



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 18, 2021 – 05:09 PM EDT

PDB ID : 7S2Y
Title : SAMHD1 HD domain bound to CNDAC
Authors : Digianantonio, K.M.; Xiong, Y.
Deposited on : 2021-09-04
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
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) : 2.23.2

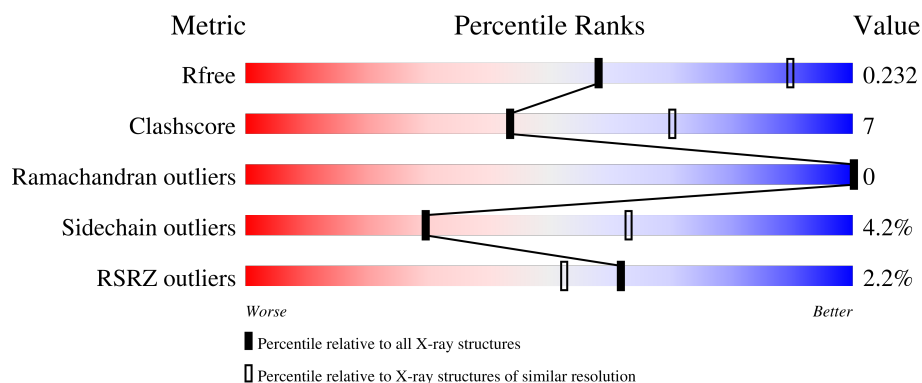
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	550	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>15%</div> <div>•</div> <div>13%</div> </div> </div>
1	B	550	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>10%</div> <div>•</div> <div>13%</div> </div> </div>
1	C	550	<div> <div>0%</div> <div> <div></div> <div>75%</div> <div>11%</div> <div>•</div> <div>13%</div> </div> </div>
1	D	550	<div> <div>0%</div> <div> <div></div> <div>75%</div> <div>12%</div> <div>•</div> <div>13%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16311 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	481	Total	C	N	O	S	0	5	0
			3979	2542	696	721	20			
1	B	481	Total	C	N	O	S	0	3	0
			3964	2537	690	717	20			
1	C	481	Total	C	N	O	S	0	3	0
			3964	2537	690	717	20			
1	D	481	Total	C	N	O	S	0	5	0
			3980	2545	693	722	20			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	MET	-	expression tag	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	-	expression tag	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	-	expression tag	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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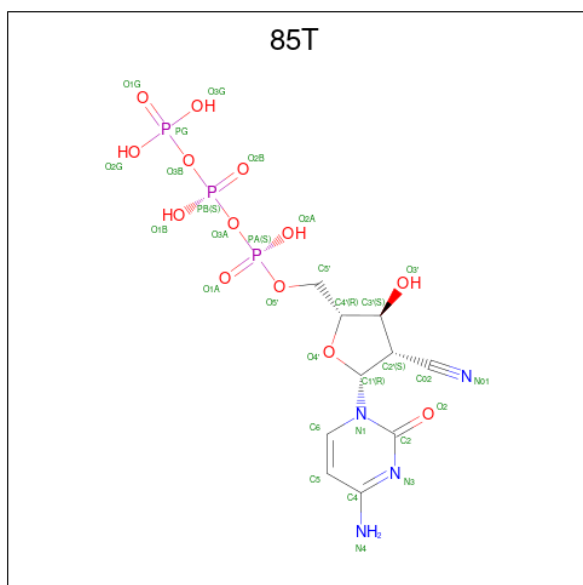
Chain	Residue	Modelled	Actual	Comment	Reference
C	106	MET	-	expression tag	UNP Q9Y3Z3
C	107	GLY	-	expression tag	UNP Q9Y3Z3
C	108	ARG	-	expression tag	UNP Q9Y3Z3
C	109	ASP	-	expression tag	UNP Q9Y3Z3
C	110	PRO	-	expression tag	UNP Q9Y3Z3
C	111	ASN	-	expression tag	UNP Q9Y3Z3
C	112	SER	-	expression tag	UNP Q9Y3Z3
C	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
C	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
D	77	MET	-	expression tag	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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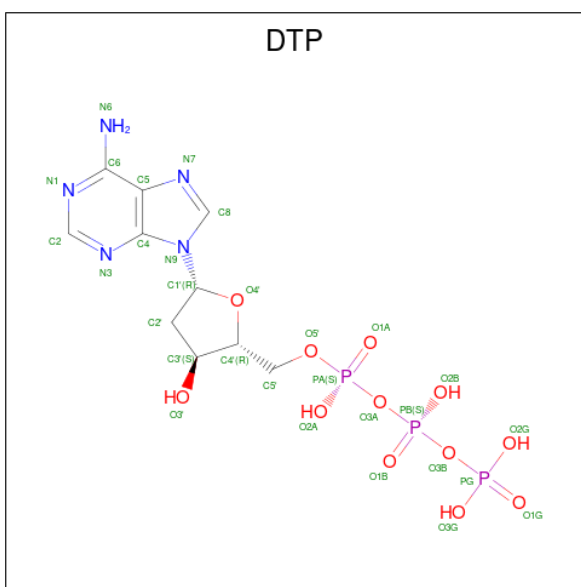
Chain	Residue	Modelled	Actual	Comment	Reference
D	110	PRO	-	expression tag	UNP Q9Y3Z3
D	111	ASN	-	expression tag	UNP Q9Y3Z3
D	112	SER	-	expression tag	UNP Q9Y3Z3
D	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
D	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3

- Molecule 2 is 4-amino-1-{2-cyano-2-deoxy-5-O-[(S)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]oxy}phosphoryl]-beta-D-arabinofuranosyl}pyrimidin-2(1H)-one (three-letter code: 85T) (formula: C₁₀H₁₅N₄O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			30	10	4	13	3		
2	B	1	Total	C	N	O	P	0	0
			30	10	4	13	3		
2	C	1	Total	C	N	O	P	0	0
			30	10	4	13	3		
2	D	1	Total	C	N	O	P	0	0
			30	10	4	13	3		

- Molecule 3 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃).

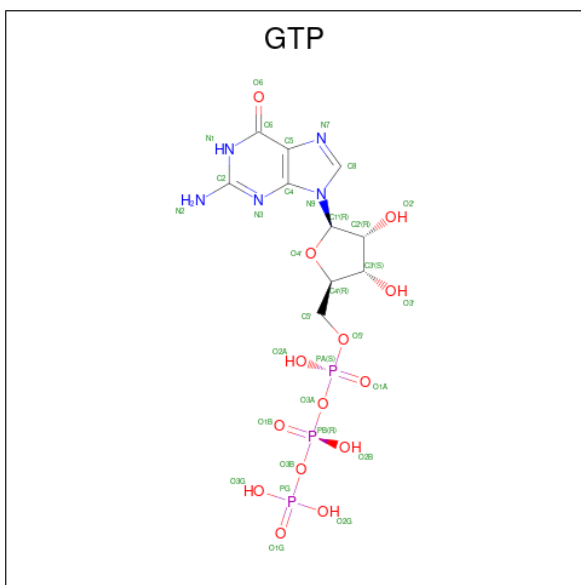


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 30	C 10	N 5	O 12	P 3	0	0
3	B	1	Total 30	C 10	N 5	O 12	P 3	0	0
3	C	1	Total 30	C 10	N 5	O 12	P 3	0	0
3	D	1	Total 30	C 10	N 5	O 12	P 3	0	0

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

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

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{14}\text{P}_3$).



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

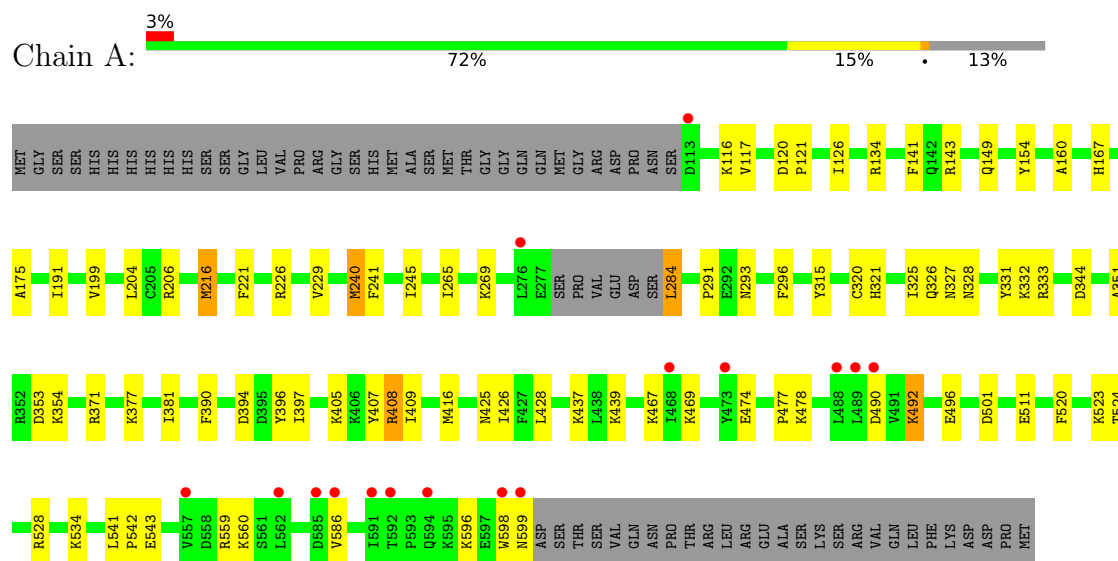
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	10	Total O 10 10	0	0
6	B	7	Total O 7 7	0	0
6	C	14	Total O 14 14	0	0
6	D	17	Total O 17 17	0	0

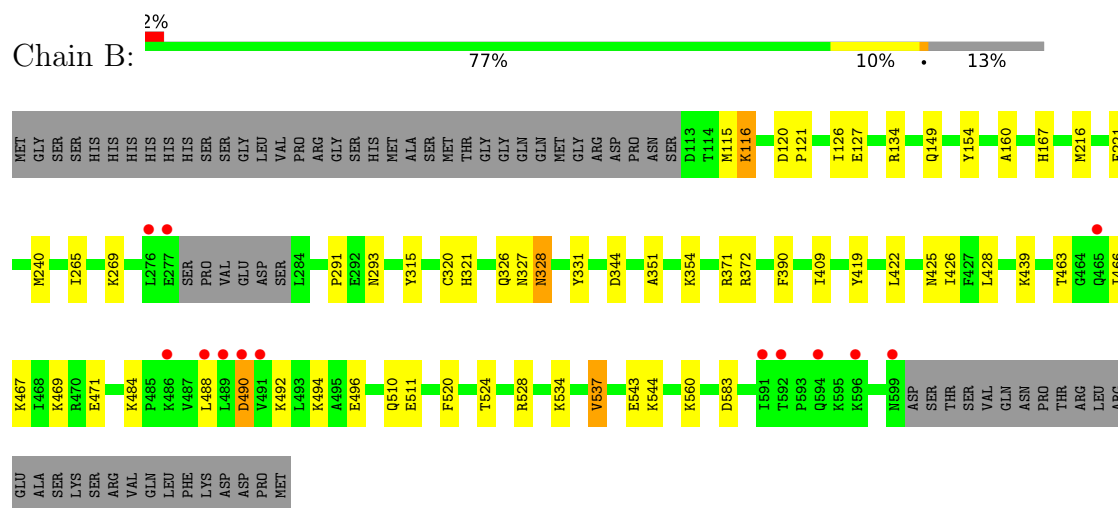
3 Residue-property plots

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

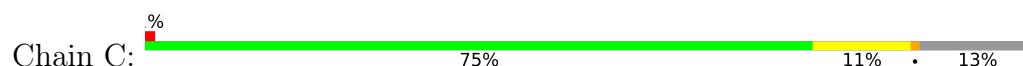
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

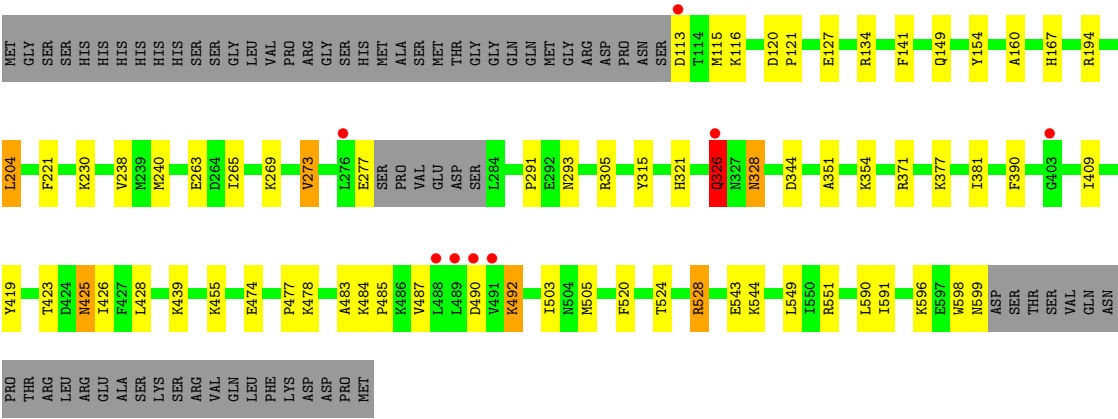


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

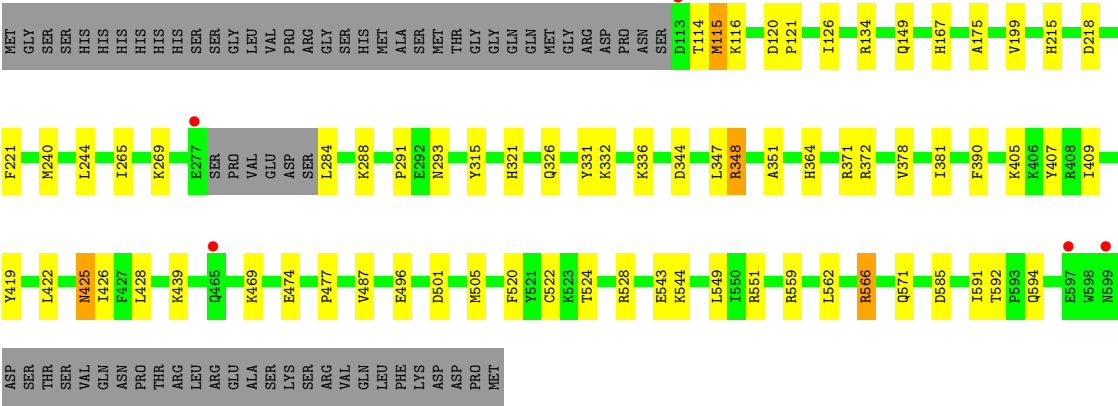
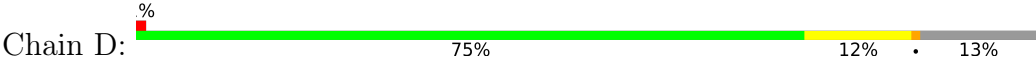


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





● Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.84Å 146.17Å 99.59Å 90.00° 114.27° 90.00°	Depositor
Resolution (Å)	50.03 – 2.80 49.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.0 (50.03-2.80) 93.0 (49.98-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.186 , 0.232 0.185 , 0.232	Depositor DCC
R_{free} test set	2482 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	60.6	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16311	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GTP, DTP, 85T

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	0.44	0/4072	0.81	2/5496 (0.0%)
1	B	0.43	0/4058	0.82	4/5478 (0.1%)
1	C	0.46	0/4058	0.83	2/5478 (0.0%)
1	D	0.48	0/4074	0.85	2/5500 (0.0%)
All	All	0.45	0/16262	0.82	10/21952 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	528	ARG	NE-CZ-NH1	-7.09	116.75	120.30
1	D	372	ARG	CB-CG-CD	-6.64	94.33	111.60
1	C	528	ARG	NE-CZ-NH1	-6.62	116.99	120.30
1	B	528	ARG	CB-CG-CD	6.19	127.70	111.60
1	A	408	ARG	CG-CD-NE	-6.17	98.84	111.80
1	D	566	ARG	CG-CD-NE	-6.01	99.17	111.80
1	A	206	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	B	528	ARG	CG-CD-NE	-5.87	99.47	111.80
1	C	326	GLN	CB-CA-C	5.54	121.48	110.40
1	B	371	ARG	CB-CG-CD	5.38	125.60	111.60

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	3979	0	3952	70	0
1	B	3964	0	3940	44	0
1	C	3964	0	3940	54	0
1	D	3980	0	3948	57	0
2	A	30	0	0	3	0
2	B	30	0	0	5	0
2	C	30	0	0	3	0
2	D	30	0	0	2	0
3	A	30	0	12	2	0
3	B	30	0	12	3	0
3	C	30	0	12	1	0
3	D	30	0	12	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	3	0	0	0	0
4	D	1	0	0	0	0
5	B	32	0	12	2	0
5	C	32	0	12	3	0
5	D	64	0	24	2	0
6	A	10	0	0	3	0
6	B	7	0	0	1	0
6	C	14	0	0	1	0
6	D	17	0	0	3	0
All	All	16311	0	15876	214	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 7.

All (214) 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:A:701:85T:C4'	2:A:701:85T:O4'	1.66	1.20
2:B:702:85T:C4'	2:B:702:85T:O4'	1.70	1.17
2:C:703:85T:O4'	2:C:703:85T:C4'	1.66	1.15
1:A:543:GLU:HG2	1:C:543:GLU:HG2	1.26	1.13
1:D:585:ASP:OD1	1:D:592:THR:HG21	1.47	1.12
1:B:543:GLU:HG2	1:D:543:GLU:HG2	1.19	1.11
1:A:371[B]:ARG:HG3	1:A:371[B]:ARG:HH11	1.09	1.06
1:A:397:ILE:HD12	1:A:397:ILE:O	1.55	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:GLN:HB3	1:D:326:GLN:NE2	1.74	1.03
1:B:328:ASN:HB3	6:D:815:HOH:O	1.62	0.98
1:A:284:LEU:HD12	1:A:284:LEU:N	1.80	0.96
1:A:523:LYS:NZ	5:C:702:GTP:O1G	2.00	0.94
1:A:371[B]:ARG:HH11	1:A:371[B]:ARG:CG	1.84	0.91
1:B:543:GLU:CG	1:D:543:GLU:HG2	2.02	0.90
1:A:390:PHE:CE2	1:A:426:ILE:HD11	2.06	0.90
1:A:371[B]:ARG:HG3	1:A:371[B]:ARG:NH1	1.83	0.89
1:D:528:ARG:HG2	1:D:528:ARG:HH11	1.35	0.89
1:B:543:GLU:HG2	1:D:543:GLU:CG	2.04	0.87
2:D:704:85T:O2B	6:D:801:HOH:O	1.93	0.85
1:A:371[B]:ARG:CG	1:A:371[B]:ARG:NH1	2.38	0.84
1:A:543:GLU:HG2	1:C:543:GLU:CG	2.08	0.81
1:A:534:LYS:HE3	1:A:542:PRO:O	1.82	0.79
1:C:503:ILE:CD1	1:C:551:ARG:NH1	2.47	0.78
1:A:534:LYS:HZ3	1:A:541:LEU:HB2	1.48	0.78
1:D:348:ARG:NH1	1:D:348:ARG:HG3	1.98	0.78
1:B:326:GLN:HB3	1:D:326:GLN:HE21	1.51	0.76
1:A:397:ILE:HD11	1:A:409:ILE:H	1.50	0.76
1:A:397:ILE:HD13	1:A:409:ILE:HG13	1.68	0.76
1:A:394:ASP:O	1:A:408:ARG:HG2	1.88	0.74
1:C:371:ARG:HD3	1:C:505:MET:HE1	1.70	0.74
1:B:115:MET:HG2	1:B:127:GLU:HB3	1.70	0.73
1:C:238:VAL:HG21	1:C:273:VAL:CG1	2.19	0.72
1:A:284:LEU:N	1:A:284:LEU:CD1	2.53	0.72
1:A:534:LYS:NZ	1:A:541:LEU:HB2	2.04	0.72
1:A:543:GLU:CG	1:C:543:GLU:HG2	2.15	0.72
1:A:397:ILE:CD1	1:A:409:ILE:HG13	2.21	0.70
1:D:116:LYS:NZ	5:D:701:GTP:O2G	2.23	0.70
1:D:528:ARG:HG2	1:D:528:ARG:NH1	2.08	0.68
1:B:326:GLN:CB	1:D:326:GLN:NE2	2.52	0.68
1:A:534:LYS:CE	1:A:542:PRO:O	2.40	0.68
1:B:321:HIS:CE1	1:C:321:HIS:CE1	2.82	0.68
1:C:503:ILE:HD12	1:C:551:ARG:NH1	2.09	0.67
2:B:702:85T:O3G	6:B:801:HOH:O	2.13	0.67
1:A:390:PHE:CE2	1:A:426:ILE:CD1	2.75	0.67
2:A:701:85T:O4'	2:A:701:85T:C5'	2.43	0.67
1:D:585:ASP:OD1	1:D:592:THR:CG2	2.37	0.67
2:C:703:85T:O1B	6:C:801:HOH:O	2.14	0.66
1:B:543:GLU:CG	1:D:543:GLU:CG	2.70	0.65
1:C:238:VAL:HG21	1:C:273:VAL:HG12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:ASN:HB2	1:D:428:LEU:HD12	1.80	0.63
1:A:390:PHE:CZ	1:A:426:ILE:HG13	2.35	0.62
1:B:534:LYS:O	1:B:537:VAL:HG23	1.98	0.62
1:D:351:ALA:O	1:D:520:PHE:HA	2.00	0.62
1:D:364:HIS:CD2	6:D:817:HOH:O	2.53	0.62
1:B:467:LYS:NZ	1:B:511[B]:GLU:OE1	2.26	0.61
1:D:348:ARG:HG3	1:D:348:ARG:HH11	1.63	0.61
1:A:326:GLN:HG2	1:A:327:ASN:N	2.15	0.60
1:C:503:ILE:CD1	1:C:551:ARG:HH11	2.14	0.60
1:A:351:ALA:O	1:A:520:PHE:HA	2.01	0.60
1:C:371:ARG:HD3	1:C:505:MET:CE	2.31	0.60
1:A:397:ILE:HG12	1:A:409:ILE:CD1	2.31	0.60
1:B:351:ALA:O	1:B:520:PHE:HA	2.02	0.59
1:C:351:ALA:O	1:C:520:PHE:HA	2.02	0.59
1:C:273:VAL:O	1:C:273:VAL:CG2	2.50	0.59
1:B:494:LYS:HB2	1:B:496:GLU:OE2	2.03	0.59
1:D:291:PRO:HG2	1:D:293:ASN:OD1	2.03	0.58
1:A:396:TYR:CE1	1:A:437:LYS:HD2	2.37	0.58
1:A:291:PRO:HG2	1:A:293:ASN:OD1	2.04	0.58
1:B:331[B]:TYR:CD1	1:B:331[B]:TYR:C	2.77	0.58
1:B:115:MET:CG	1:B:127:GLU:HB3	2.34	0.58
1:B:291:PRO:HG2	1:B:293:ASN:OD1	2.03	0.58
1:C:238:VAL:CG2	1:C:273:VAL:HG12	2.33	0.58
1:C:328:ASN:OD1	1:C:328:ASN:N	2.36	0.58
1:B:428:LEU:HD12	1:C:425:ASN:HB2	1.86	0.58
1:C:291:PRO:HG2	1:C:293:ASN:OD1	2.04	0.57
1:C:503:ILE:HD12	1:C:551:ARG:HH11	1.66	0.57
1:C:238:VAL:HG21	1:C:273:VAL:HG11	1.85	0.57
1:A:321:HIS:CE1	1:D:321:HIS:CE1	2.93	0.57
1:D:348:ARG:HH11	1:D:348:ARG:CG	2.17	0.57
1:C:127:GLU:HG3	1:D:336:LYS:HE3	1.86	0.56
1:D:371:ARG:HD3	1:D:505:MET:HE1	1.87	0.56
2:C:703:85T:C6	2:C:703:85T:C02	2.84	0.56
1:A:328:ASN:HB3	6:A:809:HOH:O	2.06	0.56
1:B:422:LEU:HD12	1:B:426:ILE:HG13	1.86	0.56
1:D:331[B]:TYR:CD1	1:D:331[B]:TYR:C	2.79	0.56
1:A:501:ASP:OD2	6:A:801:HOH:O	2.18	0.56
1:A:397:ILE:CD1	1:A:409:ILE:H	2.18	0.56
1:A:425:ASN:HB2	1:D:428:LEU:CD1	2.36	0.56
1:A:390:PHE:HE2	1:A:426:ILE:HD11	1.67	0.56
1:B:372:ARG:HG2	3:D:702:DTP:N6	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:ASN:HB2	1:C:428:LEU:HD12	1.88	0.55
1:A:226:ARG:NH2	1:A:229:VAL:HG21	2.22	0.55
1:C:426:ILE:N	1:C:426:ILE:HD12	2.21	0.55
1:A:598:TRP:O	1:A:599:ASN:HB2	2.07	0.54
1:D:293:ASN:O	1:D:347:LEU:HD12	2.08	0.54
1:D:528:ARG:NH1	1:D:528:ARG:CG	2.71	0.54
2:B:702:85T:O3G	2:B:702:85T:O1B	2.25	0.54
1:A:265:ILE:CG2	1:A:269:LYS:HE3	2.38	0.53
3:B:703:DTP:O2A	3:B:703:DTP:H8	2.09	0.53
1:A:543:GLU:CG	1:C:543:GLU:CG	2.82	0.53
2:D:704:85T:C6	2:D:704:85T:C02	2.87	0.52
1:A:397:ILE:O	1:A:397:ILE:CD1	2.43	0.51
1:D:571:GLN:NE2	1:D:594:GLN:HE22	2.09	0.51
1:C:423:THR:O	1:C:426:ILE:HD13	2.10	0.51
1:A:326:GLN:HG2	1:A:327:ASN:H	1.76	0.50
1:D:405:LYS:HD2	1:D:407:TYR:OH	2.11	0.50
1:A:428:LEU:HD12	1:D:425:ASN:HB2	1.93	0.50
1:C:487:VAL:CG2	1:C:590:LEU:HD13	2.42	0.50
1:D:371:ARG:HD3	1:D:505:MET:CE	2.42	0.50
1:D:487:VAL:HG23	1:D:591:ILE:HD11	1.94	0.50
1:B:354:LYS:CE	3:B:703:DTP:O1A	2.60	0.49
1:B:425:ASN:ND2	1:C:425:ASN:OD1	2.44	0.49
1:B:326:GLN:HG3	1:D:326:GLN:HE22	1.77	0.49
1:D:265:ILE:CG2	1:D:269:LYS:HE3	2.42	0.49
1:A:216:MET:CE	1:A:221:PHE:HB2	2.42	0.49
3:A:702:DTP:O2A	3:A:702:DTP:H8	2.13	0.49
1:C:455:LYS:HA	1:C:455:LYS:HE2	1.95	0.49
1:D:422:LEU:HD12	1:D:426:ILE:HG13	1.95	0.48
1:D:240:MET:CE	1:D:419:TYR:HD2	2.26	0.48
1:C:149:GLN:HE22	1:C:167:HIS:CD2	2.31	0.48
1:C:598:TRP:O	1:C:599:ASN:HB2	2.13	0.48
1:A:221:PHE:CE2	1:A:409:ILE:HG22	2.49	0.48
1:B:265:ILE:CG2	1:B:269:LYS:HE3	2.44	0.48
1:C:141:PHE:CZ	1:C:204:LEU:HD22	2.48	0.48
1:A:425:ASN:ND2	1:D:425:ASN:OD1	2.47	0.48
1:B:463:THR:O	1:B:466:ILE:HG13	2.13	0.47
2:B:702:85T:O4'	2:B:702:85T:C5'	2.55	0.47
1:C:381:ILE:HD12	1:C:381:ILE:HA	1.78	0.47
1:A:149:GLN:HE22	1:A:167:HIS:CD2	2.33	0.47
2:B:702:85T:O4'	2:B:702:85T:O5'	2.32	0.47
1:B:240:MET:CE	1:B:419:TYR:HD2	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:701:GTP:O3B	5:B:701:GTP:O2A	2.33	0.47
1:A:467:LYS:HE2	1:A:511[B]:GLU:OE2	2.15	0.47
1:A:120:ASP:OD1	1:A:121:PRO:HD2	2.14	0.46
1:A:154:TYR:HB2	1:A:160:ALA:O	2.15	0.46
1:B:149:GLN:HE22	1:B:167:HIS:CD2	2.34	0.46
1:B:221:PHE:CE2	1:B:409:ILE:HG22	2.50	0.46
1:C:492:LYS:HE3	1:C:492:LYS:HB3	1.68	0.46
1:C:240:MET:CE	1:C:419:TYR:HD2	2.28	0.46
1:A:221:PHE:CE1	1:A:390:PHE:HB3	2.50	0.46
5:B:701:GTP:O1A	1:C:116:LYS:HE3	2.16	0.46
1:B:583:ASP:CB	1:D:522:CYS:SG	3.04	0.46
1:A:377:LYS:HZ2	1:C:354:LYS:HE3	1.81	0.46
1:B:326:GLN:HG3	1:D:326:GLN:NE2	2.30	0.46
1:D:149:GLN:HE22	1:D:167:HIS:CD2	2.33	0.46
1:C:487:VAL:CG2	1:C:590:LEU:CD1	2.94	0.46
1:A:397:ILE:HG12	1:A:409:ILE:HD12	1.96	0.45
1:C:221:PHE:CE2	1:C:409:ILE:HG22	2.51	0.45
1:C:265:ILE:CG2	1:C:269:LYS:HE3	2.46	0.45
1:A:405:LYS:HD3	1:A:407:TYR:OH	2.16	0.45
1:A:492:LYS:HE3	1:A:492:LYS:HB2	1.70	0.45
1:C:487:VAL:HG21	1:C:590:LEU:HD12	1.99	0.45
1:C:194:ARG:NH2	1:C:263:GLU:OE1	2.44	0.45
1:D:221:PHE:CE2	1:D:409:ILE:HG22	2.51	0.45
1:A:134:ARG:HD2	1:A:134:ARG:HA	1.77	0.45
2:A:701:85T:O4'	2:A:701:85T:O5'	2.35	0.45
1:D:331[B]:TYR:CZ	1:D:332:LYS:HG3	2.51	0.45
1:B:134:ARG:HA	1:B:134:ARG:HD3	1.79	0.45
3:C:701:DTP:O1G	3:C:701:DTP:O1B	2.34	0.45
1:B:116:LYS:NZ	5:C:702:GTP:O2A	2.50	0.45
1:B:490:ASP:OD2	1:B:560:LYS:HD3	2.16	0.45
1:A:143:ARG:HD3	6:A:806:HOH:O	2.16	0.44
1:B:120:ASP:OD1	1:B:121:PRO:HD2	2.17	0.44
1:B:320:CYS:SG	1:B:327:ASN:HB2	2.57	0.44
1:D:114:THR:HB	1:D:115:MET:H	1.65	0.44
1:A:381:ILE:HD12	1:A:381:ILE:HA	1.76	0.44
1:C:426:ILE:N	1:C:426:ILE:CD1	2.81	0.44
1:D:120:ASP:OD1	1:D:121:PRO:HD2	2.16	0.44
1:C:273:VAL:O	1:C:273:VAL:HG22	2.18	0.44
1:B:221:PHE:CE1	1:B:390:PHE:HB3	2.53	0.43
1:C:221:PHE:CE1	1:C:390:PHE:HB3	2.52	0.43
1:B:494:LYS:CB	1:B:496:GLU:OE2	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:LYS:O	1:B:537:VAL:CG2	2.65	0.43
5:C:702:GTP:O2A	5:C:702:GTP:O3B	2.35	0.43
1:A:586:VAL:HG22	1:C:528:ARG:HD3	2.00	0.43
1:B:425:ASN:HB2	1:C:428:LEU:CD1	2.48	0.43
1:C:120:ASP:OD1	1:C:121:PRO:HD2	2.19	0.43
1:D:381:ILE:HD12	1:D:381:ILE:HA	1.76	0.43
1:D:562:LEU:O	1:D:566:ARG:HG3	2.19	0.43
1:B:583:ASP:HB2	1:D:522:CYS:SG	2.59	0.43
1:B:154:TYR:HB2	1:B:160:ALA:O	2.19	0.42
1:A:117:VAL:O	3:B:703:DTP:H5'1	2.19	0.42
1:C:154:TYR:HB2	1:C:160:ALA:O	2.19	0.42
1:A:126:ILE:HD13	1:A:126:ILE:HG21	1.76	0.42
1:C:483:ALA:O	1:C:485:PRO:HD3	2.20	0.42
1:A:353:ASP:OD1	1:A:354:LYS:N	2.51	0.42
1:A:141:PHE:CZ	1:A:204:LEU:HD22	2.55	0.42
1:B:126:ILE:HD13	1:B:126:ILE:HG21	1.78	0.42
1:D:221:PHE:CE1	1:D:390:PHE:HB3	2.55	0.42
1:D:571:GLN:CD	1:D:594:GLN:HE22	2.22	0.42
1:D:175:ALA:HB1	1:D:199:VAL:HG12	2.01	0.42
1:D:126:ILE:HG21	1:D:126:ILE:HD13	1.70	0.41
1:A:175:ALA:HB1	1:A:199:VAL:HG12	2.02	0.41
1:D:215:HIS:HA	1:D:218:ASP:OD1	2.19	0.41
1:D:378:VAL:HG21	5:D:703:GTP:C5'	2.50	0.41
1:C:371:ARG:CZ	1:C:549:LEU:HD11	2.51	0.41
1:A:331:TYR:CE1	1:A:332:LYS:HG3	2.54	0.41
1:B:116:LYS:HZ3	1:B:116:LYS:HG3	1.79	0.41
1:D:474:GLU:O	1:D:477:PRO:HD2	2.20	0.41
1:A:191:ILE:HD11	1:A:296:PHE:HE2	1.86	0.41
1:A:377:LYS:NZ	1:C:354:LYS:HE3	2.36	0.41
1:A:333:ARG:NH1	3:A:702:DTP:C4	2.84	0.41
1:C:273:VAL:O	1:C:273:VAL:HG23	2.20	0.41
1:A:474:GLU:O	1:A:477:PRO:HD2	2.21	0.41
1:C:377:LYS:HB3	1:C:551:ARG:HE	1.85	0.41
1:A:241:PHE:O	1:A:245:ILE:HG12	2.21	0.40
1:A:320:CYS:SG	1:A:327:ASN:HB2	2.61	0.40
1:C:474:GLU:O	1:C:477:PRO:HD2	2.21	0.40
1:D:284:LEU:C	1:D:284:LEU:HD13	2.41	0.40
1:D:371:ARG:CZ	1:D:549:LEU:HD11	2.51	0.40
1:C:326:GLN:H	1:C:326:GLN:HG2	1.62	0.40
1:A:240:MET:HG2	1:A:416:MET:SD	2.61	0.40
1:D:244:LEU:C	1:D:244:LEU:HD23	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:571:GLN:HE22	1:D:594:GLN:HE22	1.68	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	482/550 (88%)	471 (98%)	11 (2%)	0	100	100
1	B	480/550 (87%)	470 (98%)	10 (2%)	0	100	100
1	C	480/550 (87%)	470 (98%)	10 (2%)	0	100	100
1	D	482/550 (88%)	472 (98%)	10 (2%)	0	100	100
All	All	1924/2200 (88%)	1883 (98%)	41 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	432/488 (88%)	414 (96%)	18 (4%)	30	63
1	B	430/488 (88%)	414 (96%)	16 (4%)	34	68
1	C	430/488 (88%)	408 (95%)	22 (5%)	24	55
1	D	432/488 (88%)	417 (96%)	15 (4%)	36	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1724/1952 (88%)	1653 (96%)	71 (4%)	30 64

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	LYS
1	A	216	MET
1	A	240	MET
1	A	284	LEU
1	A	315	TYR
1	A	325	ILE
1	A	344	ASP
1	A	439	LYS
1	A	469	LYS
1	A	478	LYS
1	A	490	ASP
1	A	492	LYS
1	A	496	GLU
1	A	524	THR
1	A	528	ARG
1	A	559	ARG
1	A	560	LYS
1	A	596	LYS
1	B	116	LYS
1	B	216	MET
1	B	315	TYR
1	B	328	ASN
1	B	344	ASP
1	B	439	LYS
1	B	469	LYS
1	B	471	GLU
1	B	484	LYS
1	B	488	LEU
1	B	490	ASP
1	B	492	LYS
1	B	510	GLN
1	B	524	THR
1	B	537	VAL
1	B	544	LYS
1	C	113	ASP
1	C	115	MET
1	C	134	ARG

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Mol	Chain	Res	Type
1	C	204	LEU
1	C	230	LYS
1	C	273	VAL
1	C	277	GLU
1	C	305	ARG
1	C	315	TYR
1	C	326	GLN
1	C	328	ASN
1	C	344	ASP
1	C	425	ASN
1	C	439	LYS
1	C	478	LYS
1	C	484	LYS
1	C	490	ASP
1	C	492	LYS
1	C	524	THR
1	C	544	LYS
1	C	591	ILE
1	C	596	LYS
1	D	115	MET
1	D	134	ARG
1	D	288	LYS
1	D	315	TYR
1	D	344	ASP
1	D	348	ARG
1	D	425	ASN
1	D	439	LYS
1	D	469	LYS
1	D	496	GLU
1	D	501	ASP
1	D	524	THR
1	D	544	LYS
1	D	551	ARG
1	D	559	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	A	233	HIS
1	A	321	HIS
1	A	425	ASN

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Mol	Chain	Res	Type
1	B	149	GLN
1	B	322	HIS
1	B	425	ASN
1	C	235	GLN
1	C	321	HIS
1	C	322	HIS
1	C	425	ASN
1	D	149	GLN
1	D	215	HIS
1	D	235	GLN
1	D	322	HIS
1	D	326	GLN
1	D	364	HIS
1	D	425	ASN
1	D	571	GLN
1	D	577	ASN
1	D	594	GLN

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 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GTP	D	701	4	26,34,34	1.03	2 (7%)	33,54,54	2.29	10 (30%)
3	DTP	B	703	4	26,32,32	0.69	0	30,50,50	1.10	3 (10%)
2	85T	D	704	4	23,31,31	3.48	11 (47%)	26,48,48	2.27	9 (34%)
5	GTP	D	703	4	26,34,34	1.07	2 (7%)	33,54,54	2.37	6 (18%)
3	DTP	C	701	4	26,32,32	0.78	1 (3%)	30,50,50	1.09	2 (6%)
5	GTP	B	701	4	26,34,34	1.10	1 (3%)	33,54,54	2.13	7 (21%)
3	DTP	D	702	4	26,32,32	0.93	1 (3%)	30,50,50	0.94	1 (3%)
3	DTP	A	702	4	26,32,32	0.66	0	30,50,50	1.08	2 (6%)
2	85T	A	701	4	23,31,31	3.84	7 (30%)	26,48,48	1.73	8 (30%)
2	85T	C	703	4	23,31,31	3.55	5 (21%)	26,48,48	1.88	6 (23%)
2	85T	B	702	4	23,31,31	4.06	9 (39%)	26,48,48	2.05	9 (34%)
5	GTP	C	702	4	26,34,34	1.09	1 (3%)	33,54,54	2.33	8 (24%)

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
5	GTP	D	701	4	-	5/18/38/38	0/3/3/3
3	DTP	B	703	4	-	7/18/34/34	0/3/3/3
2	85T	D	704	4	-	4/20/40/40	0/2/2/2
5	GTP	D	703	4	-	9/18/38/38	0/3/3/3
3	DTP	C	701	4	-	6/18/34/34	0/3/3/3
5	GTP	B	701	4	-	4/18/38/38	0/3/3/3
3	DTP	D	702	4	-	2/18/34/34	0/3/3/3
3	DTP	A	702	4	-	7/18/34/34	0/3/3/3
2	85T	A	701	4	-	3/20/40/40	0/2/2/2
2	85T	C	703	4	-	3/20/40/40	0/2/2/2
2	85T	B	702	4	-	8/20/40/40	0/2/2/2
5	GTP	C	702	4	-	6/18/38/38	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	702	85T	O4'-C4'	11.30	1.70	1.45
2	B	702	85T	O4'-C1'	-10.93	1.25	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	85T	C3'-C4'	-10.43	1.26	1.53
2	D	704	85T	C3'-C4'	-9.82	1.27	1.53
2	A	701	85T	O4'-C1'	-9.73	1.27	1.41
2	C	703	85T	O4'-C4'	9.71	1.66	1.45
2	A	701	85T	O4'-C4'	9.60	1.66	1.45
2	B	702	85T	C3'-C4'	-9.53	1.28	1.53
2	C	703	85T	C3'-C4'	-9.30	1.29	1.53
2	D	704	85T	O4'-C4'	7.68	1.62	1.45
2	C	703	85T	O4'-C1'	-7.65	1.30	1.41
2	D	704	85T	O4'-C1'	-7.28	1.30	1.41
2	C	703	85T	C2'-C02	-4.69	1.39	1.46
5	B	701	GTP	C6-N1	4.24	1.40	1.33
5	D	703	GTP	C6-N1	4.07	1.40	1.33
5	C	702	GTP	C6-N1	3.94	1.39	1.33
2	D	704	85T	C2'-C02	-3.57	1.41	1.46
3	D	702	DTP	PG-O1G	3.32	1.61	1.50
2	D	704	85T	O3'-C3'	3.31	1.50	1.43
2	D	704	85T	C4-N4	3.28	1.44	1.35
2	A	701	85T	PA-O5'	3.16	1.72	1.59
5	D	701	GTP	C6-N1	3.09	1.38	1.33
2	A	701	85T	C4-N4	2.96	1.43	1.35
2	D	704	85T	PG-O2G	-2.90	1.43	1.54
2	C	703	85T	PA-O5'	2.78	1.70	1.59
2	B	702	85T	C4-N4	2.63	1.42	1.35
2	B	702	85T	C2-N3	-2.55	1.33	1.38
5	D	701	GTP	C8-N7	-2.48	1.30	1.34
2	A	701	85T	O3'-C3'	2.46	1.48	1.43
2	A	701	85T	C2-N3	-2.45	1.33	1.38
2	B	702	85T	PA-O5'	2.27	1.68	1.59
2	B	702	85T	C2'-C02	-2.23	1.43	1.46
2	B	702	85T	O3'-C3'	2.18	1.48	1.43
2	D	704	85T	C6-N1	2.16	1.38	1.35
5	D	703	GTP	C8-N7	-2.16	1.30	1.34
3	C	701	DTP	PG-O1G	2.14	1.57	1.50
2	B	702	85T	C6-N1	2.12	1.38	1.35
2	D	704	85T	C4-N3	2.10	1.39	1.35
2	D	704	85T	C2-N3	-2.09	1.34	1.38
2	D	704	85T	PA-O5'	2.01	1.67	1.59

All (71) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	702	GTP	C5-C6-N1	-8.71	111.52	123.43
5	D	703	GTP	C5-C6-N1	-8.58	111.70	123.43
5	D	701	GTP	C5-C6-N1	-8.27	112.12	123.43
5	B	701	GTP	C5-C6-N1	-8.04	112.44	123.43
2	D	704	85T	PB-O3B-PG	-6.29	111.24	132.83
5	D	703	GTP	C6-N1-C2	6.01	125.49	115.93
5	C	702	GTP	C6-N1-C2	5.54	124.73	115.93
5	D	701	GTP	C6-N1-C2	5.37	124.46	115.93
5	B	701	GTP	C6-N1-C2	5.32	124.38	115.93
2	C	703	85T	PB-O3B-PG	-4.92	115.95	132.83
2	A	701	85T	C2-N3-C4	4.59	121.00	116.34
2	C	703	85T	PB-O3A-PA	-4.37	117.82	132.83
2	D	704	85T	O3'-C3'-C2'	-4.29	99.92	112.17
2	B	702	85T	C5-C4-N3	4.19	126.55	121.72
5	C	702	GTP	O3G-PG-O3B	-4.17	90.66	104.64
5	D	703	GTP	O3'-C3'-C4'	-4.13	99.10	111.05
2	C	703	85T	C2-N3-C4	4.11	120.50	116.34
2	D	704	85T	O2G-PG-O1G	-4.02	94.95	110.68
2	B	702	85T	N4-C4-N3	-3.49	110.97	116.49
2	B	702	85T	O3G-PG-O2G	3.47	120.91	107.64
2	B	702	85T	PB-O3B-PG	-3.43	121.07	132.83
2	D	704	85T	PB-O3A-PA	-3.40	121.16	132.83
2	D	704	85T	N4-C4-N3	3.35	121.78	116.49
5	C	702	GTP	O2G-PG-O3B	3.25	115.55	104.64
2	B	702	85T	O2G-PG-O3B	-3.19	93.93	104.64
5	D	703	GTP	N3-C2-N1	-3.17	122.99	127.22
5	D	701	GTP	PB-O3B-PG	-3.00	122.53	132.83
5	D	701	GTP	C2-N3-C4	-3.00	111.93	115.36
2	D	704	85T	O2G-PG-O3B	2.99	114.67	104.64
3	C	701	DTP	C5-C6-N6	2.89	124.75	120.35
2	A	701	85T	PB-O3A-PA	-2.87	122.97	132.83
3	D	702	DTP	C5-C6-N6	2.84	124.66	120.35
5	D	703	GTP	C2-N3-C4	-2.81	112.14	115.36
2	B	702	85T	O5'-PA-O1A	-2.71	98.49	109.07
5	B	701	GTP	N3-C2-N1	-2.70	123.62	127.22
5	B	701	GTP	PA-O3A-PB	-2.66	123.69	132.83
2	C	703	85T	O3'-C3'-C2'	-2.54	104.90	112.17
3	C	701	DTP	PB-O3B-PG	-2.53	124.14	132.83
5	C	702	GTP	N3-C2-N1	-2.47	123.92	127.22
2	D	704	85T	C5-C4-N4	-2.46	116.86	121.14
2	A	701	85T	PB-O3B-PG	-2.44	124.45	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	702	85T	O3'-C3'-C2'	-2.43	105.23	112.17
5	D	701	GTP	N3-C2-N1	-2.43	123.98	127.22
5	C	702	GTP	C2-N3-C4	-2.41	112.61	115.36
2	A	701	85T	O4'-C4'-C5'	-2.40	101.47	109.37
2	D	704	85T	C2-N3-C4	2.37	118.74	116.34
5	D	701	GTP	C3'-C2'-C1'	2.35	104.52	100.98
2	C	703	85T	O3G-PG-O3B	2.32	112.42	104.64
5	B	701	GTP	O2G-PG-O3B	-2.32	96.85	104.64
2	D	704	85T	PA-O5'-C5'	-2.32	108.10	121.68
5	B	701	GTP	C2-N3-C4	-2.30	112.73	115.36
2	A	701	85T	C2'-C02-N01	-2.26	175.41	177.87
3	B	703	DTP	O3'-C3'-C2'	2.26	118.99	110.90
5	D	703	GTP	N2-C2-N3	2.24	121.45	117.79
2	B	702	85T	C6-N1-C2	2.22	124.72	121.20
3	B	703	DTP	C2'-C1'-N9	2.22	119.38	114.27
2	A	701	85T	O3'-C3'-C4'	-2.22	104.64	111.05
3	A	702	DTP	C5-C6-N6	2.20	123.69	120.35
5	D	701	GTP	N2-C2-N3	2.19	121.36	117.79
5	B	701	GTP	C6-C5-C4	-2.17	118.72	120.80
5	D	701	GTP	O3G-PG-O3B	-2.12	97.54	104.64
2	B	702	85T	O3G-PG-O3B	2.11	111.72	104.64
5	C	702	GTP	N2-C2-N3	2.10	121.21	117.79
5	C	702	GTP	C1'-N9-C4	2.10	130.33	126.64
5	D	701	GTP	C1'-N9-C4	2.08	130.30	126.64
3	B	703	DTP	C5-C6-N6	2.08	123.51	120.35
2	C	703	85T	O5'-PA-O1A	-2.07	100.98	109.07
2	A	701	85T	O3'-C3'-C2'	-2.04	106.35	112.17
2	A	701	85T	PA-O5'-C5'	-2.03	109.77	121.68
3	A	702	DTP	O3G-PG-O3B	2.03	111.44	104.64
5	D	701	GTP	O3'-C3'-C4'	-2.00	105.27	111.05

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	85T	O4'-C4'-C5'-O5'
2	B	702	85T	PB-O3B-PG-O2G
2	B	702	85T	PB-O3B-PG-O3G
2	B	702	85T	O4'-C4'-C5'-O5'
2	C	703	85T	C3'-C4'-C5'-O5'
2	C	703	85T	O4'-C4'-C5'-O5'
3	A	702	DTP	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
3	A	702	DTP	C5'-O5'-PA-O1A
3	A	702	DTP	C5'-O5'-PA-O2A
3	A	702	DTP	C5'-O5'-PA-O3A
3	A	702	DTP	O4'-C4'-C5'-O5'
3	A	702	DTP	C3'-C4'-C5'-O5'
3	B	703	DTP	PB-O3B-PG-O2G
3	B	703	DTP	C5'-O5'-PA-O2A
3	B	703	DTP	C5'-O5'-PA-O3A
3	B	703	DTP	O4'-C4'-C5'-O5'
3	B	703	DTP	C3'-C4'-C5'-O5'
3	C	701	DTP	PB-O3B-PG-O2G
3	C	701	DTP	C5'-O5'-PA-O3A
5	D	703	GTP	PB-O3B-PG-O3G
5	D	703	GTP	C5'-O5'-PA-O2A
2	A	701	85T	C3'-C4'-C5'-O5'
2	B	702	85T	C3'-C4'-C5'-O5'
2	D	704	85T	O4'-C4'-C5'-O5'
3	C	701	DTP	O4'-C4'-C5'-O5'
2	D	704	85T	C3'-C4'-C5'-O5'
3	C	701	DTP	C3'-C4'-C5'-O5'
5	B	701	GTP	PG-O3B-PB-O1B
5	D	701	GTP	PG-O3B-PB-O1B
5	C	702	GTP	C4'-C5'-O5'-PA
2	D	704	85T	C5'-O5'-PA-O3A
5	D	703	GTP	C5'-O5'-PA-O3A
3	B	703	DTP	PG-O3B-PB-O1B
5	C	702	GTP	PB-O3A-PA-O2A
5	D	703	GTP	PB-O3A-PA-O2A
5	D	703	GTP	C4'-C5'-O5'-PA
3	B	703	DTP	C5'-O5'-PA-O1A
3	C	701	DTP	C5'-O5'-PA-O1A
3	C	701	DTP	C5'-O5'-PA-O2A
5	C	702	GTP	C5'-O5'-PA-O2A
5	D	703	GTP	C5'-O5'-PA-O1A
2	A	701	85T	PG-O3B-PB-O1B
2	B	702	85T	PG-O3B-PB-O1B
5	D	701	GTP	PB-O3A-PA-O2A
5	D	703	GTP	PG-O3B-PB-O2B
5	B	701	GTP	C4'-C5'-O5'-PA
5	D	701	GTP	C4'-C5'-O5'-PA
2	B	702	85T	PB-O3A-PA-O1A
3	A	702	DTP	PB-O3B-PG-O1G

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Mol	Chain	Res	Type	Atoms
3	D	702	DTP	PB-O3B-PG-O2G
3	D	702	DTP	PB-O3B-PG-O3G
5	C	702	GTP	C5'-O5'-PA-O3A
2	B	702	85T	PB-O3A-PA-O2A
2	C	703	85T	PG-O3B-PB-O1B
5	B	701	GTP	PG-O3B-PB-O2B
5	B	701	GTP	PA-O3A-PB-O2B
5	C	702	GTP	PB-O3A-PA-O1A
5	D	701	GTP	PG-O3B-PB-O2B
5	D	701	GTP	PB-O3A-PA-O1A
5	D	703	GTP	PB-O3A-PA-O1A
2	D	704	85T	C5'-O5'-PA-O1A
5	C	702	GTP	C5'-O5'-PA-O1A
2	B	702	85T	PB-O3B-PG-O1G
5	D	703	GTP	PB-O3B-PG-O1G

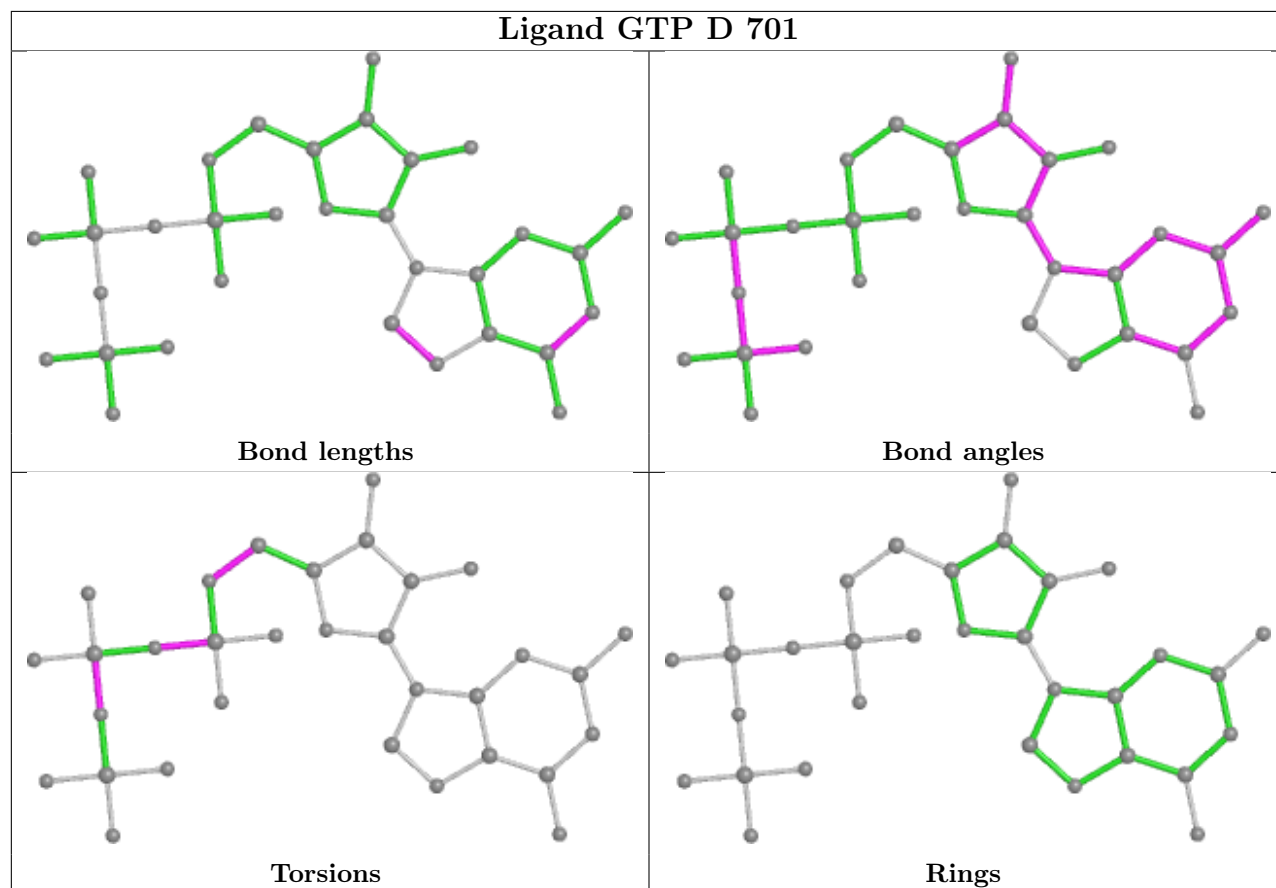
There are no ring outliers.

12 monomers are involved in 27 short contacts:

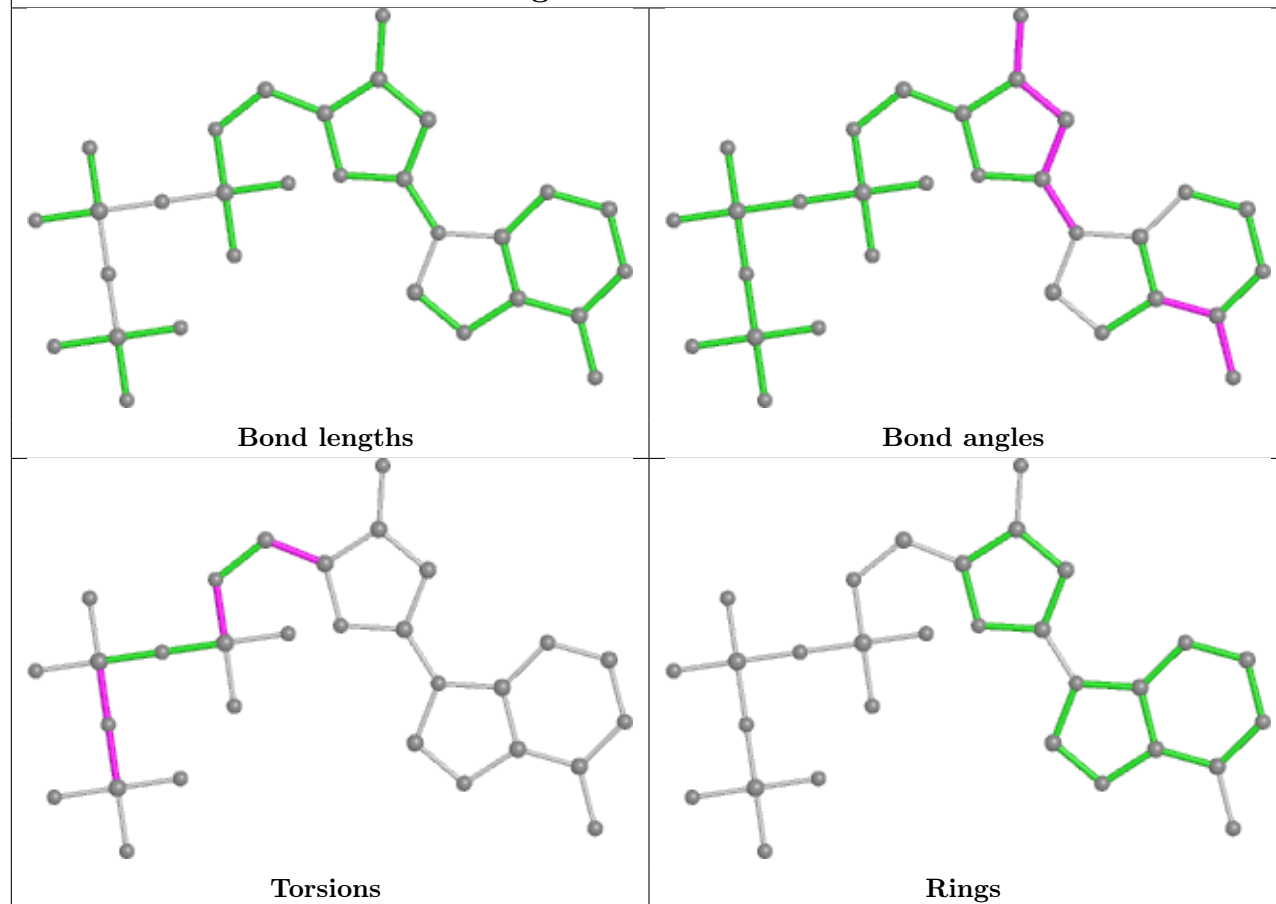
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	701	GTP	1	0
3	B	703	DTP	3	0
2	D	704	85T	2	0
5	D	703	GTP	1	0
3	C	701	DTP	1	0
5	B	701	GTP	2	0
3	D	702	DTP	1	0
3	A	702	DTP	2	0
2	A	701	85T	3	0
2	C	703	85T	3	0
2	B	702	85T	5	0
5	C	702	GTP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

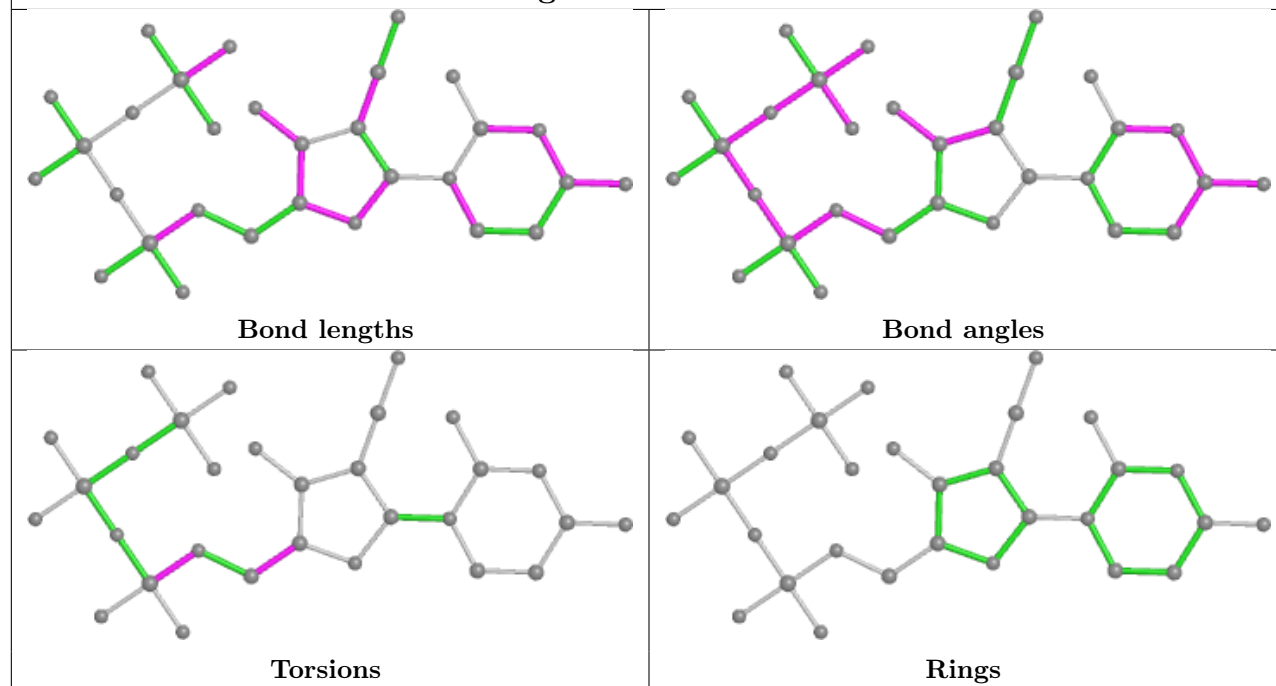
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

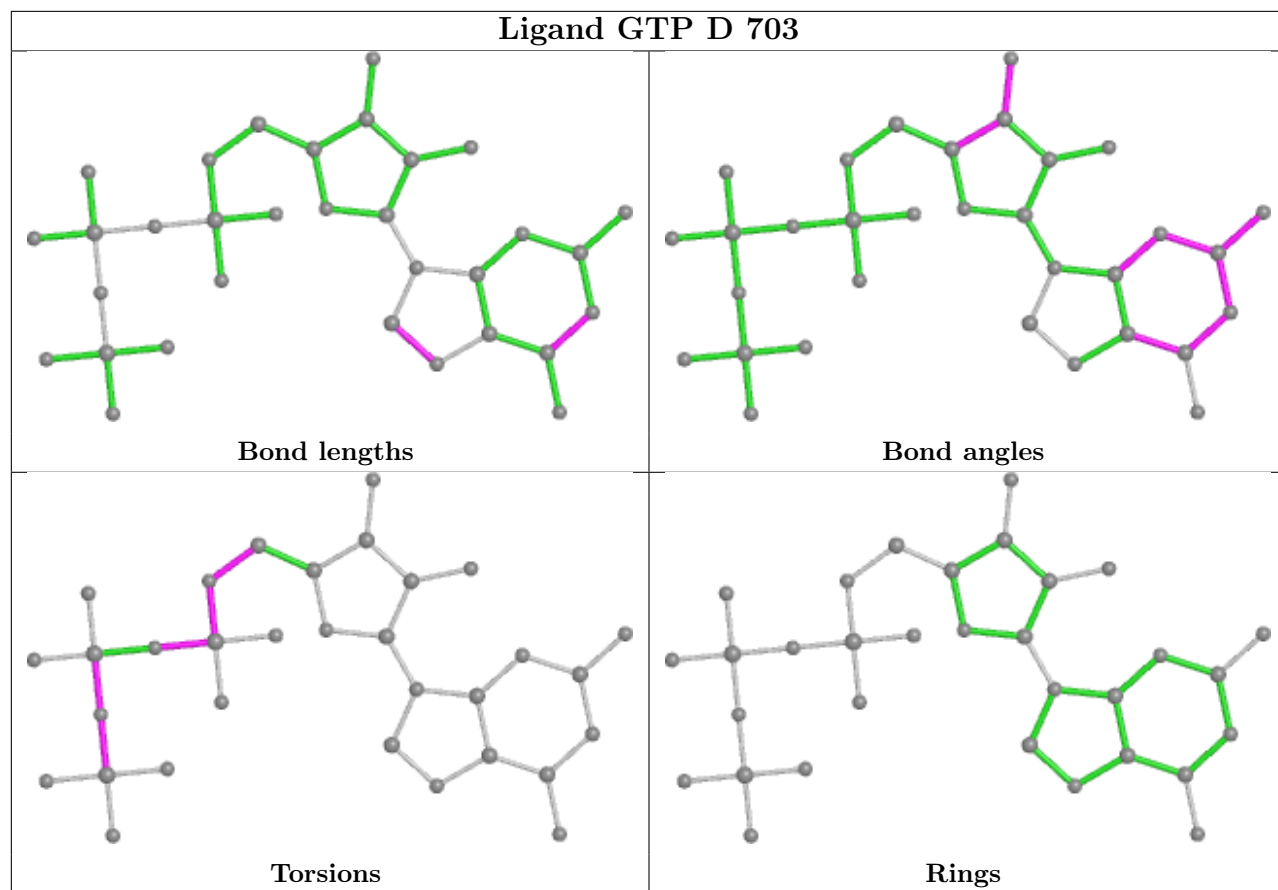


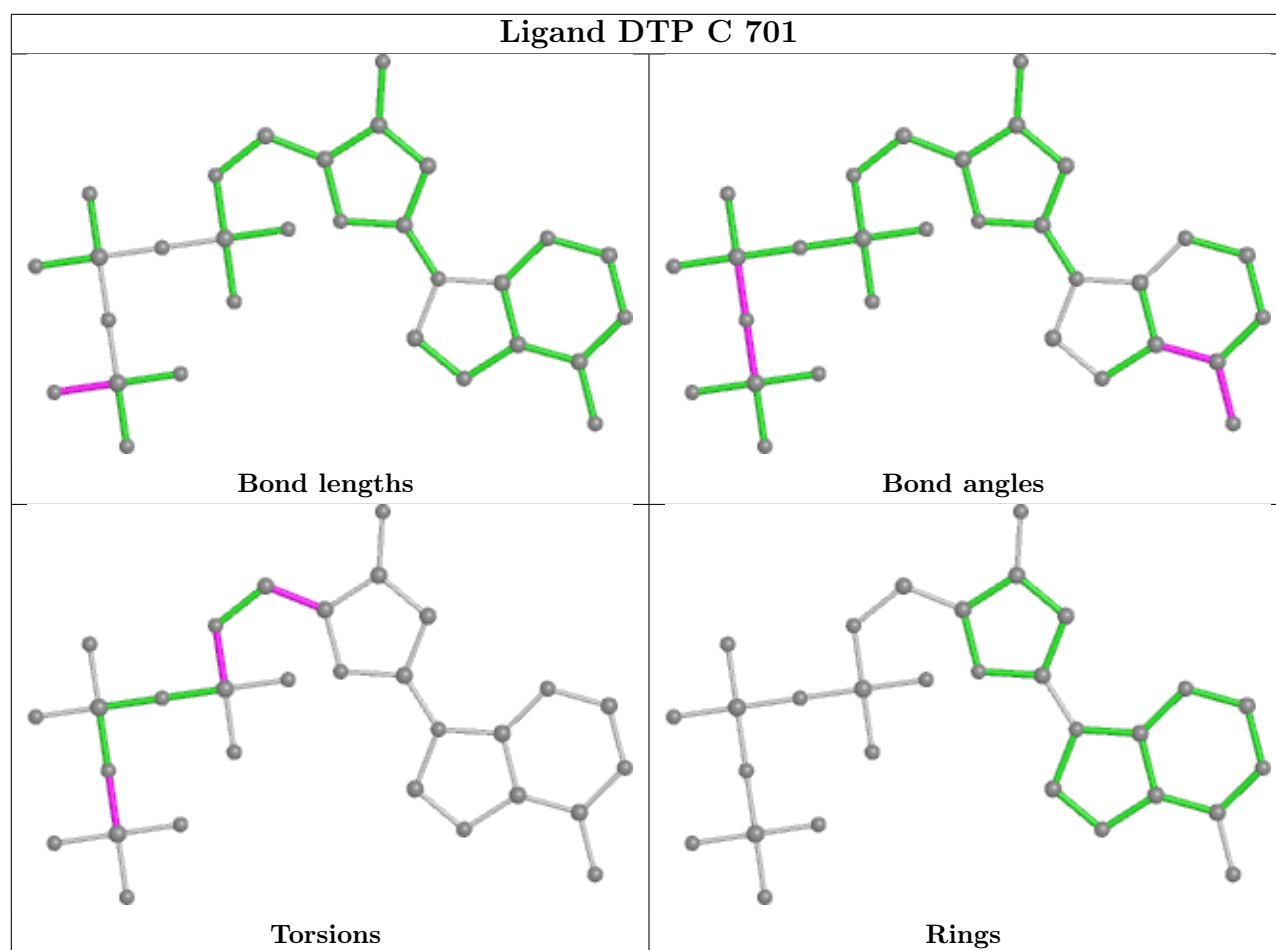
Ligand DTP B 703

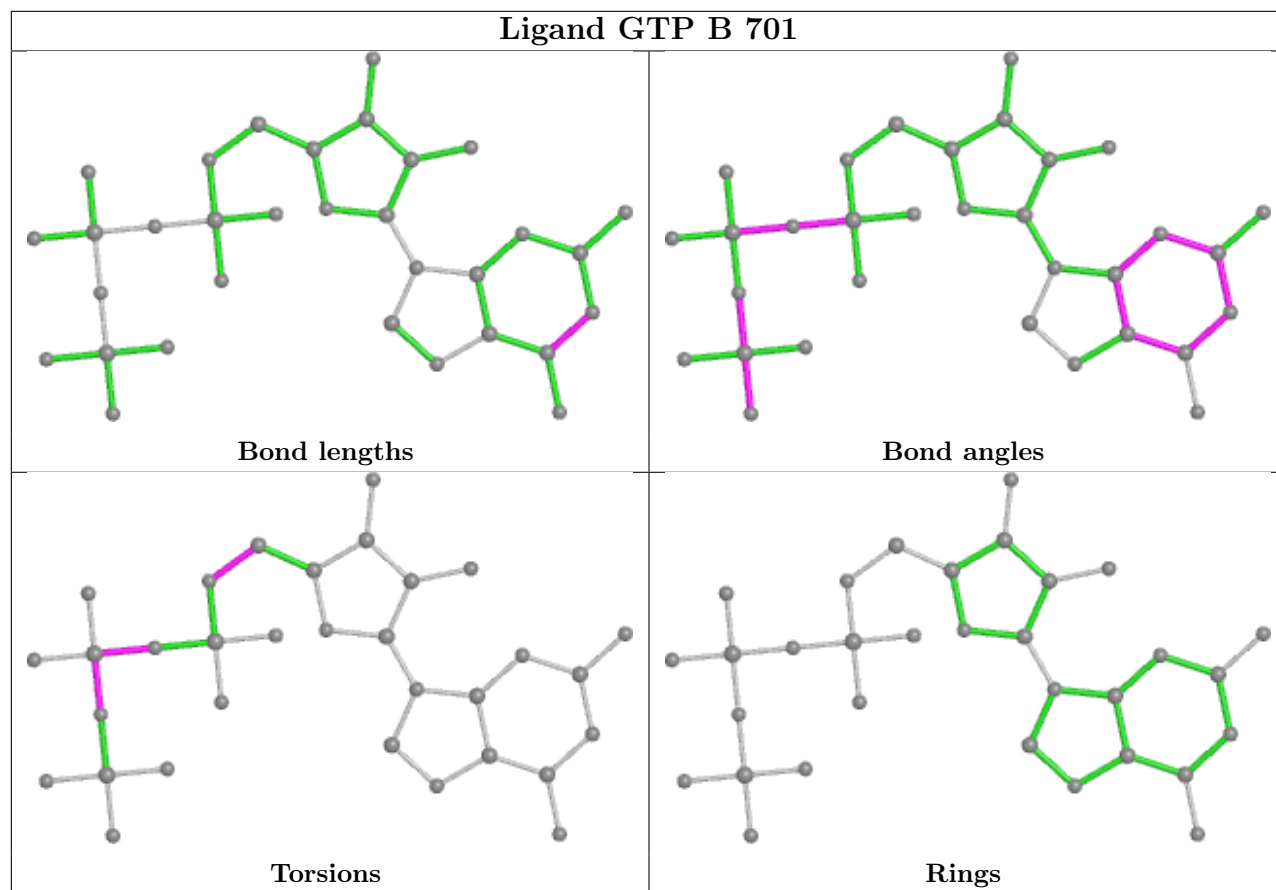


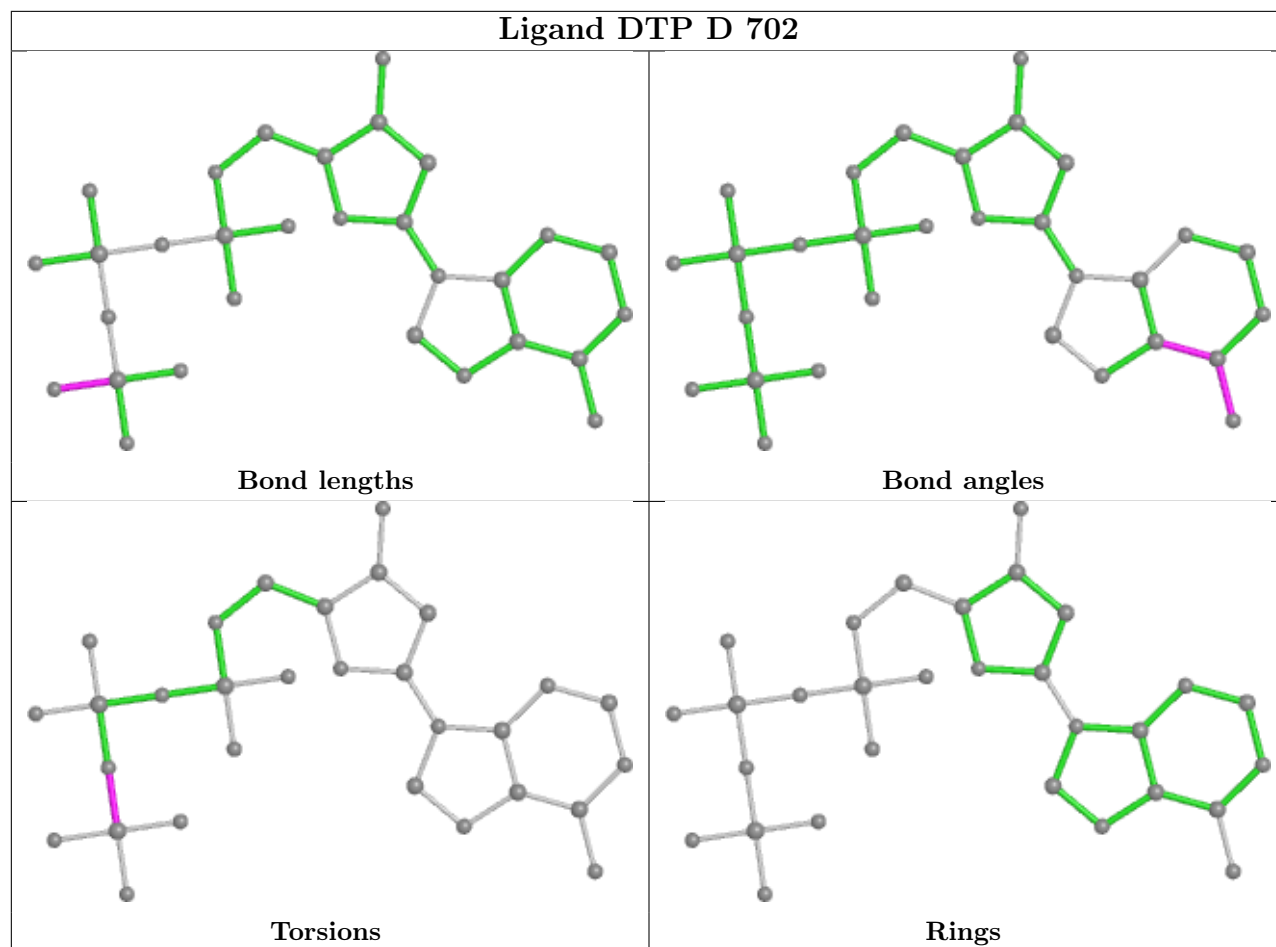
Ligand 85T D 704



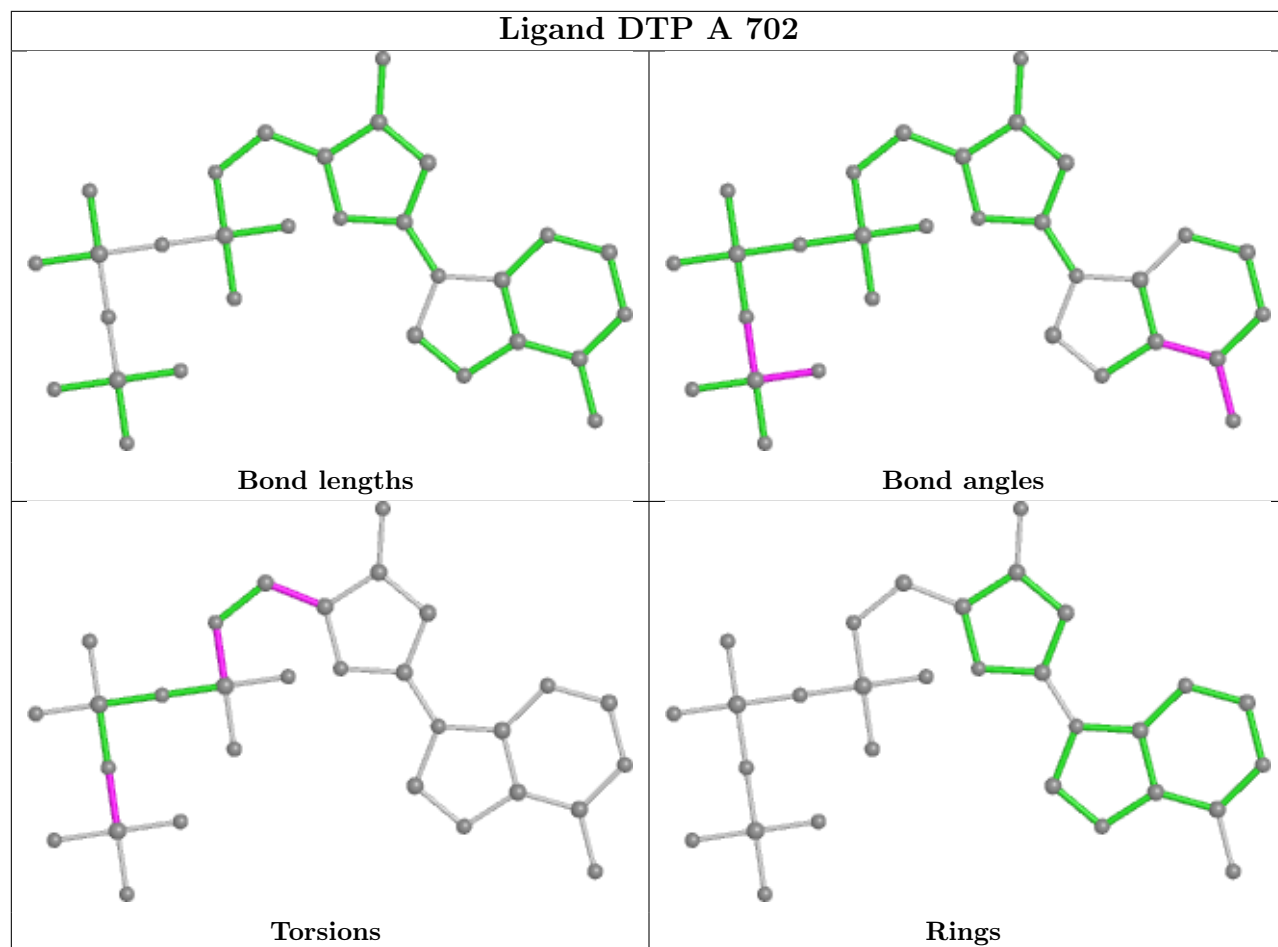




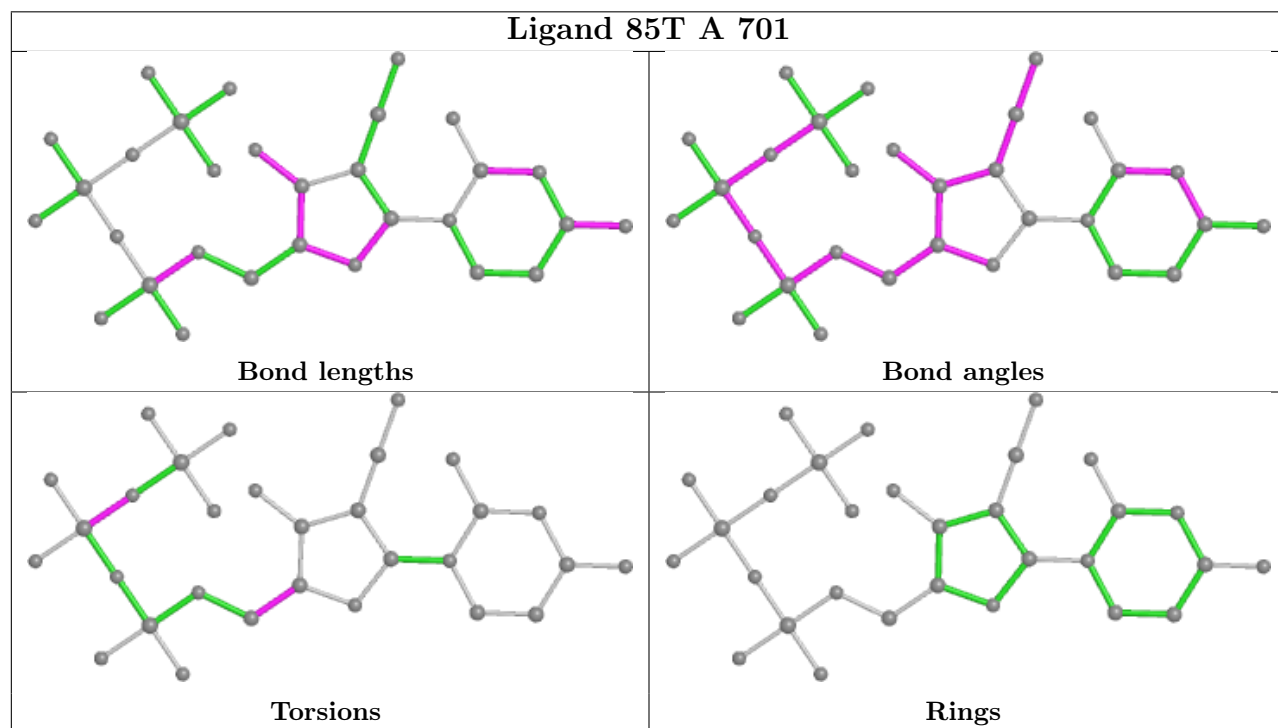




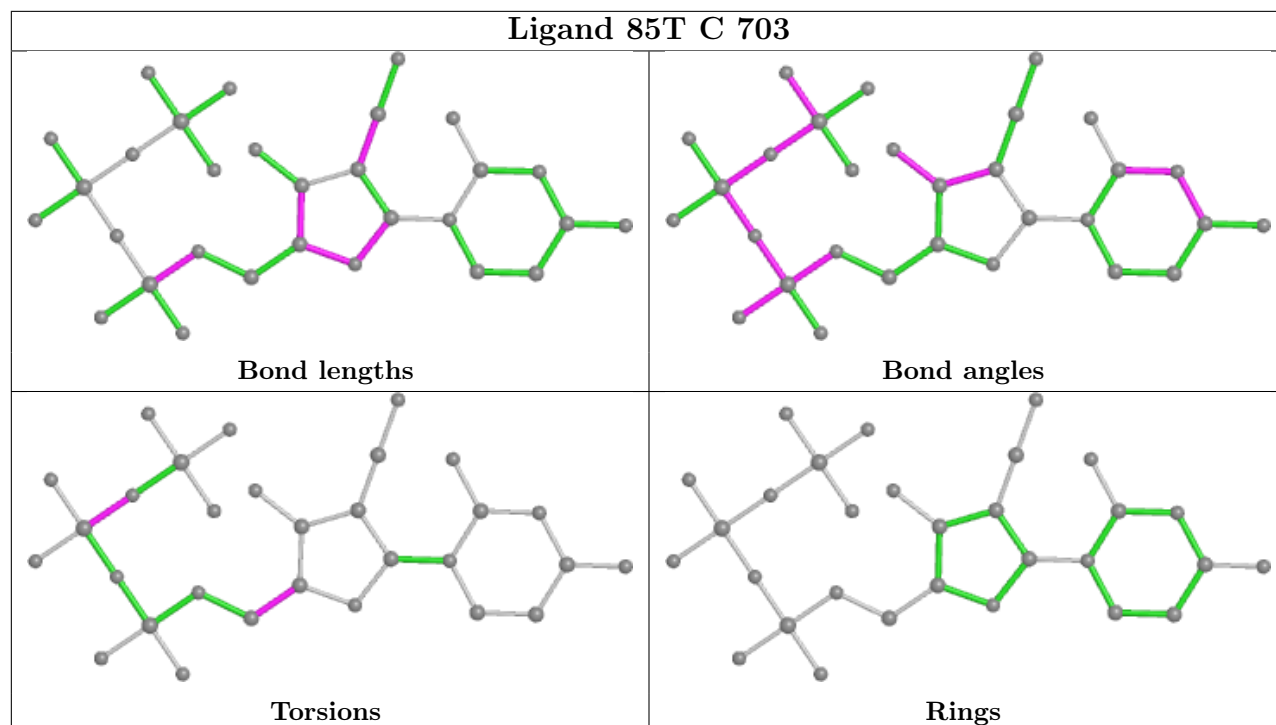
Ligand DTP A 702



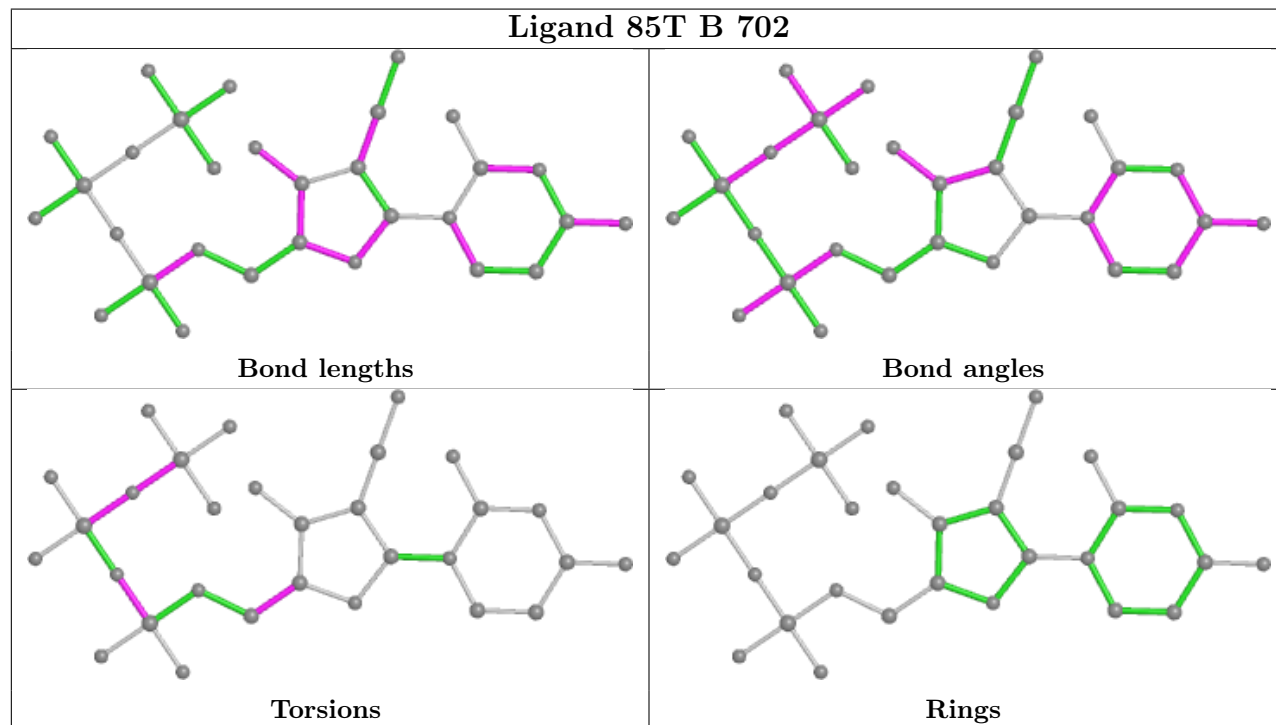
Ligand 85T A 701

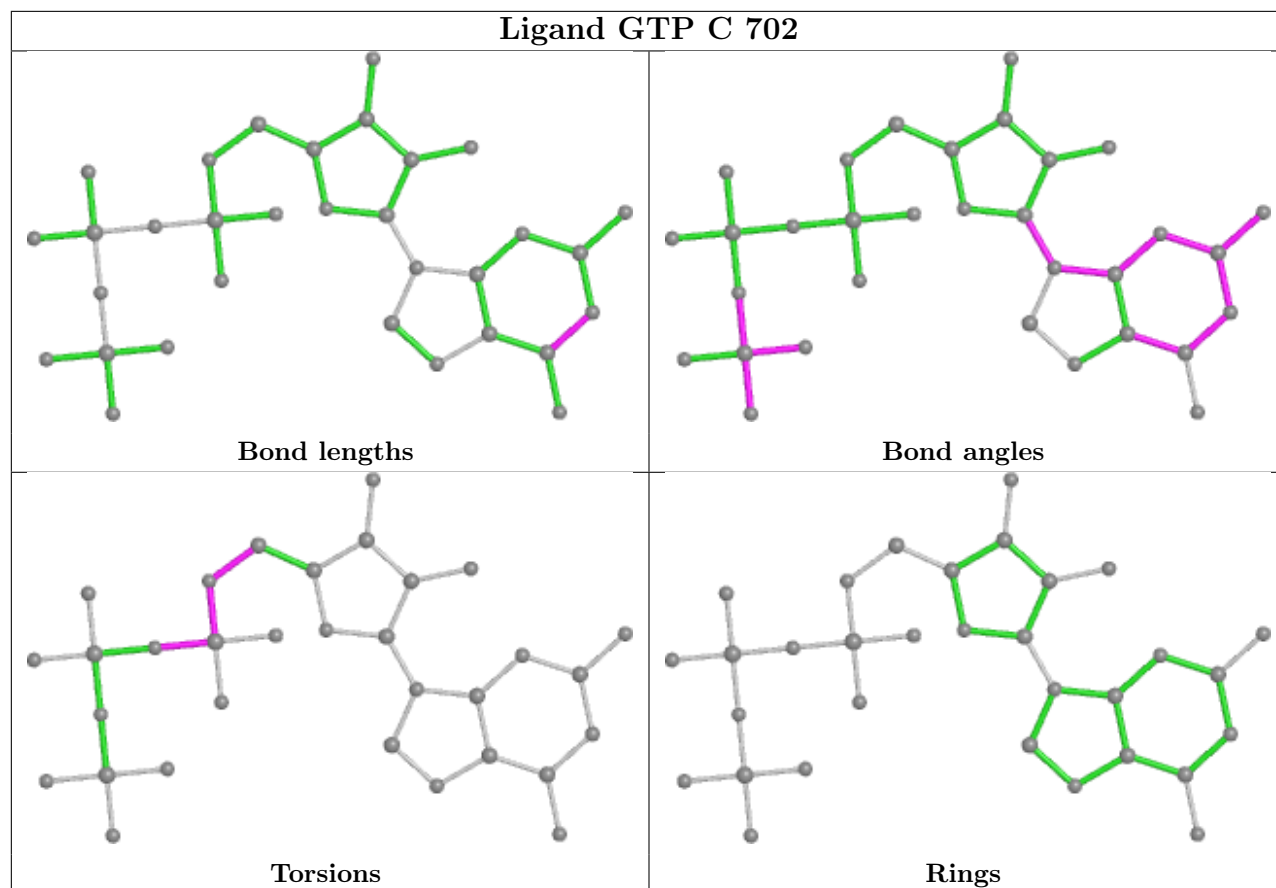


Ligand 85T C 703



Ligand 85T B 702





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	481/550 (87%)	-0.24	16 (3%)	46 36	34, 67, 132, 164	0
1	B	481/550 (87%)	-0.30	13 (2%)	54 44	32, 67, 126, 167	0
1	C	481/550 (87%)	-0.39	8 (1%)	70 63	35, 66, 109, 148	0
1	D	481/550 (87%)	-0.45	5 (1%)	82 77	31, 59, 95, 172	0
All	All	1924/2200 (87%)	-0.35	42 (2%)	62 52	31, 64, 120, 172	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	113	ASP	7.2
1	B	465	GLN	5.7
1	A	592	THR	5.4
1	B	490	ASP	5.1
1	B	276	LEU	4.8
1	C	490	ASP	4.5
1	A	598	TRP	4.3
1	C	488	LEU	4.1
1	A	599	ASN	4.0
1	C	276	LEU	3.8
1	B	488	LEU	3.7
1	C	113	ASP	3.3
1	D	277	GLU	3.2
1	D	113	ASP	3.2
1	B	491	VAL	3.1
1	A	488	LEU	3.0
1	A	276	LEU	3.0
1	B	594	GLN	3.0
1	A	562	LEU	2.9
1	A	489	LEU	2.8
1	B	592	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	490	ASP	2.8
1	B	277	GLU	2.7
1	A	591	ILE	2.6
1	B	591	ILE	2.6
1	B	596	LYS	2.5
1	A	473	TYR	2.4
1	B	599	ASN	2.4
1	A	594	GLN	2.3
1	A	585	ASP	2.3
1	A	586	VAL	2.3
1	C	403	GLY	2.2
1	C	489	LEU	2.2
1	A	557	VAL	2.2
1	D	597	GLU	2.2
1	D	465	GLN	2.1
1	D	599	ASN	2.1
1	C	326	GLN	2.1
1	C	491	VAL	2.1
1	B	486	LYS	2.1
1	B	489	LEU	2.0
1	A	468	ILE	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	D	705	1/1	0.95	0.11	33,33,33,33	0
4	MG	C	705	1/1	0.96	0.12	30,30,30,30	0

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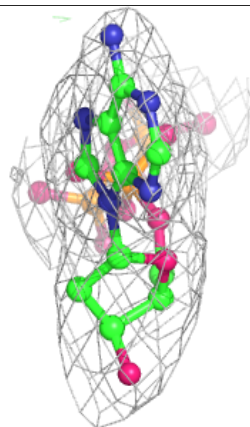
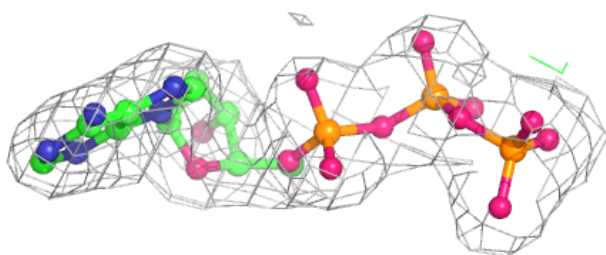
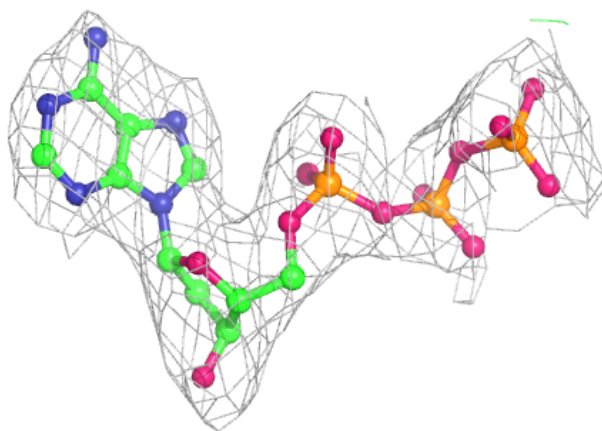
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	C	704	1/1	0.96	0.19	27,27,27,27	0
4	MG	B	705	1/1	0.97	0.14	31,31,31,31	0
4	MG	A	703	1/1	0.97	0.14	38,38,38,38	0
3	DTP	B	703	30/30	0.98	0.12	33,39,45,46	0
3	DTP	D	702	30/30	0.98	0.15	35,41,50,51	0
2	85T	A	701	30/30	0.98	0.12	42,47,55,57	0
4	MG	B	704	1/1	0.98	0.07	46,46,46,46	0
2	85T	B	702	30/30	0.98	0.14	43,53,59,67	0
2	85T	C	703	30/30	0.98	0.16	45,53,61,66	0
2	85T	D	704	30/30	0.98	0.14	46,52,57,65	0
4	MG	C	706	1/1	0.98	0.24	37,37,37,37	0
3	DTP	A	702	30/30	0.98	0.12	36,42,45,47	0
5	GTP	B	701	32/32	0.98	0.14	42,50,55,57	0
5	GTP	C	702	32/32	0.98	0.11	37,43,47,50	0
5	GTP	D	701	32/32	0.98	0.13	43,47,50,53	0
5	GTP	D	703	32/32	0.98	0.13	37,42,48,50	0
3	DTP	C	701	30/30	0.99	0.14	35,39,43,44	0
4	MG	A	704	1/1	0.99	0.18	56,56,56,56	0

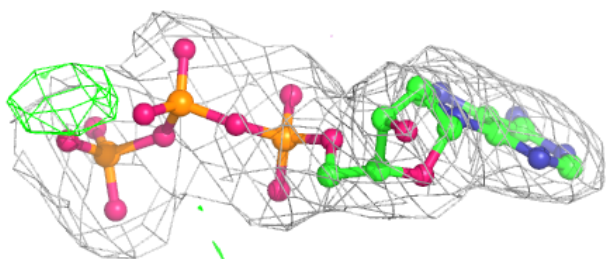
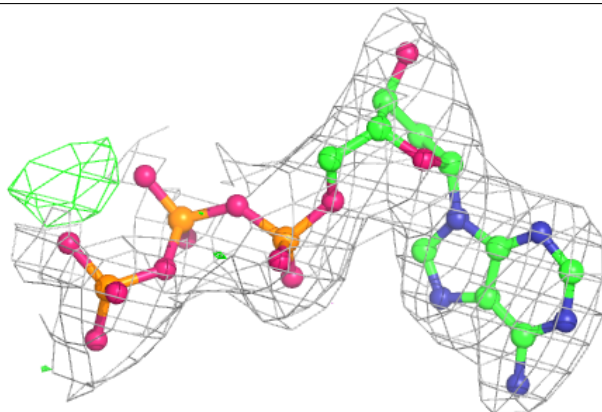
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

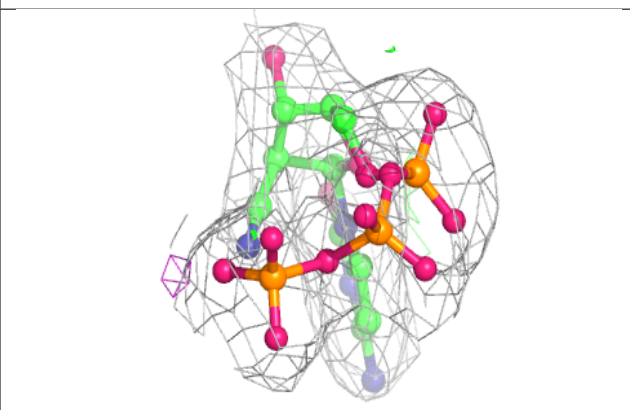
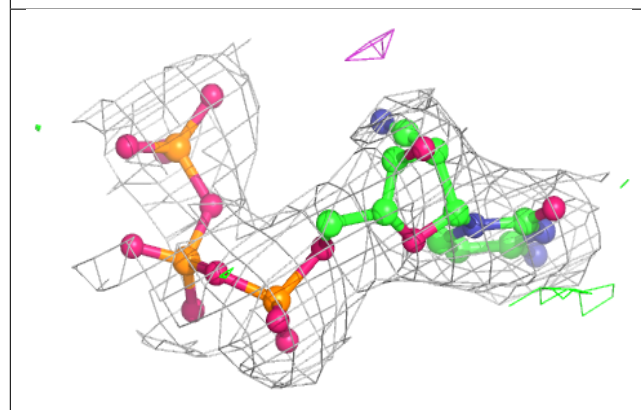
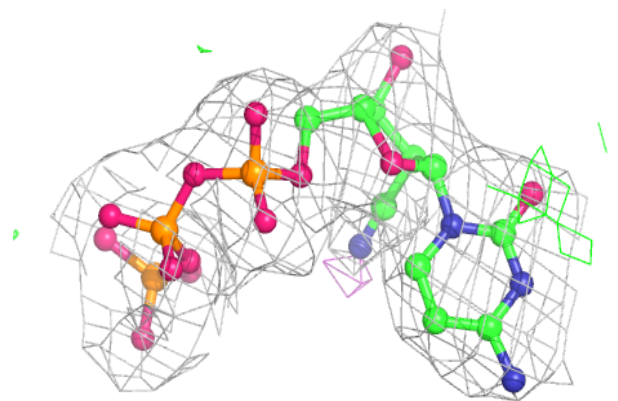
**Electron density around DTP D 702:**

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

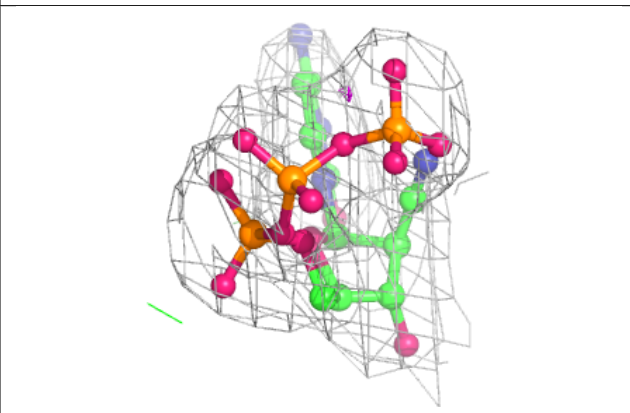
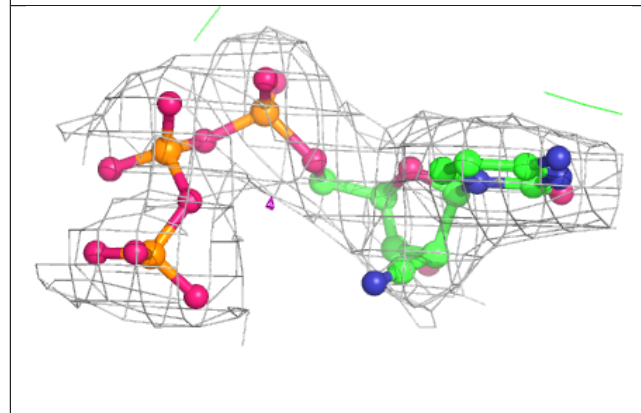
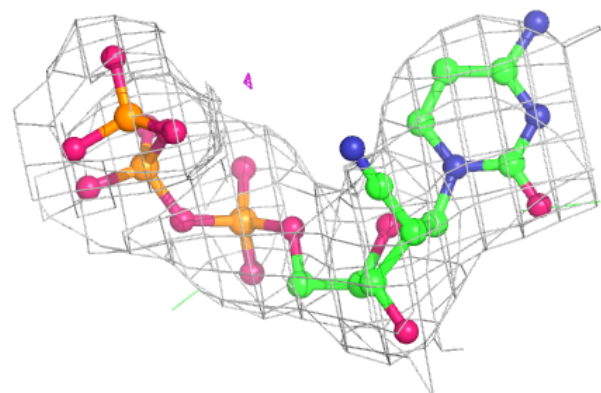


Electron density around 85T A 701:

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

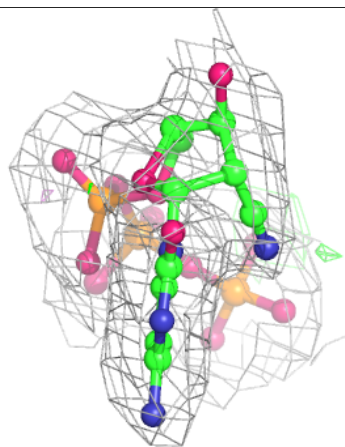
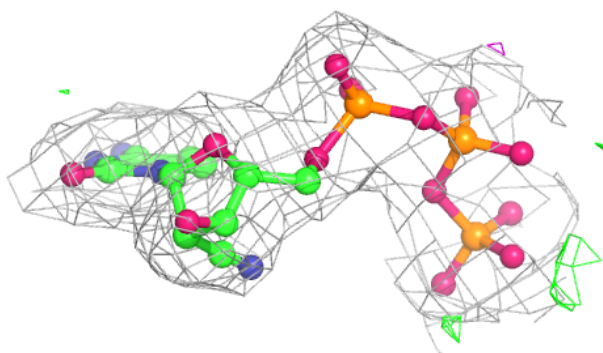
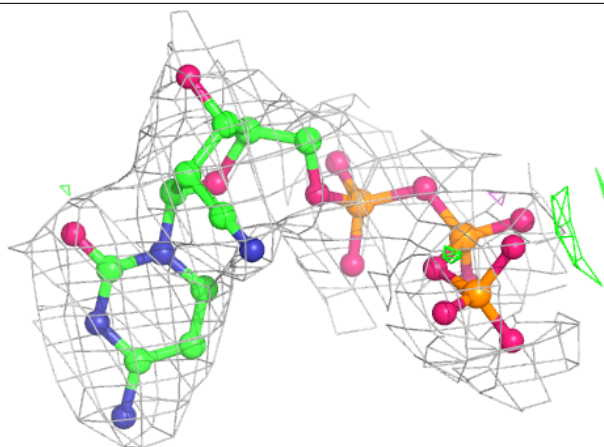
**Electron density around 85T B 702:**

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

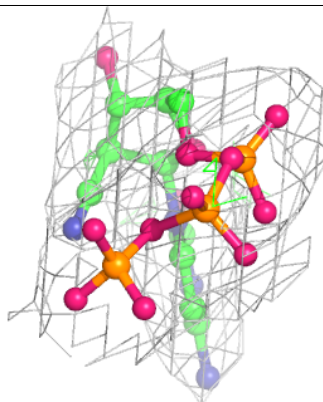
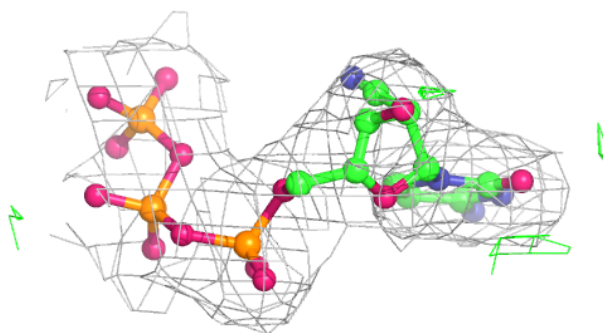
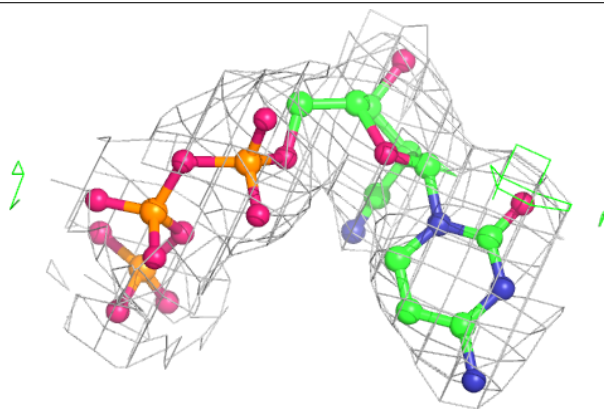


Electron density around 85T C 703:

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

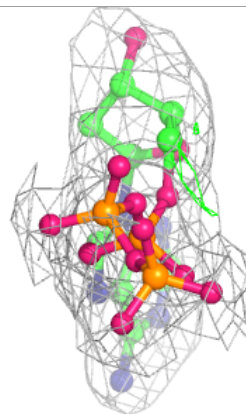
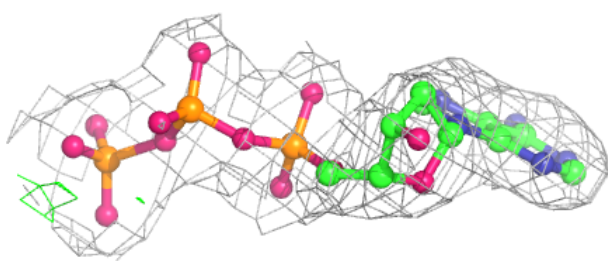
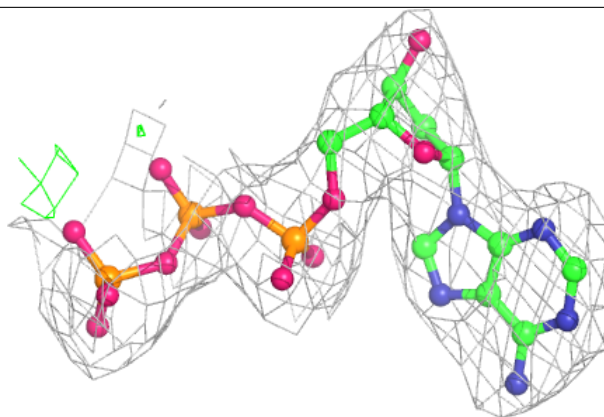
**Electron density around 85T D 704:**

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

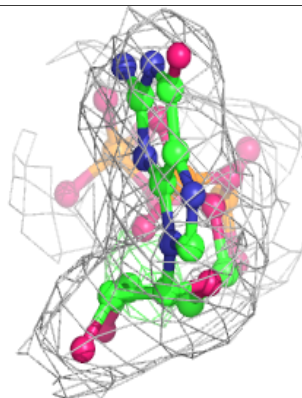
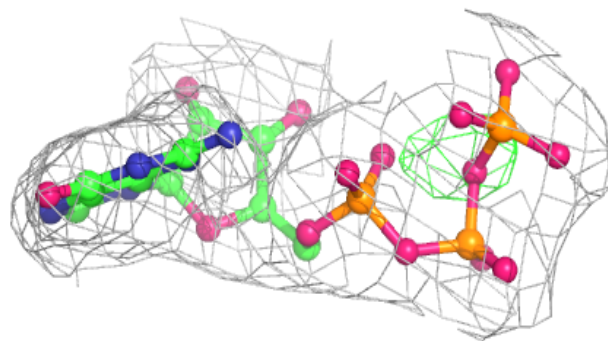
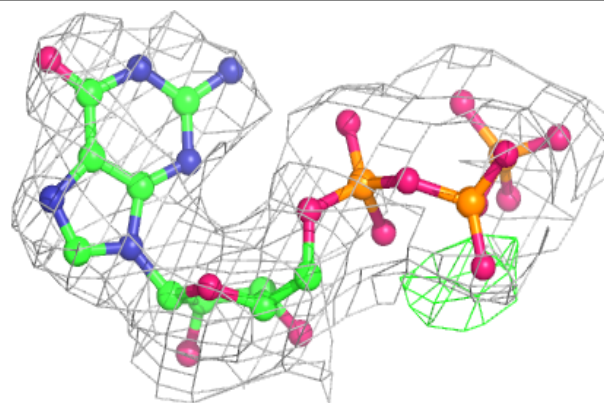


Electron density around DTP A 702:

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

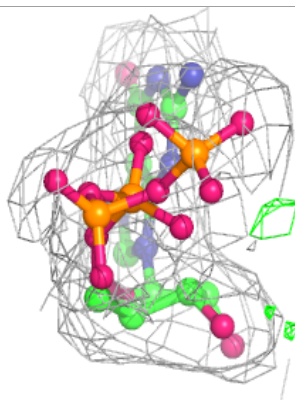
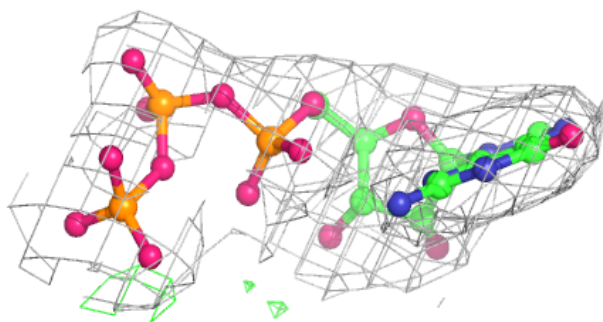
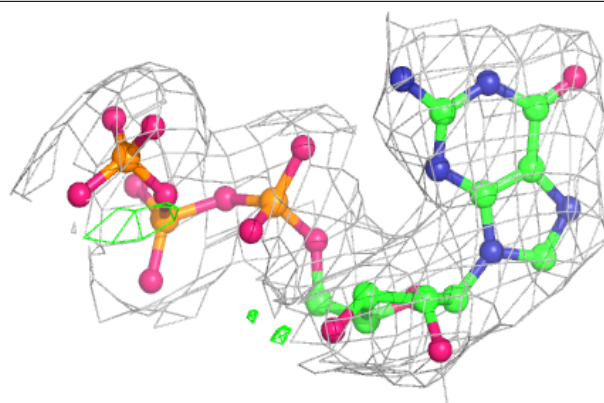
**Electron density around GTP B 701:**

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

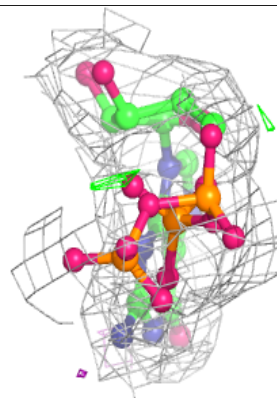
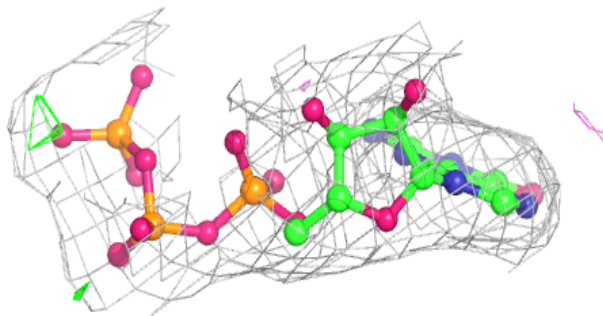
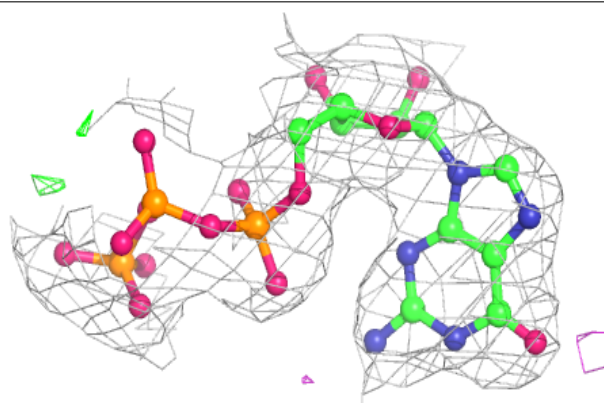


Electron density around GTP C 702:

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

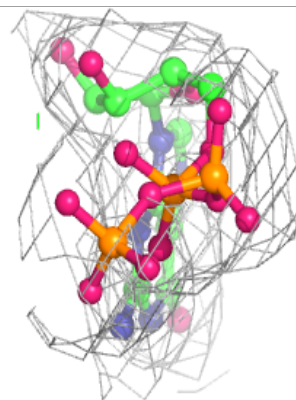
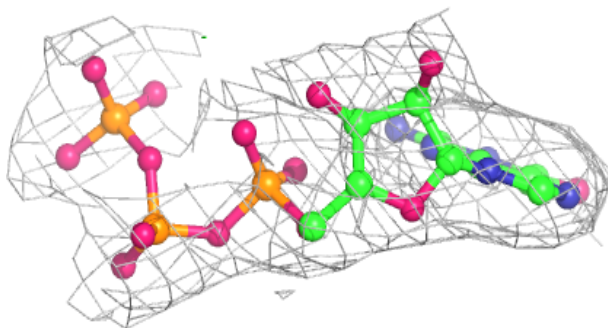
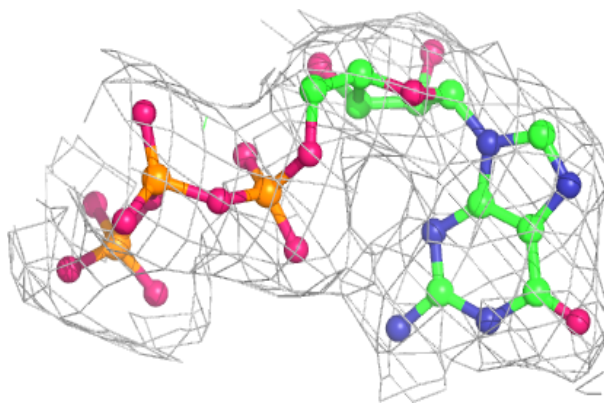
**Electron density around GTP D 701:**

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

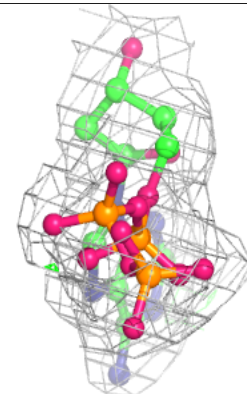
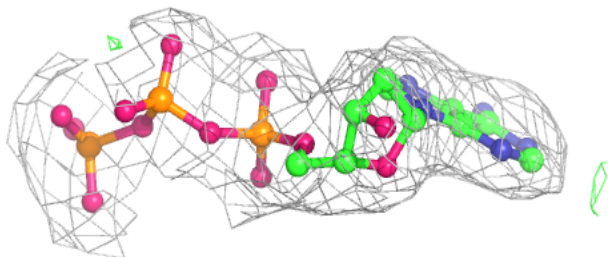
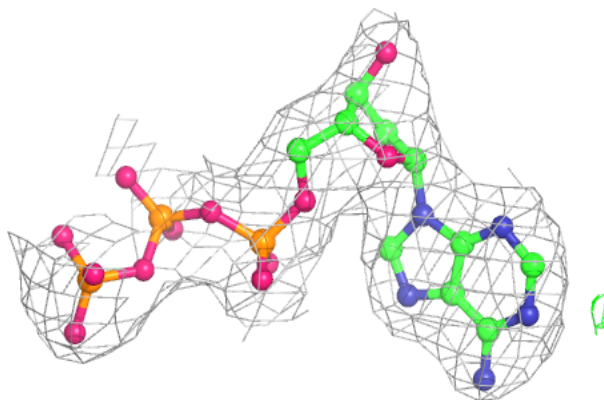


Electron density around GTP D 703:

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

**Electron density around DTP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.