



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:13 PM UTC

PDB ID : 6DW5 / pdb_00006dw5
Title : SAMHD1 Bound to Gemcitabine-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 : 1.93 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

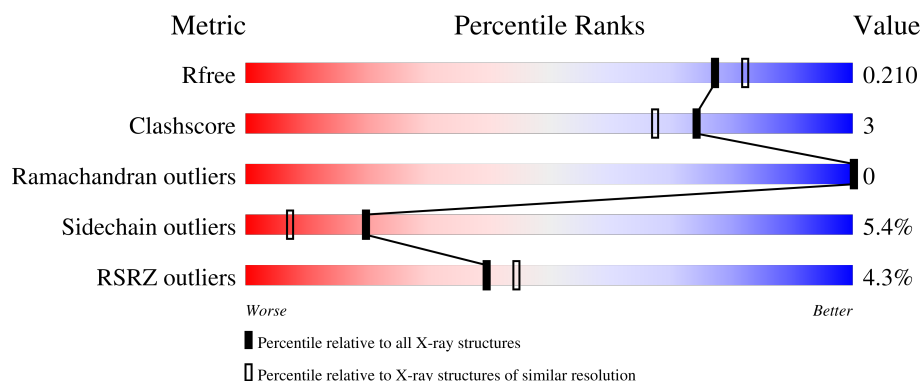
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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}	180053	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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 $\leq 5\%$. 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	4% 73% 10% 15%
1	B	550	7% 75% 10% 13%
1	C	550	3% 75% 11% 13%
1	D	550	% 78% 8% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	NI	C	701	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16603 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	468	Total	C	N	O	S	0	0	0
			3825	2445	667	693	20			
1	B	480	Total	C	N	O	S	0	0	0
			3925	2513	684	708	20			
1	C	481	Total	C	N	O	S	0	0	0
			3933	2517	685	711	20			
1	D	481	Total	C	N	O	S	0	1	0
			3940	2522	687	711	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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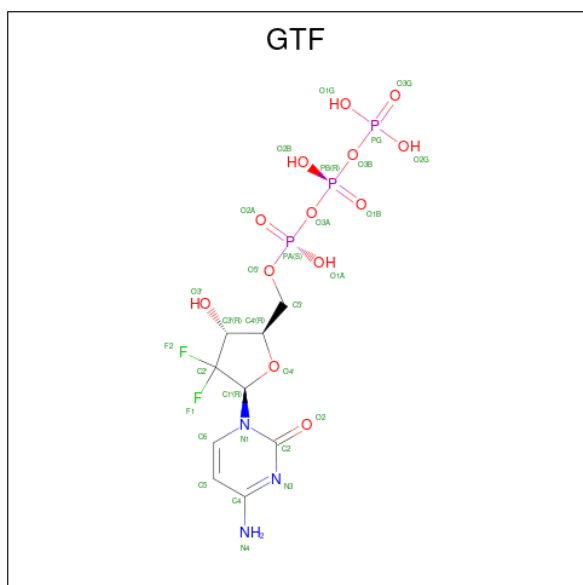
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C	106	MET	-	expression tag	UNP Q9Y3Z3
C	107	GLY	-	expression tag	UNP Q9Y3Z3
C	108	ARG	-	expression tag	UNP Q9Y3Z3
C	109	ASP	-	expression tag	UNP Q9Y3Z3
C	110	PRO	-	expression tag	UNP Q9Y3Z3
C	111	ASN	-	expression tag	UNP Q9Y3Z3
C	112	SER	-	expression 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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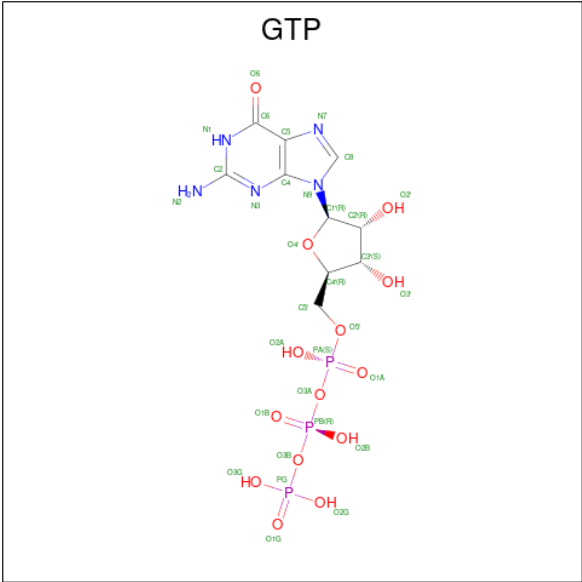
Chain	Residue	Modelled	Actual	Comment	Reference
D	110	PRO	-	expression tag	UNP Q9Y3Z3
D	111	ASN	-	expression tag	UNP Q9Y3Z3
D	112	SER	-	expression tag	UNP Q9Y3Z3
D	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
D	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3

- Molecule 2 is 2'-deoxy-2',2'-difluorocytidine 5'-(tetrahydrogen triphosphate) (CCD ID: GTF) (formula: $C_9H_{14}F_2N_3O_{13}P_3$).



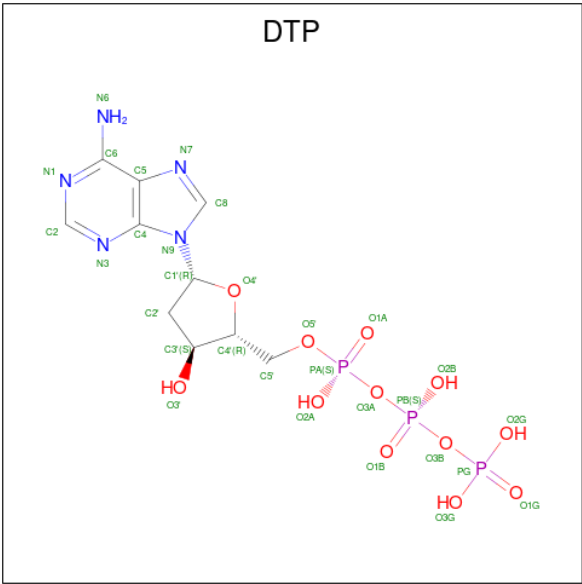
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	P	0	0
			30	9	2	3	13	3		
2	B	1	Total	C	F	N	O	P	0	0
			30	9	2	3	13	3		
2	C	1	Total	C	F	N	O	P	0	0
			30	9	2	3	13	3		
2	D	1	Total	C	F	N	O	P	0	0
			30	9	2	3	13	3		

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: 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	B	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	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 4 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃)



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 (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		
6	B	1	Total	Na	0	0
			1	1		
6	C	2	Total	Na	0	0
			2	2		

- Molecule 7 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Ni	0	0
			1	1		

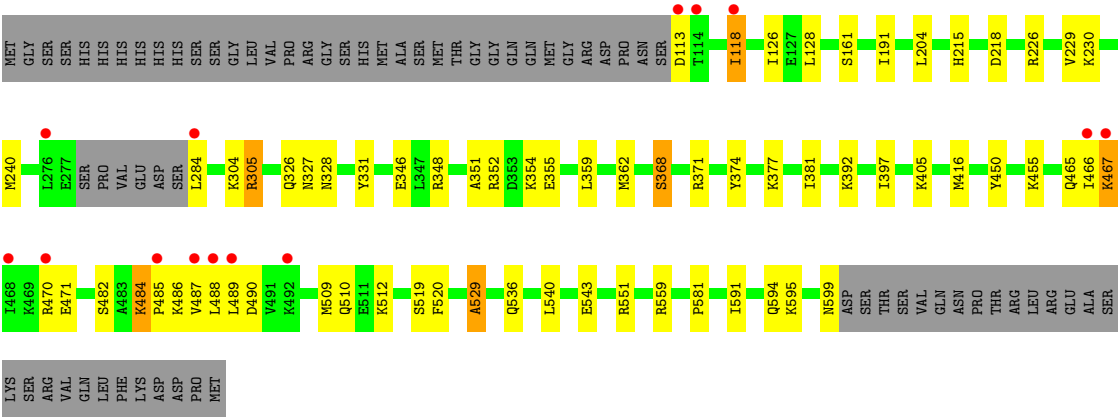
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	164	Total	O	0	0
			164	164		

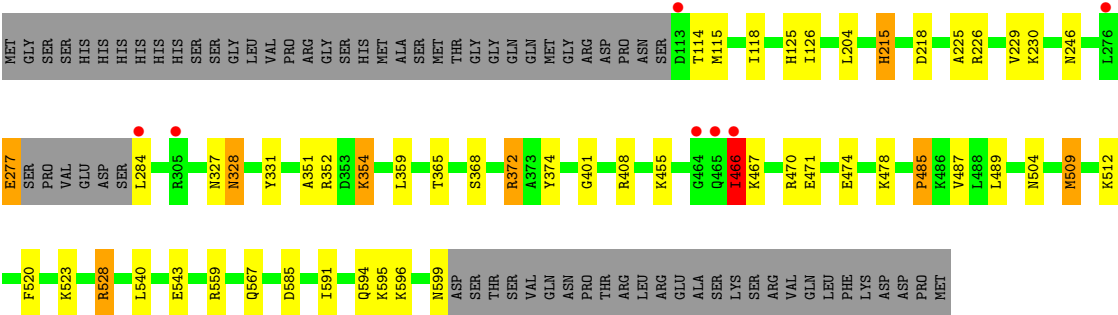
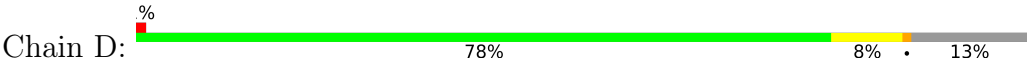
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	138	Total 138	O 138	0	0
8	C	137	Total 137	O 137	0	0
8	D	158	Total 158	O 158	0	0



● 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, α , β , γ	80.69Å 142.90Å 98.91Å 90.00° 113.92° 90.00°	Depositor
Resolution (Å)	90.41 – 1.93 90.41 – 1.93	Depositor EDS
% Data completeness (in resolution range)	97.0 (90.41-1.93) 97.0 (90.41-1.93)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.173 , 0.205 0.181 , 0.210	Depositor DCC
R_{free} test set	7434 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16603	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.37	10/3913 (0.3%)	1.23	20/5279 (0.4%)
1	B	1.29	7/4017 (0.2%)	1.20	16/5422 (0.3%)
1	C	1.30	9/4025 (0.2%)	1.20	9/5433 (0.2%)
1	D	1.40	16/4036 (0.4%)	1.21	11/5448 (0.2%)
All	All	1.34	42/15991 (0.3%)	1.21	56/21582 (0.3%)

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	327	ASN	C-O	-11.61	1.09	1.24
1	A	161	SER	CB-OG	8.22	1.58	1.42
1	D	328	ASN	CA-C	7.96	1.63	1.52
1	B	371	ARG	CZ-NH2	7.56	1.43	1.33
1	A	327	ASN	C-O	-7.27	1.15	1.24
1	C	191	ILE	C-O	-7.08	1.17	1.24
1	A	538	SER	N-CA	6.91	1.55	1.46
1	C	328	ASN	C-O	6.81	1.32	1.23
1	D	408	ARG	CD-NE	6.73	1.55	1.46
1	C	161	SER	CB-OG	6.72	1.55	1.42
1	D	485	PRO	CA-C	6.45	1.60	1.52
1	A	246	ASN	C-O	-6.29	1.16	1.24
1	C	529	ALA	CA-C	-6.10	1.45	1.52
1	B	161	SER	CB-OG	6.09	1.54	1.42
1	D	115	MET	CA-C	6.03	1.60	1.52
1	A	582	GLN	C-O	6.00	1.31	1.23
1	C	392	LYS	C-O	-5.99	1.16	1.24
1	A	347	LEU	C-O	-5.92	1.16	1.24
1	B	466	ILE	CA-CB	5.84	1.60	1.54
1	D	225	ALA	C-O	-5.83	1.17	1.24
1	D	327	ASN	CA-C	5.82	1.60	1.52
1	D	327	ASN	CG-ND2	5.75	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	408	ARG	CZ-NH1	5.56	1.40	1.32
1	C	368	SER	CB-OG	-5.54	1.31	1.42
1	B	191	ILE	C-O	-5.54	1.18	1.24
1	B	302	SER	CA-C	-5.54	1.46	1.52
1	D	246	ASN	C-O	-5.44	1.17	1.24
1	D	204	LEU	CB-CG	-5.43	1.42	1.53
1	A	466	ILE	CA-CB	5.39	1.60	1.54
1	D	509	MET	C-O	5.39	1.30	1.23
1	D	218	ASP	C-O	-5.36	1.17	1.24
1	A	479	GLU	C-O	-5.29	1.17	1.24
1	C	362	MET	CA-C	5.27	1.59	1.52
1	B	368	SER	CB-OG	-5.24	1.31	1.42
1	A	581	PRO	CA-C	5.16	1.58	1.52
1	B	597	GLU	N-CA	5.14	1.52	1.46
1	D	125	HIS	C-O	-5.12	1.17	1.24
1	C	581	PRO	CA-C	5.11	1.59	1.52
1	D	504	ASN	C-O	-5.09	1.17	1.24
1	D	401	GLY	C-O	-5.08	1.17	1.23
1	C	218	ASP	C-O	-5.04	1.17	1.24
1	A	395	ASP	C-O	-5.03	1.17	1.24

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	466	ILE	N-CA-CB	10.45	124.58	110.26
1	B	594	GLN	CB-CA-C	-8.14	97.79	110.81
1	B	485	PRO	N-CA-C	7.84	124.03	113.84
1	A	485	PRO	CA-C-N	7.83	131.10	120.54
1	A	485	PRO	C-N-CA	7.83	131.10	120.54
1	A	408	ARG	CG-CD-NE	-7.04	96.52	112.00
1	A	305	ARG	CB-CG-CD	6.99	127.36	111.30
1	A	582	GLN	N-CA-C	-6.98	100.11	110.23
1	C	304	LYS	CD-CE-NZ	6.61	133.06	111.90
1	A	535	ASN	CB-CA-C	-6.52	97.45	110.42
1	A	371	ARG	CA-CB-CG	-6.31	101.48	114.10
1	B	371	ARG	NE-CZ-NH1	-6.30	115.20	121.50
1	B	354	LYS	CB-CA-C	-6.25	98.33	110.46
1	A	354	LYS	CB-CA-C	-6.11	98.61	110.46
1	A	485	PRO	N-CA-C	6.11	125.05	112.47
1	C	466	ILE	CB-CA-C	-6.05	101.37	111.29
1	D	204	LEU	CB-CA-C	-5.96	100.90	110.79
1	C	485	PRO	N-CA-C	5.94	121.29	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	354	LYS	CB-CA-C	-5.90	99.02	110.46
1	B	328	ASN	N-CA-C	5.87	120.14	112.92
1	C	467	LYS	N-CA-CB	5.82	119.92	110.43
1	A	215	HIS	N-CA-C	5.77	119.42	112.38
1	B	204	LEU	CB-CA-C	-5.71	101.32	110.79
1	B	230	LYS	CB-CG-CD	5.69	124.39	111.30
1	B	327	ASN	CA-C-O	-5.65	114.24	120.69
1	D	226	ARG	NE-CZ-NH2	5.65	124.29	119.20
1	D	372	ARG	CG-CD-NE	5.60	124.31	112.00
1	A	204	LEU	CB-CA-C	-5.55	101.57	110.79
1	A	580	LYS	CA-C-N	-5.51	114.10	119.78
1	A	580	LYS	C-N-CA	-5.51	114.10	119.78
1	D	215	HIS	N-CA-C	5.47	119.05	112.38
1	A	471	GLU	CA-CB-CG	5.46	125.03	114.10
1	D	328	ASN	N-CA-CB	-5.42	101.95	110.46
1	D	528	ARG	CG-CD-NE	5.42	123.91	112.00
1	C	204	LEU	CB-CA-C	-5.37	101.87	110.79
1	B	551	ARG	NE-CZ-NH1	-5.36	116.14	121.50
1	B	222	ILE	N-CA-CB	5.35	113.87	110.50
1	B	230	LYS	CA-CB-CG	5.34	124.79	114.10
1	D	585	ASP	N-CA-C	5.33	118.88	112.38
1	B	594	GLN	CA-CB-CG	5.33	124.75	114.10
1	C	215	HIS	N-CA-C	5.30	118.84	112.38
1	D	489	LEU	N-CA-C	5.29	117.03	108.41
1	B	215	HIS	N-CA-C	5.28	118.82	112.38
1	A	352	ARG	CG-CD-NE	-5.27	100.41	112.00
1	B	576	ARG	CA-CB-CG	5.27	124.64	114.10
1	C	551	ARG	NE-CZ-NH1	-5.26	116.24	121.50
1	A	371	ARG	CD-NE-CZ	5.20	131.68	124.40
1	A	585	ASP	N-CA-C	5.20	117.23	109.59
1	C	226	ARG	NE-CZ-NH2	5.13	123.81	119.20
1	C	352	ARG	NE-CZ-NH1	-5.11	116.39	121.50
1	A	327	ASN	CA-C-O	-5.08	114.69	120.58
1	A	226	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	B	226	ARG	NE-CZ-NH2	5.06	123.76	119.20
1	B	352	ARG	CG-CD-NE	-5.04	100.92	112.00
1	D	352	ARG	CG-CD-NE	-5.01	100.98	112.00
1	A	479	GLU	CB-CG-CD	-5.00	104.10	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3825	0	3806	24	2
1	B	3925	0	3917	30	0
1	C	3933	0	3921	29	0
1	D	3940	0	3928	19	2
2	A	30	0	10	3	0
2	B	30	0	10	3	0
2	C	30	0	10	3	0
2	D	30	0	9	6	0
3	A	32	0	12	0	0
3	B	64	0	24	0	0
3	D	32	0	12	0	0
4	A	30	0	12	0	0
4	B	30	0	12	1	0
4	C	30	0	12	1	0
4	D	30	0	12	0	0
5	A	4	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	1	0	0	0	0
6	B	1	0	0	0	0
6	C	2	0	0	0	0
7	C	1	0	0	0	0
8	A	164	0	0	1	0
8	B	138	0	0	1	0
8	C	137	0	0	3	0
8	D	158	0	0	0	0
All	All	16603	0	15707	98	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (98) 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:C:705:GTF:O4'	2:C:705:GTF:C1'	1.71	1.26
2:A:701:GTF:O4'	2:A:701:GTF:C1'	1.69	1.21
2:D:702:GTF:O4'	2:D:702:GTF:C1'	1.69	1.20
2:B:701:GTF:O4'	2:B:701:GTF:C1'	1.68	1.17
1:D:215:HIS:CE1	2:D:702:GTF:O1A	2.20	0.94
1:A:534:LYS:HE3	1:A:542:PRO:O	1.78	0.83
1:A:543:GLU:HG3	1:C:543:GLU:HG3	1.61	0.81
1:A:558:ASP:OD2	1:A:560:LYS:HG2	1.83	0.77
1:B:371:ARG:HD2	1:B:505:MET:HE2	1.66	0.77
1:D:215:HIS:NE2	2:D:702:GTF:O1A	2.20	0.74
1:B:371:ARG:CD	1:B:505:MET:HE2	2.25	0.66
1:B:140:GLN:CG	1:B:240:MET:HE1	2.27	0.65
1:A:543:GLU:CG	1:C:543:GLU:HG3	2.28	0.64
1:D:591:ILE:O	1:D:594:GLN:HG2	1.97	0.64
1:C:591:ILE:O	1:C:594:GLN:HG2	1.98	0.63
1:A:470:ARG:C	1:A:470:ARG:HD3	2.24	0.62
1:B:591:ILE:O	1:B:594:GLN:HG2	2.00	0.61
1:B:534:LYS:O	1:B:537:VAL:HG22	2.01	0.61
1:C:374:TYR:CE1	2:C:705:GTF:F1	2.45	0.60
1:B:140:GLN:HG3	1:B:240:MET:HE1	1.84	0.59
1:A:326:GLN:HG2	1:C:327:ASN:O	2.03	0.58
1:C:326:GLN:NE2	8:C:801:HOH:O	2.21	0.58
1:A:371:ARG:HG3	1:A:505:MET:HE3	1.87	0.57
1:D:374:TYR:CE1	2:D:702:GTF:F1	2.51	0.54
1:D:509:MET:HE2	1:D:512:LYS:HE3	1.89	0.54
1:A:326:GLN:OE1	1:C:326:GLN:OE1	2.27	0.53
1:B:537:VAL:HG23	1:B:541:LEU:CD1	2.38	0.53
1:A:470:ARG:HD3	1:A:471:GLU:N	2.24	0.53
1:C:487:VAL:HG13	1:C:489:LEU:HG	1.89	0.53
1:A:380:ASN:OD1	8:A:801:HOH:O	2.19	0.52
1:D:215:HIS:HE1	2:D:702:GTF:O1A	1.82	0.52
1:C:509:MET:HE2	1:C:512:LYS:HE3	1.90	0.52
1:D:595:LYS:O	1:D:599:ASN:ND2	2.43	0.51
1:A:374:TYR:CE1	2:A:701:GTF:F1	2.53	0.51
1:B:374:TYR:CE1	2:B:701:GTF:F1	2.53	0.51
1:C:595:LYS:O	1:C:599:ASN:ND2	2.43	0.51
1:A:239:MET:HE2	1:A:416:MET:HE3	1.92	0.51
1:B:185:LYS:NZ	8:B:804:HOH:O	2.42	0.51
1:C:305:ARG:HG2	1:C:348:ARG:NH1	2.26	0.51
1:B:328:ASN:HB3	1:D:328:ASN:HB3	1.92	0.50
1:D:487:VAL:HG21	1:D:567:GLN:HG3	1.93	0.50
1:C:374:TYR:CZ	2:C:705:GTF:F1	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:GLU:OE2	1:B:336:LYS:HE2	2.12	0.49
1:C:118:ILE:CD1	1:C:128:LEU:HD11	2.43	0.49
1:B:509:MET:HE2	1:B:512:LYS:HE3	1.94	0.48
1:B:240:MET:HG2	1:B:416:MET:SD	2.53	0.48
2:A:701:GTF:F2	2:A:701:GTF:H5'	2.04	0.48
1:C:240:MET:HE2	1:C:416:MET:SD	2.55	0.47
1:D:215:HIS:NE2	2:D:702:GTF:PA	2.88	0.47
1:D:328:ASN:CG	1:D:365:THR:HG1	2.16	0.47
1:B:331:TYR:CD1	1:B:331:TYR:C	2.92	0.47
1:A:331:TYR:C	1:A:331:TYR:CD1	2.92	0.47
1:D:331:TYR:C	1:D:331:TYR:CD1	2.93	0.46
1:C:354:LYS:HG3	1:C:355:GLU:OE2	2.16	0.46
1:A:455:LYS:HG2	1:A:557:VAL:HG12	1.96	0.46
1:D:485:PRO:HB2	1:D:487:VAL:HG22	1.98	0.45
1:C:371:ARG:NH2	8:C:811:HOH:O	2.49	0.45
1:B:537:VAL:HG23	1:B:541:LEU:HD12	1.99	0.45
1:B:537:VAL:CG2	1:B:541:LEU:CD1	2.95	0.45
1:C:331:TYR:C	1:C:331:TYR:CD1	2.95	0.45
1:C:351:ALA:O	1:C:520:PHE:HA	2.16	0.45
1:D:351:ALA:O	1:D:520:PHE:HA	2.17	0.45
1:B:490:ASP:OD2	1:B:490:ASP:N	2.50	0.44
1:C:118:ILE:HD11	1:C:128:LEU:CD1	2.47	0.44
1:D:277:GLU:OE1	1:D:277:GLU:C	2.60	0.44
1:A:381:ILE:HD12	1:A:381:ILE:HA	1.91	0.44
1:C:482:SER:O	1:C:484:LYS:HE2	2.17	0.44
1:B:143:ARG:HD2	1:B:420:THR:HA	1.99	0.44
1:B:537:VAL:HG23	1:B:541:LEU:HD11	2.00	0.44
1:A:543:GLU:CG	1:C:543:GLU:CG	2.95	0.44
2:B:701:GTF:F2	2:B:701:GTF:C6	2.56	0.43
1:B:140:GLN:HB3	1:B:240:MET:HE2	2.00	0.43
1:A:543:GLU:HG3	1:C:543:GLU:CG	2.40	0.43
1:A:351:ALA:O	1:A:520:PHE:HA	2.18	0.43
1:B:468:ILE:HD12	1:B:550:ILE:HD11	2.00	0.43
1:D:118:ILE:HG23	1:D:126:ILE:HG12	2.01	0.43
1:C:377:LYS:NZ	8:C:808:HOH:O	2.42	0.43
1:A:126:ILE:HD13	1:A:126:ILE:HG21	1.65	0.43
1:B:139:PRO:HD3	1:C:450:TYR:CE1	2.54	0.43
1:D:277:GLU:C	1:D:277:GLU:CD	2.87	0.43
4:B:704:DTP:N6	1:D:372:ARG:HG2	2.34	0.43
1:A:582:GLN:HG2	1:C:536:GLN:NE2	2.34	0.42
1:B:537:VAL:CG2	1:B:541:LEU:HD11	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:GLN:H	1:A:465:GLN:CD	2.27	0.42
1:C:381:ILE:HD12	1:C:381:ILE:HA	1.95	0.42
1:A:277:GLU:OE1	1:A:277:GLU:C	2.62	0.42
1:B:351:ALA:O	1:B:520:PHE:HA	2.20	0.42
1:B:463:THR:O	1:B:466:ILE:HD12	2.19	0.42
1:C:126:ILE:HD13	1:C:126:ILE:HG21	1.62	0.42
1:C:519:SER:HB3	1:C:529:ALA:HB1	2.03	0.41
1:B:118:ILE:CD1	1:B:128:LEU:HD11	2.51	0.41
1:B:541:LEU:HB3	1:B:542:PRO:HD2	2.02	0.41
1:C:354:LYS:NZ	4:C:702:DTP:O1A	2.54	0.41
1:A:244:LEU:C	1:A:244:LEU:HD23	2.46	0.41
1:B:244:LEU:C	1:B:244:LEU:HD23	2.46	0.41
1:D:126:ILE:HG21	1:D:126:ILE:HD13	1.74	0.41
1:B:126:ILE:HD13	1:B:126:ILE:HG21	1.66	0.40
1:B:369:LEU:HD23	1:B:369:LEU:HA	1.93	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:ASP:OD2	1:D:466:ILE:CD1[1_455]	1.73	0.47
1:A:472:ASP:OD2	1:D:466:ILE:CG1[1_455]	2.18	0.02

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	464/550 (84%)	456 (98%)	8 (2%)	0	100	100
1	B	476/550 (86%)	468 (98%)	8 (2%)	0	100	100
1	C	477/550 (87%)	466 (98%)	11 (2%)	0	100	100
1	D	478/550 (87%)	472 (99%)	6 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1895/2200 (86%)	1862 (98%)	33 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	415/488 (85%)	391 (94%)	24 (6%)	18	6
1	B	426/488 (87%)	402 (94%)	24 (6%)	19	7
1	C	427/488 (88%)	404 (95%)	23 (5%)	20	7
1	D	428/488 (88%)	407 (95%)	21 (5%)	22	9
All	All	1696/1952 (87%)	1604 (95%)	92 (5%)	20	7

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	MET
1	A	184	GLU
1	A	230	LYS
1	A	235	GLN
1	A	277	GLU
1	A	284	LEU
1	A	305	ARG
1	A	354	LYS
1	A	359	LEU
1	A	368	SER
1	A	405	LYS
1	A	425	ASN
1	A	465	GLN
1	A	470	ARG
1	A	471	GLU
1	A	474	GLU
1	A	478	LYS

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Mol	Chain	Res	Type
1	A	488	LEU
1	A	490	ASP
1	A	492	LYS
1	A	494	LYS
1	A	559	ARG
1	A	560	LYS
1	A	586	VAL
1	B	118	ILE
1	B	193	GLU
1	B	229	VAL
1	B	230	LYS
1	B	240	MET
1	B	262	GLU
1	B	277	GLU
1	B	284	LEU
1	B	305	ARG
1	B	354	LYS
1	B	368	SER
1	B	405	LYS
1	B	426	ILE
1	B	463	THR
1	B	465	GLN
1	B	470	ARG
1	B	471	GLU
1	B	478	LYS
1	B	488	LEU
1	B	490	ASP
1	B	492	LYS
1	B	576	ARG
1	B	579	THR
1	B	596	LYS
1	C	113	ASP
1	C	118	ILE
1	C	229	VAL
1	C	230	LYS
1	C	284	LEU
1	C	305	ARG
1	C	346	GLU
1	C	359	LEU
1	C	368	SER
1	C	397	ILE
1	C	405	LYS

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Mol	Chain	Res	Type
1	C	455	LYS
1	C	465	GLN
1	C	467	LYS
1	C	470	ARG
1	C	471	GLU
1	C	484	LYS
1	C	486	LYS
1	C	488	LEU
1	C	490	ASP
1	C	510	GLN
1	C	540	LEU
1	C	559	ARG
1	D	114	THR
1	D	229	VAL
1	D	230	LYS
1	D	277	GLU
1	D	284	LEU
1	D	354	LYS
1	D	359	LEU
1	D	368	SER
1	D	455	LYS
1	D	466	ILE
1	D	467	LYS
1	D	470	ARG
1	D	471	GLU
1	D	474	GLU
1	D	478	LYS
1	D	523	LYS
1	D	528	ARG
1	D	540	LEU
1	D	543	GLU
1	D	559	ARG
1	D	596	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	A	163	ASN
1	A	248	ASN
1	A	326	GLN
1	A	364	HIS

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Mol	Chain	Res	Type
1	A	367	ASN
1	A	370	HIS
1	A	375	GLN
1	A	380	ASN
1	A	465	GLN
1	A	510	GLN
1	A	571	GLN
1	B	149	GLN
1	B	321	HIS
1	B	370	HIS
1	B	375	GLN
1	B	380	ASN
1	B	465	GLN
1	B	527	ASN
1	B	567	GLN
1	B	577	ASN
1	C	149	GLN
1	C	163	ASN
1	C	235	GLN
1	C	370	HIS
1	C	375	GLN
1	C	380	ASN
1	C	465	GLN
1	C	510	GLN
1	C	535	ASN
1	C	571	GLN
1	C	594	GLN
1	D	149	GLN
1	D	235	GLN
1	D	248	ASN
1	D	326	GLN
1	D	364	HIS
1	D	370	HIS
1	D	375	GLN
1	D	380	ASN
1	D	539	GLN
1	D	571	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 15 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$
2	GTF	A	701	5	28,31,31	6.53	18 (64%)	39,50,50	2.88	14 (35%)
4	DTP	D	701	5	31,32,32	2.06	8 (25%)	46,50,50	1.93	12 (26%)
4	DTP	A	703	5	31,32,32	1.77	7 (22%)	46,50,50	1.78	15 (32%)
3	GTP	A	702	5	33,34,34	1.77	4 (12%)	50,54,54	1.72	11 (22%)
2	GTF	C	705	-	28,31,31	6.90	18 (64%)	39,50,50	2.97	15 (38%)
4	DTP	B	704	5	31,32,32	2.04	7 (22%)	46,50,50	2.01	14 (30%)
2	GTF	B	701	5	28,31,31	5.99	17 (60%)	39,50,50	2.51	13 (33%)
2	GTF	D	702	5	28,31,31	6.10	16 (57%)	39,50,50	2.51	13 (33%)
3	GTP	B	703	5	33,34,34	1.63	9 (27%)	50,54,54	1.62	13 (26%)
4	DTP	C	702	5	31,32,32	1.76	9 (29%)	46,50,50	1.55	8 (17%)
3	GTP	B	702	5	33,34,34	2.21	9 (27%)	50,54,54	1.24	4 (8%)
3	GTP	D	703	5	33,34,34	1.57	6 (18%)	50,54,54	1.79	13 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GTF	A	701	5	-	4/22/42/42	0/2/2/2
4	DTP	D	701	5	-	3/22/34/34	0/3/3/3
4	DTP	A	703	5	-	2/22/34/34	0/3/3/3
3	GTP	A	702	5	-	4/22/38/38	0/3/3/3
2	GTF	C	705	-	-	5/22/42/42	0/2/2/2
4	DTP	B	704	5	-	5/22/34/34	0/3/3/3
2	GTF	B	701	5	-	6/22/42/42	0/2/2/2
2	GTF	D	702	5	-	5/22/42/42	0/2/2/2
3	GTP	B	703	5	-	6/22/38/38	0/3/3/3
4	DTP	C	702	5	-	2/22/34/34	0/3/3/3
3	GTP	B	702	5	-	7/22/38/38	0/3/3/3
3	GTP	D	703	5	-	1/22/38/38	0/3/3/3

All (128) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	705	GTF	PB-O3B	20.20	1.81	1.59
2	C	705	GTF	O4'-C1'	18.80	1.71	1.42
2	A	701	GTF	PB-O3B	18.48	1.79	1.59
2	A	701	GTF	O4'-C1'	17.48	1.69	1.42
2	D	702	GTF	PB-O3B	17.43	1.78	1.59
2	D	702	GTF	O4'-C1'	17.12	1.69	1.42
2	B	701	GTF	PB-O3B	16.35	1.77	1.59
2	B	701	GTF	O4'-C1'	16.29	1.68	1.42
2	C	705	GTF	PA-O3A	12.21	1.72	1.59
2	C	705	GTF	PB-O3A	9.97	1.70	1.59
2	B	701	GTF	PA-O3A	9.43	1.69	1.59
2	A	701	GTF	PA-O3A	9.38	1.69	1.59
2	D	702	GTF	C2-N3	8.53	1.53	1.36
2	B	701	GTF	PB-O3A	8.48	1.68	1.59
2	A	701	GTF	C4-N3	8.15	1.50	1.34
2	A	701	GTF	C2-N3	8.14	1.52	1.36
2	C	705	GTF	C2-N1	7.98	1.56	1.40
2	A	701	GTF	C2-N1	7.87	1.56	1.40
2	D	702	GTF	C2-N1	7.57	1.55	1.40
2	D	702	GTF	PA-O3A	7.50	1.67	1.59
2	A	701	GTF	PB-O3A	7.40	1.67	1.59
4	B	704	DTP	PB-O3A	7.36	1.67	1.59
3	B	702	GTP	PB-O3B	-7.31	1.51	1.59
4	D	701	DTP	PB-O3A	7.30	1.67	1.59
2	C	705	GTF	C2-N3	7.05	1.50	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	GTF	C6-N1	7.00	1.54	1.38
2	A	701	GTF	C6-N1	6.81	1.54	1.38
2	A	701	GTF	C6-C5	6.77	1.50	1.35
3	A	702	GTP	PA-O3A	6.72	1.66	1.59
2	B	701	GTF	C2-N1	6.61	1.53	1.40
2	C	705	GTF	C6-C5	6.49	1.50	1.35
2	D	702	GTF	C6-C5	5.98	1.48	1.35
2	D	702	GTF	O3'-C3'	-5.92	1.31	1.42
2	D	702	GTF	C6-N1	5.90	1.52	1.38
2	B	701	GTF	C6-C5	5.86	1.48	1.35
2	B	701	GTF	C2-N3	5.85	1.48	1.36
2	A	701	GTF	C4'-C3'	5.82	1.63	1.53
2	B	701	GTF	O4'-C4'	-5.71	1.32	1.45
2	C	705	GTF	C6-N1	5.38	1.50	1.38
2	C	705	GTF	C4-N3	5.35	1.45	1.34
2	B	701	GTF	C4-N3	5.31	1.45	1.34
2	D	702	GTF	O4'-C4'	-5.21	1.33	1.45
2	C	705	GTF	O4'-C4'	-5.21	1.33	1.45
2	D	702	GTF	C4-N3	5.05	1.44	1.34
2	D	702	GTF	C4'-C3'	5.01	1.62	1.53
2	B	701	GTF	C4'-C3'	4.96	1.62	1.53
2	D	702	GTF	PB-O3A	4.91	1.64	1.59
4	A	703	DTP	C5-C4	4.72	1.47	1.39
4	C	702	DTP	C5-N7	-4.57	1.30	1.39
3	D	703	GTP	PA-O3A	4.49	1.64	1.59
3	B	702	GTP	PA-O3A	4.40	1.64	1.59
2	C	705	GTF	C4'-C3'	4.32	1.61	1.53
4	D	701	DTP	PA-O3A	-3.90	1.55	1.59
2	A	701	GTF	F2-C2'	3.76	1.45	1.37
2	A	701	GTF	O4'-C4'	-3.71	1.36	1.45
2	B	701	GTF	C4-N4	3.62	1.42	1.33
4	A	703	DTP	C5-N7	-3.47	1.32	1.39
3	D	703	GTP	C4-N9	-3.47	1.29	1.38
2	C	705	GTF	C1'-N1	3.45	1.55	1.46
2	D	702	GTF	C4-N4	3.43	1.42	1.33
3	B	702	GTP	C6-N1	-3.41	1.32	1.38
4	B	704	DTP	C5-C4	3.40	1.45	1.39
4	D	701	DTP	C5-C4	3.29	1.45	1.39
3	B	703	GTP	PA-O3A	3.22	1.63	1.59
2	A	701	GTF	C5-C4	3.22	1.50	1.42
3	B	702	GTP	PB-O3A	-3.20	1.56	1.59
2	B	701	GTF	C5-C4	3.16	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	DTP	PB-O3B	-3.09	1.56	1.59
3	B	703	GTP	C4-N9	-3.09	1.30	1.38
4	B	704	DTP	C8-N7	3.07	1.37	1.31
4	D	701	DTP	C5-N7	-3.06	1.33	1.39
4	A	703	DTP	PA-O3A	3.01	1.62	1.59
4	B	704	DTP	PB-O3B	-3.01	1.56	1.59
2	C	705	GTF	F2-C2'	3.00	1.43	1.37
3	B	703	GTP	PG-O3G	-3.00	1.43	1.54
4	C	702	DTP	C4-N9	-2.97	1.31	1.37
2	A	701	GTF	PA-O5'	2.92	1.70	1.59
3	B	703	GTP	C6-N1	-2.88	1.33	1.38
4	C	702	DTP	PB-O3B	-2.86	1.56	1.59
3	B	702	GTP	C5-C4	2.84	1.46	1.38
2	A	701	GTF	C5'-C4'	2.81	1.60	1.51
2	B	701	GTF	F2-C2'	2.80	1.43	1.37
2	D	702	GTF	C1'-N1	2.80	1.53	1.46
2	A	701	GTF	C1'-N1	2.78	1.53	1.46
2	C	705	GTF	C5-C4	2.77	1.49	1.42
2	A	701	GTF	O3'-C3'	-2.73	1.37	1.42
4	D	701	DTP	C5-C6	2.69	1.48	1.41
4	B	704	DTP	C8-N9	-2.68	1.33	1.37
4	C	702	DTP	O4'-C1'	2.66	1.48	1.42
2	B	701	GTF	PA-O5'	2.65	1.69	1.59
3	A	702	GTP	O4'-C1'	2.62	1.48	1.42
3	B	703	GTP	PB-O3A	2.61	1.62	1.59
2	C	705	GTF	F1-C2'	2.60	1.42	1.37
3	B	703	GTP	PB-O2B	-2.58	1.43	1.55
3	B	702	GTP	C4-N9	-2.55	1.31	1.38
4	C	702	DTP	C2-N1	-2.53	1.29	1.33
4	D	701	DTP	C4-N9	-2.53	1.32	1.37
3	A	702	GTP	O6-C6	2.51	1.28	1.23
4	D	701	DTP	C6-N1	-2.51	1.28	1.35
3	B	702	GTP	O4'-C4'	-2.50	1.39	1.45
2	C	705	GTF	C5'-C4'	2.49	1.59	1.51
2	D	702	GTF	F2-C2'	2.49	1.42	1.37
2	A	701	GTF	C4-N4	2.39	1.39	1.33
4	B	704	DTP	C5-C6	2.39	1.47	1.41
2	B	701	GTF	O3'-C3'	-2.38	1.38	1.42
3	D	703	GTP	PG-O2G	-2.35	1.46	1.54
2	D	702	GTF	C5-C4	2.32	1.48	1.42
3	B	703	GTP	O2'-C2'	2.28	1.48	1.43
4	A	703	DTP	O3'-C3'	2.28	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	GTP	O4'-C1'	2.27	1.47	1.42
4	C	702	DTP	C3'-C4'	-2.27	1.47	1.53
4	C	702	DTP	PG-O2G	-2.27	1.46	1.54
2	C	705	GTF	PA-O5'	2.26	1.68	1.59
3	B	703	GTP	O6-C6	2.26	1.27	1.23
4	B	704	DTP	O4'-C4'	-2.23	1.40	1.45
2	C	705	GTF	PG-O2G	-2.22	1.46	1.54
4	A	703	DTP	PA-O2A	-2.19	1.45	1.55
3	B	702	GTP	PG-O3G	-2.19	1.46	1.54
3	D	703	GTP	PB-O2B	-2.17	1.45	1.55
4	C	702	DTP	C8-N7	2.16	1.35	1.31
2	B	701	GTF	C5'-C4'	2.16	1.58	1.51
4	A	703	DTP	C2-N3	2.13	1.37	1.33
4	D	701	DTP	PB-O2B	-2.13	1.45	1.55
3	D	703	GTP	PA-O2A	-2.13	1.45	1.55
3	B	703	GTP	PB-O3B	-2.13	1.57	1.59
3	D	703	GTP	C5-C4	2.11	1.44	1.38
4	C	702	DTP	PB-O3A	2.10	1.61	1.59
3	A	702	GTP	O4'-C4'	-2.03	1.40	1.45

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	GTF	F2-C2'-F1	10.51	118.17	105.55
2	B	701	GTF	O4'-C1'-N1	9.83	117.05	108.23
2	A	701	GTF	O4'-C1'-N1	8.82	116.14	108.23
2	C	705	GTF	O4'-C1'-N1	8.79	116.12	108.23
2	C	705	GTF	F2-C2'-F1	7.22	114.21	105.55
2	C	705	GTF	O3A-PA-O2A	-7.20	89.04	110.70
2	D	702	GTF	O2B-PB-O3B	6.68	125.33	107.27
4	B	704	DTP	C4-N9-C8	6.63	112.70	105.74
2	D	702	GTF	O4'-C1'-N1	6.28	113.86	108.23
2	D	702	GTF	C5'-C4'-C3'	-5.46	107.18	116.11
3	D	703	GTP	C5-C4-N3	-5.04	120.36	128.39
2	A	701	GTF	O1A-PA-O5'	5.04	130.39	107.57
2	D	702	GTF	F2-C2'-F1	4.87	111.39	105.55
4	D	701	DTP	C5-C4-N3	-4.46	120.57	126.72
4	D	701	DTP	C5-N7-C8	4.43	110.42	103.45
2	C	705	GTF	O2G-PG-O3B	4.43	119.50	104.64
4	D	701	DTP	N9-C8-N7	-4.43	107.66	113.94
3	D	703	GTP	N9-C4-N3	4.33	134.62	125.95
3	A	702	GTP	C5-C4-N3	-4.27	121.59	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	GTF	O2-C2-N1	4.13	127.00	118.90
2	B	701	GTF	N4-C4-N3	-4.03	110.71	117.91
2	B	701	GTF	O2B-PB-O3B	4.00	118.08	107.27
4	B	704	DTP	O2A-PA-O3A	3.95	117.96	107.27
2	C	705	GTF	O2-C2-N3	-3.85	116.25	122.33
4	A	703	DTP	C5-C4-N3	-3.84	121.43	126.72
2	C	705	GTF	O1A-PA-O3A	3.82	117.61	107.27
4	D	701	DTP	N3-C4-N9	3.82	133.66	127.17
2	C	705	GTF	O5'-PA-O2A	3.82	124.06	108.94
3	B	703	GTP	O2B-PB-O3B	3.80	117.56	107.27
2	C	705	GTF	O2B-PB-O3B	3.78	117.50	107.27
3	A	702	GTP	O2G-PG-O3B	3.76	117.24	104.64
3	D	703	GTP	C2-N3-C4	3.75	118.76	112.30
2	A	701	GTF	O4'-C4'-C3'	-3.67	99.66	104.46
3	A	702	GTP	C2-N3-C4	3.66	118.60	112.30
4	C	702	DTP	N6-C6-N1	3.64	126.49	118.38
4	A	703	DTP	N3-C4-N9	3.61	133.31	127.17
3	B	703	GTP	N9-C4-N3	3.61	133.16	125.95
2	D	702	GTF	O3A-PB-O1B	-3.57	99.95	110.70
4	C	702	DTP	O2A-PA-O3A	3.54	116.85	107.27
4	C	702	DTP	O3A-PA-O1A	-3.54	100.05	110.70
2	C	705	GTF	C5-C4-N3	3.51	127.23	121.32
2	D	702	GTF	O1G-PG-O3G	3.48	124.40	110.83
4	B	704	DTP	N3-C4-N9	3.39	132.94	127.17
2	D	702	GTF	O2G-PG-O3B	-3.35	93.41	104.64
4	D	701	DTP	C4-C5-N7	-3.33	106.77	110.58
4	D	701	DTP	C4-N9-C8	3.32	109.22	105.74
2	B	701	GTF	O5'-PA-O2A	3.31	122.06	108.94
3	B	702	GTP	N9-C4-N3	3.28	132.51	125.95
4	B	704	DTP	N9-C8-N7	-3.28	109.29	113.94
2	B	701	GTF	F2-C2'-F1	3.21	109.40	105.55
3	B	703	GTP	C8-N9-C4	3.19	112.00	106.03
2	C	705	GTF	O3B-PB-O1B	3.17	120.24	110.70
4	D	701	DTP	C2'-C1'-N9	3.17	122.07	114.63
3	D	703	GTP	O2B-PB-O3B	3.15	115.78	107.27
2	D	702	GTF	O2-C2-N3	-3.15	117.37	122.33
3	A	702	GTP	O6-C6-N1	3.13	126.00	120.11
2	A	701	GTF	O1G-PG-O3G	-3.11	98.71	110.83
4	A	703	DTP	O3G-PG-O1G	3.09	122.89	110.83
2	B	701	GTF	O1A-PA-O3A	-3.09	98.92	107.27
2	A	701	GTF	O3A-PA-O2A	-3.05	101.53	110.70
3	B	703	GTP	C5-C4-N3	-3.03	123.57	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	702	DTP	C5-C6-N6	-3.02	115.80	123.29
2	A	701	GTF	O1G-PG-O3B	2.99	114.65	104.64
2	C	705	GTF	F2-C2'-C3'	-2.94	103.68	111.45
4	D	701	DTP	O3A-PA-O1A	2.92	119.49	110.70
4	B	704	DTP	O3A-PB-O1B	-2.91	101.95	110.70
3	A	702	GTP	O6-C6-C5	-2.90	118.87	126.53
2	B	701	GTF	O2G-PG-O1G	2.90	118.67	107.80
4	A	703	DTP	O2A-PA-O1A	2.88	125.83	112.44
2	D	702	GTF	F2-C2'-C3'	-2.87	103.85	111.45
3	A	702	GTP	O2A-PA-O1A	2.86	125.75	112.44
3	D	703	GTP	C8-N9-C4	2.86	111.39	106.03
4	B	704	DTP	C2-N1-C6	2.86	123.43	118.73
4	B	704	DTP	N6-C6-N1	2.83	124.69	118.38
4	D	701	DTP	O4'-C1'-N9	-2.83	102.89	107.96
2	A	701	GTF	O1A-PA-O2A	-2.82	99.33	112.44
4	A	703	DTP	O3A-PB-O1B	-2.80	102.28	110.70
4	A	703	DTP	O3B-PB-O1B	2.78	119.06	110.70
4	C	702	DTP	C2'-C3'-C4'	2.78	108.44	102.80
3	A	702	GTP	O3G-PG-O2G	2.75	118.12	107.80
2	A	701	GTF	O2G-PG-O1G	2.75	118.10	107.80
3	B	702	GTP	C5-C4-N3	-2.74	124.02	128.39
2	A	701	GTF	O1A-PA-O3A	2.72	114.64	107.27
4	C	702	DTP	C2'-C1'-N9	2.71	120.98	114.63
3	A	702	GTP	N9-C4-N3	2.67	131.30	125.95
4	A	703	DTP	C4-C5-N7	-2.67	107.53	110.58
4	D	701	DTP	O2A-PA-O3A	-2.67	100.06	107.27
4	A	703	DTP	C5-N7-C8	2.67	107.64	103.45
4	C	702	DTP	O2G-PG-O1G	2.64	121.13	110.83
3	B	703	GTP	O6-C6-N1	2.62	125.03	120.11
3	B	703	GTP	C2-N3-C4	2.61	116.80	112.30
4	B	704	DTP	N3-C2-N1	-2.61	124.63	128.58
2	D	702	GTF	C5-C4-N3	2.60	125.71	121.32
2	C	705	GTF	O3'-C3'-C4'	2.57	118.48	112.79
3	B	703	GTP	C4'-O4'-C1'	-2.56	103.81	109.47
4	A	703	DTP	O4'-C1'-N9	-2.56	103.36	107.96
3	D	703	GTP	O2'-C2'-C1'	-2.56	101.31	110.10
2	D	702	GTF	C4-N3-C2	-2.52	116.29	120.26
4	D	701	DTP	O3G-PG-O1G	2.52	120.66	110.83
2	B	701	GTF	O2-C2-N3	-2.51	118.37	122.33
3	D	703	GTP	O3G-PG-O2G	2.49	117.15	107.80
3	B	703	GTP	O3G-PG-O2G	2.47	117.08	107.80
2	A	701	GTF	O2-C2-N1	2.47	123.74	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	703	GTP	O6-C6-C5	-2.46	120.04	126.53
3	B	702	GTP	O3G-PG-O2G	2.43	116.91	107.80
3	D	703	GTP	O2A-PA-O3A	2.43	113.83	107.27
4	C	702	DTP	N9-C8-N7	-2.42	110.50	113.94
2	B	701	GTF	N1-C2-N3	-2.40	114.63	118.80
4	B	704	DTP	C5-C4-N9	-2.40	103.19	105.81
3	A	702	GTP	O5'-C5'-C4'	2.39	117.14	108.99
3	D	703	GTP	O2A-PA-O5'	-2.39	96.73	107.57
3	B	703	GTP	O3B-PG-O1G	-2.39	98.47	111.04
4	A	703	DTP	O2A-PA-O3A	-2.39	100.82	107.27
4	B	704	DTP	O3G-PG-O2G	2.38	116.73	107.80
3	B	703	GTP	O3A-PB-O1B	-2.37	103.57	110.70
2	B	701	GTF	C5-C4-N4	2.35	124.74	120.63
2	C	705	GTF	C4-N3-C2	-2.33	116.59	120.26
4	A	703	DTP	N6-C6-N1	2.32	123.54	118.38
3	D	703	GTP	C3'-C2'-C1'	2.30	105.82	101.46
2	D	702	GTF	N4-C4-N3	-2.29	113.81	117.91
3	D	703	GTP	N9-C8-N7	-2.29	109.16	113.40
2	D	702	GTF	O3A-PA-O2A	-2.28	103.85	110.70
2	C	705	GTF	N4-C4-N3	-2.27	113.85	117.91
4	B	704	DTP	O3A-PA-O1A	-2.24	103.96	110.70
3	B	703	GTP	O2A-PA-O3A	2.24	113.33	107.27
3	A	702	GTP	O3'-C3'-C4'	-2.23	104.68	111.08
4	A	703	DTP	C4-N9-C8	2.23	108.08	105.74
3	A	702	GTP	O4'-C4'-C5'	-2.19	102.31	109.33
3	B	702	GTP	O2A-PA-O1A	2.17	122.55	112.44
4	B	704	DTP	C5-C6-N6	-2.17	117.91	123.29
2	A	701	GTF	N1-C2-N3	-2.17	115.04	118.80
2	A	701	GTF	C1'-N1-C6	2.16	123.40	121.26
2	A	701	GTF	F2-C2'-C3'	-2.14	105.79	111.45
2	C	705	GTF	O2-C2-N1	2.14	123.08	118.90
2	B	701	GTF	O1A-PA-O2A	-2.10	102.68	112.44
4	A	703	DTP	C2'-C1'-N9	2.10	119.55	114.63
4	D	701	DTP	O3'-C3'-C2'	-2.10	103.60	110.88
4	B	704	DTP	O2A-PA-O1A	2.09	122.19	112.44
4	A	703	DTP	O3G-PG-O3B	-2.08	97.67	104.64
3	B	703	GTP	O6-C6-C5	-2.08	121.05	126.53
4	B	704	DTP	C5-C4-N3	-2.07	123.87	126.72
3	D	703	GTP	C4-C5-N7	-2.06	107.40	110.67
2	B	701	GTF	O1G-PG-O3G	-2.06	102.82	110.83
4	A	703	DTP	C4-N9-C1'	-2.04	118.30	126.50
3	B	703	GTP	C1'-N9-C8	-2.04	120.94	126.73

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	GTF	C5'-O5'-PA-O1A
2	A	701	GTF	C5'-O5'-PA-O3A
2	B	701	GTF	C5'-O5'-PA-O2A
2	B	701	GTF	C5'-O5'-PA-O3A
2	C	705	GTF	PB-O3A-PA-O5'
2	C	705	GTF	C5'-O5'-PA-O1A
2	C	705	GTF	C5'-O5'-PA-O3A
2	D	702	GTF	PB-O3B-PG-O1G
3	B	702	GTP	PB-O3B-PG-O2G
4	B	704	DTP	PB-O3B-PG-O2G
4	B	704	DTP	PB-O3B-PG-O3G
4	D	701	DTP	PB-O3B-PG-O3G
2	D	702	GTF	C3'-C4'-C5'-O5'
2	D	702	GTF	O4'-C4'-C5'-O5'
2	C	705	GTF	C4'-C5'-O5'-PA
2	B	701	GTF	C3'-C4'-C5'-O5'
4	C	702	DTP	PB-O3A-PA-O1A
2	D	702	GTF	C4'-C5'-O5'-PA
4	A	703	DTP	PB-O3B-PG-O3G
2	A	701	GTF	O4'-C1'-N1-C2
3	A	702	GTP	C4'-C5'-O5'-PA
2	B	701	GTF	PB-O3A-PA-O2A
2	A	701	GTF	C4'-C5'-O5'-PA
3	B	702	GTP	C4'-C5'-O5'-PA
3	B	703	GTP	C4'-C5'-O5'-PA
3	B	703	GTP	C5'-O5'-PA-O3A
2	B	701	GTF	C4'-C5'-O5'-PA
2	D	702	GTF	PB-O3B-PG-O3G
3	B	702	GTP	PB-O3B-PG-O1G
3	B	702	GTP	PG-O3B-PB-O2B
3	B	703	GTP	PG-O3B-PB-O2B
3	B	703	GTP	PB-O3A-PA-O2A
4	C	702	DTP	PB-O3A-PA-O2A
3	A	702	GTP	PG-O3B-PB-O1B
3	B	702	GTP	PG-O3B-PB-O1B
3	B	703	GTP	PB-O3B-PG-O1G
4	B	704	DTP	PB-O3B-PG-O1G
3	D	703	GTP	C4'-C5'-O5'-PA
3	B	702	GTP	PB-O3A-PA-O1A
3	B	703	GTP	PG-O3B-PB-O1B

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

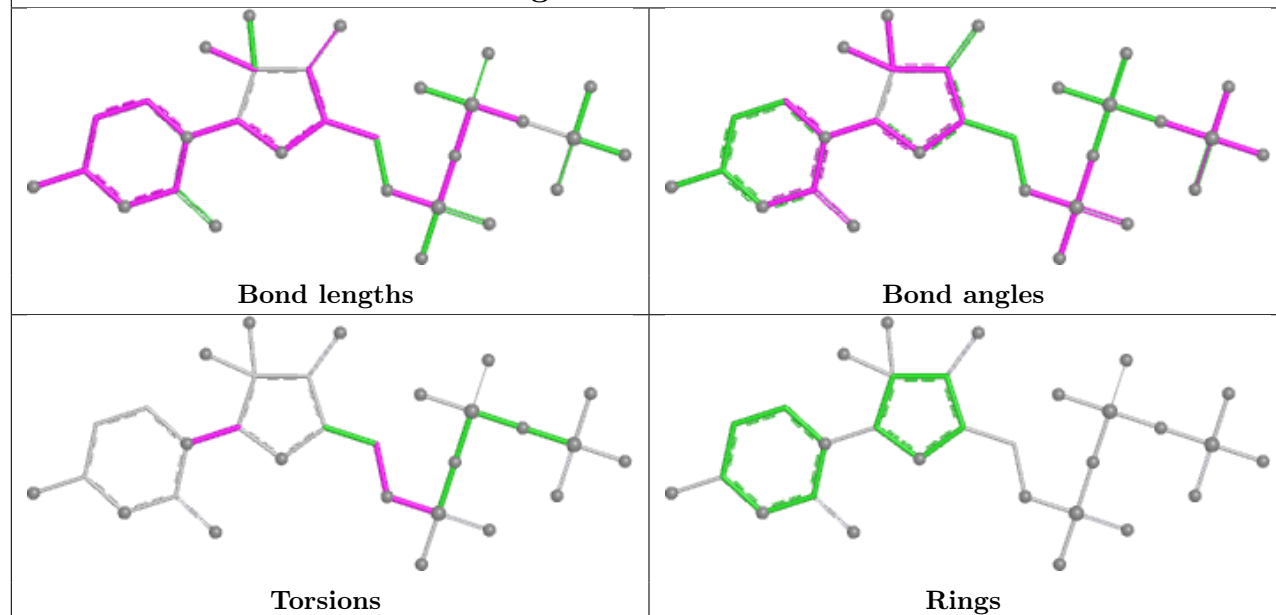
There are no ring outliers.

6 monomers are involved in 17 short contacts:

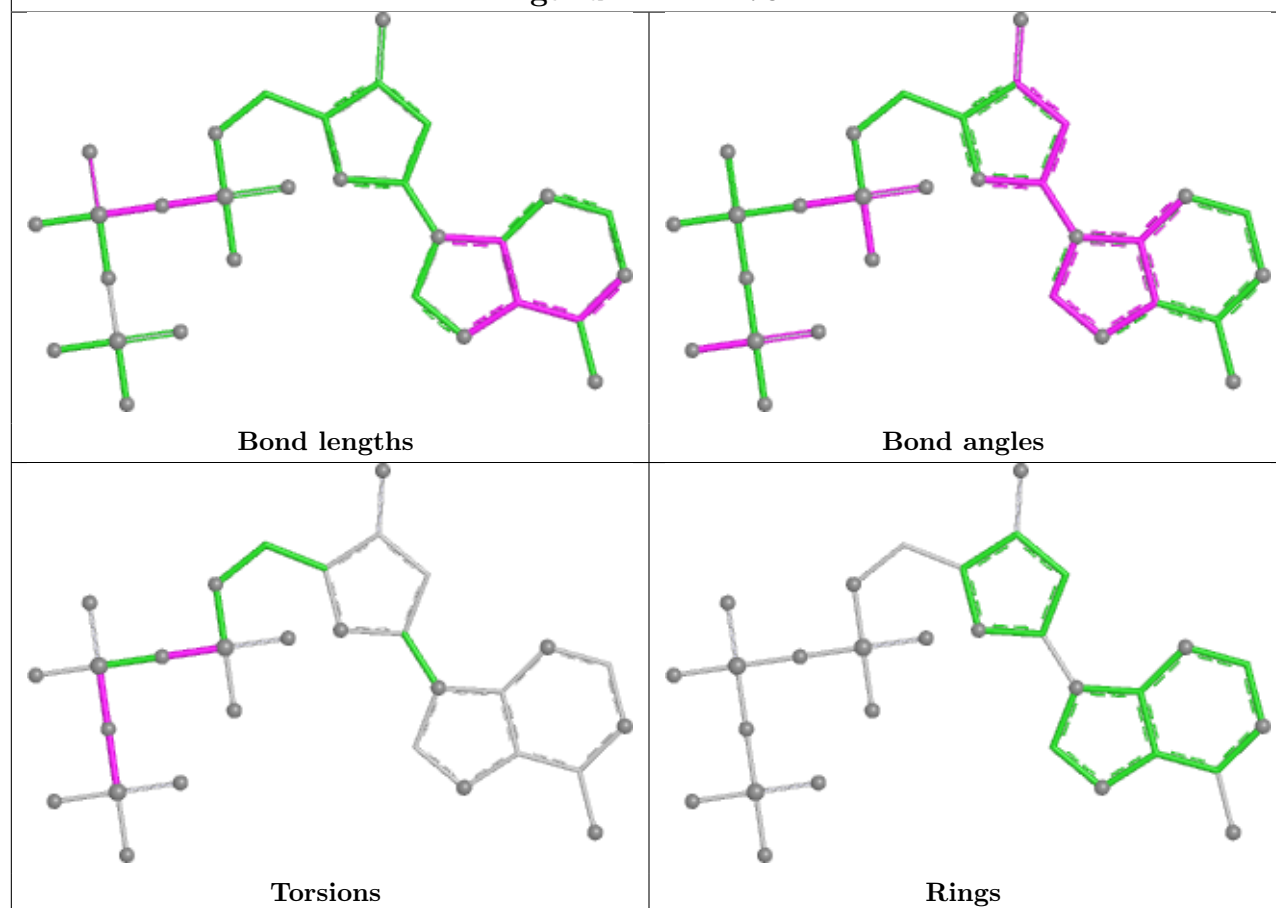
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	GTF	3	0
2	C	705	GTF	3	0
4	B	704	DTP	1	0
2	B	701	GTF	3	0
2	D	702	GTF	6	0
4	C	702	DTP	1	0

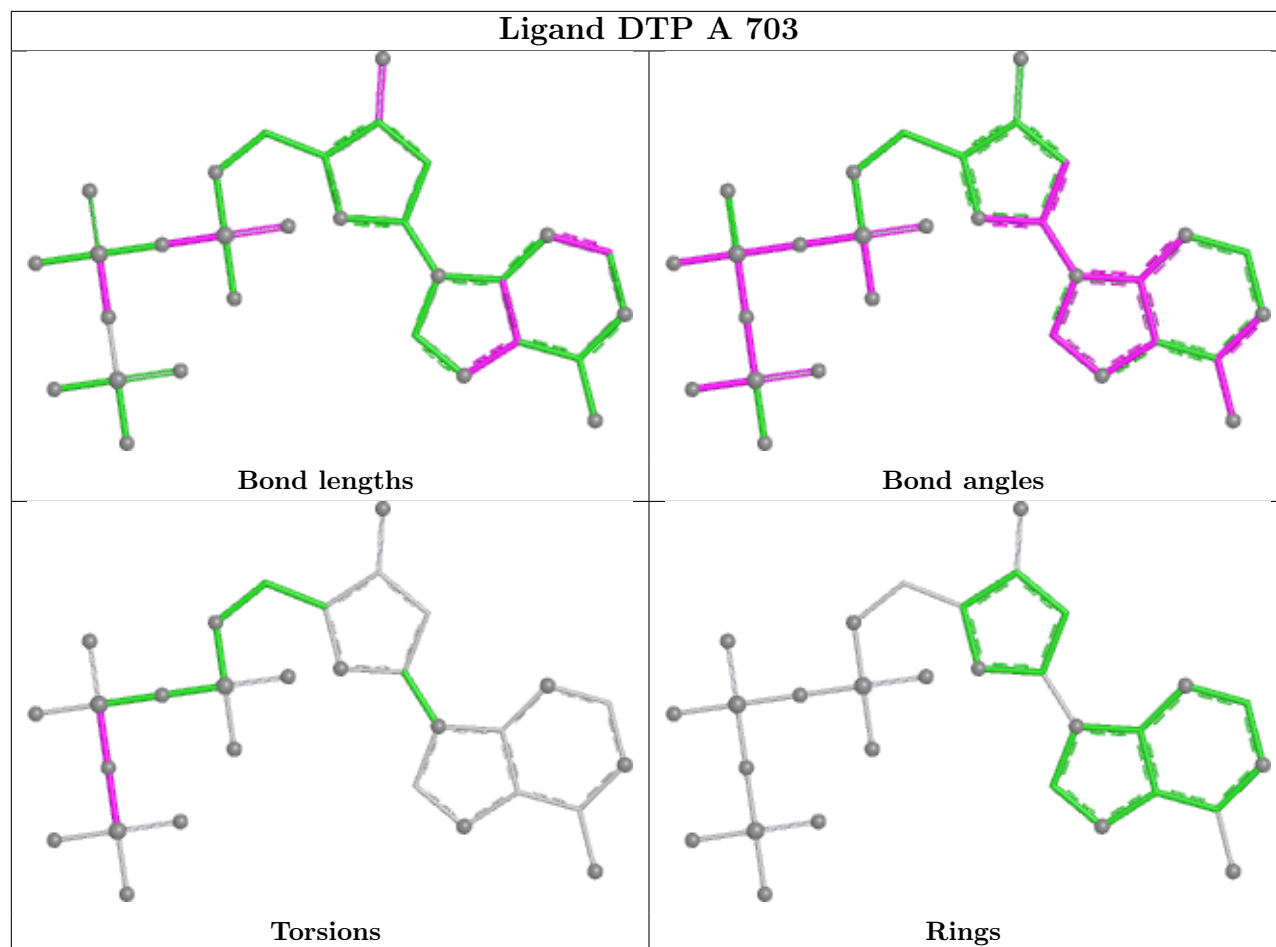
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 GTF A 701

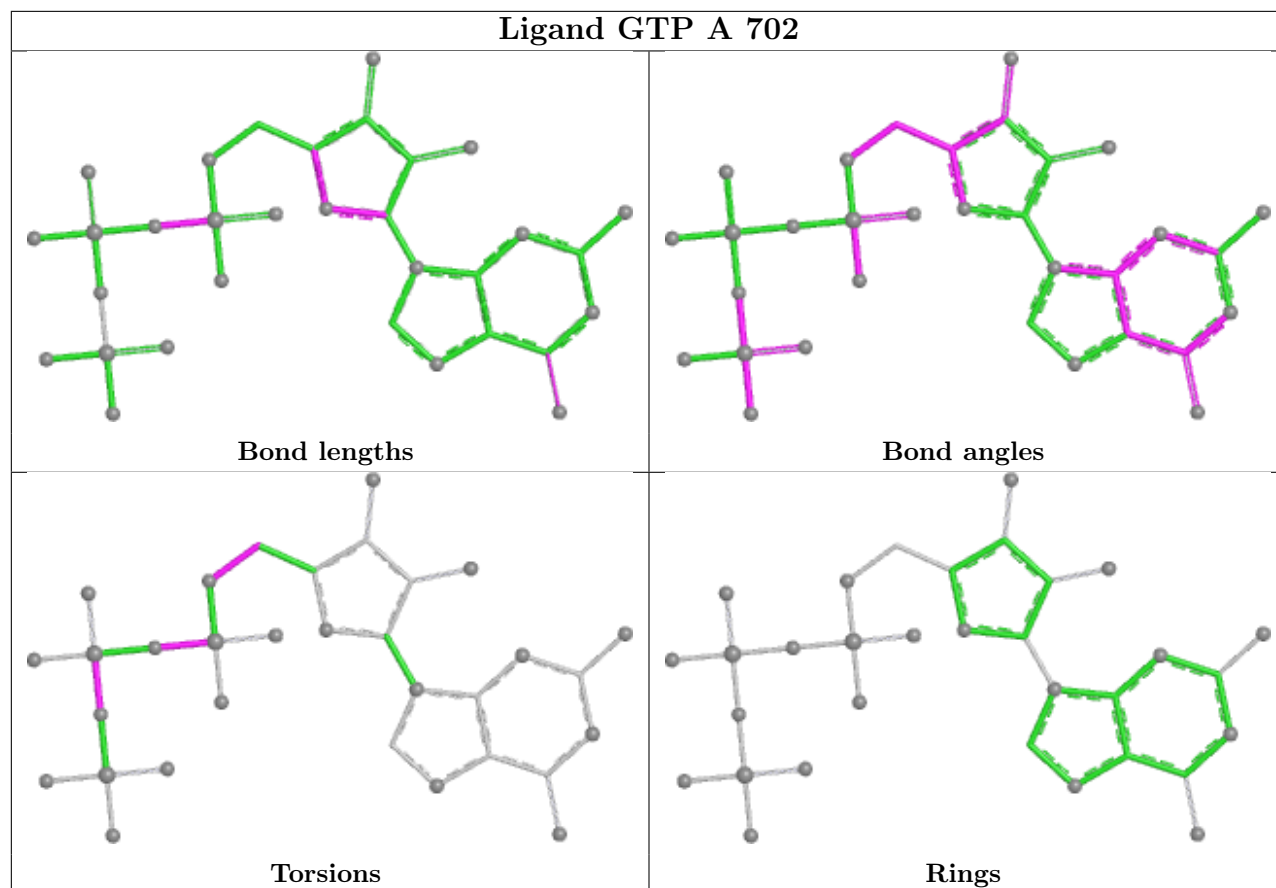


Ligand DTP D 701

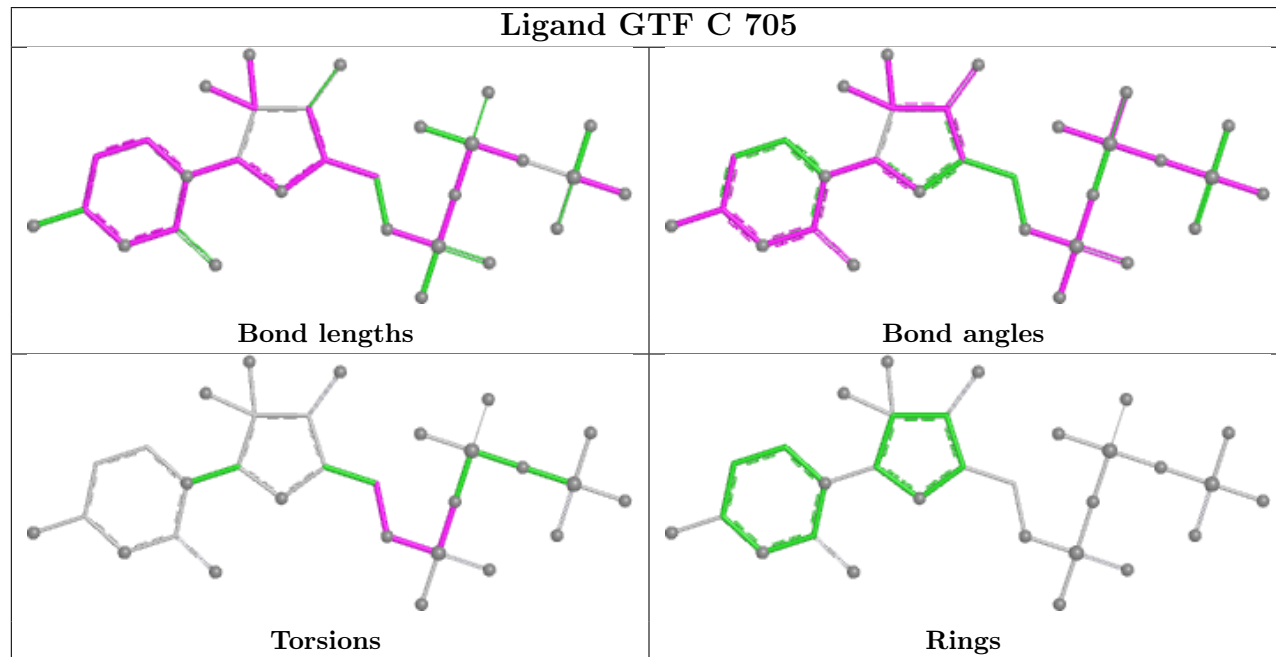




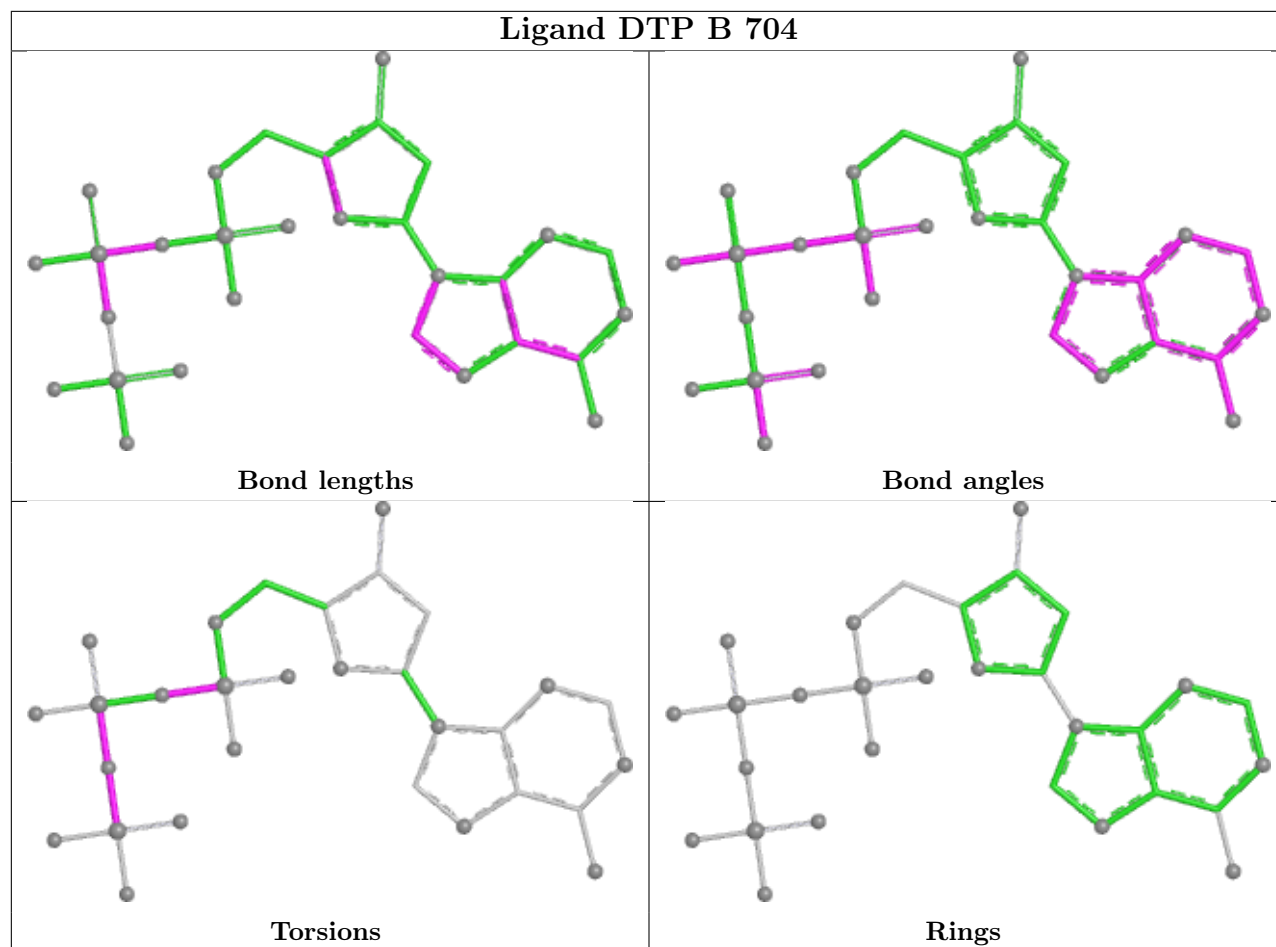
Ligand GTP A 702



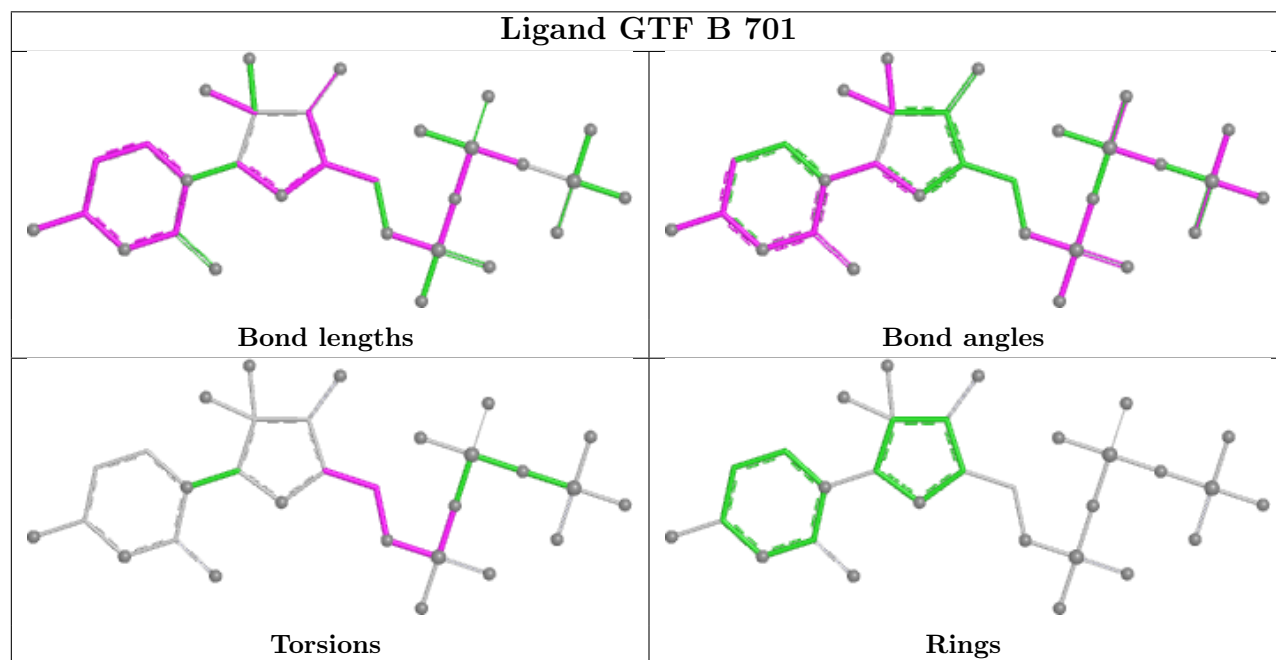
Ligand GTF C 705



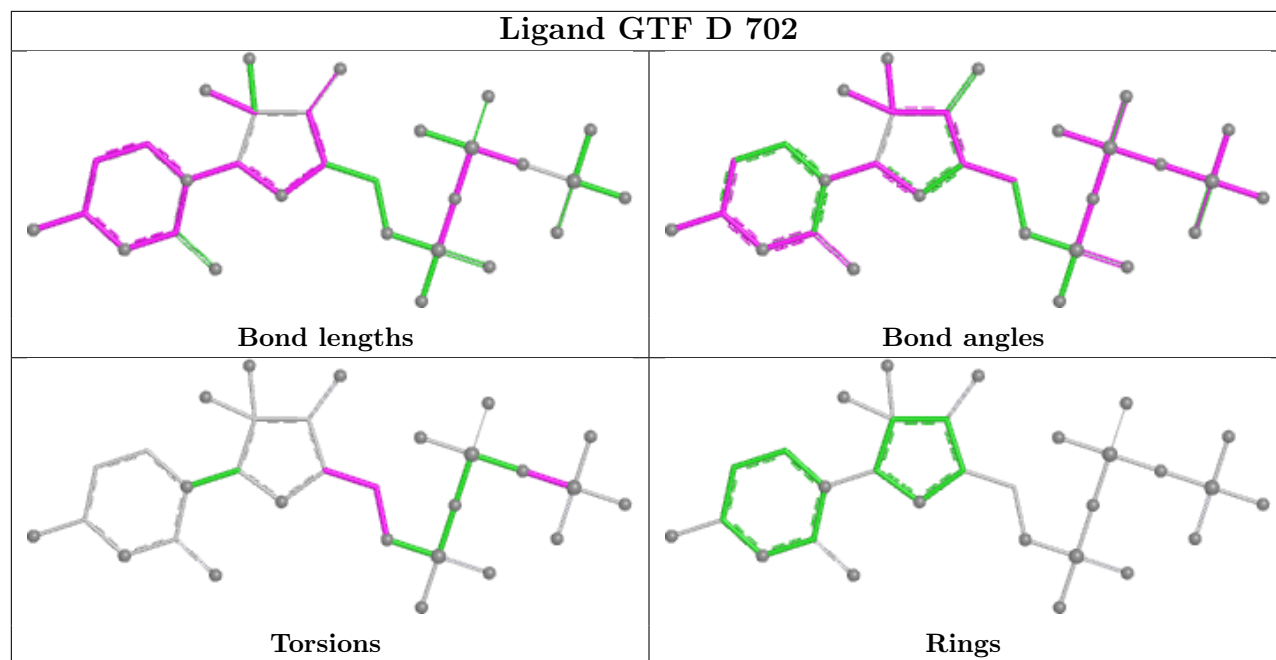
Ligand DTP B 704



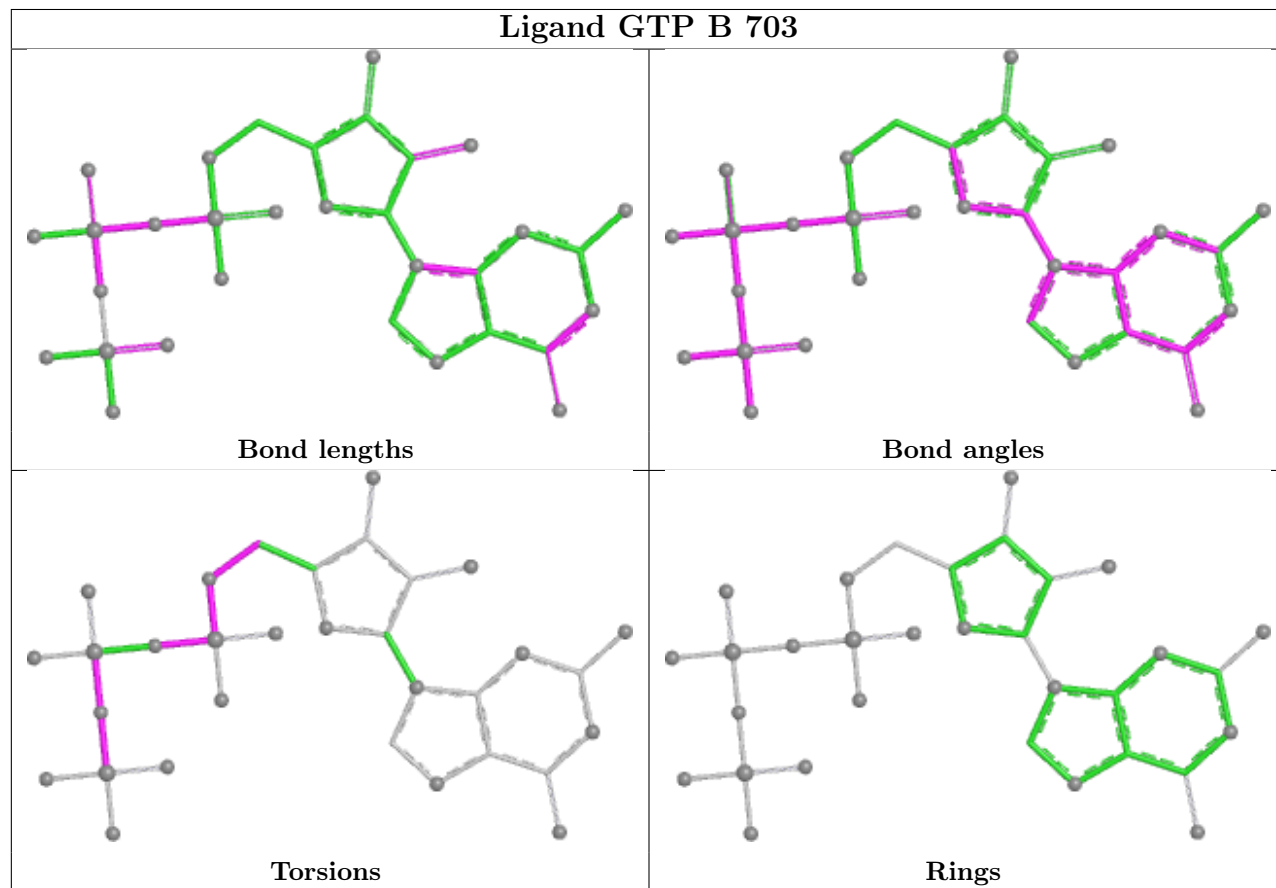
Ligand GTF B 701

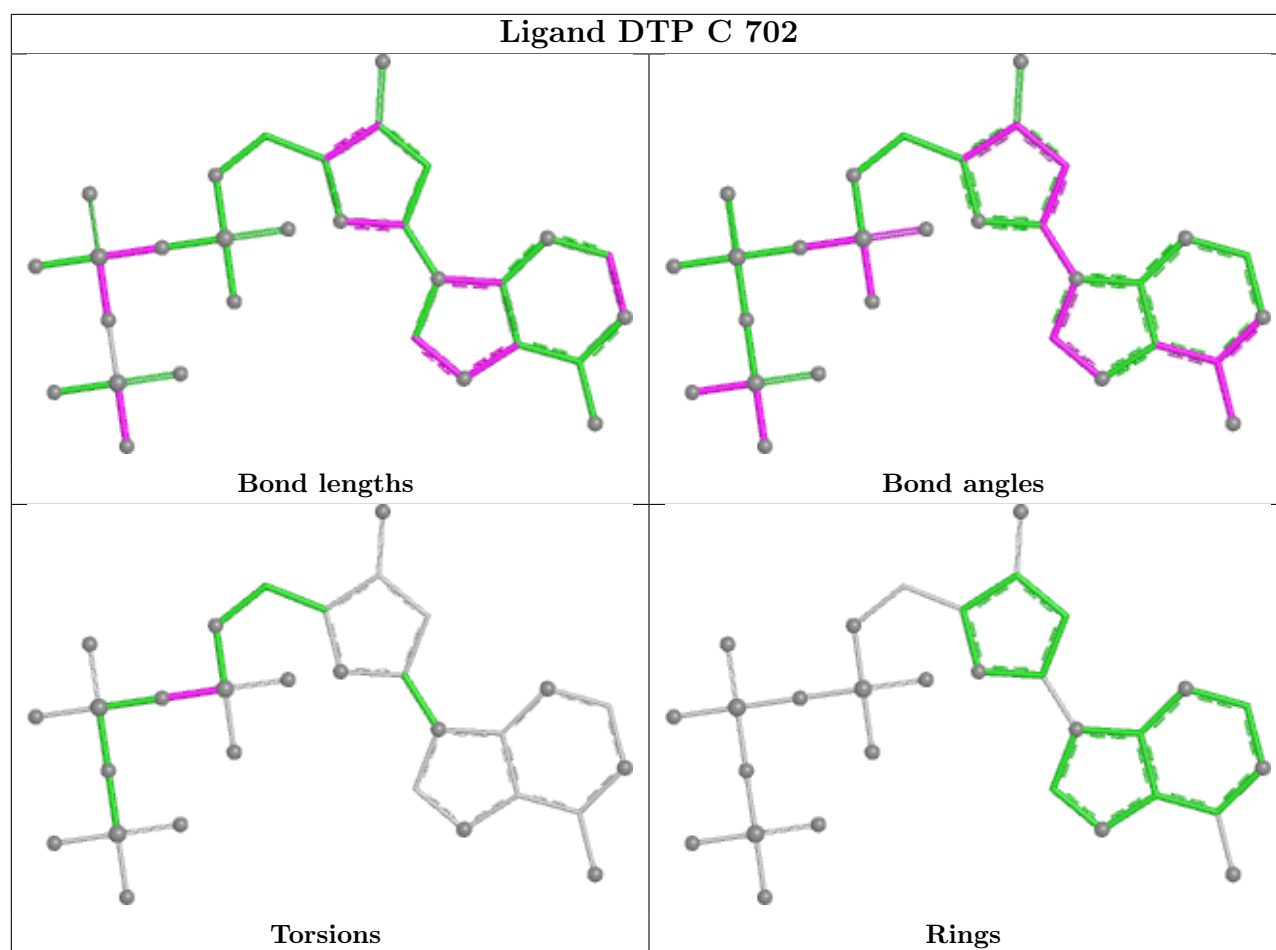


Ligand GTF D 702

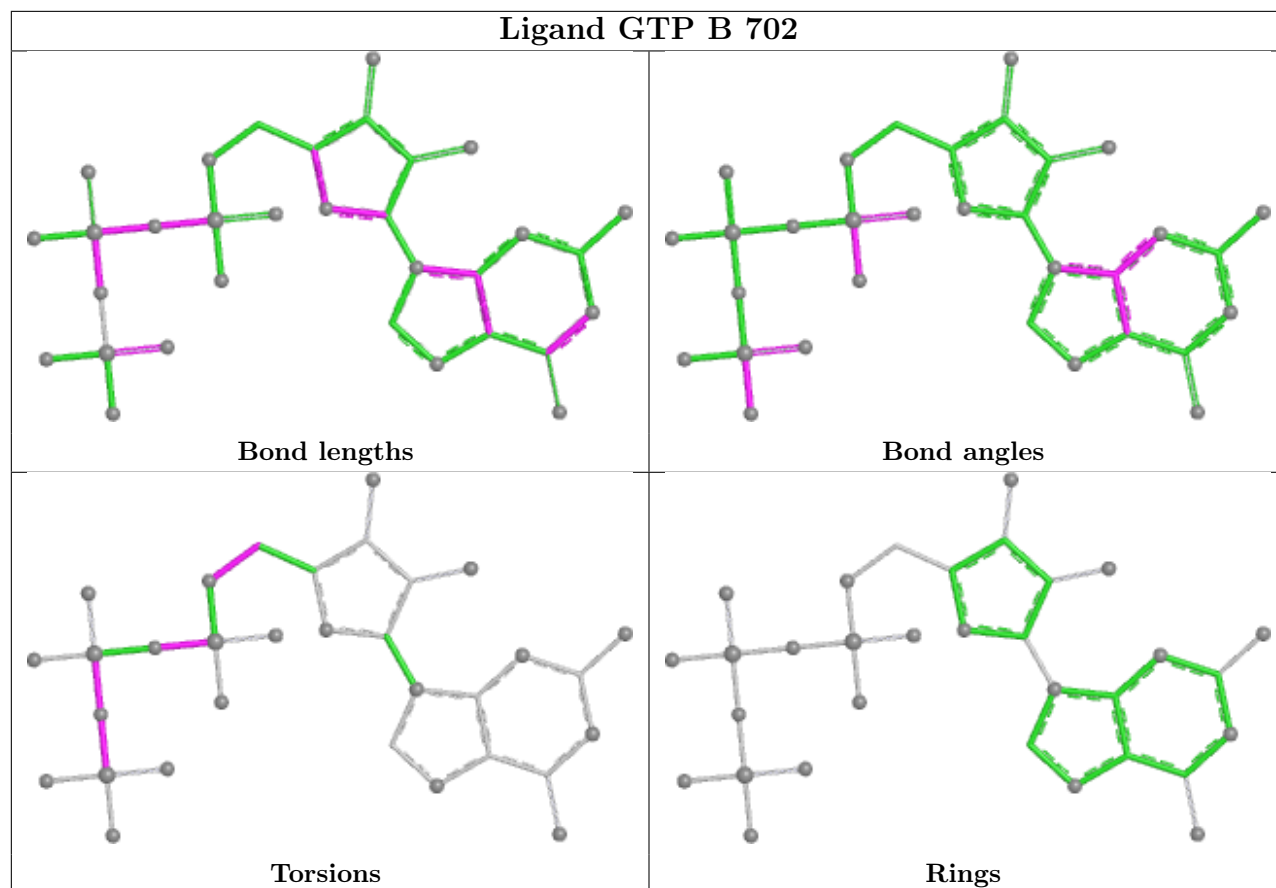


Ligand GTP B 703

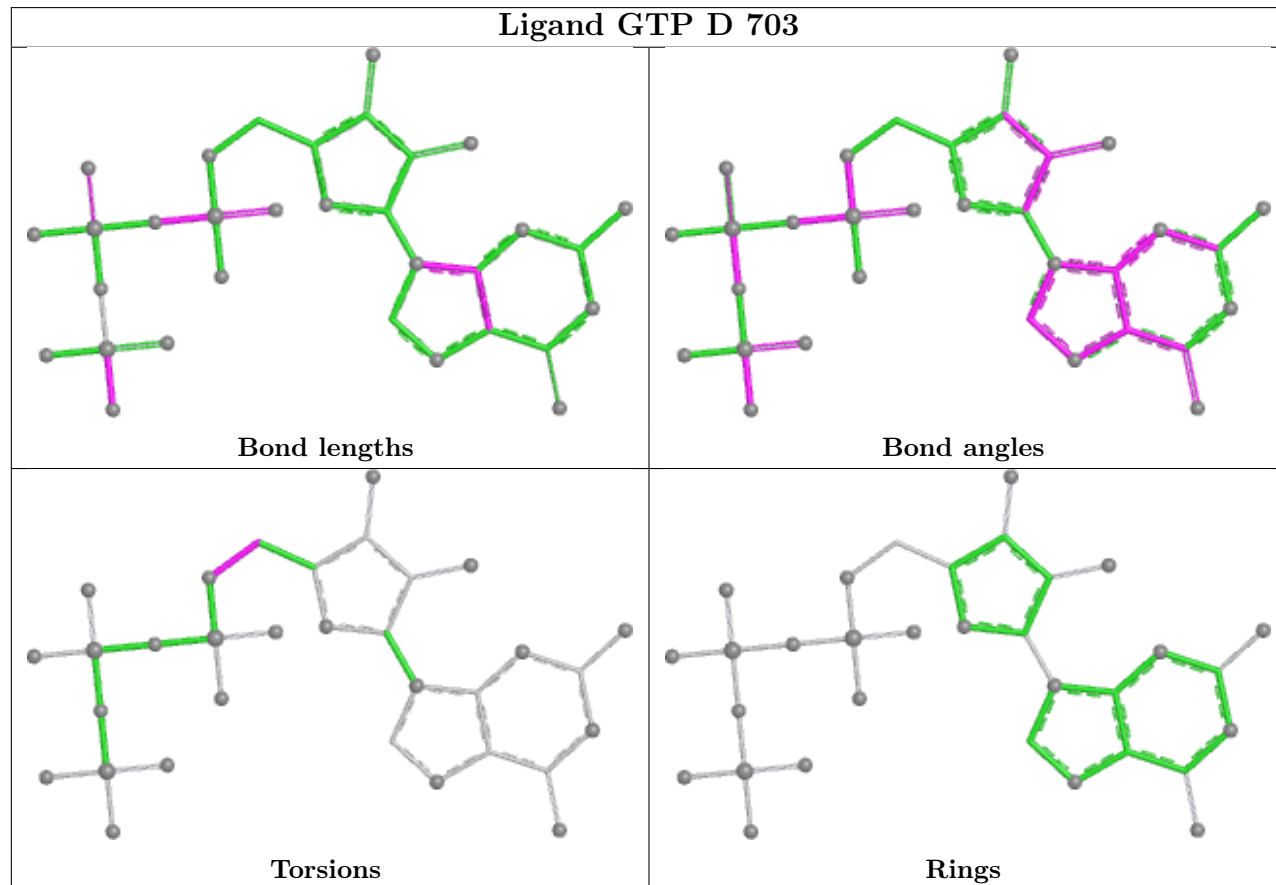




Ligand GTP B 702



Ligand GTP D 703



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	468/550 (85%)	0.07	21 (4%) 38 43	14, 32, 67, 102	0
1	B	480/550 (87%)	0.33	41 (8%) 16 18	18, 37, 84, 118	0
1	C	481/550 (87%)	0.08	14 (2%) 53 60	18, 35, 73, 105	0
1	D	481/550 (87%)	-0.07	7 (1%) 72 78	14, 31, 58, 108	1 (0%)
All	All	1910/2200 (86%)	0.10	83 (4%) 40 44	14, 33, 73, 118	1 (0%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	466	ILE	5.7
1	C	466	ILE	5.7
1	B	466	ILE	5.0
1	B	284	LEU	4.6
1	D	276	LEU	4.6
1	A	586	VAL	4.1
1	B	587	ILE	4.1
1	A	284	LEU	4.1
1	B	591	ILE	4.0
1	B	579	THR	3.9
1	A	584	GLY	3.8
1	B	574	ALA	3.8
1	B	598	TRP	3.8
1	A	276	LEU	3.7
1	B	586	VAL	3.7
1	B	570	VAL	3.6
1	B	276	LEU	3.6
1	B	114	THR	3.4
1	B	590	LEU	3.4
1	D	113	ASP	3.4
1	C	284	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	486	LYS	3.3
1	B	581	PRO	3.3
1	A	466	ILE	3.3
1	A	488	LEU	3.3
1	C	114	THR	3.3
1	B	597	GLU	3.2
1	D	464	GLY	3.1
1	B	487	VAL	3.1
1	A	114	THR	3.1
1	B	463	THR	3.1
1	C	488	LEU	3.0
1	B	488	LEU	3.0
1	D	284	LEU	2.9
1	C	487	VAL	2.8
1	B	584	GLY	2.8
1	A	470	ARG	2.8
1	B	489	LEU	2.8
1	C	276	LEU	2.7
1	C	485	PRO	2.7
1	A	583	ASP	2.7
1	D	465	GLN	2.7
1	A	487	VAL	2.7
1	A	585	ASP	2.6
1	B	589	PRO	2.6
1	B	580	LYS	2.6
1	B	599	ASN	2.6
1	B	573	CYS	2.6
1	A	262	GLU	2.6
1	B	593	PRO	2.5
1	C	489	LEU	2.5
1	B	596	LYS	2.5
1	C	492	LYS	2.5
1	B	485	PRO	2.5
1	C	467	LYS	2.5
1	B	582	GLN	2.5
1	B	594	GLN	2.4
1	A	115	MET	2.4
1	B	595	LYS	2.4
1	B	577	ASN	2.3
1	B	583	ASP	2.3
1	A	465	GLN	2.3
1	B	569	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	491	VAL	2.2
1	B	575	ASP	2.2
1	B	475	SER	2.2
1	B	588	ALA	2.2
1	C	468	ILE	2.2
1	A	463	THR	2.2
1	B	464	GLY	2.2
1	B	578	PHE	2.1
1	B	478	LYS	2.1
1	B	126	ILE	2.1
1	A	537	VAL	2.1
1	B	481	ALA	2.1
1	C	113	ASP	2.1
1	C	118	ILE	2.1
1	A	533	THR	2.1
1	A	464	GLY	2.1
1	A	492	LYS	2.0
1	B	537	VAL	2.0
1	C	470	ARG	2.0
1	D	305	ARG	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 oligosaccharides 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, 95th 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
7	NI	C	701	1/1	0.71	0.46	239,239,239,239	0
2	GTF	A	701	30/30	0.79	0.14	23,50,75,85	0
2	GTF	B	701	30/30	0.80	0.14	30,58,94,110	0

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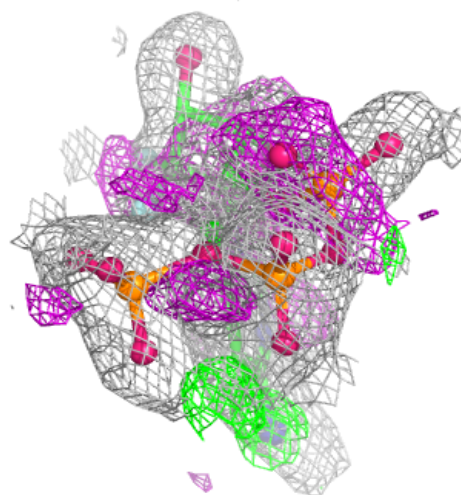
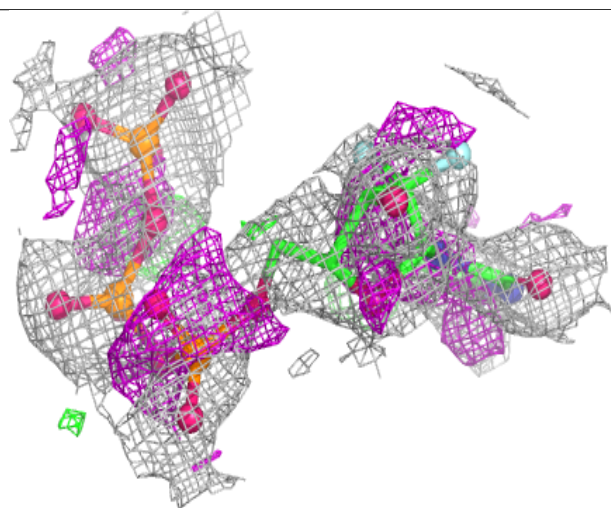
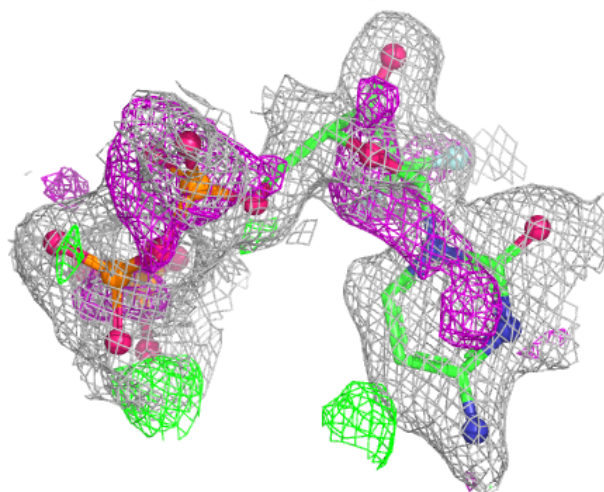
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GTF	C	705	30/30	0.81	0.13	32,51,67,81	0
2	GTF	D	702	30/30	0.86	0.12	25,45,67,70	0
5	MG	D	705	1/1	0.87	0.13	57,57,57,57	0
5	MG	D	704	1/1	0.87	0.14	57,57,57,57	0
6	NA	C	706	1/1	0.89	0.10	56,56,56,56	0
5	MG	A	708	1/1	0.90	0.28	53,53,53,53	0
6	NA	B	705	1/1	0.90	0.16	40,40,40,40	0
5	MG	A	707	1/1	0.91	0.26	62,62,62,62	0
6	NA	C	707	1/1	0.92	0.13	39,39,39,39	0
5	MG	B	706	1/1	0.92	0.09	66,66,66,66	0
5	MG	D	706	1/1	0.93	0.24	49,49,49,49	0
6	NA	A	706	1/1	0.95	0.09	37,37,37,37	0
3	GTP	B	702	32/32	0.99	0.03	18,21,29,29	0
3	GTP	B	703	32/32	0.99	0.04	21,23,30,30	0
5	MG	C	703	1/1	0.99	0.02	18,18,18,18	0
5	MG	C	704	1/1	0.99	0.02	22,22,22,22	0
3	GTP	D	703	32/32	0.99	0.03	15,18,26,27	0
4	DTP	A	703	30/30	0.99	0.04	18,21,25,26	0
4	DTP	B	704	30/30	0.99	0.03	15,19,22,24	0
4	DTP	C	702	30/30	0.99	0.03	13,16,19,19	0
4	DTP	D	701	30/30	0.99	0.04	17,21,24,25	0
5	MG	A	704	1/1	0.99	0.02	24,24,24,24	0
5	MG	A	705	1/1	0.99	0.02	20,20,20,20	0
3	GTP	A	702	32/32	0.99	0.04	14,16,21,21	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.

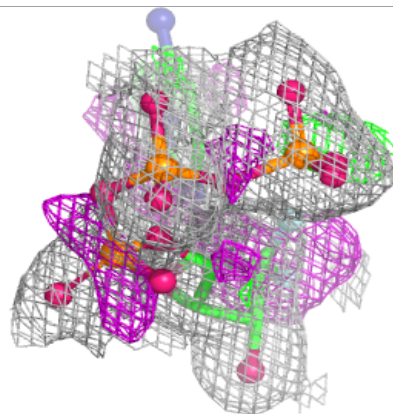
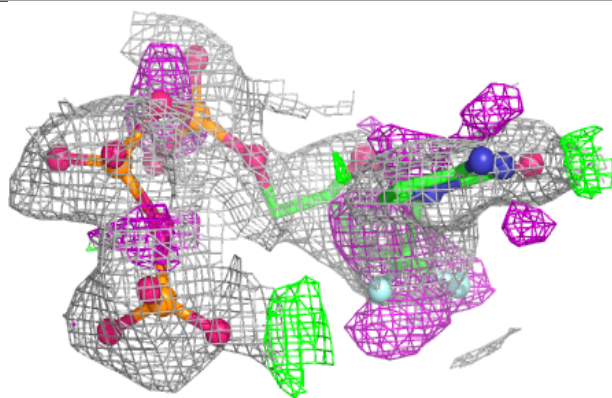
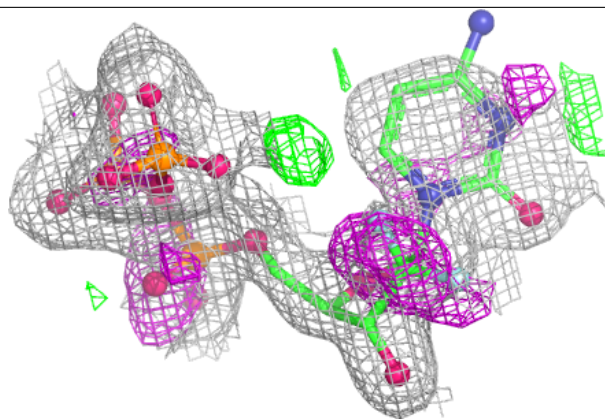
Electron density around GTF A 701:

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



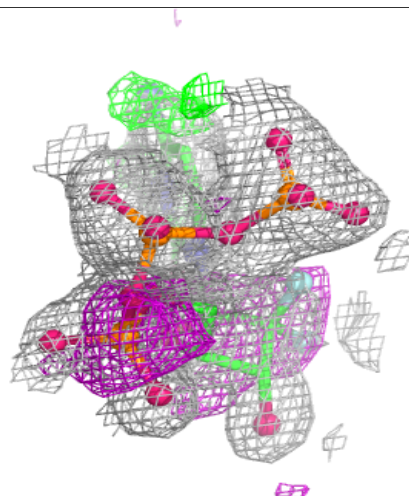
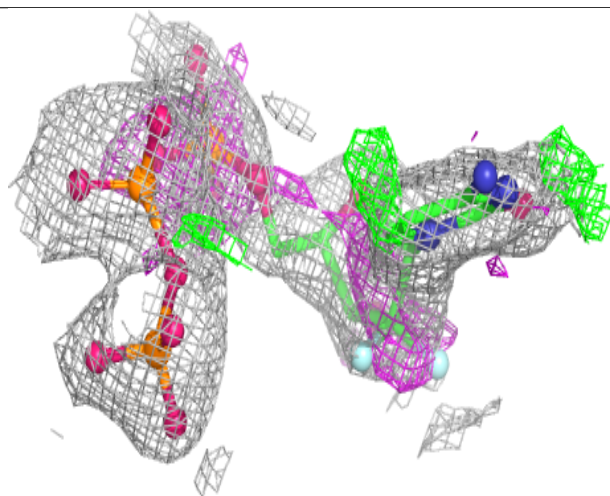
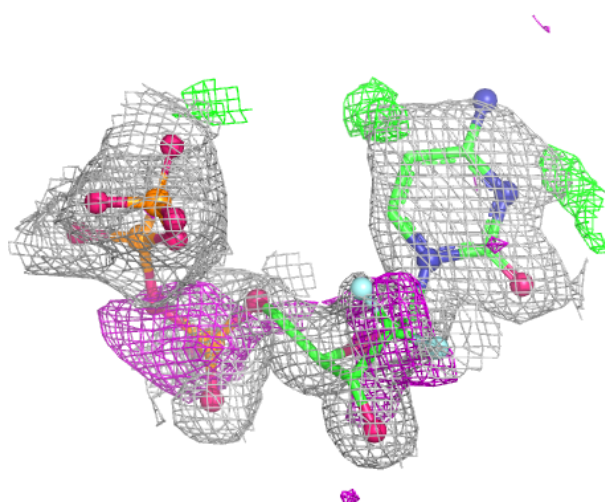
Electron density around GTF B 701:

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



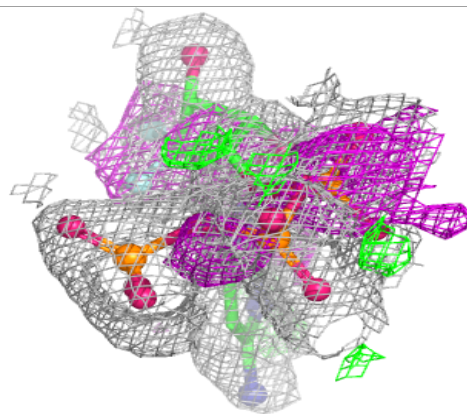
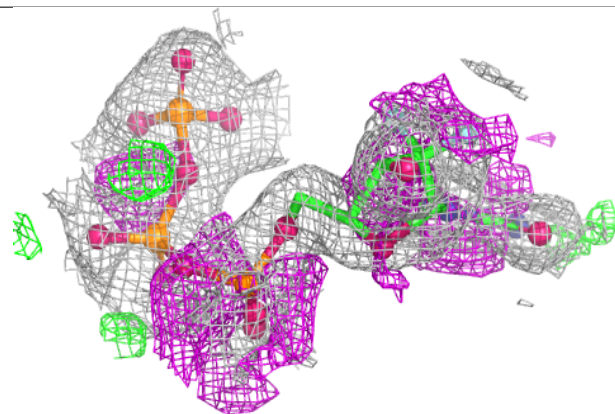
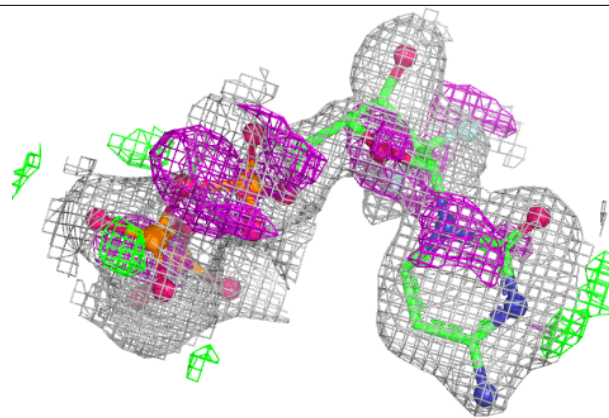
Electron density around GTF C 705:

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

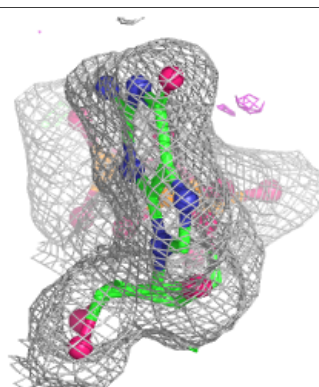
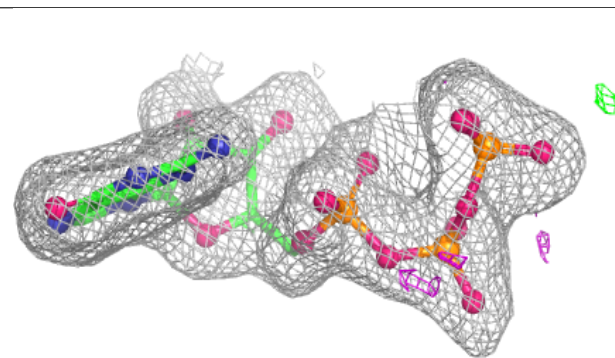
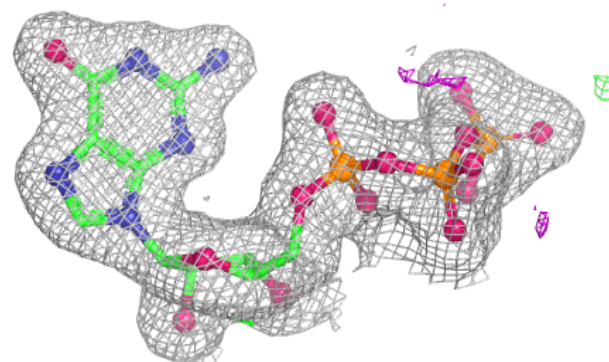


Electron density around GTF D 702:

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

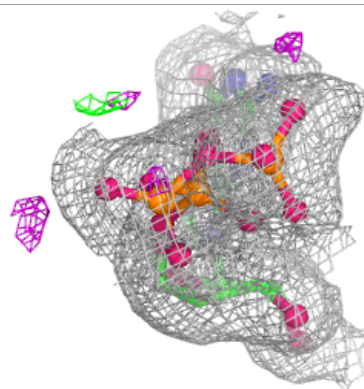
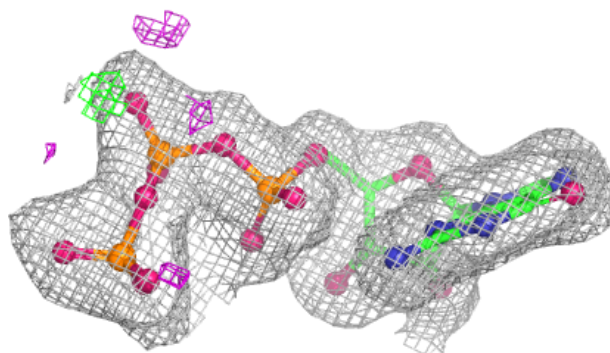
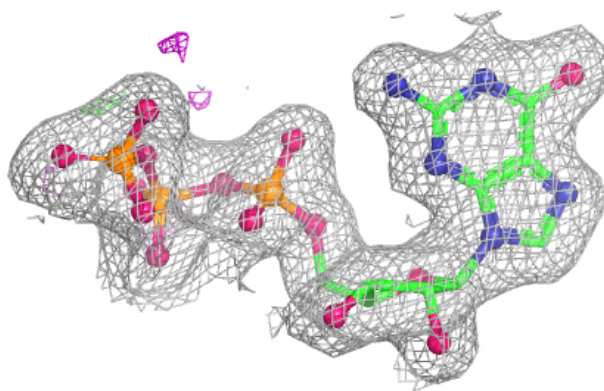
**Electron density around GTP B 702:**

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

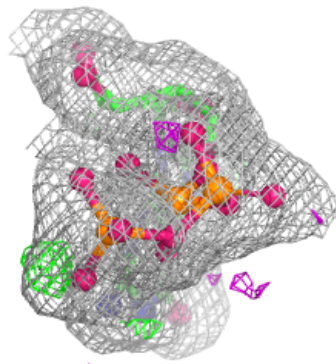
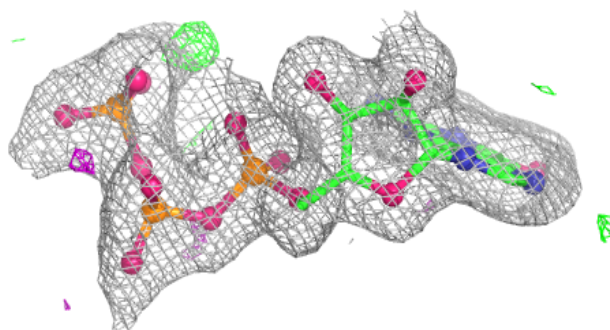
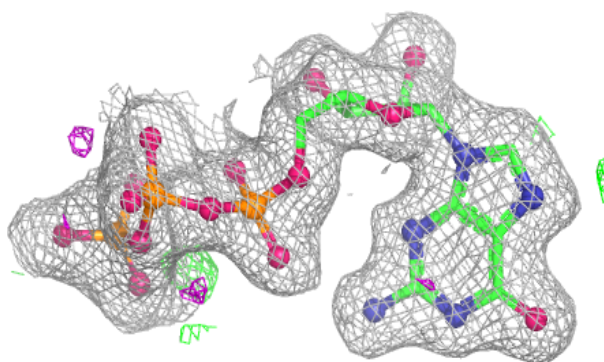


Electron density around GTP B 703:

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

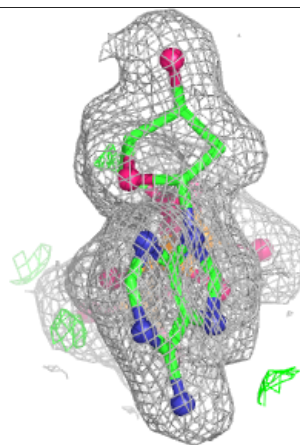
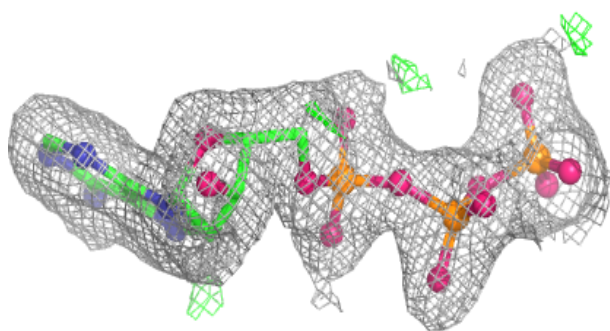
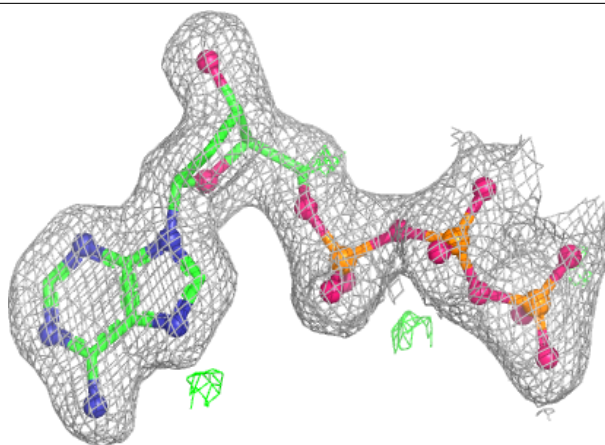
**Electron density around GTP D 703:**

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

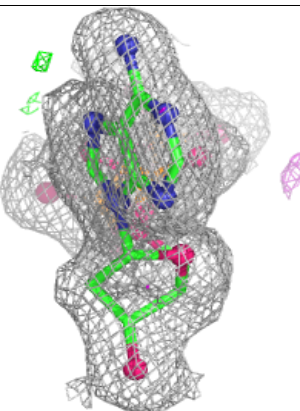
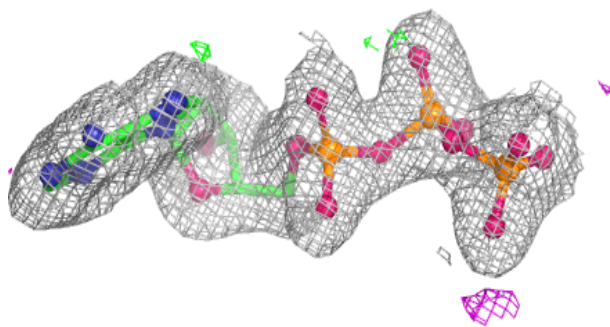
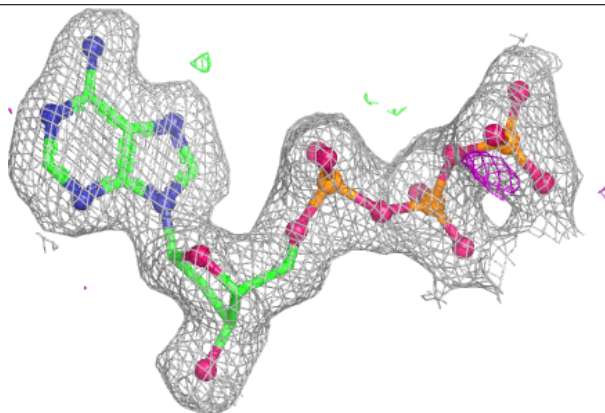


Electron density around DTP A 703:

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

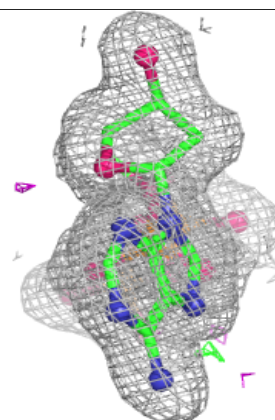
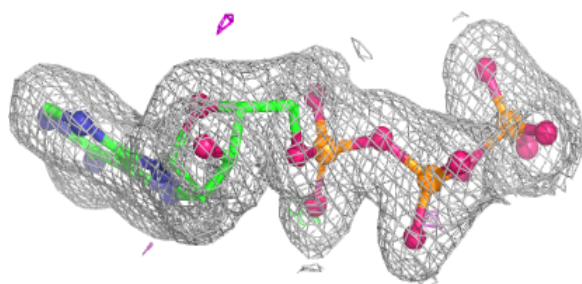
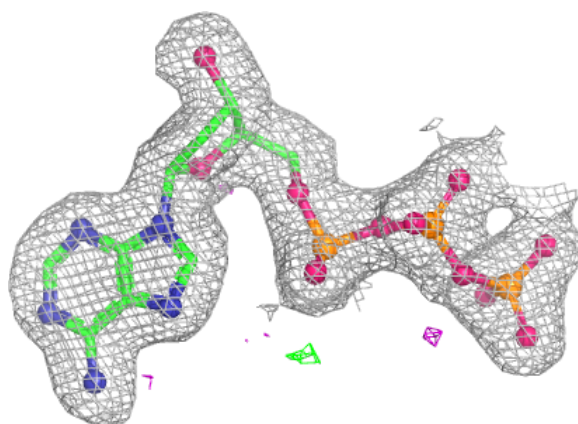
**Electron density around DTP B 704:**

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

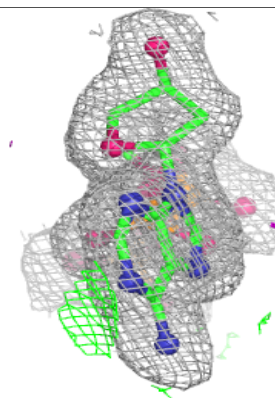
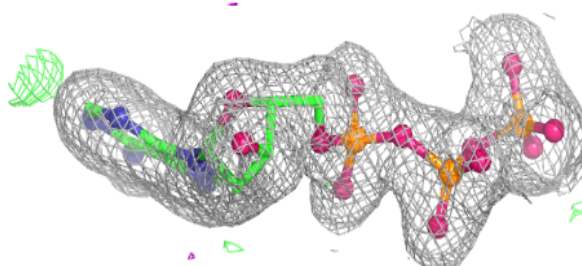
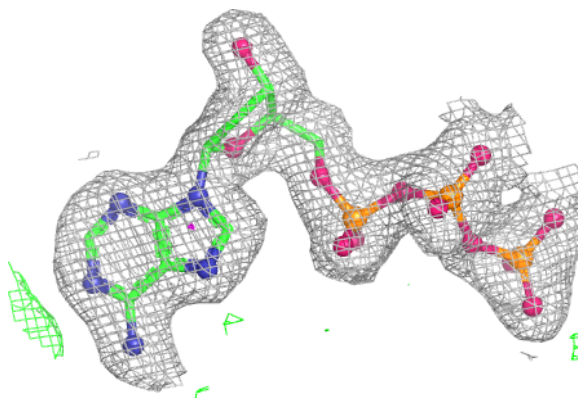


Electron density around DTP C 702:

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

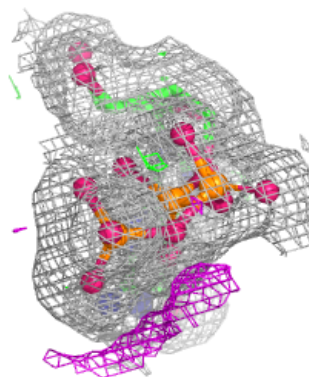
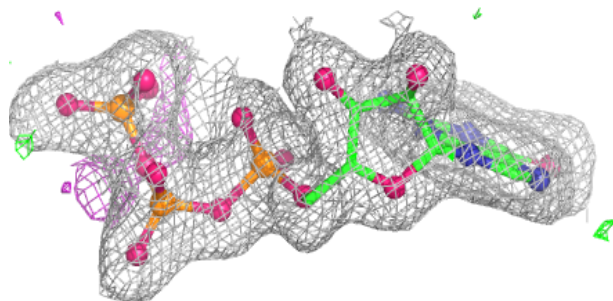
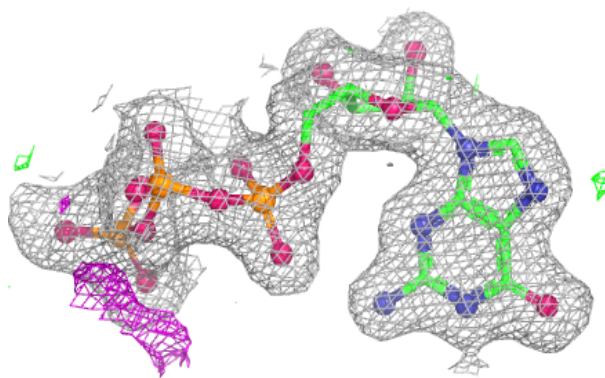
**Electron density around DTP D 701:**

$2mF_o-DF_c$ (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.