437	LYS
1	B	439	LYS
1	B	447	GLN
1	B	467	LYS
1	B	469	LYS
1	B	470	ARG
1	B	486	LYS
1	B	488	LEU
1	B	490	ASP
1	B	524	THR
1	B	559	ARG
1	B	562	LEU
1	B	594	GLN
1	A	115	MET
1	A	118	ILE
1	A	193	GLU
1	A	230	LYS
1	A	284	LEU
1	A	288	LYS
1	A	315	TYR
1	A	327	ASN

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Mol	Chain	Res	Type
1	A	398	GLU
1	A	406	LYS
1	A	478	LYS
1	A	484	LYS
1	A	492	LYS
1	A	499	ILE
1	A	511	GLU
1	A	522[A]	CYS
1	A	522[B]	CYS
1	A	534	LYS
1	A	556	LYS
1	A	577	ASN
1	A	590	LEU
1	A	594	GLN
1	A	595	LYS
1	A	596	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	190	GLN
1	D	235	GLN
1	D	425	ASN
1	D	571	GLN
1	D	594	GLN
1	C	149	GLN
1	C	235	GLN
1	C	328	ASN
1	C	425	ASN
1	C	535	ASN
1	C	539	GLN
1	C	594	GLN
1	C	599	ASN
1	B	149	GLN
1	B	190	GLN
1	B	235	GLN
1	B	322	HIS
1	B	326	GLN
1	B	504	ASN
1	B	517	HIS
1	B	535	ASN
1	B	539	GLN

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Mol	Chain	Res	Type
1	B	594	GLN
1	A	326	GLN
1	A	535	ASN
1	A	539	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	DTP	B	701	4	26,32,32	1.46	4 (15%)	30,50,50	1.24	5 (16%)
3	DTP	C	704	4	26,32,32	1.21	2 (7%)	30,50,50	1.55	4 (13%)
2	HF4	D	701	4	26,30,30	2.79	8 (30%)	39,47,47	1.57	9 (23%)
2	HF4	B	703	4	26,30,30	2.55	9 (34%)	39,47,47	1.85	9 (23%)
3	DTP	A	703	4	26,32,32	1.06	1 (3%)	30,50,50	1.27	2 (6%)
5	GTP	B	702	4	26,34,34	1.39	5 (19%)	32,54,54	1.64	6 (18%)
3	DTP	D	702	4	26,32,32	1.04	0	30,50,50	1.63	7 (23%)
2	HF4	C	701	4	26,30,30	2.49	9 (34%)	39,47,47	1.41	6 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	GTP	A	702	4	26,34,34	1.48	4 (15%)	32,54,54	1.46	7 (21%)
5	GTP	C	703	4	26,34,34	1.33	3 (11%)	32,54,54	1.42	5 (15%)
5	GTP	D	704	4	26,34,34	1.34	3 (11%)	32,54,54	1.14	1 (3%)
2	HF4	A	705	4	26,30,30	2.86	9 (34%)	39,47,47	1.49	8 (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
3	DTP	B	701	4	-	4/18/34/34	0/3/3/3
3	DTP	C	704	4	-	3/18/34/34	0/3/3/3
2	HF4	D	701	4	-	7/22/38/38	0/2/2/2
2	HF4	B	703	4	-	4/22/38/38	0/2/2/2
3	DTP	A	703	4	-	2/18/34/34	0/3/3/3
5	GTP	B	702	4	-	4/18/38/38	0/3/3/3
3	DTP	D	702	4	-	2/18/34/34	0/3/3/3
2	HF4	C	701	4	-	6/22/38/38	0/2/2/2
5	GTP	A	702	4	-	3/18/38/38	0/3/3/3
5	GTP	C	703	4	-	6/18/38/38	0/3/3/3
5	GTP	D	704	4	-	2/18/38/38	0/3/3/3
2	HF4	A	705	4	-	4/22/38/38	0/2/2/2

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	HF4	O2-C2	10.24	1.42	1.23
2	A	705	HF4	O2-C2	10.21	1.42	1.23
2	C	701	HF4	O2-C2	8.38	1.39	1.23
2	B	703	HF4	O2-C2	7.52	1.37	1.23
2	D	701	HF4	C4-N4	5.38	1.46	1.33
2	B	703	HF4	C6-C5	5.01	1.46	1.35
2	A	705	HF4	C2-N3	4.66	1.45	1.36
2	A	705	HF4	C4-N4	4.07	1.43	1.33
2	A	705	HF4	C6-C5	4.05	1.44	1.35
2	B	703	HF4	C2-N3	3.79	1.44	1.36
3	B	701	DTP	C2-N1	3.72	1.40	1.33
2	B	703	HF4	C2'-C3'	-3.71	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	705	HF4	C2'-C3'	-3.58	1.43	1.53
5	A	702	GTP	O4'-C1'	3.52	1.46	1.41
2	C	701	HF4	O4'-C1'	3.52	1.50	1.42
2	B	703	HF4	C6-N1	3.48	1.46	1.38
2	D	701	HF4	C2'-C3'	-3.39	1.44	1.53
2	C	701	HF4	C4-N4	3.35	1.41	1.33
3	B	701	DTP	C5-C4	3.35	1.49	1.40
2	C	701	HF4	C2-N3	3.20	1.42	1.36
5	B	702	GTP	O4'-C1'	3.18	1.45	1.41
2	D	701	HF4	C2-N3	3.14	1.42	1.36
3	C	704	DTP	C2-N3	3.03	1.37	1.32
5	B	702	GTP	O6-C6	3.03	1.29	1.23
2	B	703	HF4	C4-N4	3.01	1.41	1.33
2	A	705	HF4	O4'-C1'	3.00	1.49	1.42
2	D	701	HF4	O4'-C1'	2.91	1.48	1.42
2	A	705	HF4	C6-N1	2.90	1.45	1.38
5	D	704	GTP	C6-N1	-2.86	1.33	1.37
5	D	704	GTP	C2'-C1'	-2.86	1.49	1.53
2	C	701	HF4	C4-N3	2.73	1.40	1.34
3	C	704	DTP	C5-C4	2.73	1.48	1.40
2	C	701	HF4	C2'-C3'	-2.61	1.46	1.53
2	C	701	HF4	C6-N1	2.58	1.44	1.38
5	A	702	GTP	PG-O3G	-2.57	1.45	1.54
5	D	704	GTP	O4'-C1'	2.50	1.44	1.41
5	A	702	GTP	C6-N1	-2.49	1.34	1.37
5	C	703	GTP	C6-N1	-2.42	1.34	1.37
2	B	703	HF4	PG-O1G	-2.40	1.45	1.54
5	A	702	GTP	C5-C6	-2.39	1.42	1.47
5	C	703	GTP	C2-N3	2.36	1.38	1.33
2	D	701	HF4	PG-O1G	-2.34	1.45	1.54
5	B	702	GTP	C6-N1	-2.32	1.34	1.37
2	B	703	HF4	C1'-N1	-2.31	1.40	1.47
2	C	701	HF4	C2'-C1'	-2.25	1.46	1.53
2	D	701	HF4	PA-O5'	2.22	1.68	1.59
3	A	703	DTP	C4-N3	-2.19	1.32	1.35
3	B	701	DTP	C1'-N9	-2.16	1.43	1.49
2	D	701	HF4	PA-O1A	-2.15	1.45	1.55
2	A	705	HF4	PA-O5'	2.14	1.68	1.59
2	B	703	HF4	O4'-C1'	2.11	1.47	1.42
5	C	703	GTP	C2'-C1'	-2.09	1.50	1.53
2	C	701	HF4	O4'-C4'	2.08	1.49	1.45
5	B	702	GTP	C2-N3	2.07	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	702	GTP	O3'-C3'	2.06	1.47	1.43
2	A	705	HF4	PA-O1A	-2.05	1.45	1.55
3	B	701	DTP	O4'-C4'	2.04	1.49	1.45

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	702	GTP	C3'-C2'-C1'	5.15	108.74	100.98
2	B	703	HF4	O2-C2-N3	-4.89	114.37	122.33
2	D	701	HF4	PB-O3B-PG	-4.54	117.23	132.83
2	C	701	HF4	PB-O3B-PG	-4.44	117.60	132.83
5	C	703	GTP	C3'-C2'-C1'	4.33	107.50	100.98
3	D	702	DTP	N3-C2-N1	-3.99	122.44	128.68
2	B	703	HF4	PA-O3A-PB	-3.98	119.17	132.83
2	B	703	HF4	C3'-C2'-C1'	3.91	108.84	101.43
3	C	704	DTP	O3G-PG-O2G	3.89	122.51	107.64
5	A	702	GTP	O3G-PG-O2G	3.89	122.49	107.64
2	B	703	HF4	PB-O3B-PG	-3.75	119.96	132.83
2	A	705	HF4	PA-O3A-PB	-3.71	120.11	132.83
5	C	703	GTP	C8-N7-C5	3.65	109.94	102.99
5	B	702	GTP	PA-O3A-PB	-3.64	120.33	132.83
2	A	705	HF4	PB-O3B-PG	-3.57	120.56	132.83
3	A	703	DTP	N3-C2-N1	-3.57	123.10	128.68
3	C	704	DTP	N6-C6-N1	3.57	125.98	118.57
3	D	702	DTP	O2A-PA-O1A	3.56	129.85	112.24
2	B	703	HF4	O2G-PG-O3B	3.53	116.48	104.64
2	D	701	HF4	O1G-PG-O3B	3.29	115.66	104.64
2	D	701	HF4	C3'-C2'-C1'	2.98	107.09	101.43
2	D	701	HF4	O4'-C1'-N1	2.76	114.67	108.36
5	C	703	GTP	O3G-PG-O3B	2.72	113.77	104.64
2	C	701	HF4	PA-O3A-PB	-2.70	123.56	132.83
5	A	702	GTP	C3'-C2'-C1'	2.66	104.99	100.98
2	D	701	HF4	PA-O3A-PB	-2.63	123.80	132.83
3	B	701	DTP	O2A-PA-O1A	2.61	125.17	112.24
2	B	703	HF4	C6-N1-C2	-2.60	115.98	120.49
3	C	704	DTP	O2G-PG-O3B	-2.60	95.92	104.64
2	C	701	HF4	O1G-PG-O3B	2.57	113.27	104.64
3	A	703	DTP	O2A-PA-O1A	2.55	124.87	112.24
2	A	705	HF4	C5-C4-N4	2.54	124.57	120.57
5	B	702	GTP	O3G-PG-O3B	2.52	113.09	104.64
3	B	701	DTP	O3G-PG-O2G	2.51	117.24	107.64
2	C	701	HF4	C4'-O4'-C1'	-2.48	104.00	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	703	GTP	PA-O3A-PB	-2.44	124.45	132.83
3	C	704	DTP	O2A-PA-O1A	2.44	124.31	112.24
5	B	702	GTP	O4'-C1'-C2'	-2.43	103.37	106.93
3	D	702	DTP	N6-C6-N1	2.42	123.61	118.57
3	B	701	DTP	C2'-C1'-N9	2.37	119.74	114.27
2	A	705	HF4	C3'-C2'-C1'	2.36	105.92	101.43
2	B	703	HF4	C5-C4-N4	2.34	124.25	120.57
2	A	705	HF4	O2-C2-N3	-2.34	118.53	122.33
2	A	705	HF4	N4-C4-N3	-2.32	113.89	117.97
2	D	701	HF4	O2G-PG-O3B	2.31	112.39	104.64
2	D	701	HF4	C6-N1-C2	-2.31	116.49	120.49
2	C	701	HF4	O2G-PG-O3B	2.29	112.31	104.64
2	B	703	HF4	N1-C2-N3	2.27	122.95	118.81
5	C	703	GTP	C5-C6-N1	2.22	117.87	113.95
2	A	705	HF4	C4'-O4'-C1'	-2.21	104.60	109.47
5	A	702	GTP	O3G-PG-O3B	-2.19	97.29	104.64
5	B	702	GTP	O2G-PG-O1G	2.16	119.15	110.68
5	D	704	GTP	O4'-C1'-C2'	2.15	110.07	106.93
3	D	702	DTP	O2G-PG-O1G	2.15	119.10	110.68
2	A	705	HF4	O4'-C1'-N1	2.14	113.26	108.36
3	D	702	DTP	O3G-PG-O2G	2.12	115.73	107.64
3	D	702	DTP	PA-O3A-PB	2.12	140.10	132.83
5	B	702	GTP	C8-N7-C5	2.11	107.00	102.99
3	B	701	DTP	C4-C5-N7	-2.10	107.21	109.40
5	A	702	GTP	O2A-PA-O1A	2.09	122.60	112.24
2	C	701	HF4	O2-C2-N3	-2.09	118.94	122.33
2	D	701	HF4	O5'-C5'-C4'	2.06	116.09	108.99
5	A	702	GTP	O2'-C2'-C1'	-2.06	103.25	110.85
5	A	702	GTP	PA-O3A-PB	-2.04	125.84	132.83
3	B	701	DTP	O2G-PG-O3B	-2.03	97.82	104.64
3	D	702	DTP	C2-N1-C6	2.01	122.19	118.75
2	B	703	HF4	N4-C4-N3	-2.01	114.44	117.97
5	A	702	GTP	N2-C2-N1	2.00	120.98	116.71
2	D	701	HF4	O2-C2-N3	-2.00	119.08	122.33

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	701	HF4	C5'-O5'-PA-O2A
2	D	701	HF4	C4'-C5'-O5'-PA
2	A	705	HF4	PB-O3A-PA-O5'

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Mol	Chain	Res	Type	Atoms
3	B	701	DTP	PB-O3B-PG-O2G
3	B	701	DTP	PB-O3B-PG-O3G
5	C	703	GTP	PB-O3B-PG-O3G
2	C	701	HF4	C3'-C4'-C5'-O5'
2	C	701	HF4	O4'-C4'-C5'-O5'
2	B	703	HF4	C3'-C4'-C5'-O5'
2	B	703	HF4	O4'-C4'-C5'-O5'
2	C	701	HF4	C4'-C5'-O5'-PA
2	B	703	HF4	C4'-C5'-O5'-PA
2	A	705	HF4	C4'-C5'-O5'-PA
2	D	701	HF4	PB-O3A-PA-O5'
2	B	703	HF4	PB-O3A-PA-O5'
2	C	701	HF4	PB-O3B-PG-O2G
3	D	702	DTP	PB-O3B-PG-O2G
3	A	703	DTP	PB-O3B-PG-O3G
2	D	701	HF4	C5'-O5'-PA-O3A
3	C	704	DTP	PG-O3B-PB-O2B
5	B	702	GTP	PG-O3B-PB-O2B
5	B	702	GTP	C4'-C5'-O5'-PA
2	D	701	HF4	C5'-O5'-PA-O1A
5	A	702	GTP	C4'-C5'-O5'-PA
2	D	701	HF4	C3'-C4'-C5'-O5'
2	A	705	HF4	C3'-C4'-C5'-O5'
5	B	702	GTP	PG-O3B-PB-O1B
5	B	702	GTP	PB-O3A-PA-O2A
5	D	704	GTP	C4'-C5'-O5'-PA
5	C	703	GTP	C4'-C5'-O5'-PA
3	D	702	DTP	PB-O3B-PG-O1G
3	C	704	DTP	PG-O3B-PB-O1B
3	B	701	DTP	PG-O3B-PB-O1B
3	A	703	DTP	PG-O3B-PB-O1B
5	C	703	GTP	PG-O3B-PB-O1B
5	C	703	GTP	PG-O3B-PB-O2B
2	A	705	HF4	O4'-C4'-C5'-O5'
5	C	703	GTP	PB-O3B-PG-O1G
5	A	702	GTP	C5'-O5'-PA-O3A
2	C	701	HF4	PG-O3B-PB-O1B
2	C	701	HF4	PG-O3B-PB-O2B
3	C	704	DTP	PB-O3A-PA-O2A
3	B	701	DTP	PB-O3A-PA-O1A
5	D	704	GTP	PB-O3A-PA-O2A
5	C	703	GTP	PB-O3A-PA-O1A

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Mol	Chain	Res	Type	Atoms
5	A	702	GTP	PG-O3B-PB-O1B
2	D	701	HF4	O4'-C4'-C5'-O5'

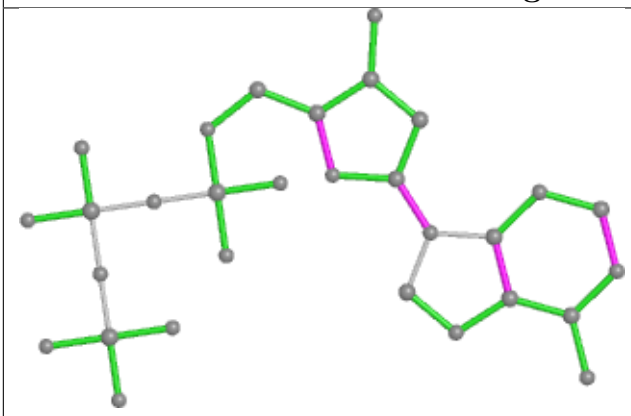
There are no ring outliers.

1 monomer is involved in 1 short contact:

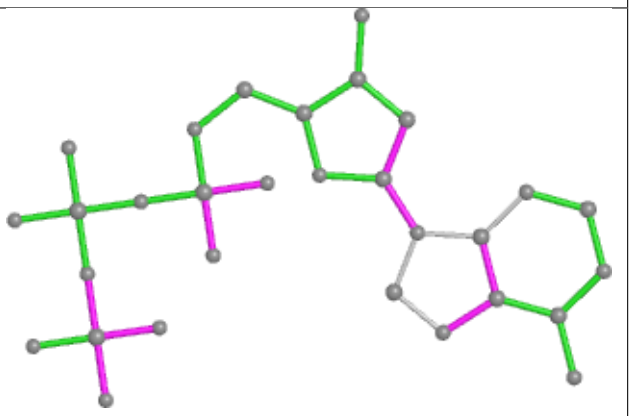
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	701	HF4	1	0

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 then 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.

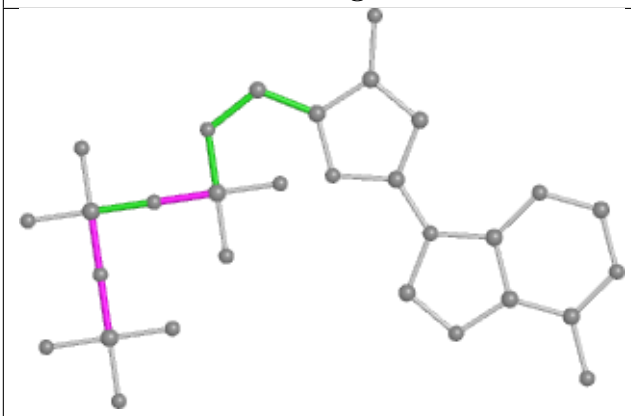
Ligand DTP B 701



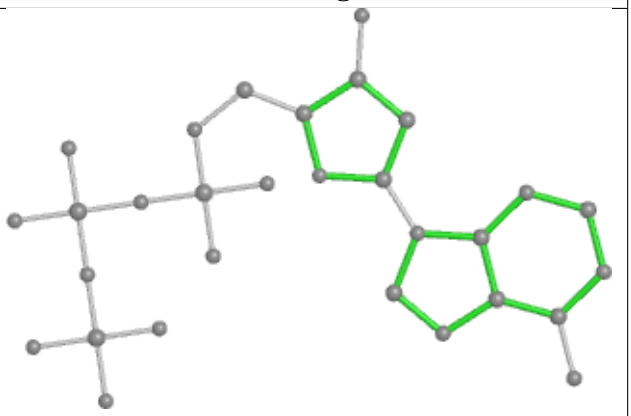
Bond lengths



Bond angles

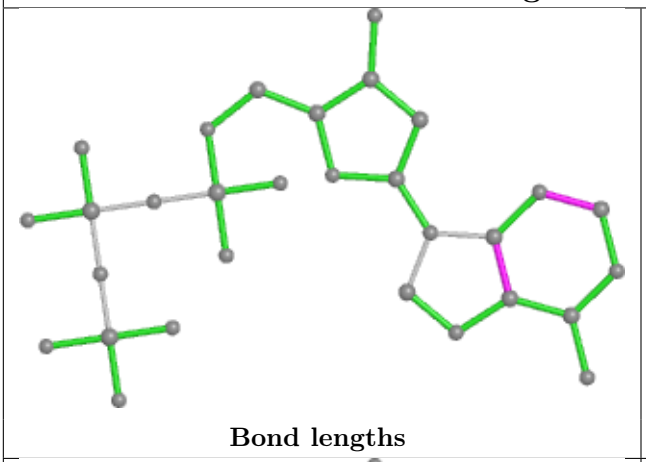


Torsions

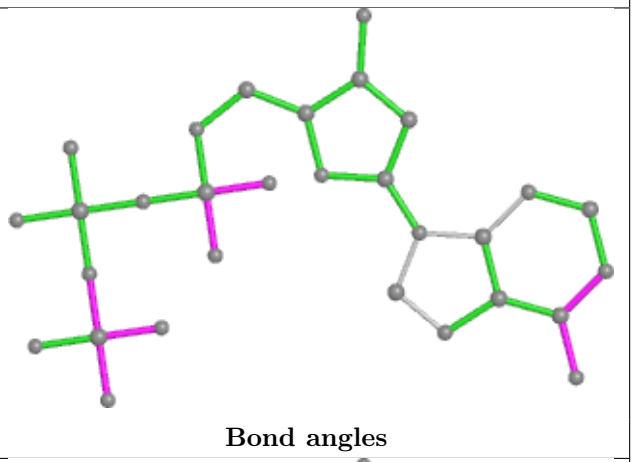


Rings

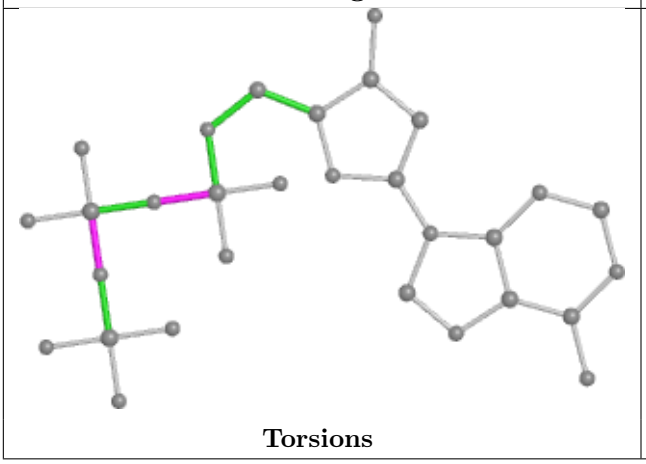
Ligand DTP C 704



Bond lengths



Bond angles



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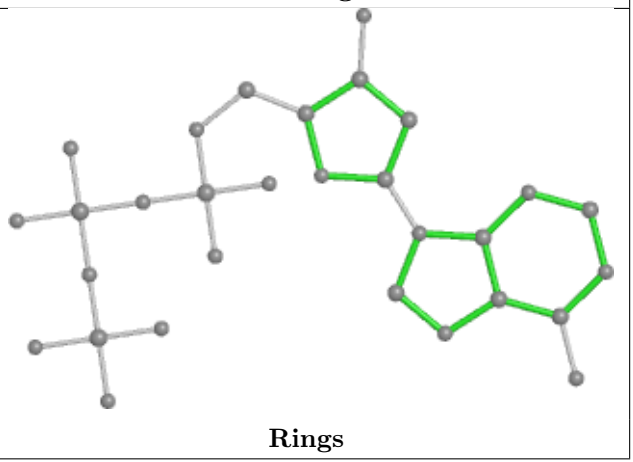
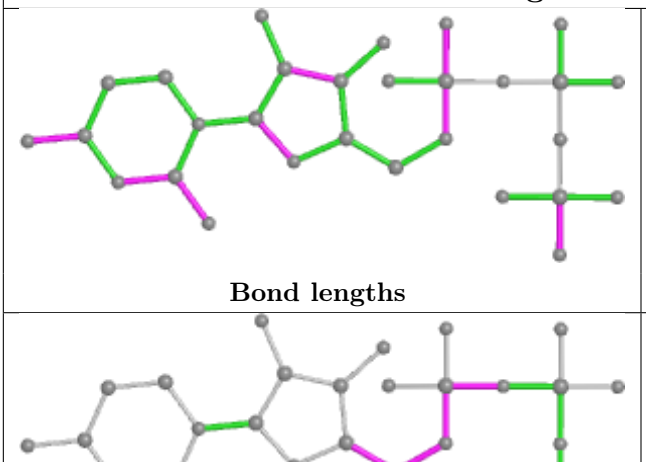
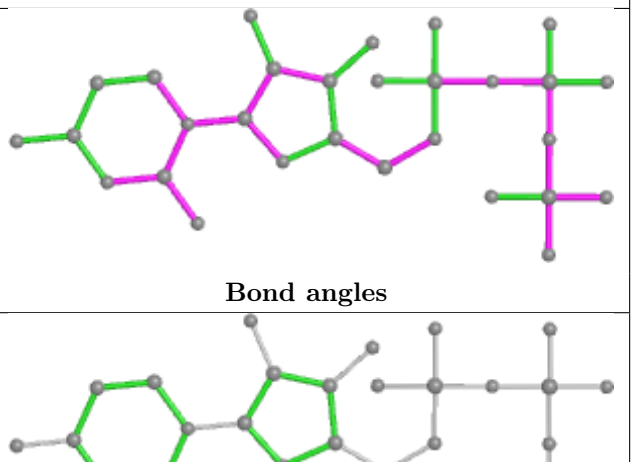


Rings

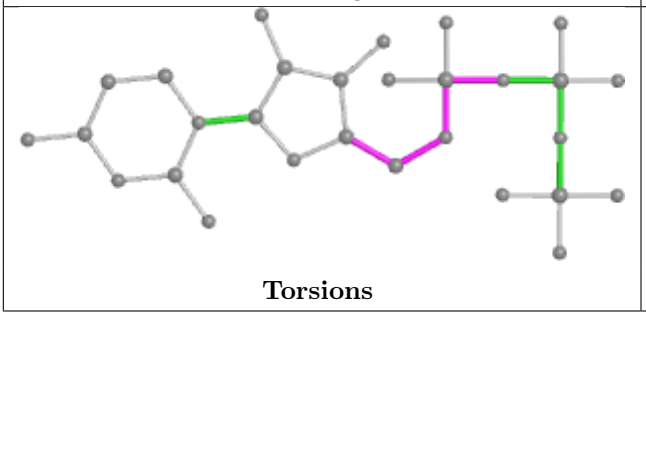
Ligand HF4 D 701



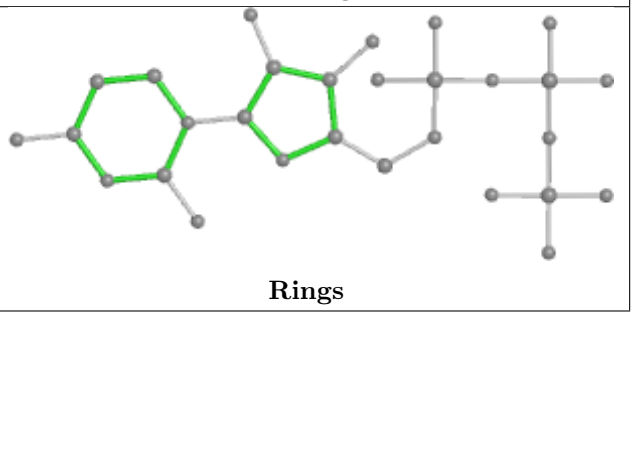
Bond lengths



Bond angles

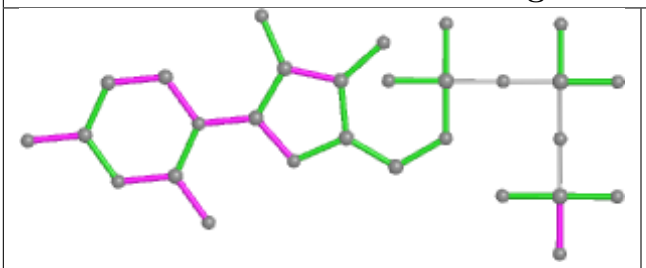


Torsions

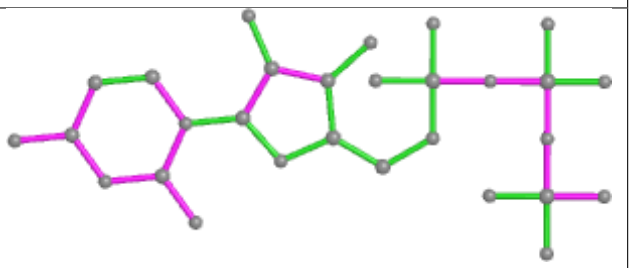


Rings

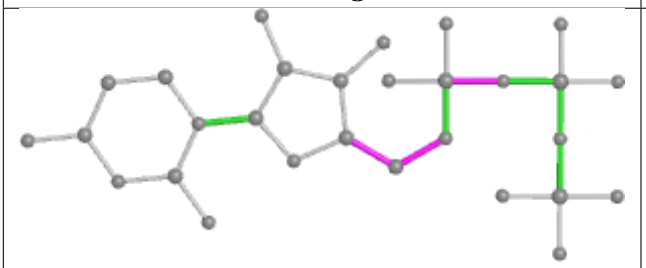
Ligand HF4 B 703



Bond lengths



Bond angles



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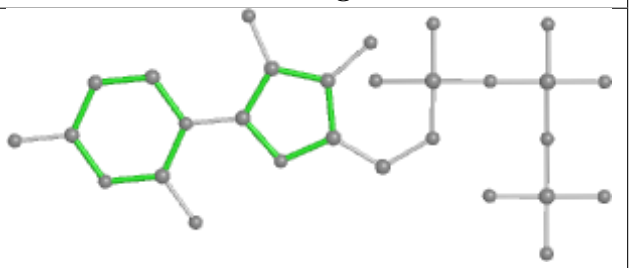
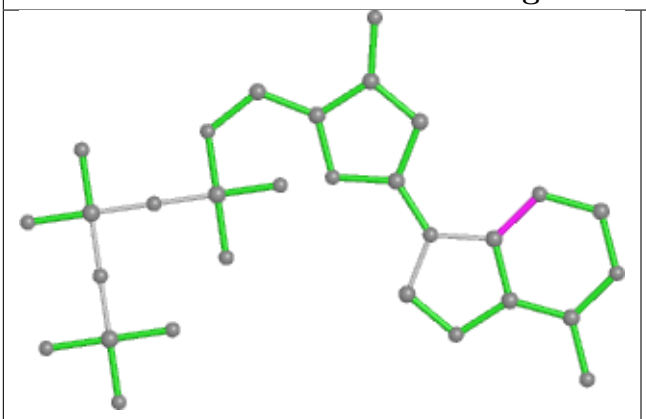
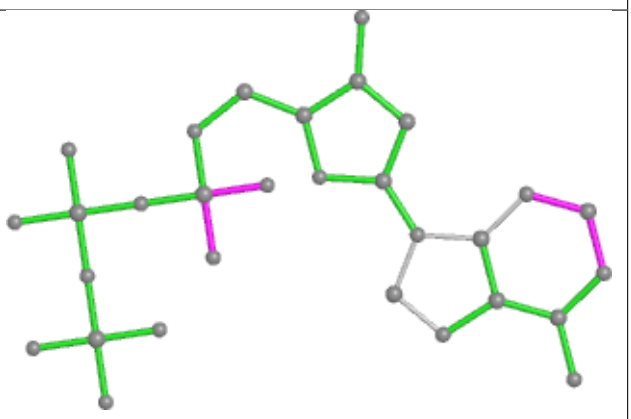


Rings

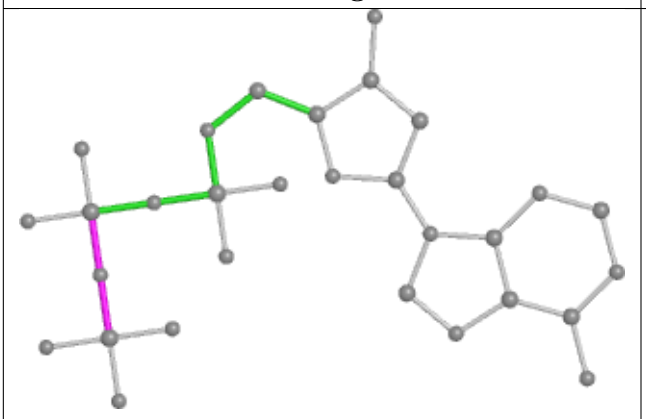
Ligand DTP A 703



Bond lengths



Bond angles



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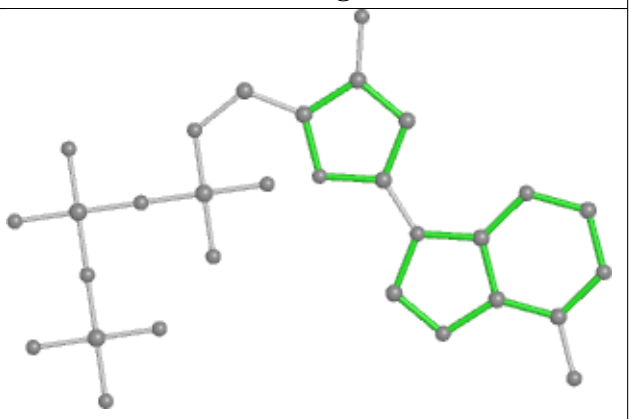
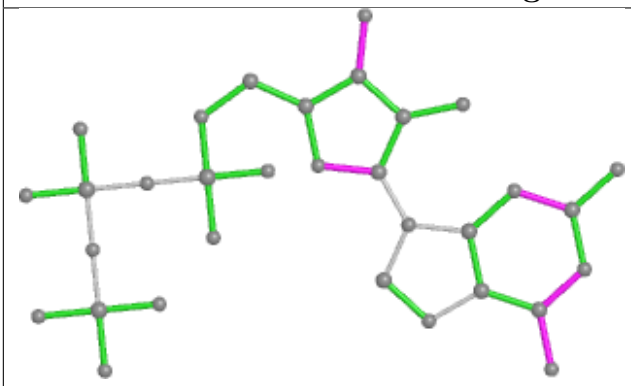


Rings

Ligand GTP B 702



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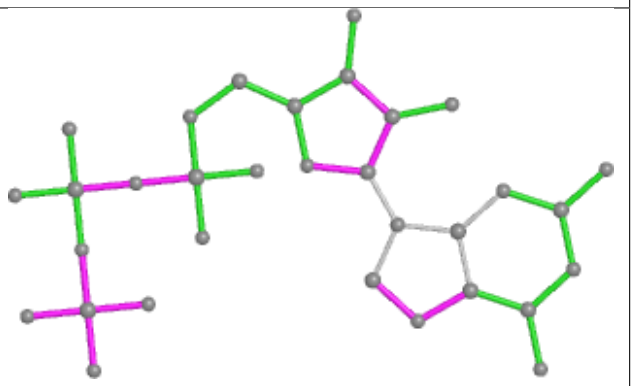
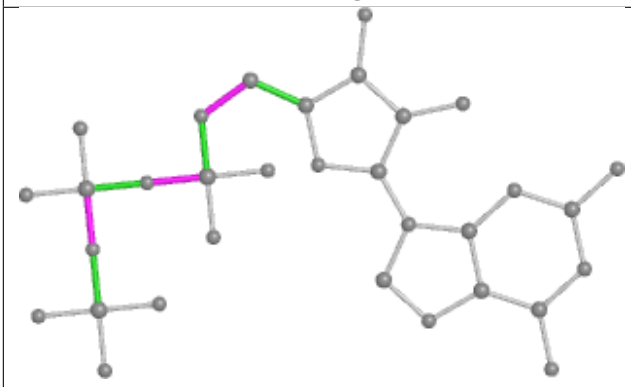
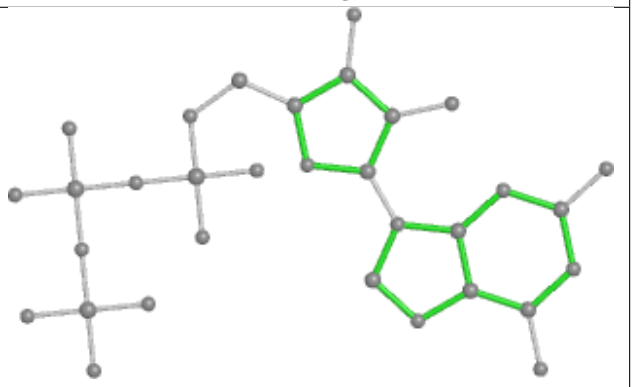


Bond angles

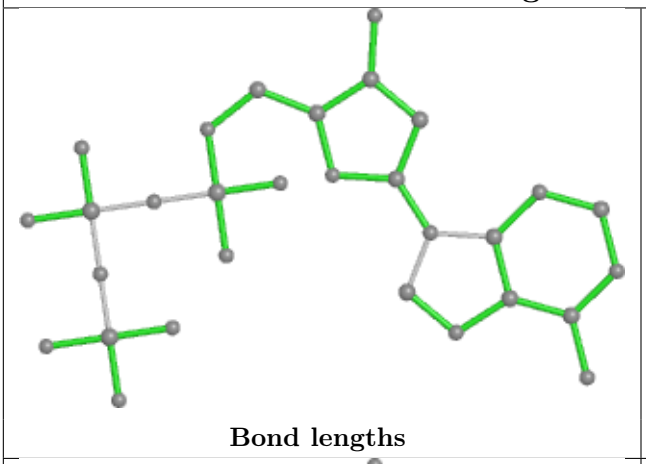


Torsions

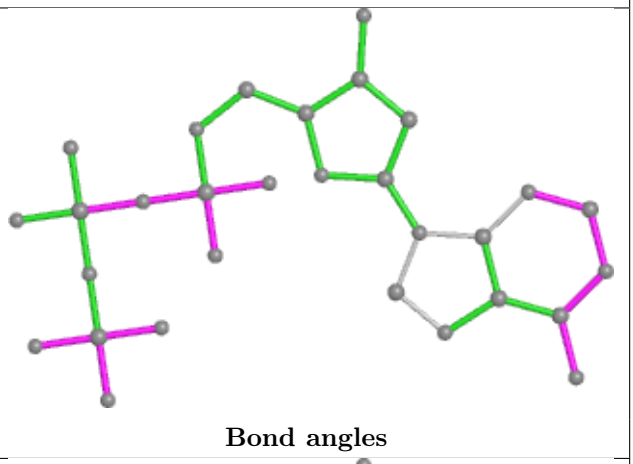


Rings

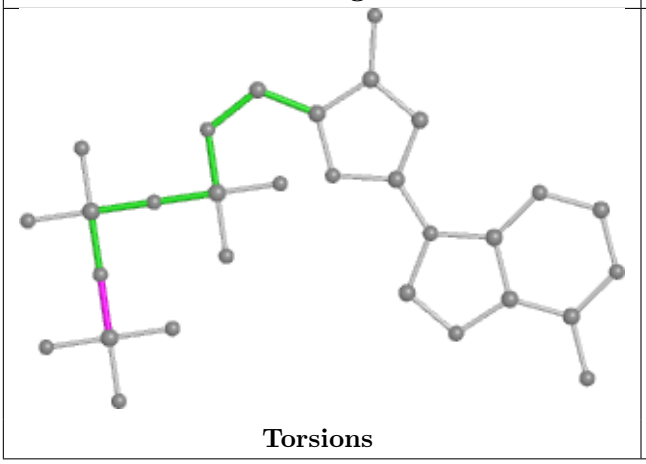
Ligand DTP D 702



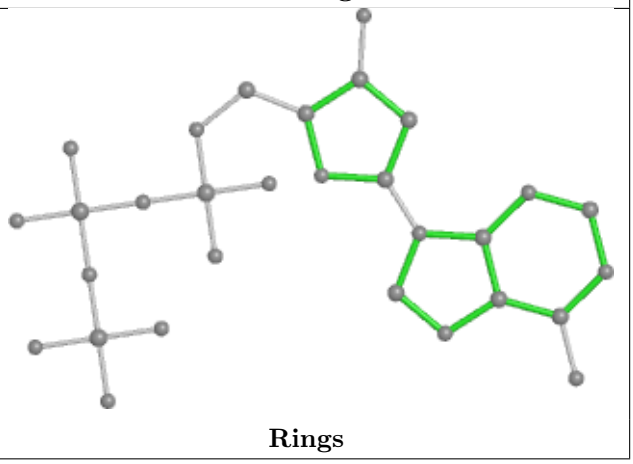
Bond lengths



Bond angles

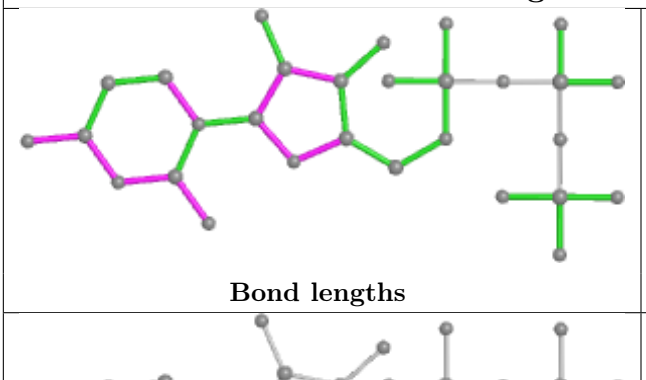


Torsions

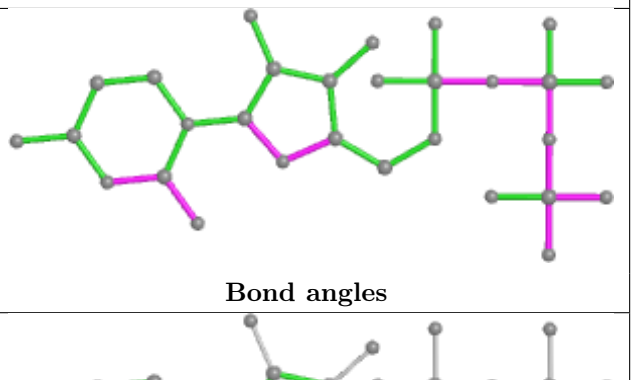


Rings

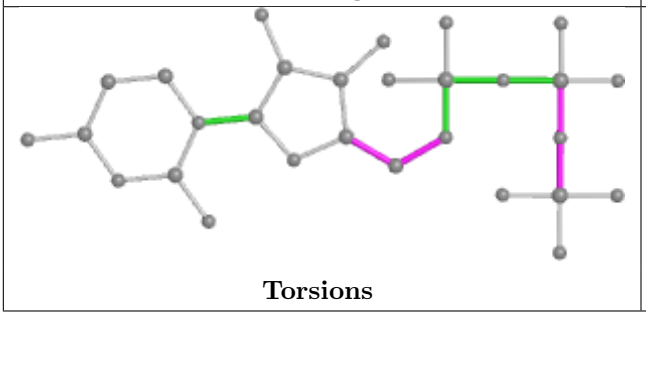
Ligand HF4 C 701



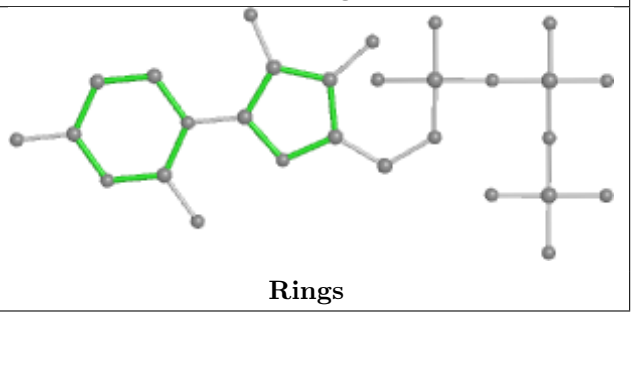
Bond lengths



Bond angles

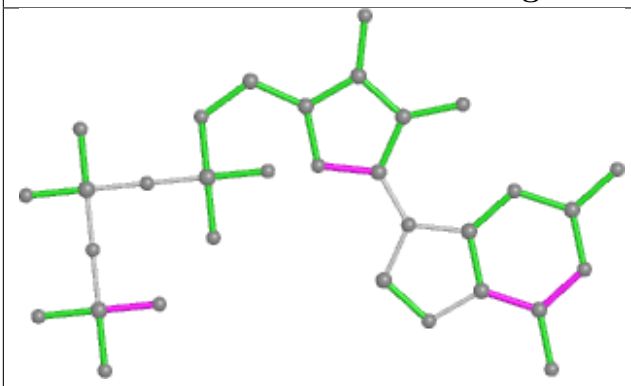


Torsions

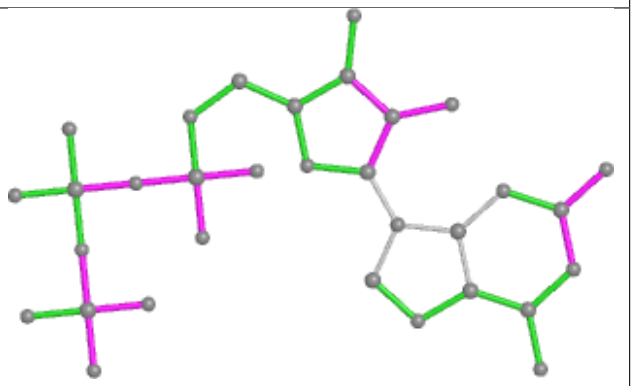


Rings

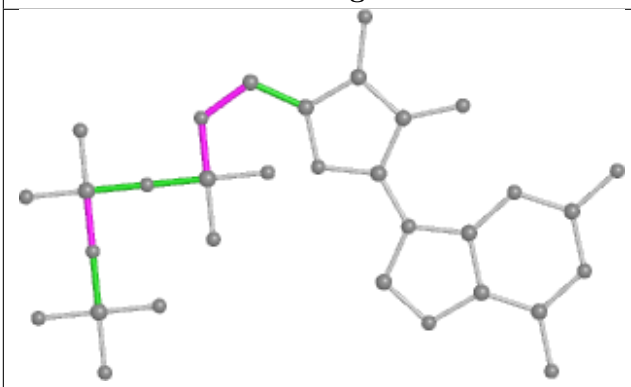
Ligand GTP A 702



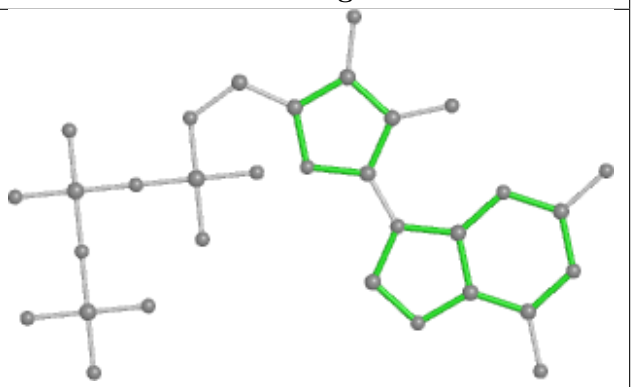
Bond lengths



Bond angles

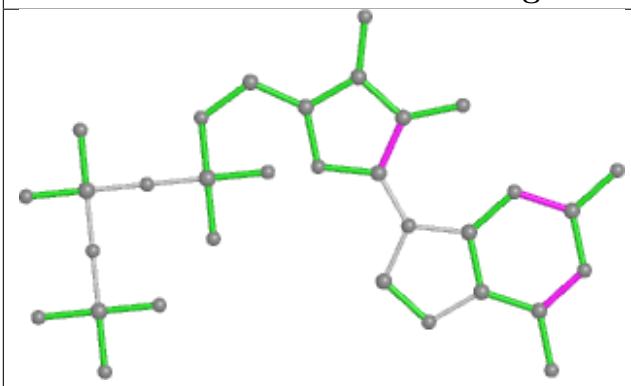


Torsions

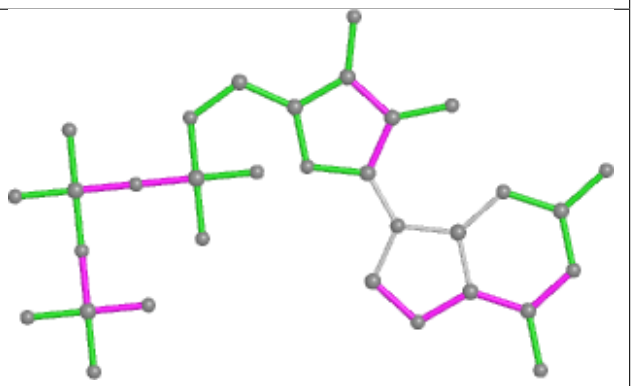


Rings

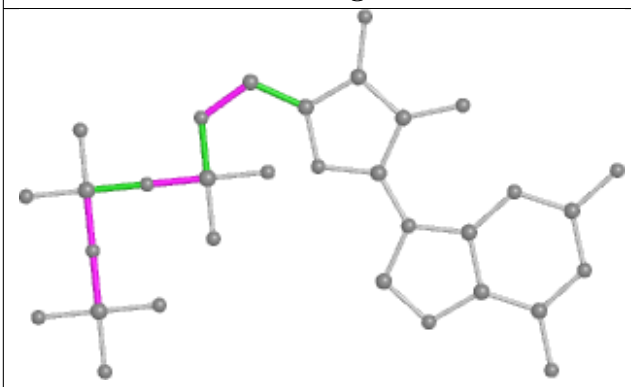
Ligand GTP C 703



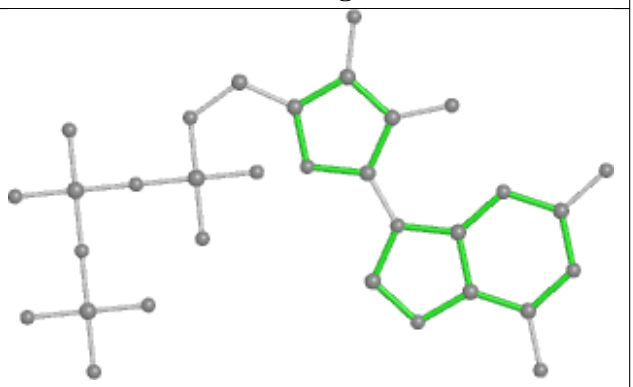
Bond lengths



Bond angles

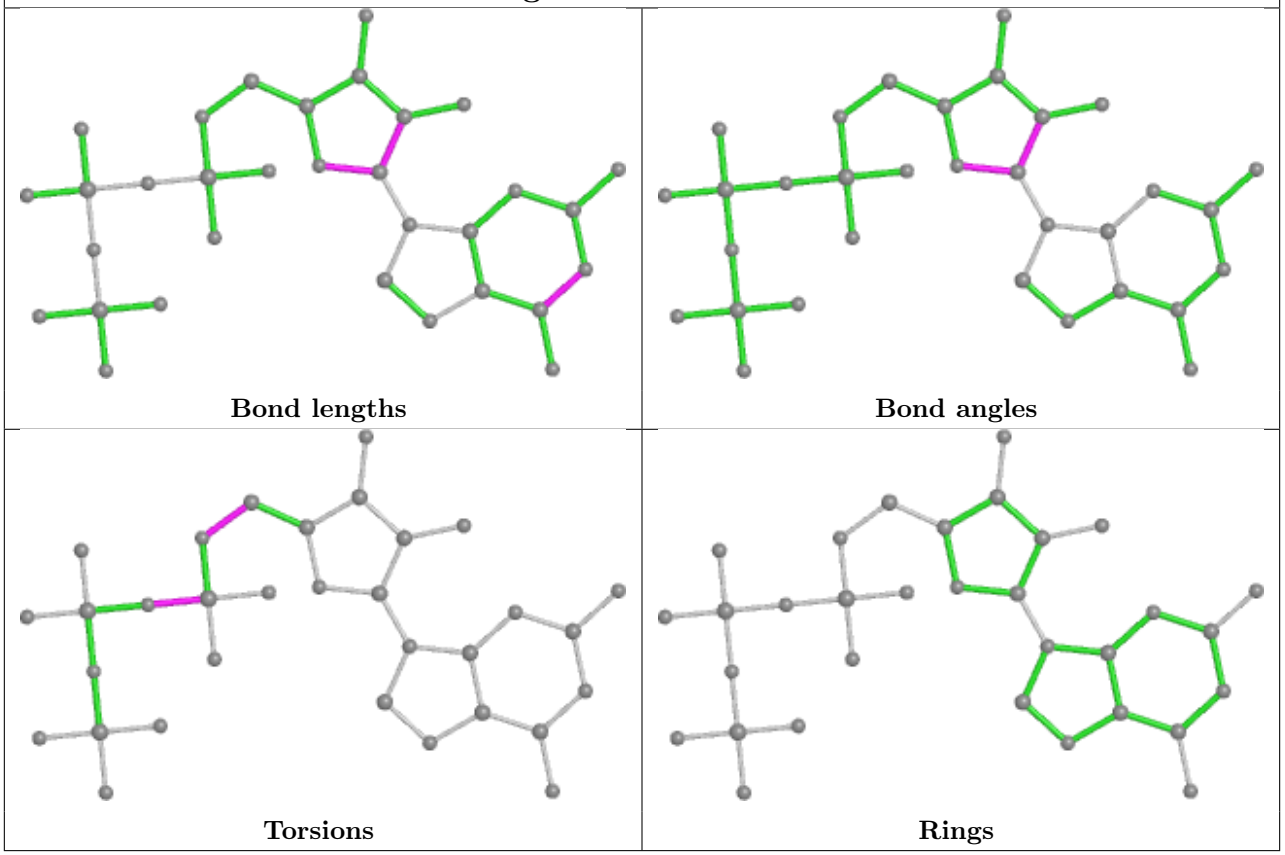


Torsions

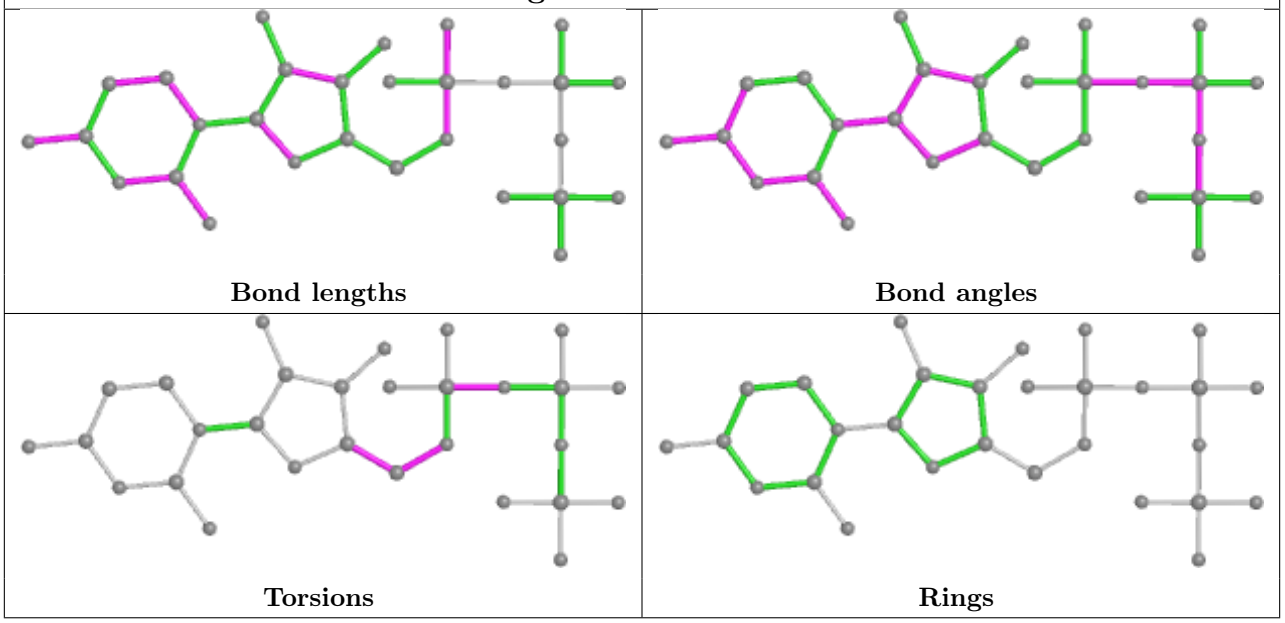


Rings

Ligand GTP D 704



Ligand HF4 A 705



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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	480/550 (87%)	-0.04	14 (2%)	51	49	18, 42, 80, 105	0
1	B	480/550 (87%)	-0.01	24 (5%)	28	27	20, 42, 76, 106	0
1	C	479/550 (87%)	-0.02	10 (2%)	63	61	21, 43, 73, 104	0
1	D	480/550 (87%)	-0.26	7 (1%)	73	72	15, 35, 62, 86	0
All	All	1919/2200 (87%)	-0.08	55 (2%)	51	49	15, 40, 73, 106	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	488	LEU	8.2
1	C	599	ASN	5.6
1	C	488	LEU	4.8
1	B	490	ASP	4.6
1	A	599	ASN	4.6
1	B	599	ASN	4.3
1	C	114	THR	4.3
1	D	490	ASP	4.3
1	B	594	GLN	3.8
1	A	465	GLN	3.6
1	B	284	LEU	3.6
1	B	491	VAL	3.5
1	B	277	GLU	3.4
1	D	465	GLN	3.4
1	B	560	LYS	3.3
1	A	490	ASP	3.1
1	B	562	LEU	3.1
1	C	597	GLU	3.1
1	D	596	LYS	3.1
1	A	486	LYS	3.0
1	A	466	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	487	VAL	2.9
1	A	345	ASN	2.9
1	B	465	GLN	2.9
1	B	484	LYS	2.9
1	B	559	ARG	2.8
1	A	472	ASP	2.8
1	C	490	ASP	2.8
1	D	113	ASP	2.7
1	A	596	LYS	2.7
1	B	262	GLU	2.6
1	B	563	TYR	2.6
1	D	284	LEU	2.5
1	C	403	GLY	2.5
1	A	488	LEU	2.5
1	B	494	LYS	2.4
1	B	285	TRP	2.4
1	B	590	LEU	2.4
1	D	599	ASN	2.3
1	C	589	PRO	2.3
1	A	585	ASP	2.2
1	C	326	GLN	2.2
1	B	486	LYS	2.2
1	A	471	GLU	2.2
1	B	592	THR	2.2
1	B	276	LEU	2.2
1	A	487	VAL	2.2
1	C	596	LYS	2.2
1	B	489	LEU	2.2
1	A	598	TRP	2.2
1	D	262	GLU	2.1
1	B	345	ASN	2.1
1	B	230	LYS	2.1
1	A	342	GLU	2.0
1	C	590	LEU	2.0

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)

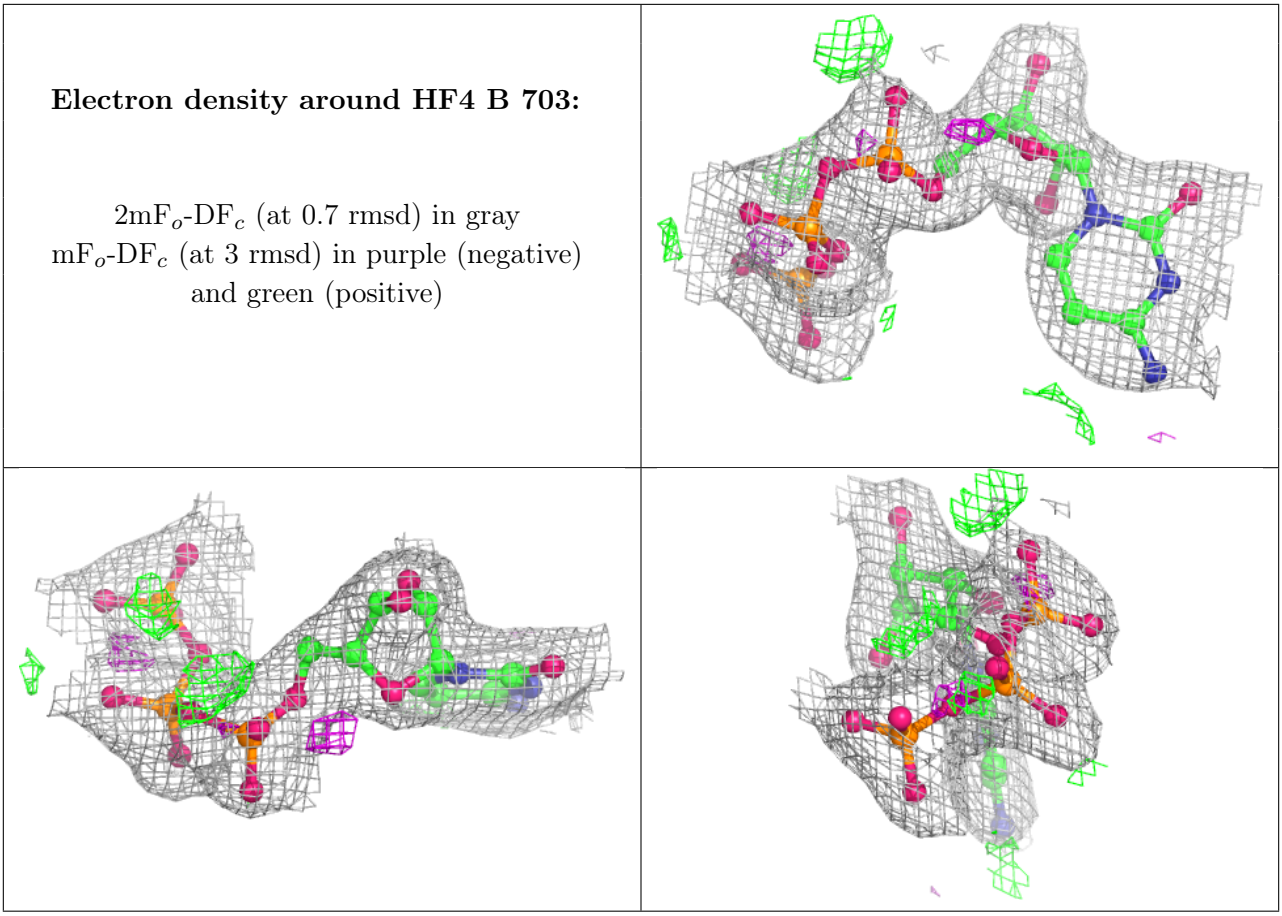
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	B	704	1/1	0.52	0.09	58,58,58,58	0
4	MG	A	706	1/1	0.67	0.10	64,64,64,64	0
4	MG	D	705	1/1	0.73	0.15	66,66,66,66	0
4	MG	C	705	1/1	0.90	0.22	79,79,79,79	0
4	MG	C	702	1/1	0.96	0.04	35,35,35,35	0
2	HF4	B	703	29/29	0.97	0.09	27,31,42,46	0
2	HF4	C	701	29/29	0.97	0.10	31,39,54,56	0
2	HF4	A	705	29/29	0.98	0.09	29,34,52,56	0
2	HF4	D	701	29/29	0.98	0.10	22,28,42,47	0
5	GTP	D	704	32/32	0.98	0.09	18,22,28,31	0
5	GTP	C	703	32/32	0.98	0.09	25,29,33,34	0
5	GTP	B	702	32/32	0.98	0.09	22,25,29,30	0
3	DTP	A	703	30/30	0.99	0.10	20,21,24,25	0
4	MG	A	701	1/1	0.99	0.08	26,26,26,26	0
4	MG	A	704	1/1	0.99	0.07	26,26,26,26	0
4	MG	D	703	1/1	0.99	0.09	25,25,25,25	0
3	DTP	D	702	30/30	0.99	0.12	21,24,28,29	0
3	DTP	C	704	30/30	0.99	0.12	20,23,27,28	0
3	DTP	B	701	30/30	0.99	0.11	18,20,24,25	0
5	GTP	A	702	32/32	0.99	0.10	19,21,29,33	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.

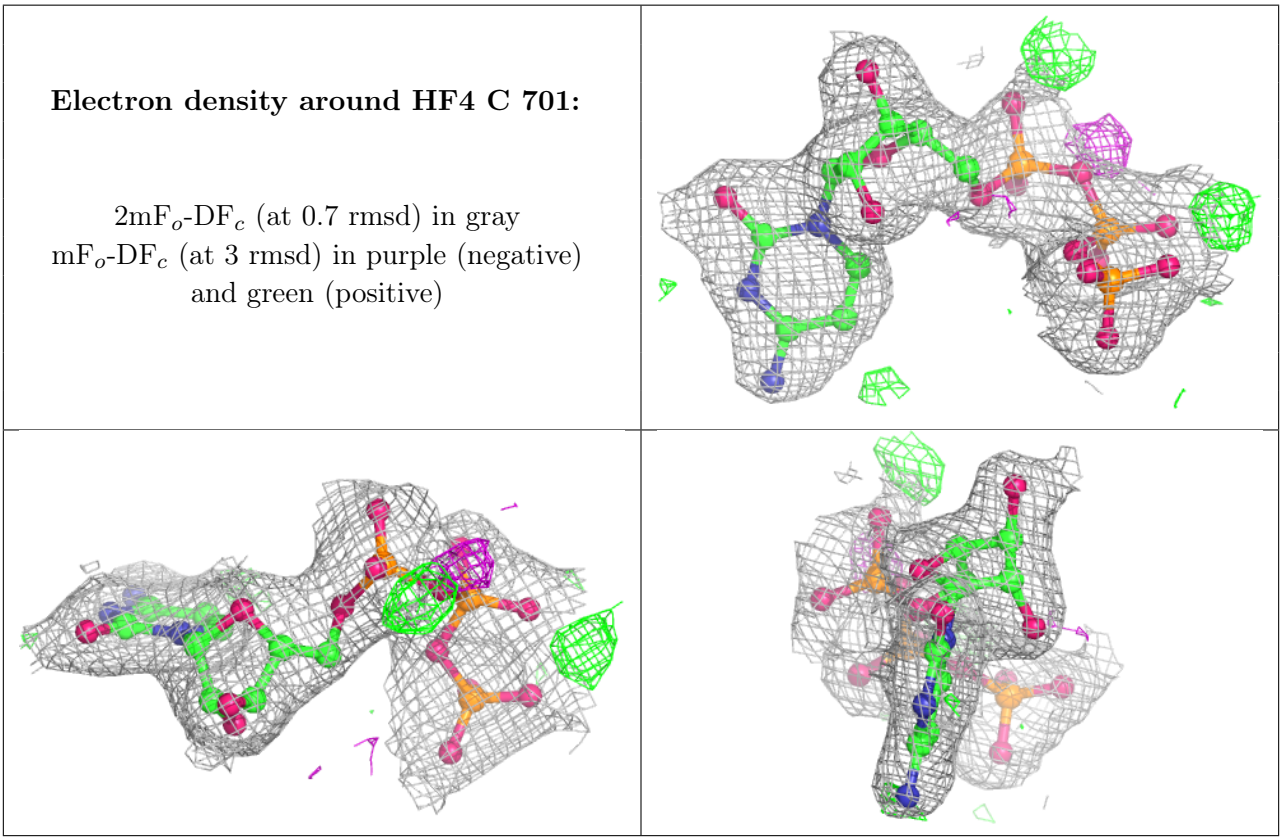
Electron density around HF4 B 703:

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



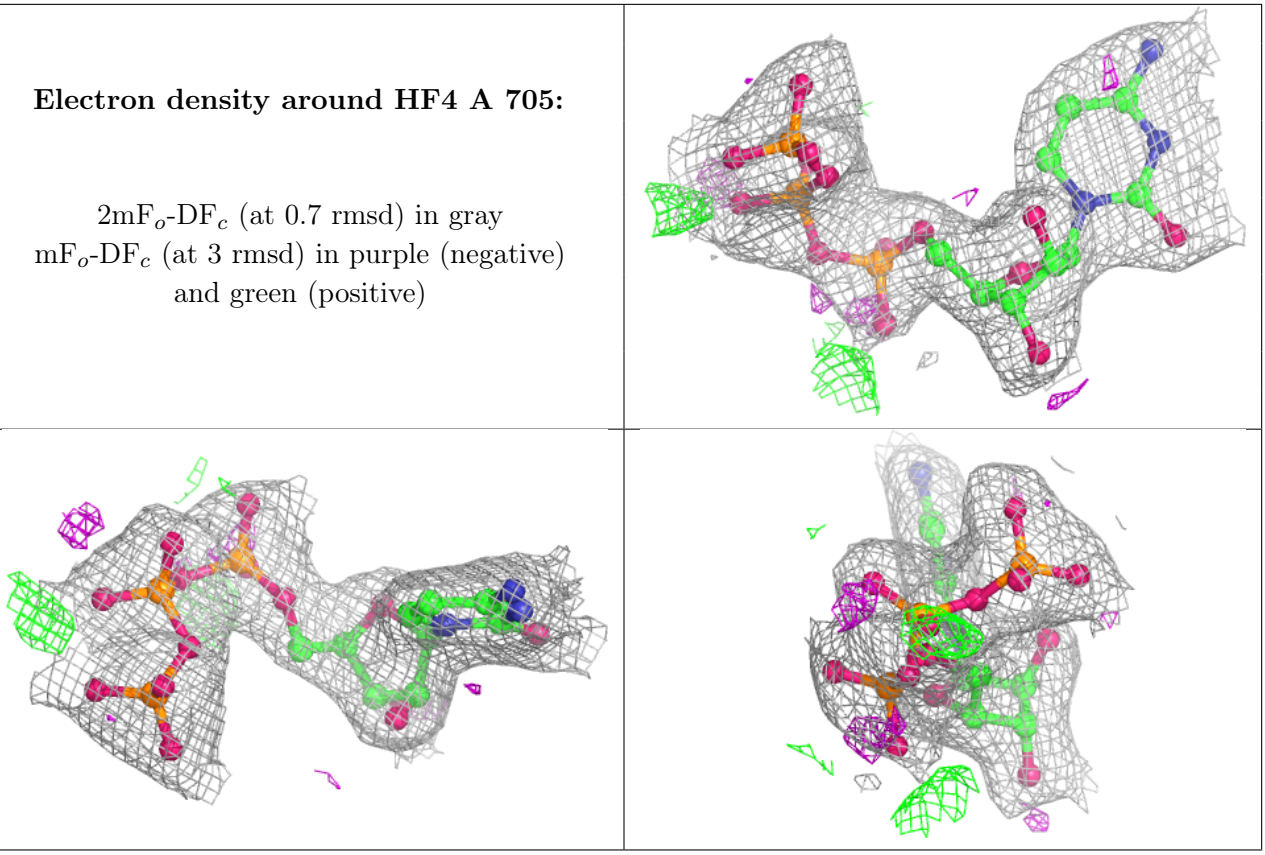
Electron density around HF4 C 701:

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



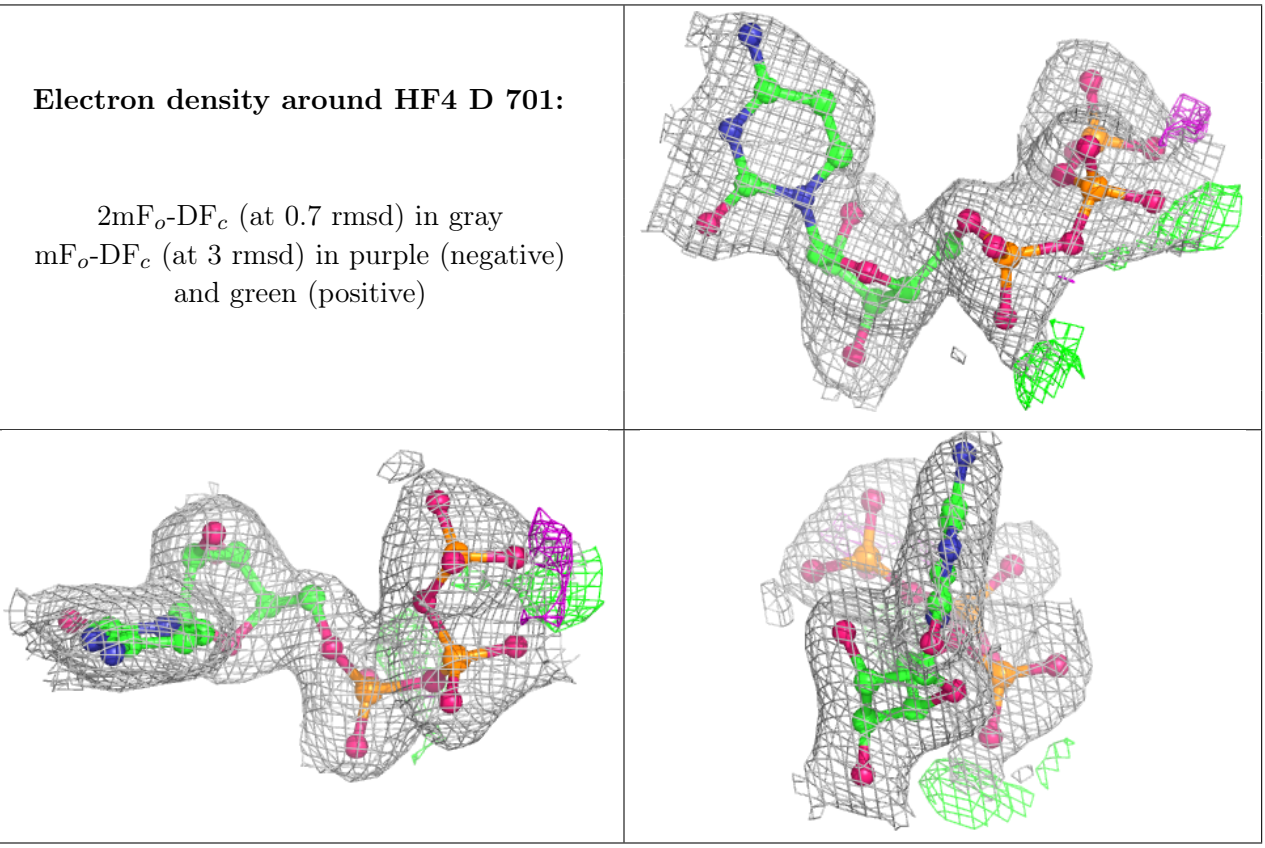
Electron density around HF4 A 705:

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



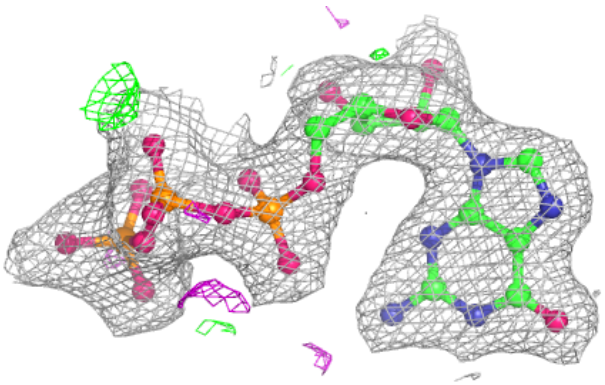
Electron density around HF4 D 701:

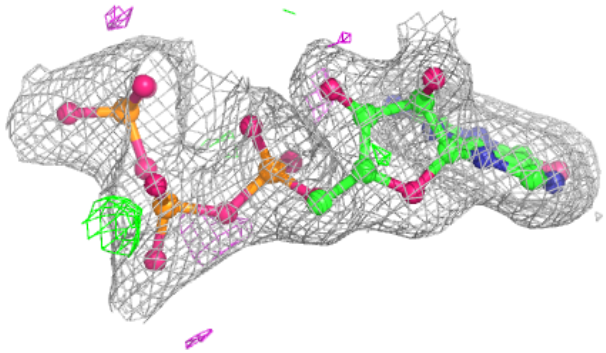
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

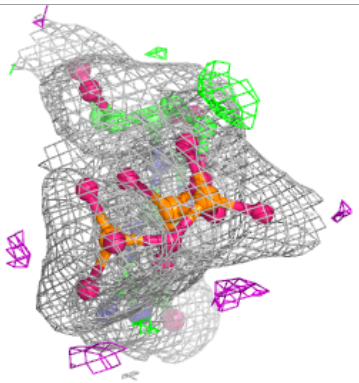


Electron density around GTP D 704:

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

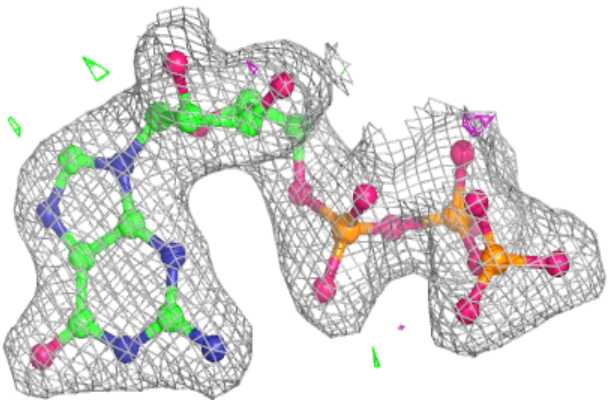


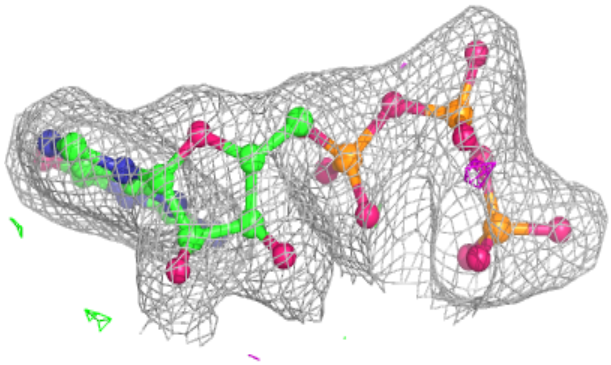


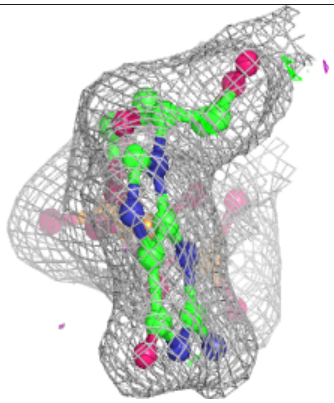


Electron density around GTP C 703:

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

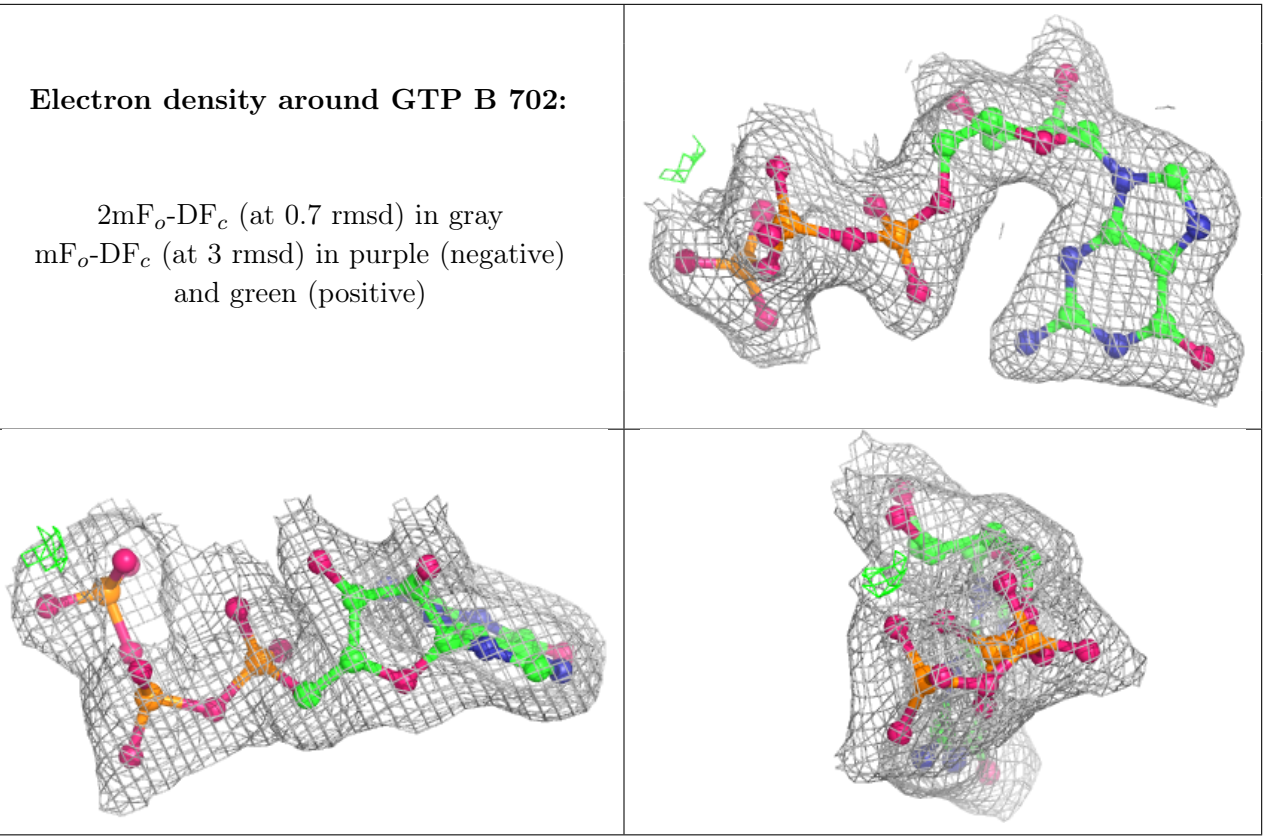






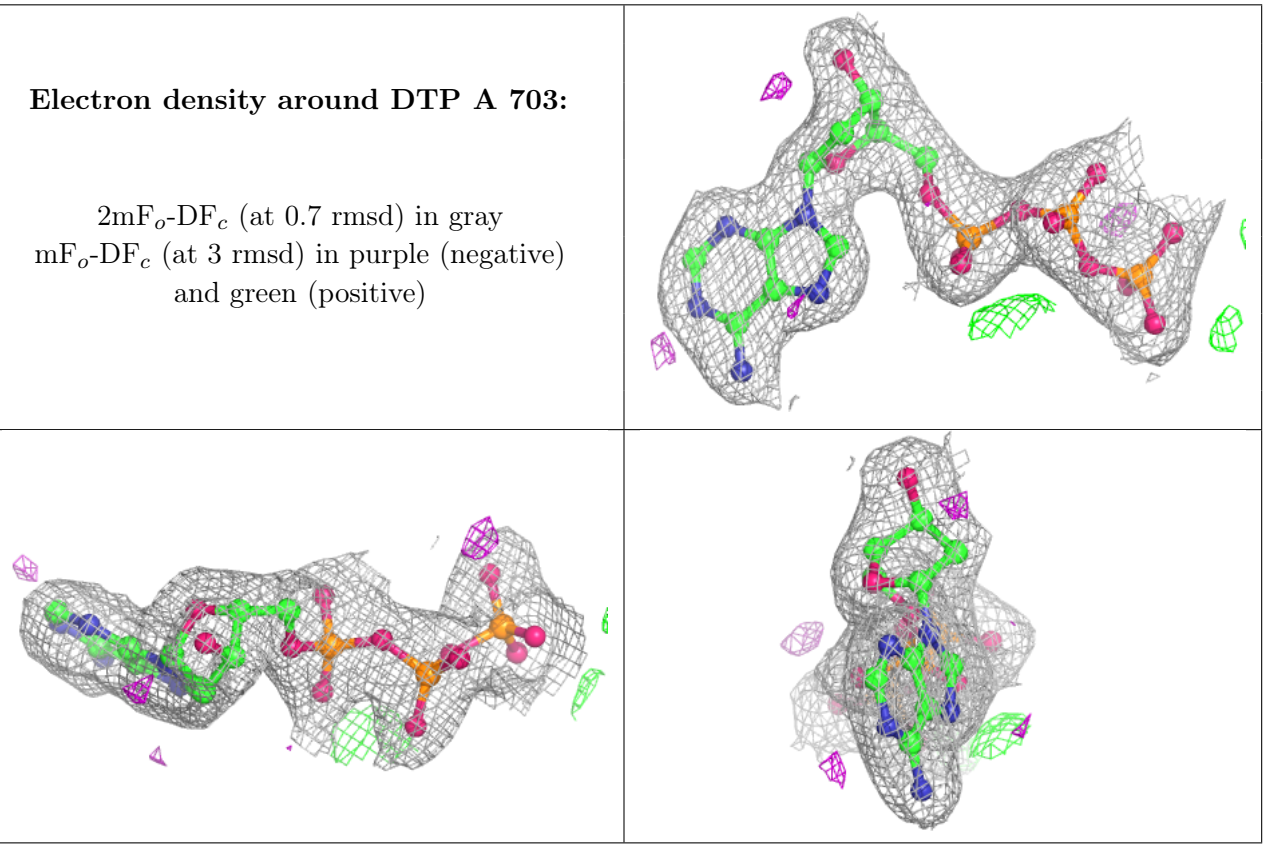
Electron density around GTP B 702:

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



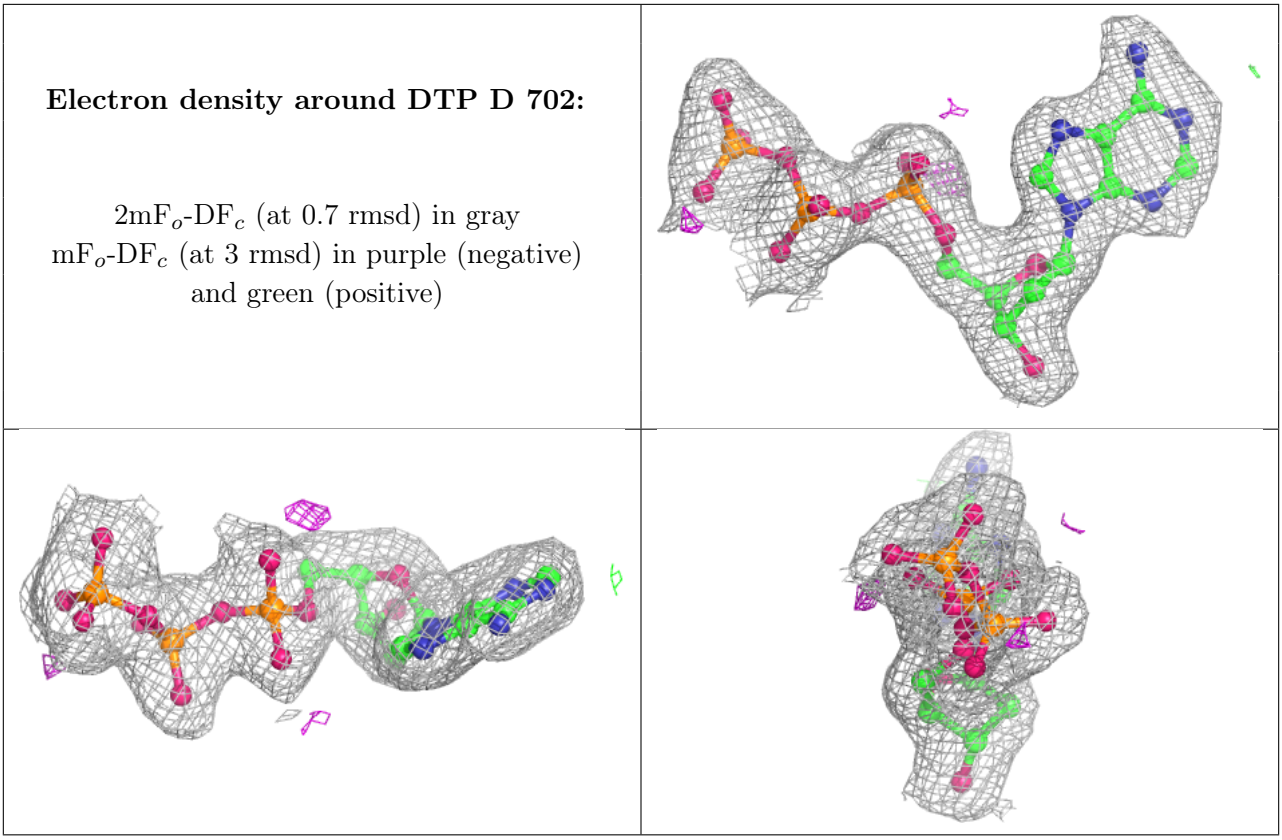
Electron density around DTP A 703:

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



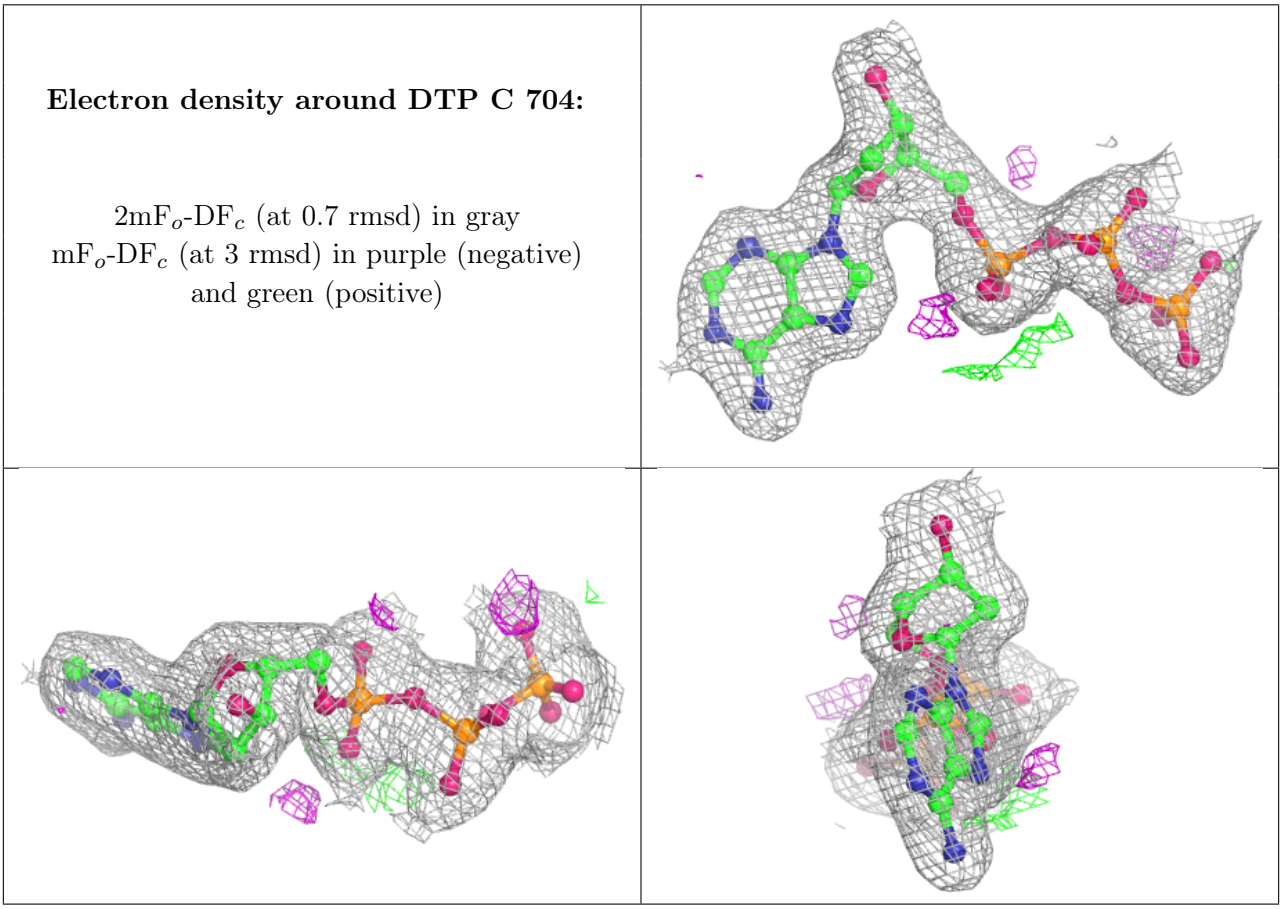
Electron density around DTP D 702:

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



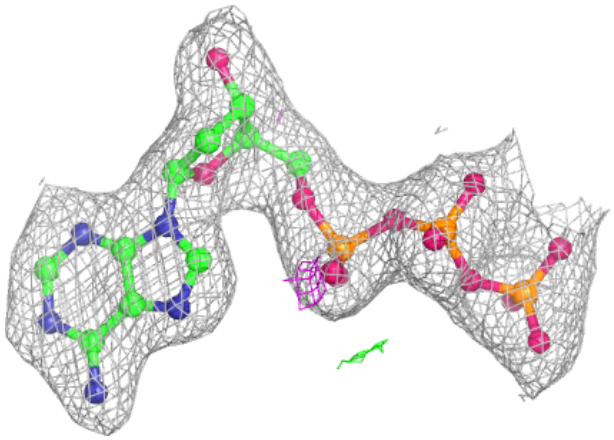
Electron density around DTP C 704:

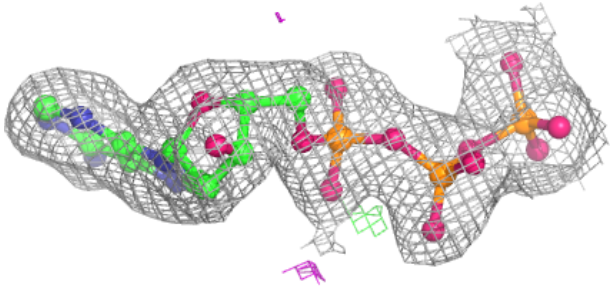
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

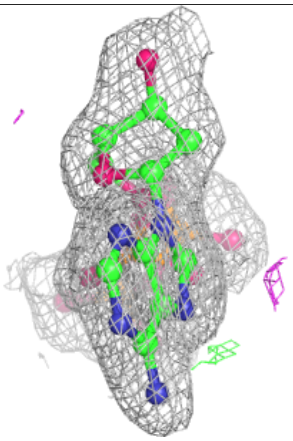


Electron density around DTP B 701:

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

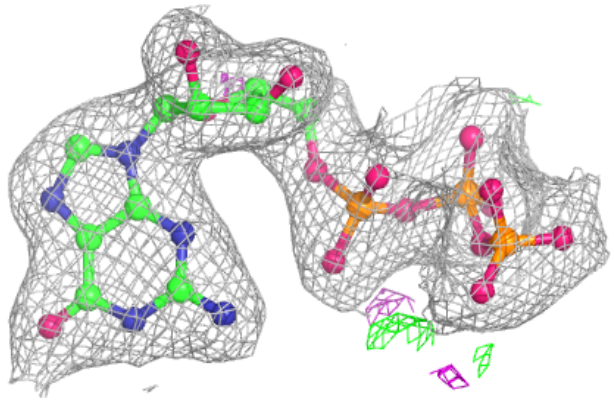


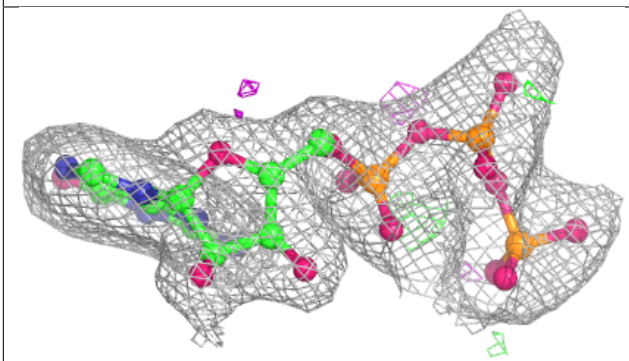


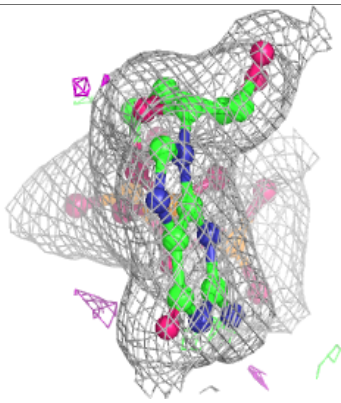


Electron density around GTP A 702:

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







6.5 Other polymers (i)

There are no such residues in this entry.