wwPDB X-ray Structure Validation Summary Report (i)

Sep 17, 2023 – 07:11 AM EDT

PDB ID	:	4TNX
Title	:	Structure basis of cellular dNTP regulation, SAMHD1-GTP-dGTP complex
Authors	:	Ji, X.; Tang, C.; Zhao, Q.; Wang, W.; Xiong, Y.
Deposited on	:	2014-06-05
Resolution	:	2.31 Å(reported)

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

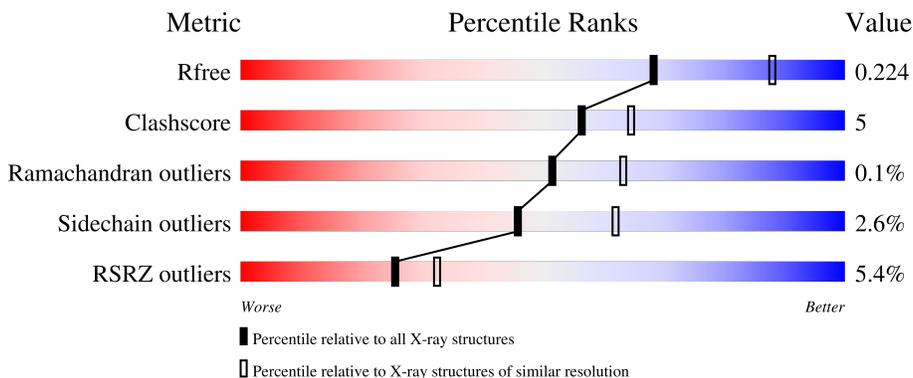|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.31 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	Percentile Ranks	Value
Rfree		0.224
Clashscore		5
Ramachandran outliers		0.1%
Sidechain outliers		2.6%
RSRZ outliers		5.4%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	514	2% / 82% 10% · 6%
1	B	514	5% / 84% 8% · 7%
1	C	514	10% / 84% 9% · 6%
1	D	514	4% / 84% 10% · 6%

2   Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 16322 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 3956	C 2529	N 689	O 717	S 21	0	3	0
1	B	479	Total 3940	C 2521	N 686	O 712	S 21	0	3	0
1	C	481	Total 3947	C 2524	N 688	O 714	S 21	0	2	0
1	D	483	Total 3961	C 2531	N 690	O 719	S 21	0	2	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
A	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
B	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
B	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
C	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
C	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
D	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
D	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3

- Molecule 2 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

DGT

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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

GTP

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

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

- Molecule 5 is TRIPHOSPHATE (three-letter code: 3PO) (formula: $H_5O_{10}P_3$).
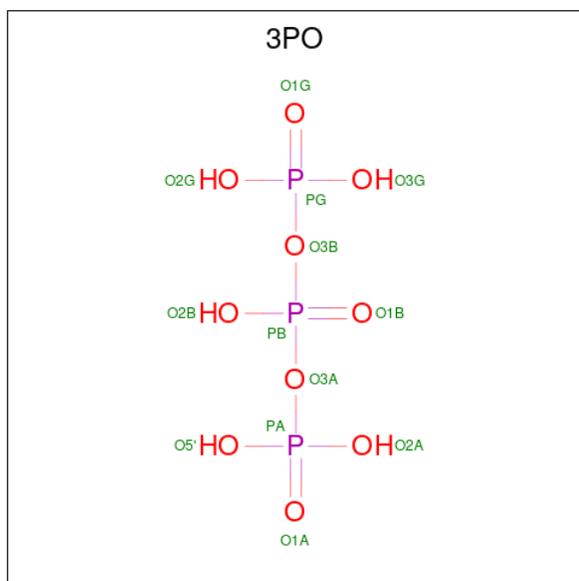
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			13	10	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	80	Total 80	O 80	0	0
6	B	49	Total 49	O 49	0	0
6	C	47	Total 47	O 47	0	0
6	D	73	Total 73	O 73	0	0

3 Residue-property plots ⓘ

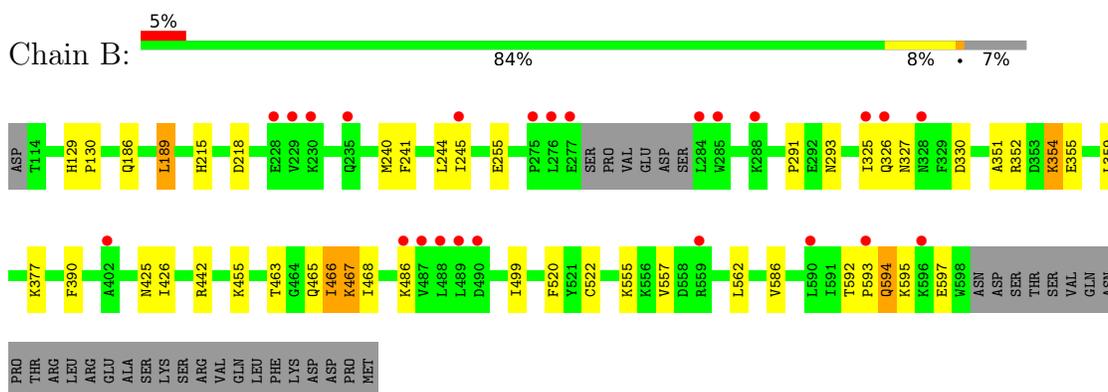These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.
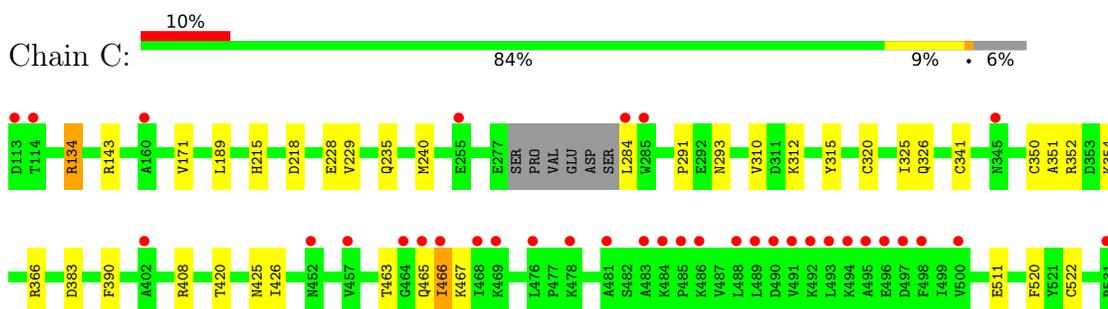
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1
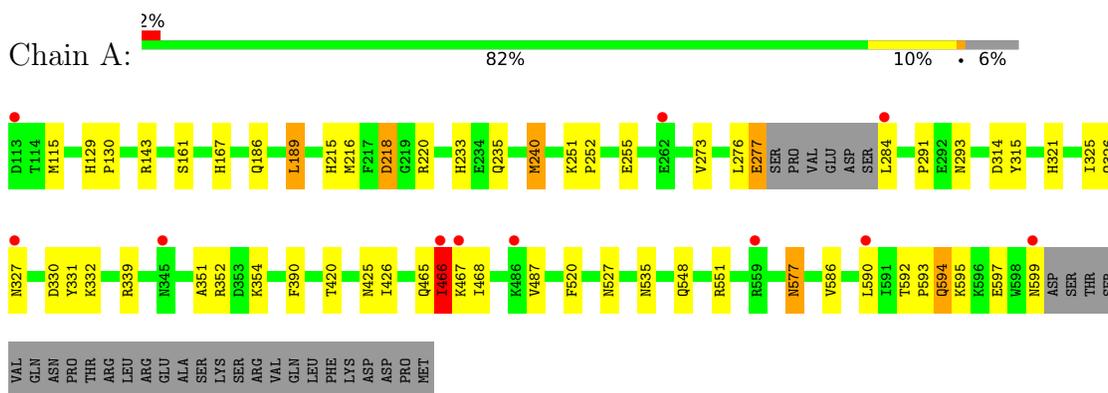
Chain A:

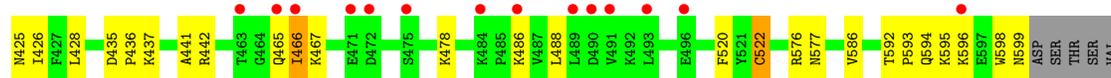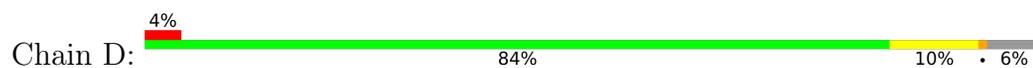• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain B:

• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain C:

K534 R551 C554 K555 K556 V557 D558 S561 L562 Y563 Y568 F569 V570 A588 P589 L590 I591 T592 P593 Q594 K595 K596 E597 W598 N599 ASP SER THR SER VAL GLN ASN PRO THR ARG LEU ARG GLU ALA SER LYS SER ARG VAL GLN LEU PHE LYS ASP ASP PRO MET

• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain D:

4%

84% 10% • 6%

D113 T114 M115 L128 H129 P130 Q186 L189 R206 D218 M240 K251 P252 E255 V273 E277 SER PRO VAL GLU D282 S283 L284 P291 E292 N293 H321 H322 I325 Q326 N327 N328 N345 A351 R352 D353 K354 E355 F390 L391 K392 Y396

N425 I426 F427 L428 D435 P436 K437 A441 R442 T463 G464 Q465 I466 K467 E471 D472 S475 K478 K484 P485 K486 V487 L488 L489 D490 V491 K492 L493 E496 F520 Y521 C522 R576 N577 V586 T592 P593 Q594 K595 K596 E597 W598 N599 ASP SER THR SER VAL

GLN ASN PRO THR ARG LEU ARG GLU ALA SER LYS SER ARG VAL GLN LEU PHE LYS ASP ASP PRO MET

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	80.89Å 140.73Å 97.60Å 90.00° 114.71° 90.00°	Depositor
Resolution (Å)	50.00 – 2.31 47.82 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.31) 99.2 (47.82-2.31)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.188 , 0.226 0.192 , 0.224	Depositor DCC
R_{free} test set	4335 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	40.8	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.6	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16322	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: GTP, DGT, 3PO, MG

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	0.76	1/4048 (0.0%)	0.81	5/5464 (0.1%)
1	B	0.69	1/4032 (0.0%)	0.77	4/5442 (0.1%)
1	C	0.65	0/4039	0.76	5/5452 (0.1%)
1	D	0.76	1/4053 (0.0%)	0.82	7/5471 (0.1%)
All	All	0.72	3/16172 (0.0%)	0.79	21/21829 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	355	GLU	CD-OE2	6.14	1.32	1.25
1	A	161	SER	CB-OG	5.90	1.50	1.42
1	D	355	GLU	CD-OE1	5.41	1.31	1.25

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	MET	CG-SD-CE	-8.38	86.80	100.20
1	A	551	ARG	NE-CZ-NH2	6.96	123.78	120.30
1	D	218	ASP	CB-CG-OD2	6.76	124.39	118.30
1	A	218	ASP	CB-CG-OD2	6.55	124.19	118.30
1	B	330	ASP	CB-CG-OD2	-6.45	112.49	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3956	0	3935	56	0
1	B	3940	0	3925	35	0
1	C	3947	0	3930	34	0
1	D	3961	0	3939	47	0
2	A	31	0	12	4	0
2	B	31	0	12	1	0
2	C	31	0	12	1	0
2	D	31	0	12	2	0
3	A	64	0	24	0	0
3	B	32	0	12	0	0
3	C	32	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
5	A	13	0	0	1	0
6	A	80	0	0	4	0
6	B	49	0	0	0	0
6	C	47	0	0	2	0
6	D	73	0	0	6	0
All	All	16322	0	15825	158	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 5.

The worst 5 of 158 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:577:ASN:ND2	1:D:595:LYS:HZ1	1.60	1.00
1:D:596:LYS:HB3	6:D:907:HOH:O	1.63	0.98
1:A:597:GLU:OE1	1:A:597:GLU:N	1.97	0.96
1:A:216:MET:HA	6:A:869:HOH:O	1.67	0.94
1:D:577:ASN:ND2	1:D:595:LYS:NZ	2.19	0.89

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	480/514 (93%)	474 (99%)	5 (1%)	1 (0%)	47	58
1	B	478/514 (93%)	470 (98%)	8 (2%)	0	100	100
1	C	479/514 (93%)	474 (99%)	5 (1%)	0	100	100
1	D	481/514 (94%)	474 (98%)	7 (2%)	0	100	100
All	All	1918/2056 (93%)	1892 (99%)	25 (1%)	1 (0%)	51	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	466	ILE

5.3.2 Protein sidechains ⓘ

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	430/459 (94%)	419 (97%)	11 (3%)	46	62
1	B	428/459 (93%)	419 (98%)	9 (2%)	53	70
1	C	429/459 (94%)	417 (97%)	12 (3%)	43	59
1	D	431/459 (94%)	418 (97%)	13 (3%)	41	56
All	All	1718/1836 (94%)	1673 (97%)	45 (3%)	46	62

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	467	LYS
1	D	273	VAL
1	C	511	GLU
1	D	189	LEU
1	D	283	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	322	HIS
1	D	577	ASN
1	A	577	ASN
1	B	425	ASN
1	C	322	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	3PO	A	705	-	8,12,12	0.65	0	15,20,20	1.49	4 (26%)
3	GTP	A	702	4	26,34,34	0.94	2 (7%)	32,54,54	1.19	4 (12%)
2	DGT	B	703	4	26,33,33	1.25	2 (7%)	32,52,52	1.35	5 (15%)
2	DGT	A	701	4	26,33,33	0.98	2 (7%)	32,52,52	1.46	4 (12%)
2	DGT	C	703	4	26,33,33	0.73	0	32,52,52	1.71	7 (21%)
3	GTP	A	704	4	26,34,34	1.10	3 (11%)	32,54,54	1.53	7 (21%)
3	GTP	B	701	4	26,34,34	1.09	3 (11%)	32,54,54	1.63	7 (21%)
2	DGT	D	800	4	26,33,33	1.12	1 (3%)	32,52,52	1.46	6 (18%)
3	GTP	C	704	4	26,34,34	0.78	0	32,54,54	1.67	7 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	3PO	A	705	-	-	2/12/12/12	-
3	GTP	A	702	4	-	2/18/38/38	0/3/3/3
2	DGT	B	703	4	-	4/18/34/34	0/3/3/3
2	DGT	A	701	4	-	2/18/34/34	0/3/3/3
2	DGT	C	703	4	-	3/18/34/34	0/3/3/3
3	GTP	A	704	4	-	7/18/38/38	0/3/3/3
3	GTP	B	701	4	-	2/18/38/38	0/3/3/3
2	DGT	D	800	4	-	2/18/34/34	0/3/3/3
3	GTP	C	704	4	-	5/18/38/38	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	800	DGT	C6-N1	-3.66	1.32	1.37
2	B	703	DGT	C6-N1	-3.25	1.33	1.37
3	B	701	GTP	O4'-C1'	2.66	1.44	1.41
2	B	703	DGT	C2-N1	-2.56	1.31	1.37
3	A	702	GTP	C5-C4	2.50	1.49	1.43

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	704	GTP	C3'-C2'-C1'	4.42	107.63	100.98
3	B	701	GTP	PA-O3A-PB	-3.82	119.71	132.83
2	C	703	DGT	O6-C6-C5	-3.77	117.01	124.37
3	B	701	GTP	C3'-C2'-C1'	3.72	106.58	100.98
2	A	701	DGT	N2-C2-N3	-3.64	112.65	119.74

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	DGT	PB-O3B-PG-O1G
2	C	703	DGT	PB-O3B-PG-O1G
2	D	800	DGT	PB-O3B-PG-O1G
3	A	704	GTP	PB-O3B-PG-O2G
3	A	704	GTP	PB-O3B-PG-O3G

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	705	3PO	1	0
2	B	703	DGT	1	0
2	A	701	DGT	4	0
2	C	703	DGT	1	0
2	D	800	DGT	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 3PO A 705

Bond lengths

Bond angles

Torsions

Rings

Ligand GTP A 702

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT B 703

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT A 701

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT C 703

Bond lengths

Bond angles

Torsions

Rings

Ligand GTP A 704

Bond lengths

Bond angles

Torsions

Rings

Ligand GTP B 701

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT D 800

Bond lengths

Bond angles

Torsions

Rings

Ligand GTP C 704

Bond lengths

Bond angles

Torsions

Rings

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, 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(Å²)	Q<0.9
1	A	481/514 (93%)	-0.01	11 (2%)	60	67	27, 44, 71, 98	0
1	B	479/514 (93%)	0.18	24 (5%)	28	36	32, 54, 86, 113	0
1	C	481/514 (93%)	0.42	49 (10%)	6	10	32, 55, 101, 129	0
1	D	483/514 (93%)	0.06	20 (4%)	37	44	28, 45, 86, 112	0
All	All	1924/2056 (93%)	0.17	104 (5%)	25	32	27, 50, 88, 129	0

The worst 5 of 104 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	488	LEU	6.7
1	A	466	ILE	6.4
1	C	490	ASP	6.4
1	C	493	LEU	6.3
1	C	485	PRO	6.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	3PO	A	705	13/13	0.88	0.21	62,89,154,155	0
4	MG	C	702	1/1	0.93	0.06	49,49,49,49	0
4	MG	B	702	1/1	0.93	0.10	49,49,49,49	0
4	MG	A	703	1/1	0.96	0.10	34,34,34,34	0
3	GTP	A	704	32/32	0.98	0.10	29,30,32,32	0
3	GTP	B	701	32/32	0.98	0.09	37,40,44,45	0
3	GTP	C	704	32/32	0.98	0.10	36,43,49,50	0
2	DGT	A	701	31/31	0.98	0.13	31,34,38,39	0
2	DGT	B	703	31/31	0.98	0.14	29,30,34,36	0
4	MG	C	701	1/1	0.98	0.07	43,43,43,43	0
2	DGT	C	703	31/31	0.98	0.13	37,40,48,49	0
2	DGT	D	800	31/31	0.98	0.13	34,36,38,38	0
3	GTP	A	702	32/32	0.99	0.10	30,31,34,35	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 3PO A 705:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
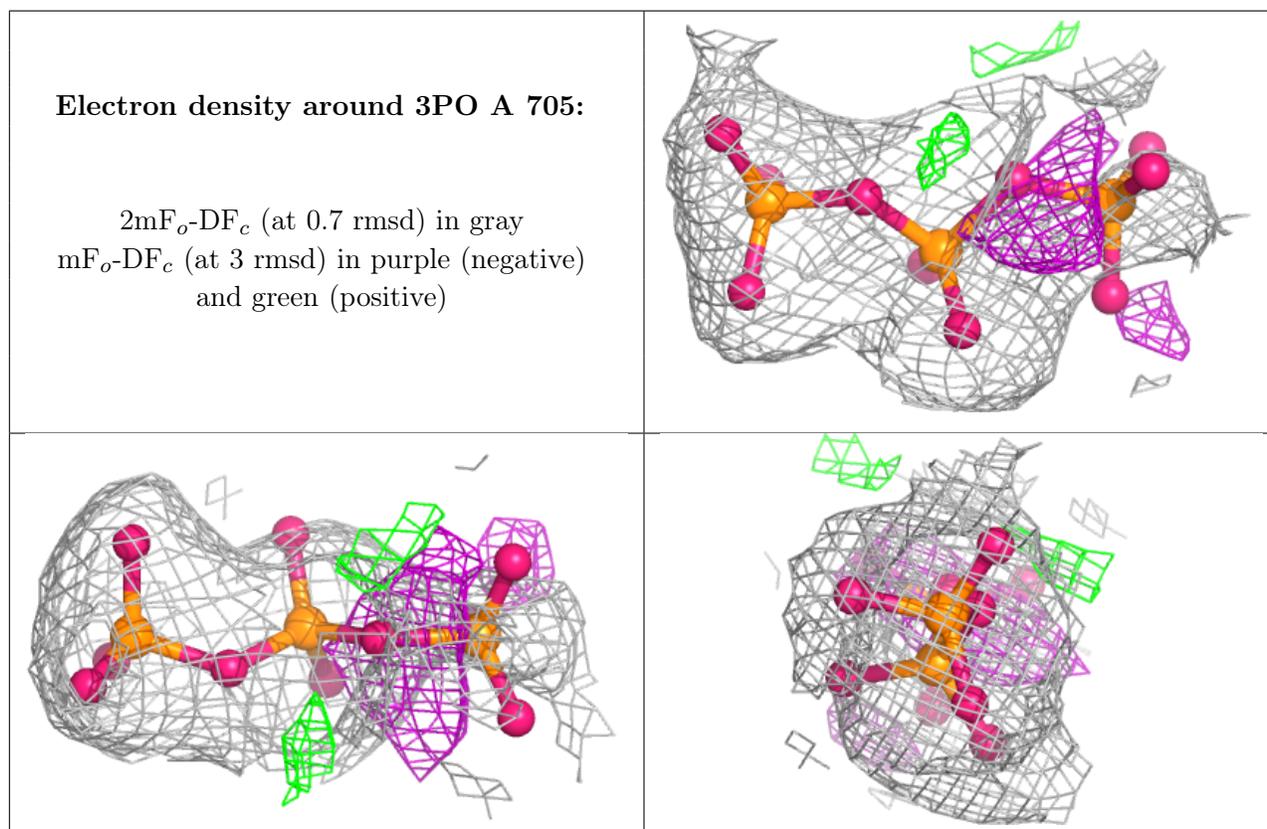
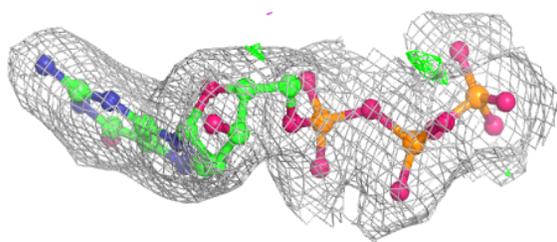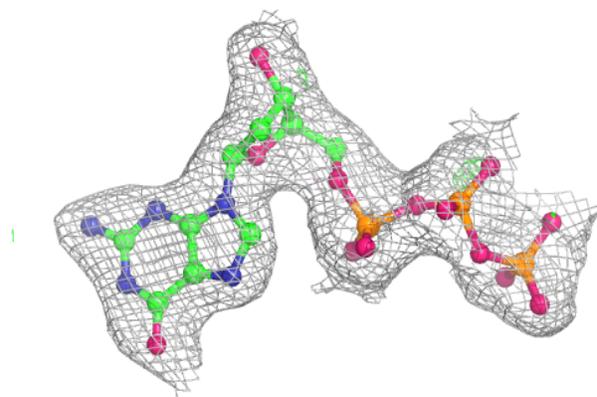**Electron density around GTP A 704:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
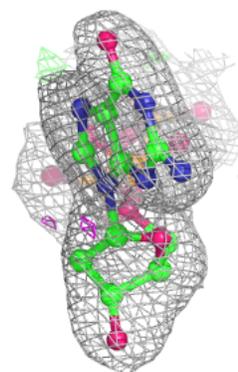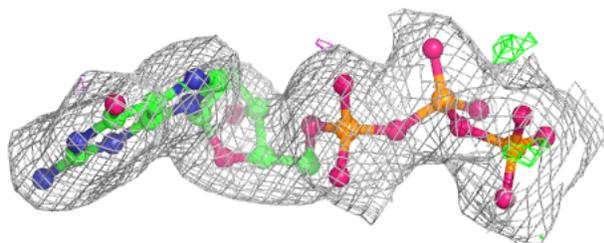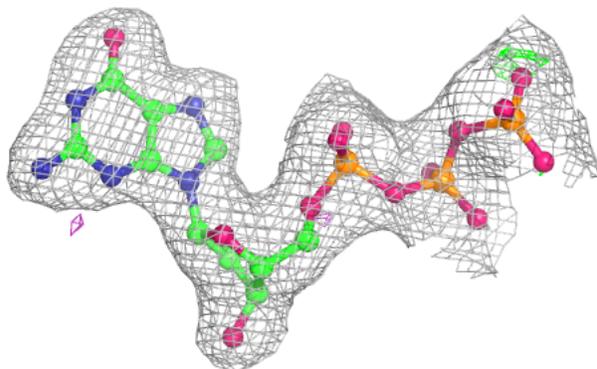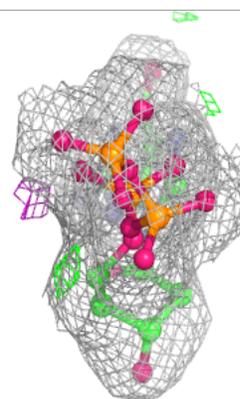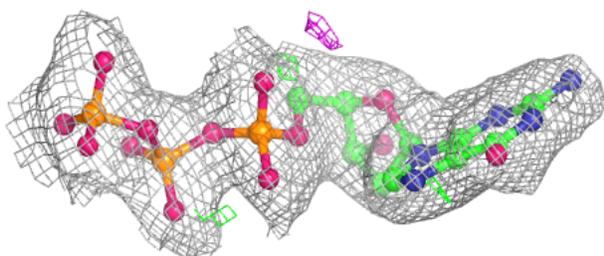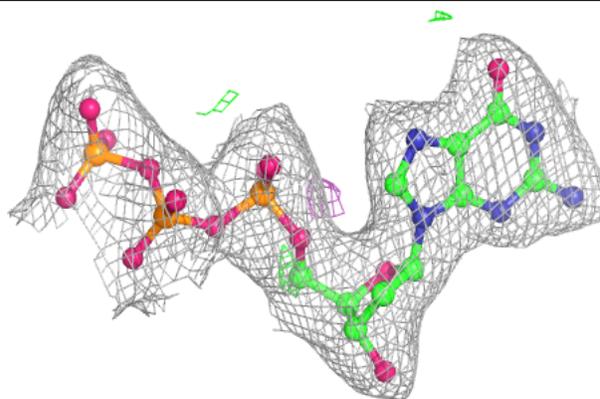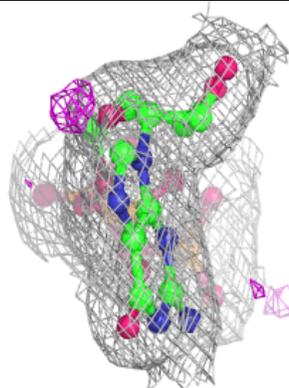and green (positive)
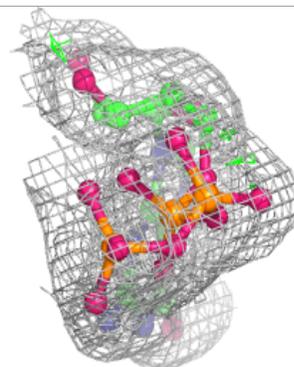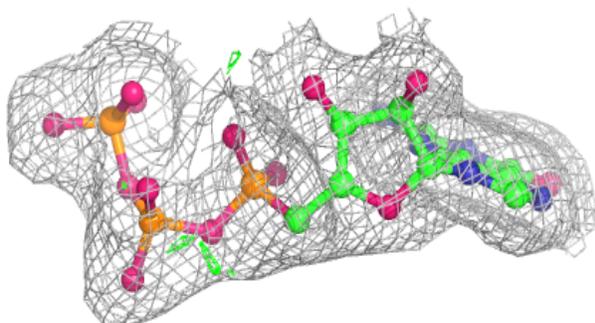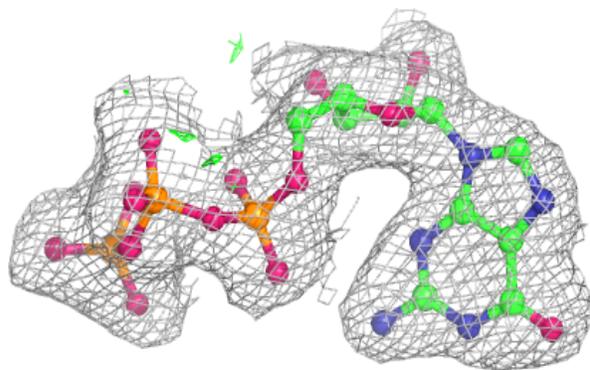
Electron density around GTP B 701:

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

Electron density around GTP C 704:

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

Electron density around DGT A 701:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
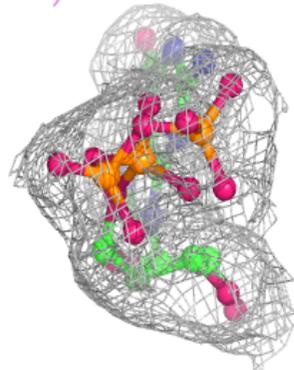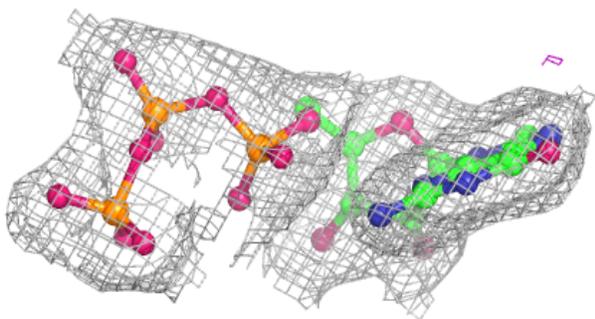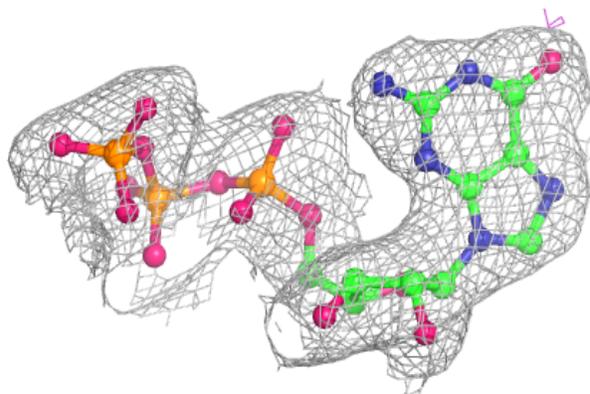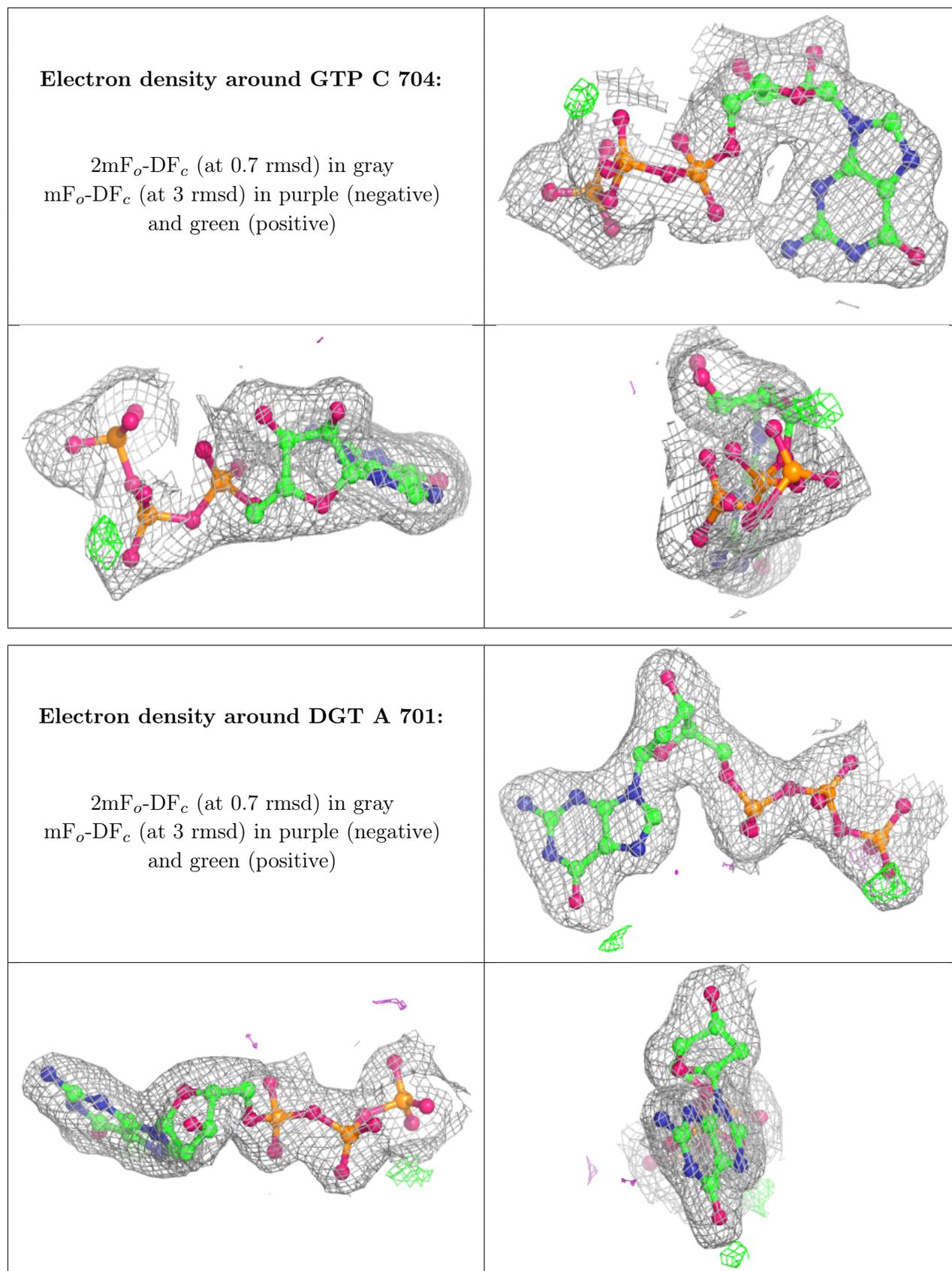
Electron density around DGT B 703:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
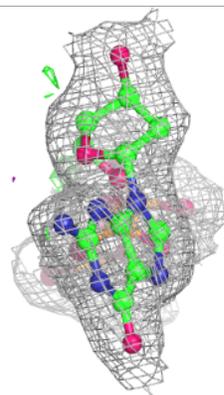
Electron density around DGT C 703:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
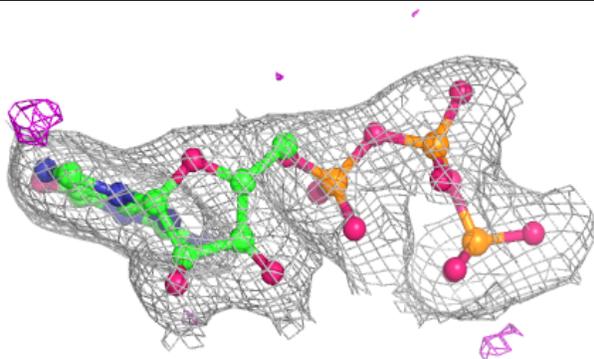mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
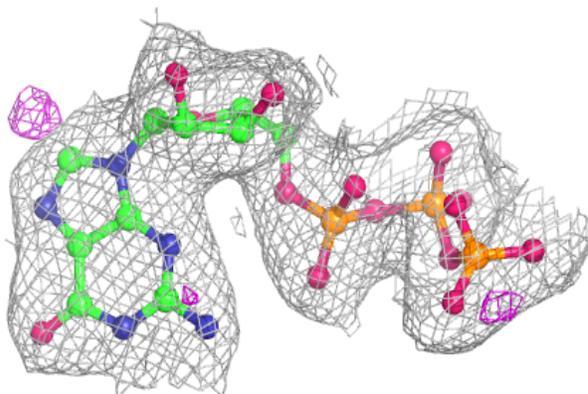and green (positive)

Electron density around DGT D 800:

$2mF_o-DF_c$ (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)

6.5 Other polymers ⓘ

There are no such residues in this entry.