



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:32 PM UTC

PDB ID : 6DW4 / pdb_00006dw4
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.; Ferreira, 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) 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

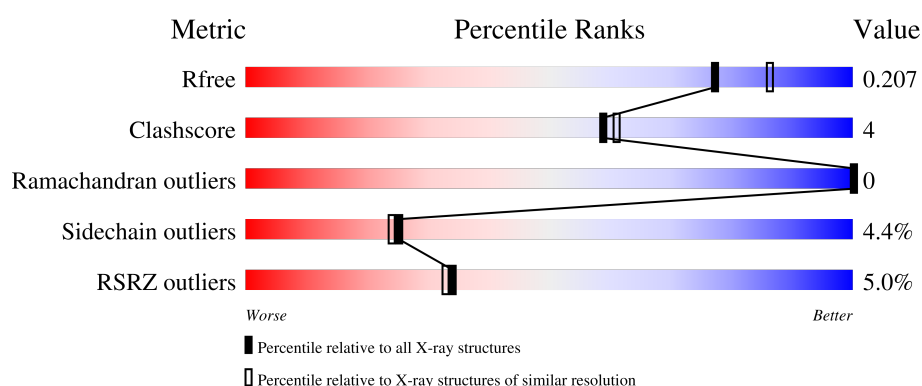
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 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	8% 77% 9% • 13%
1	B	550	5% 77% 9% • 13%
1	C	550	3% 78% 9% • 13%
1	D	550	2% 77% 9% • 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
5	NA	C	707	-	-	-	X

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

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

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

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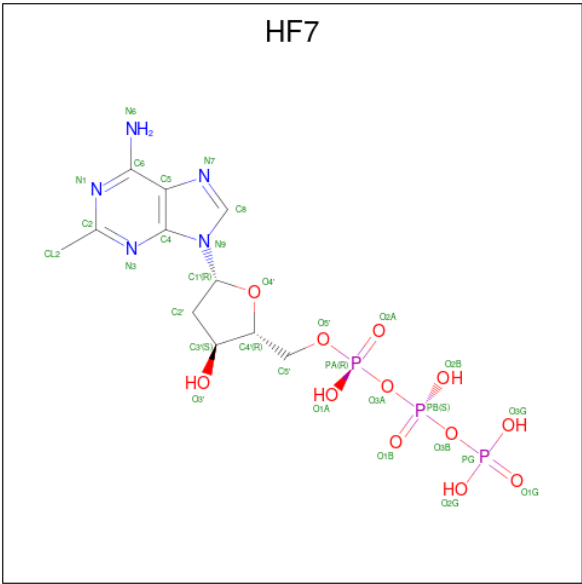
Chain	Residue	Modelled	Actual	Comment	Reference
B	106	MET	-	expression tag	UNP Q9Y3Z3
B	107	GLY	-	expression tag	UNP Q9Y3Z3
B	108	ARG	-	expression tag	UNP Q9Y3Z3
B	109	ASP	-	expression tag	UNP Q9Y3Z3
B	110	PRO	-	expression tag	UNP Q9Y3Z3
B	111	ASN	-	expression tag	UNP Q9Y3Z3
B	112	SER	-	expression tag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

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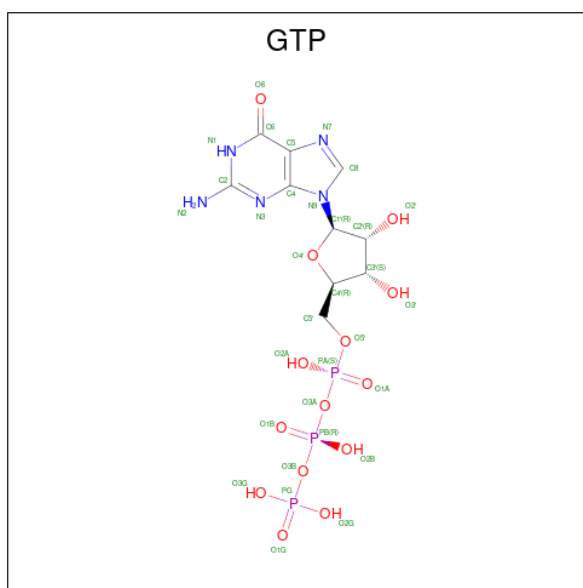
Chain	Residue	Modelled	Actual	Comment	Reference
A	110	PRO	-	expression tag	UNP Q9Y3Z3
A	111	ASN	-	expression tag	UNP Q9Y3Z3
A	112	SER	-	expression tag	UNP Q9Y3Z3
A	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
A	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3

- Molecule 2 is 2'-deoxy-2-methyladenosine 5'-(tetrahydrogen triphosphate) (CCD ID: HF7) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	D	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	C	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	C	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	A	1	Total	C	N	O	P	0	0
			31	11	5	12	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	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 (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

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

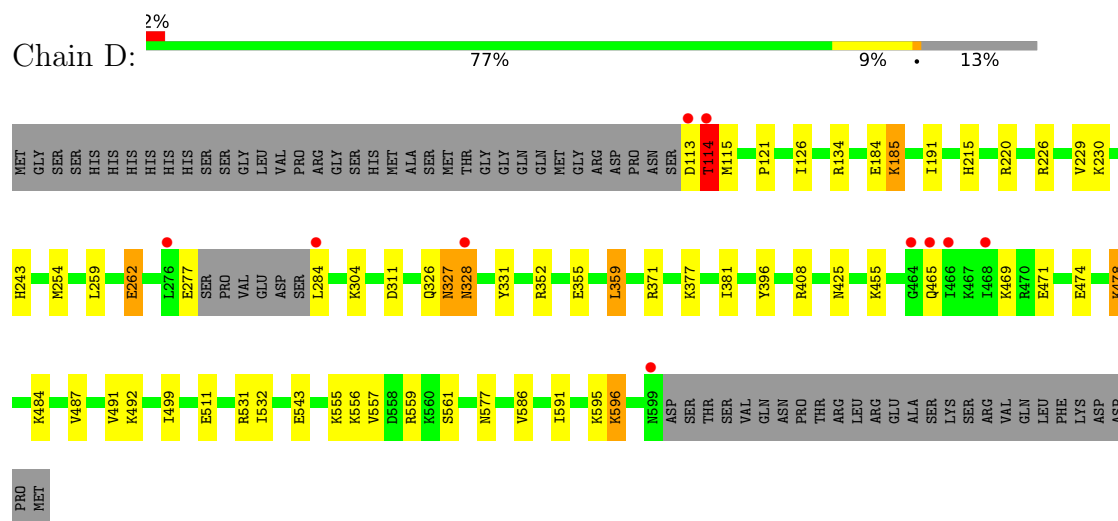
- Molecule 6 is water.

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

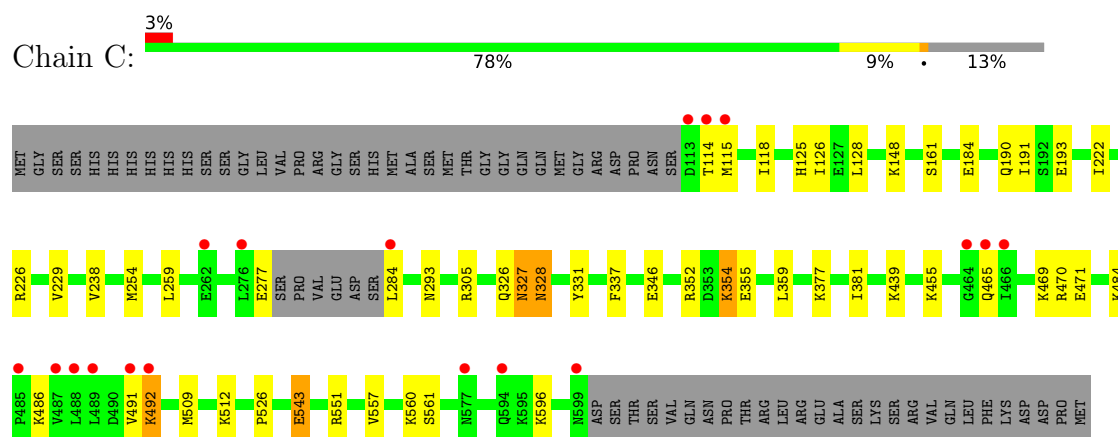
3 Residue-property plots [i](#)

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

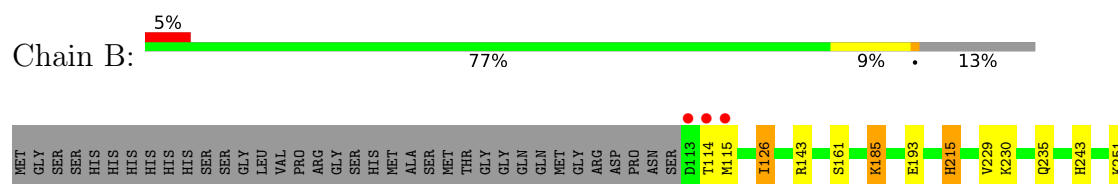
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

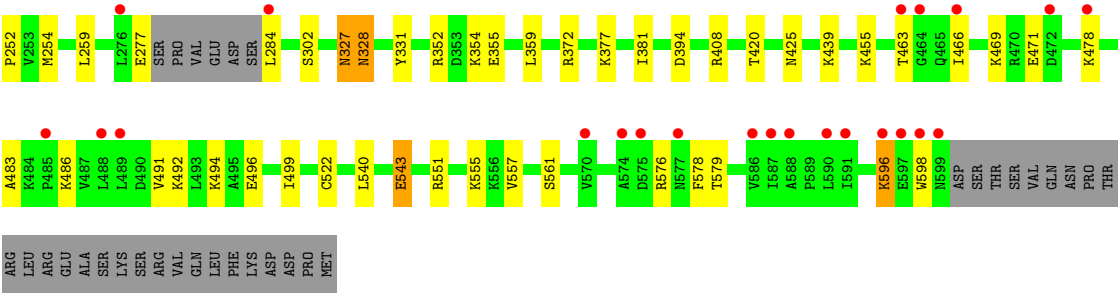


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

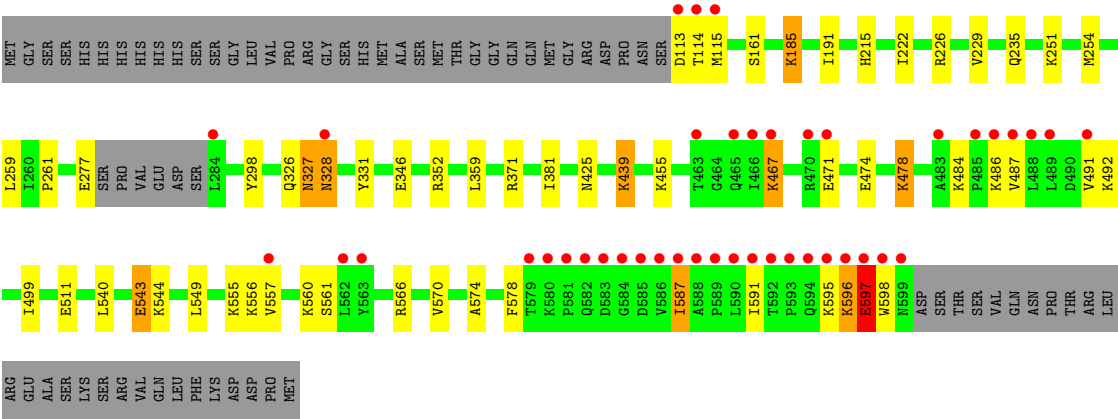
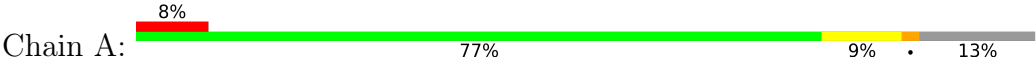


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





● Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.32Å 142.27Å 98.44Å 90.00° 114.08° 90.00°	Depositor
Resolution (Å)	89.87 – 1.99 89.87 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.0 (89.87-1.99) 94.9 (89.87-2.00)	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 (4.76%)	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)	0.33 , 40.8	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, NA, HF7, GTP

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	1.30	5/4040 (0.1%)	1.16	11/5453 (0.2%)
1	B	1.24	5/4040 (0.1%)	1.10	7/5453 (0.1%)
1	C	1.26	13/4051 (0.3%)	1.13	4/5468 (0.1%)
1	D	1.29	11/4062 (0.3%)	1.12	9/5483 (0.2%)
All	All	1.27	34/16193 (0.2%)	1.13	31/21857 (0.1%)

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 (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	327	ASN	C-O	-9.51	1.12	1.24
1	A	161	SER	CB-OG	9.32	1.60	1.42
1	A	327	ASN	C-O	-7.94	1.14	1.24
1	D	532	ILE	C-O	-7.57	1.15	1.24
1	C	327	ASN	C-O	-7.19	1.15	1.24
1	C	327	ASN	CA-C	6.89	1.61	1.52
1	B	161	SER	CB-OG	6.74	1.55	1.42
1	D	327	ASN	CA-C	6.74	1.61	1.52
1	C	125	HIS	C-O	-6.64	1.16	1.24
1	A	191	ILE	C-O	-6.58	1.17	1.24
1	C	526	PRO	N-CA	-6.40	1.39	1.47
1	A	327	ASN	CA-C	6.39	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	304	LYS	C-O	-6.12	1.16	1.24
1	C	161	SER	CB-OG	6.10	1.54	1.42
1	B	327	ASN	C-O	-6.08	1.16	1.24
1	D	191	ILE	C-O	-6.00	1.18	1.24
1	C	191	ILE	C-O	-5.82	1.18	1.24
1	C	222	ILE	CA-C	5.76	1.57	1.52
1	C	190	GLN	C-O	-5.70	1.16	1.23
1	C	328	ASN	CA-C	5.68	1.61	1.52
1	A	222	ILE	CA-C	5.58	1.57	1.52
1	C	184	GLU	C-O	-5.57	1.17	1.24
1	B	328	ASN	CA-C	5.53	1.60	1.52
1	D	121	PRO	C-O	-5.53	1.17	1.24
1	D	327	ASN	CG-ND2	5.46	1.44	1.33
1	D	531	ARG	C-O	-5.40	1.17	1.23
1	D	371	ARG	C-O	-5.39	1.17	1.24
1	B	302	SER	C-O	-5.38	1.17	1.23
1	D	184	GLU	C-O	-5.31	1.18	1.24
1	C	238	VAL	CA-CB	5.30	1.60	1.54
1	C	352	ARG	CA-C	5.20	1.59	1.52
1	C	354	LYS	C-O	-5.16	1.17	1.24
1	D	243	HIS	CA-C	5.02	1.59	1.52
1	B	243	HIS	CA-C	5.01	1.59	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	596	LYS	N-CA-C	7.36	120.18	111.71
1	A	352	ARG	CG-CD-NE	-6.52	97.65	112.00
1	C	328	ASN	N-CA-C	6.50	120.91	112.92
1	D	596	LYS	N-CA-C	6.41	119.25	111.82
1	C	543	GLU	CB-CG-CD	6.30	123.32	112.60
1	B	352	ARG	CG-CD-NE	-6.30	98.14	112.00
1	D	328[A]	ASN	N-CA-C	6.26	121.06	113.17
1	D	328[B]	ASN	N-CA-C	6.26	121.06	113.17
1	C	352	ARG	NE-CZ-NH2	-6.15	113.67	119.20
1	A	226	ARG	NE-CZ-NH2	6.08	124.67	119.20
1	A	328	ASN	N-CA-C	6.02	120.32	112.92
1	D	114	THR	N-CA-CB	5.96	119.57	110.70
1	A	597	GLU	CA-CB-CG	5.82	125.74	114.10
1	B	543	GLU	CB-CG-CD	5.75	122.37	112.60
1	A	215	HIS	N-CA-C	5.71	119.34	112.38
1	A	543	GLU	CB-CG-CD	5.63	122.17	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	352	ARG	CG-CD-NE	-5.55	99.80	112.00
1	D	215	HIS	N-CA-C	5.53	119.12	112.38
1	B	328	ASN	N-CA-C	5.46	119.93	112.88
1	B	543	GLU	N-CA-CB	5.41	118.88	110.44
1	D	226	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	B	215	HIS	N-CA-C	5.34	118.90	112.38
1	A	439	LYS	CD-CE-NZ	5.33	128.94	111.90
1	A	596	LYS	N-CA-C	5.26	118.95	112.54
1	A	587	ILE	CB-CA-C	5.24	126.45	111.42
1	B	576	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	D	220	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	A	439	LYS	CB-CG-CD	5.17	123.18	111.30
1	A	235	GLN	CB-CG-CD	5.15	121.36	112.60
1	D	262	GLU	N-CA-C	-5.14	105.37	110.97
1	C	226	ARG	NE-CZ-NH2	5.05	123.75	119.20

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3948	0	3930	42	0
1	B	3948	0	3930	32	0
1	C	3958	0	3936	29	1
1	D	3970	0	3944	38	1
2	A	62	0	0	3	0
2	B	62	0	0	4	0
2	C	62	0	0	2	0
2	D	62	0	0	3	0
3	A	32	0	12	0	0
3	B	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	12	0
6	D	229	0	0	21	0
All	All	17077	0	15788	141	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 (141) 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:D:511[A]:GLU:H	1:D:511[A]:GLU:CD	1.56	1.09
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
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:D:328[B]:ASN:ND2	6:D:801:HOH:O	1.93	0.99
1:C:354:LYS:HE2	6:C:801:HOH:O	1.59	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
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:511[A]:GLU:CD	1:D:511[A]:GLU:N	2.34	0.85
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:909:HOH:O	1:B:328:ASN:HB3	1.80	0.82
1:D:328[B]:ASN:CG	6:D:801:HOH:O	2.17	0.81
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:B:578:PHE:C	6:B:801:HOH:O	2.25	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
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:D:455:LYS:HG2	1:D:557:VAL:HG12	1.76	0.67
1:B:455:LYS:HG2	1:B:557:VAL:HG12	1.75	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:ARG:HE	1:A:587:ILE:HG13	1.68	0.56
1:D:254:MET:CE	6:D:1029:HOH:O	2.40	0.56
1:D:474:GLU:O	1:D:478:LYS:NZ	2.34	0.55
1:A:574:ALA:HA	1:A:595:LYS:HE3	1.88	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:B:215:HIS:NE2	2:B:703:HF7:O2A	2.42	0.53
1:A:327:ASN:HA	6:A:848:HOH:O	2.08	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:D:327:ASN:HA	6:D:851:HOH:O	2.11	0.51
1:B:491:VAL:HG21	1:B:561:SER:HA	1.92	0.51
1:C:354:LYS:NZ	6:C:801:HOH:O	2.04	0.51
1:D:511[A]:GLU:N	1:D:511[A]:GLU:OE2	2.40	0.50
1:C:254:MET:HE3	1:C:259:LEU:HD23	1.93	0.50
1:D:114:THR:HG22	6:D:1002:HOH:O	2.11	0.50
2:C:701:HF7:O1A	6:C:804:HOH:O	2.19	0.50
1:A:574:ALA:O	1:A:595:LYS:CE	2.59	0.50
1:A:566:ARG:CZ	1:A:587:ILE:HD11	2.44	0.48
1:B:331:TYR:CD2	1:B:331:TYR:C	2.92	0.47
1:D:331:TYR:CD2	1:D:331:TYR:C	2.93	0.47
1:D:487:VAL:HG23	1:D:591:ILE:HD11	1.97	0.47
1:C:327:ASN:O	1:A:326:GLN:HG2	2.15	0.47
1:A:261:PRO:HD2	6:A:850:HOH:O	2.15	0.47
1:B:254:MET:HE3	1:B:259:LEU:HD23	1.97	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:D:134:ARG:CD	6:D:1014:HOH:O	2.64	0.46
1:C:354:LYS:HG3	1:C:355:GLU:OE2	2.16	0.46
1:A:331:TYR:CD2	1:A:331:TYR:C	2.93	0.46
1:D:586:VAL:CG1	1:B:522[A]:CYS:SG	2.97	0.46
1:B:579:THR:C	6:B:801:HOH:O	2.58	0.46
1:A:467:LYS:HE3	6:A:861:HOH:O	2.16	0.45
1:C:331:TYR:CD2	1:C:331:TYR:C	2.94	0.45
1:D:381:ILE:HD12	1:D:381:ILE:HA	1.87	0.45
1:C:115:MET:SD	1:C:115:MET:C	3.00	0.45
1:C:148:LYS:NZ	6:C:810:HOH:O	2.44	0.45
1:D:408:ARG:NH2	6:D:806:HOH:O	2.30	0.45
1:C:126:ILE:HD13	1:C:126:ILE:HG21	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:ASP:O	1:B:408:ARG:HD2	2.17	0.44
1:B:115:MET:C	1:B:115:MET:SD	3.00	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:A:254:MET:HE3	1:A:259:LEU:HD23	1.99	0.43
1:A:115:MET:C	1:A:115:MET:SD	3.02	0.43
1:D:254:MET:HE3	1:D:259:LEU:HD23	2.00	0.42
1:B:251:LYS:HB2	1:B:252:PRO:HD3	2.01	0.42
1:A:346:GLU:HA	6:A:833:HOH:O	2.18	0.42
1:C:346:GLU:CD	6:C:836:HOH:O	2.62	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:D:499:ILE:HD11	1:D:555:LYS:HE2	2.02	0.41
1:A:185:LYS:HE2	6:A:995:HOH:O	2.19	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: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
2:D:702:HF7:N6	1:B:372:ARG:HG2	2.35	0.41
1:B:126:ILE:HD13	1:B:126:ILE:HG21	1.64	0.41
1:D:262:GLU:H	1:D:262:GLU:CD	2.29	0.41
1:B:551:ARG:NH1	6:B:825:HOH:O	2.52	0.41
1:D:115:MET:C	1:D:115:MET:SD	3.03	0.41
1:A:566:ARG:CZ	1:A:587:ILE:HG13	2.51	0.41
1:B:381:ILE:HD12	1:B:381:ILE:HA	1.89	0.41
1:A:381:ILE:HD12	1:A:381:ILE:HA	1.83	0.41
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:509:MET:HE2	1:C:512:LYS:HD2	2.04	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%)	410 (96%)	19 (4%)	25	24
1	B	429/488 (88%)	407 (95%)	22 (5%)	21	19
1	C	430/488 (88%)	413 (96%)	17 (4%)	28	27
1	D	432/488 (88%)	414 (96%)	18 (4%)	26	25
All	All	1720/1952 (88%)	1644 (96%)	76 (4%)	25	24

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	113	ASP
1	D	114	THR
1	D	185	LYS
1	D	229	VAL
1	D	230	LYS
1	D	277	GLU
1	D	284	LEU
1	D	359	LEU
1	D	377	LYS
1	D	465	GLN
1	D	469	LYS
1	D	471	GLU
1	D	478	LYS
1	D	484	LYS
1	D	492	LYS
1	D	556	LYS
1	D	559	ARG
1	D	596	LYS
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	469	LYS
1	C	470	ARG
1	C	471	GLU
1	C	484	LYS
1	C	486	LYS
1	C	492	LYS
1	C	560	LYS
1	C	596	LYS
1	B	114	THR
1	B	126	ILE
1	B	185	LYS
1	B	193	GLU
1	B	229	VAL
1	B	230	LYS
1	B	277	GLU
1	B	284	LEU

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Mol	Chain	Res	Type
1	B	359	LEU
1	B	377	LYS
1	B	425	ASN
1	B	439	LYS
1	B	463	THR
1	B	469	LYS
1	B	471	GLU
1	B	478	LYS
1	B	486	LYS
1	B	492	LYS
1	B	494	LYS
1	B	496	GLU
1	B	540	LEU
1	B	596	LYS
1	A	113	ASP
1	A	114	THR
1	A	185	LYS
1	A	229	VAL
1	A	277	GLU
1	A	359	LEU
1	A	439	LYS
1	A	467	LYS
1	A	471	GLU
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	556	LYS
1	A	560	LYS
1	A	596	LYS
1	A	597	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	163	ASN
1	D	447	GLN
1	D	452	ASN
1	D	571	GLN
1	D	594	GLN

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Mol	Chain	Res	Type
1	C	149	GLN
1	C	163	ASN
1	C	190	GLN
1	C	248	ASN
1	C	367	ASN
1	C	527	ASN
1	C	535	ASN
1	C	539	GLN
1	C	571	GLN
1	C	594	GLN
1	B	149	GLN
1	B	190	GLN
1	B	235	GLN
1	B	248	ASN
1	B	321	HIS
1	B	364	HIS
1	B	367	ASN
1	B	535	ASN
1	B	571	GLN
1	B	594	GLN
1	A	149	GLN
1	A	163	ASN
1	A	321	HIS
1	A	326	GLN
1	A	364	HIS
1	A	375	GLN
1	A	380	ASN
1	A	425	ASN
1	A	447	GLN
1	A	452	ASN
1	A	510	GLN
1	A	567	GLN
1	A	571	GLN
1	A	594	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
2	HF7	C	704	4	32,33,33	2.28	12 (37%)	48,52,52	2.23	15 (31%)
2	HF7	B	703	4	32,33,33	2.81	9 (28%)	48,52,52	2.65	12 (25%)
3	GTP	C	703	4	33,34,34	1.86	6 (18%)	50,54,54	1.97	15 (30%)
3	GTP	B	702	4	33,34,34	1.82	5 (15%)	50,54,54	1.68	12 (24%)
3	GTP	A	702	4	33,34,34	1.55	9 (27%)	50,54,54	1.62	10 (20%)
3	GTP	D	703	4	33,34,34	1.67	6 (18%)	50,54,54	1.42	7 (14%)
2	HF7	B	701	4	32,33,33	1.60	9 (28%)	48,52,52	2.23	11 (22%)
2	HF7	D	701	4	32,33,33	2.99	15 (46%)	48,52,52	2.62	20 (41%)
2	HF7	A	703	4	32,33,33	2.07	10 (31%)	48,52,52	2.17	13 (27%)
2	HF7	C	701	4	32,33,33	2.40	11 (34%)	48,52,52	2.29	14 (29%)
2	HF7	D	702	4	32,33,33	2.19	10 (31%)	48,52,52	2.95	14 (29%)
2	HF7	A	705	4	32,33,33	2.78	12 (37%)	48,52,52	2.72	17 (35%)

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	HF7	C	704	4	-	3/22/34/34	0/3/3/3
2	HF7	B	703	4	-	3/22/34/34	0/3/3/3
3	GTP	C	703	4	-	5/22/38/38	0/3/3/3
3	GTP	B	702	4	-	6/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GTP	A	702	4	-	5/22/38/38	0/3/3/3
3	GTP	D	703	4	-	4/22/38/38	0/3/3/3
2	HF7	B	701	4	-	5/22/34/34	0/3/3/3
2	HF7	D	701	4	-	4/22/34/34	0/3/3/3
2	HF7	A	703	4	-	2/22/34/34	0/3/3/3
2	HF7	C	701	4	-	3/22/34/34	0/3/3/3
2	HF7	D	702	4	-	2/22/34/34	0/3/3/3
2	HF7	A	705	4	-	2/22/34/34	0/3/3/3

All (114) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	HF7	PB-O3B	10.19	1.70	1.59
2	B	703	HF7	PB-O3B	7.74	1.67	1.59
2	A	705	HF7	PB-O3B	7.51	1.67	1.59
2	B	703	HF7	PA-O3A	7.09	1.67	1.59
2	A	705	HF7	PA-O3A	6.73	1.66	1.59
3	B	702	GTP	PB-O3A	6.70	1.66	1.59
2	A	703	HF7	C6-N1	-6.49	1.26	1.35
2	D	702	HF7	PB-O3A	6.09	1.66	1.59
2	A	705	HF7	C6-N6	5.97	1.49	1.34
3	C	703	GTP	PA-O3A	5.74	1.65	1.59
2	C	701	HF7	PB-O3B	5.73	1.65	1.59
2	C	701	HF7	PA-O3A	5.46	1.65	1.59
2	B	703	HF7	C6-N6	5.44	1.48	1.34
2	C	704	HF7	PB-O3A	5.32	1.65	1.59
3	C	703	GTP	PB-O3B	-5.06	1.54	1.59
3	D	703	GTP	PA-O3A	5.01	1.64	1.59
2	D	701	HF7	CL2-C2	5.01	1.63	1.49
2	D	702	HF7	C6-N6	4.93	1.46	1.34
2	C	704	HF7	O4'-C1'	4.92	1.53	1.42
2	D	701	HF7	C6-N6	4.88	1.46	1.34
2	A	705	HF7	PB-O3A	4.67	1.64	1.59
2	C	704	HF7	C2-N1	-4.53	1.26	1.34
2	A	705	HF7	C5-N7	4.42	1.47	1.39
2	C	701	HF7	C5-N7	4.40	1.47	1.39
2	C	701	HF7	C6-N6	4.39	1.45	1.34
2	D	702	HF7	C6-N1	-4.38	1.29	1.35
2	B	703	HF7	C5-N7	4.34	1.47	1.39
2	D	701	HF7	PB-O3A	4.28	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	HF7	PA-O3A	4.13	1.64	1.59
2	A	703	HF7	O4'-C1'	4.12	1.51	1.42
2	B	703	HF7	C8-N7	3.95	1.39	1.31
2	D	701	HF7	C6-N1	3.89	1.40	1.35
3	A	702	GTP	O6-C6	3.88	1.30	1.23
2	C	704	HF7	C3'-C4'	-3.74	1.43	1.53
2	B	703	HF7	CL2-C2	3.71	1.59	1.49
2	D	701	HF7	C5-N7	3.66	1.45	1.39
2	B	703	HF7	C2-N3	3.55	1.40	1.34
3	D	703	GTP	C5-C4	3.53	1.48	1.38
3	B	702	GTP	PG-O2G	-3.49	1.41	1.54
2	B	703	HF7	C6-N1	3.49	1.39	1.35
2	B	703	HF7	PA-O5'	3.36	1.72	1.59
2	A	705	HF7	C4-N9	-3.28	1.30	1.37
2	C	704	HF7	C2-N3	-3.28	1.28	1.34
2	A	705	HF7	C2-N3	3.25	1.39	1.34
2	D	702	HF7	C5-N7	3.17	1.44	1.39
2	D	702	HF7	C5-C4	3.16	1.44	1.39
3	B	702	GTP	PB-O3B	-3.15	1.56	1.59
2	C	701	HF7	CL2-C2	3.12	1.58	1.49
2	C	701	HF7	C4-N3	-3.06	1.30	1.34
2	C	701	HF7	O3'-C3'	3.03	1.49	1.43
2	D	701	HF7	C5-C4	3.01	1.44	1.39
2	A	703	HF7	PB-O3A	2.99	1.62	1.59
3	A	702	GTP	C5-C4	2.99	1.47	1.38
3	D	703	GTP	PB-O3A	2.97	1.62	1.59
3	A	702	GTP	C5-N7	-2.94	1.33	1.39
3	B	702	GTP	C4-N9	-2.92	1.30	1.38
2	C	704	HF7	O4'-C4'	2.86	1.51	1.45
2	A	703	HF7	C6-N6	2.85	1.41	1.34
2	A	703	HF7	C5-C4	2.85	1.44	1.39
2	D	702	HF7	PG-O3G	-2.85	1.44	1.54
2	C	701	HF7	O4'-C1'	2.84	1.48	1.42
2	B	701	HF7	C4-N3	-2.82	1.30	1.34
2	A	703	HF7	PB-O2B	-2.82	1.42	1.55
2	D	701	HF7	O4'-C1'	2.80	1.48	1.42
2	C	704	HF7	PA-O3A	-2.79	1.56	1.59
2	C	704	HF7	C6-N6	2.78	1.41	1.34
3	C	703	GTP	C5-C4	2.77	1.46	1.38
2	C	704	HF7	PB-O1B	-2.75	1.41	1.50
3	D	703	GTP	C8-N7	2.75	1.40	1.32
2	B	701	HF7	PB-O2B	-2.73	1.42	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	705	HF7	O4'-C1'	2.66	1.48	1.42
2	D	702	HF7	C3'-C4'	-2.57	1.46	1.53
2	C	701	HF7	PA-O5'	2.56	1.69	1.59
2	C	701	HF7	C8-N7	2.52	1.36	1.31
2	C	701	HF7	PG-O2G	-2.51	1.45	1.54
3	D	703	GTP	C6-N1	-2.50	1.34	1.38
3	C	703	GTP	C5'-C4'	2.50	1.59	1.51
2	A	703	HF7	PG-O3G	-2.49	1.45	1.54
2	A	703	HF7	PA-O3A	-2.44	1.56	1.59
3	B	702	GTP	C6-N1	-2.42	1.34	1.38
2	D	701	HF7	C2'-C3'	-2.40	1.46	1.52
2	B	701	HF7	PA-O3A	2.39	1.62	1.59
2	C	704	HF7	C2'-C3'	-2.38	1.46	1.52
2	B	701	HF7	C5-N7	2.37	1.43	1.39
3	A	702	GTP	PB-O2B	-2.34	1.44	1.55
2	B	701	HF7	PG-O2G	-2.29	1.46	1.54
2	D	701	HF7	C8-N7	2.29	1.36	1.31
3	C	703	GTP	C4-N9	-2.27	1.32	1.38
3	A	702	GTP	C4-N9	-2.26	1.32	1.38
2	D	701	HF7	PB-O2B	-2.23	1.45	1.55
2	A	705	HF7	PA-O5'	2.22	1.68	1.59
3	C	703	GTP	C5-N7	-2.22	1.34	1.39
2	B	701	HF7	C6-N1	-2.19	1.32	1.35
2	C	704	HF7	C5-N7	2.18	1.43	1.39
3	A	702	GTP	PG-O3G	-2.18	1.46	1.54
2	D	702	HF7	O4'-C1'	2.17	1.47	1.42
2	D	701	HF7	C2-N1	2.17	1.37	1.34
2	A	703	HF7	C4-N3	-2.17	1.31	1.34
3	A	702	GTP	PG-O2G	-2.17	1.46	1.54
3	A	702	GTP	PA-O2A	-2.15	1.45	1.55
2	B	701	HF7	C8-N9	-2.15	1.33	1.37
2	D	702	HF7	C2'-C1'	-2.14	1.46	1.52
2	D	701	HF7	PG-O2G	-2.12	1.46	1.54
2	C	704	HF7	CL2-C2	2.11	1.55	1.49
2	B	701	HF7	PG-O3G	-2.11	1.46	1.54
2	A	705	HF7	C6-N1	2.10	1.37	1.35
2	A	705	HF7	CL2-C2	2.09	1.55	1.49
2	A	705	HF7	C4-N3	-2.07	1.31	1.34
2	D	701	HF7	PA-O1A	-2.07	1.45	1.55
3	A	702	GTP	O3'-C3'	-2.06	1.37	1.43
2	D	702	HF7	PG-O2G	-2.05	1.47	1.54
2	B	701	HF7	C6-N6	2.05	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	703	HF7	PB-O1B	-2.04	1.43	1.50
3	D	703	GTP	PB-O1B	2.03	1.57	1.50

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	702	HF7	C5-C4-N3	-9.25	117.43	127.18
2	B	703	HF7	C4-N9-C8	8.95	115.14	105.74
2	D	702	HF7	N3-C4-N9	8.39	137.64	126.99
2	A	705	HF7	C4-N9-C8	8.35	114.51	105.74
2	B	701	HF7	C5-C4-N3	-7.77	118.99	127.18
2	A	703	HF7	C5-C4-N3	-7.36	119.43	127.18
2	D	702	HF7	C4-N9-C8	7.21	113.31	105.74
2	D	701	HF7	CL2-C2-N1	6.92	127.48	117.13
2	B	703	HF7	N3-C4-N9	6.77	135.58	126.99
2	C	701	HF7	N6-C6-N1	6.74	126.12	117.03
2	A	705	HF7	N3-C4-N9	6.66	135.44	126.99
2	B	703	HF7	N6-C6-N1	6.63	125.97	117.03
2	D	701	HF7	N1-C2-N3	-6.57	114.17	125.77
2	D	702	HF7	C4-C5-N7	-6.34	103.33	110.58
2	B	701	HF7	N3-C4-N9	6.32	135.01	126.99
2	A	705	HF7	N6-C6-N1	6.23	125.43	117.03
2	A	703	HF7	N3-C4-N9	6.13	134.77	126.99
2	C	704	HF7	N3-C4-N9	6.10	134.73	126.99
2	A	705	HF7	C5-C4-N3	-5.86	121.01	127.18
2	C	701	HF7	C4-N9-C8	5.81	111.84	105.74
2	D	702	HF7	C5-N7-C8	5.65	112.33	103.45
2	D	701	HF7	C2-N1-C6	5.62	126.75	118.10
2	D	701	HF7	C4-N9-C8	5.57	111.58	105.74
2	D	702	HF7	N9-C8-N7	-5.53	106.10	113.94
2	C	704	HF7	C5-C4-N3	-5.47	121.42	127.18
2	C	704	HF7	C4-N9-C8	5.38	111.39	105.74
3	C	703	GTP	C6-C5-N7	5.38	140.08	130.29
2	B	701	HF7	C4-N9-C8	5.11	111.11	105.74
2	C	701	HF7	CL2-C2-N1	4.94	124.52	117.13
2	A	703	HF7	O4'-C1'-N9	-4.89	99.17	107.96
3	A	702	GTP	C5-C4-N3	-4.88	120.62	128.39
2	B	703	HF7	C5-C4-N3	-4.81	122.12	127.18
3	D	703	GTP	C5-C4-N3	-4.77	120.80	128.39
2	D	701	HF7	N6-C6-N1	4.77	123.46	117.03
2	D	701	HF7	O1A-PA-O5'	4.71	128.93	107.57
2	C	701	HF7	N3-C4-N9	4.70	132.96	126.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	704	HF7	CL2-C2-N3	4.52	123.89	117.13
2	B	703	HF7	C5-C6-N6	-4.42	112.35	123.29
2	A	705	HF7	CL2-C2-N1	4.37	123.66	117.13
3	A	702	GTP	N9-C4-N3	4.32	134.59	125.95
2	C	701	HF7	C5-C4-N3	-4.22	122.73	127.18
2	B	703	HF7	N1-C2-N3	-4.22	118.33	125.77
2	B	703	HF7	CL2-C2-N3	4.19	123.41	117.13
2	A	705	HF7	O2B-PB-O3A	4.16	118.53	107.27
2	D	702	HF7	CL2-C2-N1	-4.15	110.92	117.13
2	A	705	HF7	C5-C6-N6	-4.14	113.03	123.29
2	D	702	HF7	N1-C2-N3	4.00	132.82	125.77
2	C	701	HF7	N1-C2-N3	-3.98	118.75	125.77
2	C	704	HF7	C2-N1-C6	3.98	124.22	118.10
3	B	702	GTP	N9-C4-N3	3.98	133.90	125.95
3	C	703	GTP	O2B-PB-O3B	3.94	117.92	107.27
2	D	701	HF7	O2B-PB-O3B	3.92	117.86	107.27
2	C	704	HF7	N6-C6-N1	3.86	122.24	117.03
2	A	703	HF7	CL2-C2-N1	-3.84	111.37	117.13
3	C	703	GTP	C2-N3-C4	3.83	118.89	112.30
2	C	701	HF7	C5-C6-N6	-3.77	113.94	123.29
2	B	701	HF7	C4-C5-N7	-3.73	106.32	110.58
3	B	702	GTP	C5-C4-N3	-3.73	122.46	128.39
2	B	703	HF7	N9-C8-N7	-3.68	108.71	113.94
2	B	701	HF7	O1A-PA-O3A	3.63	117.08	107.27
2	A	705	HF7	N9-C8-N7	-3.62	108.80	113.94
3	A	702	GTP	C2-N3-C4	3.62	118.53	112.30
3	D	703	GTP	N9-C4-N3	3.60	133.14	125.95
2	A	705	HF7	O1A-PA-O2A	-3.57	95.82	112.44
3	C	703	GTP	C4-C5-N7	-3.53	105.08	110.67
2	A	705	HF7	O2G-PG-O3B	3.49	116.33	104.64
2	A	703	HF7	C4-N9-C8	3.45	109.36	105.74
3	C	703	GTP	C8-N7-C5	3.42	110.36	104.26
2	D	701	HF7	O3G-PG-O3B	3.42	116.11	104.64
3	D	703	GTP	O3G-PG-O2G	3.39	120.52	107.80
3	C	703	GTP	C5-C4-N3	-3.39	122.99	128.39
3	C	703	GTP	N9-C4-N3	3.37	132.69	125.95
2	C	701	HF7	N9-C8-N7	-3.32	109.23	113.94
2	C	701	HF7	O4'-C1'-N9	3.27	113.84	107.96
2	B	703	HF7	O2B-PB-O3B	3.24	116.04	107.27
2	C	704	HF7	C2'-C3'-C4'	3.23	109.36	102.80
2	B	703	HF7	C5-C4-N9	-3.23	102.30	105.81
3	A	702	GTP	O3G-PG-O2G	3.11	119.47	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	HF7	O3A-PA-O2A	-3.11	101.35	110.70
3	B	702	GTP	O2B-PB-O3B	3.11	115.67	107.27
2	A	705	HF7	O1A-PA-O5'	3.10	121.60	107.57
2	D	702	HF7	O1A-PA-O3A	-3.09	98.92	107.27
2	D	701	HF7	O3A-PB-O1B	-3.04	101.56	110.70
3	B	702	GTP	C2-N3-C4	3.04	117.53	112.30
2	C	704	HF7	N9-C8-N7	-3.02	109.65	113.94
3	B	702	GTP	C3'-C2'-C1'	2.94	107.02	101.46
3	B	702	GTP	C8-N9-C4	2.92	111.50	106.03
2	C	704	HF7	O4'-C1'-N9	-2.92	102.72	107.96
2	B	701	HF7	O2B-PB-O3A	2.91	115.15	107.27
2	A	705	HF7	O3A-PA-O2A	-2.87	102.07	110.70
2	A	705	HF7	O1A-PA-O3A	2.87	115.03	107.27
2	D	701	HF7	O1A-PA-O2A	-2.87	99.10	112.44
2	D	702	HF7	C6-C5-C4	2.86	121.08	117.18
2	A	703	HF7	C4-C5-N7	-2.84	107.33	110.58
2	D	701	HF7	C6-C5-N7	2.82	137.53	132.09
3	D	703	GTP	C3'-C2'-C1'	2.80	106.76	101.46
2	C	704	HF7	O1A-PA-O3A	2.77	114.76	107.27
2	B	701	HF7	N6-C6-N1	2.77	120.76	117.03
2	B	701	HF7	O4'-C1'-N9	-2.75	103.02	107.96
2	A	705	HF7	O3A-PB-O1B	-2.72	102.51	110.70
3	C	703	GTP	O3G-PG-O3B	2.68	113.63	104.64
2	A	703	HF7	N1-C2-N3	2.66	130.45	125.77
2	B	701	HF7	N9-C8-N7	-2.65	110.17	113.94
2	A	703	HF7	O2B-PB-O3A	2.65	114.44	107.27
3	C	703	GTP	C6-C5-C4	-2.65	114.84	118.83
2	D	701	HF7	O2G-PG-O3G	-2.64	97.89	107.80
2	B	703	HF7	C4-N9-C1'	-2.55	116.27	126.50
2	D	701	HF7	N3-C4-N9	2.54	130.22	126.99
2	C	701	HF7	O3G-PG-O3B	2.54	113.15	104.64
3	D	703	GTP	O6-C6-N1	2.53	124.87	120.11
3	B	702	GTP	O3A-PB-O1B	-2.53	103.10	110.70
2	C	701	HF7	O2G-PG-O3B	2.52	113.07	104.64
2	D	702	HF7	O2B-PB-O3B	2.51	114.06	107.27
2	D	701	HF7	O3A-PA-O2A	-2.50	103.18	110.70
2	A	703	HF7	C6-C5-C4	2.49	120.58	117.18
3	C	703	GTP	C8-N9-C4	2.48	110.68	106.03
2	D	702	HF7	O2G-PG-O3B	2.48	112.95	104.64
2	D	701	HF7	C4-N9-C1'	-2.48	116.57	126.50
2	A	703	HF7	C2'-C1'-N9	2.47	120.43	114.63
2	B	701	HF7	O3G-PG-O3B	2.47	112.92	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	703	GTP	O5'-PA-O1A	2.46	118.69	108.94
2	C	701	HF7	C2-N1-C6	2.45	121.86	118.10
3	B	702	GTP	C5-C6-N1	2.41	119.39	113.25
3	C	703	GTP	O2'-C2'-C1'	-2.38	101.91	110.10
2	C	704	HF7	CL2-C2-N1	-2.38	113.57	117.13
3	B	702	GTP	C6-C5-N7	2.38	134.61	130.29
2	A	703	HF7	O3A-PA-O2A	2.37	117.84	110.70
2	D	701	HF7	N9-C8-N7	-2.37	110.58	113.94
2	B	703	HF7	O1A-PA-O2A	-2.36	101.47	112.44
3	C	703	GTP	O3A-PB-O1B	-2.36	103.62	110.70
3	A	702	GTP	C8-N7-C5	2.34	108.43	104.26
2	A	705	HF7	N1-C2-N3	-2.33	121.65	125.77
2	A	705	HF7	C5-C4-N9	-2.31	103.30	105.81
2	A	703	HF7	O1A-PA-O3A	-2.30	101.05	107.27
2	C	701	HF7	O3G-PG-O1G	-2.29	101.89	110.83
3	C	703	GTP	N9-C8-N7	-2.26	109.21	113.40
3	D	703	GTP	O5'-C5'-C4'	2.25	116.67	108.99
2	D	701	HF7	C5-C4-N3	-2.24	124.82	127.18
2	D	701	HF7	C6-C5-C4	-2.24	114.12	117.18
2	C	701	HF7	O3A-PB-O1B	2.23	117.40	110.70
3	B	702	GTP	C2-N1-C6	-2.21	121.11	125.11
2	C	704	HF7	N1-C2-N3	-2.19	121.90	125.77
3	A	702	GTP	C3'-C2'-C1'	2.18	105.58	101.46
3	A	702	GTP	C4-C5-N7	-2.16	107.24	110.67
2	D	701	HF7	C5-C6-N6	-2.16	117.94	123.29
2	D	701	HF7	C4-C5-N7	-2.16	108.12	110.58
3	A	702	GTP	N9-C8-N7	-2.15	109.41	113.40
2	C	704	HF7	O3A-PA-O2A	-2.14	104.26	110.70
3	A	702	GTP	C8-N9-C4	2.14	110.03	106.03
2	A	705	HF7	C4-C5-N7	-2.13	108.14	110.58
2	C	704	HF7	O3G-PG-O3B	2.11	111.72	104.64
3	B	702	GTP	O6-C6-C5	-2.10	121.00	126.53
3	C	703	GTP	O3B-PB-O1B	2.09	116.98	110.70
2	A	703	HF7	N9-C8-N7	-2.09	110.98	113.94
3	B	702	GTP	O2'-C2'-C1'	-2.08	102.95	110.10
3	C	703	GTP	O4'-C4'-C3'	-2.07	101.04	105.15
2	C	704	HF7	O2G-PG-O1G	-2.07	102.78	110.83
2	D	702	HF7	C2-N1-C6	-2.06	114.92	118.10
2	D	702	HF7	C3'-C2'-C1'	2.05	107.61	102.60
3	A	702	GTP	O2'-C2'-C1'	-2.02	103.14	110.10

There are no chirality outliers.

All (44) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
2	C	704	HF7	PA-O3A-PB-O2B
3	A	702	GTP	PB-O3A-PA-O2A

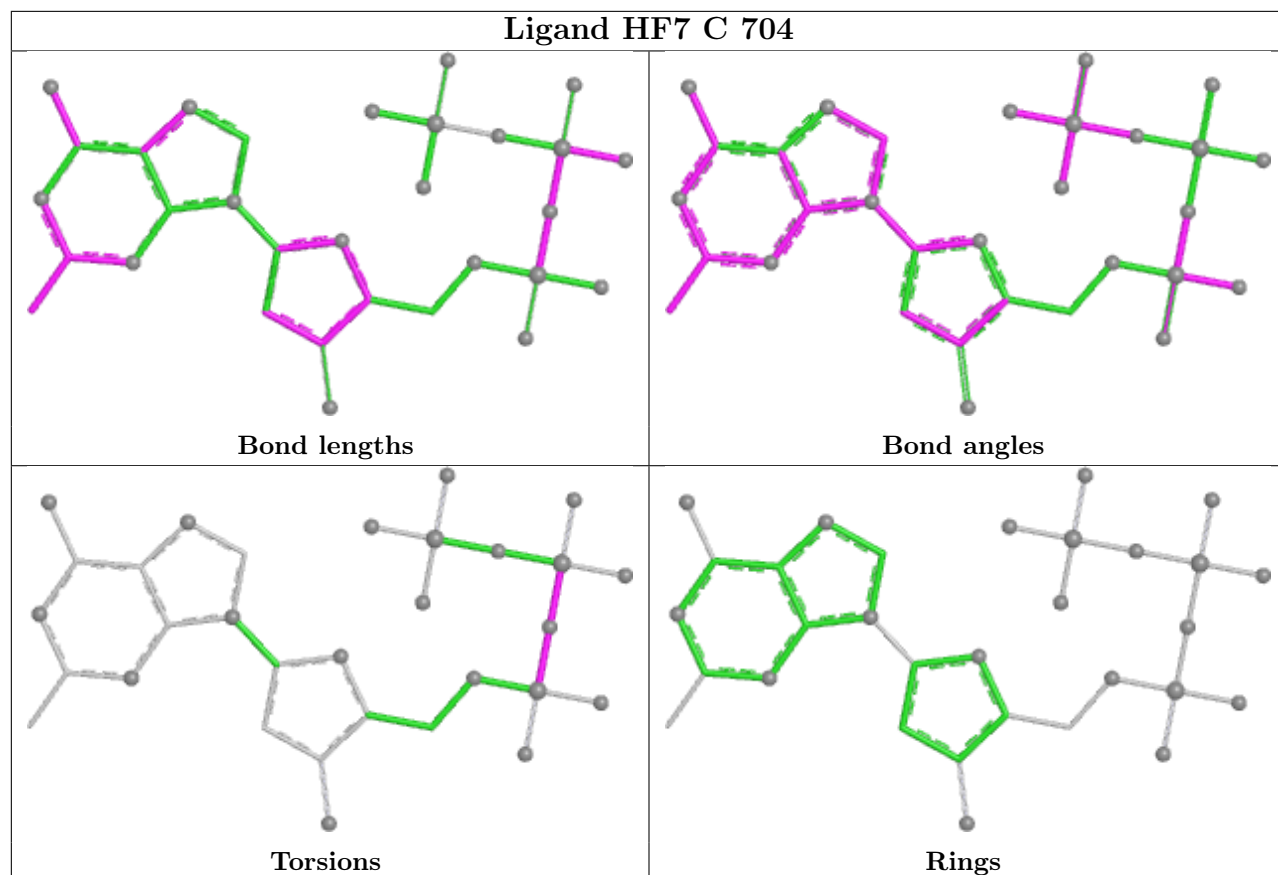
There are no ring outliers.

8 monomers are involved in 12 short contacts:

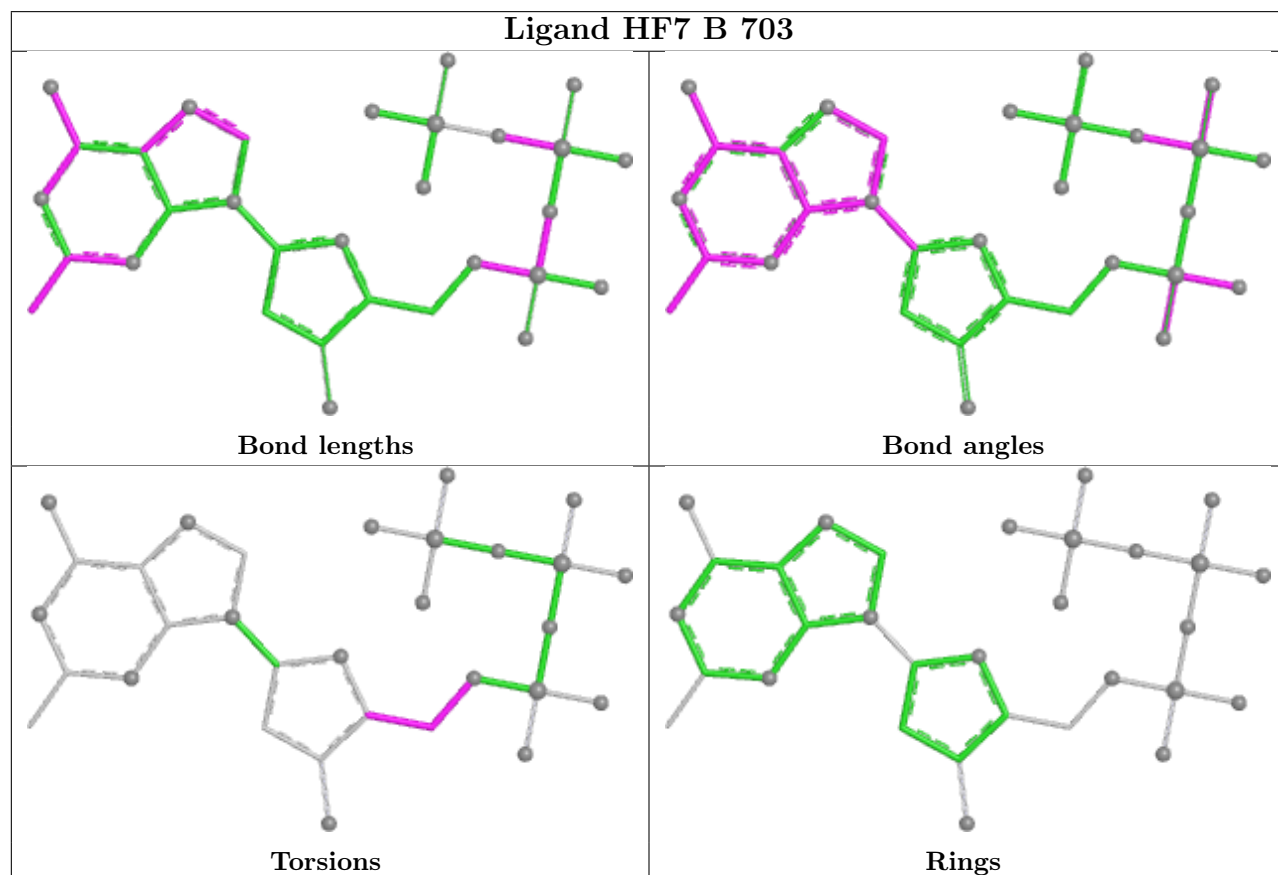
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	704	HF7	1	0
2	B	703	HF7	3	0
2	B	701	HF7	1	0
2	D	701	HF7	1	0
2	A	703	HF7	1	0
2	C	701	HF7	1	0
2	D	702	HF7	2	0
2	A	705	HF7	2	0

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

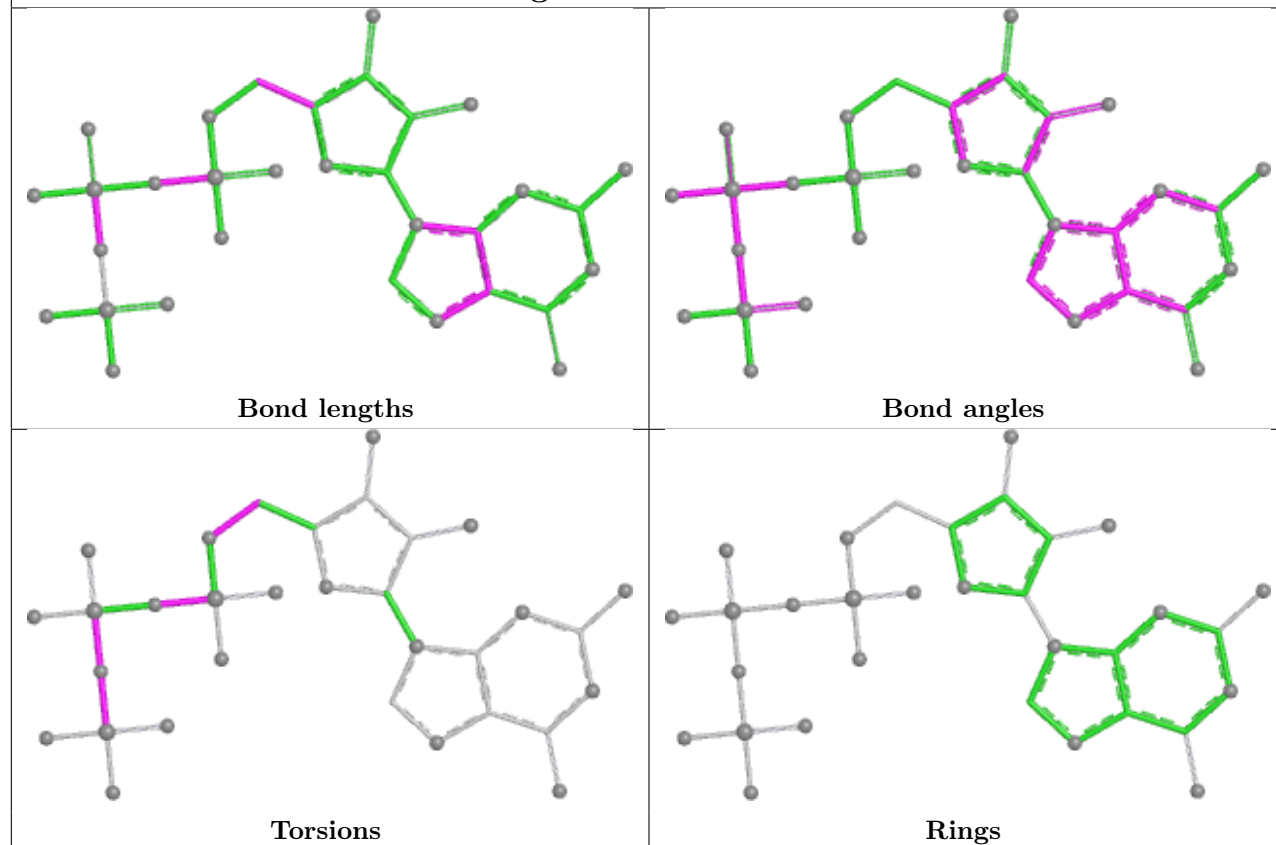
Ligand HF7 C 704



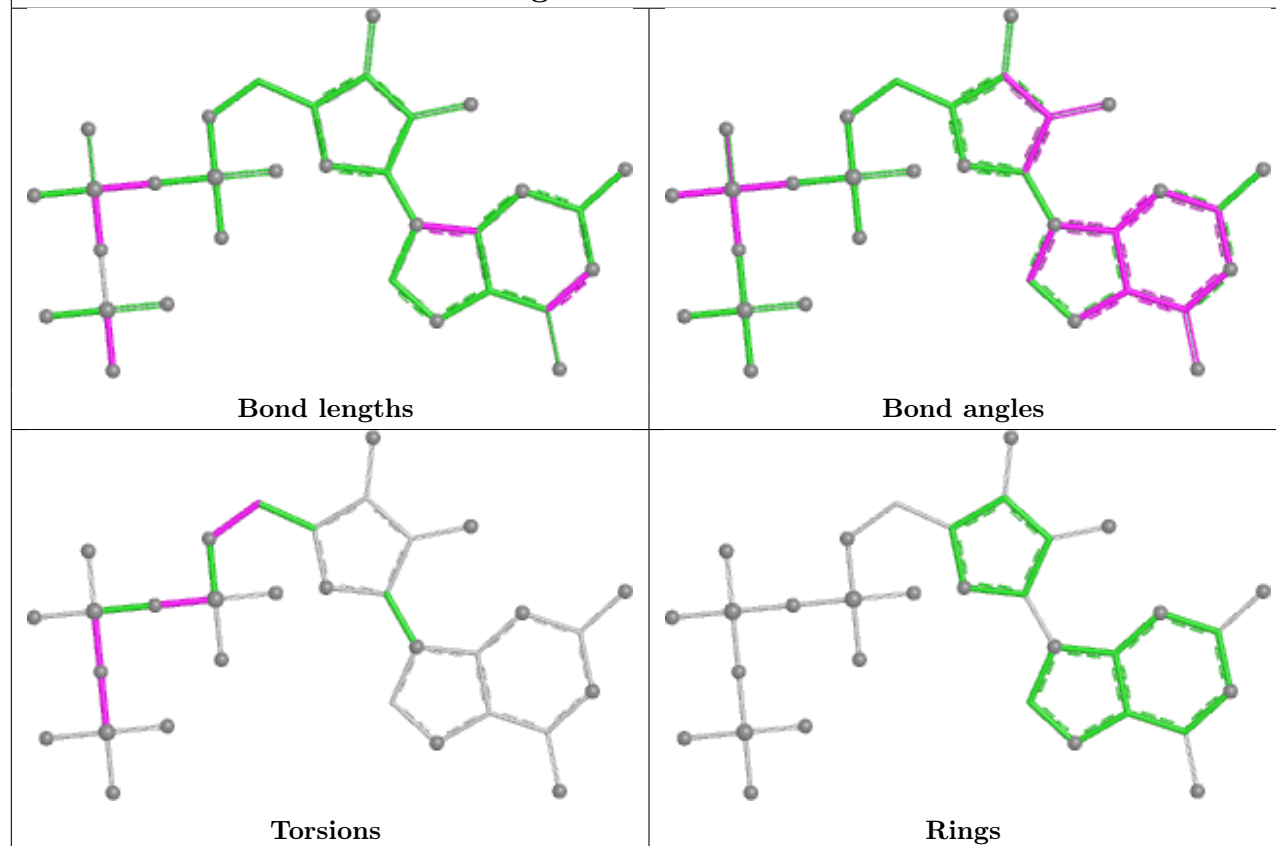
Ligand HF7 B 703



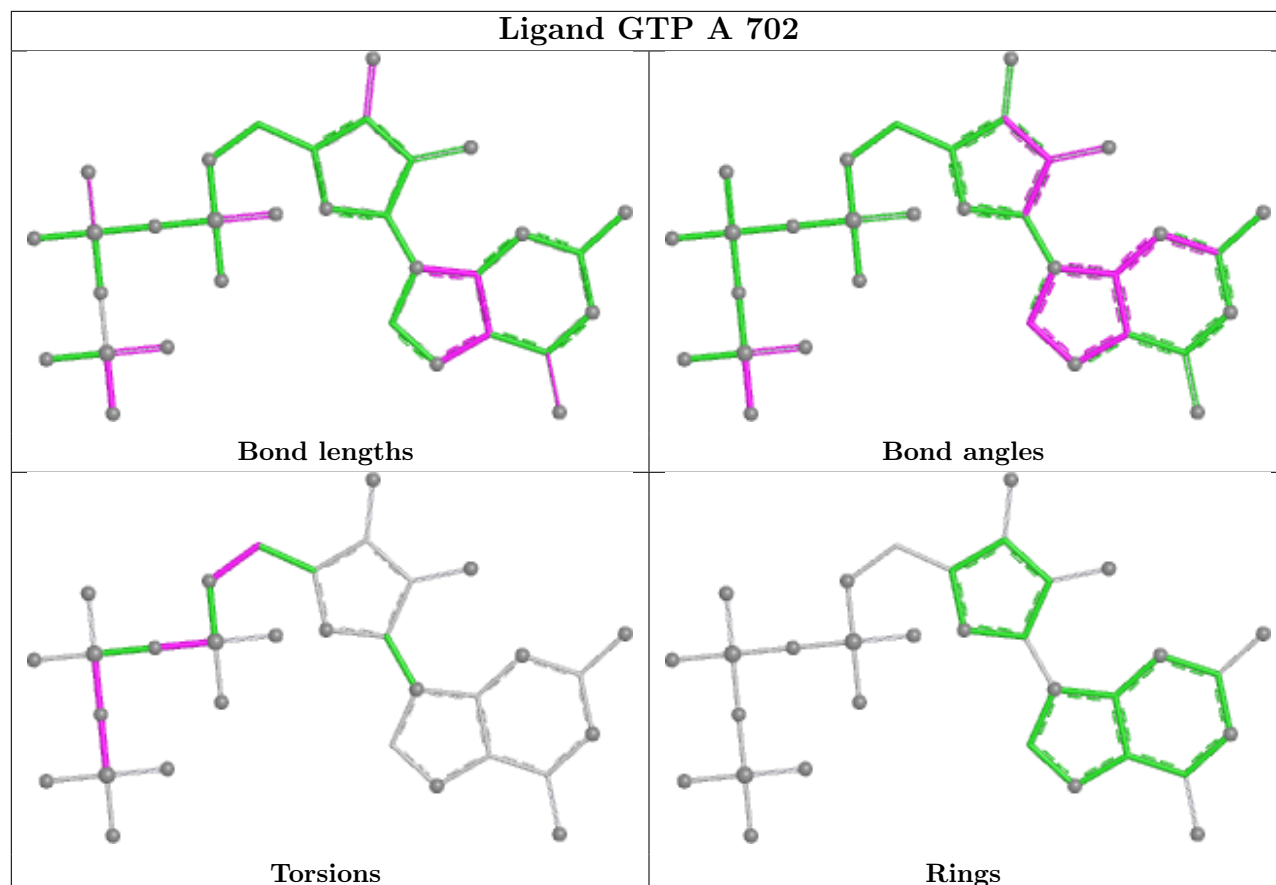
Ligand GTP C 703



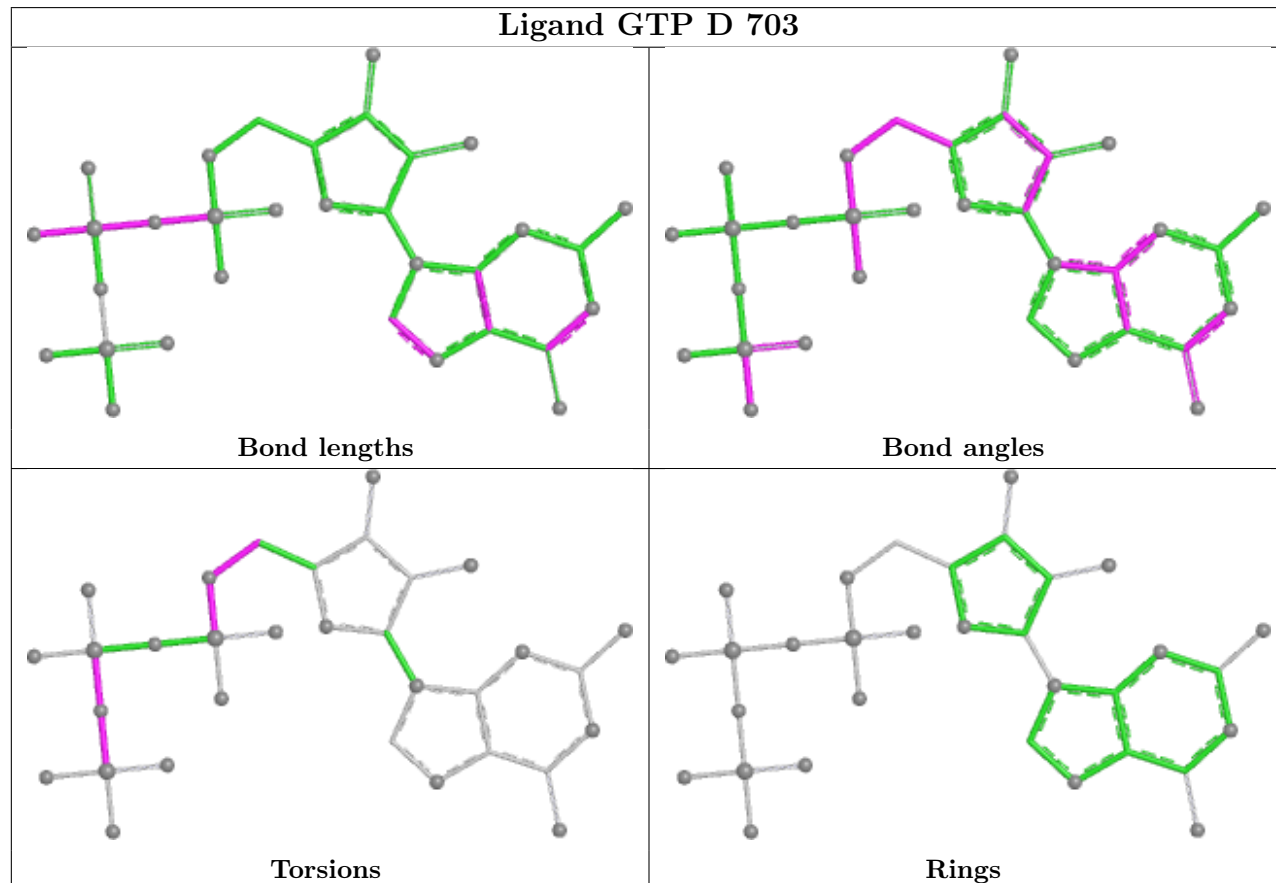
Ligand GTP B 702



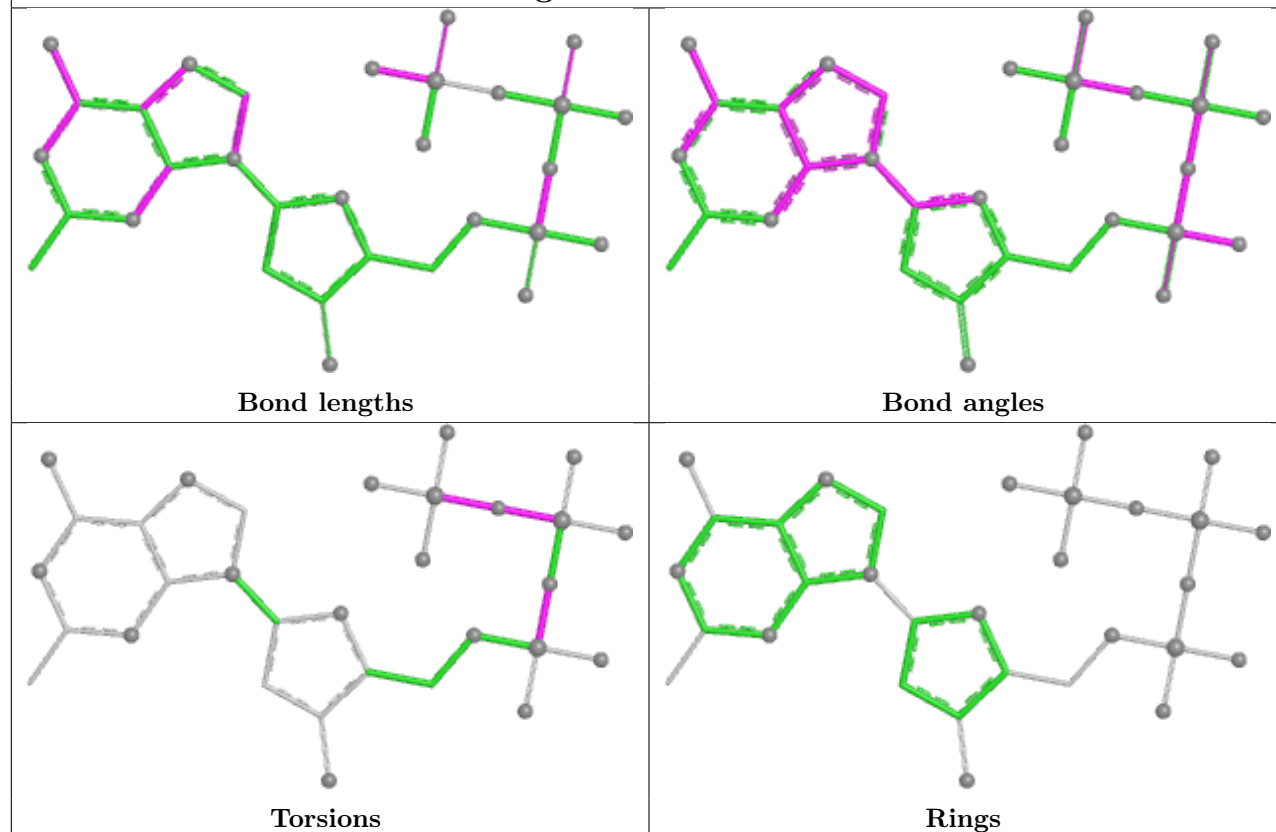
Ligand GTP A 702



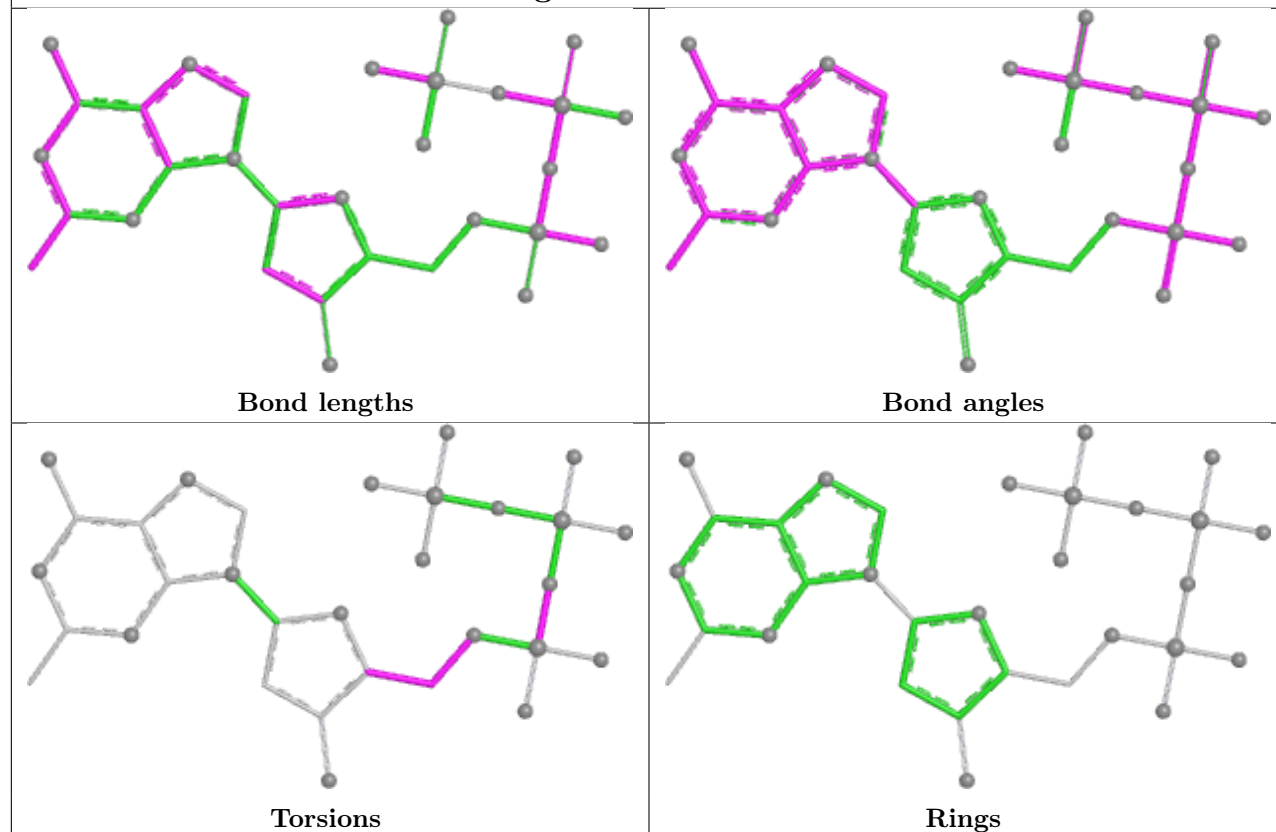
Ligand GTP D 703



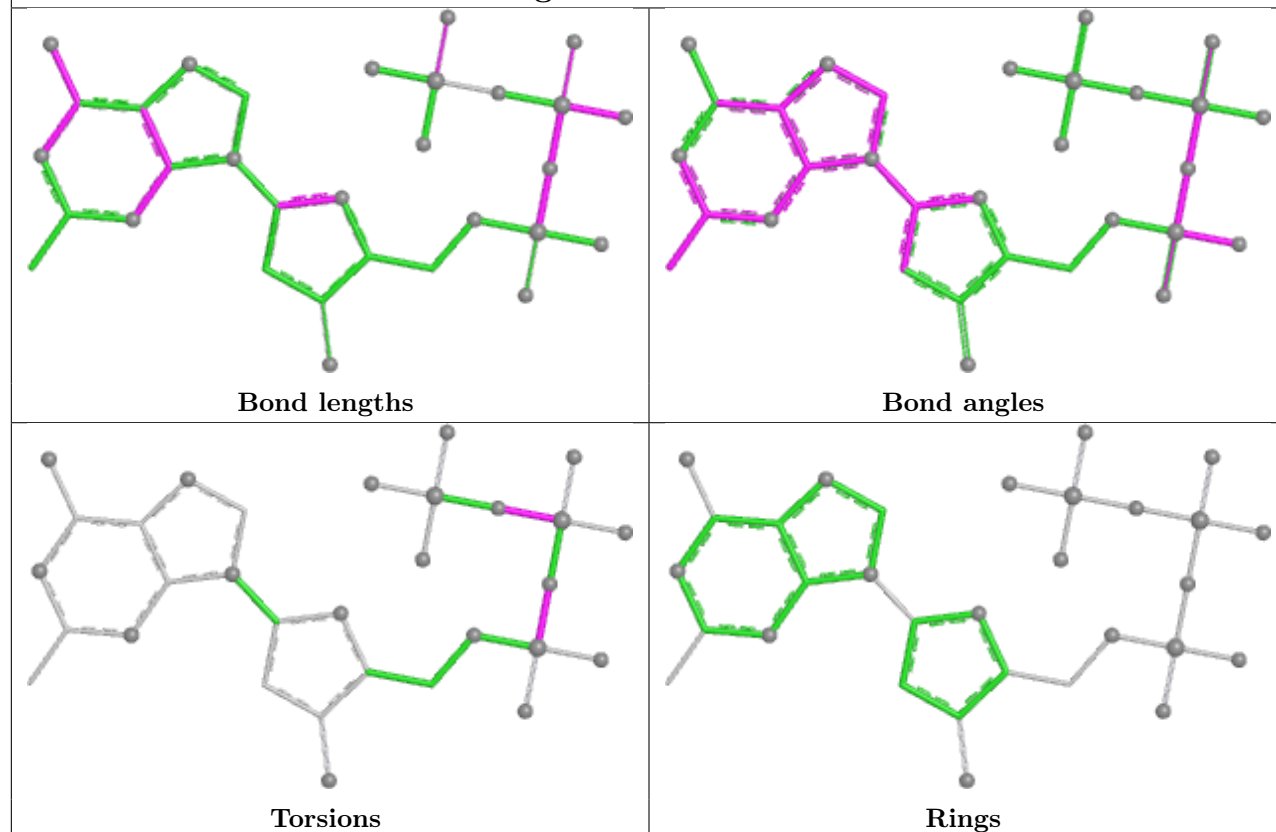
Ligand HF7 B 701



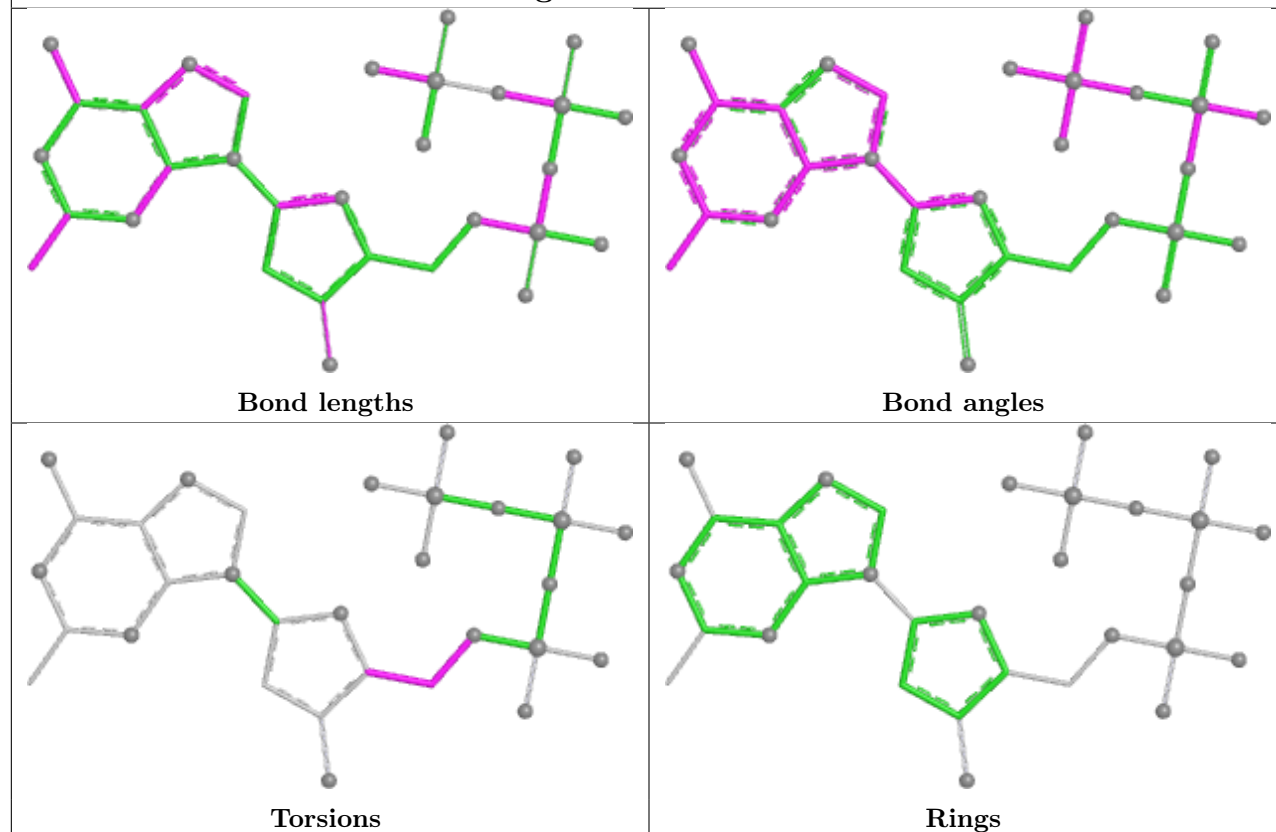
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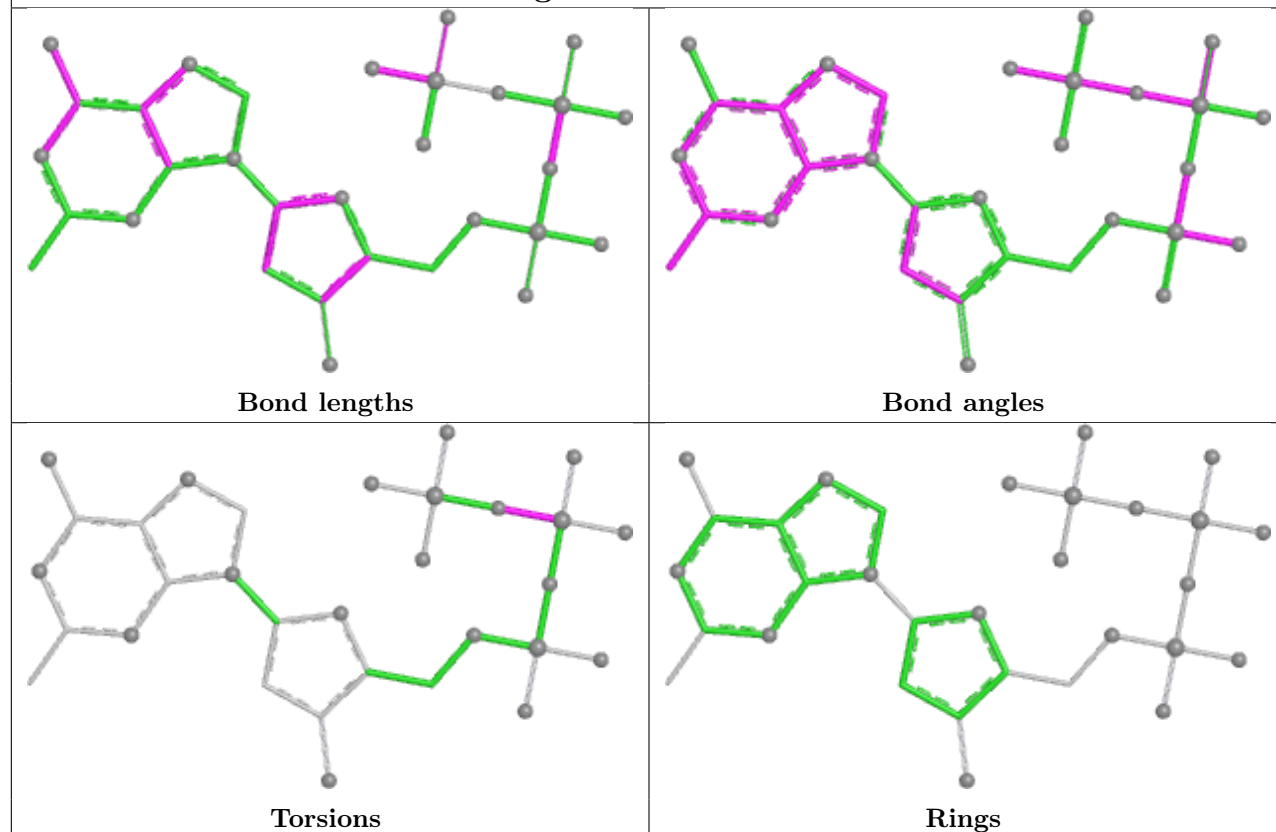
Ligand HF7 A 703



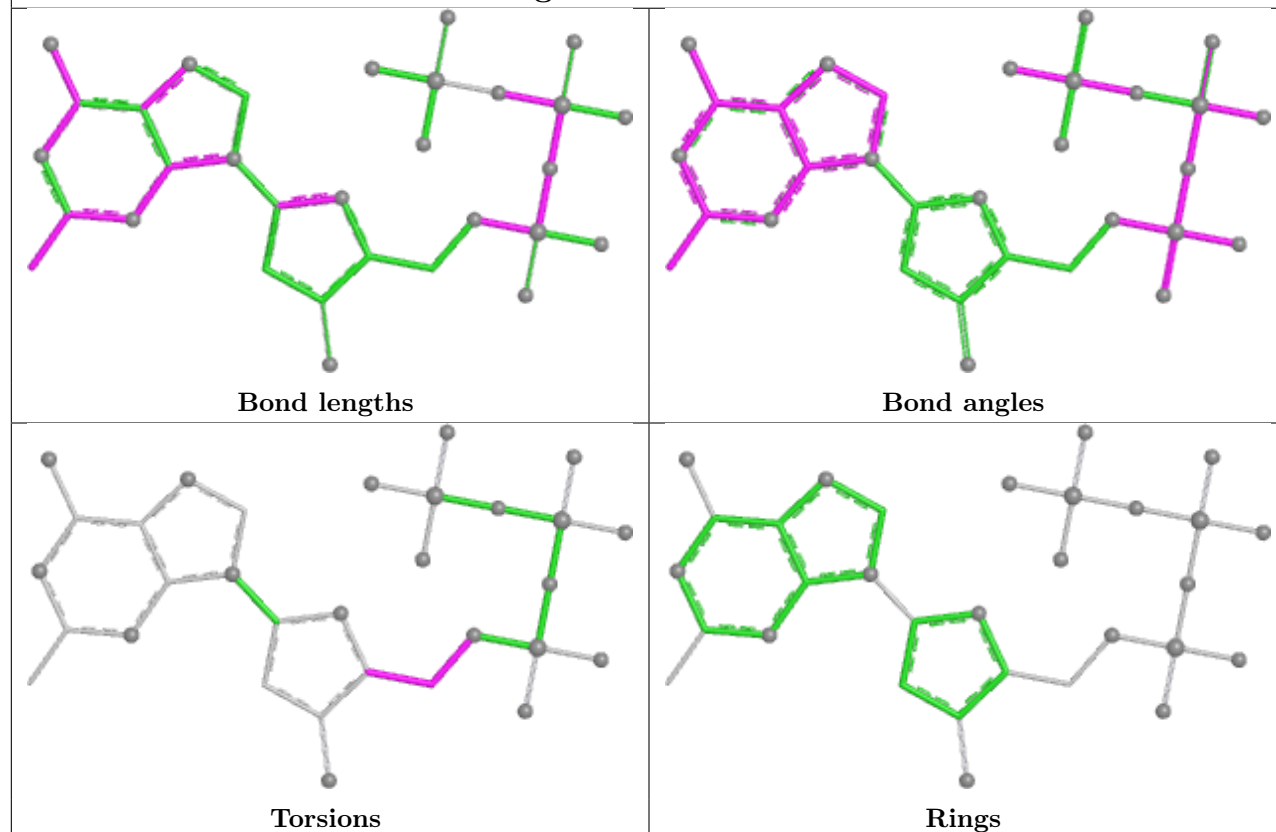
Ligand HF7 C 701



Ligand HF7 D 702



Ligand HF7 A 705



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.26	42 (8%)	16 15	11, 26, 82, 224	2 (0%)
1	B	481/550 (87%)	0.21	26 (5%)	31 30	13, 30, 62, 92	2 (0%)
1	C	481/550 (87%)	0.07	18 (3%)	45 44	10, 27, 63, 104	3 (0%)
1	D	481/550 (87%)	-0.08	10 (2%)	63 63	11, 25, 53, 93	5 (1%)
All	All	1924/2200 (87%)	0.12	96 (4%)	34 33	10, 27, 64, 224	12 (0%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	591	ILE	9.0
1	A	587	ILE	8.4
1	A	590	LEU	6.7
1	A	584	GLY	6.7
1	C	466	ILE	5.9
1	A	598	TRP	5.8
1	A	586	VAL	5.7
1	A	466	ILE	5.5
1	A	588	ALA	5.4
1	D	466	ILE	5.3
1	C	114	THR	5.2
1	C	465	GLN	5.0
1	D	284	LEU	4.9
1	C	115	MET	4.8
1	A	114	THR	4.8
1	A	284	LEU	4.6
1	C	487	VAL	4.3
1	C	464	GLY	4.2
1	A	489	LEU	4.1
1	D	113	ASP	4.1
1	A	593	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	284	LEU	4.0
1	D	465	GLN	3.9
1	B	114	THR	3.9
1	A	488	LEU	3.8
1	C	489	LEU	3.8
1	A	583	ASP	3.8
1	A	595	LYS	3.8
1	A	592	THR	3.7
1	A	594	GLN	3.7
1	C	488	LEU	3.7
1	A	562	LEU	3.7
1	B	599	ASN	3.7
1	B	463	THR	3.6
1	B	488	LEU	3.6
1	C	485	PRO	3.5
1	A	491	VAL	3.5
1	B	284	LEU	3.5
1	A	589	PRO	3.4
1	B	466	ILE	3.4
1	A	115	MET	3.4
1	A	113	ASP	3.4
1	A	487	VAL	3.3
1	B	587	ILE	3.3
1	B	115	MET	3.3
1	C	577	ASN	3.3
1	A	597	GLU	3.3
1	C	491	VAL	3.3
1	A	463	THR	3.2
1	B	598	TRP	3.1
1	C	113	ASP	3.0
1	B	591	ILE	3.0
1	B	596	LYS	3.0
1	D	468	ILE	3.0
1	A	486	LYS	2.9
1	D	464	GLY	2.9
1	B	586	VAL	2.9
1	B	574	ALA	2.9
1	A	596	LYS	2.9
1	B	464	GLY	2.8
1	B	485	PRO	2.8
1	A	563	TYR	2.7
1	C	599	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	581	PRO	2.7
1	A	585	ASP	2.7
1	C	276	LEU	2.7
1	C	492	LYS	2.6
1	D	276	LEU	2.6
1	B	597	GLU	2.6
1	A	582	GLN	2.6
1	B	472	ASP	2.5
1	A	557	VAL	2.5
1	D	599	ASN	2.4
1	A	579	THR	2.4
1	A	485	PRO	2.4
1	A	483	ALA	2.4
1	D	328[A]	ASN	2.4
1	A	470	ARG	2.3
1	D	114	THR	2.3
1	B	489	LEU	2.3
1	A	580	LYS	2.3
1	B	577	ASN	2.3
1	A	467	LYS	2.3
1	B	588	ALA	2.2
1	B	478	LYS	2.2
1	C	594	GLN	2.2
1	A	328	ASN	2.2
1	A	471	GLU	2.2
1	B	575	ASP	2.2
1	A	465	GLN	2.1
1	B	590	LEU	2.1
1	B	113	ASP	2.1
1	C	262	GLU	2.1
1	B	570	VAL	2.0
1	B	276	LEU	2.0
1	A	599	ASN	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

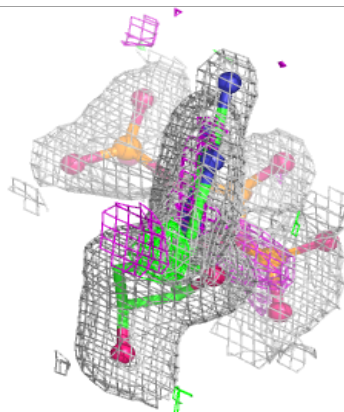
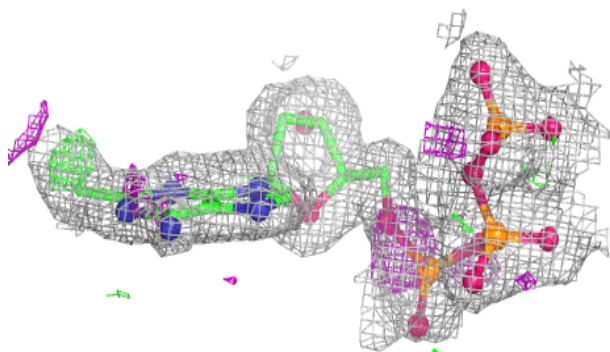
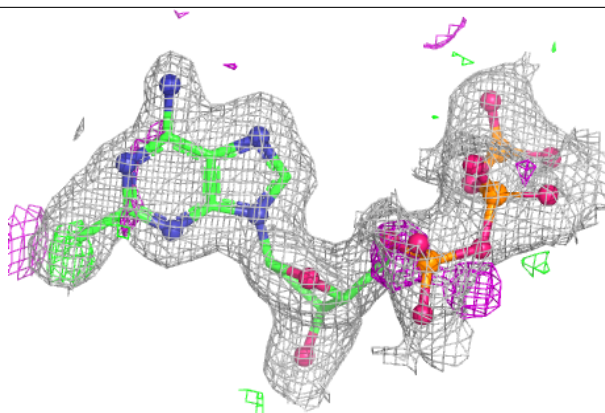
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	0.67	0.60	93,93,93,93	0
2	HF7	B	703	31/31	0.94	0.08	20,28,39,44	0
2	HF7	D	701	31/31	0.95	0.07	13,22,31,35	0
2	HF7	A	705	31/31	0.96	0.06	15,24,30,34	0
2	HF7	C	701	31/31	0.96	0.06	17,25,33,36	0
3	GTP	C	703	32/32	0.98	0.04	13,16,22,24	0
4	MG	B	704	1/1	0.98	0.06	35,35,35,35	0
4	MG	A	706	1/1	0.98	0.03	30,30,30,30	0
2	HF7	A	703	31/31	0.98	0.04	14,17,19,21	0
2	HF7	D	702	31/31	0.99	0.04	13,16,19,22	0
3	GTP	B	702	32/32	0.99	0.04	17,18,24,25	0
3	GTP	A	702	32/32	0.99	0.03	13,15,23,24	0
4	MG	D	704	1/1	0.99	0.06	24,24,24,24	0
4	MG	C	702	1/1	0.99	0.03	20,20,20,20	0
4	MG	C	705	1/1	0.99	0.02	15,15,15,15	0
4	MG	C	706	1/1	0.99	0.04	36,36,36,36	0
2	HF7	C	704	31/31	0.99	0.04	10,13,16,16	0
4	MG	A	701	1/1	0.99	0.03	16,16,16,16	0
4	MG	A	704	1/1	0.99	0.02	18,18,18,18	0
2	HF7	B	701	31/31	0.99	0.03	13,16,18,21	0
3	GTP	D	703	32/32	0.99	0.04	11,13,17,18	0

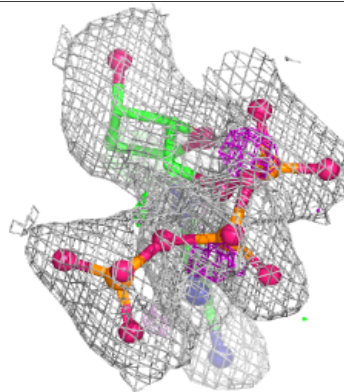
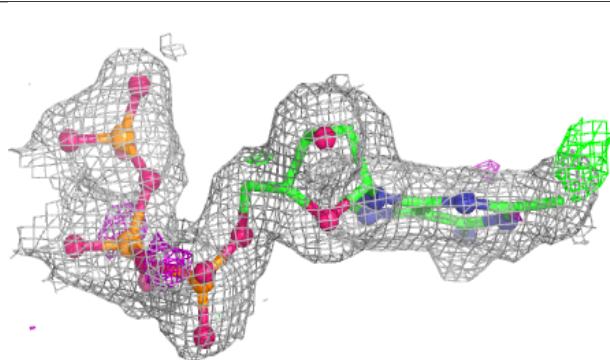
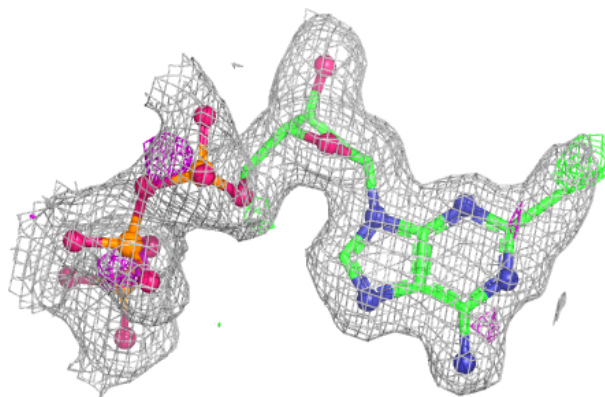
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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)

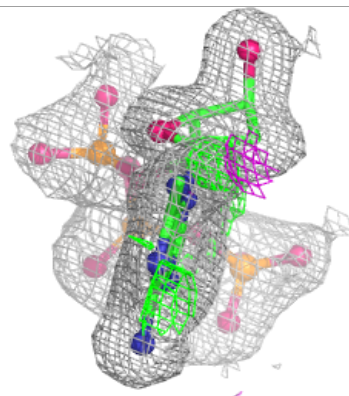
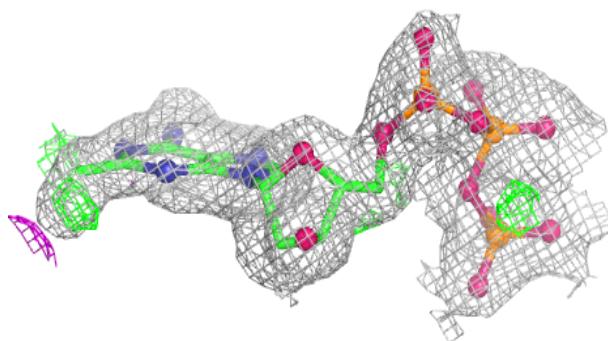
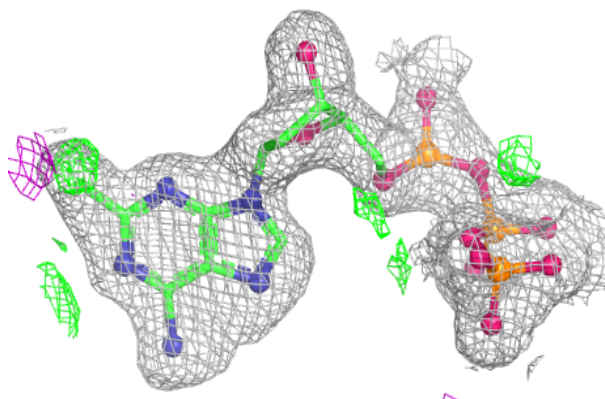
**Electron density around HF7 D 701:**

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

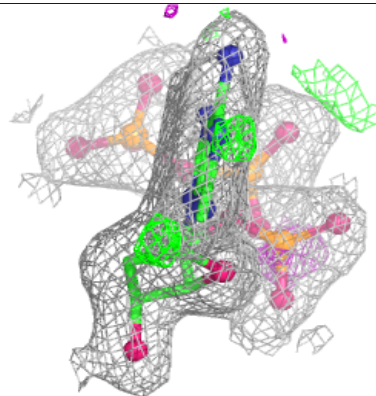
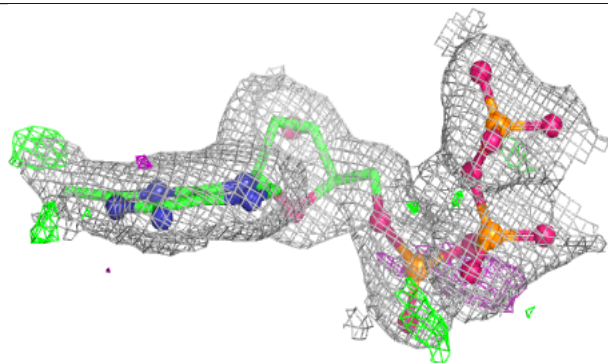
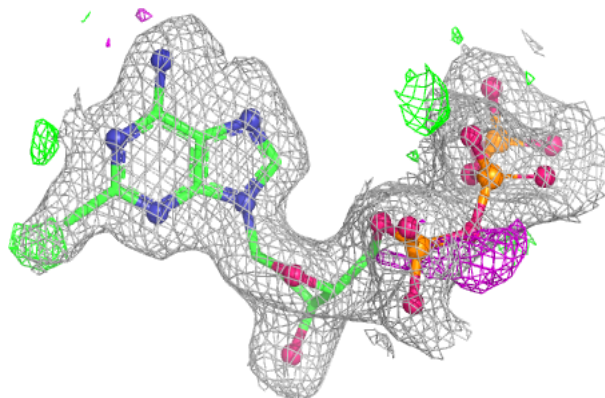


Electron density around HF7 A 705:

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

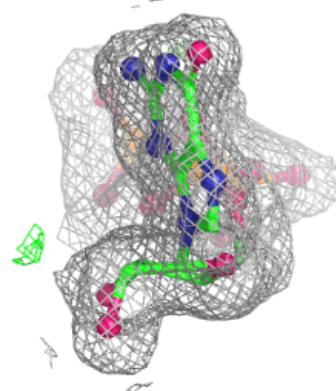
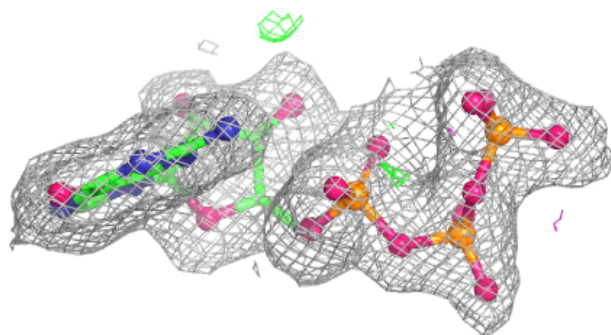
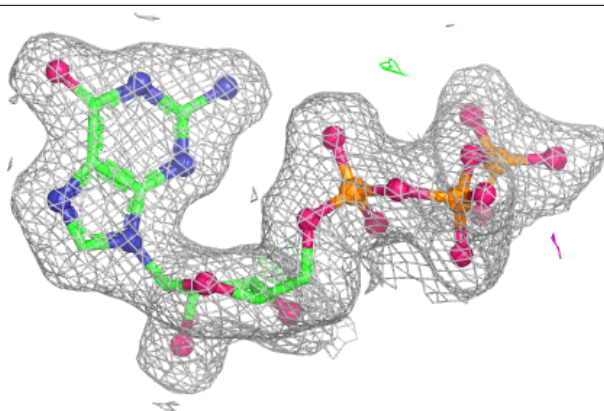
**Electron density around HF7 C 701:**

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

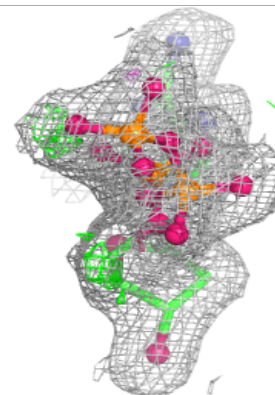
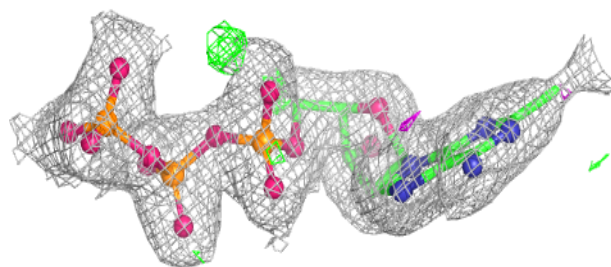
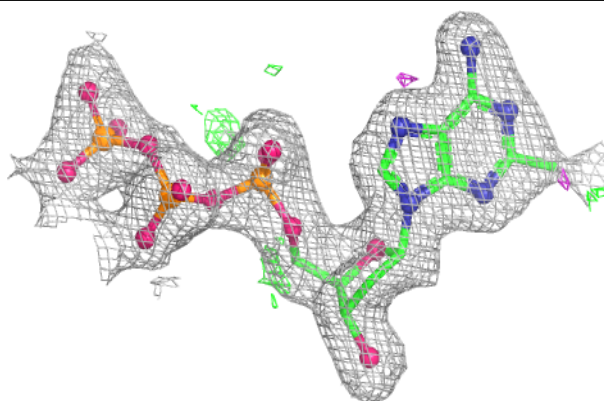


Electron density around GTP C 703:

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

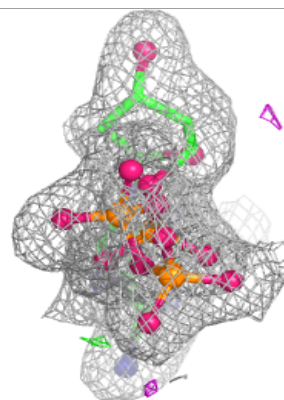
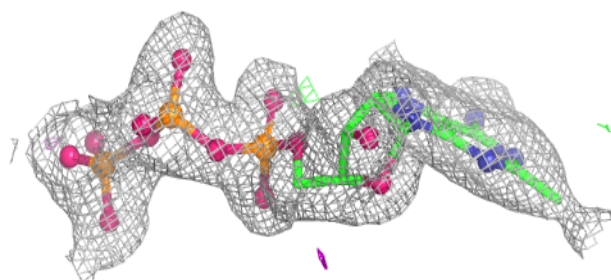
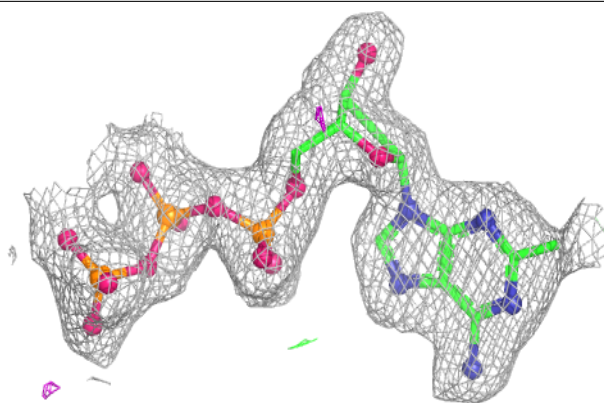
**Electron density around HF7 A 703:**

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

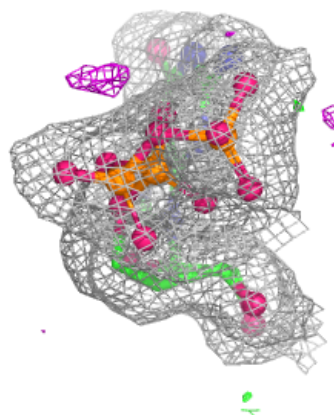
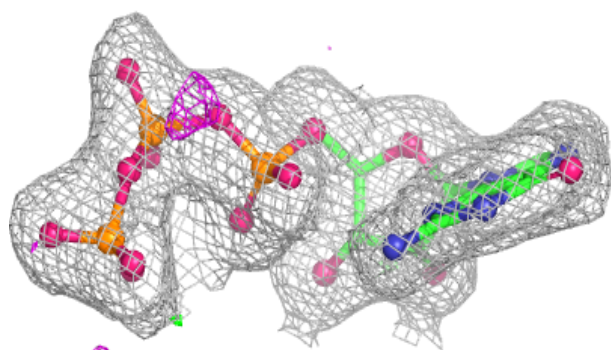
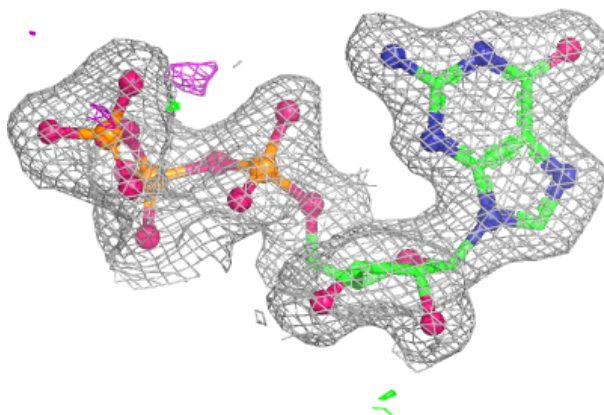


Electron density around HF7 D 702:

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

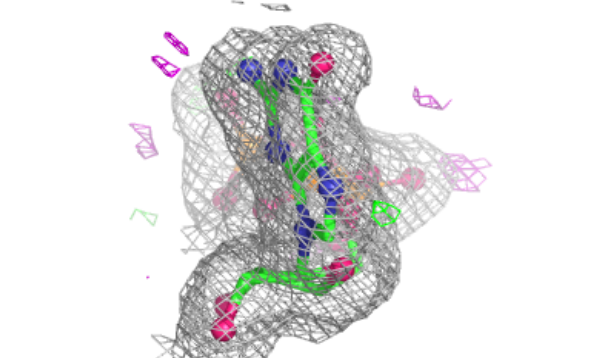
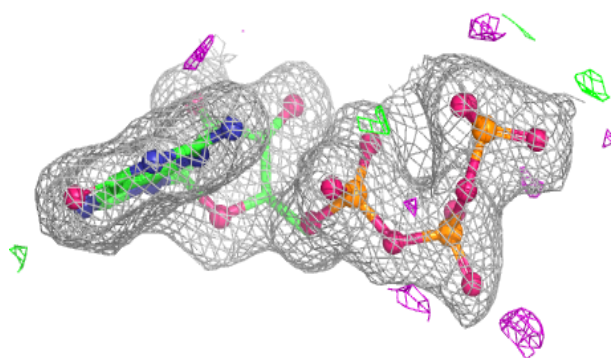
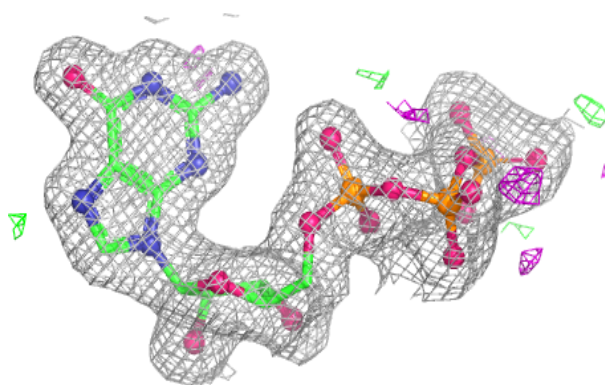
**Electron density around GTP B 702:**

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

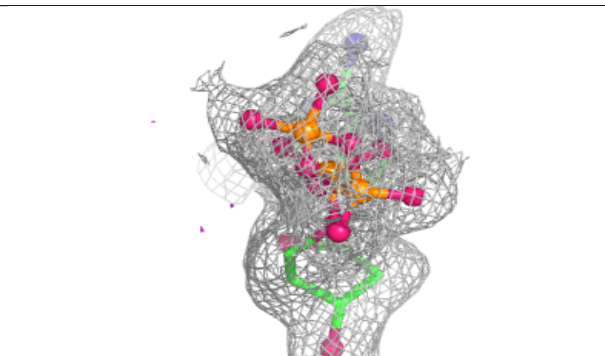
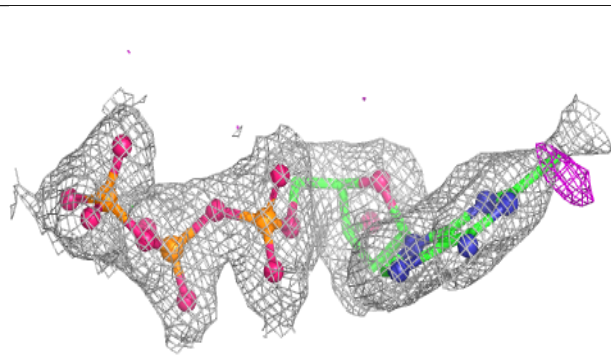
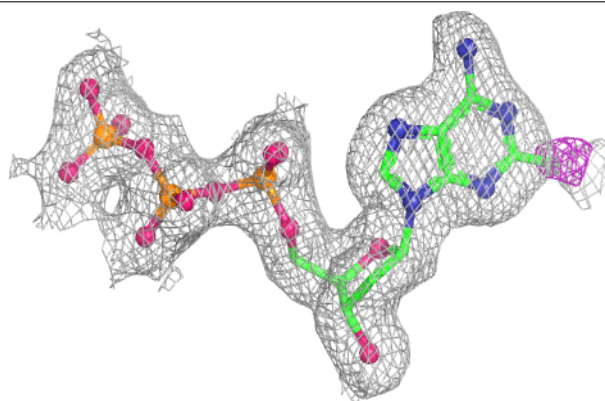


Electron density around GTP A 702:

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

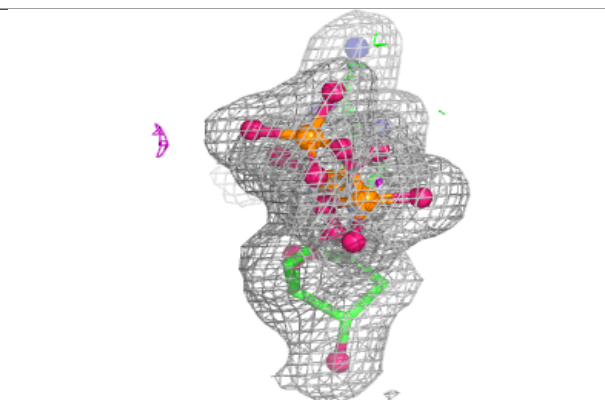
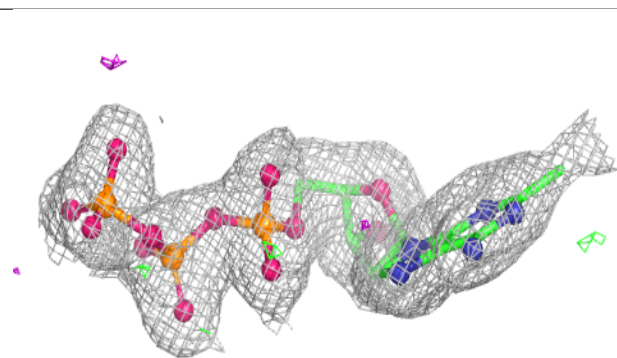
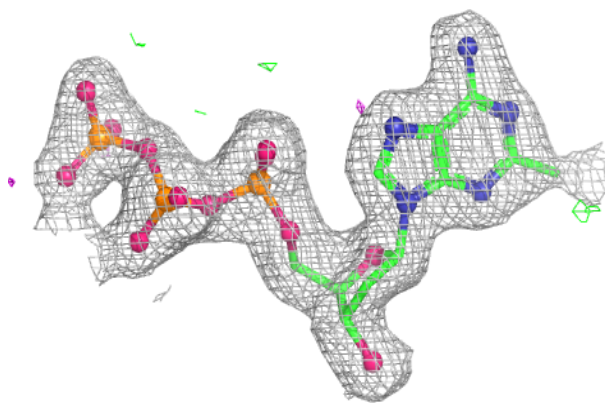
**Electron density around HF7 C 704:**

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

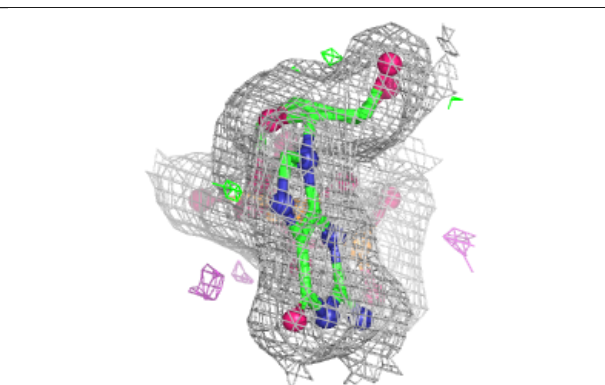
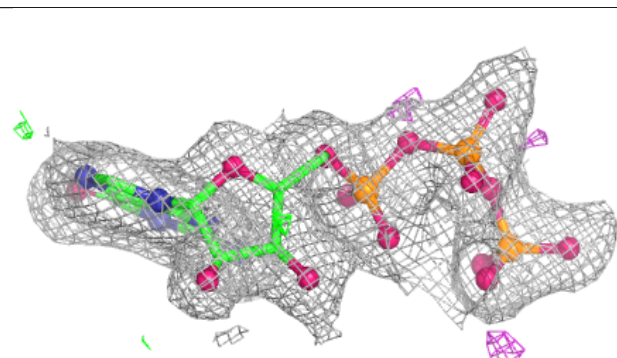
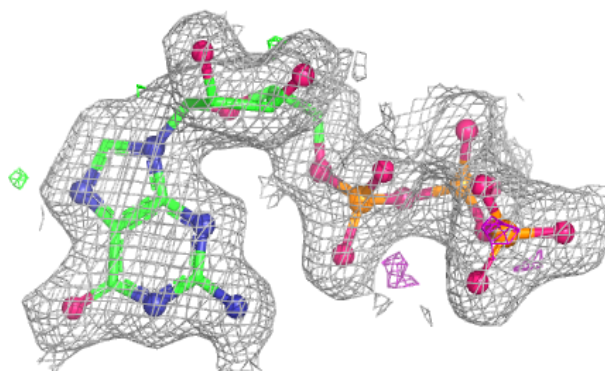


Electron density around HF7 B 701:

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

**Electron density around GTP D 703:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.