Full wwPDB X-ray Structure Validation Report ⓘ

Mar 3, 2024 – 05:33 PM EST

PDB ID	:	6DW7
Title	:	SAMHD1 without Catalytic Nucleotides
Authors	:	Knecht, K.M.; Buzovetsky, O.; Schneider, C.; Thomas, D.; Srikanth, V.; Kaderali, L.; Tofoleanu, F.; Reiss, K.; Ferreiros, N.; Geisslinger, G.; Batista, V.S.; Ji, X.; Cinatl, J.; Keppler, O.T.; Xiong, Y.
Deposited on	:	2018-06-26
Resolution	:	2.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

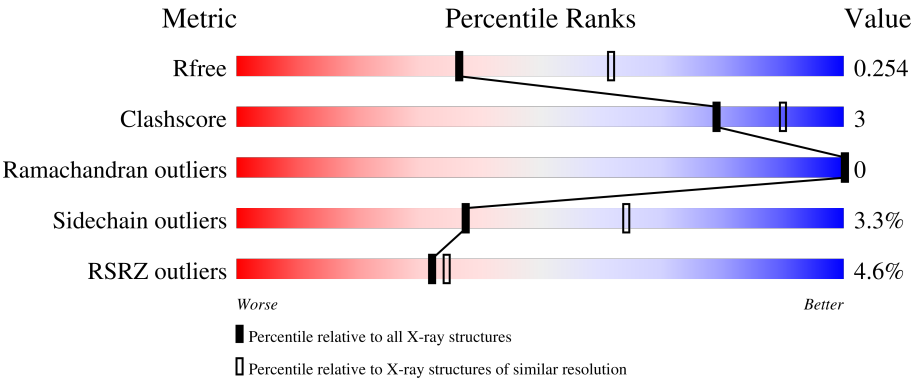
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	550	6% 78% 8% • 13%
1	B	550	5% 81% 6% • 13%
1	C	550	3% 81% 5% • 13%
1	D	550	% 80% 7% • 13%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 16049 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	0	0
			3924	2512	684	708	20			
1	B	481	Total	C	N	O	S	0	0	0
			3933	2517	685	711	20			
1	C	481	Total	C	N	O	S	0	0	0
			3933	2517	685	711	20			
1	D	481	Total	C	N	O	S	0	0	0
			3933	2517	685	711	20			

There are 152 discrepancies between the modelled and reference sequences:

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

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

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

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

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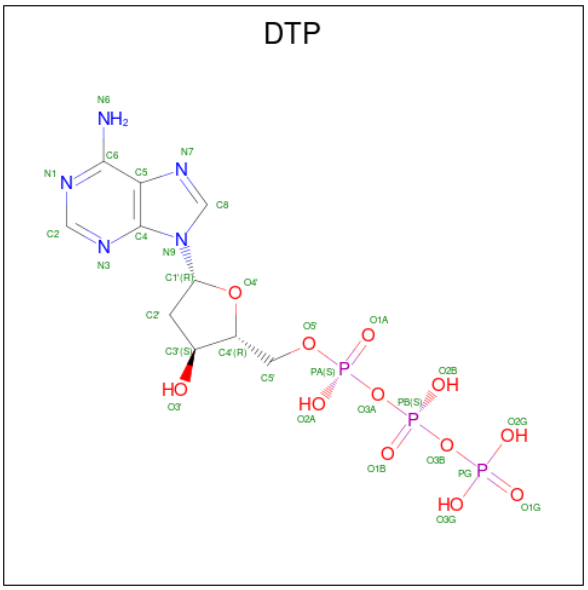
Chain	Residue	Modelled	Actual	Comment	Reference
D	110	PRO	-	expression tag	UNP Q9Y3Z3
D	111	ASN	-	expression tag	UNP Q9Y3Z3
D	112	SER	-	expression tag	UNP Q9Y3Z3
D	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
D	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3

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



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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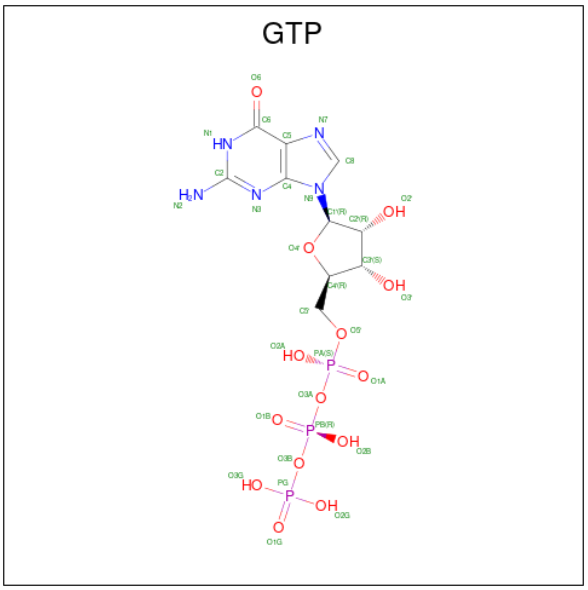
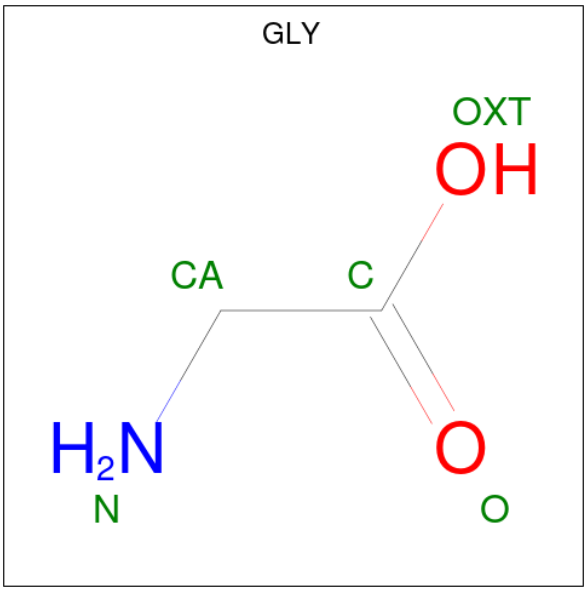
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	2	Total Mg 2 2	0	0

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 5 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$).

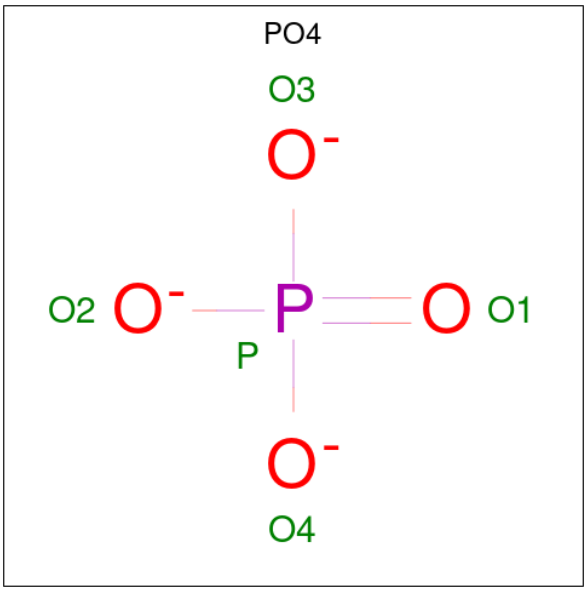


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 5 2 1 2	0	0
5	C	1	Total C N O 5 2 1 2	0	0

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

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

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 8 is water.

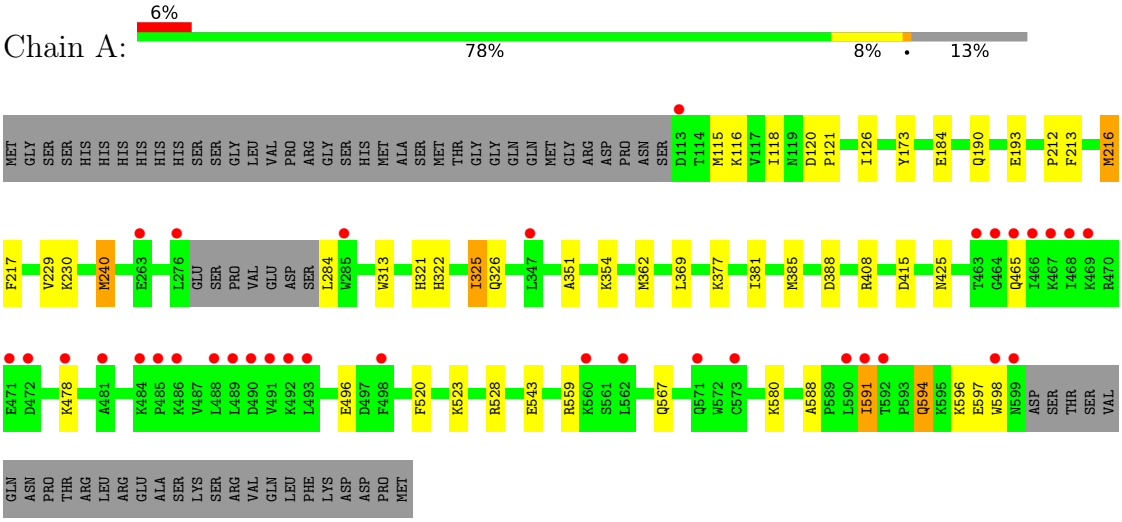
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	14	Total O 14 14	0	0
8	B	18	Total O 18 18	0	0
8	C	13	Total O 13 13	0	0
8	D	11	Total O 11 11	0	0

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.

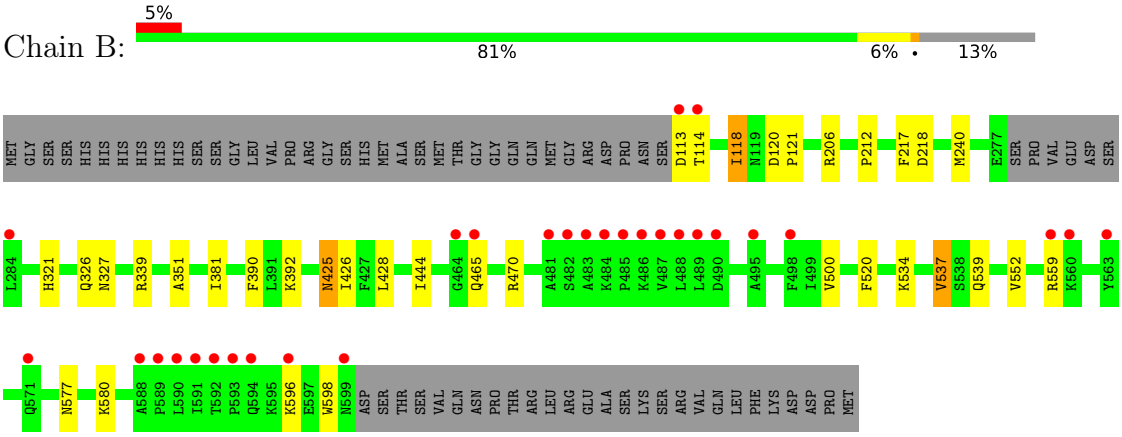
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain A:



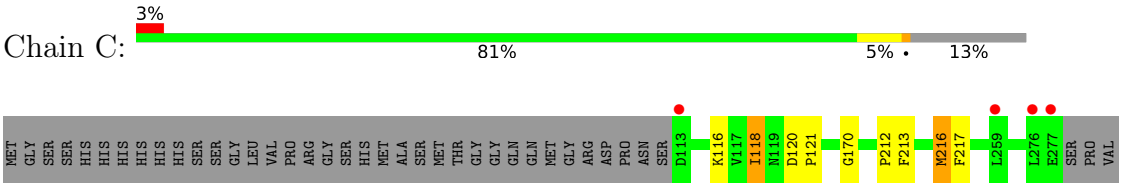
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

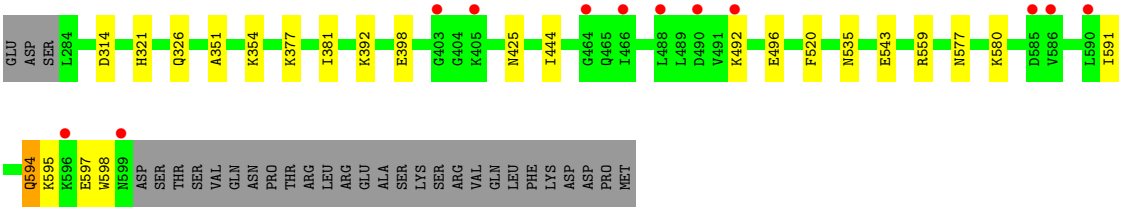
Chain B:



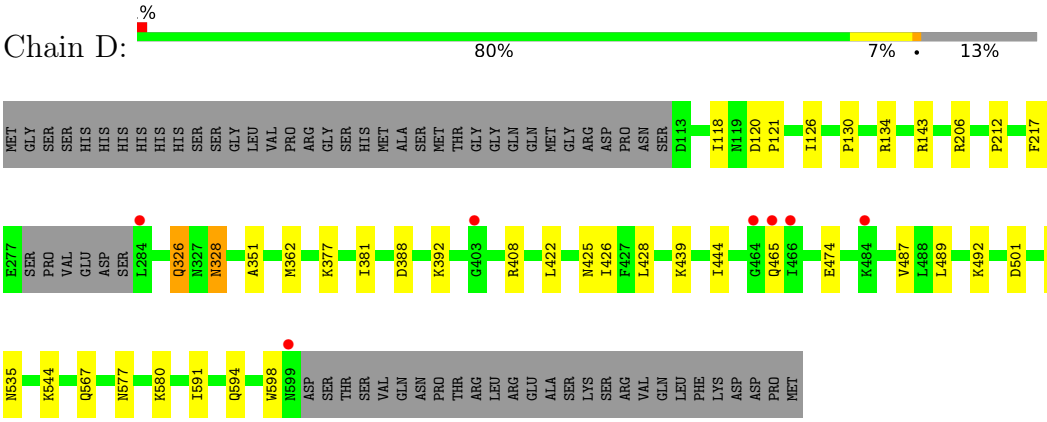
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain C:





• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.55Å 146.37Å 98.93Å 90.00° 113.67° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 36.68 – 2.45	Depositor EDS
% Data completeness (in resolution range)	94.7 (50.00-2.50) 94.7 (36.68-2.45)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.212 , 0.250 0.216 , 0.254	Depositor DCC
R_{free} test set	4009 reflections (5.25%)	wwPDB-VP
Wilson B-factor (Å^2)	50.9	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 33.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16049	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, DTP, MG, PO4, 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	0.61	0/4016	0.82	5/5421 (0.1%)
1	B	0.59	0/4025	0.80	3/5433 (0.1%)
1	C	0.58	0/4025	0.76	0/5433
1	D	0.60	0/4025	0.80	6/5433 (0.1%)
All	All	0.60	0/16091	0.80	14/21720 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	218	ASP	CB-CG-OD1	9.74	127.06	118.30
1	D	218	ASP	CB-CG-OD1	6.57	124.21	118.30
1	D	239	MET	CA-CB-CG	6.41	124.20	113.30
1	B	206	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	A	415	ASP	CB-CG-OD2	6.04	123.74	118.30
1	D	388	ASP	CB-CG-OD1	6.04	123.73	118.30
1	D	206	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	A	415	ASP	CB-CG-OD1	-5.93	112.96	118.30
1	A	240	MET	CG-SD-CE	-5.51	91.38	100.20
1	A	388	ASP	CB-CG-OD2	5.35	123.12	118.30
1	A	385	MET	CG-SD-CE	5.34	108.75	100.20
1	D	501	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	B	113	ASP	CB-CG-OD2	5.24	123.01	118.30
1	D	218	ASP	CB-CG-OD2	-5.12	113.69	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3924	0	3915	36	0
1	B	3933	0	3921	19	0
1	C	3933	0	3921	24	0
1	D	3933	0	3921	22	0
2	A	30	0	12	0	0
2	B	30	0	12	0	0
2	C	30	0	12	1	0
2	D	30	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
4	A	32	0	12	0	0
4	B	32	0	12	1	0
4	C	32	0	12	4	0
4	D	32	0	12	1	0
5	A	5	0	2	0	0
5	C	5	0	2	0	0
6	A	2	0	0	0	0
6	C	1	0	0	0	0
7	D	5	0	0	0	0
8	A	14	0	0	0	0
8	B	18	0	0	1	0
8	C	13	0	0	0	0
8	D	11	0	0	1	0
All	All	16049	0	15778	90	0

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

All (90) 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:A:588:ALA:HB1	1:A:591:ILE:HG12	1.40	1.01
1:A:588:ALA:HB1	1:A:591:ILE:CG1	1.90	1.00
1:A:543:GLU:HG2	1:C:543:GLU:HG3	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:GLN:OE1	1:A:591:ILE:HD11	1.82	0.80
1:D:487:VAL:HG21	1:D:567:GLN:HG3	1.64	0.79
1:A:313:TRP:HE1	1:A:362:MET:CE	1.97	0.75
1:B:392:LYS:HE2	1:B:444:ILE:HD11	1.68	0.74
1:C:392:LYS:HE2	1:C:444:ILE:HD11	1.68	0.73
1:A:588:ALA:HB1	1:A:591:ILE:HG13	1.71	0.71
1:A:126:ILE:HD13	1:A:173:TYR:HB2	1.72	0.71
1:A:523:LYS:HE3	8:B:813:HOH:O	1.92	0.69
1:A:543:GLU:CG	1:C:543:GLU:HG3	2.24	0.66
1:A:116:LYS:CB	1:A:116:LYS:NZ	2.60	0.65
1:A:425:ASN:HB2	1:D:428:LEU:HD13	1.80	0.63
1:A:543:GLU:HG2	1:C:543:GLU:CG	2.28	0.61
1:D:328:ASN:OD1	1:D:328:ASN:N	2.31	0.60
1:A:313:TRP:HE1	1:A:362:MET:HE3	1.66	0.59
1:A:588:ALA:CB	1:A:591:ILE:HG12	2.24	0.59
1:A:116:LYS:HB2	1:A:116:LYS:HZ2	1.68	0.59
1:A:313:TRP:NE1	1:A:362:MET:CE	2.67	0.58
1:B:539:GLN:HG2	1:D:544:LYS:HD3	1.86	0.57
1:B:425:ASN:ND2	1:C:425:ASN:OD1	2.36	0.56
1:D:212:PRO:HD2	1:D:217:PHE:CD1	2.40	0.56
1:A:591:ILE:N	1:A:591:ILE:HD13	2.20	0.56
1:C:213:PHE:HB2	1:C:216:MET:HG2	1.89	0.55
1:C:212:PRO:HD2	1:C:217:PHE:CD1	2.41	0.55
1:A:213:PHE:HB2	1:A:216:MET:HG2	1.87	0.55
1:B:212:PRO:HD2	1:B:217:PHE:CD1	2.42	0.55
1:A:212:PRO:HD2	1:A:217:PHE:CD1	2.42	0.55
1:C:116:LYS:NZ	4:C:704:GTP:O1G	2.34	0.54
1:A:126:ILE:HD13	1:A:173:TYR:CB	2.37	0.54
1:B:534:LYS:O	1:B:537:VAL:HG23	2.07	0.54
1:A:591:ILE:O	1:A:594:GLN:HG2	2.08	0.54
1:B:118:ILE:HG12	4:B:702:GTP:O2'	2.07	0.53
2:C:701:DTP:O2B	4:D:701:GTP:H5"	2.08	0.53
1:C:591:ILE:O	1:C:594:GLN:HG2	2.10	0.52
1:A:116:LYS:CB	1:A:116:LYS:HZ2	2.22	0.51
1:C:213:PHE:CB	1:C:216:MET:HG2	2.42	0.50
1:D:392:LYS:HE2	1:D:444:ILE:HD11	1.94	0.49
1:B:539:GLN:CG	1:D:544:LYS:HD3	2.42	0.49
1:A:313:TRP:HE1	1:A:362:MET:HE1	1.74	0.49
1:B:390:PHE:CZ	1:B:426:ILE:CG2	2.96	0.49
1:B:120:ASP:OD1	1:B:121:PRO:HD2	2.13	0.48
1:D:130:PRO:O	1:D:134:ARG:HG2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:ASN:HB2	1:D:428:LEU:CD1	2.43	0.48
1:D:120:ASP:OD1	1:D:121:PRO:HD2	2.13	0.48
1:C:120:ASP:OD1	1:C:121:PRO:HD2	2.14	0.47
1:A:120:ASP:OD1	1:A:121:PRO:HD2	2.14	0.47
1:D:422:LEU:HD12	1:D:426:ILE:HG13	1.95	0.47
1:A:597:GLU:OE1	1:A:597:GLU:N	2.26	0.47
1:B:428:LEU:HD13	1:C:425:ASN:HB2	1.97	0.46
1:A:213:PHE:CB	1:A:216:MET:HG2	2.44	0.46
1:D:143:ARG:HD3	8:D:802:HOH:O	2.15	0.46
1:C:381:ILE:HD12	1:C:381:ILE:HA	1.84	0.46
1:A:580:LYS:HD2	1:A:598:TRP:HB3	1.97	0.46
1:B:327:ASN:O	1:D:326:GLN:HB3	2.16	0.46
1:B:381:ILE:HD12	1:B:381:ILE:HA	1.84	0.46
1:D:535:ASN:OD1	1:D:535:ASN:N	2.49	0.45
1:C:170:GLY:HA3	1:C:314:ASP:OD2	2.15	0.45
1:B:351:ALA:O	1:B:520:PHE:HA	2.16	0.45
1:A:325:ILE:HG13	1:A:326:GLN:N	2.32	0.45
1:A:351:ALA:O	1:A:520:PHE:HA	2.16	0.45
1:B:390:PHE:CZ	1:B:426:ILE:HG23	2.52	0.45
1:D:351:ALA:O	1:D:520:PHE:HA	2.17	0.45
1:D:381:ILE:HD12	1:D:381:ILE:HA	1.83	0.45
1:C:392:LYS:HE2	1:C:444:ILE:CD1	2.41	0.44
1:C:351:ALA:O	1:C:520:PHE:HA	2.17	0.44
1:B:534:LYS:O	1:B:537:VAL:CG2	2.65	0.44
1:B:580:LYS:HD2	1:B:598:TRP:HB3	2.00	0.44
1:B:392:LYS:HE2	1:B:444:ILE:CD1	2.42	0.44
1:C:580:LYS:HD2	1:C:598:TRP:HB3	2.00	0.43
1:D:580:LYS:HD2	1:D:598:TRP:HB3	2.01	0.43
1:D:487:VAL:HG23	1:D:489:LEU:CD2	2.49	0.43
1:C:535:ASN:OD1	1:C:535:ASN:N	2.49	0.43
1:D:487:VAL:HG13	1:D:591:ILE:HD11	2.00	0.43
1:D:326:GLN:HE21	1:D:326:GLN:HB2	1.73	0.42
1:D:422:LEU:CD1	1:D:426:ILE:HG13	2.50	0.42
1:A:321:HIS:HD2	1:A:322:HIS:CE1	2.38	0.42
1:A:381:ILE:HD12	1:A:381:ILE:HA	1.84	0.42
1:A:588:ALA:O	1:A:591:ILE:HG12	2.19	0.42
1:C:595:LYS:HE3	1:C:597:GLU:OE1	2.19	0.42
1:C:116:LYS:HE3	4:C:704:GTP:HN22	1.85	0.41
1:A:354:LYS:HE3	1:A:354:LYS:HB2	1.86	0.41
1:C:118:ILE:HG12	4:C:704:GTP:O2'	2.21	0.41
1:B:321:HIS:CE1	1:C:321:HIS:CE1	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:LYS:HZ3	1:C:354:LYS:HD2	1.86	0.40
1:A:369:LEU:HD23	1:A:369:LEU:HA	1.81	0.40
1:C:116:LYS:HE3	4:C:704:GTP:O1A	2.21	0.40
1:D:126:ILE:HG21	1:D:126:ILE:HD13	1.84	0.40
1:B:500:VAL:HG22	1:B:552:VAL:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	476/550 (86%)	469 (98%)	7 (2%)	0	100	100
1	B	477/550 (87%)	470 (98%)	7 (2%)	0	100	100
1	C	477/550 (87%)	470 (98%)	7 (2%)	0	100	100
1	D	477/550 (87%)	471 (99%)	6 (1%)	0	100	100
All	All	1907/2200 (87%)	1880 (99%)	27 (1%)	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	426/488 (87%)	406 (95%)	20 (5%)	26	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	427/488 (88%)	415 (97%)	12 (3%)	43 70
1	C	427/488 (88%)	417 (98%)	10 (2%)	50 76
1	D	427/488 (88%)	412 (96%)	15 (4%)	36 62
All	All	1707/1952 (87%)	1650 (97%)	57 (3%)	38 64

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	MET
1	A	118	ILE
1	A	184	GLU
1	A	190	GLN
1	A	193	GLU
1	A	216	MET
1	A	229	VAL
1	A	230	LYS
1	A	240	MET
1	A	284	LEU
1	A	325	ILE
1	A	408	ARG
1	A	465	GLN
1	A	478	LYS
1	A	496	GLU
1	A	528	ARG
1	A	559	ARG
1	A	591	ILE
1	A	594	GLN
1	A	596	LYS
1	B	114	THR
1	B	118	ILE
1	B	240	MET
1	B	326	GLN
1	B	339	ARG
1	B	425	ASN
1	B	465	GLN
1	B	470	ARG
1	B	537	VAL
1	B	559	ARG
1	B	577	ASN
1	B	596	LYS
1	C	118	ILE

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Mol	Chain	Res	Type
1	C	216	MET
1	C	326	GLN
1	C	377	LYS
1	C	398	GLU
1	C	492	LYS
1	C	496	GLU
1	C	559	ARG
1	C	577	ASN
1	C	594	GLN
1	D	118	ILE
1	D	239	MET
1	D	326	GLN
1	D	328	ASN
1	D	362	MET
1	D	377	LYS
1	D	408	ARG
1	D	425	ASN
1	D	439	LYS
1	D	465	GLN
1	D	474	GLU
1	D	492	LYS
1	D	528	ARG
1	D	577	ASN
1	D	594	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	321	HIS
1	A	452	ASN
1	A	571	GLN
1	A	594	GLN
1	B	322	HIS
1	C	235	GLN
1	C	321	HIS
1	C	322	HIS
1	C	326	GLN
1	D	235	GLN
1	D	322	HIS
1	D	326	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

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 7 are monoatomic - leaving 11 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	DTP	B	703	3	26,32,32	1.08	2 (7%)	30,50,50	1.48	5 (16%)
2	DTP	A	701	3	26,32,32	0.92	1 (3%)	30,50,50	1.74	7 (23%)
5	GLY	C	705	-	4,4,4	1.00	0	3,4,4	1.87	2 (66%)
4	GTP	A	703	3	26,34,34	0.99	1 (3%)	32,54,54	1.49	7 (21%)
2	DTP	C	701	3	26,32,32	0.90	1 (3%)	30,50,50	1.80	7 (23%)
7	PO4	D	703	-	4,4,4	0.78	0	6,6,6	0.66	0
5	GLY	A	704	-	4,4,4	0.92	0	3,4,4	2.05	2 (66%)
4	GTP	B	702	3	26,34,34	1.25	4 (15%)	32,54,54	1.45	4 (12%)
2	DTP	D	702	3	26,32,32	0.99	2 (7%)	30,50,50	1.51	6 (20%)
4	GTP	C	704	3	26,34,34	1.00	1 (3%)	32,54,54	1.45	4 (12%)
4	GTP	D	701	3	26,34,34	1.01	1 (3%)	32,54,54	1.39	5 (15%)

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	DTP	B	703	3	-	3/18/34/34	0/3/3/3
2	DTP	A	701	3	-	3/18/34/34	0/3/3/3
5	GLY	C	705	-	-	0/2/2/2	-
4	GTP	A	703	3	-	4/18/38/38	0/3/3/3
2	DTP	C	701	3	-	4/18/34/34	0/3/3/3
5	GLY	A	704	-	-	0/2/2/2	-
4	GTP	B	702	3	-	4/18/38/38	0/3/3/3
2	DTP	D	702	3	-	5/18/34/34	0/3/3/3
4	GTP	C	704	3	-	9/18/38/38	0/3/3/3
4	GTP	D	701	3	-	6/18/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	702	GTP	C6-N1	-3.23	1.33	1.37
4	C	704	GTP	C6-N1	-2.82	1.33	1.37
2	B	703	DTP	C2-N3	2.79	1.36	1.32
4	A	703	GTP	C6-N1	-2.78	1.33	1.37
2	A	701	DTP	C5-C4	2.67	1.48	1.40
4	B	702	GTP	O4'-C1'	2.41	1.44	1.41
2	B	703	DTP	C5-N7	-2.34	1.31	1.39
2	D	702	DTP	C5-C4	2.22	1.46	1.40
2	C	701	DTP	C1'-N9	-2.18	1.42	1.49
4	D	701	GTP	O6-C6	2.10	1.27	1.23
2	D	702	DTP	PG-O3G	-2.09	1.46	1.54
4	B	702	GTP	C2'-C1'	-2.03	1.50	1.53
4	B	702	GTP	O4'-C4'	-2.00	1.40	1.45

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	703	DTP	N3-C2-N1	-4.33	121.91	128.68
4	B	702	GTP	PA-O3A-PB	-4.03	119.00	132.83
2	A	701	DTP	N3-C2-N1	-3.92	122.55	128.68
4	A	703	GTP	O3G-PG-O2G	3.87	122.42	107.64
2	A	701	DTP	C2-N1-C6	3.84	125.32	118.75
2	C	701	DTP	O4'-C1'-C2'	3.72	113.27	106.25
4	C	704	GTP	C3'-C2'-C1'	3.57	106.35	100.98
2	C	701	DTP	O2A-PA-O1A	3.53	129.70	112.24
4	C	704	GTP	PA-O3A-PB	-3.46	120.94	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	701	DTP	N3-C2-N1	-3.33	123.48	128.68
2	C	701	DTP	PB-O3B-PG	-3.21	121.81	132.83
2	D	702	DTP	N3-C2-N1	-3.18	123.70	128.68
4	D	701	GTP	PB-O3B-PG	-2.94	122.73	132.83
2	D	702	DTP	N6-C6-N1	2.86	124.51	118.57
4	A	703	GTP	PA-O3A-PB	-2.81	123.19	132.83
4	C	704	GTP	C5-C6-N1	2.81	118.91	113.95
4	D	701	GTP	C8-N7-C5	2.80	108.33	102.99
2	D	702	DTP	C2'-C3'-C4'	2.80	108.59	102.76
2	A	701	DTP	C4-C5-N7	-2.79	106.49	109.40
4	B	702	GTP	PB-O3B-PG	-2.79	123.26	132.83
2	A	701	DTP	C5-C6-N6	2.76	124.55	120.35
4	D	701	GTP	O3G-PG-O2G	2.72	118.05	107.64
2	C	701	DTP	O3G-PG-O2G	2.69	117.90	107.64
2	D	702	DTP	O2A-PA-O1A	2.65	125.34	112.24
4	A	703	GTP	C8-N7-C5	2.64	108.01	102.99
5	C	705	GLY	OXT-C-O	-2.55	116.95	123.30
2	A	701	DTP	O2A-PA-O1A	2.50	124.61	112.24
5	A	704	GLY	OXT-C-CA	2.50	123.39	113.45
2	B	703	DTP	C2'-C3'-C4'	2.45	107.86	102.76
5	A	704	GLY	OXT-C-O	-2.42	117.26	123.30
4	B	702	GTP	C8-N7-C5	2.39	107.55	102.99
2	B	703	DTP	O2A-PA-O1A	2.38	124.00	112.24
4	A	703	GTP	N2-C2-N3	-2.37	115.11	119.74
2	B	703	DTP	O3G-PG-O2G	2.36	116.67	107.64
2	D	702	DTP	O2G-PG-O1G	2.35	119.87	110.68
2	C	701	DTP	O2G-PG-O3B	-2.35	96.77	104.64
4	D	701	GTP	C3'-C2'-C1'	2.29	104.43	100.98
2	A	701	DTP	O3G-PG-O2G	2.27	116.32	107.64
2	A	701	DTP	C2'-C1'-N9	2.23	119.42	114.27
4	D	701	GTP	C2-N1-C6	-2.22	121.01	125.10
4	B	702	GTP	O2B-PB-O1B	2.21	123.15	112.24
2	B	703	DTP	C4-C5-N7	-2.20	107.11	109.40
2	C	701	DTP	C3'-C2'-C1'	-2.18	97.07	102.54
2	D	702	DTP	C2-N1-C6	2.16	122.45	118.75
4	C	704	GTP	O2'-C2'-C1'	-2.12	103.03	110.85
4	A	703	GTP	O4'-C1'-C2'	2.07	109.95	106.93
4	A	703	GTP	O2B-PB-O1B	2.04	122.32	112.24
4	A	703	GTP	O3G-PG-O3B	-2.02	97.87	104.64
5	C	705	GLY	OXT-C-CA	2.00	121.41	113.45

There are no chirality outliers.

All (38) torsion outliers are listed below:

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

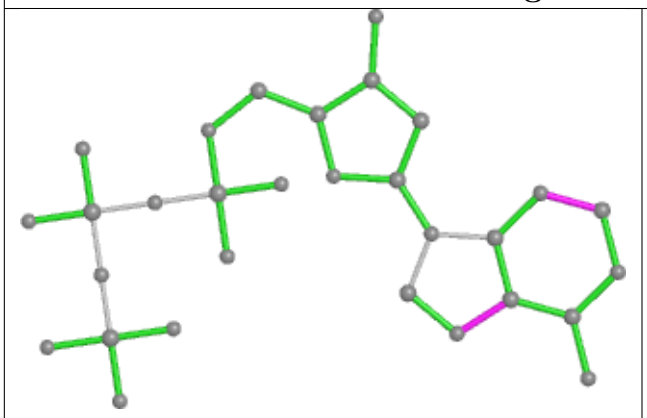
There are no ring outliers.

4 monomers are involved in 6 short contacts:

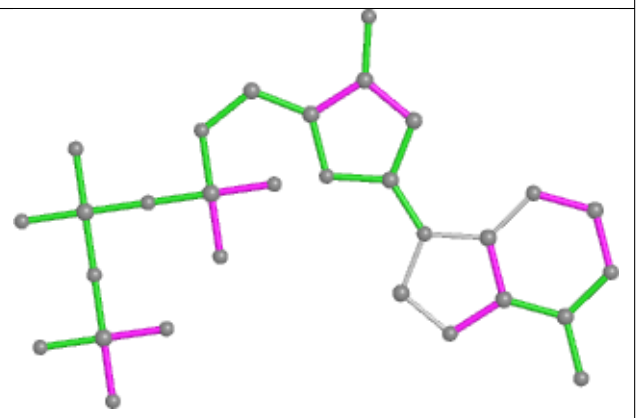
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	701	DTP	1	0
4	B	702	GTP	1	0
4	C	704	GTP	4	0
4	D	701	GTP	1	0

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

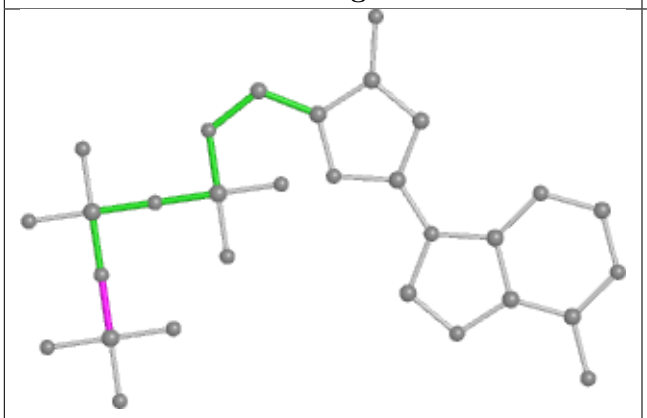
Ligand DTP B 703



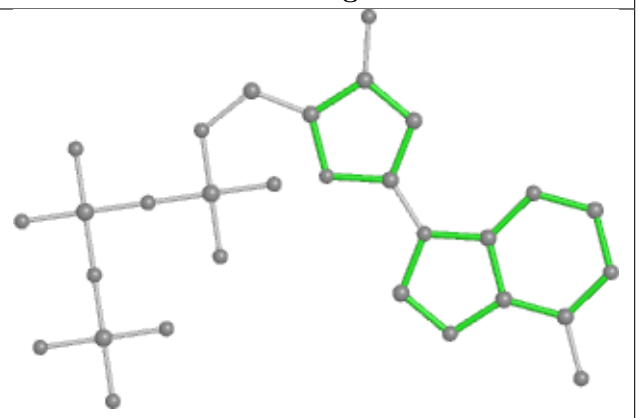
Bond lengths



Bond angles

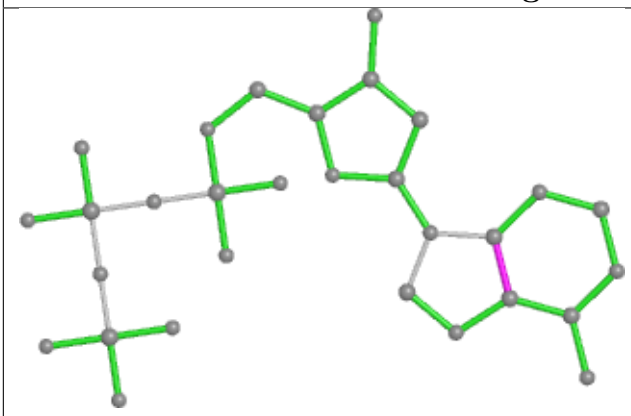


Torsions

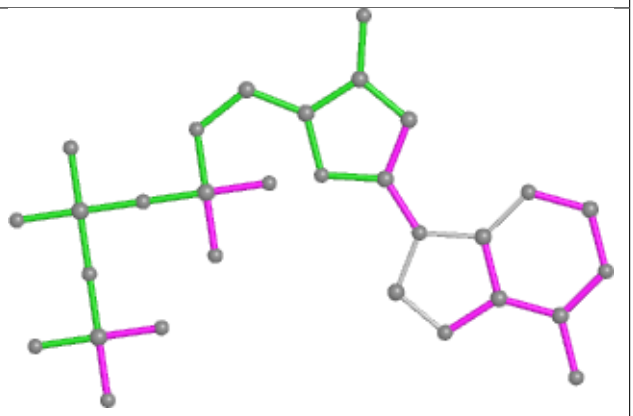


Rings

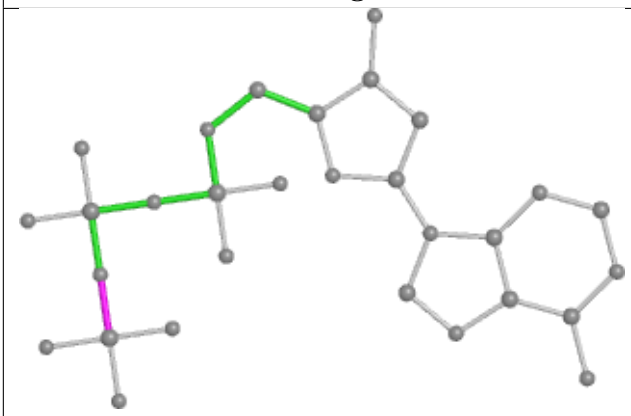
Ligand DTP A 701



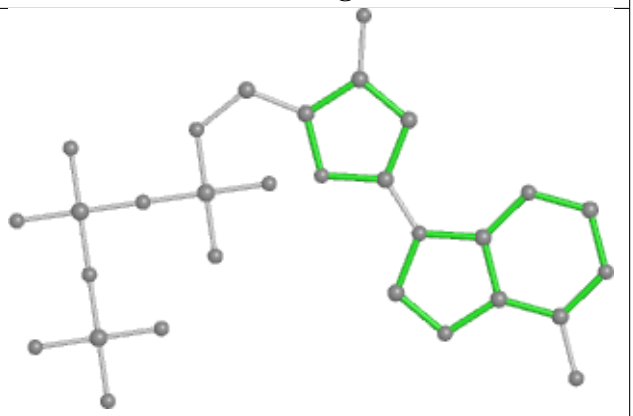
Bond lengths



Bond angles

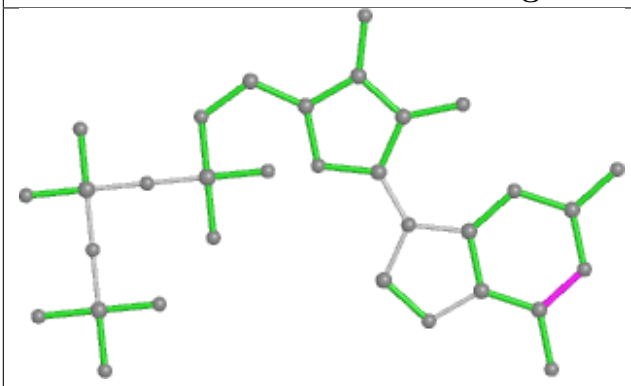


Torsions

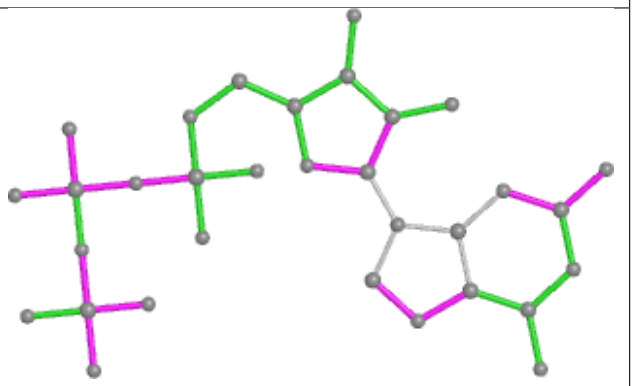


Rings

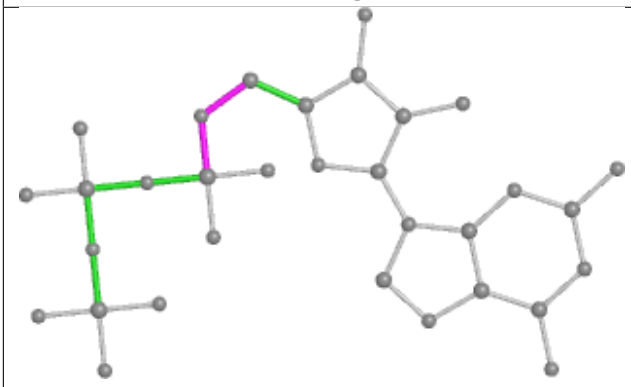
Ligand GTP A 703



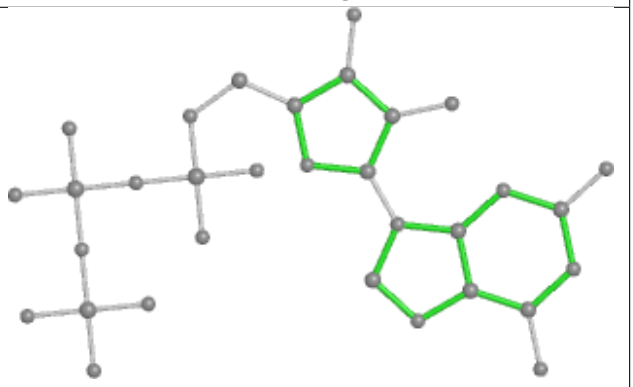
Bond lengths



Bond angles

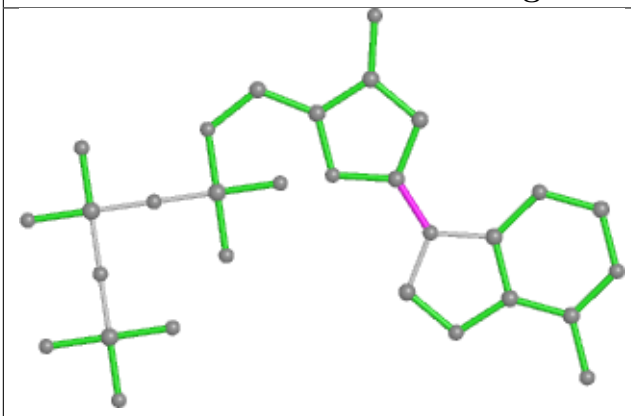


Torsions

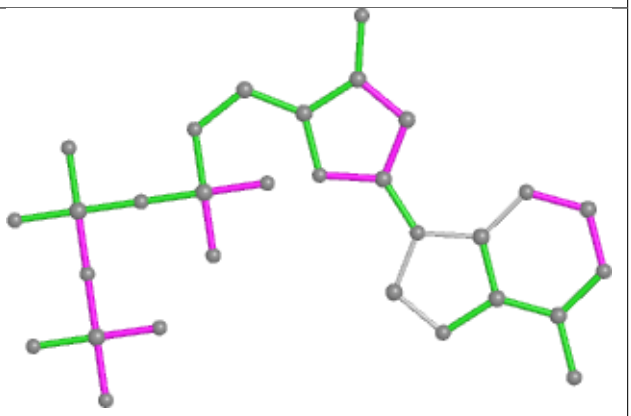


Rings

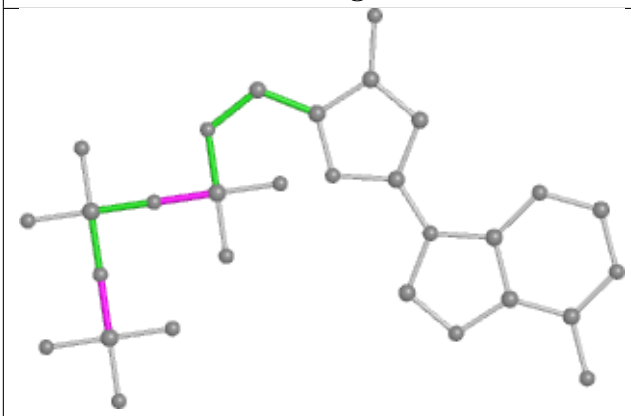
Ligand DTP C 701



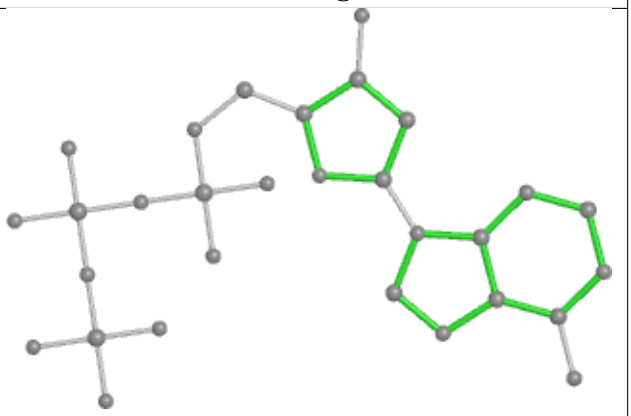
Bond lengths



Bond angles

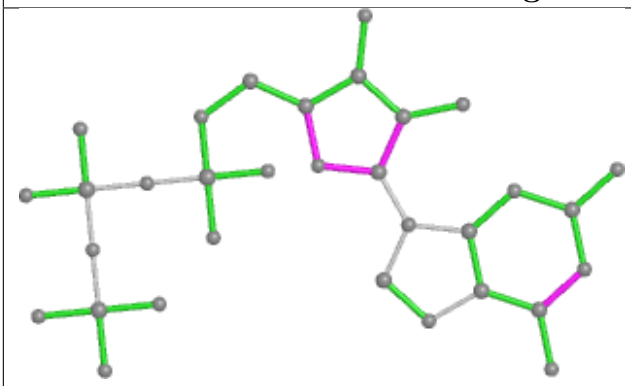


Torsions

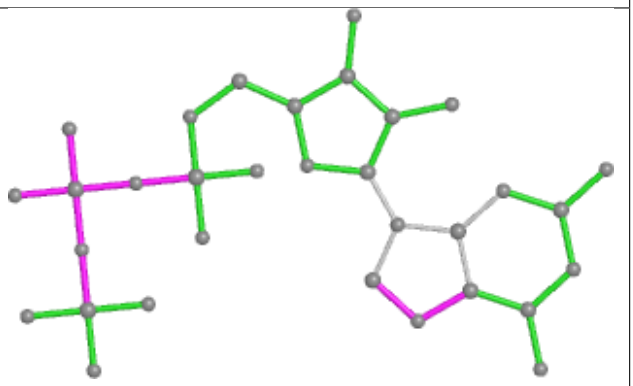


Rings

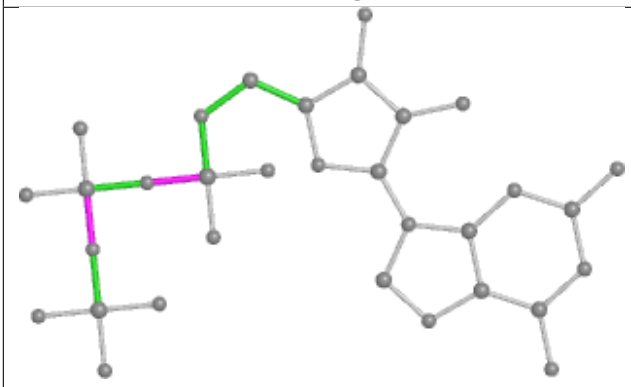
Ligand GTP B 702



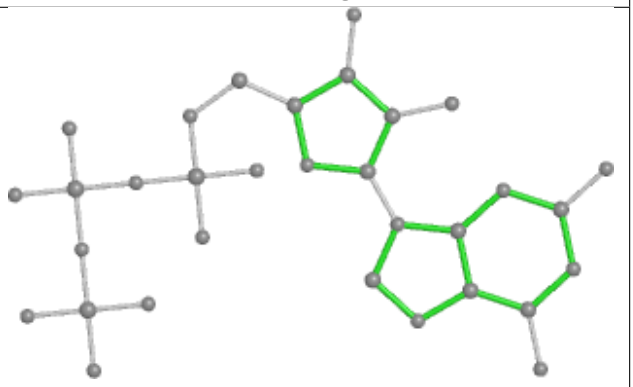
Bond lengths



Bond angles

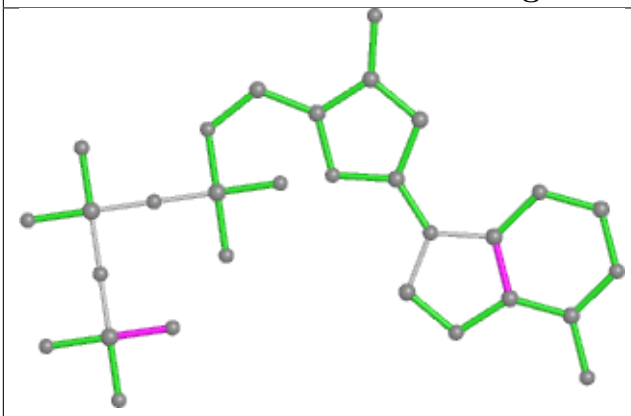


Torsions



Rings

Ligand DTP D 702



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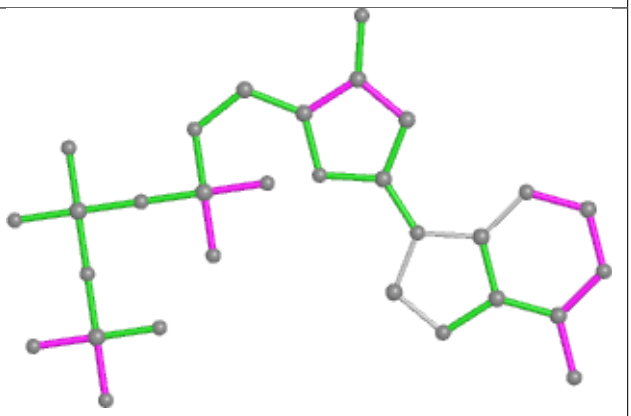
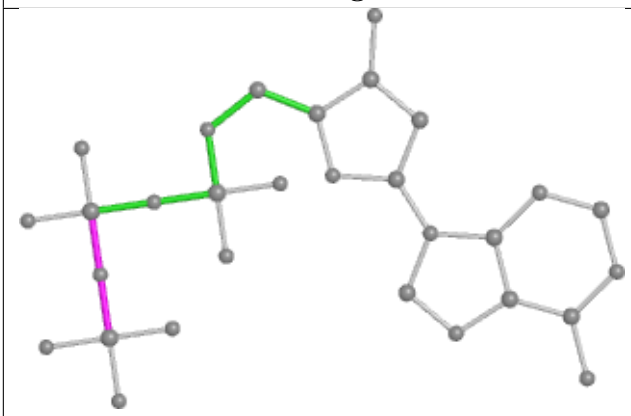
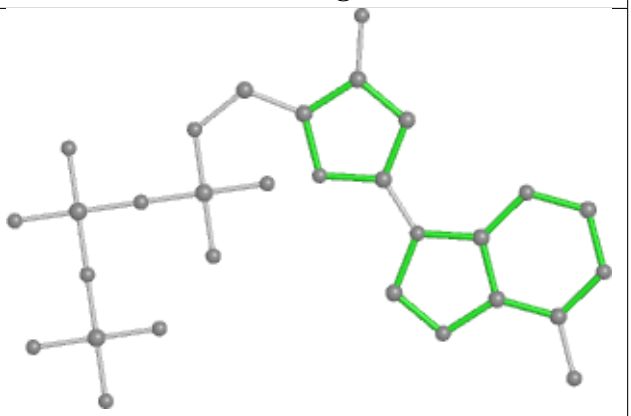


Bond angles

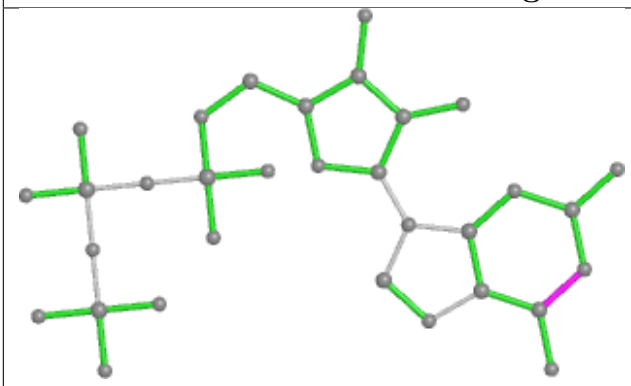


Torsions

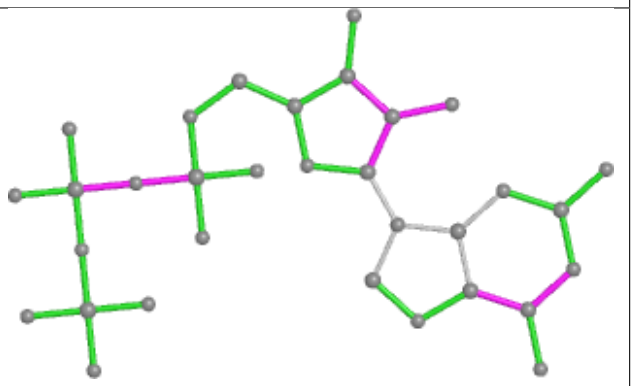


Rings

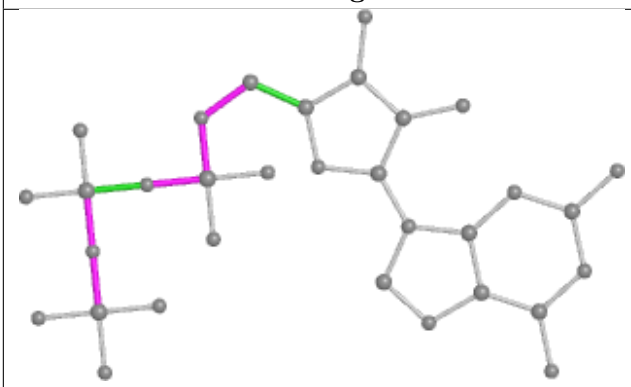
Ligand GTP C 704



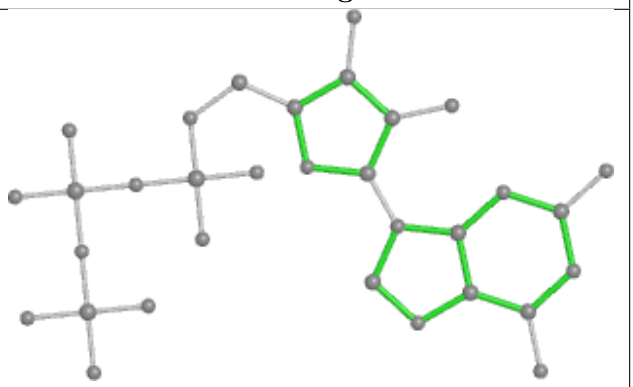
Bond lengths



Bond angles

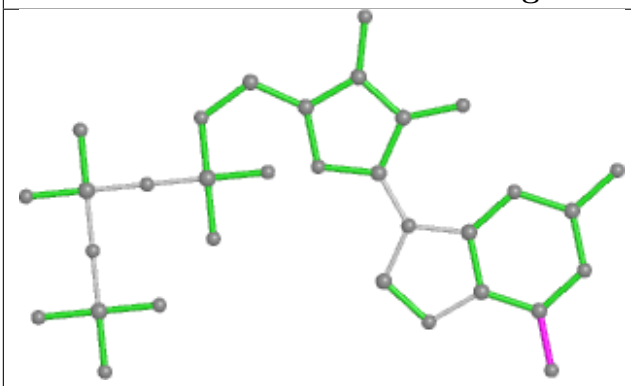


Torsions

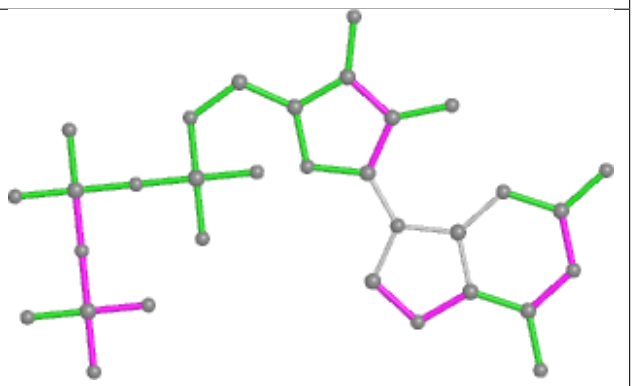


Rings

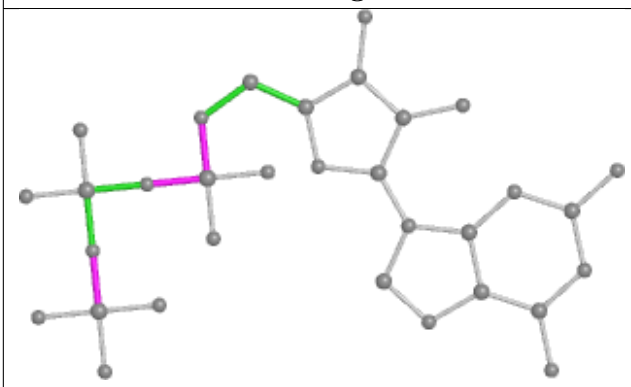
Ligand GTP D 701



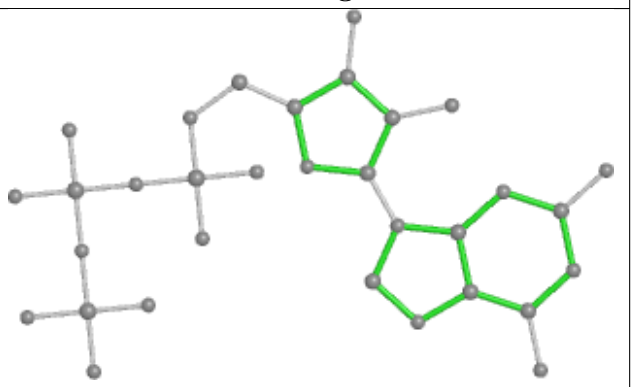
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	480/550 (87%)	0.21	35 (7%)	15	15	29, 65, 121, 159	0
1	B	481/550 (87%)	0.21	30 (6%)	20	21	30, 63, 123, 163	0
1	C	481/550 (87%)	0.02	16 (3%)	46	50	33, 64, 111, 147	0
1	D	481/550 (87%)	-0.03	7 (1%)	73	75	29, 59, 100, 145	0
All	All	1923/2200 (87%)	0.10	88 (4%)	32	34	29, 62, 117, 163	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	596	LYS	7.6
1	D	465	GLN	6.0
1	A	463	THR	5.8
1	A	488	LEU	5.3
1	B	465	GLN	5.3
1	A	490	ASP	5.2
1	D	464	GLY	5.2
1	B	599	ASN	5.0
1	B	590	LEU	4.9
1	D	403	GLY	4.8
1	B	591	ILE	4.8
1	A	485	PRO	4.6
1	B	485	PRO	4.6
1	B	490	ASP	4.6
1	B	593	PRO	4.5
1	A	465	GLN	4.4
1	A	486	LYS	4.3
1	C	113	ASP	4.3
1	A	493	LEU	4.3
1	B	488	LEU	4.2
1	A	468	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	594	GLN	4.1
1	A	492	LYS	4.1
1	C	590	LEU	4.1
1	A	276	LEU	4.1
1	B	498	PHE	4.0
1	B	563	TYR	3.9
1	C	464	GLY	3.8
1	A	464	GLY	3.7
1	A	481	ALA	3.6
1	A	491	VAL	3.6
1	B	486	LYS	3.6
1	B	487	VAL	3.5
1	A	471	GLU	3.3
1	A	113	ASP	3.3
1	A	592	THR	3.3
1	D	284	LEU	3.3
1	B	592	THR	3.2
1	B	559	ARG	3.2
1	B	284	LEU	3.2
1	A	573	CYS	3.1
1	A	562	LEU	3.1
1	A	598	TRP	3.1
1	B	560	LYS	3.0
1	D	599	ASN	3.0
1	B	484	LYS	3.0
1	C	586	VAL	3.0
1	A	599	ASN	3.0
1	A	591	ILE	2.9
1	C	488	LEU	2.9
1	B	571	GLN	2.8
1	A	466	ILE	2.8
1	C	466	ILE	2.8
1	B	114	THR	2.8
1	B	483	ALA	2.7
1	C	490	ASP	2.7
1	C	276	LEU	2.7
1	C	277	GLU	2.7
1	C	599	ASN	2.6
1	A	478	LYS	2.6
1	B	588	ALA	2.6
1	B	596	LYS	2.6
1	A	571	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	498	PHE	2.5
1	B	589	PRO	2.5
1	A	484	LYS	2.5
1	A	489	LEU	2.4
1	B	489	LEU	2.4
1	B	113	ASP	2.4
1	B	495	ALA	2.4
1	A	347	LEU	2.4
1	A	285	TRP	2.3
1	C	585	ASP	2.3
1	B	481	ALA	2.3
1	D	466	ILE	2.2
1	D	484	LYS	2.2
1	A	472	ASP	2.2
1	C	259	LEU	2.2
1	C	405	LYS	2.1
1	B	464	GLY	2.1
1	A	590	LEU	2.1
1	A	467	LYS	2.1
1	A	469	LYS	2.1
1	A	263	GLU	2.1
1	C	403	GLY	2.0
1	C	492	LYS	2.0
1	A	560	LYS	2.0
1	B	482	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

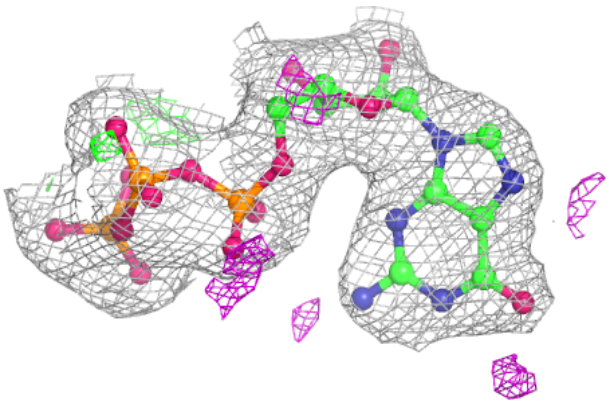
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

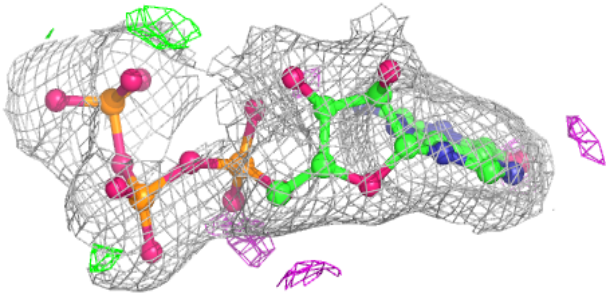
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NA	C	706	1/1	0.66	0.19	68,68,68,68	0
6	NA	A	705	1/1	0.84	0.37	74,74,74,74	0
5	GLY	A	704	5/5	0.85	0.22	75,76,80,83	0
5	GLY	C	705	5/5	0.91	0.23	60,63,69,70	0
6	NA	A	706	1/1	0.92	0.12	74,74,74,74	0
3	MG	C	702	1/1	0.93	0.14	35,35,35,35	0
3	MG	C	703	1/1	0.94	0.12	43,43,43,43	0
3	MG	B	701	1/1	0.94	0.11	48,48,48,48	0
3	MG	A	702	1/1	0.94	0.17	47,47,47,47	0
7	PO4	D	703	5/5	0.94	0.23	94,104,112,112	0
4	GTP	D	701	32/32	0.97	0.13	36,45,54,65	0
2	DTP	A	701	30/30	0.98	0.13	34,38,45,46	0
4	GTP	A	703	32/32	0.98	0.14	29,40,47,52	0
4	GTP	C	704	32/32	0.98	0.11	34,46,54,56	0
2	DTP	C	701	30/30	0.98	0.12	24,37,49,50	0
2	DTP	D	702	30/30	0.98	0.12	30,35,45,51	0
2	DTP	B	703	30/30	0.99	0.13	28,31,36,38	0
4	GTP	B	702	32/32	0.99	0.12	30,38,48,57	0

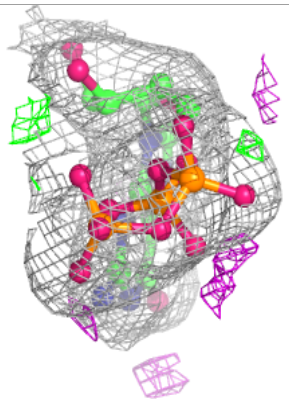
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GTP 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)

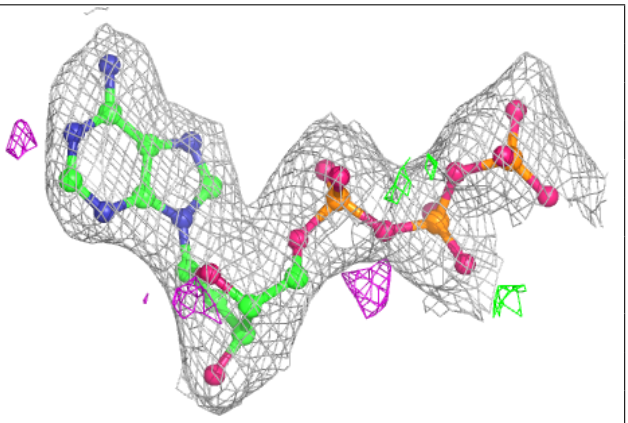


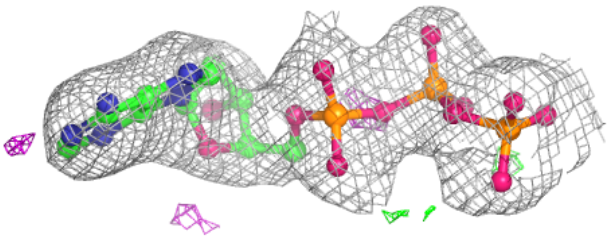


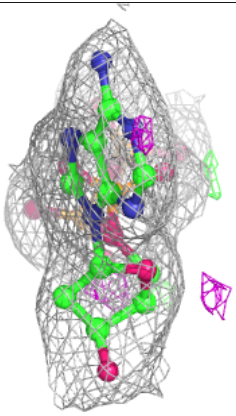


Electron density around DTP A 701:

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

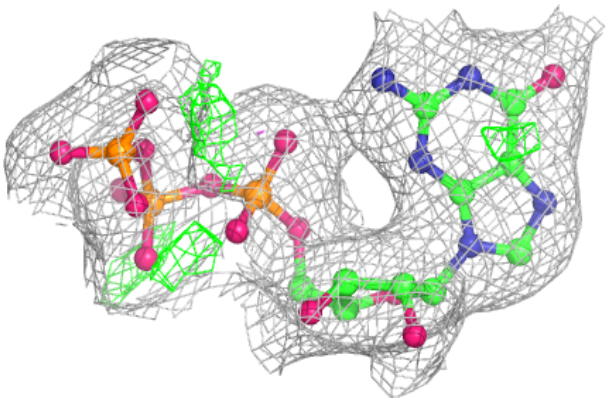


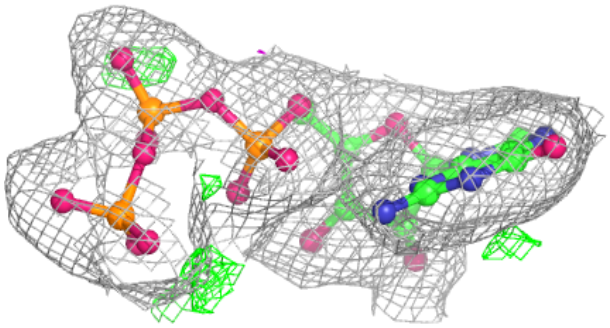


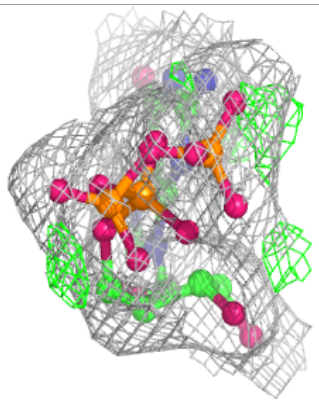


Electron density around GTP A 703:

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

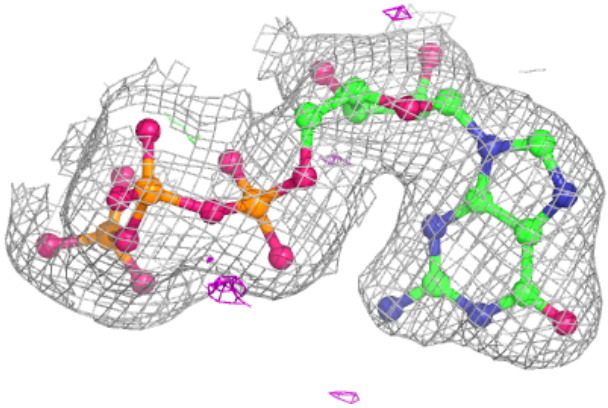


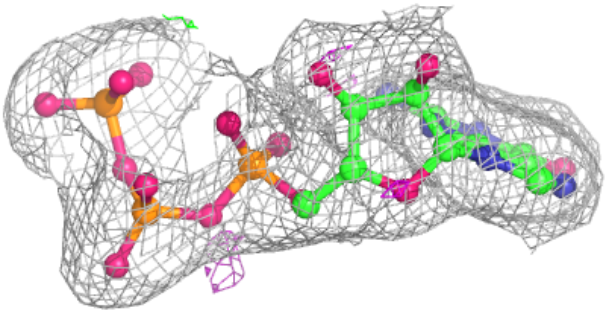


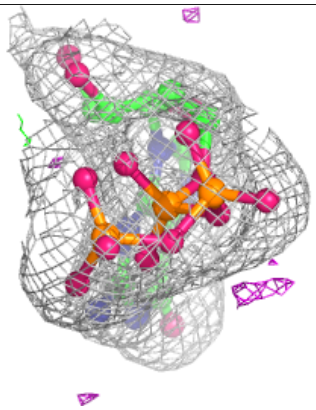


Electron density around GTP C 704:

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

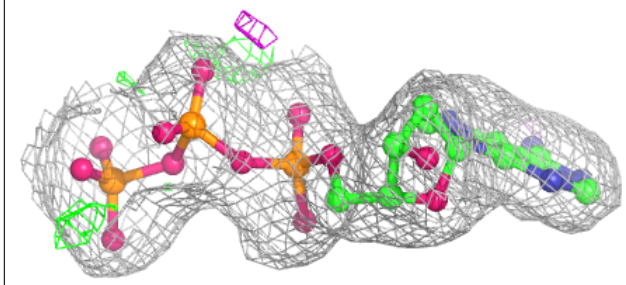


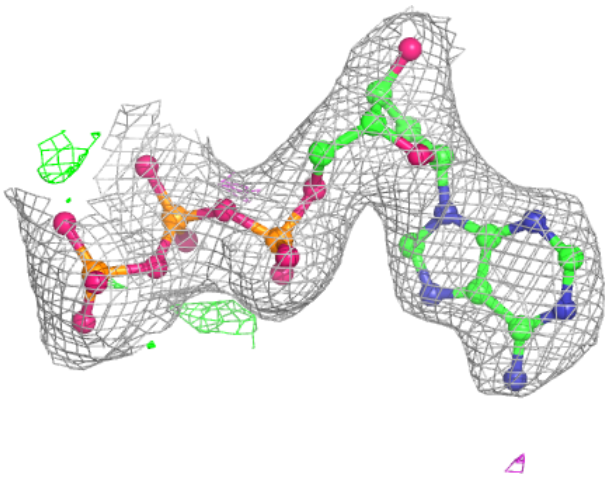


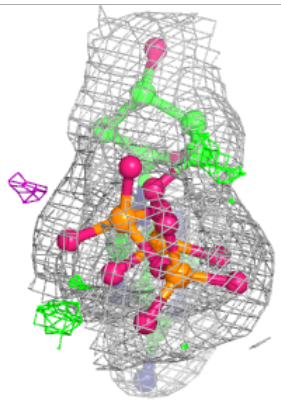


Electron density around DTP C 701:

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

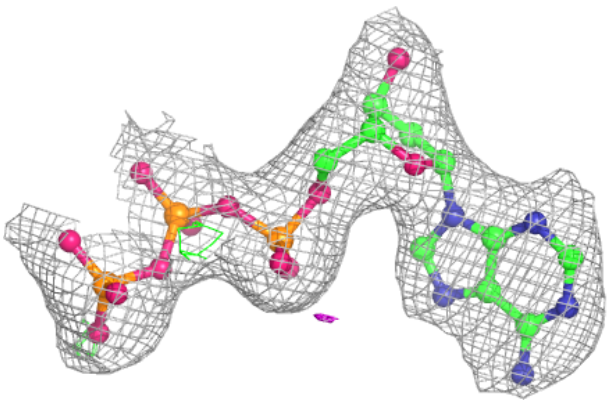


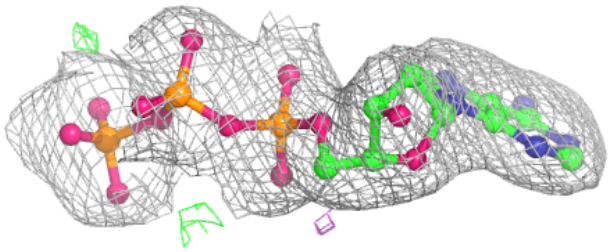


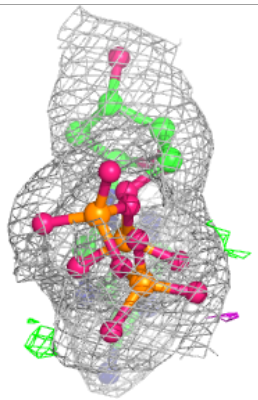


Electron density around DTP D 702:

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

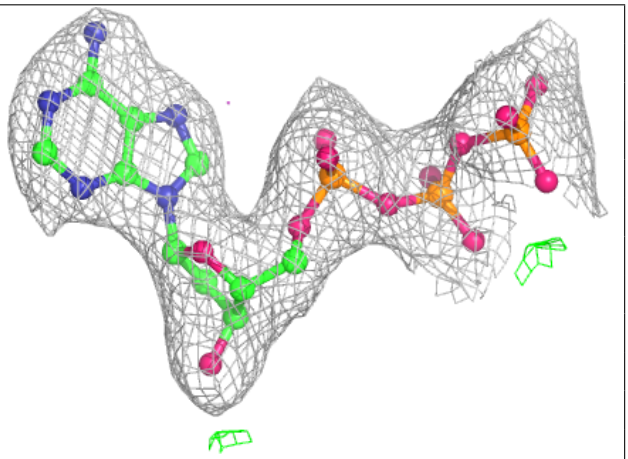


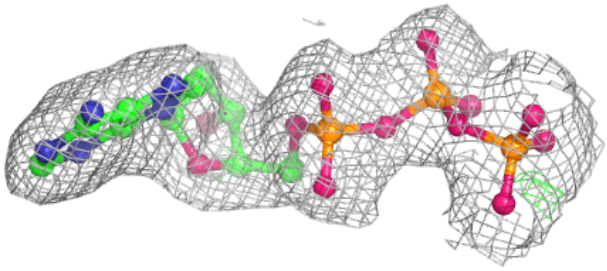


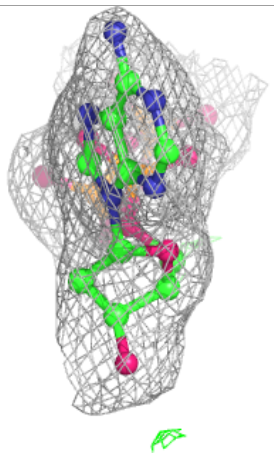


Electron density around DTP B 703:

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

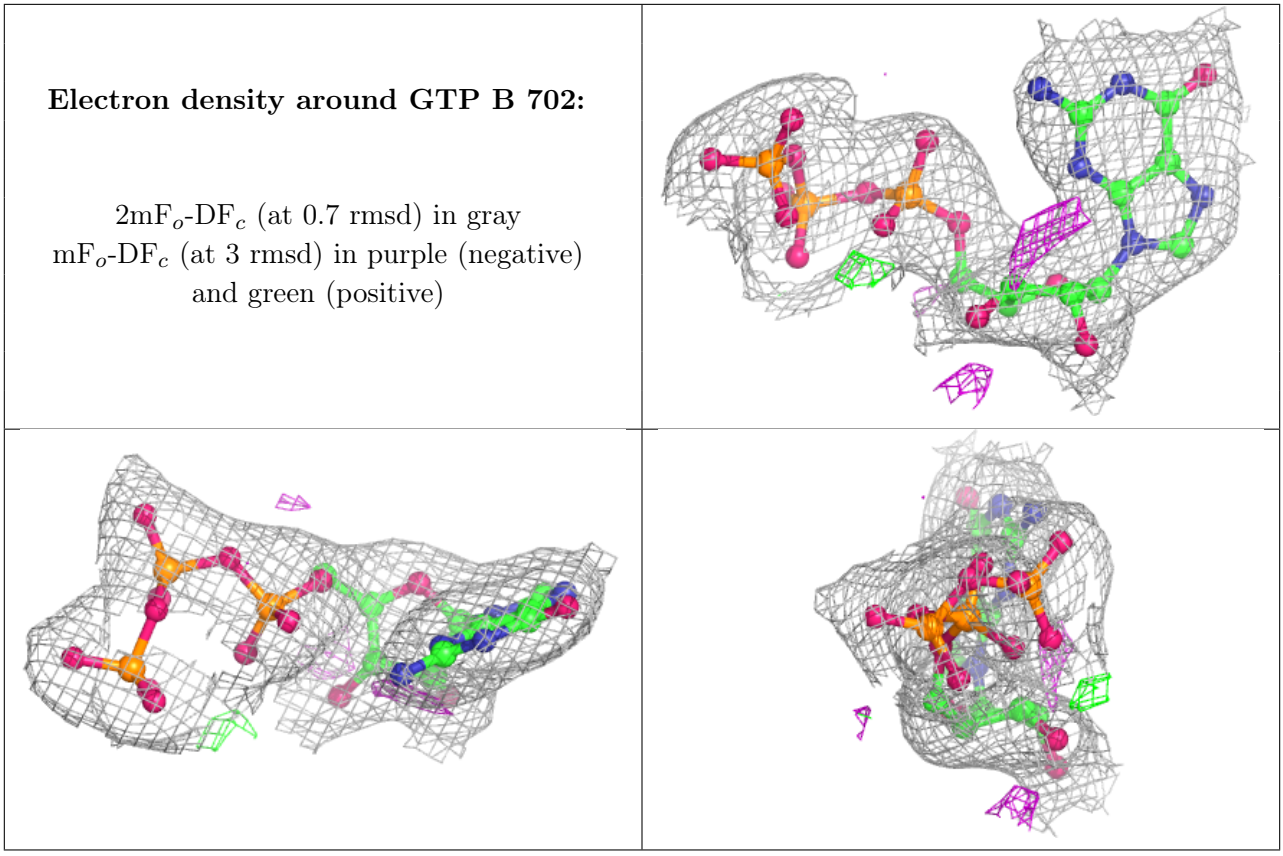






Electron density around GTP B 702:

$2mF_o$-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.