



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 02:32 pm BST

PDB ID : 6DW4
Title : SAMHD1 Bound to Cladribine-TP in the Catalytic Pocket and Allosteric 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 : 1.99 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 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 : 2.11
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) : 2.11

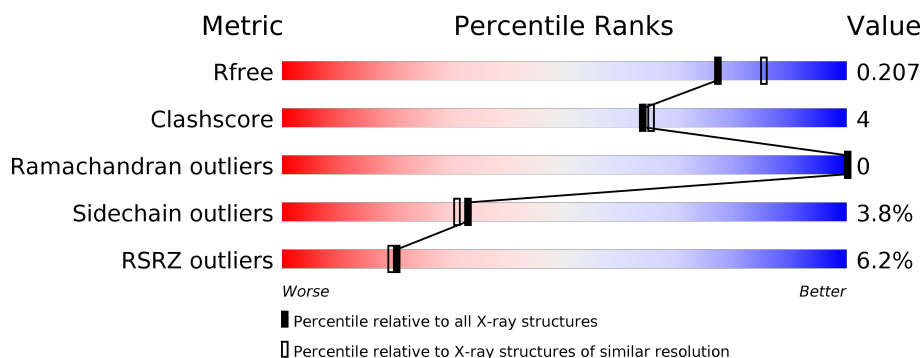
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	550	<div> <div>8%</div> <div> <div></div> <div>74%</div> <div>12%</div> <div>•</div> <div>13%</div> </div> </div>
1	B	550	<div> <div>6%</div> <div> <div></div> <div>75%</div> <div>11%</div> <div>•</div> <div>13%</div> </div> </div>
1	C	550	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>8%</div> <div>•</div> <div>13%</div> </div> </div>
1	D	550	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>11%</div> <div>•</div> <div>13%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17077 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	481	Total	C	N	O	S	0	5	0
			3970	2536	692	721	21			
1	C	481	Total	C	N	O	S	0	3	0
			3958	2531	690	716	21			
1	B	481	Total	C	N	O	S	0	2	0
			3948	2525	687	715	21			
1	A	481	Total	C	N	O	S	0	2	0
			3948	2525	687	715	21			

There are 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

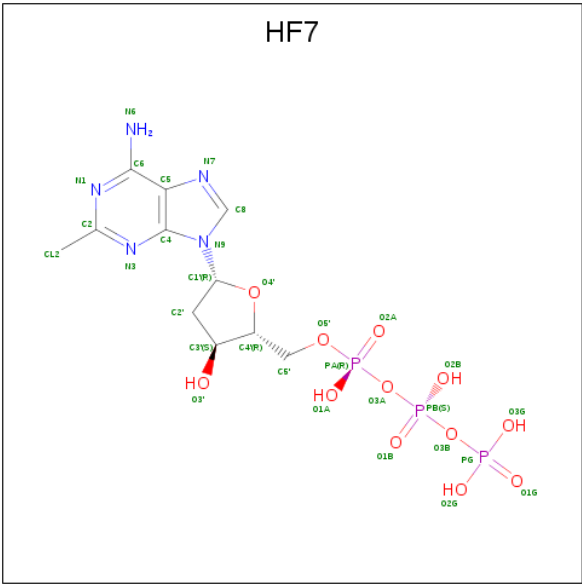
Chain	Residue	Modelled	Actual	Comment	Reference
B	106	MET	-	expression tag	UNP Q9Y3Z3
B	107	GLY	-	expression tag	UNP Q9Y3Z3
B	108	ARG	-	expression tag	UNP Q9Y3Z3
B	109	ASP	-	expression tag	UNP Q9Y3Z3
B	110	PRO	-	expression tag	UNP Q9Y3Z3
B	111	ASN	-	expression tag	UNP Q9Y3Z3
B	112	SER	-	expression tag	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

Continued on next page...

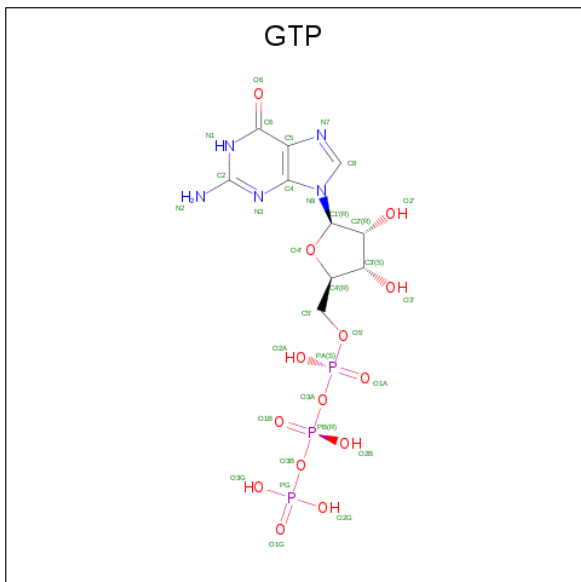
Continued from previous page...

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 2'-deoxy-2-methyladenosine 5'-(tetrahydrogen triphosphate) (three-letter code: HF7) (formula: C₁₁H₁₈N₅O₁₂P₃).



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



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

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

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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Na 1 1	0	0

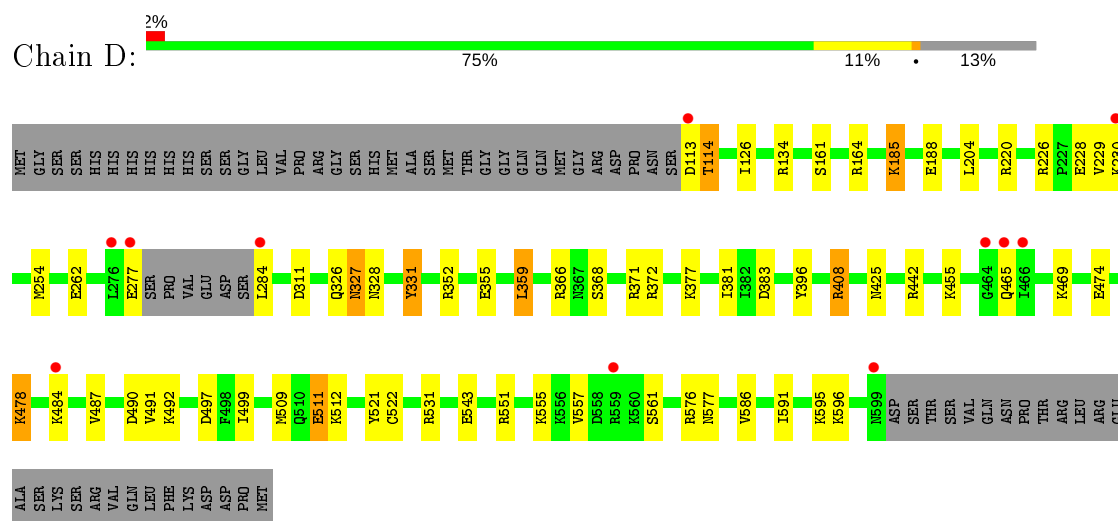
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	229	Total O 229 229	0	0
6	C	219	Total O 219 219	0	0
6	B	187	Total O 187 187	0	0
6	A	233	Total O 233 233	0	0

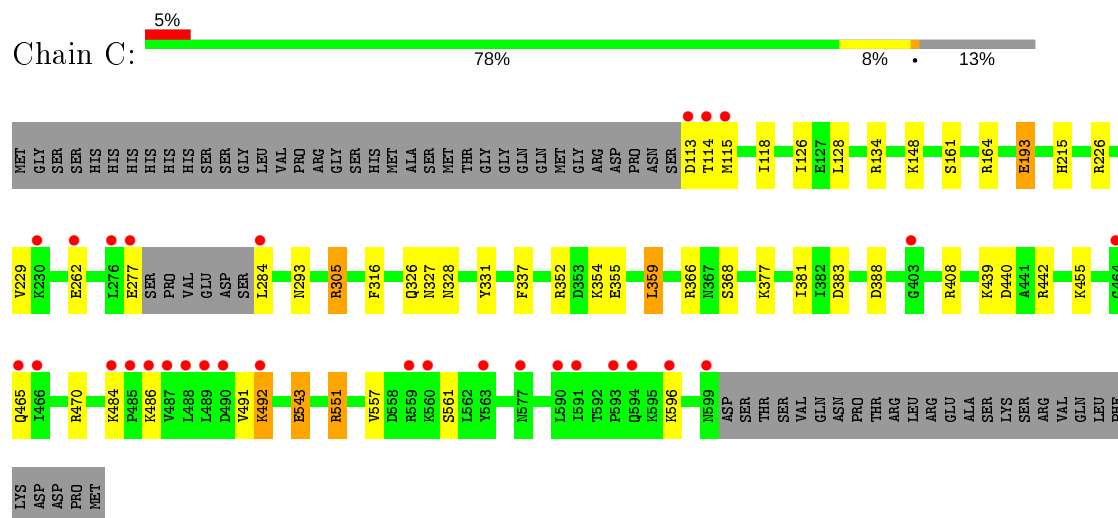
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

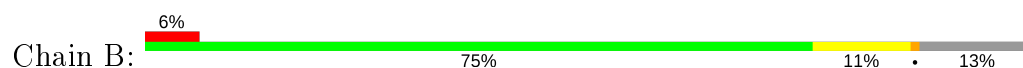
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

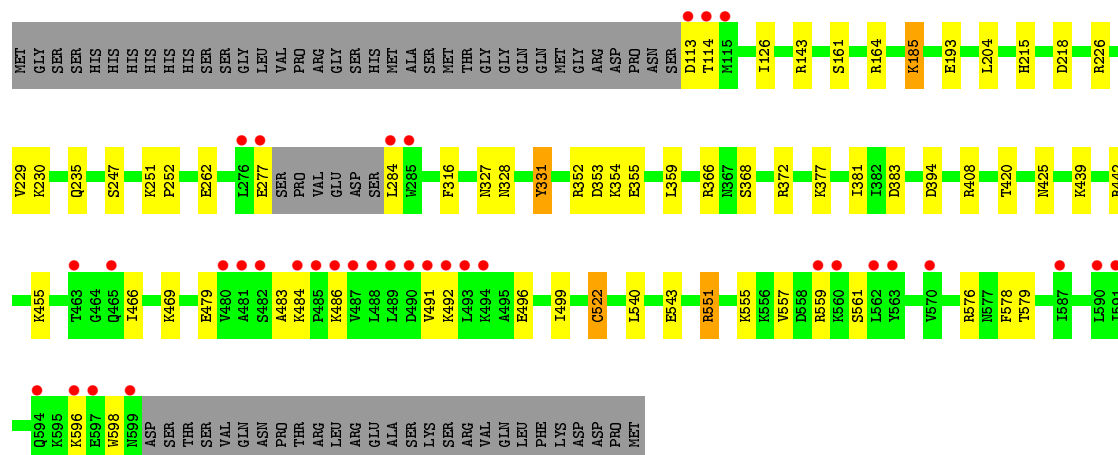


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

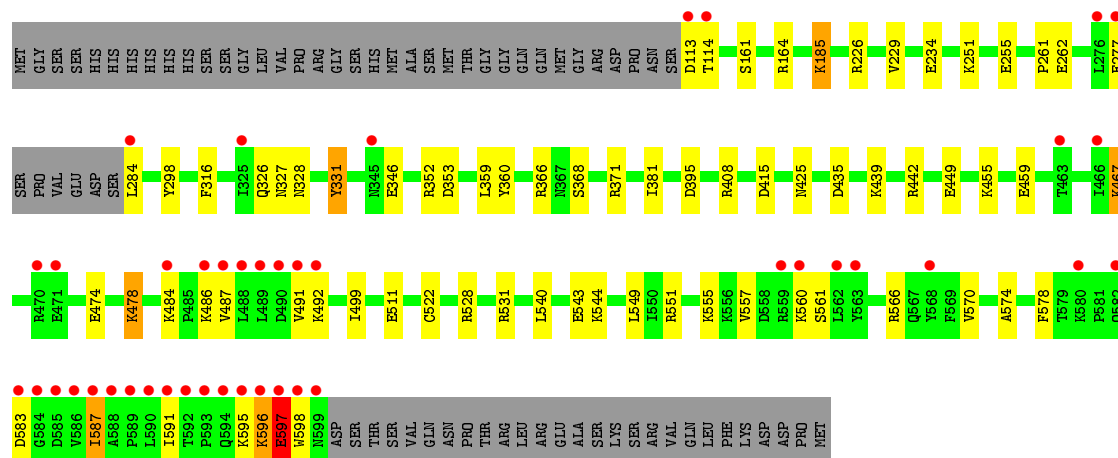


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.32Å 142.27Å 98.44Å 90.00° 114.08° 90.00°	Depositor
Resolution (Å)	89.87 – 1.99 45.50 – 1.99	Depositor EDS
% Data completeness (in resolution range)	95.0 (89.87-1.99) 95.0 (45.50-1.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.169 , 0.202 0.177 , 0.207	Depositor DCC
R_{free} test set	6512 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17077	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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: GTP, NA, MG, HF7

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	1.07	10/4040 (0.2%)	1.10	25/5453 (0.5%)
1	B	1.00	8/4040 (0.2%)	1.02	19/5453 (0.3%)
1	C	1.00	5/4051 (0.1%)	1.06	17/5468 (0.3%)
1	D	1.04	9/4062 (0.2%)	1.06	23/5483 (0.4%)
All	All	1.03	32/16193 (0.2%)	1.06	84/21857 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	SER	CB-OG	14.26	1.60	1.42
1	B	161	SER	CB-OG	10.29	1.55	1.42
1	C	161	SER	CB-OG	9.30	1.54	1.42
1	B	522[A]	CYS	CB-SG	-8.13	1.68	1.82
1	B	522[B]	CYS	CB-SG	-8.13	1.68	1.82
1	A	262	GLU	CG-CD	7.78	1.63	1.51
1	D	161	SER	CB-OG	7.33	1.51	1.42
1	A	262	GLU	CD-OE2	6.95	1.33	1.25
1	D	522[A]	CYS	CB-SG	-6.94	1.70	1.82
1	D	522[B]	CYS	CB-SG	-6.94	1.70	1.82
1	A	459	GLU	CG-CD	6.82	1.62	1.51
1	A	522[A]	CYS	CB-SG	-6.39	1.71	1.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	522[B]	CYS	CB-SG	-6.39	1.71	1.82
1	D	188	GLU	CD-OE2	6.34	1.32	1.25
1	B	368	SER	CB-OG	-6.03	1.34	1.42
1	B	262	GLU	CD-OE1	5.99	1.32	1.25
1	D	228	GLU	CD-OE2	5.85	1.32	1.25
1	C	262	GLU	CG-CD	5.77	1.60	1.51
1	D	327	ASN	C-O	-5.73	1.12	1.23
1	B	496	GLU	CG-CD	5.68	1.60	1.51
1	C	368	SER	CB-OG	-5.67	1.34	1.42
1	C	543	GLU	CD-OE1	5.64	1.31	1.25
1	D	262	GLU	CG-CD	5.50	1.60	1.51
1	B	247	SER	CB-OG	-5.47	1.35	1.42
1	A	360	TYR	CG-CD2	-5.42	1.32	1.39
1	D	368	SER	CB-OG	-5.39	1.35	1.42
1	D	521	TYR	CE1-CZ	-5.33	1.31	1.38
1	A	234	GLU	CD-OE1	5.16	1.31	1.25
1	C	193	GLU	CD-OE1	5.09	1.31	1.25
1	A	368	SER	CB-OG	-5.07	1.35	1.42
1	A	255	GLU	CD-OE1	5.07	1.31	1.25
1	B	161	SER	CA-CB	5.03	1.60	1.52

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	352	ARG	NE-CZ-NH2	-13.27	113.67	120.30
1	C	442	ARG	NE-CZ-NH1	11.55	126.08	120.30
1	D	442	ARG	NE-CZ-NH1	10.87	125.74	120.30
1	B	442	ARG	NE-CZ-NH1	10.80	125.70	120.30
1	A	442	ARG	NE-CZ-NH1	10.07	125.33	120.30
1	A	442	ARG	NE-CZ-NH2	-9.23	115.69	120.30
1	A	226	ARG	NE-CZ-NH2	8.75	124.67	120.30
1	D	372	ARG	NE-CZ-NH1	-7.58	116.51	120.30
1	A	366	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	A	439	LYS	CD-CE-NZ	7.50	128.94	111.70
1	D	226	ARG	NE-CZ-NH2	7.48	124.04	120.30
1	A	587	ILE	CB-CA-C	7.43	126.45	111.60
1	D	490	ASP	CB-CG-OD2	-7.14	111.87	118.30
1	B	576	ARG	NE-CZ-NH2	7.13	123.86	120.30
1	D	220	ARG	NE-CZ-NH2	7.12	123.86	120.30
1	C	226	ARG	NE-CZ-NH2	6.89	123.75	120.30
1	A	352	ARG	CG-CD-NE	-6.74	97.65	111.80
1	C	134	ARG	NE-CZ-NH1	-6.63	116.98	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	442	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	B	352	ARG	CG-CD-NE	-6.50	98.14	111.80
1	D	371	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	D	490	ASP	CB-CG-OD1	6.34	124.01	118.30
1	B	383	ASP	CB-CG-OD1	6.31	123.98	118.30
1	A	551	ARG	NE-CZ-NH1	-6.26	117.17	120.30
1	D	204	LEU	CA-CB-CG	6.22	129.60	115.30
1	C	383	ASP	CB-CG-OD1	6.21	123.89	118.30
1	D	185	LYS	CD-CE-NZ	6.20	125.97	111.70
1	A	408	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	D	164	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	A	583	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	395	ASP	CB-CG-OD1	6.09	123.78	118.30
1	B	442	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	A	353	ASP	CB-CG-OD1	6.03	123.73	118.30
1	A	551	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	D	512	LYS	CD-CE-NZ	-5.94	98.05	111.70
1	A	531	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	164	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	D	366	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	C	366	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	C	134	ARG	NE-CZ-NH2	5.79	123.20	120.30
1	C	164	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	B	353	ASP	CB-CG-OD1	5.72	123.45	118.30
1	D	352	ARG	CG-CD-NE	-5.72	99.80	111.80
1	D	497	ASP	CB-CG-OD2	5.63	123.37	118.30
1	D	551	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	D	408	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	597	GLU	CA-CB-CG	5.61	125.74	113.40
1	B	204	LEU	CA-CB-CG	5.60	128.18	115.30
1	B	551	ARG	NE-CZ-NH2	5.59	123.10	120.30
1	B	551	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	C	366	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	D	576	ARG	NE-CZ-NH2	5.51	123.06	120.30
1	A	185	LYS	CD-CE-NZ	5.51	124.38	111.70
1	B	366	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	C	442	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	C	316	PHE	CB-CG-CD1	5.49	124.64	120.80
1	C	388	ASP	CB-CG-OD1	5.47	123.23	118.30
1	C	551	ARG	NE-CZ-NH2	5.47	123.04	120.30
1	B	226	ARG	NE-CZ-NH2	5.47	123.03	120.30
1	A	316	PHE	CB-CG-CD1	5.45	124.61	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	551	ARG	NE-CZ-NH1	-5.43	117.58	120.30
1	A	528	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	596	LYS	CD-CE-NZ	5.38	124.07	111.70
1	B	164	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	435	ASP	CB-CG-OD1	5.33	123.09	118.30
1	C	359	LEU	CB-CG-CD2	5.30	120.02	111.00
1	B	366	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	415	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	449	GLU	OE1-CD-OE2	5.27	129.63	123.30
1	C	440	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	B	559	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	B	185	LYS	CD-CE-NZ	5.21	123.69	111.70
1	B	316	PHE	CB-CG-CD1	5.21	124.45	120.80
1	A	316	PHE	CB-CG-CD2	-5.16	117.19	120.80
1	C	305	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	B	218	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	A	284	LEU	CB-CG-CD1	5.09	119.66	111.00
1	D	531	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	D	509	MET	CG-SD-CE	5.05	108.28	100.20
1	C	408	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	B	479	GLU	OE1-CD-OE2	5.01	129.32	123.30
1	B	164	ARG	NE-CZ-NH2	-5.00	117.80	120.30
1	D	226	ARG	NE-CZ-NH1	-5.00	117.80	120.30
1	D	383	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	598	TRP	Peptide
1	C	337	PHE	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3948	0	3930	40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3948	0	3930	31	0
1	C	3958	0	3936	27	1
1	D	3970	0	3944	35	1
2	A	62	0	0	3	0
2	B	62	0	0	5	0
2	C	62	0	0	3	0
2	D	62	0	0	3	0
3	A	32	0	12	0	0
3	B	32	0	12	0	0
3	C	32	0	12	0	0
3	D	32	0	12	0	0
4	A	3	0	0	0	0
4	B	1	0	0	0	0
4	C	3	0	0	0	0
4	D	1	0	0	0	0
5	C	1	0	0	0	0
6	A	233	0	0	23	0
6	B	187	0	0	16	0
6	C	219	0	0	11	0
6	D	229	0	0	21	0
All	All	17077	0	15788	133	1

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 4.

All (133) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:MET:SD	6:D:1029:HOH:O	1.97	1.20
1:A:425:ASN:ND2	6:A:801:HOH:O	1.76	1.07
1:C:354:LYS:CE	6:C:801:HOH:O	2.02	1.05
1:D:511[A]:GLU:H	1:D:511[A]:GLU:CD	1.56	1.05
2:D:702:HF7:CL2	6:D:824:HOH:O	2.08	1.02
2:B:701:HF7:CL2	6:B:830:HOH:O	2.06	1.02
1:A:578:PHE:O	6:A:802:HOH:O	1.77	1.00
1:A:598:TRP:CH2	6:A:930:HOH:O	2.14	1.00
1:C:354:LYS:HE2	6:C:801:HOH:O	1.59	0.99
1:D:328[B]:ASN:ND2	6:D:801:HOH:O	1.93	0.99
2:C:704:HF7:CL2	6:C:816:HOH:O	2.11	0.99
1:C:543:GLU:HG3	1:A:543:GLU:HG3	1.46	0.97
1:C:118:ILE:HD11	1:C:128:LEU:HD11	1.50	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:705:HF7:O2A	6:A:803:HOH:O	1.87	0.92
2:A:703:HF7:CL2	6:A:839:HOH:O	2.16	0.92
1:A:595:LYS:HD3	6:A:1012:HOH:O	1.73	0.88
1:C:328:ASN:HB3	6:A:942:HOH:O	1.72	0.87
1:B:578:PHE:O	6:B:801:HOH:O	1.91	0.87
1:D:328[B]:ASN:OD1	6:D:801:HOH:O	1.92	0.86
1:D:586:VAL:HG11	1:B:522[A]:CYS:SG	2.18	0.83
1:D:511[B]:GLU:OE1	6:D:802:HOH:O	1.94	0.83
6:D:909:HOH:O	1:B:328:ASN:HB3	1.80	0.82
1:D:511[A]:GLU:N	1:D:511[A]:GLU:CD	2.34	0.80
2:B:703:HF7:O1A	6:B:802:HOH:O	1.99	0.80
1:D:185:LYS:HE2	6:D:966:HOH:O	1.82	0.80
1:C:305:ARG:HD2	6:C:973:HOH:O	1.81	0.79
1:A:566:ARG:NE	1:A:587:ILE:HG13	1.98	0.78
1:C:118:ILE:HD11	1:C:128:LEU:CD1	2.16	0.76
1:D:577[B]:ASN:OD1	1:D:595:LYS:NZ	2.18	0.75
1:A:251:LYS:HD2	6:A:807:HOH:O	1.87	0.75
2:D:701:HF7:O2A	6:D:803:HOH:O	2.02	0.75
1:D:311:ASP:OD2	6:D:804:HOH:O	2.05	0.74
1:B:578:PHE:C	6:B:801:HOH:O	2.25	0.74
2:B:703:HF7:CL2	6:B:961:HOH:O	2.35	0.74
1:A:455:LYS:HG2	1:A:557:VAL:HG12	1.70	0.73
1:A:598:TRP:HH2	6:A:930:HOH:O	1.64	0.72
1:C:118:ILE:CD1	1:C:128:LEU:HD11	2.19	0.71
1:A:425:ASN:OD1	6:A:804:HOH:O	2.07	0.71
1:B:185:LYS:HE2	6:B:912:HOH:O	1.91	0.70
1:C:326:GLN:O	6:C:802:HOH:O	2.08	0.70
1:C:115:MET:HB2	6:C:1011:HOH:O	1.91	0.69
1:A:595:LYS:HG3	1:A:597:GLU:OE1	1.91	0.69
1:B:455:LYS:HG2	1:B:557:VAL:HG12	1.75	0.67
1:D:455:LYS:HG2	1:D:557:VAL:HG12	1.76	0.67
1:D:328[B]:ASN:CG	6:D:801:HOH:O	2.17	0.67
1:C:455:LYS:HG2	1:C:557:VAL:HG12	1.77	0.66
1:D:543:GLU:HG3	1:B:543:GLU:HG3	1.77	0.66
1:C:293:ASN:OD1	6:C:803:HOH:O	2.14	0.66
1:D:185:LYS:CE	6:D:966:HOH:O	2.43	0.65
1:A:298:TYR:O	6:A:805:HOH:O	2.14	0.65
1:A:511[B]:GLU:HG2	6:A:861:HOH:O	1.97	0.65
1:C:543:GLU:CG	1:A:543:GLU:HG3	2.25	0.64
1:A:328:ASN:HB2	6:A:891:HOH:O	1.97	0.64
1:A:598:TRP:HZ2	6:A:802:HOH:O	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:425:ASN:ND2	6:D:805:HOH:O	2.23	0.62
1:A:595:LYS:HD2	6:A:814:HOH:O	1.98	0.62
2:A:705:HF7:CL2	6:A:999:HOH:O	2.47	0.62
1:B:185:LYS:CE	6:B:912:HOH:O	2.46	0.61
1:C:326:GLN:HG2	1:A:326:GLN:HG2	1.83	0.61
1:D:185:LYS:NZ	6:D:808:HOH:O	2.34	0.60
1:D:326:GLN:HG2	1:B:327:ASN:O	2.03	0.58
1:A:574:ALA:O	1:A:595:LYS:HE2	2.03	0.58
1:B:483:ALA:O	6:B:803:HOH:O	2.17	0.57
1:A:566:ARG:HE	1:A:587:ILE:HG13	1.68	0.56
1:B:215:HIS:HE2	2:B:703:HF7:PA	2.29	0.56
1:D:254:MET:HE3	6:D:1029:HOH:O	2.02	0.56
1:A:574:ALA:HA	1:A:595:LYS:HE3	1.88	0.55
1:D:474:GLU:O	1:D:478:LYS:NZ	2.34	0.55
1:B:355:GLU:OE1	6:B:804:HOH:O	2.18	0.55
1:A:491:VAL:HG21	1:A:561:SER:HA	1.88	0.54
1:A:474:GLU:O	1:A:478:LYS:NZ	2.35	0.54
1:A:327:ASN:HA	6:A:848:HOH:O	2.08	0.53
1:D:511[A]:GLU:N	1:D:511[A]:GLU:OE2	2.40	0.53
1:C:326:GLN:HG2	1:A:326:GLN:CG	2.39	0.53
1:C:491:VAL:HG21	1:C:561:SER:HA	1.89	0.53
1:B:215:HIS:NE2	2:B:703:HF7:O2A	2.42	0.52
1:B:491:VAL:HG21	1:B:561:SER:HA	1.92	0.51
1:D:327:ASN:HA	6:D:851:HOH:O	2.11	0.51
1:C:354:LYS:NZ	6:C:801:HOH:O	2.04	0.51
1:D:114:THR:HG22	6:D:1002:HOH:O	2.11	0.50
1:A:574:ALA:O	1:A:595:LYS:CE	2.59	0.50
2:C:701:HF7:O1A	6:C:804:HOH:O	2.19	0.50
1:A:566:ARG:CZ	1:A:587:ILE:HD11	2.44	0.48
1:C:327:ASN:O	1:A:326:GLN:HG2	2.15	0.47
1:D:487:VAL:HG23	1:D:591:ILE:HD11	1.97	0.47
1:A:261:PRO:HD2	6:A:850:HOH:O	2.15	0.47
1:A:487:VAL:HG23	1:A:591:ILE:HD11	1.96	0.47
1:D:491:VAL:HG21	1:D:561:SER:HA	1.97	0.46
1:B:355:GLU:HG3	6:B:804:HOH:O	2.15	0.46
1:C:354:LYS:HG3	1:C:355:GLU:OE2	2.16	0.46
1:D:134:ARG:CD	6:D:1014:HOH:O	2.64	0.46
1:D:586:VAL:CG1	1:B:522[A]:CYS:SG	2.97	0.46
1:A:467:LYS:HE3	6:A:861:HOH:O	2.16	0.45
1:D:381:ILE:HA	1:D:381:ILE:HD12	1.87	0.45
1:C:148:LYS:NZ	6:C:810:HOH:O	2.44	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:ILE:HD13	1:C:126:ILE:HG21	1.64	0.45
1:D:408:ARG:NH2	6:D:806:HOH:O	2.30	0.45
1:B:394:ASP:O	1:B:408:ARG:HD2	2.17	0.44
1:B:466:ILE:HA	6:B:963:HOH:O	2.18	0.44
1:B:143:ARG:HD2	1:B:420:THR:HA	2.00	0.44
1:C:381:ILE:HD12	1:C:381:ILE:HA	1.89	0.44
1:D:126:ILE:HD13	1:D:126:ILE:HG21	1.78	0.43
1:B:499:ILE:HD11	1:B:555:LYS:HE2	2.01	0.43
1:D:114:THR:CG2	6:D:1002:HOH:O	2.67	0.43
1:A:371:ARG:NH2	1:A:549:LEU:HD11	2.33	0.43
1:B:331:TYR:CD2	1:B:331:TYR:C	2.92	0.43
1:A:346:GLU:HA	6:A:833:HOH:O	2.18	0.42
1:B:251:LYS:HB2	1:B:252:PRO:HD3	2.01	0.42
1:D:331:TYR:CD2	1:D:331:TYR:C	2.93	0.42
1:B:543:GLU:HG3	6:B:824:HOH:O	2.19	0.42
1:A:570:VAL:HG13	6:A:930:HOH:O	2.19	0.42
1:A:499:ILE:HD11	1:A:555:LYS:HE2	2.01	0.42
1:B:354:LYS:HE2	6:B:940:HOH:O	2.19	0.42
1:B:235:GLN:HG3	6:B:935:HOH:O	2.20	0.42
1:A:185:LYS:HE2	6:A:995:HOH:O	2.19	0.41
1:D:499:ILE:HD11	1:D:555:LYS:HE2	2.02	0.41
1:C:118:ILE:CD1	1:C:128:LEU:CD1	2.91	0.41
1:C:551:ARG:NH1	6:C:824:HOH:O	2.53	0.41
1:A:331:TYR:C	1:A:331:TYR:CD2	2.93	0.41
1:D:326:GLN:CG	1:B:327:ASN:O	2.67	0.41
1:D:359:LEU:HD13	6:D:975:HOH:O	2.20	0.41
1:B:126:ILE:HG21	1:B:126:ILE:HD13	1.64	0.41
2:D:702:HF7:N6	1:B:372:ARG:HG2	2.35	0.41
1:B:579:THR:C	6:B:801:HOH:O	2.58	0.41
1:B:551:ARG:NH1	6:B:825:HOH:O	2.52	0.41
1:A:566:ARG:CZ	1:A:587:ILE:HG13	2.51	0.41
1:A:381:ILE:HA	1:A:381:ILE:HD12	1.83	0.41
1:B:381:ILE:HA	1:B:381:ILE:HD12	1.89	0.41
1:C:215:HIS:HE2	2:C:701:HF7:PA	2.44	0.40
1:C:331:TYR:CD2	1:C:331:TYR:C	2.94	0.40
1:D:355:GLU:HB3	6:D:975:HOH:O	2.20	0.40
1:A:185:LYS:CE	6:A:995:HOH:O	2.70	0.40
1:C:115:MET:C	1:C:115:MET:SD	3.00	0.40

All (1) 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:D:396:TYR:OH	1:C:492:LYS:CG[1_556]	2.14	0.06

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	479/550 (87%)	470 (98%)	9 (2%)	0	100	100
1	B	479/550 (87%)	471 (98%)	8 (2%)	0	100	100
1	C	480/550 (87%)	472 (98%)	8 (2%)	0	100	100
1	D	482/550 (88%)	475 (98%)	7 (2%)	0	100	100
All	All	1920/2200 (87%)	1888 (98%)	32 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	429/488 (88%)	413 (96%)	16 (4%)	34	32
1	B	429/488 (88%)	411 (96%)	18 (4%)	30	27
1	C	430/488 (88%)	415 (96%)	15 (4%)	36	35
1	D	432/488 (88%)	415 (96%)	17 (4%)	32	30
All	All	1720/1952 (88%)	1654 (96%)	66 (4%)	33	31

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	113	ASP
1	D	114	THR
1	D	229	VAL
1	D	230	LYS
1	D	277	GLU
1	D	284	LEU
1	D	331	TYR
1	D	359	LEU
1	D	377	LYS
1	D	465	GLN
1	D	469	LYS
1	D	478	LYS
1	D	484	LYS
1	D	492	LYS
1	D	511[A]	GLU
1	D	511[B]	GLU
1	D	596	LYS
1	C	113	ASP
1	C	114	THR
1	C	193	GLU
1	C	229	VAL
1	C	277	GLU
1	C	284	LEU
1	C	359	LEU
1	C	377	LYS
1	C	439	LYS
1	C	465	GLN
1	C	470	ARG
1	C	484	LYS
1	C	486	LYS
1	C	492	LYS
1	C	596	LYS
1	B	113	ASP
1	B	114	THR
1	B	193	GLU
1	B	229	VAL
1	B	230	LYS
1	B	277	GLU
1	B	284	LEU
1	B	331	TYR
1	B	359	LEU
1	B	377	LYS
1	B	425	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	439	LYS
1	B	469	LYS
1	B	484	LYS
1	B	486	LYS
1	B	492	LYS
1	B	540	LEU
1	B	596	LYS
1	A	113	ASP
1	A	114	THR
1	A	229	VAL
1	A	277	GLU
1	A	331	TYR
1	A	359	LEU
1	A	467	LYS
1	A	478	LYS
1	A	484	LYS
1	A	486	LYS
1	A	492	LYS
1	A	540	LEU
1	A	544	LYS
1	A	560	LYS
1	A	596	LYS
1	A	597	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	322	HIS
1	D	364	HIS
1	D	510	GLN
1	D	535	ASN
1	C	190	GLN
1	C	322	HIS
1	C	364	HIS
1	C	510	GLN
1	C	535	ASN
1	C	539	GLN
1	B	235	GLN
1	B	535	ASN
1	A	233	HIS
1	A	326	GLN
1	A	364	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	425	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 9 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	GTP	C	703	4	26,34,34	1.51	5 (19%)	33,54,54	2.46	10 (30%)
2	HF7	C	701	4	27,33,33	1.79	8 (29%)	33,52,52	2.18	11 (33%)
2	HF7	A	705	4	27,33,33	1.78	9 (33%)	33,52,52	2.23	10 (30%)
2	HF7	B	701	4	27,33,33	1.37	4 (14%)	33,52,52	1.54	4 (12%)
2	HF7	D	701	4	27,33,33	1.95	9 (33%)	33,52,52	2.90	12 (36%)
2	HF7	D	702	4	27,33,33	1.64	7 (25%)	33,52,52	1.85	8 (24%)
2	HF7	C	704	4	27,33,33	2.13	9 (33%)	33,52,52	2.26	9 (27%)
2	HF7	A	703	4	27,33,33	1.78	7 (25%)	33,52,52	1.77	6 (18%)
2	HF7	B	703	4	27,33,33	1.91	8 (29%)	33,52,52	2.31	8 (24%)
3	GTP	A	702	4	26,34,34	1.46	8 (30%)	33,54,54	2.27	9 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GTP	B	702	4	26,34,34	1.29	2 (7%)	33,54,54	1.83	7 (21%)
3	GTP	D	703	4	26,34,34	1.47	3 (11%)	33,54,54	2.21	7 (21%)

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	GTP	C	703	4	-	5/18/38/38	0/3/3/3
2	HF7	C	701	4	-	3/18/34/34	0/3/3/3
2	HF7	A	705	4	-	2/18/34/34	0/3/3/3
2	HF7	B	701	4	-	5/18/34/34	0/3/3/3
2	HF7	D	701	4	-	4/18/34/34	0/3/3/3
2	HF7	D	702	4	-	2/18/34/34	0/3/3/3
2	HF7	C	704	4	-	2/18/34/34	0/3/3/3
2	HF7	A	703	4	-	2/18/34/34	0/3/3/3
2	HF7	B	703	4	-	3/18/34/34	0/3/3/3
3	GTP	A	702	4	-	4/18/38/38	0/3/3/3
3	GTP	B	702	4	-	6/18/38/38	0/3/3/3
3	GTP	D	703	4	-	4/18/38/38	0/3/3/3

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	704	HF7	O4'-C1'	4.90	1.53	1.42
2	D	701	HF7	CL2-C2	4.80	1.63	1.49
2	C	704	HF7	C2-N1	-4.33	1.26	1.34
2	A	705	HF7	C6-N6	4.22	1.49	1.34
2	A	703	HF7	C6-N1	-4.13	1.26	1.33
2	A	703	HF7	O4'-C1'	4.11	1.51	1.42
3	D	703	GTP	O4'-C1'	3.87	1.46	1.41
2	B	703	HF7	C6-N6	3.85	1.48	1.34
2	C	704	HF7	C3'-C4'	-3.57	1.43	1.53
2	B	703	HF7	CL2-C2	3.56	1.59	1.49
2	D	701	HF7	C6-N1	3.51	1.40	1.33
2	D	702	HF7	C6-N6	3.49	1.46	1.34
2	C	701	HF7	C4-N3	-3.46	1.30	1.35
2	D	701	HF7	C6-N6	3.46	1.46	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	703	HF7	C2-N3	3.44	1.40	1.34
3	B	702	GTP	PG-O2G	-3.38	1.41	1.54
2	B	703	HF7	PA-O5'	3.28	1.72	1.59
2	B	701	HF7	C4-N3	-3.26	1.30	1.35
2	B	703	HF7	C6-N1	3.22	1.39	1.33
3	C	703	GTP	C8-N7	-3.19	1.29	1.34
2	A	705	HF7	C2-N3	3.15	1.39	1.34
2	C	704	HF7	C2-N3	-3.12	1.28	1.34
2	C	701	HF7	C6-N6	3.12	1.45	1.34
3	D	703	GTP	C8-N7	3.12	1.40	1.34
2	C	701	HF7	CL2-C2	3.00	1.58	1.49
2	C	701	HF7	O3'-C3'	2.99	1.49	1.43
3	C	703	GTP	C6-C5	2.91	1.46	1.41
3	D	703	GTP	C5-C4	2.85	1.48	1.40
2	C	704	HF7	O4'-C4'	2.84	1.51	1.45
2	C	701	HF7	O4'-C1'	2.83	1.48	1.42
2	D	701	HF7	O4'-C1'	2.80	1.48	1.42
2	A	703	HF7	PB-O2B	-2.78	1.42	1.55
2	D	702	HF7	PG-O3G	-2.76	1.44	1.54
2	A	703	HF7	C4-N3	-2.72	1.31	1.35
2	C	704	HF7	PB-O1B	-2.72	1.41	1.50
2	B	701	HF7	PB-O2B	-2.69	1.42	1.55
2	A	705	HF7	O4'-C1'	2.66	1.48	1.42
2	A	705	HF7	C4-N3	-2.64	1.31	1.35
2	D	702	HF7	C6-N1	-2.58	1.29	1.33
2	B	703	HF7	C8-N7	2.56	1.39	1.34
2	B	703	HF7	C4-N3	-2.56	1.31	1.35
3	C	703	GTP	O4'-C1'	2.56	1.44	1.41
3	A	702	GTP	O6-C6	2.53	1.30	1.24
2	C	701	HF7	PA-O5'	2.50	1.69	1.59
2	D	702	HF7	C3'-C4'	-2.46	1.46	1.53
2	C	701	HF7	PG-O2G	-2.43	1.45	1.54
2	A	703	HF7	PG-O3G	-2.41	1.45	1.54
3	C	703	GTP	C5'-C4'	2.40	1.59	1.51
2	C	704	HF7	C4-N3	-2.32	1.32	1.35
2	D	701	HF7	C2'-C3'	-2.31	1.46	1.52
3	A	702	GTP	C6-C5	2.30	1.45	1.41
3	A	702	GTP	PB-O2B	-2.30	1.44	1.55
2	C	704	HF7	C2'-C3'	-2.28	1.46	1.52
3	A	702	GTP	C5-C4	2.28	1.47	1.40
2	A	705	HF7	C8-N7	-2.23	1.30	1.34
2	B	701	HF7	PG-O2G	-2.22	1.46	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	705	HF7	C6-N1	2.20	1.37	1.33
2	D	701	HF7	PB-O2B	-2.20	1.45	1.55
2	A	705	HF7	PA-O5'	2.17	1.68	1.59
3	A	702	GTP	O3'-C3'	-2.17	1.37	1.43
2	D	702	HF7	O4'-C1'	2.17	1.47	1.42
2	D	702	HF7	C4-N3	-2.15	1.32	1.35
3	B	702	GTP	C8-N7	-2.13	1.30	1.34
3	A	702	GTP	PA-O2A	-2.12	1.45	1.55
3	A	702	GTP	PG-O3G	-2.11	1.46	1.54
2	D	701	HF7	C2-N1	2.11	1.37	1.34
3	A	702	GTP	PG-O2G	-2.10	1.46	1.54
2	D	702	HF7	C2'-C1'	-2.08	1.46	1.52
2	D	701	HF7	PG-O2G	-2.05	1.46	1.54
2	A	703	HF7	C6-N6	2.05	1.41	1.34
2	B	701	HF7	PG-O3G	-2.05	1.46	1.54
2	A	705	HF7	C5-N7	2.05	1.47	1.39
3	C	703	GTP	C5-C4	2.04	1.46	1.40
2	C	701	HF7	C5-N7	2.04	1.47	1.39
2	D	701	HF7	PA-O1A	-2.04	1.45	1.55
2	C	704	HF7	CL2-C2	2.03	1.55	1.49
2	A	703	HF7	PB-O1B	-2.02	1.43	1.50
2	B	703	HF7	C5-N7	2.01	1.47	1.39
2	A	705	HF7	CL2-C2	2.01	1.55	1.49

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	703	GTP	C5-C6-N1	-7.82	112.73	123.43
2	C	704	HF7	C5-C6-N1	-7.56	116.04	121.01
3	A	702	GTP	C5-C6-N1	-7.32	113.42	123.43
2	B	703	HF7	C2-N3-C4	7.20	121.37	115.52
2	D	701	HF7	C2-N3-C4	7.07	121.27	115.52
2	D	701	HF7	CL2-C2-N1	6.62	127.48	117.15
2	D	701	HF7	N3-C2-N1	-6.33	114.17	125.73
3	C	703	GTP	C6-C5-C4	-6.24	114.84	120.80
2	C	701	HF7	C2-N3-C4	6.08	120.46	115.52
3	A	702	GTP	C6-N1-C2	6.02	125.50	115.93
3	C	703	GTP	C6-N1-C2	5.84	125.21	115.93
2	D	702	HF7	C4-C5-N7	-5.82	103.33	109.40
3	D	703	GTP	C6-N1-C2	5.82	125.17	115.93
2	A	703	HF7	C5-C6-N1	-5.61	117.33	121.01
2	D	701	HF7	C2-N1-C6	5.56	126.75	118.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	HF7	C2-N3-C4	5.52	120.01	115.52
3	C	703	GTP	C5-C6-N1	-5.43	116.00	123.43
2	A	705	HF7	C2-N3-C4	5.42	119.92	115.52
2	B	703	HF7	C5-C6-N6	-5.27	112.35	120.35
2	C	704	HF7	C2-N3-C4	5.22	119.76	115.52
2	A	705	HF7	C5-C6-N6	-4.82	113.03	120.35
2	C	701	HF7	CL2-C2-N1	4.72	124.52	117.15
2	D	701	HF7	O1A-PA-O5'	4.56	128.93	107.75
2	A	705	HF7	PB-O3B-PG	-4.54	117.23	132.83
3	B	702	GTP	C6-C5-C4	-4.43	116.57	120.80
2	C	704	HF7	CL2-C2-N3	4.33	123.89	117.16
2	C	701	HF7	C5-C6-N6	-4.22	113.94	120.35
2	A	705	HF7	CL2-C2-N1	4.17	123.66	117.15
3	C	703	GTP	C4-C5-N7	-4.14	105.08	109.40
2	B	703	HF7	N3-C2-N1	-4.05	118.33	125.73
2	B	703	HF7	CL2-C2-N3	4.01	123.41	117.16
3	B	702	GTP	C3'-C2'-C1'	4.01	107.02	100.98
2	D	702	HF7	CL2-C2-N1	-3.99	110.92	117.15
3	C	703	GTP	N3-C2-N1	-3.94	121.97	127.22
2	C	704	HF7	C2-N1-C6	3.94	124.22	118.08
2	B	703	HF7	PB-O3A-PA	-3.93	119.34	132.83
2	D	702	HF7	N3-C2-N1	3.88	132.82	125.73
2	A	705	HF7	PB-O3A-PA	-3.85	119.60	132.83
3	D	703	GTP	C3'-C2'-C1'	3.84	106.76	100.98
2	C	701	HF7	N3-C2-N1	-3.83	118.75	125.73
2	D	701	HF7	C5-C6-N1	-3.73	118.56	121.01
2	A	703	HF7	CL2-C2-N1	-3.70	111.37	117.15
2	D	701	HF7	PB-O3B-PG	-3.55	120.63	132.83
3	A	702	GTP	N3-C2-N1	-3.54	122.49	127.22
2	A	705	HF7	O2G-PG-O3B	3.49	116.33	104.64
2	A	703	HF7	C2-N3-C4	-3.43	112.73	115.52
2	D	701	HF7	O3G-PG-O3B	3.42	116.11	104.64
2	D	701	HF7	PB-O3A-PA	-3.37	121.25	132.83
3	D	703	GTP	O3G-PG-O2G	3.37	120.52	107.64
2	C	701	HF7	N6-C6-N1	3.33	126.12	117.07
2	A	705	HF7	O1A-PA-O2A	-3.32	95.82	112.24
2	B	703	HF7	N6-C6-N1	3.28	125.97	117.07
3	B	702	GTP	C6-N1-C2	3.26	121.11	115.93
3	B	702	GTP	N3-C2-N1	-3.24	122.90	127.22
3	B	702	GTP	PA-O3A-PB	-3.20	121.86	132.83
2	C	704	HF7	C2'-C3'-C4'	3.17	109.36	102.76
3	A	702	GTP	PA-O3A-PB	-3.10	122.17	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	GTP	O3G-PG-O2G	3.10	119.47	107.64
3	C	703	GTP	C2-N3-C4	3.09	118.89	115.36
3	C	703	GTP	PA-O3A-PB	-3.08	122.26	132.83
2	A	705	HF7	N6-C6-N1	3.07	125.43	117.07
3	A	702	GTP	C3'-C2'-C1'	3.06	105.58	100.98
2	B	701	HF7	C5-C6-N1	-3.01	119.03	121.01
2	A	705	HF7	O1A-PA-O5'	2.98	121.60	107.75
2	B	701	HF7	C4-C5-N7	-2.96	106.32	109.40
3	B	702	GTP	C5-C6-N1	-2.95	119.39	123.43
2	A	703	HF7	C5-C6-N6	2.85	124.68	120.35
2	B	703	HF7	PB-O3B-PG	-2.83	123.11	132.83
3	D	703	GTP	PA-O3A-PB	-2.78	123.27	132.83
3	A	702	GTP	C2-N3-C4	2.78	118.53	115.36
2	C	701	HF7	PB-O3B-PG	-2.74	123.42	132.83
3	C	703	GTP	O3G-PG-O3B	2.68	113.63	104.64
2	A	703	HF7	C2'-C1'-N9	2.67	120.43	114.27
2	D	701	HF7	O1A-PA-O2A	-2.66	99.10	112.24
2	A	703	HF7	N3-C2-N1	2.58	130.45	125.73
2	D	701	HF7	O2G-PG-O3G	-2.55	97.89	107.64
2	C	701	HF7	O3G-PG-O3B	2.54	113.15	104.64
2	C	701	HF7	O2G-PG-O3B	2.52	113.07	104.64
2	D	702	HF7	O2G-PG-O3B	2.48	112.95	104.64
2	B	701	HF7	O3G-PG-O3B	2.47	112.92	104.64
3	D	703	GTP	O5'-PA-O1A	2.46	118.69	109.07
2	C	701	HF7	C2-N1-C6	2.42	121.86	118.08
3	C	703	GTP	O2'-C2'-C1'	-2.42	101.91	110.85
2	C	701	HF7	PB-O3A-PA	-2.42	124.53	132.83
2	D	701	HF7	N6-C6-N1	2.35	123.46	117.07
2	C	704	HF7	CL2-C2-N1	-2.29	113.57	117.15
2	D	702	HF7	C5-C6-N1	-2.25	119.53	121.01
2	C	701	HF7	O3G-PG-O1G	-2.24	101.89	110.68
2	A	705	HF7	N3-C2-N1	-2.23	121.65	125.73
3	D	703	GTP	O5'-C5'-C4'	2.23	116.67	108.99
2	B	703	HF7	O1A-PA-O2A	-2.18	101.47	112.24
3	B	702	GTP	O2'-C2'-C1'	-2.14	102.95	110.85
2	D	702	HF7	C2'-C1'-N9	2.13	119.18	114.27
2	C	704	HF7	O3G-PG-O3B	2.11	111.72	104.64
2	C	704	HF7	N3-C2-N1	-2.10	121.90	125.73
3	A	702	GTP	O2'-C2'-C1'	-2.09	103.14	110.85
3	A	702	GTP	C4-C5-N7	-2.07	107.24	109.40
3	C	703	GTP	O4'-C4'-C3'	-2.06	101.04	105.11
2	D	702	HF7	C2-N1-C6	-2.03	114.92	118.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	702	HF7	C3'-C2'-C1'	2.03	107.61	102.54
2	C	704	HF7	O2G-PG-O1G	-2.02	102.78	110.68

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	701	HF7	PB-O3A-PA-O5'
3	B	702	GTP	PB-O3B-PG-O3G
3	D	703	GTP	PB-O3B-PG-O3G
2	C	701	HF7	C3'-C4'-C5'-O5'
2	D	701	HF7	C3'-C4'-C5'-O5'
2	B	703	HF7	C3'-C4'-C5'-O5'
2	B	703	HF7	O4'-C4'-C5'-O5'
2	C	701	HF7	C4'-C5'-O5'-PA
3	B	702	GTP	PG-O3B-PB-O1B
2	D	701	HF7	C4'-C5'-O5'-PA
3	B	702	GTP	C4'-C5'-O5'-PA
3	D	703	GTP	C4'-C5'-O5'-PA
3	B	702	GTP	PB-O3B-PG-O1G
2	B	701	HF7	PB-O3B-PG-O3G
2	B	701	HF7	PB-O3A-PA-O1A
2	B	701	HF7	PG-O3B-PB-O1B
2	D	702	HF7	PG-O3B-PB-O2B
2	A	703	HF7	PB-O3A-PA-O2A
3	A	702	GTP	PG-O3B-PB-O1B
2	A	705	HF7	C4'-C5'-O5'-PA
2	B	703	HF7	C4'-C5'-O5'-PA
3	D	703	GTP	C5'-O5'-PA-O1A
3	C	703	GTP	C4'-C5'-O5'-PA
2	D	701	HF7	O4'-C4'-C5'-O5'
2	A	705	HF7	C3'-C4'-C5'-O5'
3	C	703	GTP	PG-O3B-PB-O2B
3	B	702	GTP	PG-O3B-PB-O2B
3	B	702	GTP	PB-O3A-PA-O2A
3	A	702	GTP	C4'-C5'-O5'-PA
2	C	701	HF7	O4'-C4'-C5'-O5'
2	C	704	HF7	PB-O3A-PA-O2A
3	C	703	GTP	PB-O3B-PG-O1G
2	B	701	HF7	PB-O3B-PG-O2G
3	A	702	GTP	PB-O3B-PG-O2G
3	C	703	GTP	PG-O3B-PB-O1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	703	GTP	PB-O3A-PA-O1A
2	B	701	HF7	PB-O3A-PA-O2A
2	D	702	HF7	PG-O3B-PB-O1B
2	C	704	HF7	PB-O3A-PA-O1A
2	A	703	HF7	PG-O3B-PB-O2B
3	A	702	GTP	PG-O3B-PB-O2B
3	D	703	GTP	PG-O3B-PB-O2B

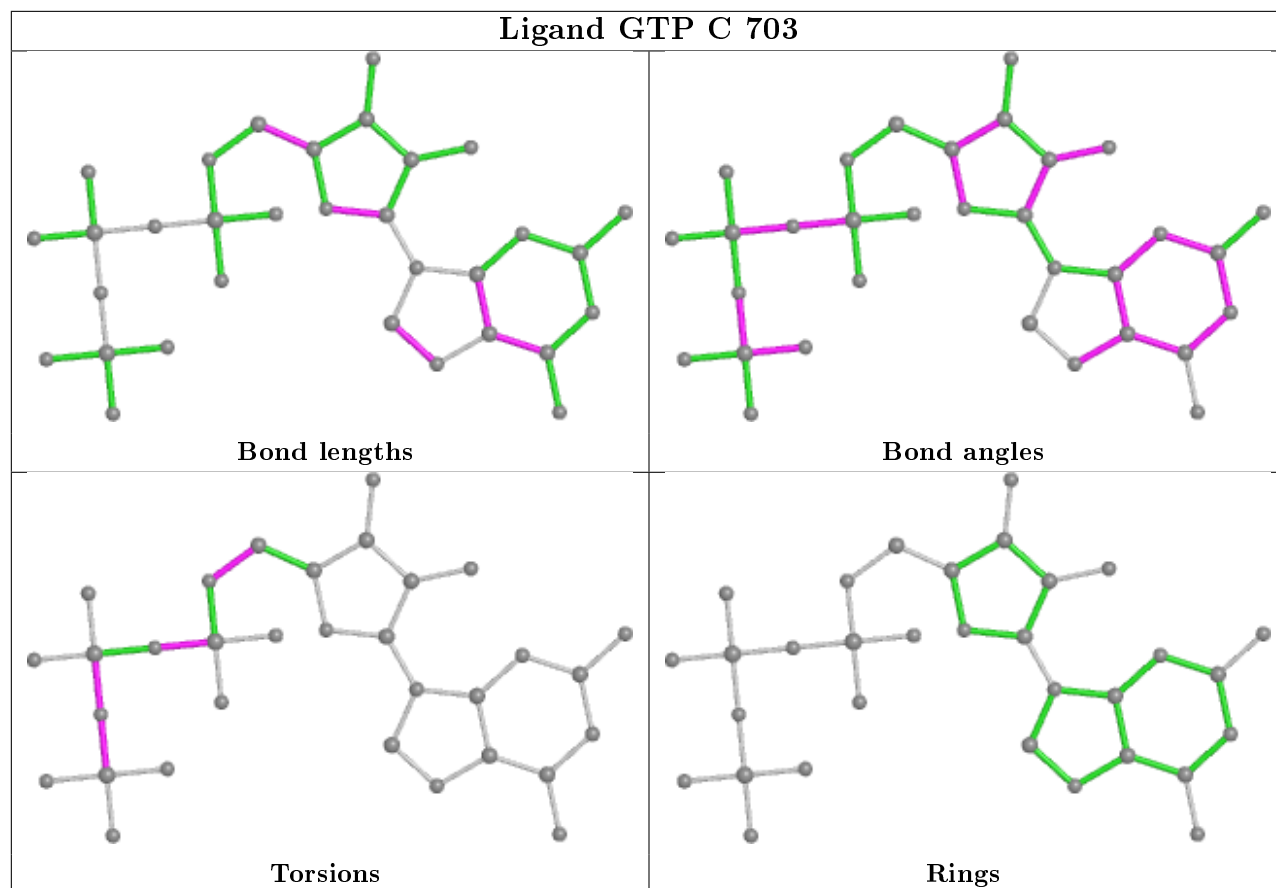
There are no ring outliers.

8 monomers are involved in 14 short contacts:

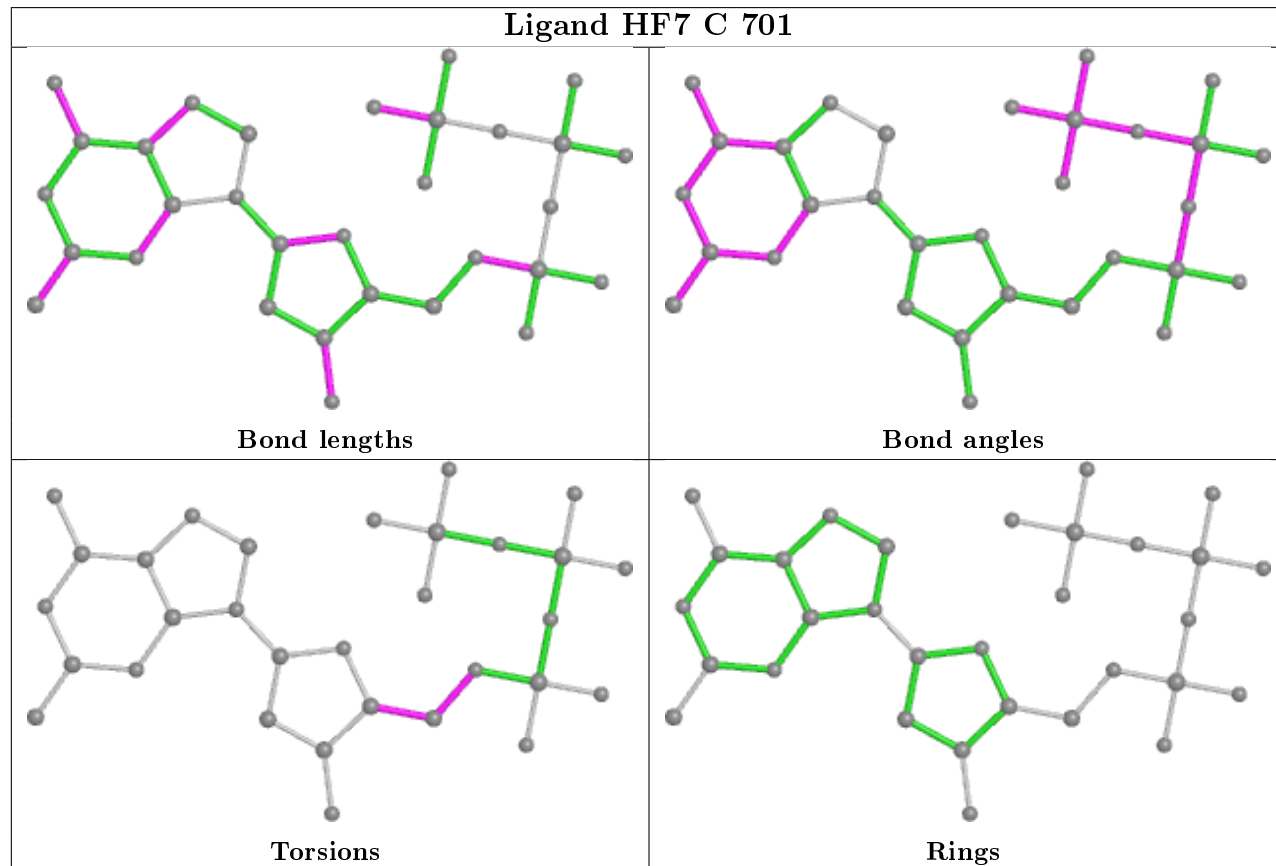
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	701	HF7	2	0
2	A	705	HF7	2	0
2	B	701	HF7	1	0
2	D	701	HF7	1	0
2	D	702	HF7	2	0
2	C	704	HF7	1	0
2	A	703	HF7	1	0
2	B	703	HF7	4	0

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

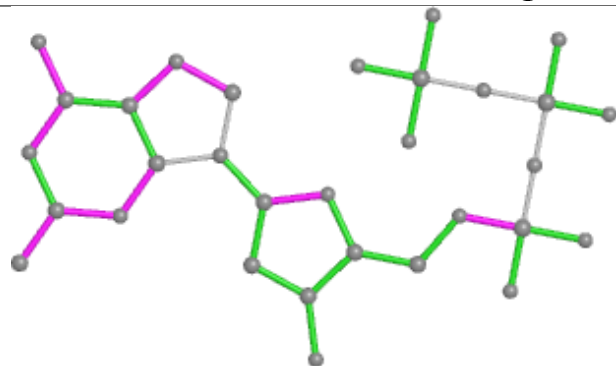
Ligand GTP C 703



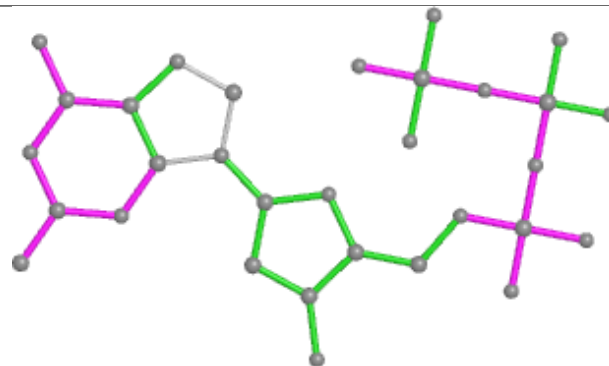
Ligand HF7 C 701



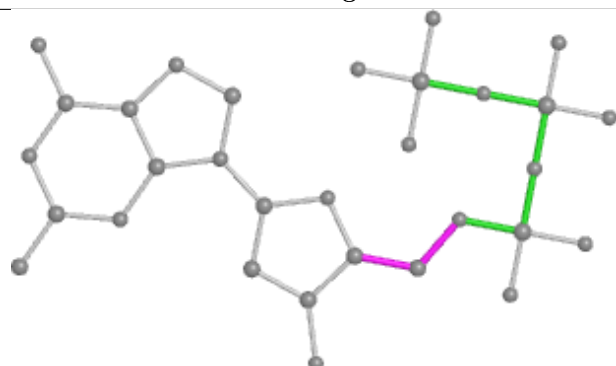
Ligand HF7 A 705



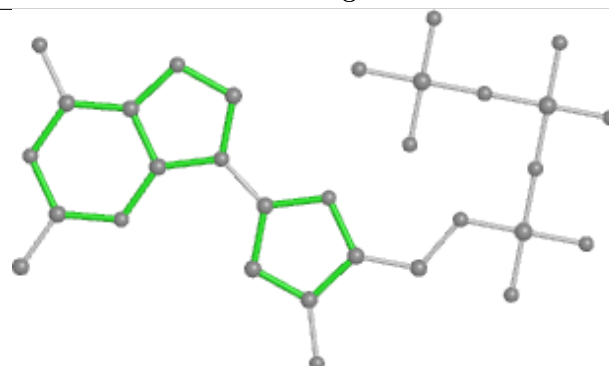
Bond lengths



Bond angles

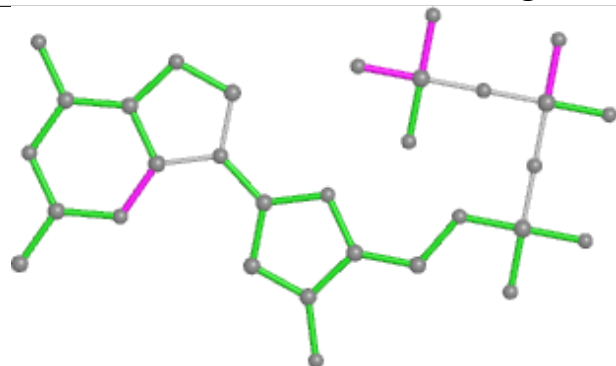


Torsions

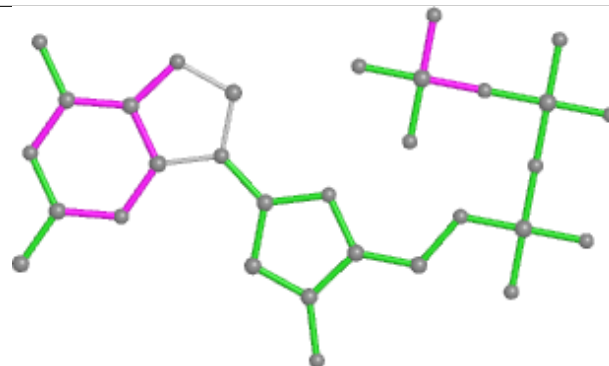


Rings

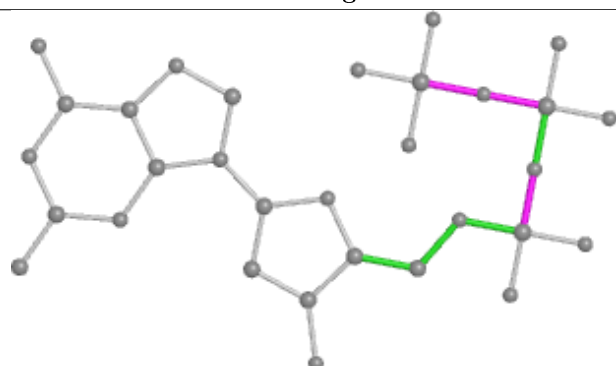
Ligand HF7 B 701



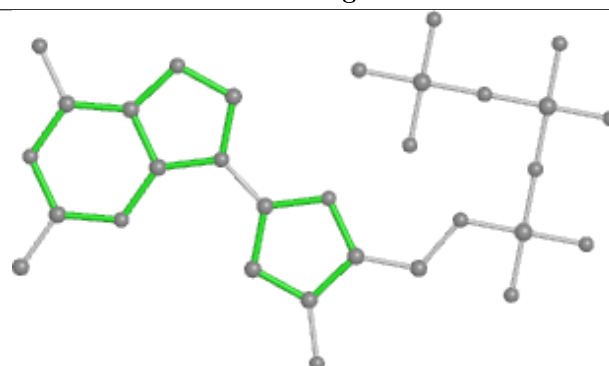
Bond lengths



Bond angles

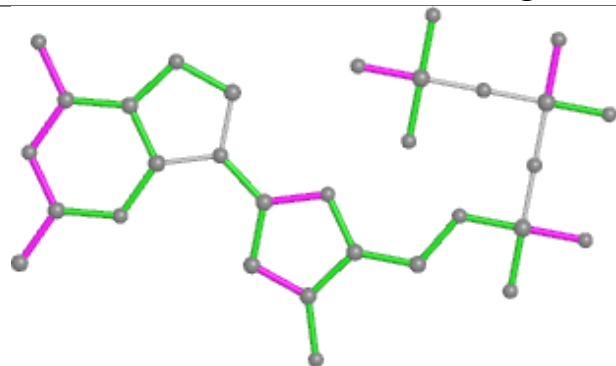


Torsions

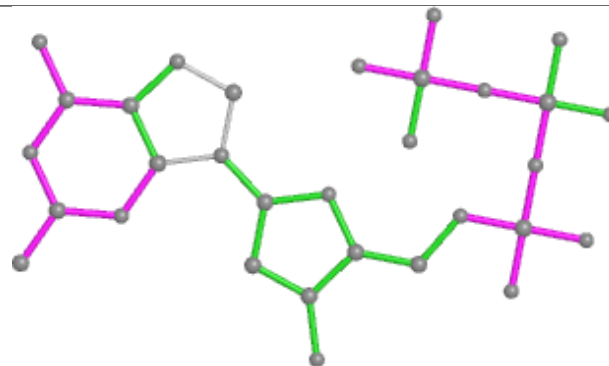


Rings

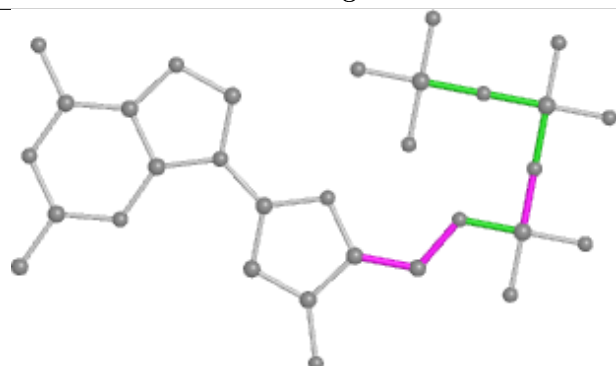
Ligand HF7 D 701



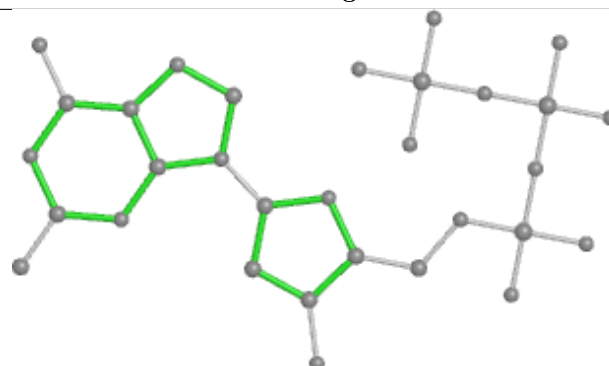
Bond lengths



Bond angles

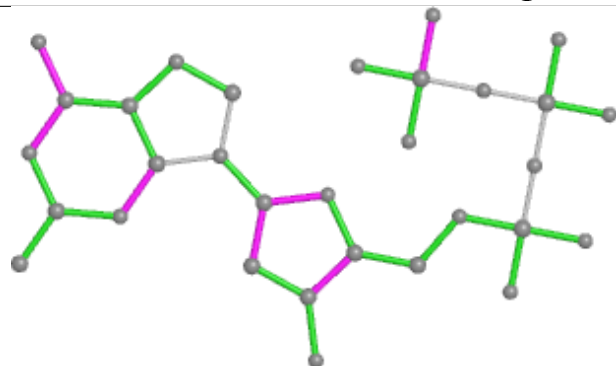


Torsions

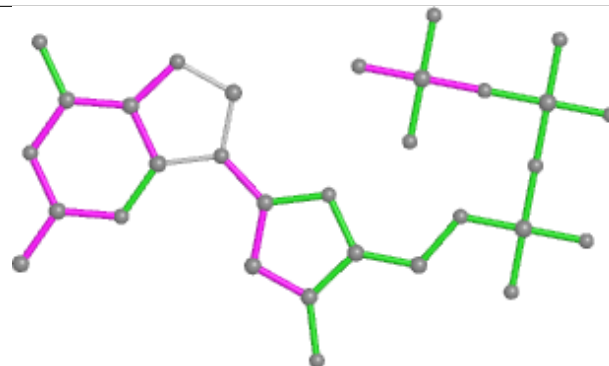


Rings

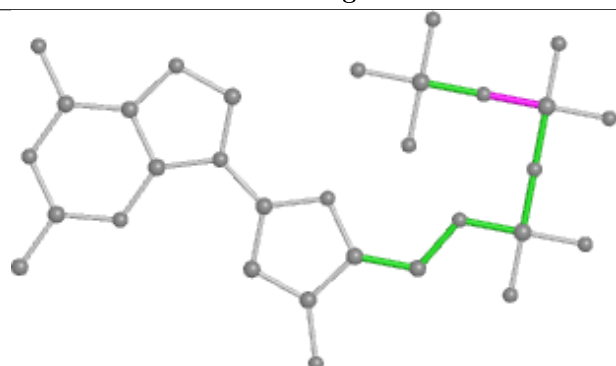
Ligand HF7 D 702



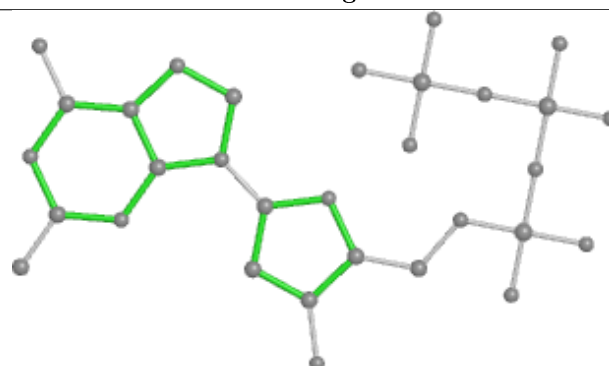
Bond lengths



Bond angles

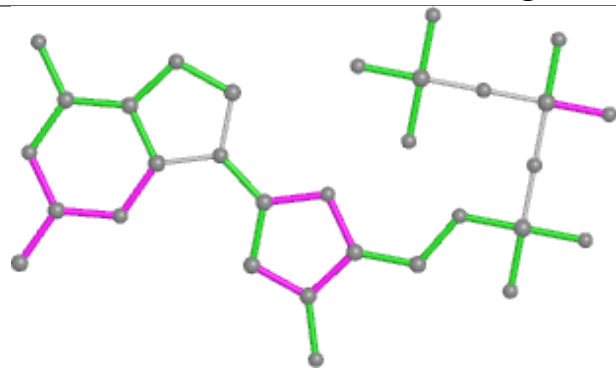


Torsions

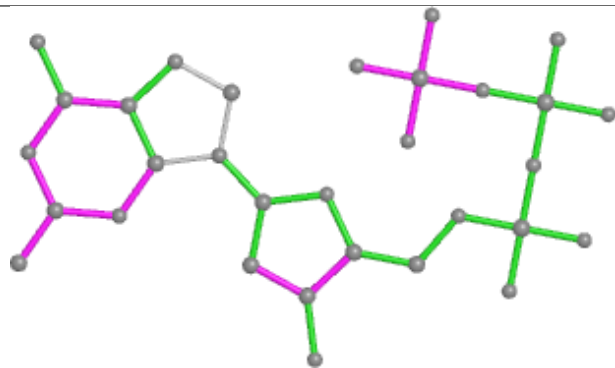


Rings

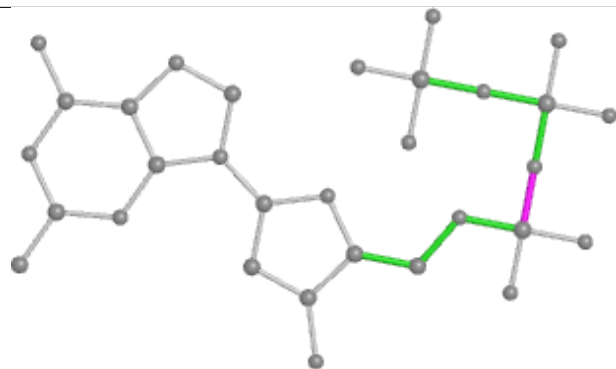
Ligand HF7 C 704



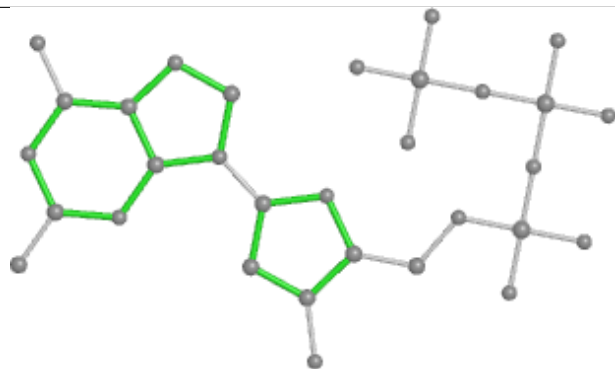
Bond lengths



Bond angles

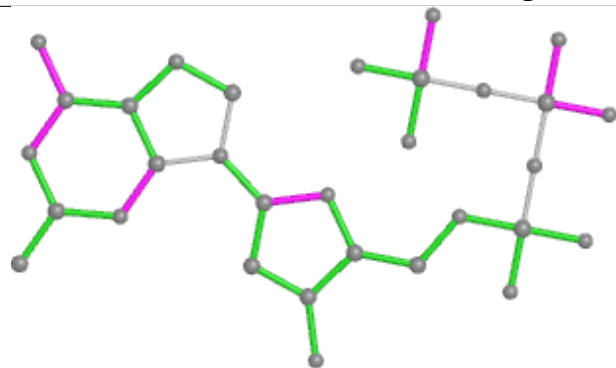


Torsions

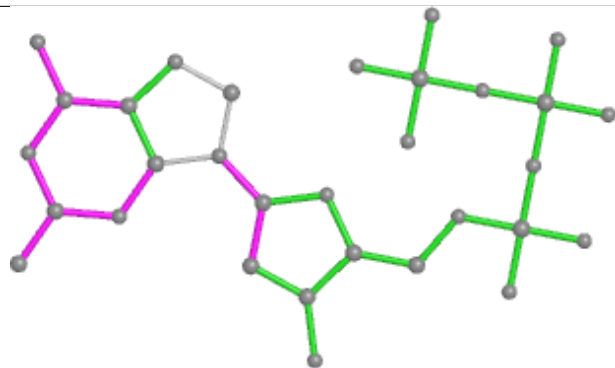


Rings

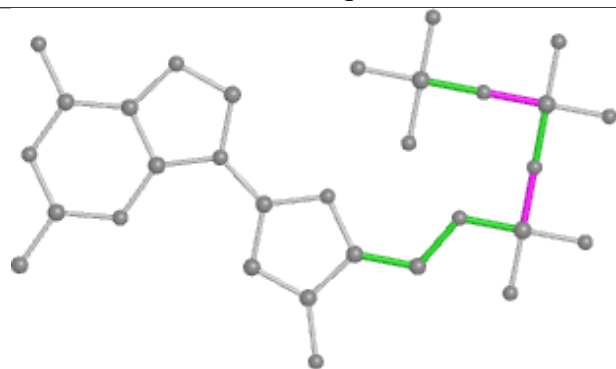
Ligand HF7 A 703



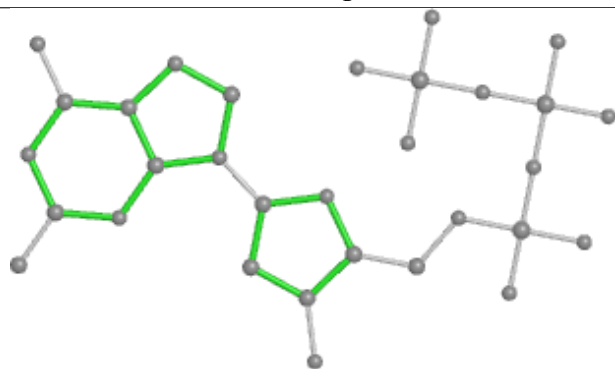
Bond lengths



Bond angles

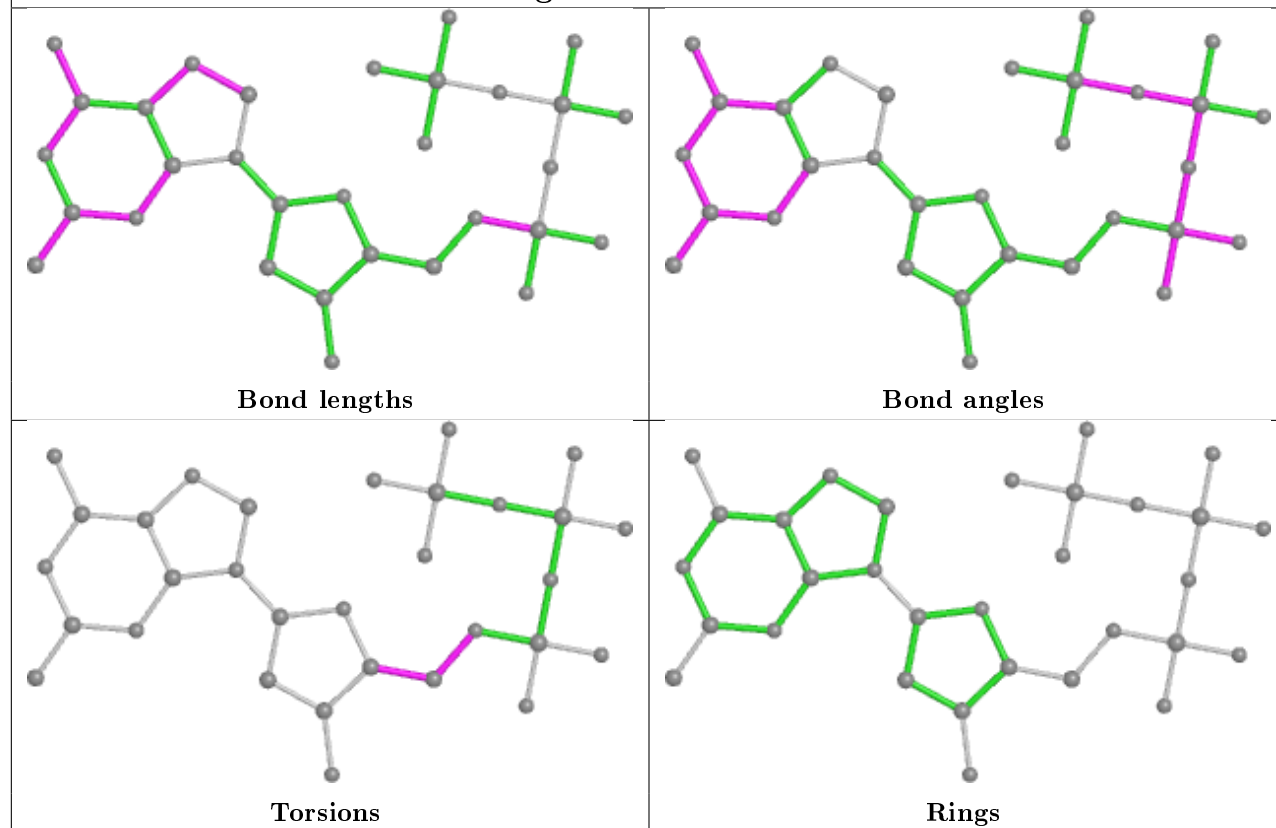


Torsions

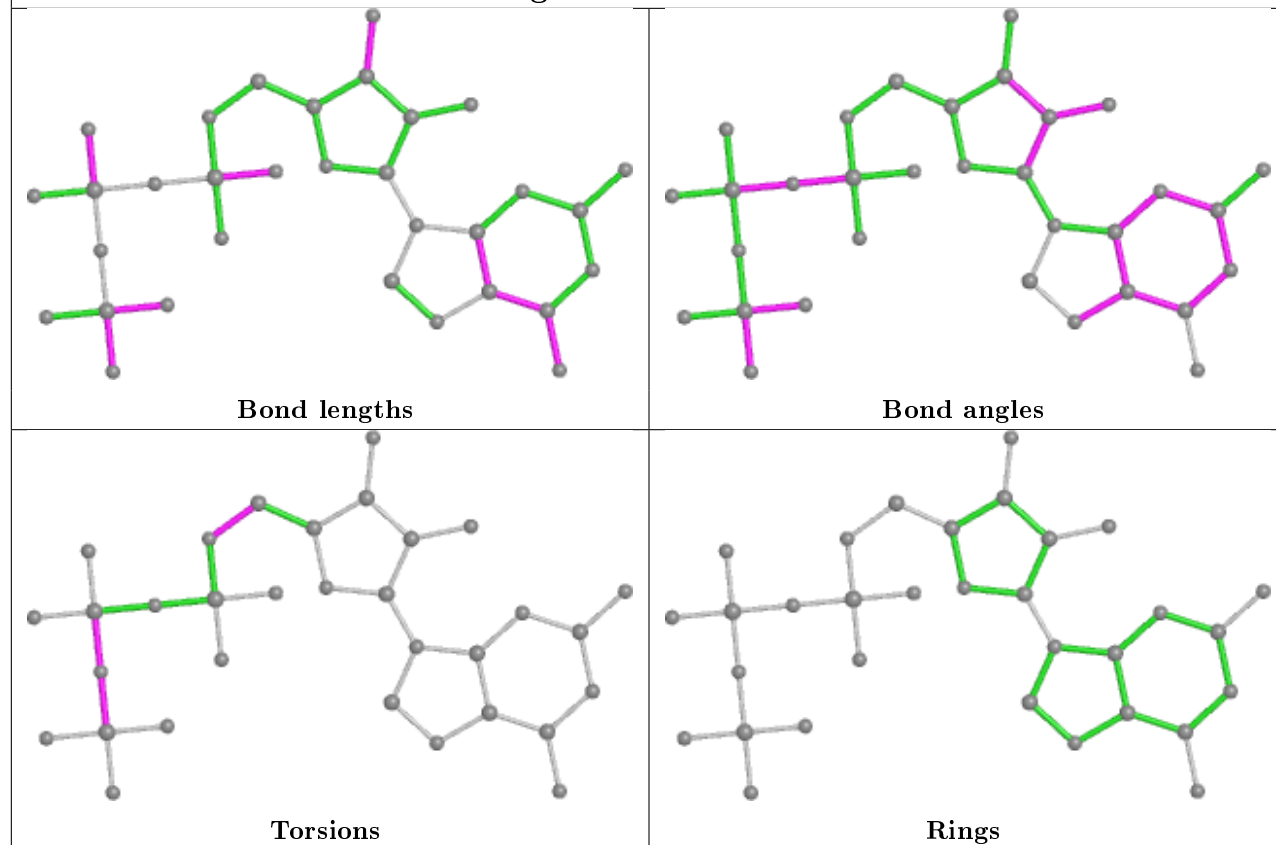


Rings

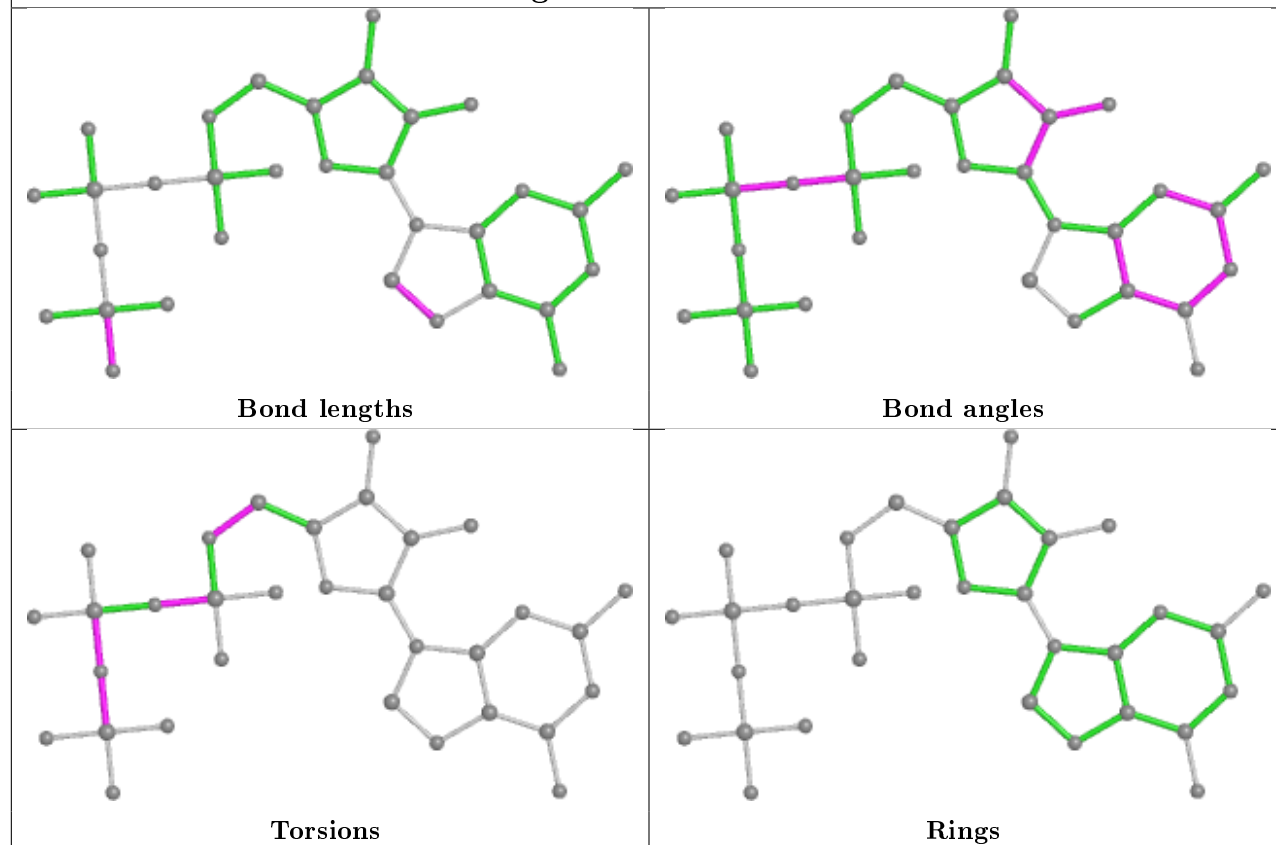
Ligand HF7 B 703



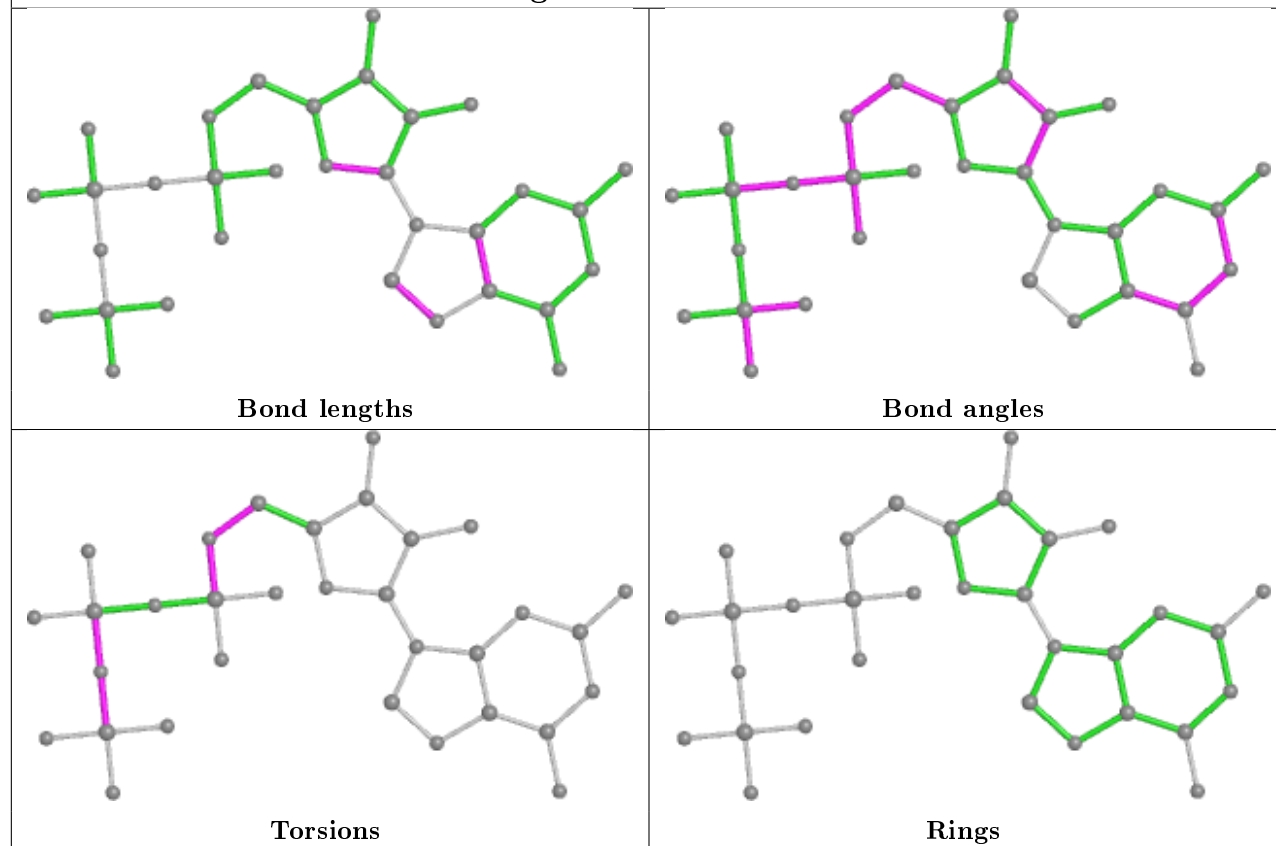
Ligand GTP A 702



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	481/550 (87%)	0.56	43 (8%) 9 8	11, 26, 82, 224	0
1	B	481/550 (87%)	0.14	35 (7%) 15 14	13, 30, 62, 92	0
1	C	481/550 (87%)	0.03	30 (6%) 20 19	14, 27, 63, 104	0
1	D	481/550 (87%)	-0.14	11 (2%) 60 59	11, 25, 53, 93	0
All	All	1924/2200 (87%)	0.15	119 (6%) 20 19	11, 27, 64, 224	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	591	ILE	29.0
1	A	584	GLY	25.4
1	A	590	LEU	24.8
1	A	589	PRO	19.4
1	A	586	VAL	18.1
1	A	598	TRP	17.3
1	A	588	ALA	17.0
1	A	587	ILE	15.6
1	A	592	THR	14.2
1	A	585	ASP	14.1
1	A	593	PRO	13.1
1	C	488	LEU	13.0
1	A	596	LYS	11.0
1	A	488	LEU	10.9
1	A	594	GLN	10.1
1	B	488	LEU	8.8
1	C	487	VAL	8.6
1	A	597	GLU	8.5
1	D	113	ASP	7.1
1	A	599	ASN	6.8
1	C	465	GLN	6.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	491	VAL	6.6
1	A	583	ASP	6.6
1	A	284	LEU	6.3
1	A	595	LYS	6.3
1	A	466	ILE	6.3
1	C	113	ASP	6.0
1	D	465	GLN	5.8
1	C	466	ILE	5.8
1	C	492	LYS	5.7
1	C	599	ASN	5.7
1	A	489	LEU	5.7
1	D	599	ASN	5.3
1	C	277	GLU	5.2
1	A	490	ASP	5.2
1	A	277	GLU	4.8
1	C	486	LYS	4.7
1	A	486	LYS	4.7
1	C	490	ASP	4.6
1	D	466	ILE	4.6
1	A	487	VAL	4.6
1	D	464	GLY	4.4
1	A	563	TYR	4.3
1	B	487	VAL	4.3
1	D	277	GLU	4.3
1	B	486	LYS	4.2
1	B	591	ILE	4.2
1	A	114	THR	4.2
1	A	113	ASP	4.2
1	B	491	VAL	4.2
1	B	113	ASP	4.1
1	B	590	LEU	4.0
1	B	490	ASP	4.0
1	B	599	ASN	4.0
1	B	484	LYS	4.0
1	B	114	THR	3.9
1	D	284	LEU	3.8
1	B	277	GLU	3.7
1	B	284	LEU	3.7
1	A	562	LEU	3.5
1	C	114	THR	3.5
1	A	582	GLN	3.5
1	C	284	LEU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	276	LEU	3.4
1	C	464	GLY	3.4
1	C	485	PRO	3.4
1	B	481	ALA	3.4
1	C	230	LYS	3.3
1	C	590	LEU	3.2
1	B	559	ARG	3.2
1	C	489	LEU	3.1
1	B	276	LEU	3.0
1	A	492	LYS	3.0
1	B	492	LYS	3.0
1	A	559	ARG	2.9
1	C	559	ARG	2.8
1	A	345	ASN	2.8
1	B	489	LEU	2.7
1	C	115	MET	2.7
1	A	484	LYS	2.7
1	C	560	LYS	2.7
1	D	276	LEU	2.7
1	B	562	LEU	2.6
1	C	484	LYS	2.6
1	D	230	LYS	2.6
1	C	262	GLU	2.6
1	B	285	TRP	2.6
1	A	463	THR	2.6
1	C	593	PRO	2.5
1	A	471	GLU	2.5
1	A	568	TYR	2.5
1	C	594	GLN	2.5
1	D	559	ARG	2.5
1	B	597	GLU	2.5
1	C	563	TYR	2.4
1	A	560	LYS	2.4
1	C	577	ASN	2.4
1	C	596	LYS	2.4
1	B	485	PRO	2.4
1	B	596	LYS	2.4
1	C	276	LEU	2.4
1	B	594	GLN	2.4
1	B	494	LYS	2.4
1	B	560	LYS	2.3
1	B	563	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	493	LEU	2.3
1	B	463	THR	2.3
1	B	482	SER	2.3
1	B	115	MET	2.2
1	B	587	ILE	2.2
1	C	591	ILE	2.2
1	B	465	GLN	2.2
1	B	480	VAL	2.2
1	A	325	ILE	2.2
1	D	484	LYS	2.1
1	B	570	VAL	2.1
1	C	403	GLY	2.1
1	A	580	LYS	2.1
1	A	470	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
5	NA	C	707	1/1	0.90	0.50	93,93,93,93	0
2	HF7	B	703	31/31	0.95	0.09	20,28,39,44	0
2	HF7	C	701	31/31	0.96	0.08	17,25,33,36	0
2	HF7	D	701	31/31	0.96	0.09	13,22,31,35	0
4	MG	B	704	1/1	0.97	0.04	35,35,35,35	0
2	HF7	A	705	31/31	0.97	0.07	15,24,30,34	0
4	MG	A	706	1/1	0.98	0.05	30,30,30,30	0
4	MG	D	704	1/1	0.99	0.02	24,24,24,24	0
4	MG	A	701	1/1	0.99	0.02	16,16,16,16	0

Continued on next page...

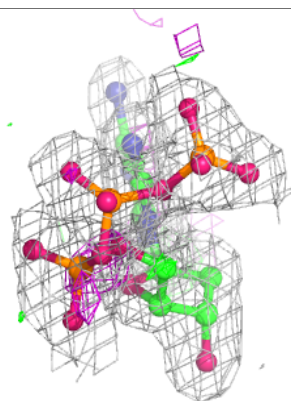
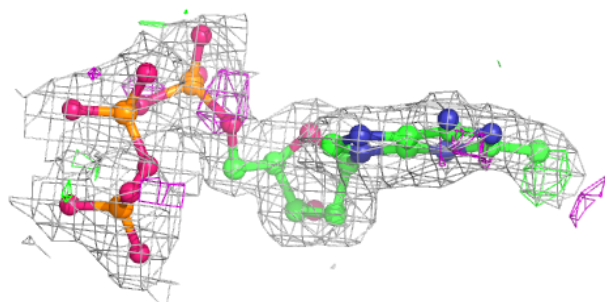
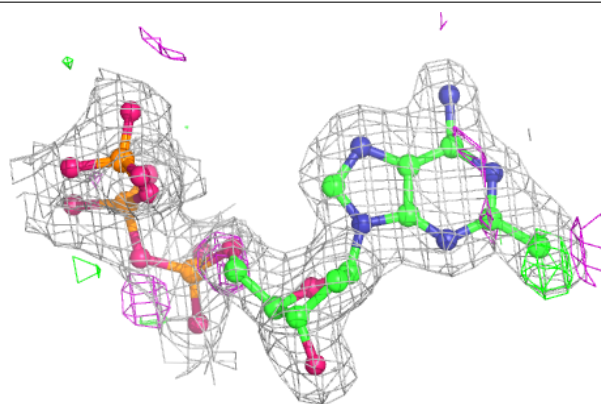
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	HF7	D	702	31/31	0.99	0.08	13,16,19,22	0
4	MG	C	706	1/1	0.99	0.02	36,36,36,36	0
4	MG	C	702	1/1	0.99	0.07	20,20,20,20	0
2	HF7	C	704	31/31	0.99	0.09	10,13,16,16	0
2	HF7	A	703	31/31	0.99	0.08	14,17,19,21	0
2	HF7	B	701	31/31	0.99	0.08	13,16,18,21	0
4	MG	C	705	1/1	0.99	0.05	15,15,15,15	0
3	GTP	C	703	32/32	0.99	0.07	13,16,22,24	0
3	GTP	A	702	32/32	0.99	0.07	13,15,23,24	0
3	GTP	B	702	32/32	0.99	0.06	17,18,24,25	0
3	GTP	D	703	32/32	0.99	0.06	11,13,17,18	0
4	MG	A	704	1/1	1.00	0.02	18,18,18,18	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.

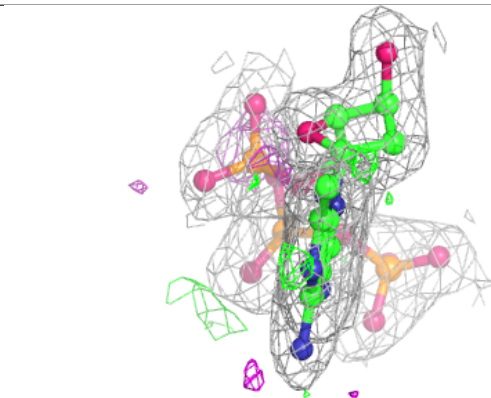
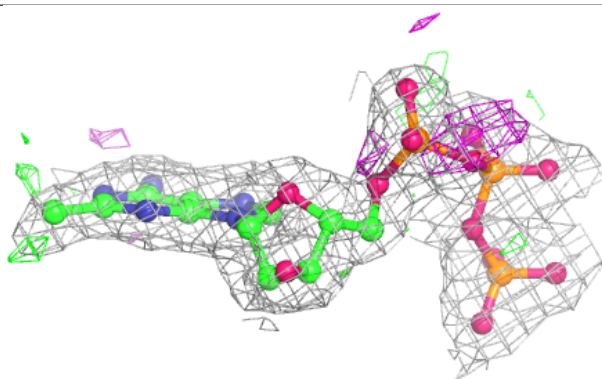
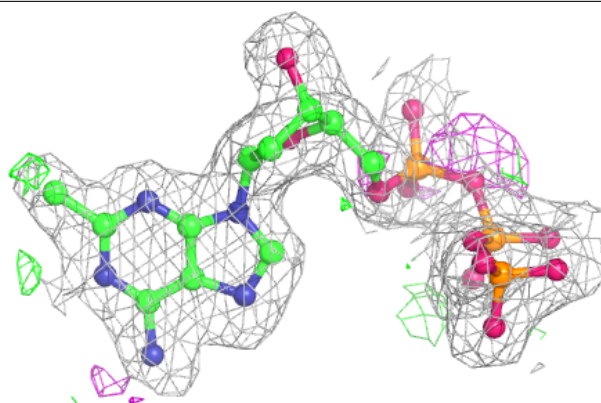
Electron density around HF7 B 703:

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

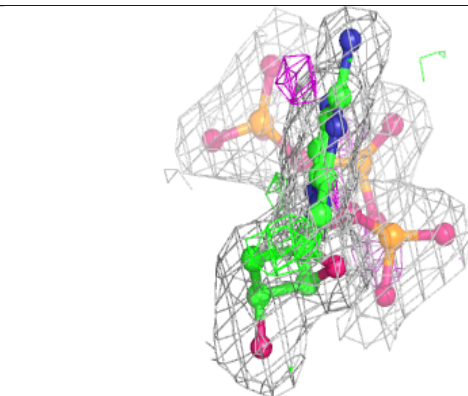
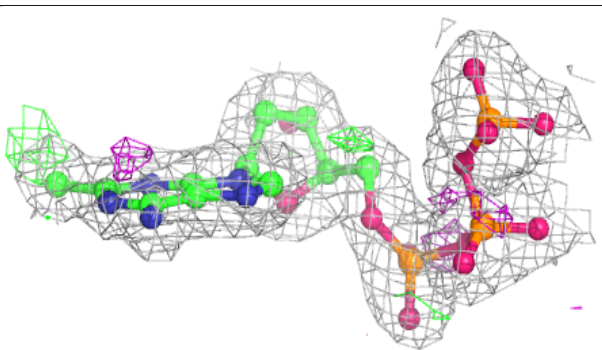
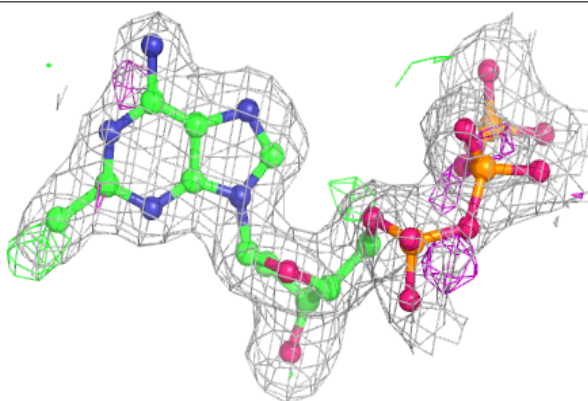


Electron density around HF7 C 701:

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

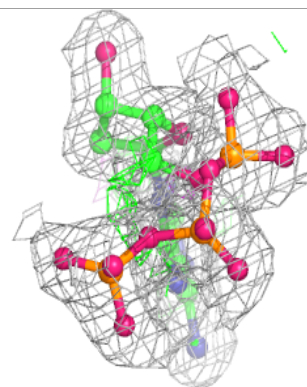
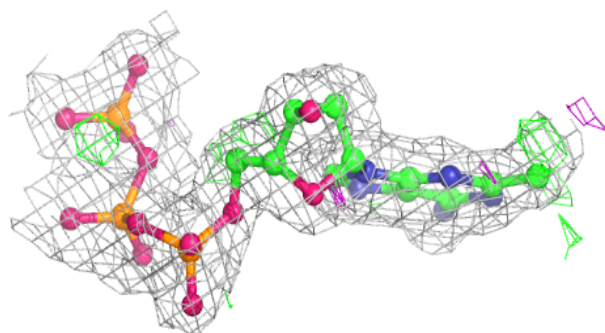
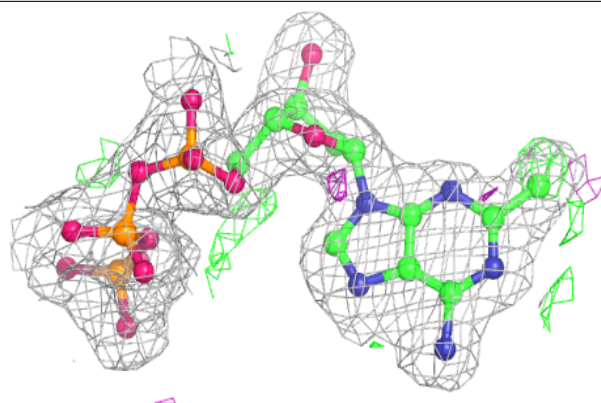
**Electron density around HF7 D 701:**

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

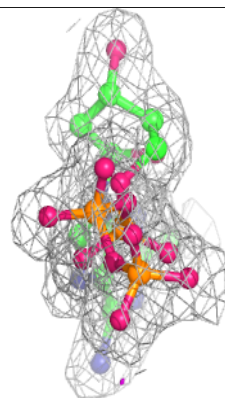
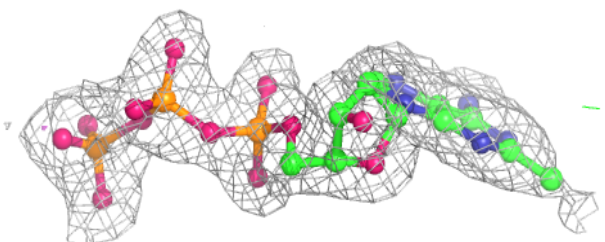
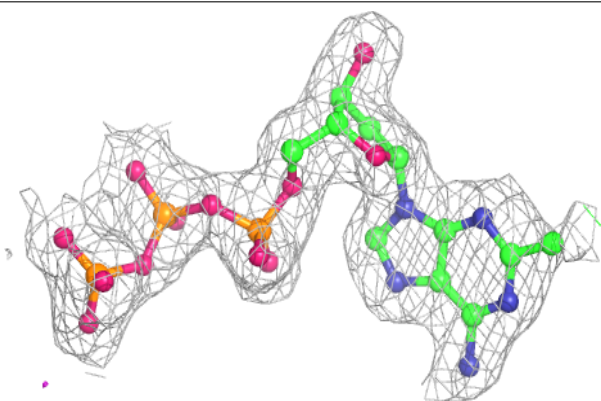


Electron density around HF7 A 705:

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

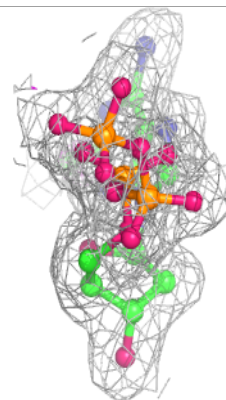
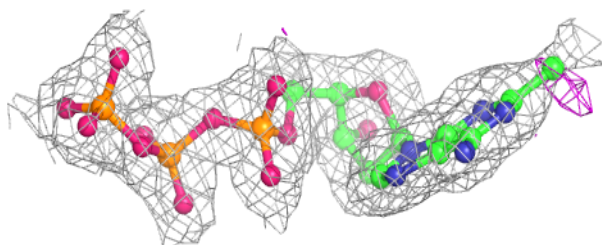
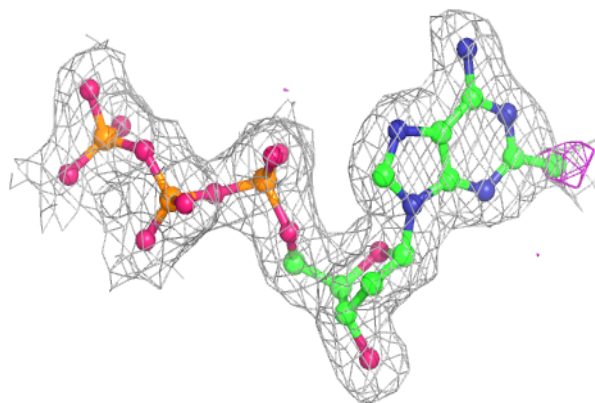
**Electron density around HF7 D 702:**

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

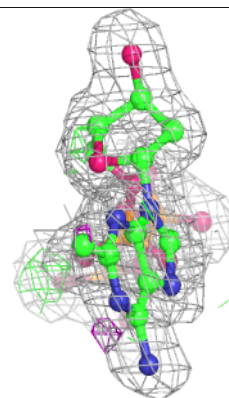
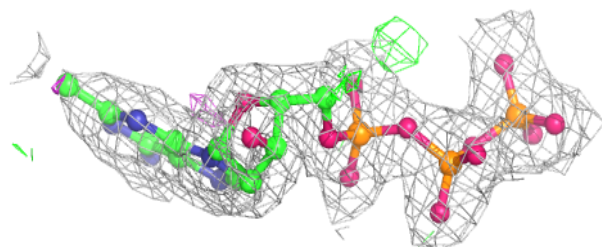
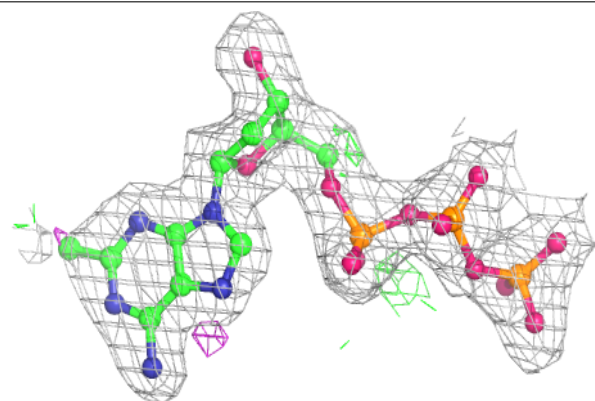


Electron density around HF7 C 704:

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

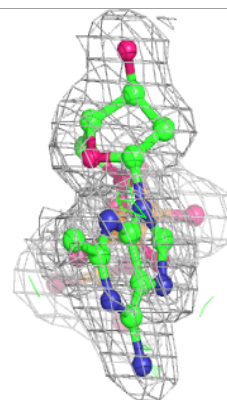
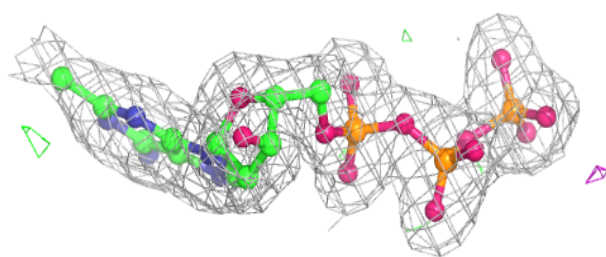
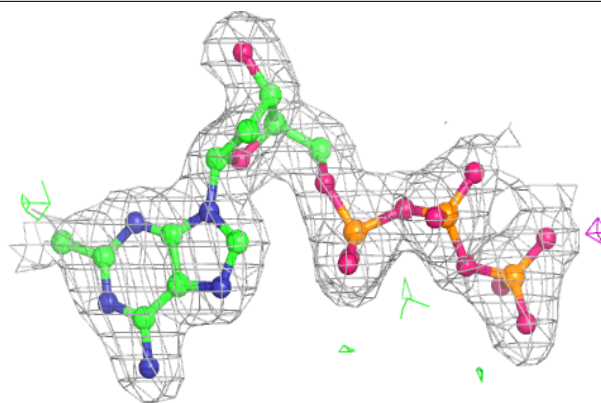
**Electron density around HF7 A 703:**

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

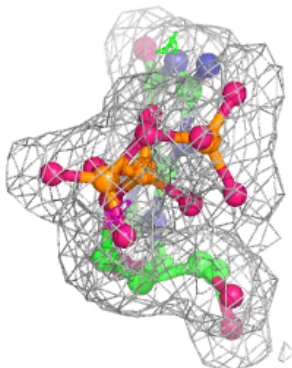
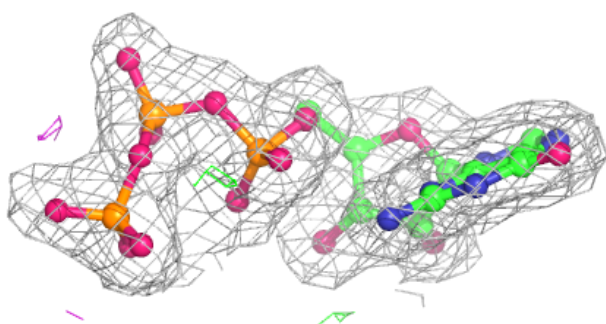
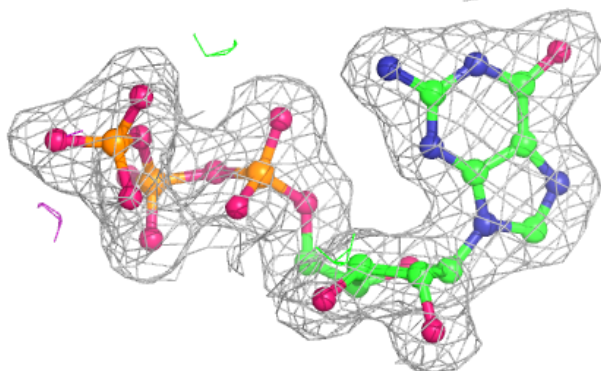


Electron density around HF7 B 701:

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

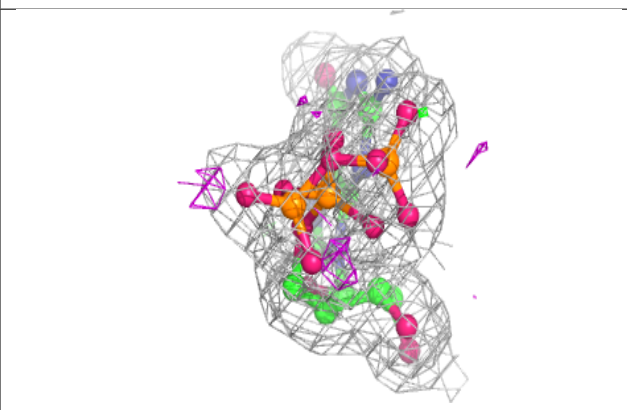
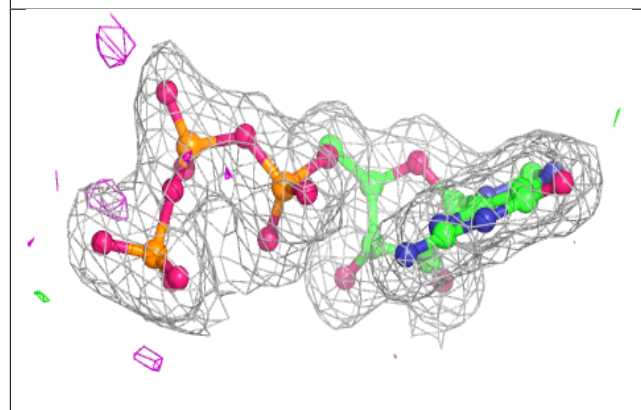
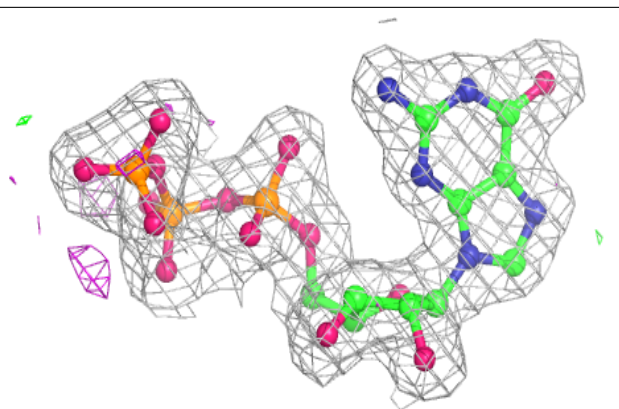
**Electron density around GTP C 703:**

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

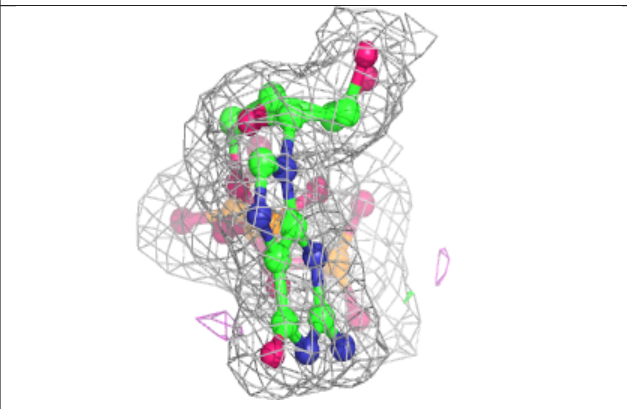
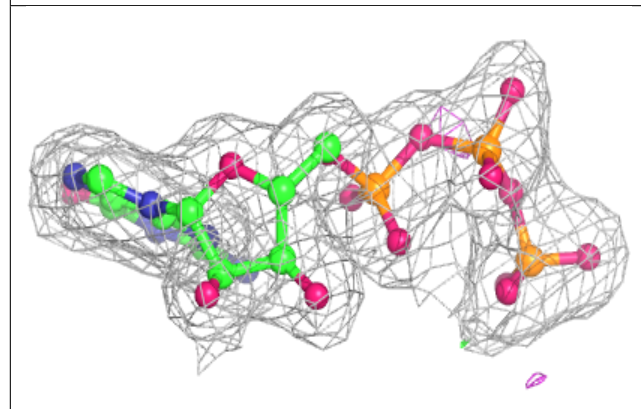
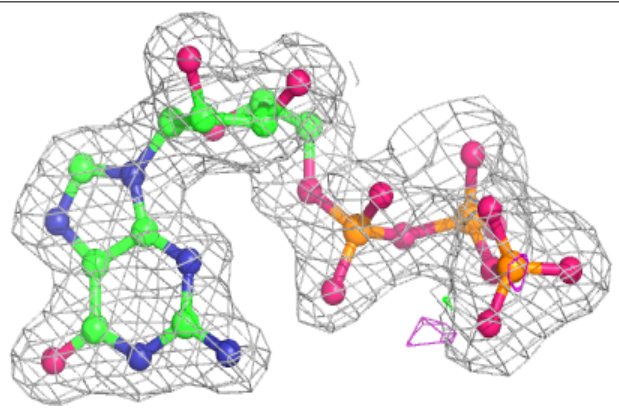


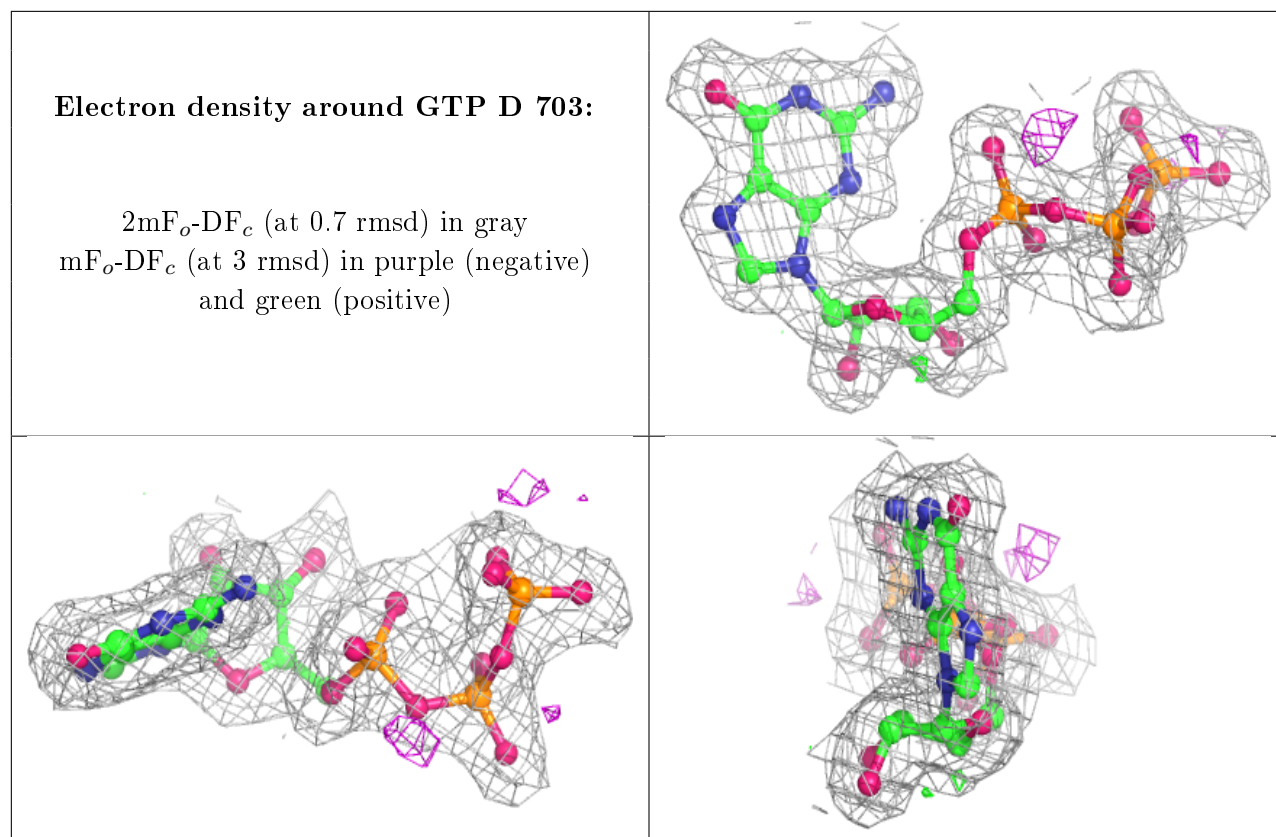
Electron density around GTP A 702:

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

**Electron density around GTP 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.