Full wwPDB X-ray Structure Validation Report (i)

Mar 3, 2024 – 08:45 PM EST

PDB ID	:	6DWK
Title	:	SAMHD1 Bound to Fludarabine-TP in the Catalytic Pocket
Authors	:	Knecht, K.M.; Buzovetsky, O.; Schneider, C.; Thomas, D.; Srikanth, V.; Kaderali, L.; Tofoleanu, F.; Reiss, K.; Ferreiros, N.; Geisslinger, G.; Batista, V.S.; Ji, X.; Cinatl, J.; Keppler, O.T.; Xiong, Y.
Deposited on	:	2018-06-26
Resolution	:	2.30 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 (i) 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 (i)) were used in the production of this report:

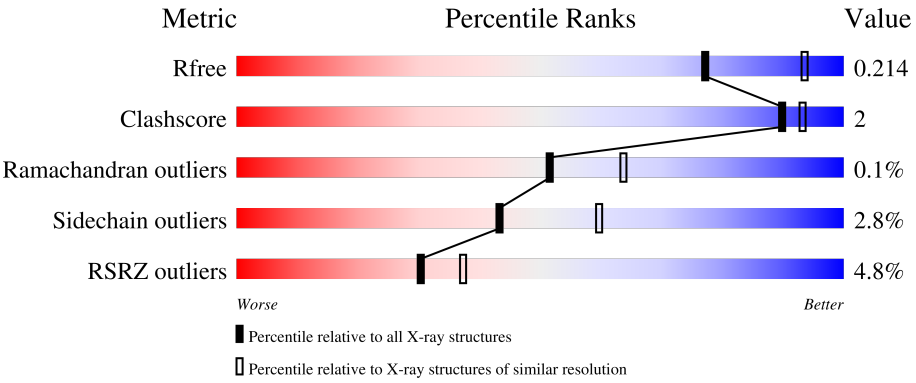
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	5% 81% 6% • 13%
1	B	550	5% 79% 7% • 13%
1	C	550	5% 78% 7% • 13%
1	D	550	2% 78% 8% • 13%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MG	B	710	-	-	-	X
7	GLY	C	710	-	X	-	-
7	GLY	C	714	-	X	-	-
7	GLY	D	713	-	X	-	X

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 16439 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	2	0
			3939	2523	687	709	20			
1	B	478	Total	C	N	O	S	0	0	0
			3908	2502	681	705	20			
1	C	478	Total	C	N	O	S	0	2	0
			3921	2511	683	707	20			
1	D	478	Total	C	N	O	S	0	0	0
			3908	2502	681	705	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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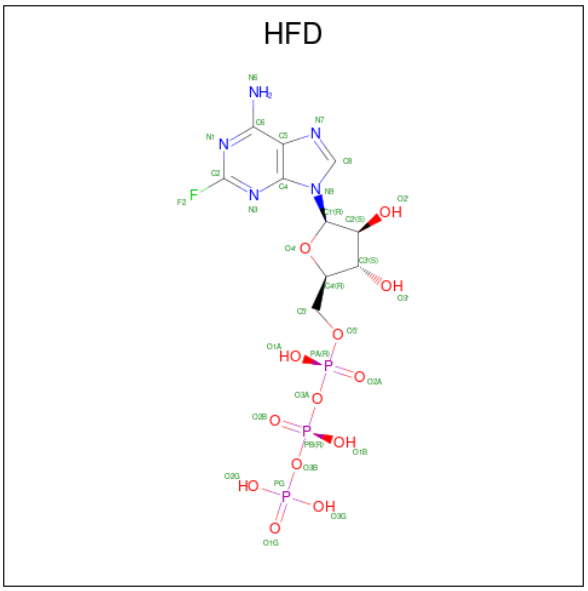
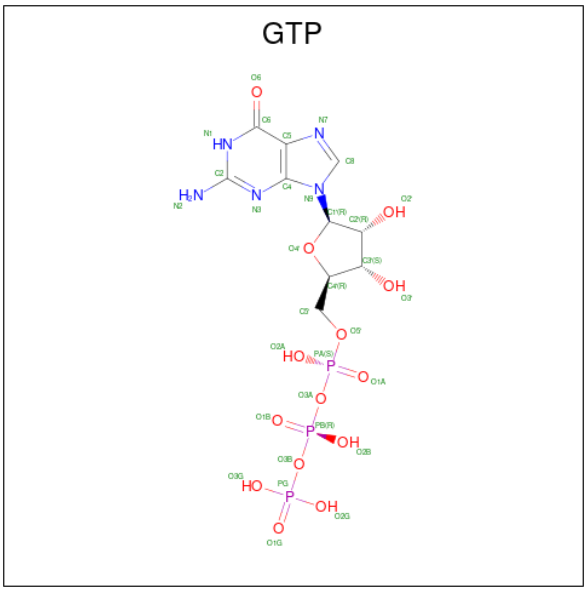
Chain	Residue	Modelled	Actual	Comment	Reference
D	110	PRO	-	expression tag	UNP Q9Y3Z3
D	111	ASN	-	expression tag	UNP Q9Y3Z3
D	112	SER	-	expression tag	UNP Q9Y3Z3
D	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
D	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3

- Molecule 2 is 2-fluoro-9-{5-O-[(R)-hydroxy{[(R)-hydroxy(phosphonooxy)phosphoryl]oxy}phosphoryl]-beta-D-arabinofuranosyl}-9H-purin-6-a mine (three-letter code: HFD) (formula: $C_{10}H_{15}FN_5O_{13}P_3$).



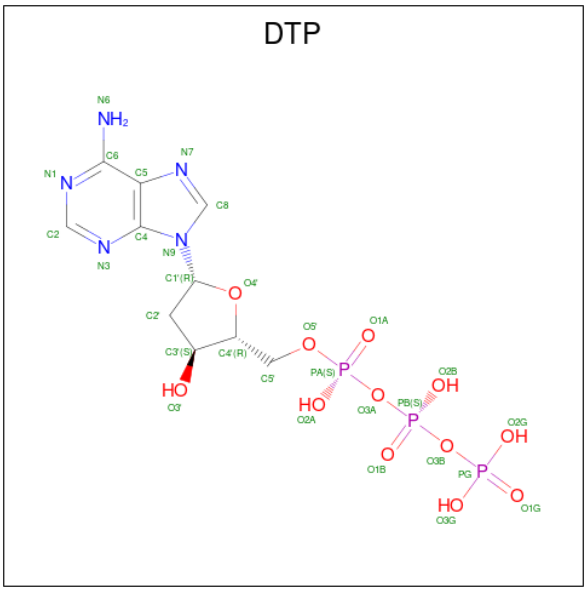
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	P	0	0
			32	10	1	5	13	3		
2	B	1	Total	C	F	N	O	P	0	0
			32	10	1	5	13	3		
2	C	1	Total	C	F	N	O	P	0	0
			32	10	1	5	13	3		
2	D	1	Total	C	F	N	O	P	0	0
			32	10	1	5	13	3		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	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		
3	B	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		

- Molecule 4 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
4	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
4	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
4	C	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
4	D	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

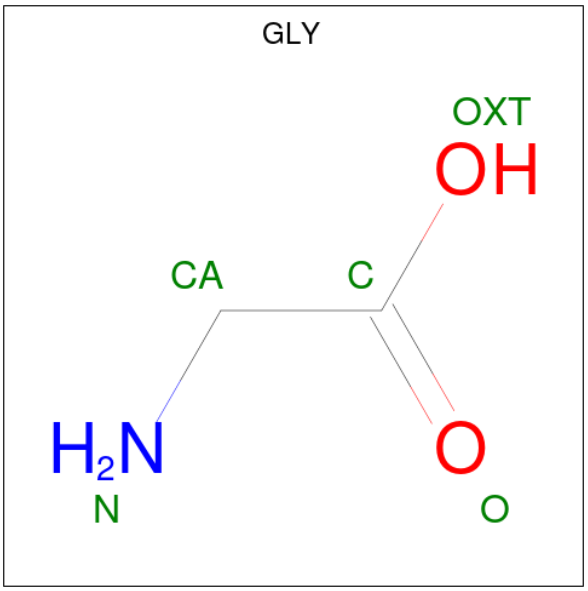
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

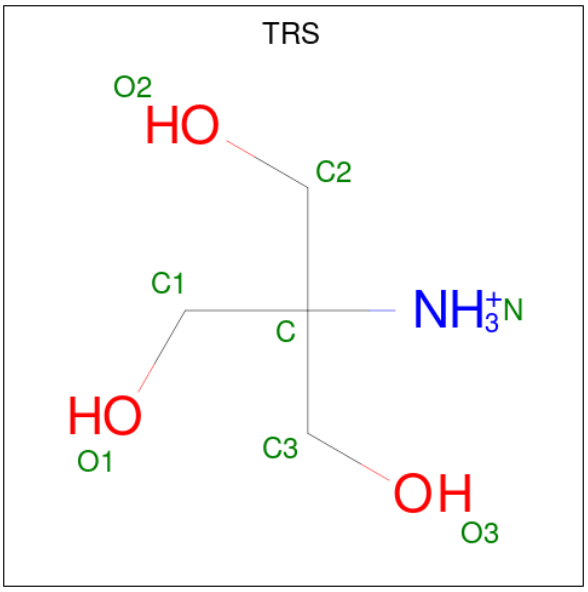
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	7	Total	Na	0	0
			7	7		
6	B	6	Total	Na	0	0
			6	6		
6	C	4	Total	Na	0	0
			4	4		
6	D	6	Total	Na	0	0
			6	6		

- Molecule 7 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$).



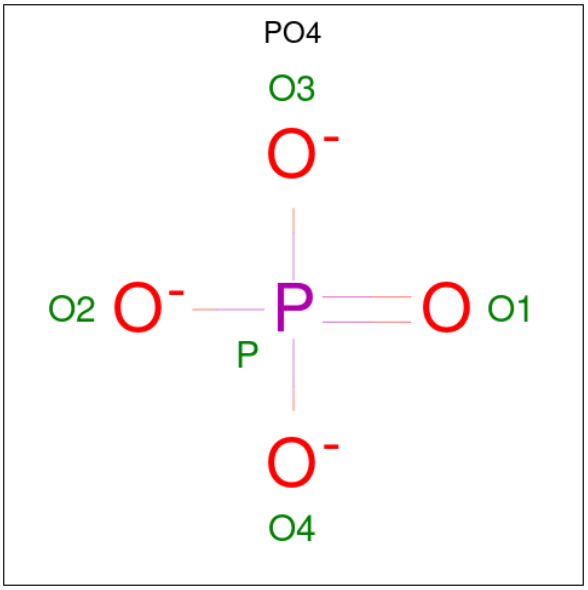
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O 5 2 1 2	0	0
7	B	1	Total C N O 5 2 1 2	0	0
7	B	1	Total C N O 5 2 1 2	0	0
7	C	1	Total C N O 5 2 1 2	0	0
7	C	1	Total C N O 5 2 1 2	0	0
7	C	1	Total C N O 5 2 1 2	0	0
7	C	1	Total C N O 5 2 1 2	0	0
7	C	1	Total C N O 5 2 1 2	0	0
7	D	1	Total C N O 5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

- Molecule 8 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C N O 8 4 1 3	0	0
8	B	1	Total C N O 8 4 1 3	0	0

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 10 is water.

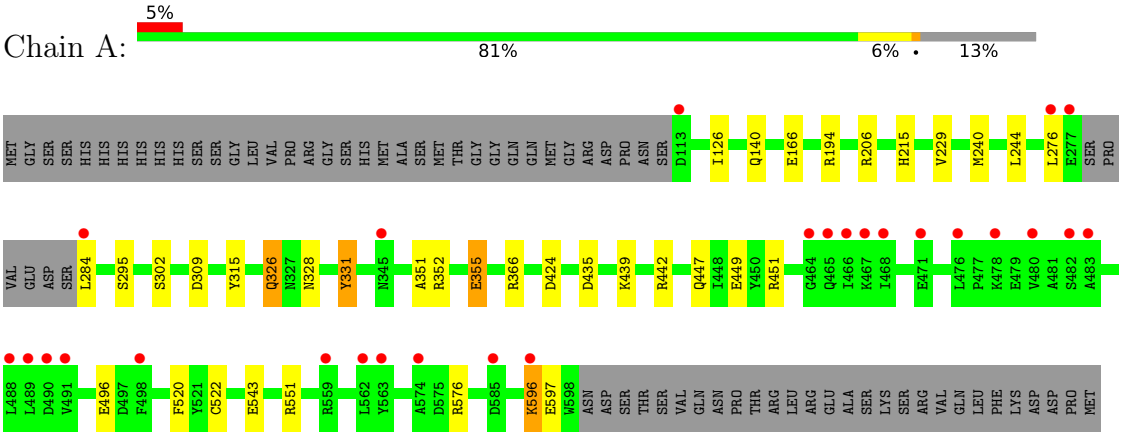
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	54	Total O 54 54	0	0
10	B	81	Total O 81 81	0	0
10	C	46	Total O 46 46	0	0
10	D	93	Total O 93 93	0	0

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.

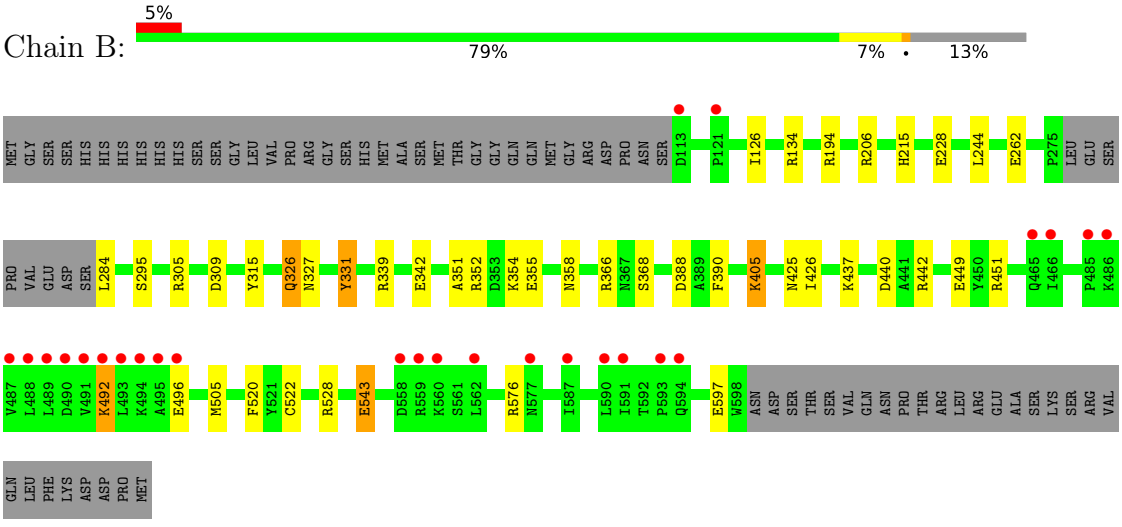
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain A:



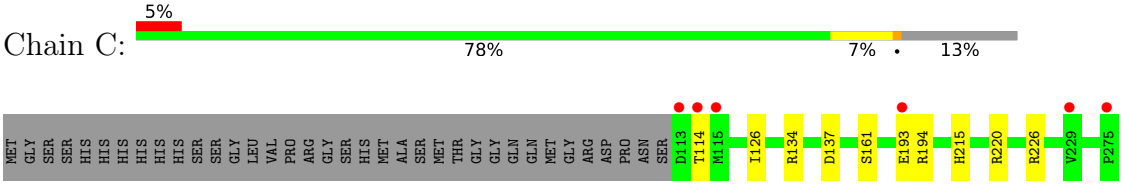
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

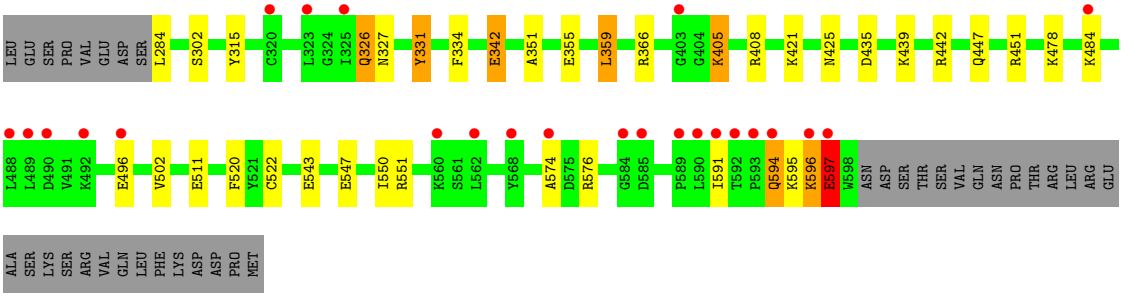
Chain B:



• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

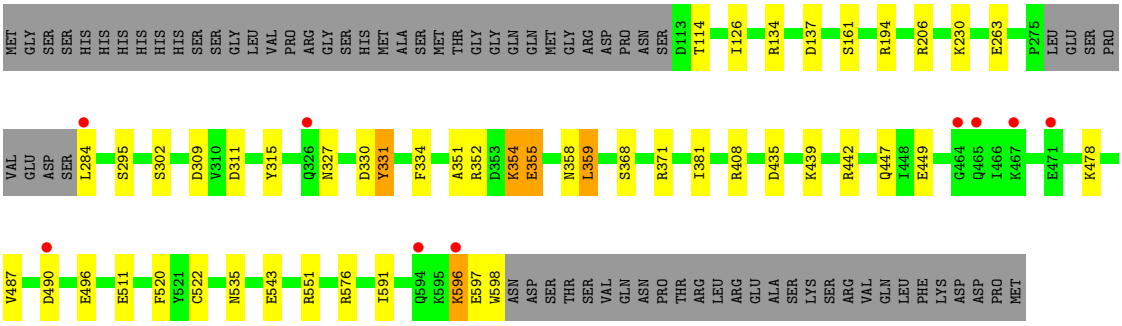
Chain C:





• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.69Å 146.67Å 99.13Å 90.00° 114.53° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 48.90 – 2.28	Depositor EDS
% Data completeness (in resolution range)	96.3 (50.00-2.30) 96.3 (48.90-2.28)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.176 , 0.212 0.181 , 0.214	Depositor DCC
R_{free} test set	5169 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	34.8	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16439	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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: DTP, TRS, MG, HFD, NA, GTP, PO4

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	1.01	7/4039 (0.2%)	1.01	14/5452 (0.3%)
1	B	1.03	11/4000 (0.3%)	1.04	21/5399 (0.4%)
1	C	0.99	7/4020 (0.2%)	1.04	17/5426 (0.3%)
1	D	1.07	13/4000 (0.3%)	1.04	17/5399 (0.3%)
All	All	1.02	38/16059 (0.2%)	1.03	69/21676 (0.3%)

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	A	0	1

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	528	ARG	NE-CZ	13.97	1.51	1.33
1	C	355	GLU	CD-OE1	10.31	1.36	1.25
1	A	449	GLU	CD-OE1	10.29	1.36	1.25
1	A	449	GLU	CD-OE2	8.81	1.35	1.25
1	C	355	GLU	CD-OE2	7.87	1.34	1.25
1	B	388	ASP	CB-CG	7.17	1.66	1.51
1	D	449	GLU	CD-OE2	7.08	1.33	1.25
1	D	490	ASP	CB-CG	7.00	1.66	1.51
1	B	368	SER	CB-OG	-6.72	1.33	1.42
1	D	511	GLU	CD-OE1	6.60	1.32	1.25
1	D	447	GLN	CG-CD	6.60	1.66	1.51
1	C	447	GLN	CG-CD	6.39	1.65	1.51
1	C	326	GLN	CG-CD	6.13	1.65	1.51
1	B	327	ASN	CG-ND2	6.12	1.48	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	161	SER	CB-OG	6.11	1.50	1.42
1	C	161	SER	CB-OG	5.99	1.50	1.42
1	A	355	GLU	CD-OE1	5.90	1.32	1.25
1	A	424	ASP	CB-CG	5.87	1.64	1.51
1	C	342	GLU	CG-CD	5.80	1.60	1.51
1	B	342	GLU	CD-OE2	5.67	1.31	1.25
1	B	354	LYS	C-O	-5.56	1.12	1.23
1	D	263	GLU	CD-OE1	5.55	1.31	1.25
1	B	228	GLU	CG-CD	5.41	1.60	1.51
1	C	496	GLU	CG-CD	5.36	1.59	1.51
1	D	496	GLU	CD-OE2	5.30	1.31	1.25
1	D	354	LYS	C-O	-5.29	1.13	1.23
1	D	295	SER	CB-OG	-5.26	1.35	1.42
1	B	331	TYR	CZ-OH	5.24	1.46	1.37
1	B	528	ARG	CZ-NH1	-5.22	1.26	1.33
1	D	368	SER	CB-OG	-5.21	1.35	1.42
1	D	511	GLU	CD-OE2	5.17	1.31	1.25
1	A	166	GLU	CG-CD	5.14	1.59	1.51
1	A	302	SER	CB-OG	-5.14	1.35	1.42
1	D	355	GLU	CG-CD	5.10	1.59	1.51
1	D	302	SER	CB-OG	-5.06	1.35	1.42
1	B	543	GLU	CG-CD	5.05	1.59	1.51
1	B	449	GLU	CD-OE2	5.01	1.31	1.25
1	A	355	GLU	CG-CD	5.00	1.59	1.51

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	339	ARG	NE-CZ-NH2	-10.94	114.83	120.30
1	C	551	ARG	NE-CZ-NH1	-9.29	115.66	120.30
1	A	435	ASP	CB-CG-OD2	-8.89	110.30	118.30
1	B	388	ASP	CB-CG-OD2	8.87	126.28	118.30
1	C	366	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	D	371	ARG	CB-CG-CD	8.28	133.12	111.60
1	D	354	LYS	CD-CE-NZ	8.15	130.46	111.70
1	C	547	GLU	OE1-CD-OE2	-7.97	113.73	123.30
1	B	528	ARG	NE-CZ-NH1	-7.93	116.33	120.30
1	A	576	ARG	NE-CZ-NH2	7.86	124.23	120.30
1	A	442	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	C	355	GLU	OE1-CD-OE2	7.63	132.45	123.30
1	C	551	ARG	NE-CZ-NH2	7.55	124.07	120.30
1	C	442	ARG	NE-CZ-NH1	7.48	124.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	137	ASP	CB-CG-OD2	7.45	125.01	118.30
1	D	206	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	A	551	ARG	NE-CZ-NH2	7.20	123.90	120.30
1	B	442	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	C	137	ASP	CB-CG-OD2	7.01	124.61	118.30
1	A	435	ASP	CB-CG-OD1	6.98	124.58	118.30
1	D	435	ASP	CB-CG-OD1	6.96	124.56	118.30
1	B	576	ARG	NE-CZ-NH2	6.82	123.71	120.30
1	C	597	GLU	CA-CB-CG	6.66	128.05	113.40
1	B	134	ARG	NE-CZ-NH2	6.66	123.63	120.30
1	B	492	LYS	CB-CG-CD	6.63	128.84	111.60
1	B	194	ARG	CG-CD-NE	-6.55	98.05	111.80
1	D	442	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	A	442	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	C	435	ASP	CB-CG-OD1	6.34	124.01	118.30
1	C	435	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	A	366	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	C	226	ARG	NE-CZ-NH2	6.12	123.36	120.30
1	B	522	CYS	CA-CB-SG	-5.98	103.24	114.00
1	A	551	ARG	NE-CZ-NH1	-5.97	117.31	120.30
1	B	206	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	A	206	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	C	194	ARG	CG-CD-NE	-5.89	99.43	111.80
1	D	194	ARG	CG-CD-NE	-5.75	99.72	111.80
1	B	366	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	D	551	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	A	366	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	D	447	GLN	CA-CB-CG	5.57	125.65	113.40
1	D	311	ASP	CB-CG-OD1	5.54	123.28	118.30
1	D	408	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	A	596	LYS	CB-CG-CD	5.48	125.86	111.60
1	B	352	ARG	CG-CD-NE	-5.46	100.33	111.80
1	B	442	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	C	220	ARG	NE-CZ-NH2	5.39	122.99	120.30
1	D	352	ARG	CG-CD-NE	-5.38	100.50	111.80
1	B	206	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	D	330	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	C	576	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	C	522	CYS	CA-CB-SG	-5.30	104.45	114.00
1	B	309	ASP	CB-CG-OD1	5.28	123.06	118.30
1	B	305	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	C	408	ARG	CG-CD-NE	5.24	122.81	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	576	ARG	NE-CZ-NH1	-5.22	117.69	120.30
1	A	522	CYS	CA-CB-SG	-5.20	104.65	114.00
1	A	449	GLU	OE1-CD-OE2	5.16	129.49	123.30
1	D	309	ASP	CB-CG-OD1	5.12	122.91	118.30
1	D	522	CYS	CA-CB-SG	-5.10	104.83	114.00
1	A	309	ASP	CB-CG-OD1	5.09	122.88	118.30
1	B	496	GLU	OE1-CD-OE2	-5.08	117.21	123.30
1	B	405	LYS	CB-CG-CD	5.08	124.79	111.60
1	B	440	ASP	CB-CG-OD2	5.07	122.86	118.30
1	D	596	LYS	CB-CG-CD	5.03	124.69	111.60
1	B	331	TYR	CB-CG-CD1	-5.01	117.99	121.00
1	C	366	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	B	505	MET	CG-SD-CE	-5.00	92.20	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	276	LEU	Peptide

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	3939	0	3928	16	0
1	B	3908	0	3898	13	0
1	C	3921	0	3909	16	0
1	D	3908	0	3898	14	0
2	A	32	0	0	1	0
2	B	32	0	0	3	0
2	C	32	0	0	2	0
2	D	32	0	0	1	0
3	A	64	0	24	2	0
3	B	32	0	12	2	0
3	C	32	0	12	2	0
4	A	30	0	12	0	0
4	B	30	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	30	0	12	0	0
4	D	30	0	12	0	0
5	A	3	0	0	0	0
5	B	1	0	0	0	0
5	C	2	0	0	0	0
5	D	3	0	0	0	0
6	A	7	0	0	0	0
6	B	6	0	0	0	0
6	C	4	0	0	0	0
6	D	6	0	0	0	0
7	A	5	0	2	0	0
7	B	10	0	4	0	0
7	C	25	0	10	0	0
7	D	20	0	8	0	0
8	B	16	0	24	0	0
9	D	5	0	0	0	0
10	A	54	0	0	1	0
10	B	81	0	0	2	0
10	C	46	0	0	0	0
10	D	93	0	0	3	0
All	All	16439	0	15777	58	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (58) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:701:HFD:O2G	10:B:801:HOH:O	1.99	0.79
1:B:326:GLN:HG2	1:D:327:ASN:O	1.89	0.73
1:D:355:GLU:OE1	1:D:358:ASN:ND2	2.27	0.68
1:A:451:ARG:HH11	3:A:702:GTP:H5'	1.59	0.67
1:B:355:GLU:OE1	1:B:358:ASN:ND2	2.28	0.66
1:A:326:GLN:HG2	1:C:327:ASN:O	2.00	0.61
2:B:701:HFD:PG	10:B:801:HOH:O	2.61	0.58
1:A:140:GLN:HG3	1:A:240:MET:CE	2.34	0.57
1:D:351:ALA:O	1:D:520:PHE:HA	2.07	0.55
1:B:351:ALA:O	1:B:520:PHE:HA	2.07	0.55
2:C:704:HFD:PG	2:C:704:HFD:O2A	2.64	0.55
1:D:487:VAL:CG1	1:D:591:ILE:HD11	2.37	0.54
1:A:543:GLU:CG	1:C:543:GLU:HG3	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:PHE:CZ	1:B:426:ILE:CG2	2.92	0.53
3:B:702:GTP:O1B	3:B:702:GTP:O1A	2.26	0.53
1:A:351:ALA:O	1:A:520:PHE:HA	2.08	0.53
1:B:425:ASN:ND2	1:C:425:ASN:OD1	2.35	0.52
1:A:140:GLN:CG	1:A:240:MET:CE	2.87	0.52
1:C:351:ALA:O	1:C:520:PHE:HA	2.10	0.51
1:C:451:ARG:HH11	3:C:705:GTP:H5'	1.76	0.51
1:B:451:ARG:HH11	3:B:702:GTP:H5'	1.76	0.51
1:A:543:GLU:HG2	1:C:543:GLU:HG3	1.94	0.50
1:D:334:PHE:CE2	1:D:359:LEU:HD11	2.46	0.50
1:C:591:ILE:O	1:C:594:GLN:HG2	2.12	0.49
1:D:114:THR:HG23	1:D:114:THR:O	2.14	0.48
3:C:705:GTP:O1B	3:C:705:GTP:O1A	2.32	0.48
1:D:126:ILE:HD13	1:D:126:ILE:HG21	1.66	0.47
1:A:328:ASN:HB3	10:A:845:HOH:O	2.15	0.47
1:C:334:PHE:CE2	1:C:359:LEU:HD11	2.51	0.46
1:C:405:LYS:HA	1:C:405:LYS:HE2	1.98	0.46
1:B:543:GLU:HG2	1:D:543:GLU:HB2	1.99	0.45
1:B:126:ILE:HG21	1:B:126:ILE:HD13	1.68	0.45
1:D:331:TYR:OH	10:D:801:HOH:O	2.20	0.45
1:A:126:ILE:HG21	1:A:126:ILE:HD13	1.64	0.45
1:C:511[B]:GLU:CD	1:C:511[B]:GLU:H	2.20	0.45
1:A:352:ARG:HB3	1:A:355:GLU:HG3	1.98	0.44
1:C:574:ALA:O	1:C:595:LYS:NZ	2.44	0.44
1:D:331:TYR:HD2	10:D:855:HOH:O	2.00	0.43
1:B:597:GLU:OE1	1:B:597:GLU:N	2.43	0.43
2:D:703:HFD:C5'	2:D:703:HFD:O2'	2.66	0.43
1:A:597:GLU:OE1	1:A:597:GLU:N	2.44	0.43
1:B:437:LYS:HB2	1:B:437:LYS:HE3	1.91	0.43
1:C:331:TYR:CD1	1:C:331:TYR:C	2.92	0.43
1:A:451:ARG:NH1	3:A:702:GTP:H5'	2.30	0.42
1:D:331:TYR:C	1:D:331:TYR:CD1	2.92	0.42
1:B:215:HIS:HE2	2:B:701:HFD:PA	2.42	0.42
1:A:331:TYR:CD1	1:A:331:TYR:C	2.93	0.42
1:A:215[B]:HIS:CD2	2:A:701:HFD:C8	3.03	0.42
1:C:215:HIS:CD2	2:C:704:HFD:C8	3.03	0.42
1:B:244:LEU:C	1:B:244:LEU:HD23	2.40	0.41
1:B:331:TYR:CD1	1:B:331:TYR:C	2.93	0.41
1:D:597:GLU:OE1	1:D:597:GLU:N	2.43	0.41
1:D:381:ILE:HD12	1:D:381:ILE:HA	1.95	0.41
1:C:502:VAL:HG22	1:C:550:ILE:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:ILE:HG21	1:C:126:ILE:HD13	1.69	0.41
1:D:598:TRP:C	10:D:809:HOH:O	2.58	0.41
1:A:244:LEU:C	1:A:244:LEU:HD23	2.41	0.41
1:A:543:GLU:HG2	1:C:543:GLU:CG	2.51	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	478/550 (87%)	470 (98%)	8 (2%)	0	100	100
1	B	474/550 (86%)	463 (98%)	11 (2%)	0	100	100
1	C	476/550 (86%)	463 (97%)	11 (2%)	2 (0%)	34	42
1	D	474/550 (86%)	464 (98%)	10 (2%)	0	100	100
All	All	1902/2200 (86%)	1860 (98%)	40 (2%)	2 (0%)	51	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	597	GLU
1	C	596	LYS

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	428/488 (88%)	417 (97%)	11 (3%)	46	63
1	B	424/488 (87%)	417 (98%)	7 (2%)	60	76
1	C	426/488 (87%)	408 (96%)	18 (4%)	30	42
1	D	424/488 (87%)	413 (97%)	11 (3%)	46	63
All	All	1702/1952 (87%)	1655 (97%)	47 (3%)	43	60

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	194	ARG
1	A	229	VAL
1	A	284	LEU
1	A	295	SER
1	A	315	TYR
1	A	326	GLN
1	A	331	TYR
1	A	439	LYS
1	A	447	GLN
1	A	496	GLU
1	A	596	LYS
1	B	262	GLU
1	B	284	LEU
1	B	295	SER
1	B	315	TYR
1	B	326	GLN
1	B	405	LYS
1	B	492	LYS
1	C	114	THR
1	C	134	ARG
1	C	193	GLU
1	C	284	LEU
1	C	302	SER
1	C	315	TYR
1	C	326	GLN
1	C	331	TYR
1	C	342	GLU
1	C	359	LEU
1	C	405	LYS
1	C	421	LYS
1	C	439	LYS
1	C	478	LYS
1	C	484	LYS

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Mol	Chain	Res	Type
1	C	594	GLN
1	C	596	LYS
1	C	597	GLU
1	D	134	ARG
1	D	230	LYS
1	D	284	LEU
1	D	315	TYR
1	D	331	TYR
1	D	354	LYS
1	D	359	LEU
1	D	439	LYS
1	D	478	LYS
1	D	535	ASN
1	D	596	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	243	HIS
1	A	425	ASN
1	B	326	GLN
1	B	425	ASN
1	C	215	HIS
1	C	235	GLN
1	C	425	ASN
1	C	571	GLN
1	C	594	GLN
1	D	215	HIS
1	D	345	ASN
1	D	425	ASN
1	D	535	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 59 ligands modelled in this entry, 32 are monoatomic - leaving 27 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	$\#\|Z\| > 2$
8	TRS	B	713	-	7,7,7	0.51	0	9,9,9	0.72	0
4	DTP	B	703	5	26,32,32	1.31	4 (15%)	30,50,50	1.23	4 (13%)
7	GLY	D	712	-	4,4,4	1.04	0	3,4,4	1.65	1 (33%)
4	DTP	D	702	5	26,32,32	1.23	3 (11%)	30,50,50	1.20	3 (10%)
3	GTP	A	706	5	26,34,34	1.54	4 (15%)	32,54,54	1.53	5 (15%)
4	DTP	A	703	5	26,32,32	1.27	6 (23%)	30,50,50	1.43	3 (10%)
7	GLY	C	714	-	4,4,4	1.18	1 (25%)	3,4,4	1.50	1 (33%)
3	GTP	C	705	5	26,34,34	1.57	6 (23%)	32,54,54	2.17	10 (31%)
4	DTP	C	702	5	26,32,32	1.45	4 (15%)	30,50,50	1.18	3 (10%)
7	GLY	B	712	-	4,4,4	1.07	1 (25%)	3,4,4	1.43	0
2	HFD	D	703	5	27,34,34	3.08	9 (33%)	33,54,54	3.49	16 (48%)
3	GTP	B	702	5	26,34,34	1.83	7 (26%)	32,54,54	1.74	6 (18%)
2	HFD	A	701	5	27,34,34	2.77	9 (33%)	33,54,54	3.61	14 (42%)
7	GLY	C	710	-	4,4,4	0.99	0	3,4,4	2.17	2 (66%)
2	HFD	B	701	5	27,34,34	3.07	12 (44%)	33,54,54	3.43	12 (36%)
7	GLY	C	713	-	4,4,4	1.10	0	3,4,4	1.07	0
2	HFD	C	704	5	27,34,34	3.08	11 (40%)	33,54,54	3.31	19 (57%)
9	PO4	D	716	-	4,4,4	0.84	0	6,6,6	0.43	0
7	GLY	D	715	-	4,4,4	1.26	1 (25%)	3,4,4	0.58	0
7	GLY	D	714	-	4,4,4	1.04	0	3,4,4	1.89	1 (33%)
7	GLY	D	713	-	4,4,4	1.15	1 (25%)	3,4,4	2.42	2 (66%)
3	GTP	A	702	5	26,34,34	1.80	8 (30%)	32,54,54	2.01	9 (28%)
7	GLY	A	715	-	4,4,4	1.04	0	3,4,4	1.75	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	GLY	B	711	-	4,4,4	1.13	1 (25%)	3,4,4	2.53	2 (66%)
8	TRS	B	714	-	7,7,7	0.74	0	9,9,9	1.08	0
7	GLY	C	711	-	4,4,4	0.96	0	3,4,4	1.43	0
7	GLY	C	712	-	4,4,4	0.92	0	3,4,4	1.77	1 (33%)

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
8	TRS	B	713	-	-	3/9/9/9	-
4	DTP	B	703	5	-	3/18/34/34	0/3/3/3
7	GLY	D	712	-	-	2/2/2/2	-
4	DTP	D	702	5	-	4/18/34/34	0/3/3/3
3	GTP	A	706	5	-	5/18/38/38	0/3/3/3
4	DTP	A	703	5	-	2/18/34/34	0/3/3/3
7	GLY	C	714	-	-	2/2/2/2	-
3	GTP	C	705	5	-	7/18/38/38	0/3/3/3
4	DTP	C	702	5	-	5/18/34/34	0/3/3/3
7	GLY	B	712	-	-	2/2/2/2	-
2	HFD	D	703	5	-	5/18/38/38	0/3/3/3
3	GTP	B	702	5	-	8/18/38/38	0/3/3/3
2	HFD	A	701	5	-	4/18/38/38	0/3/3/3
7	GLY	C	710	-	-	2/2/2/2	-
2	HFD	B	701	5	-	8/18/38/38	0/3/3/3
7	GLY	C	713	-	-	2/2/2/2	-
2	HFD	C	704	5	-	8/18/38/38	0/3/3/3
7	GLY	D	715	-	-	2/2/2/2	-
7	GLY	D	714	-	-	2/2/2/2	-
7	GLY	D	713	-	-	2/2/2/2	-
3	GTP	A	702	5	-	8/18/38/38	0/3/3/3
7	GLY	A	715	-	-	2/2/2/2	-
7	GLY	B	711	-	-	0/2/2/2	-
8	TRS	B	714	-	-	8/9/9/9	-
7	GLY	C	711	-	-	2/2/2/2	-
7	GLY	C	712	-	-	0/2/2/2	-

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	703	HFD	O4'-C1'	11.43	1.57	1.41
2	C	704	HFD	O4'-C1'	9.79	1.54	1.41
2	B	701	HFD	C2-N3	7.63	1.38	1.31
2	B	701	HFD	O4'-C1'	7.00	1.50	1.41
2	A	701	HFD	C2-N3	6.76	1.38	1.31
2	D	703	HFD	C2-N3	6.43	1.37	1.31
2	A	701	HFD	O4'-C1'	6.33	1.49	1.41
2	C	704	HFD	C2'-C1'	-5.95	1.44	1.53
2	B	701	HFD	C2-N1	5.95	1.37	1.31
2	A	701	HFD	C2'-C1'	-5.88	1.44	1.53
2	C	704	HFD	C2-N3	5.57	1.36	1.31
2	B	701	HFD	C2'-C1'	-4.68	1.46	1.53
2	B	701	HFD	C5-C4	4.45	1.52	1.40
2	A	701	HFD	C5-C4	4.38	1.52	1.40
4	C	702	DTP	C5-C4	4.34	1.52	1.40
2	D	703	HFD	C5-C4	4.29	1.52	1.40
2	C	704	HFD	O3'-C3'	3.99	1.52	1.43
3	A	706	GTP	C6-N1	-3.91	1.32	1.37
3	B	702	GTP	PB-O1B	-3.85	1.37	1.50
3	A	702	GTP	PA-O2A	-3.83	1.37	1.55
3	C	705	GTP	C4-N3	-3.81	1.28	1.37
3	B	702	GTP	PA-O5'	-3.81	1.43	1.59
2	B	701	HFD	PA-O5'	3.72	1.74	1.59
2	A	701	HFD	C6-N6	3.70	1.47	1.34
2	C	704	HFD	C5-C4	3.53	1.50	1.40
2	B	701	HFD	C6-N6	3.52	1.46	1.34
3	A	702	GTP	PB-O2B	-3.40	1.39	1.55
2	D	703	HFD	C2-N1	3.38	1.34	1.31
2	C	704	HFD	C2'-C3'	-3.37	1.44	1.53
2	C	704	HFD	C6-N6	3.32	1.46	1.34
2	D	703	HFD	O3'-C3'	3.17	1.50	1.43
2	A	701	HFD	C2-N1	3.11	1.34	1.31
2	A	701	HFD	PA-O5'	3.11	1.71	1.59
3	A	702	GTP	PA-O1A	-3.11	1.39	1.50
3	B	702	GTP	C6-N1	-3.09	1.33	1.37
2	C	704	HFD	C2-N1	3.01	1.34	1.31
2	D	703	HFD	C6-N6	3.01	1.45	1.34
2	B	701	HFD	PG-O3G	-3.00	1.43	1.54
3	C	705	GTP	O4'-C1'	2.94	1.45	1.41
2	B	701	HFD	O3'-C3'	2.83	1.49	1.43
3	A	702	GTP	C2-N1	-2.81	1.30	1.37
3	A	702	GTP	C2-N2	-2.77	1.27	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	705	GTP	PB-O1B	-2.75	1.41	1.50
3	A	706	GTP	PA-O5'	2.74	1.70	1.59
3	A	702	GTP	O5'-C5'	-2.74	1.34	1.44
2	A	701	HFD	C2'-C3'	-2.65	1.46	1.53
4	A	703	DTP	C2-N3	2.56	1.36	1.32
4	B	703	DTP	PA-O2A	-2.52	1.43	1.55
2	D	703	HFD	PA-O5'	2.48	1.69	1.59
4	C	702	DTP	PA-O1A	-2.43	1.42	1.50
4	B	703	DTP	C8-N7	2.38	1.38	1.34
3	B	702	GTP	C5-C4	2.38	1.49	1.43
4	A	703	DTP	PA-O2A	-2.38	1.44	1.55
4	D	702	DTP	C2-N3	2.37	1.35	1.32
3	A	702	GTP	C5'-C4'	2.35	1.58	1.51
2	B	701	HFD	C4-N3	-2.33	1.32	1.35
4	B	703	DTP	C5-N7	-2.29	1.31	1.39
3	A	706	GTP	C5-C6	-2.29	1.42	1.47
3	B	702	GTP	C8-N7	2.29	1.38	1.35
2	D	703	HFD	C2'-C1'	-2.27	1.50	1.53
2	D	703	HFD	PB-O1B	-2.26	1.44	1.55
4	A	703	DTP	C5-N7	-2.24	1.31	1.39
4	B	703	DTP	O4'-C1'	2.23	1.47	1.42
4	D	702	DTP	C2'-C1'	-2.23	1.46	1.52
7	B	711	GLY	OXT-C	-2.22	1.23	1.30
7	C	714	GLY	OXT-C	-2.21	1.23	1.30
3	B	702	GTP	C4-N3	-2.21	1.32	1.37
2	C	704	HFD	PG-O2G	-2.20	1.46	1.54
4	D	702	DTP	C5-N7	-2.19	1.31	1.39
3	A	706	GTP	PB-O2B	-2.18	1.45	1.55
4	A	703	DTP	O3'-C3'	-2.18	1.38	1.43
3	C	705	GTP	PG-O3G	-2.15	1.46	1.54
2	C	704	HFD	PA-O5'	2.14	1.68	1.59
4	A	703	DTP	C5-C4	2.13	1.46	1.40
2	B	701	HFD	C2'-C3'	-2.12	1.47	1.53
7	D	715	GLY	OXT-C	-2.11	1.23	1.30
3	C	705	GTP	PA-O2A	-2.10	1.45	1.55
2	B	701	HFD	C5-N7	2.09	1.47	1.39
3	C	705	GTP	PA-O5'	-2.08	1.50	1.59
4	A	703	DTP	PG-O2G	-2.08	1.46	1.54
3	A	702	GTP	PA-O5'	-2.07	1.50	1.59
2	C	704	HFD	C5-N7	2.07	1.47	1.39
4	C	702	DTP	C5-N7	-2.07	1.32	1.39
2	A	701	HFD	PG-O2G	-2.06	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	702	DTP	C8-N7	2.04	1.38	1.34
7	D	713	GLY	OXT-C	-2.03	1.23	1.30
3	B	702	GTP	PG-O3G	-2.01	1.47	1.54
7	B	712	GLY	OXT-C	-2.01	1.24	1.30

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	703	HFD	F2-C2-N3	11.94	126.07	114.73
2	A	701	HFD	F2-C2-N3	11.73	125.87	114.73
2	B	701	HFD	F2-C2-N3	9.60	123.84	114.73
2	A	701	HFD	C5-C6-N1	-8.94	115.14	121.01
2	C	704	HFD	F2-C2-N3	8.88	123.16	114.73
2	B	701	HFD	C5-C6-N1	-8.22	115.61	121.01
2	D	703	HFD	F2-C2-N1	-7.76	107.37	114.73
2	B	701	HFD	C3'-C2'-C1'	6.85	111.29	100.98
2	A	701	HFD	F2-C2-N1	-6.55	108.52	114.73
2	A	701	HFD	C3'-C2'-C1'	6.32	110.49	100.98
2	B	701	HFD	O3G-PG-O3B	6.24	125.56	104.64
3	A	702	GTP	PA-O5'-C5'	5.45	153.62	121.68
2	B	701	HFD	C5-C6-N6	5.43	128.60	120.35
2	C	704	HFD	O5'-C5'-C4'	5.37	127.47	108.99
2	C	704	HFD	C3'-C2'-C1'	5.29	108.94	100.98
2	D	703	HFD	C5-C6-N1	-5.24	117.57	121.01
3	C	705	GTP	PA-O3A-PB	-5.06	115.45	132.83
2	C	704	HFD	C5-C6-N1	-5.00	117.72	121.01
2	C	704	HFD	O3G-PG-O3B	4.92	121.13	104.64
2	B	701	HFD	O3G-PG-O1G	-4.85	91.70	110.68
3	A	706	GTP	O3G-PG-O2G	4.55	125.02	107.64
2	B	701	HFD	C4-C5-N7	-4.49	104.72	109.40
2	C	704	HFD	O1A-PA-O2A	-4.31	90.93	112.24
2	A	701	HFD	C5-C6-N6	4.27	126.84	120.35
2	D	703	HFD	O3G-PG-O3B	4.19	118.67	104.64
2	D	703	HFD	C3'-C2'-C1'	4.17	107.26	100.98
2	C	704	HFD	O4'-C4'-C5'	-4.16	95.68	109.37
3	C	705	GTP	O2A-PA-O5'	4.15	127.02	107.75
2	D	703	HFD	C5-C6-N6	4.09	126.57	120.35
2	A	701	HFD	O2G-PG-O3B	3.89	117.69	104.64
2	C	704	HFD	N1-C2-N3	-3.89	124.99	130.51
2	B	701	HFD	F2-C2-N1	-3.89	111.05	114.73
3	B	702	GTP	PA-O5'-C5'	3.86	144.34	121.68
3	C	705	GTP	PA-O5'-C5'	3.83	144.11	121.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	HFD	N1-C2-N3	-3.81	125.10	130.51
2	A	701	HFD	O3G-PG-O3B	3.81	117.40	104.64
2	A	701	HFD	C4-C5-N7	-3.77	105.47	109.40
2	C	704	HFD	O4'-C4'-C3'	-3.74	97.72	105.11
2	D	703	HFD	PB-O3A-PA	-3.72	120.05	132.83
2	D	703	HFD	O2G-PG-O3B	3.68	116.97	104.64
2	D	703	HFD	O3'-C3'-C4'	3.66	121.64	111.05
2	C	704	HFD	O3'-C3'-C4'	3.65	121.59	111.05
2	C	704	HFD	C2-N3-C4	3.62	119.43	115.03
3	C	705	GTP	O2G-PG-O3B	3.59	116.68	104.64
3	B	702	GTP	O2A-PA-O5'	3.57	124.34	107.75
7	B	711	GLY	OXT-C-O	-3.51	114.55	123.30
7	D	713	GLY	OXT-C-O	-3.47	114.66	123.30
2	A	701	HFD	N1-C2-N3	-3.45	125.61	130.51
2	B	701	HFD	O4'-C1'-C2'	-3.45	101.88	106.93
3	A	702	GTP	C2-N1-C6	-3.44	118.77	125.10
3	B	702	GTP	O5'-PA-O1A	-3.41	95.73	109.07
2	C	704	HFD	C1'-N9-C4	-3.38	120.70	126.64
2	A	701	HFD	PB-O3B-PG	-3.38	121.23	132.83
3	C	705	GTP	O3G-PG-O3B	-3.37	93.32	104.64
2	D	703	HFD	O5'-C5'-C4'	3.36	120.56	108.99
2	C	704	HFD	O4'-C1'-C2'	-3.35	102.03	106.93
3	C	705	GTP	PB-O3B-PG	-3.27	121.61	132.83
3	B	702	GTP	C3'-C2'-C1'	3.27	105.89	100.98
2	C	704	HFD	C4-C5-N7	-3.25	106.01	109.40
3	A	702	GTP	O6-C6-C5	-3.19	118.14	124.37
4	B	703	DTP	O2A-PA-O1A	3.15	127.82	112.24
4	A	703	DTP	C2'-C1'-N9	3.13	121.49	114.27
3	A	706	GTP	O4'-C1'-C2'	3.12	111.49	106.93
3	A	702	GTP	N2-C2-N3	-3.11	113.68	119.74
2	C	704	HFD	F2-C2-N1	-3.08	111.81	114.73
4	A	703	DTP	C5-C6-N6	-3.06	115.69	120.35
4	C	702	DTP	N3-C2-N1	-3.06	123.90	128.68
4	C	702	DTP	O3G-PG-O2G	3.03	119.21	107.64
3	A	702	GTP	C5-C6-N1	2.98	119.21	113.95
3	B	702	GTP	O3G-PG-O3B	-2.97	94.68	104.64
2	D	703	HFD	C4-C5-N7	-2.95	106.33	109.40
2	A	701	HFD	O2G-PG-O1G	-2.94	99.16	110.68
3	A	702	GTP	O5'-PA-O1A	2.91	120.43	109.07
3	A	706	GTP	O2G-PG-O3B	-2.86	95.04	104.64
2	D	703	HFD	N1-C2-N3	-2.80	126.54	130.51
3	A	702	GTP	O3G-PG-O2G	2.79	118.31	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	703	HFD	O4'-C1'-C2'	-2.78	102.86	106.93
7	C	710	GLY	OXT-C-CA	2.77	124.47	113.45
4	B	703	DTP	N6-C6-N1	2.76	124.31	118.57
4	D	702	DTP	N3-C2-N1	-2.75	124.38	128.68
3	A	702	GTP	O4'-C4'-C5'	-2.69	100.52	109.37
2	C	704	HFD	O1A-PA-O5'	2.69	120.22	107.75
2	C	704	HFD	O2G-PG-O3B	2.66	113.57	104.64
7	B	711	GLY	OXT-C-CA	2.63	123.91	113.45
2	C	704	HFD	C5-C6-N6	2.60	124.31	120.35
3	C	705	GTP	O6-C6-N1	2.59	123.71	120.65
7	D	714	GLY	OXT-C-O	-2.58	116.86	123.30
2	D	703	HFD	C1'-N9-C4	-2.58	122.11	126.64
2	D	703	HFD	O1B-PB-O2B	-2.54	99.68	112.24
3	A	702	GTP	O2A-PA-O5'	-2.54	95.96	107.75
2	A	701	HFD	O4'-C1'-C2'	-2.52	103.25	106.93
4	B	703	DTP	C5-C6-N6	-2.51	116.54	120.35
4	A	703	DTP	N3-C2-N1	-2.48	124.81	128.68
2	B	701	HFD	PB-O3A-PA	-2.47	124.34	132.83
4	C	702	DTP	C2-N1-C6	2.46	122.96	118.75
2	A	701	HFD	O4'-C4'-C5'	-2.44	101.33	109.37
3	C	705	GTP	O5'-PA-O1A	-2.38	99.75	109.07
4	B	703	DTP	N3-C2-N1	-2.37	124.97	128.68
7	D	713	GLY	OXT-C-CA	2.36	122.83	113.45
7	D	712	GLY	OXT-C-O	-2.31	117.53	123.30
7	C	710	GLY	OXT-C-O	-2.30	117.57	123.30
7	A	715	GLY	OXT-C-CA	2.27	122.49	113.45
3	C	705	GTP	O5'-C5'-C4'	-2.26	101.22	108.99
3	A	706	GTP	O2B-PB-O1B	2.24	123.32	112.24
2	A	701	HFD	C1'-N9-C4	-2.23	122.73	126.64
7	C	712	GLY	OXT-C-CA	2.22	122.27	113.45
7	C	714	GLY	OXT-C-O	-2.21	117.80	123.30
4	D	702	DTP	C2'-C3'-C4'	2.20	107.34	102.76
2	B	701	HFD	C1'-N9-C4	-2.18	122.82	126.64
2	C	704	HFD	O3'-C3'-C2'	-2.13	104.93	111.82
3	A	706	GTP	O2A-PA-O5'	-2.13	97.87	107.75
3	C	705	GTP	O3G-PG-O1G	2.07	118.80	110.68
3	B	702	GTP	C8-N7-C5	2.04	106.87	102.99
4	D	702	DTP	O2A-PA-O1A	2.02	122.21	112.24
2	D	703	HFD	O1A-PA-O5'	2.02	117.11	107.75

There are no chirality outliers.

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	HFD	C5'-O5'-PA-O2A
2	A	701	HFD	C5'-O5'-PA-O1A
2	A	701	HFD	C5'-O5'-PA-O3A
2	B	701	HFD	PB-O3A-PA-O5'
2	B	701	HFD	C5'-O5'-PA-O2A
2	B	701	HFD	C5'-O5'-PA-O1A
2	C	704	HFD	C5'-O5'-PA-O3A
2	C	704	HFD	PB-O3B-PG-O3G
2	D	703	HFD	C5'-O5'-PA-O2A
2	D	703	HFD	C5'-O5'-PA-O1A
3	A	702	GTP	PB-O3B-PG-O3G
3	A	702	GTP	C5'-O5'-PA-O1A
3	A	702	GTP	O4'-C4'-C5'-O5'
3	A	706	GTP	PB-O3B-PG-O3G
3	B	702	GTP	PB-O3B-PG-O2G
3	B	702	GTP	C5'-O5'-PA-O1A
3	C	705	GTP	PB-O3B-PG-O2G
3	C	705	GTP	C5'-O5'-PA-O1A
3	C	705	GTP	C5'-O5'-PA-O2A
4	A	703	DTP	PB-O3B-PG-O3G
4	C	702	DTP	PB-O3B-PG-O2G
4	C	702	DTP	PB-O3B-PG-O3G
7	B	712	GLY	O-C-CA-N
7	B	712	GLY	OXT-C-CA-N
7	C	710	GLY	O-C-CA-N
7	C	710	GLY	OXT-C-CA-N
7	C	711	GLY	O-C-CA-N
7	C	711	GLY	OXT-C-CA-N
7	D	713	GLY	OXT-C-CA-N
7	D	715	GLY	O-C-CA-N
7	D	715	GLY	OXT-C-CA-N
8	B	713	TRS	C2-C-C1-O1
8	B	714	TRS	C2-C-C1-O1
8	B	714	TRS	N-C-C1-O1
8	B	714	TRS	N-C-C2-O2
8	B	714	TRS	N-C-C3-O3
3	B	702	GTP	C3'-C4'-C5'-O5'
3	C	705	GTP	C3'-C4'-C5'-O5'
7	C	714	GLY	O-C-CA-N
7	D	713	GLY	O-C-CA-N
7	A	715	GLY	OXT-C-CA-N
7	C	714	GLY	OXT-C-CA-N
7	D	712	GLY	OXT-C-CA-N

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Mol	Chain	Res	Type	Atoms
7	D	714	GLY	OXT-C-CA-N
3	A	702	GTP	C3'-C4'-C5'-O5'
3	B	702	GTP	O4'-C4'-C5'-O5'
3	C	705	GTP	O4'-C4'-C5'-O5'
2	B	701	HFD	C4'-C5'-O5'-PA
7	C	713	GLY	O-C-CA-N
7	C	713	GLY	OXT-C-CA-N
8	B	714	TRS	C3-C-C2-O2
8	B	714	TRS	C1-C-C3-O3
7	A	715	GLY	O-C-CA-N
2	D	703	HFD	PB-O3B-PG-O1G
2	D	703	HFD	PB-O3A-PA-O5'
7	D	712	GLY	O-C-CA-N
2	B	701	HFD	C5'-O5'-PA-O3A
3	B	702	GTP	C5'-O5'-PA-O3A
3	A	706	GTP	PG-O3B-PB-O1B
4	B	703	DTP	PG-O3B-PB-O1B
4	B	703	DTP	PB-O3A-PA-O2A
4	D	702	DTP	PG-O3B-PB-O2B
4	D	702	DTP	PB-O3A-PA-O1A
8	B	713	TRS	C3-C-C1-O1
8	B	713	TRS	N-C-C1-O1
3	B	702	GTP	C5'-O5'-PA-O2A
7	D	714	GLY	O-C-CA-N
3	A	706	GTP	C4'-C5'-O5'-PA
2	C	704	HFD	PA-O3A-PB-O3B
4	B	703	DTP	PB-O3A-PA-O1A
4	C	702	DTP	PG-O3B-PB-O2B
2	C	704	HFD	C3'-C4'-C5'-O5'
8	B	714	TRS	C3-C-C1-O1
8	B	714	TRS	C1-C-C2-O2
3	A	702	GTP	PA-O3A-PB-O1B
3	A	706	GTP	PB-O3A-PA-O1A
2	A	701	HFD	O4'-C4'-C5'-O5'
2	C	704	HFD	PB-O3B-PG-O1G
4	C	702	DTP	PB-O3B-PG-O1G
2	C	704	HFD	PB-O3B-PG-O2G
3	C	705	GTP	PB-O3B-PG-O3G
2	D	703	HFD	C5'-O5'-PA-O3A
3	A	702	GTP	C5'-O5'-PA-O3A
3	C	705	GTP	C5'-O5'-PA-O3A
2	C	704	HFD	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	B	701	HFD	PB-O3A-PA-O2A
2	B	701	HFD	PB-O3A-PA-O1A
2	B	701	HFD	PG-O3B-PB-O1B
2	C	704	HFD	PA-O3A-PB-O2B
3	A	702	GTP	PB-O3A-PA-O1A
3	A	702	GTP	PB-O3A-PA-O2A
3	A	706	GTP	PB-O3A-PA-O2A
3	B	702	GTP	PA-O3A-PB-O2B
4	A	703	DTP	PG-O3B-PB-O1B
4	C	702	DTP	PB-O3A-PA-O1A
4	D	702	DTP	PG-O3B-PB-O1B
4	D	702	DTP	PB-O3A-PA-O2A
3	B	702	GTP	PB-O3B-PG-O1G

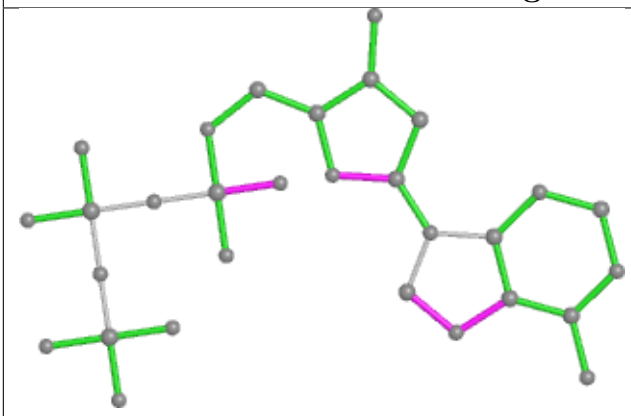
There are no ring outliers.

7 monomers are involved in 13 short contacts:

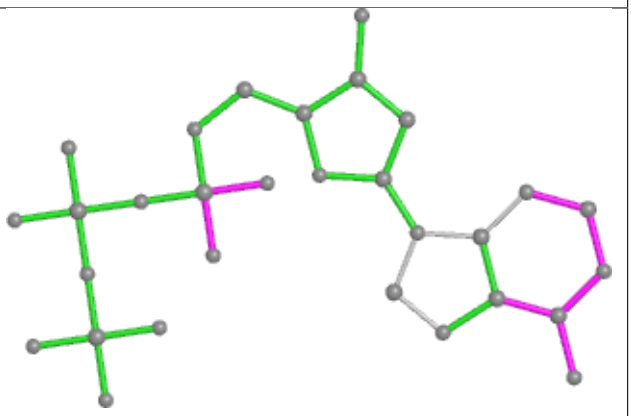
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	705	GTP	2	0
2	D	703	HFD	1	0
3	B	702	GTP	2	0
2	A	701	HFD	1	0
2	B	701	HFD	3	0
2	C	704	HFD	2	0
3	A	702	GTP	2	0

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 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.

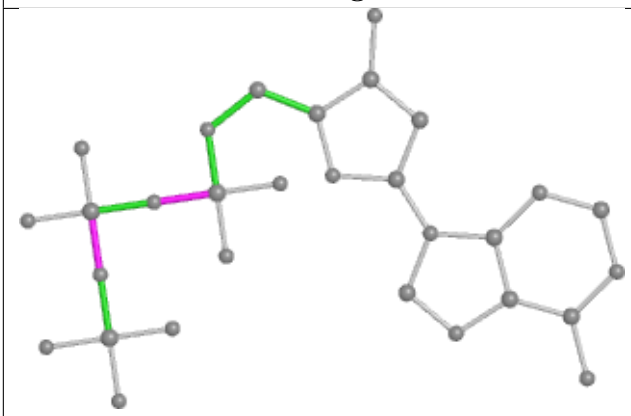
Ligand DTP B 703



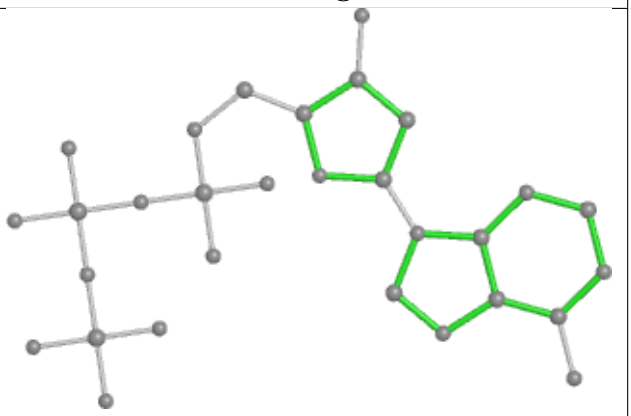
Bond lengths



Bond angles

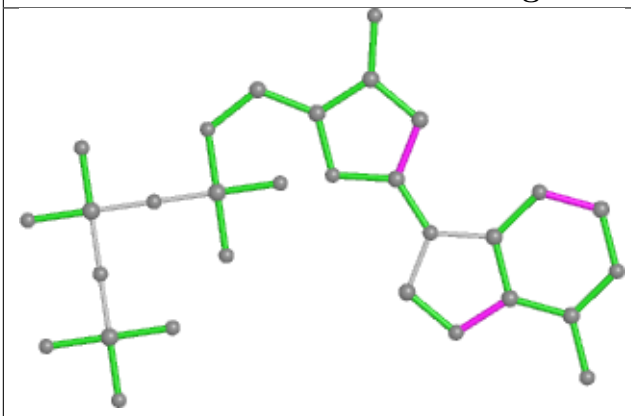


Torsions



Rings

Ligand DTP D 702



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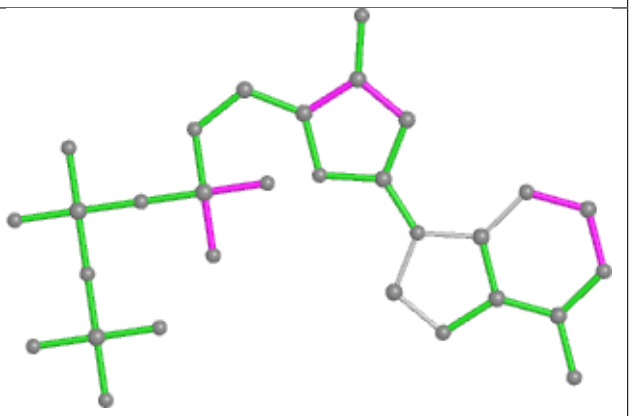
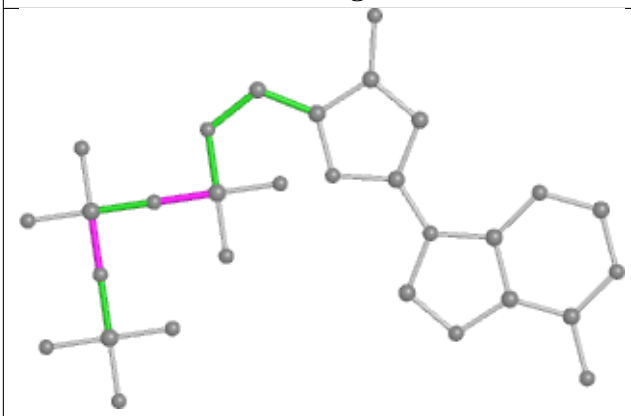


Bond angles



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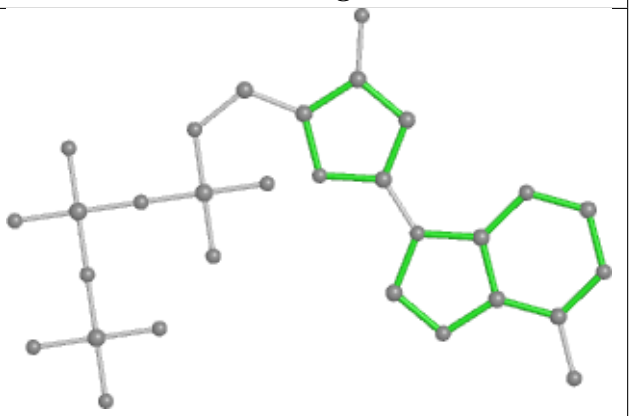
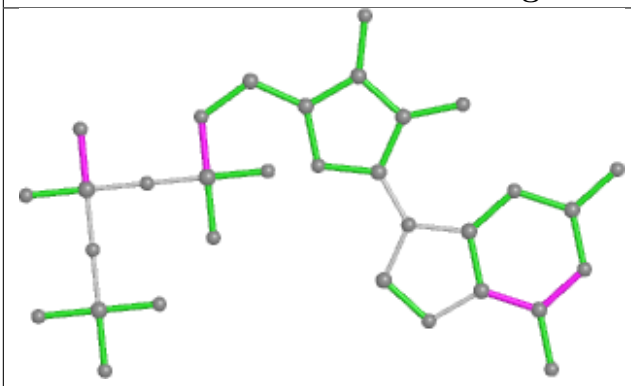
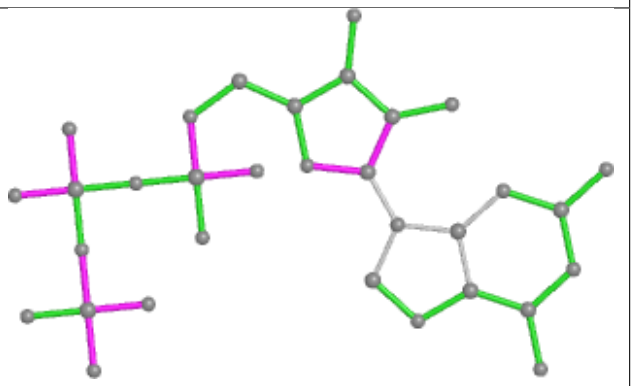


Rings

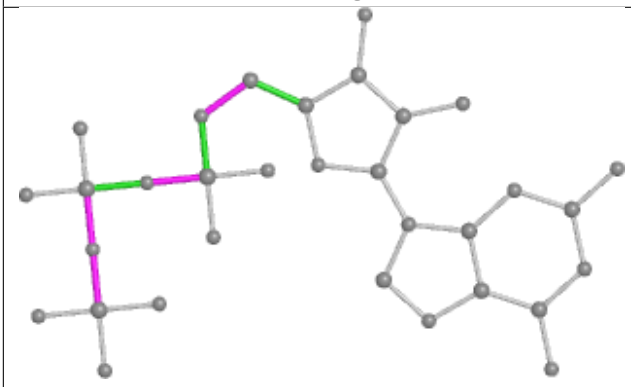
Ligand GTP A 706



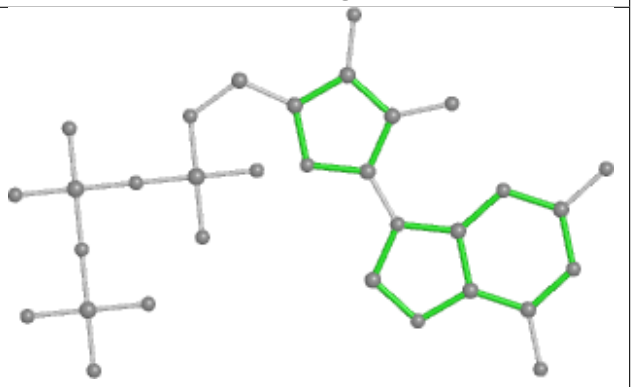
Bond lengths



Bond angles

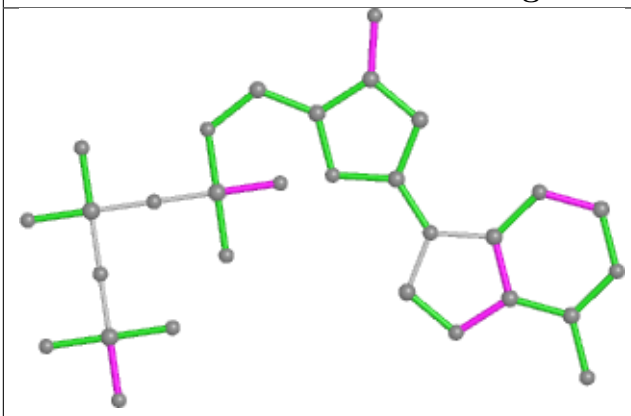


Torsions

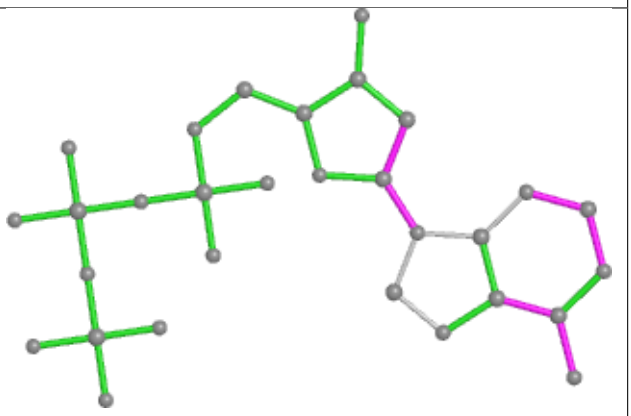


Rings

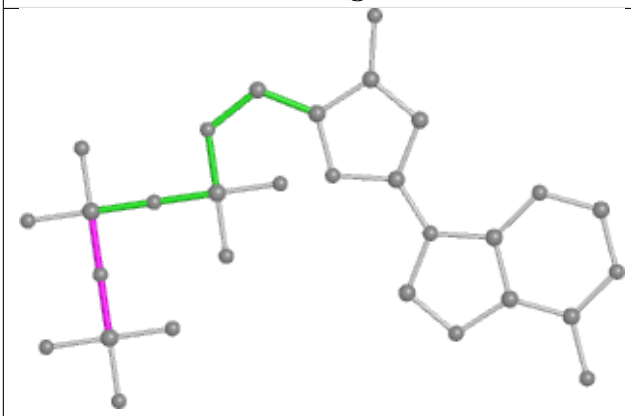
Ligand DTP A 703



Bond lengths



Bond angles



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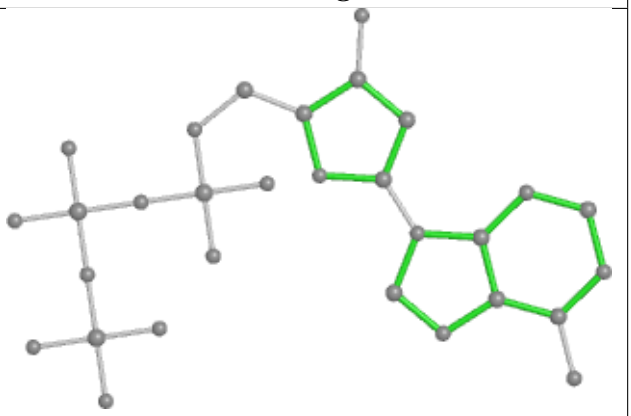
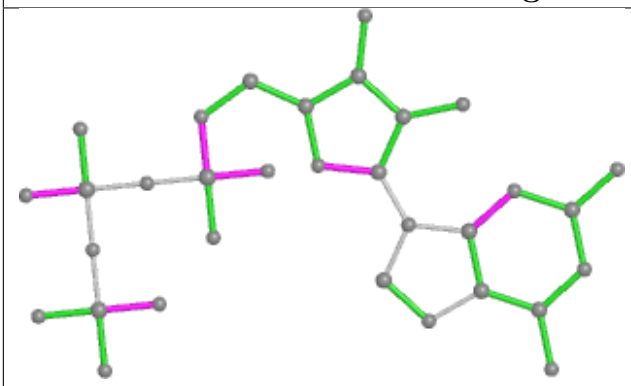
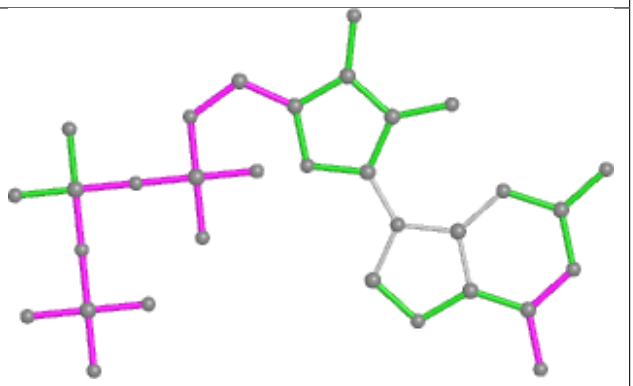


Rings

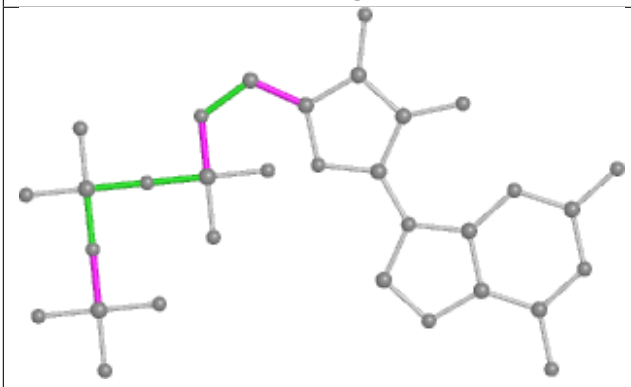
Ligand GTP C 705



Bond lengths



Bond angles



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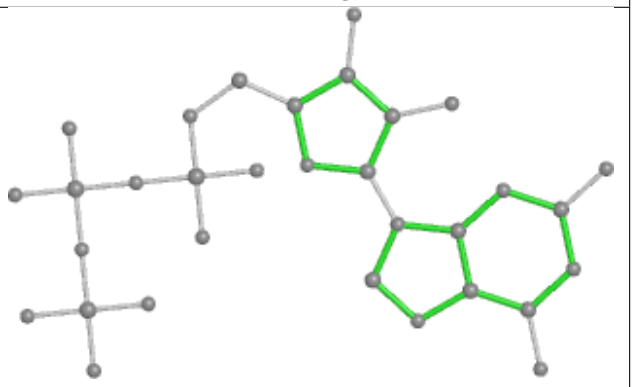
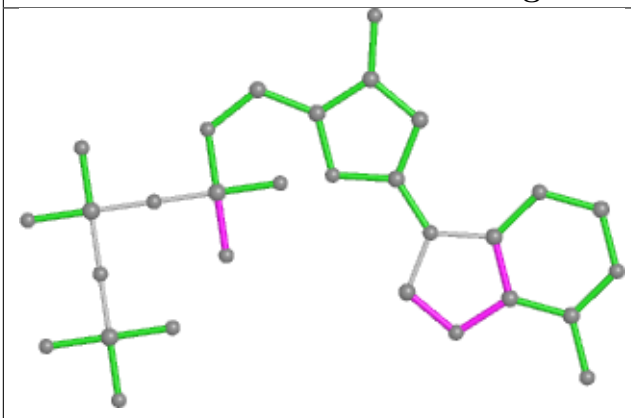


Rings

Ligand DTP C 702



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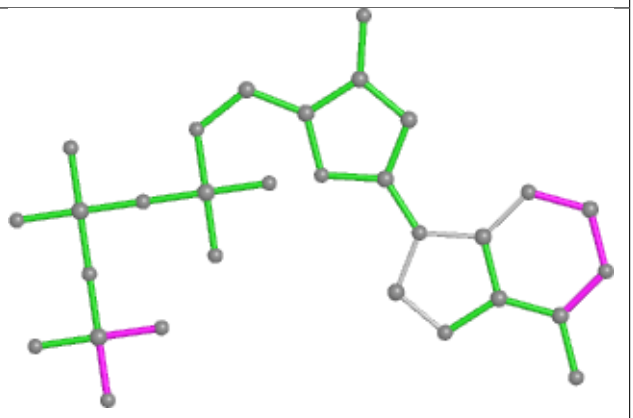

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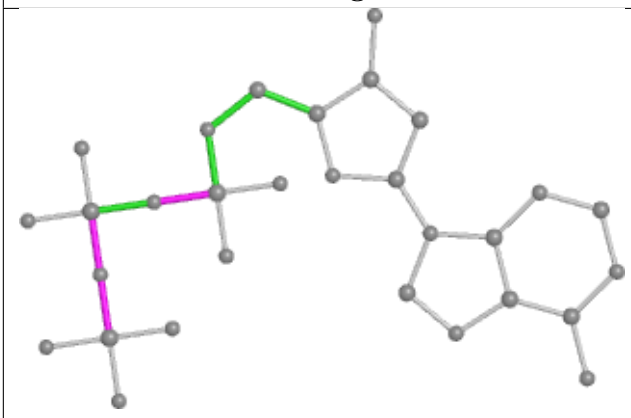

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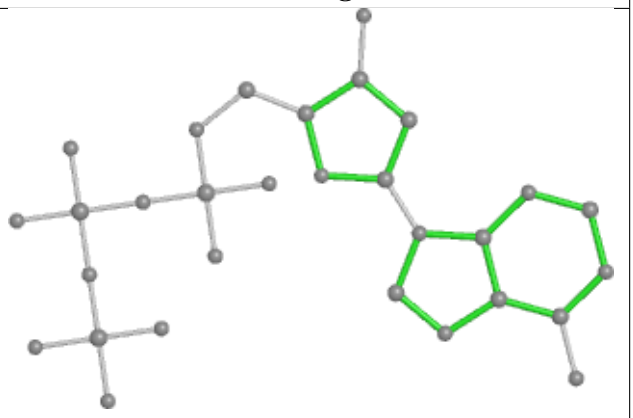
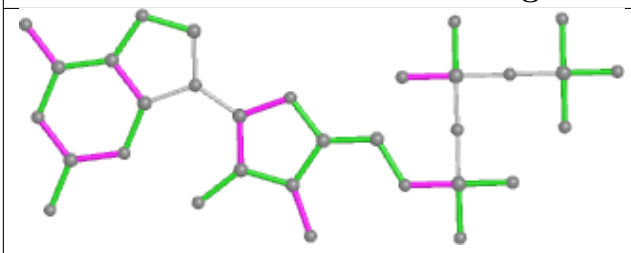


Rings

Ligand HFD D 703



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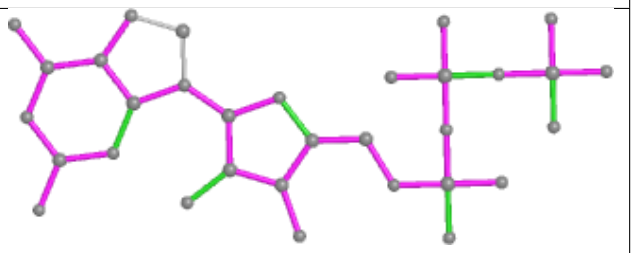
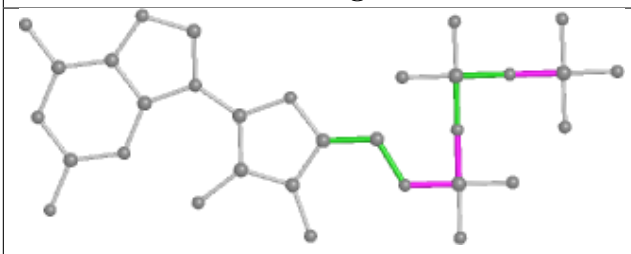


Bond angles



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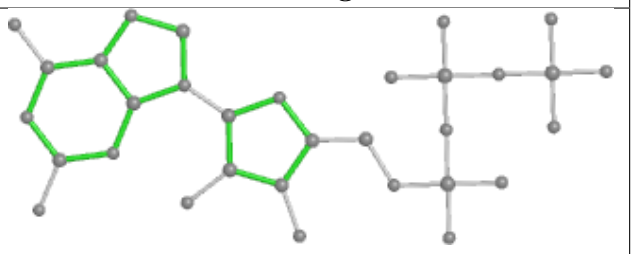
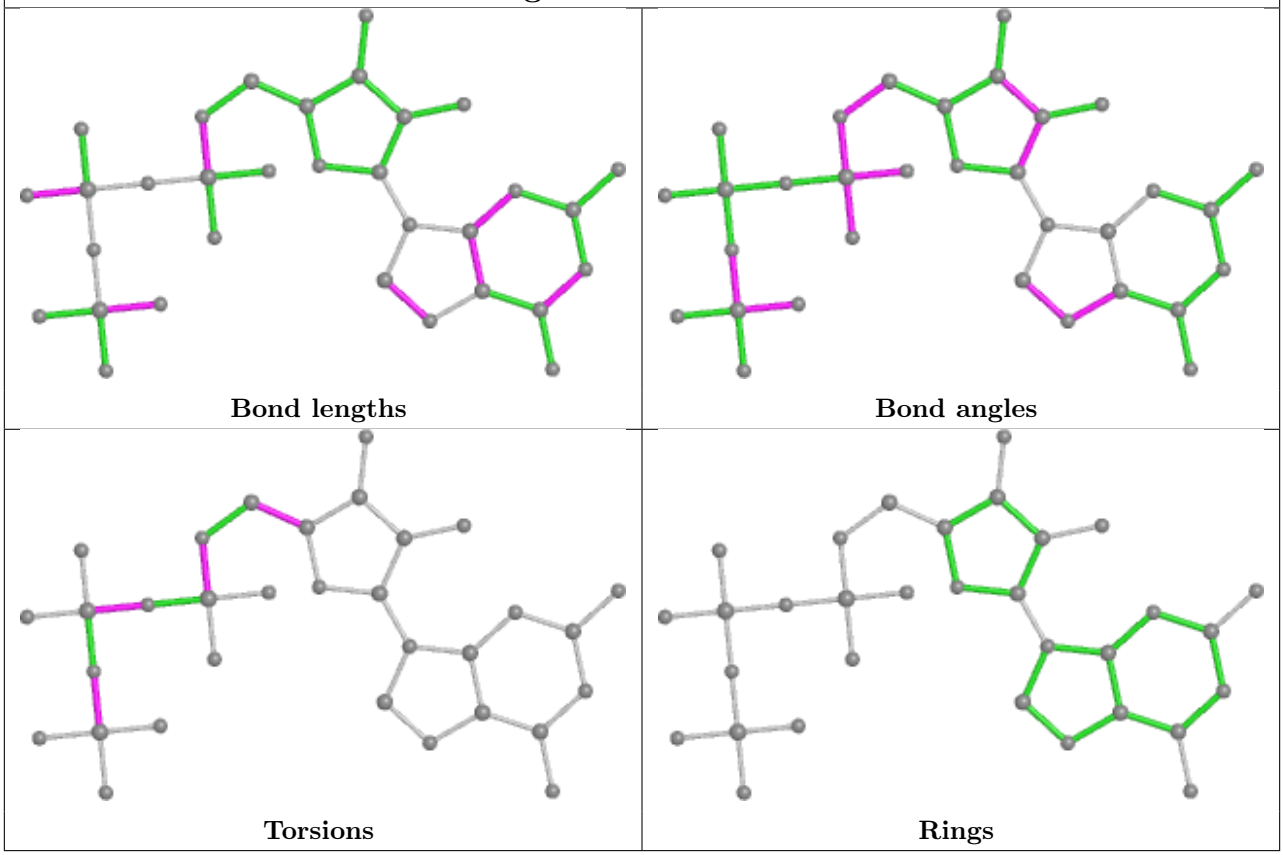
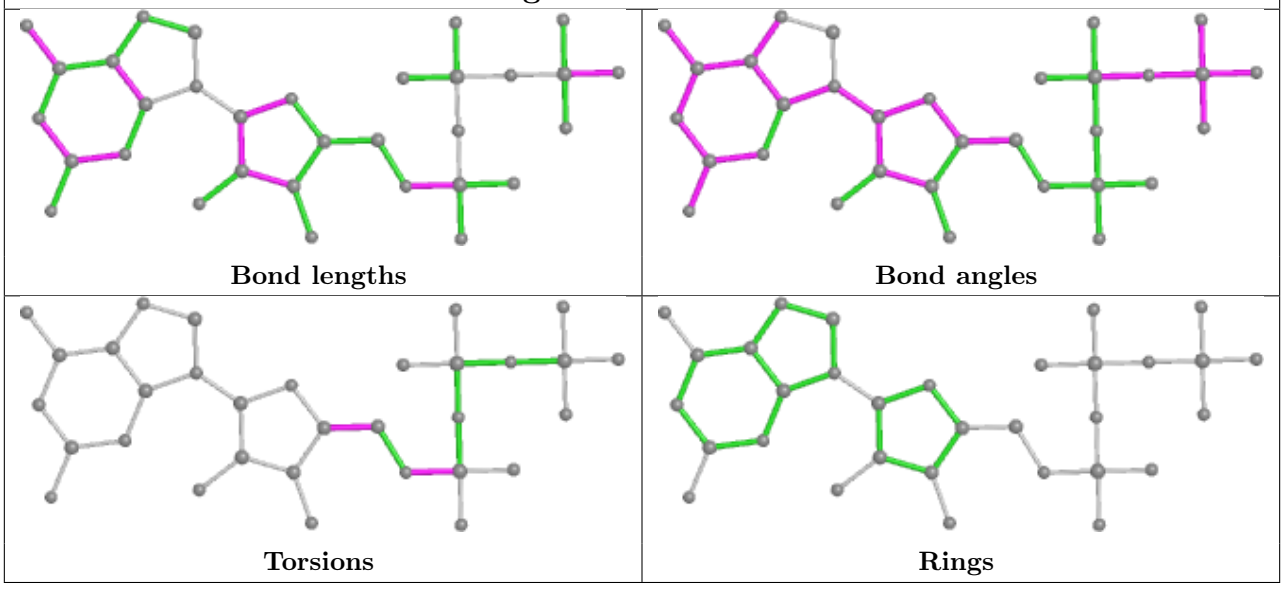


Rings

Ligand GTP B 702



Ligand HFD A 701



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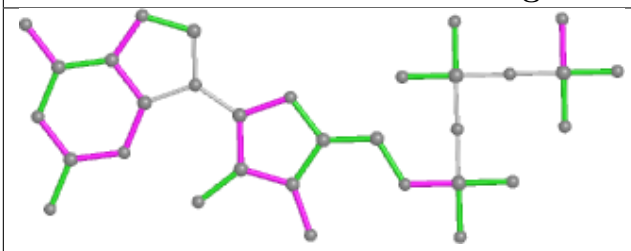
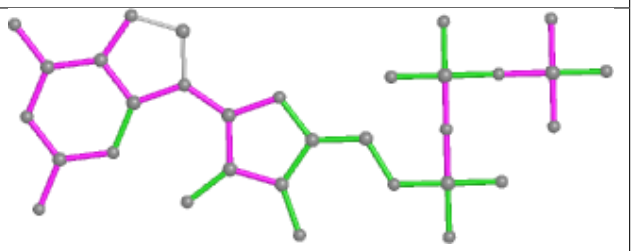
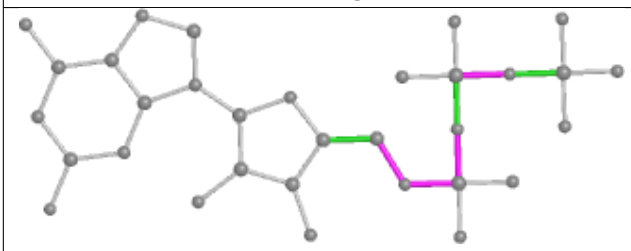


Bond lengths



Bond angles



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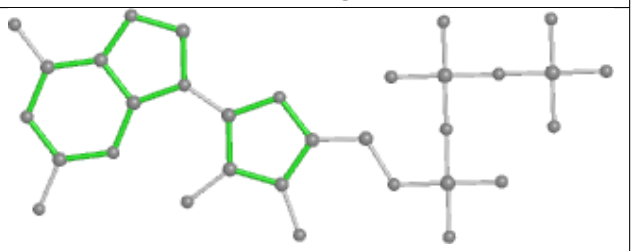
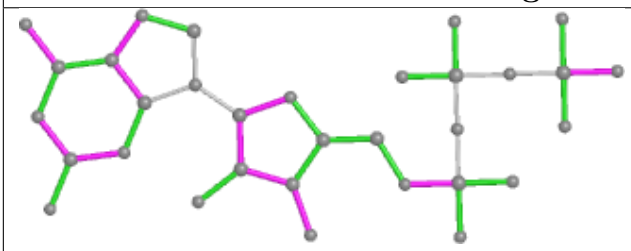
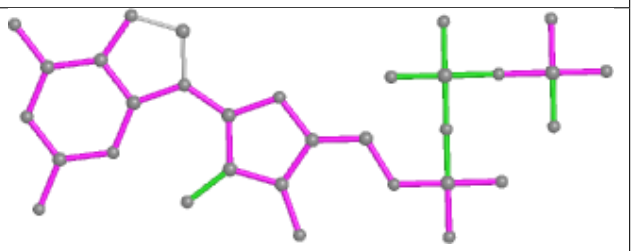


Rings

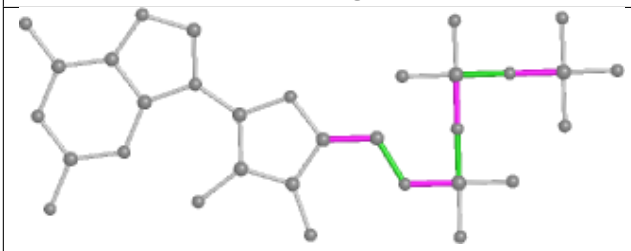
Ligand HFD C 704



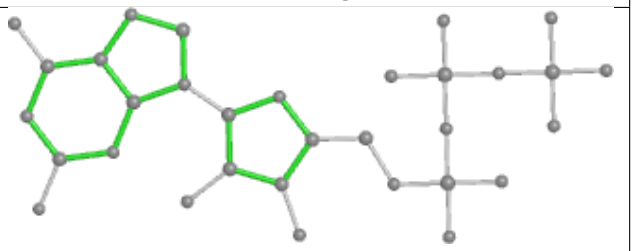
Bond lengths



Bond angles

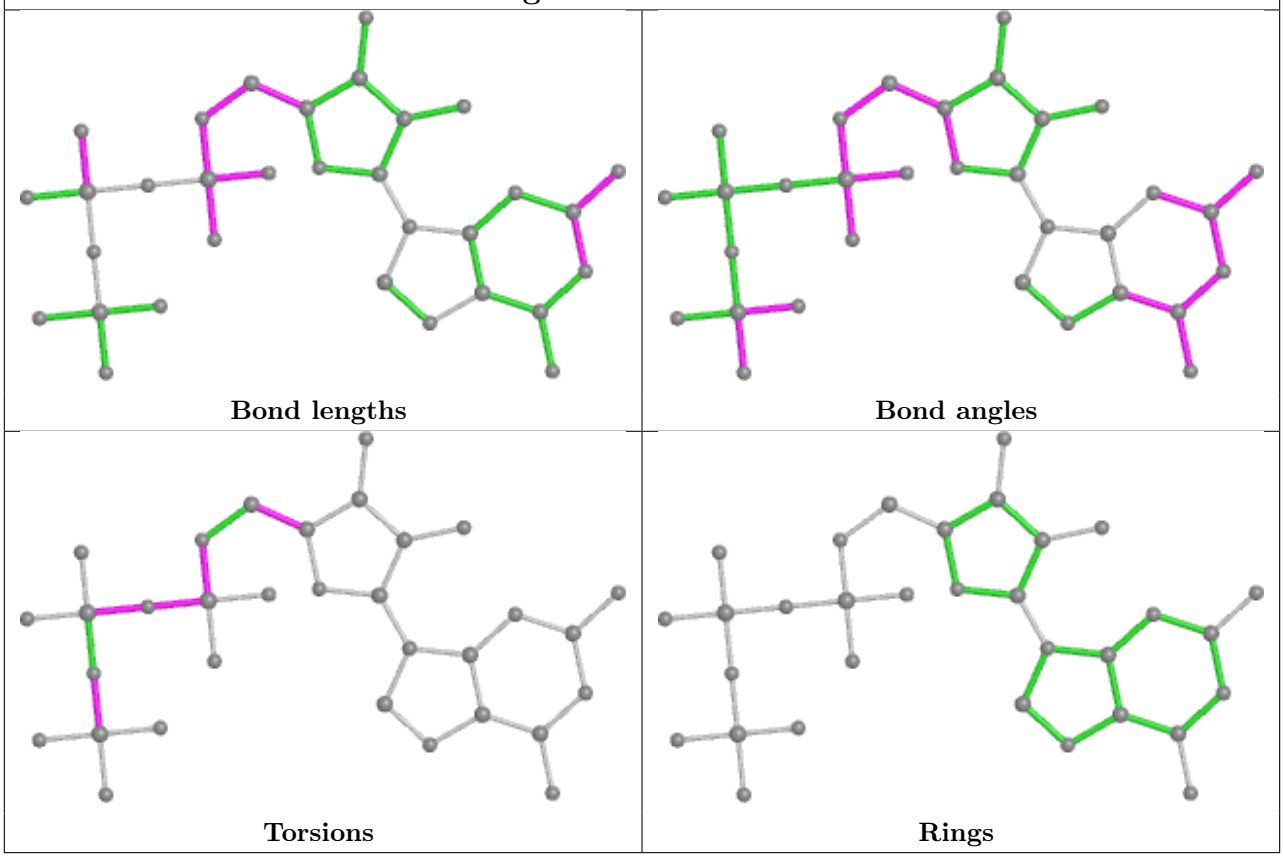


Torsions



Rings

Ligand GTP A 702



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	0.13	27 (5%)	24	30	20, 46, 86, 109	0
1	B	478/550 (86%)	0.04	26 (5%)	25	32	20, 41, 79, 107	0
1	C	478/550 (86%)	0.27	30 (6%)	20	25	23, 48, 85, 120	0
1	D	478/550 (86%)	-0.15	9 (1%)	66	73	17, 36, 68, 92	0
All	All	1914/2200 (87%)	0.07	92 (4%)	30	37	17, 42, 80, 120	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	488	LEU	8.2
1	C	113	ASP	7.3
1	C	488	LEU	7.2
1	B	487	VAL	6.4
1	B	113	ASP	6.4
1	C	593	PRO	6.0
1	C	596	LYS	5.7
1	C	592	THR	5.2
1	A	465	GLN	5.1
1	D	465	GLN	4.9
1	B	490	ASP	4.8
1	B	486	LYS	4.8
1	C	590	LEU	4.7
1	A	488	LEU	4.6
1	A	466	ILE	4.3
1	A	562	LEU	4.3
1	A	490	ASP	4.3
1	A	480	VAL	3.8
1	A	563	TYR	3.8
1	B	489	LEU	3.8
1	C	585	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	591	ILE	3.4
1	C	597	GLU	3.3
1	B	590	LEU	3.3
1	B	591	ILE	3.3
1	B	492	LYS	3.2
1	A	284	LEU	3.2
1	A	489	LEU	3.2
1	C	568	TYR	3.1
1	A	471	GLU	3.1
1	A	476	LEU	3.1
1	C	325	ILE	3.1
1	D	594	GLN	3.0
1	D	471	GLU	3.0
1	B	560	LYS	3.0
1	C	490	ASP	3.0
1	A	478	LYS	3.0
1	D	596	LYS	3.0
1	B	491	VAL	2.9
1	C	589	PRO	2.9
1	C	584	GLY	2.9
1	C	489	LEU	2.8
1	D	490	ASP	2.8
1	B	593	PRO	2.8
1	D	464	GLY	2.7
1	A	574	ALA	2.7
1	B	587	ILE	2.7
1	A	483	ALA	2.7
1	A	464	GLY	2.7
1	B	594	GLN	2.7
1	A	468	ILE	2.7
1	B	559	ARG	2.6
1	C	275	PRO	2.6
1	A	596	LYS	2.6
1	C	492	LYS	2.6
1	A	498	PHE	2.5
1	A	277	GLU	2.5
1	A	345	ASN	2.5
1	B	465	GLN	2.5
1	B	485	PRO	2.5
1	C	229	VAL	2.4
1	A	276	LEU	2.4
1	B	494	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	496	GLU	2.3
1	A	559	ARG	2.3
1	C	403	GLY	2.3
1	B	562	LEU	2.2
1	C	323	LEU	2.2
1	C	562	LEU	2.2
1	B	558	ASP	2.2
1	C	114	THR	2.2
1	B	466	ILE	2.2
1	B	493	LEU	2.2
1	B	495	ALA	2.2
1	C	115	MET	2.2
1	A	482	SER	2.2
1	A	585	ASP	2.2
1	C	320	CYS	2.1
1	D	467	LYS	2.1
1	C	193	GLU	2.1
1	C	496	GLU	2.1
1	C	594	GLN	2.1
1	D	326	GLN	2.1
1	B	121	PRO	2.1
1	C	560	LYS	2.1
1	A	491	VAL	2.1
1	A	467	LYS	2.1
1	C	484	LYS	2.1
1	C	574	ALA	2.0
1	B	577	ASN	2.0
1	D	284	LEU	2.0
1	A	113	ASP	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
7	GLY	D	714	5/5	0.45	0.17	72,81,88,92	0
7	GLY	D	713	5/5	0.50	0.55	64,67,75,92	0
7	GLY	C	713	5/5	0.60	0.30	67,69,76,77	0
8	TRS	B	713	8/8	0.62	0.20	92,100,104,106	0
6	NA	D	708	1/1	0.63	0.32	73,73,73,73	0
9	PO4	D	716	5/5	0.67	0.39	104,121,137,137	0
7	GLY	B	712	5/5	0.68	0.27	78,80,86,90	0
8	TRS	B	714	8/8	0.69	0.35	57,73,79,83	0
7	GLY	C	711	5/5	0.71	0.24	72,78,80,81	0
7	GLY	D	712	5/5	0.72	0.17	57,63,68,69	0
5	MG	B	710	1/1	0.72	0.45	67,67,67,67	0
7	GLY	C	712	5/5	0.74	0.17	67,69,76,82	0
6	NA	A	711	1/1	0.75	0.14	66,66,66,66	0
7	GLY	A	715	5/5	0.76	0.20	72,76,80,84	0
7	GLY	C	714	5/5	0.82	0.27	65,69,76,76	0
7	GLY	D	715	5/5	0.83	0.24	62,65,67,68	0
7	GLY	C	710	5/5	0.84	0.29	79,79,84,91	0
7	GLY	B	711	5/5	0.84	0.27	58,62,67,72	0
2	HFD	A	701	32/32	0.85	0.16	45,63,96,98	0
6	NA	B	709	1/1	0.85	0.21	64,64,64,64	0
2	HFD	C	704	32/32	0.86	0.16	40,65,116,119	0
6	NA	C	701	1/1	0.87	0.13	62,62,62,62	0
2	HFD	B	701	32/32	0.88	0.16	33,59,73,82	0
6	NA	D	709	1/1	0.91	0.14	51,51,51,51	0
5	MG	C	703	1/1	0.91	0.11	30,30,30,30	0
6	NA	A	713	1/1	0.92	0.32	60,60,60,60	0
6	NA	B	707	1/1	0.92	0.13	47,47,47,47	0
5	MG	D	710	1/1	0.92	0.10	78,78,78,78	0
2	HFD	D	703	32/32	0.93	0.11	32,54,81,84	0
5	MG	D	701	1/1	0.94	0.07	29,29,29,29	0
6	NA	A	710	1/1	0.94	0.23	43,43,43,43	0
6	NA	C	707	1/1	0.95	0.10	60,60,60,60	0
5	MG	C	709	1/1	0.95	0.12	69,69,69,69	0
5	MG	D	711	1/1	0.95	0.15	51,51,51,51	0
5	MG	A	704	1/1	0.96	0.09	31,31,31,31	0
6	NA	D	704	1/1	0.96	0.14	45,45,45,45	0
6	NA	D	707	1/1	0.96	0.20	52,52,52,52	0

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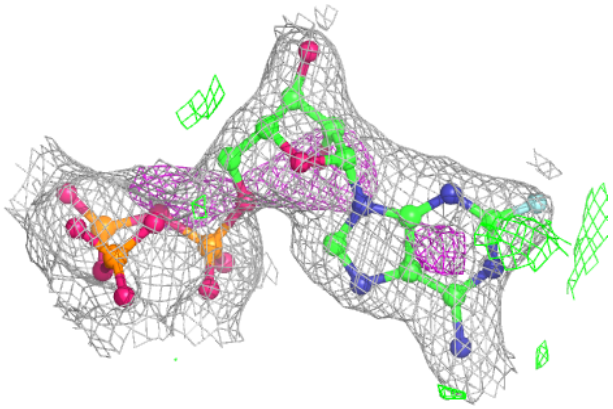
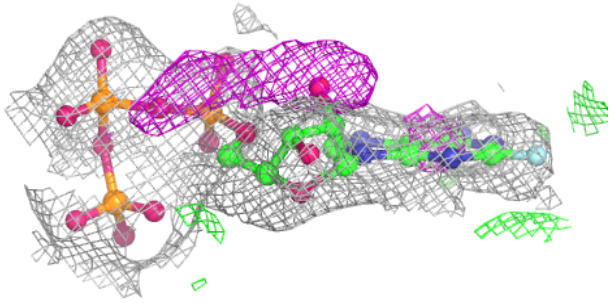
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	A	714	1/1	0.96	0.07	61,61,61,61	0
6	NA	B	704	1/1	0.97	0.09	40,40,40,40	0
6	NA	C	706	1/1	0.97	0.13	41,41,41,41	0
6	NA	B	705	1/1	0.97	0.39	47,47,47,47	0
6	NA	A	709	1/1	0.97	0.10	51,51,51,51	0
6	NA	D	705	1/1	0.97	0.08	38,38,38,38	0
6	NA	D	706	1/1	0.97	0.11	46,46,46,46	0
6	NA	B	708	1/1	0.97	0.31	53,53,53,53	0
3	GTP	C	705	32/32	0.97	0.11	26,30,37,39	0
6	NA	A	707	1/1	0.98	0.13	39,39,39,39	0
6	NA	A	712	1/1	0.98	0.17	56,56,56,56	0
6	NA	A	708	1/1	0.98	0.13	41,41,41,41	0
3	GTP	B	702	32/32	0.98	0.10	20,23,35,38	0
3	GTP	A	702	32/32	0.98	0.11	20,24,36,41	0
6	NA	B	706	1/1	0.98	0.11	42,42,42,42	0
6	NA	C	708	1/1	0.98	0.20	58,58,58,58	0
4	DTP	A	703	30/30	0.99	0.12	23,25,34,38	0
4	DTP	B	703	30/30	0.99	0.11	17,19,23,25	0
4	DTP	C	702	30/30	0.99	0.11	19,23,30,33	0
4	DTP	D	702	30/30	0.99	0.12	20,22,28,31	0
3	GTP	A	706	32/32	0.99	0.11	18,21,29,30	0
5	MG	A	705	1/1	1.00	0.07	20,20,20,20	0

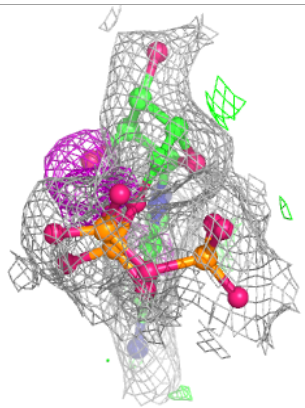
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HFD 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)

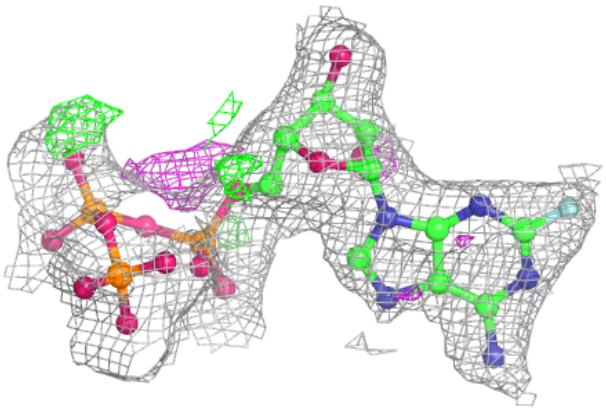


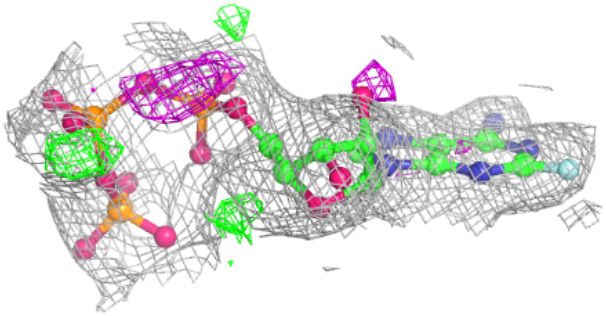


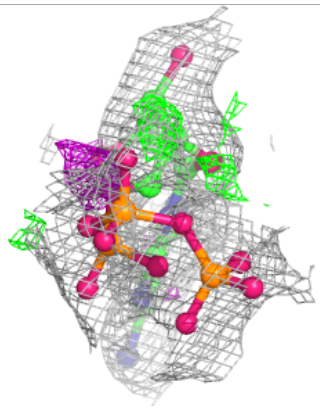


Electron density around HFD C 704:

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

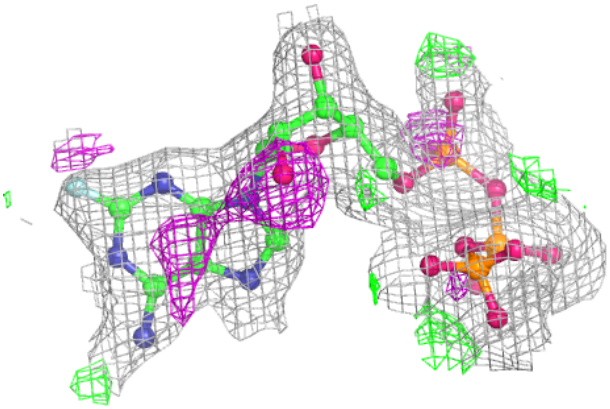


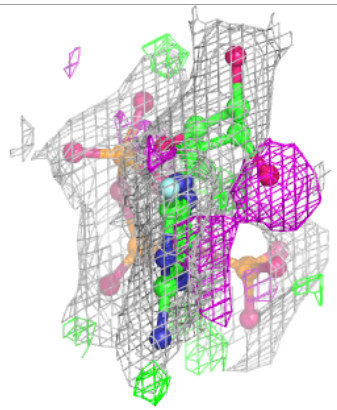




Electron density around HFD B 701:

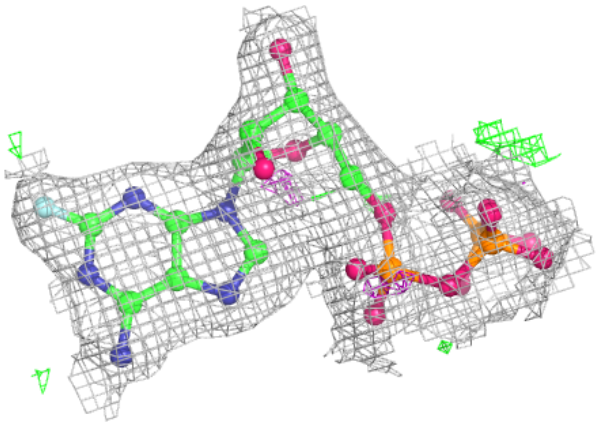
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

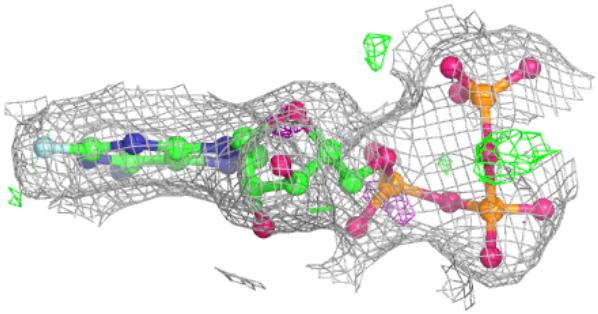


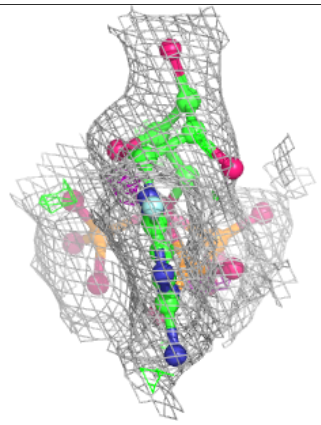


Electron density around HFD D 703:

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

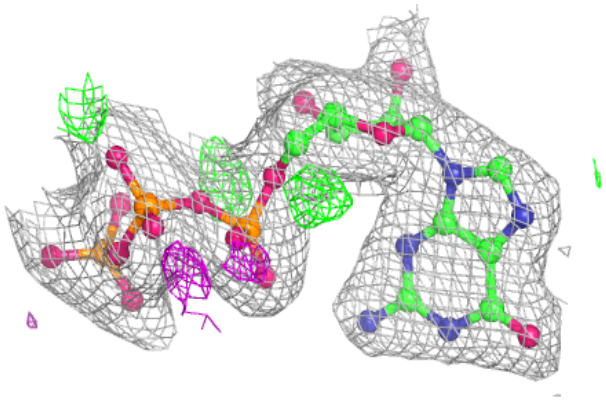


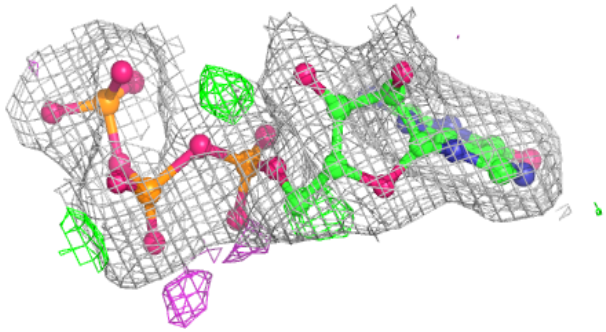


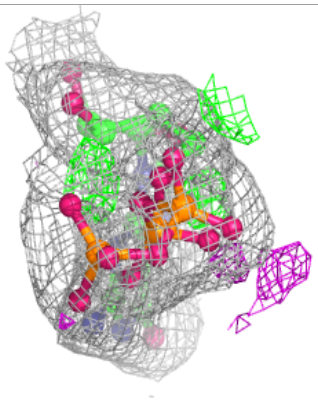


Electron density around GTP C 705:

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

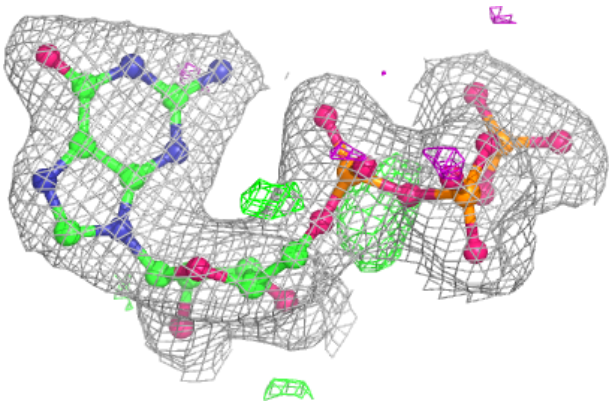


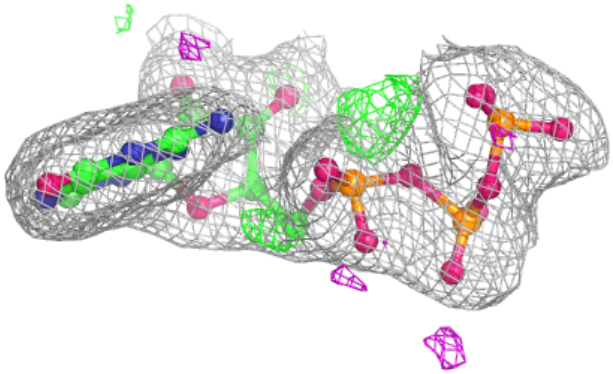


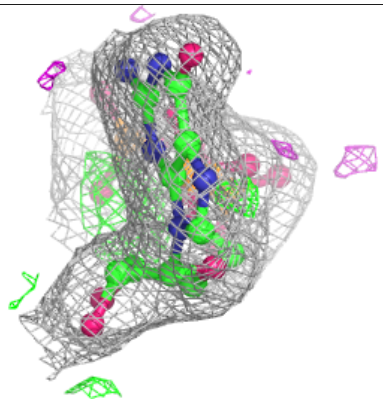


Electron density around GTP B 702:

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

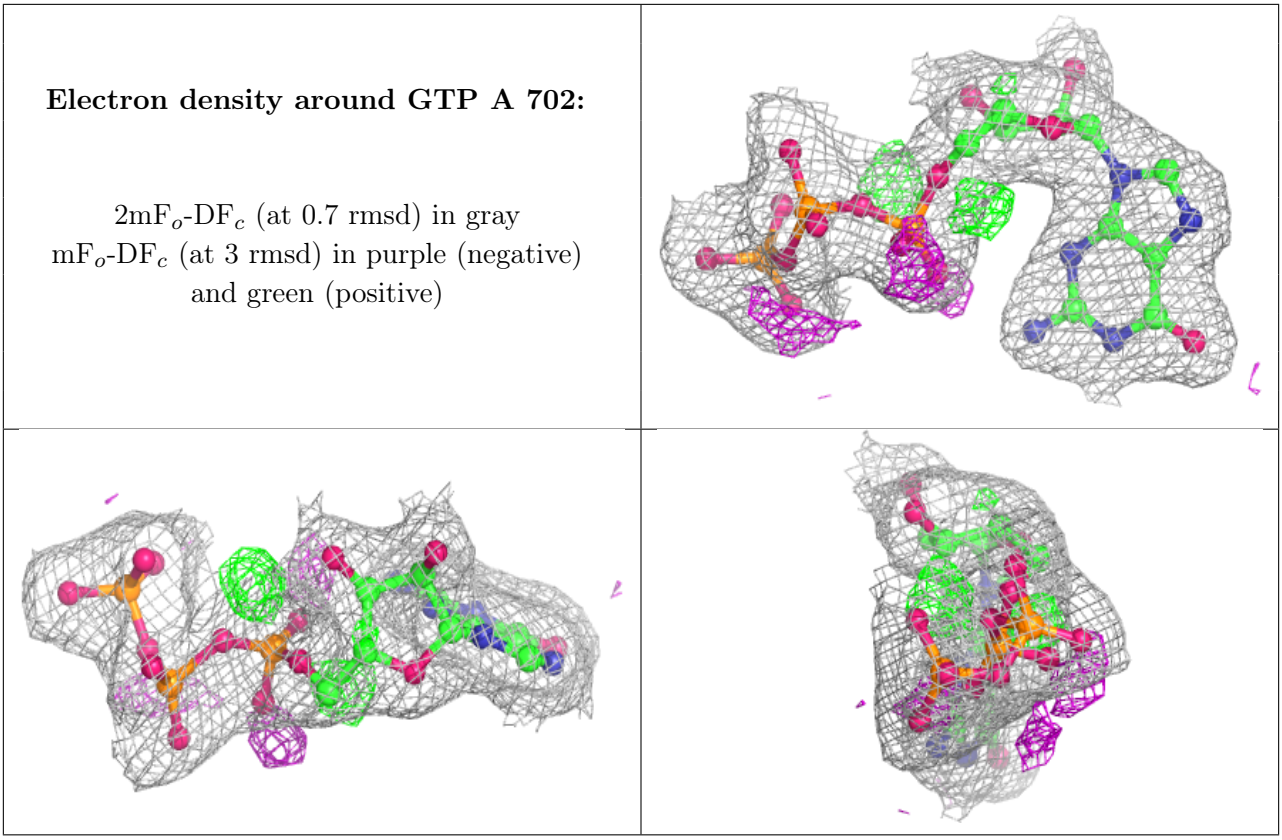






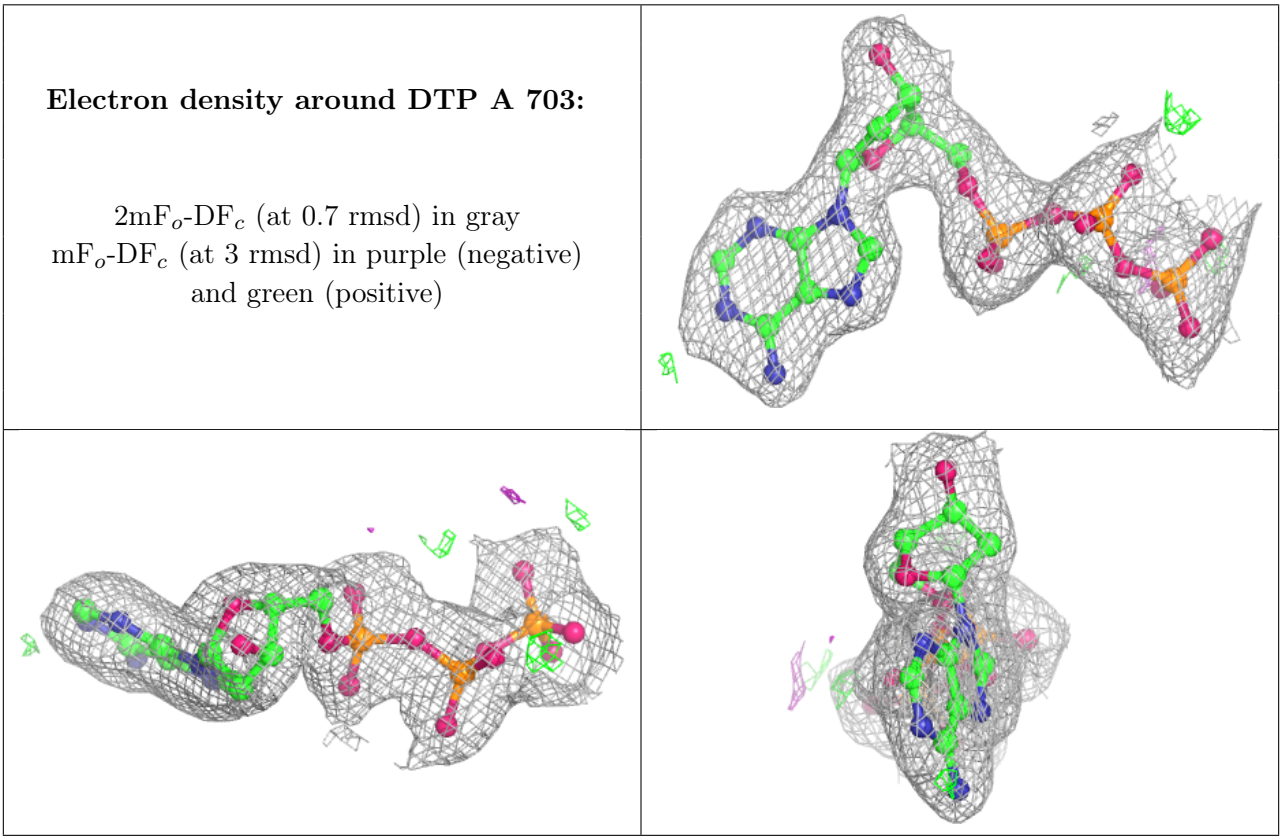
Electron density around GTP A 702:

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



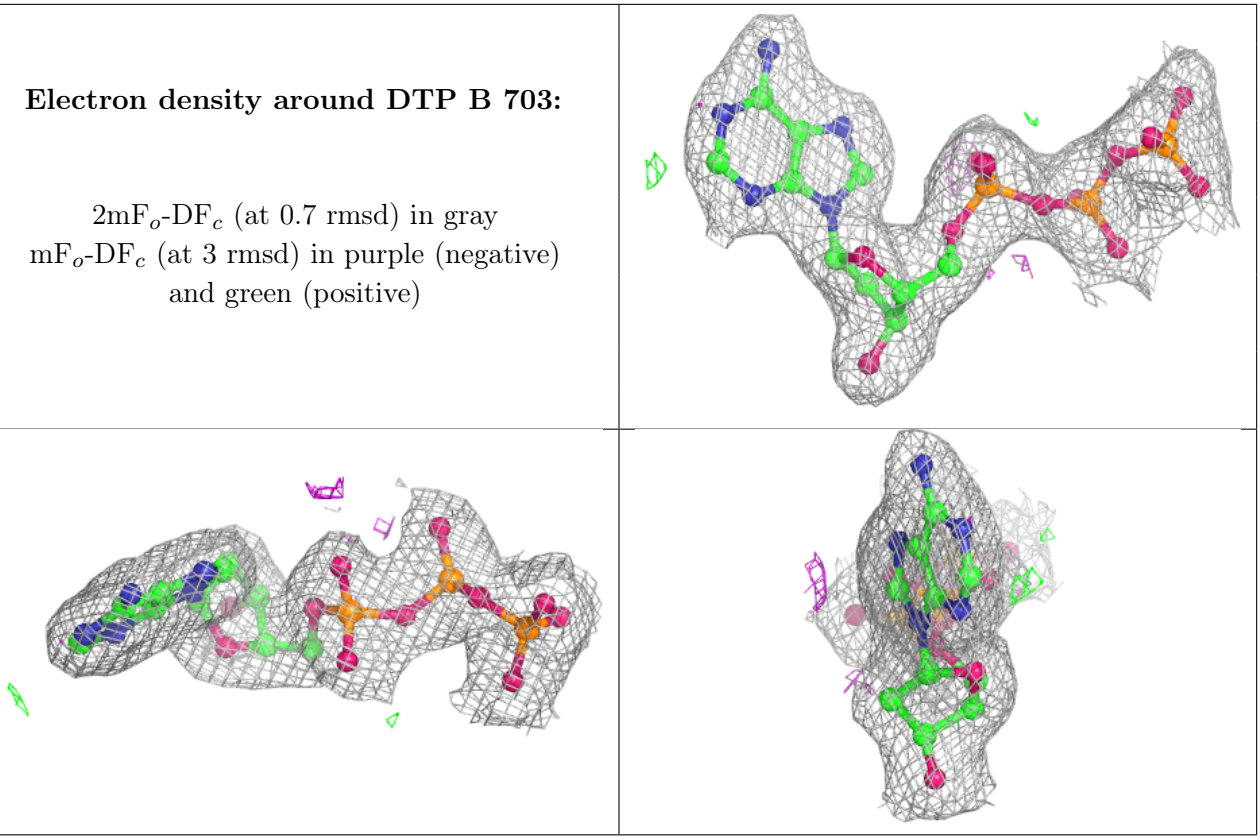
Electron density around DTP A 703:

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



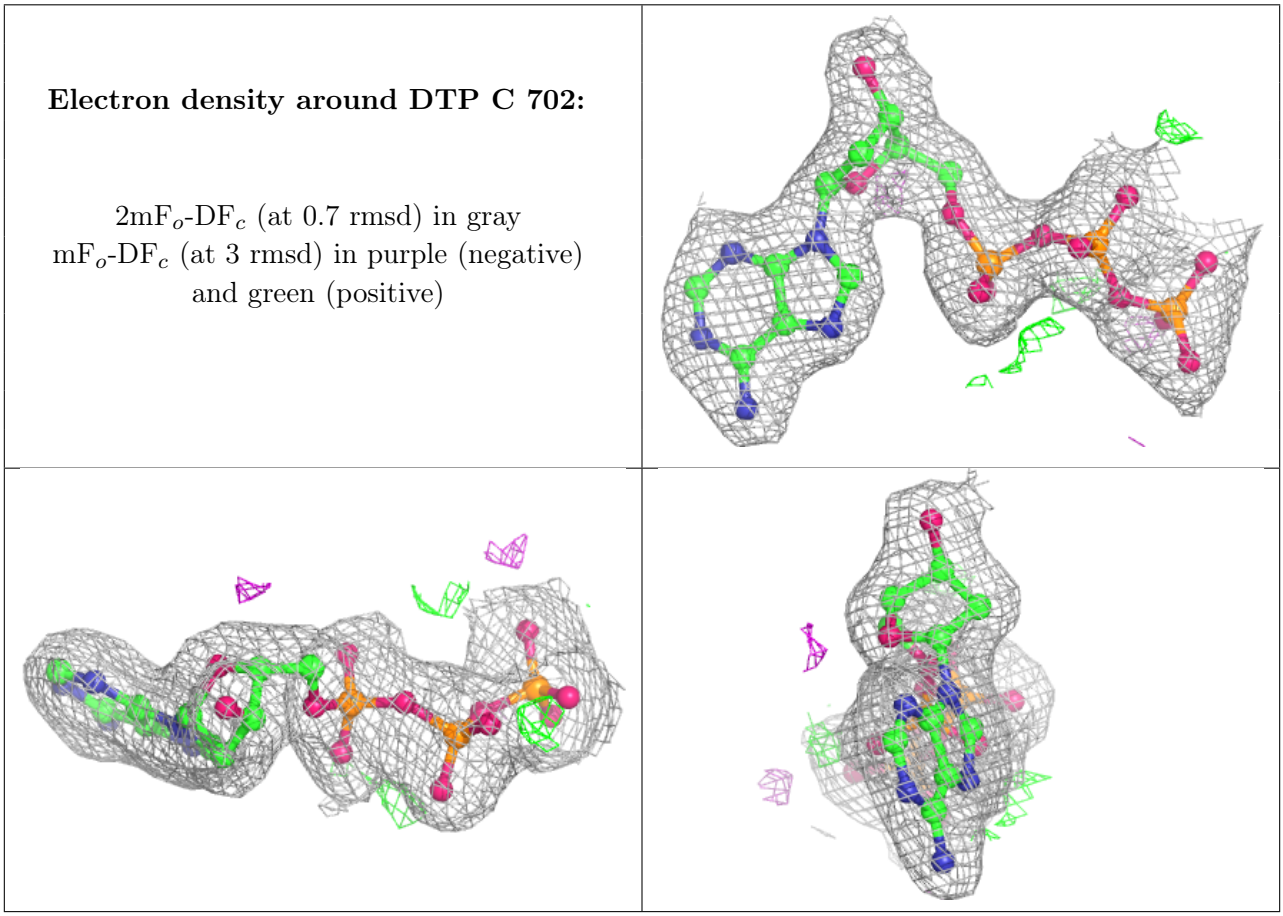
Electron density around DTP B 703:

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



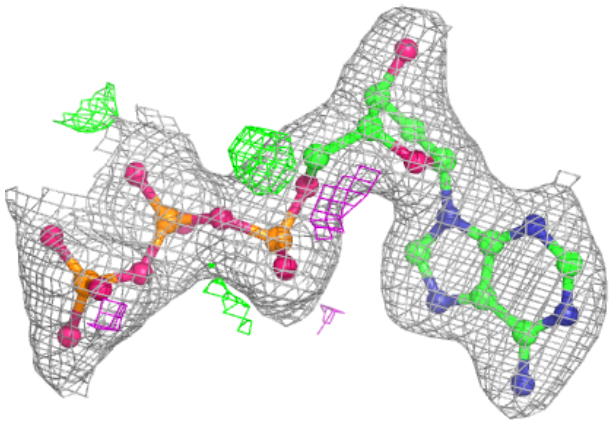
Electron density around DTP C 702:

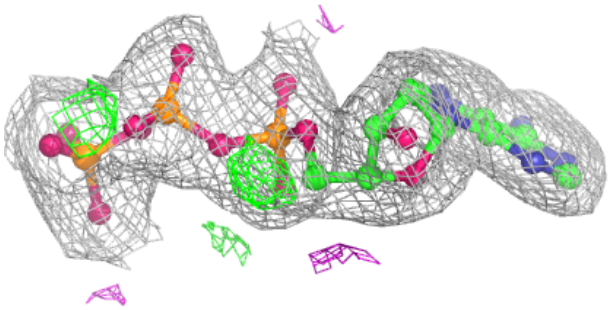
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

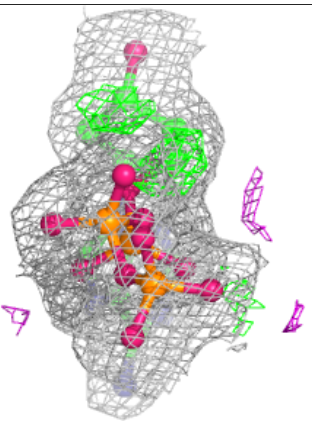


Electron density around DTP D 702:

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

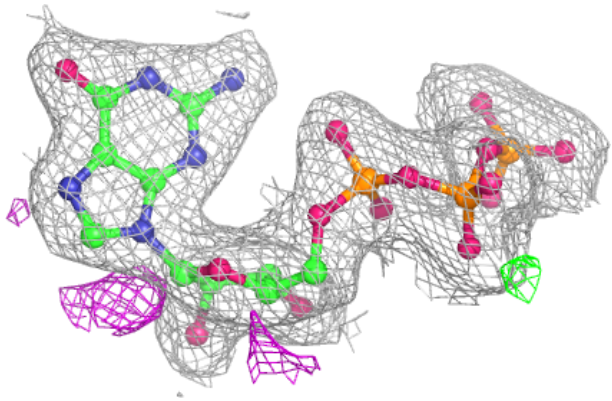


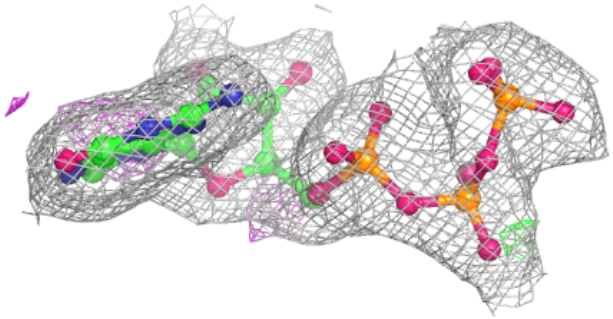


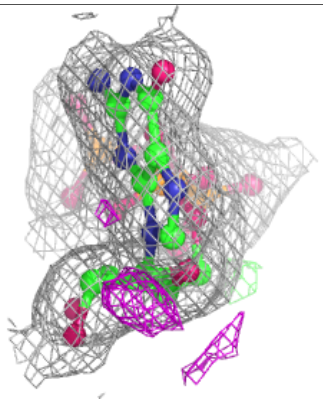


Electron density around GTP A 706:

$2mF_o$-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.