



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:12 AM UTC

PDB ID : 4TNR / pdb_00004tnr
Title : Structure basis of cellular dNTP regulation, SAMHD1-GTP-dATP-dATP complex
Authors : Ji, X.; Tang, C.; Zhao, Q.; Wang, W.; Xiong, Y.
Deposited on : 2014-06-04
Resolution : 2.75 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

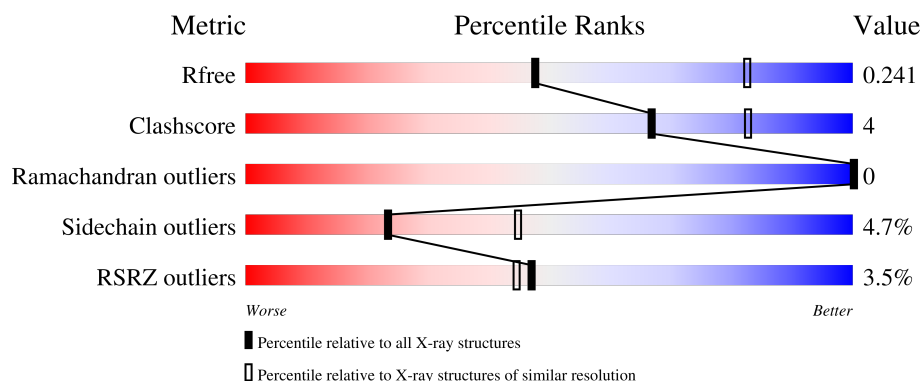
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	514	7% 80% 13% 6%
1	B	514	% 80% 13% 6%
1	C	514	4% 80% 13% 6%
1	D	514	% 81% 12% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16156 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

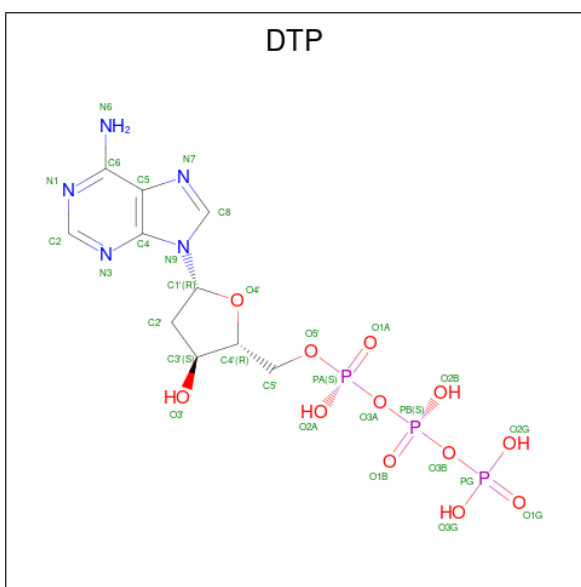
- Molecule 1 is a protein called Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	481	Total	C	N	O	S	0	2	0
			3948	2525	687	715	21			
1	C	481	Total	C	N	O	S	0	2	0
			3948	2525	687	715	21			
1	B	481	Total	C	N	O	S	0	2	0
			3948	2525	687	715	21			
1	A	481	Total	C	N	O	S	0	2	0
			3948	2525	687	715	21			

There are 8 discrepancies between the modelled and reference sequences:

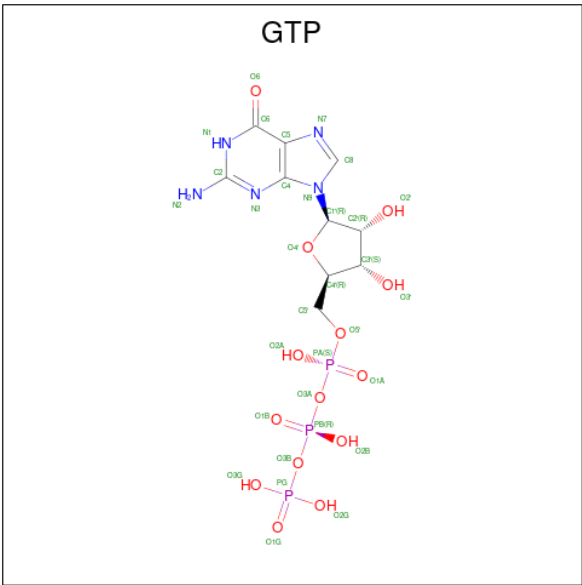
Chain	Residue	Modelled	Actual	Comment	Reference
D	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
D	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
C	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
C	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
B	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
B	207	ASN	ASP	engineered mutation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

- Molecule 2 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃)



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

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{14}\text{P}_3$).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	8	Total	O	0	0
			8	8		

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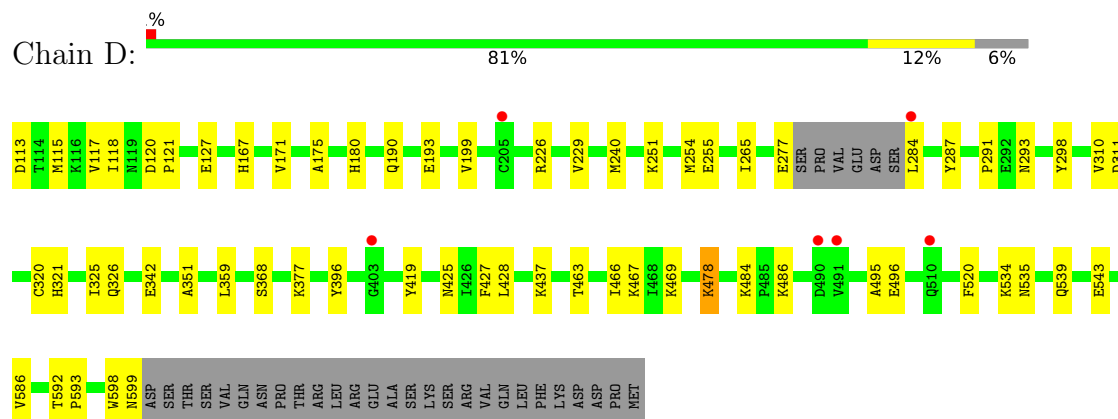
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	2	Total	O	0	0
			2	2		
5	B	9	Total	O	0	0
			9	9		
5	A	3	Total	O	0	0
			3	3		

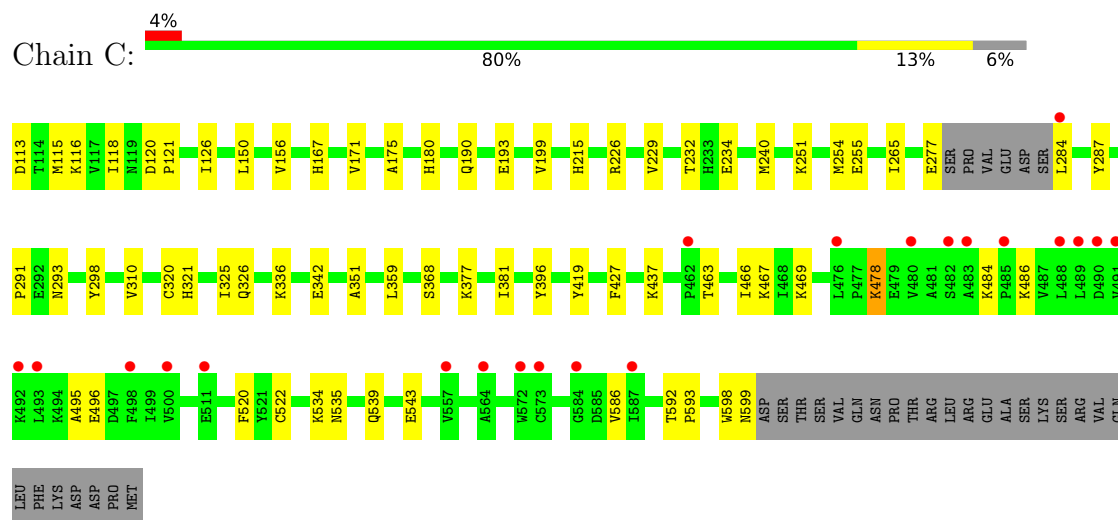
3 Residue-property plots

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.

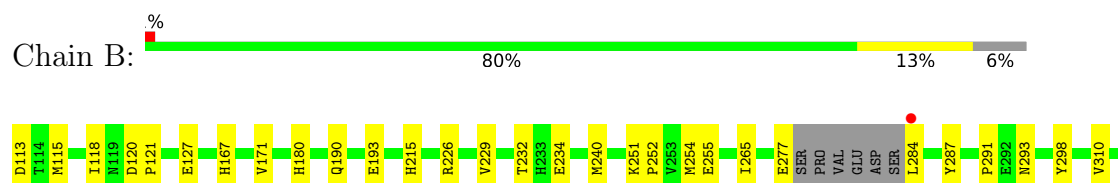
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

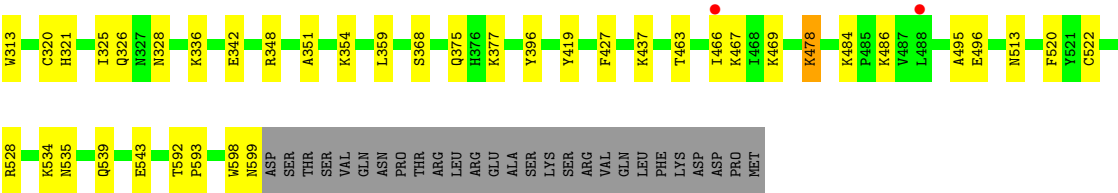


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

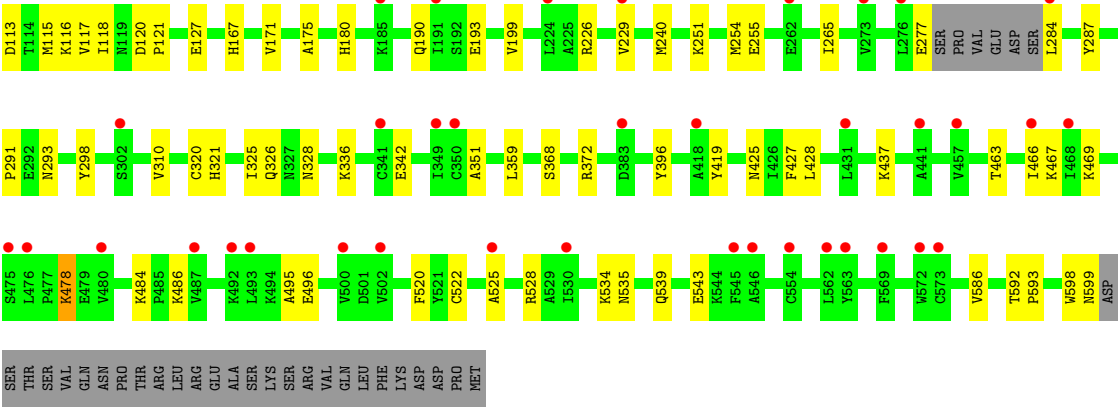
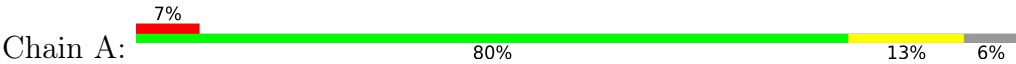


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





● 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	84.92Å 141.70Å 97.52Å 90.00° 115.40° 90.00°	Depositor
Resolution (Å)	50.00 – 2.75 50.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	96.3 (50.00-2.75) 97.7 (50.00-2.75)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.224 , 0.242 0.222 , 0.241	Depositor DCC
R_{free} test set	2775 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	65.3	Xtriage
Anisotropy	1.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 81.3	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	16156	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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 ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.84	2/4040 (0.0%)	0.93	0/5453
1	B	0.88	4/4040 (0.1%)	0.95	0/5453
1	C	0.84	0/4040	0.94	0/5453
1	D	0.90	1/4040 (0.0%)	0.95	0/5453
All	All	0.87	7/16160 (0.0%)	0.94	0/21812

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	528	ARG	CZ-NH2	9.81	1.46	1.33
1	B	528	ARG	CD-NE	6.39	1.55	1.46
1	B	328	ASN	CA-C	5.67	1.60	1.52
1	D	117	VAL	C-O	-5.32	1.18	1.24
1	B	313	TRP	N-CA	-5.18	1.40	1.46
1	A	328	ASN	CA-C	5.07	1.59	1.52
1	A	117	VAL	C-O	-5.03	1.18	1.24

There are no bond angle outliers.

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	3948	0	3930	34	0
1	B	3948	0	3930	37	0
1	C	3948	0	3930	37	0
1	D	3948	0	3930	31	0
2	A	30	0	12	2	0
2	B	60	0	24	5	0
2	C	60	0	24	4	0
2	D	60	0	24	2	0
3	A	32	0	12	0	0
3	B	32	0	12	0	0
3	C	32	0	12	1	0
3	D	32	0	12	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	3	0	0	0	0
5	B	9	0	0	1	0
5	C	2	0	0	0	0
5	D	8	0	0	0	0
All	All	16156	0	15852	118	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 4.

All (118) 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:C:377:LYS:NZ	2:A:702:DTP:O2B	1.97	0.96
1:C:326:GLN:HG2	1:A:326:GLN:HG2	1.62	0.81
1:D:326:GLN:HG2	1:B:326:GLN:HG2	1.66	0.76
1:C:215:HIS:CD2	2:C:701:DTP:C8	2.70	0.75
1:A:291:PRO:HG2	1:A:293:ASN:OD1	1.90	0.72
1:C:291:PRO:HG2	1:C:293:ASN:OD1	1.90	0.71
1:B:291:PRO:HG2	1:B:293:ASN:OD1	1.91	0.70
1:D:291:PRO:HG2	1:D:293:ASN:OD1	1.92	0.69
1:B:375:GLN:HE22	2:B:704:DTP:HN61	1.44	0.65
1:D:311:ASP:OD2	2:D:701:DTP:O1A	2.15	0.64
2:D:703:DTP:O2B	1:B:377:LYS:NZ	2.31	0.63
1:B:127:GLU:HG3	1:A:336:LYS:HE3	1.82	0.62
1:B:348:ARG:HD3	5:B:809:HOH:O	1.98	0.62
1:B:254:MET:HE1	1:B:265:ILE:HG13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:MET:HE1	1:D:265:ILE:HG13	1.85	0.59
1:D:543:GLU:HG3	1:B:543:GLU:HG3	1.85	0.58
1:A:254:MET:HE1	1:A:265:ILE:HG13	1.85	0.58
1:D:120:ASP:OD1	1:D:121:PRO:HD2	2.02	0.58
1:B:226:ARG:O	1:B:229:VAL:HG12	2.05	0.57
1:B:375:GLN:NE2	2:B:704:DTP:N6	2.49	0.57
1:D:586:VAL:HG11	1:B:522[A]:CYS:SG	2.45	0.56
1:B:287:TYR:CD1	1:B:298:TYR:CE1	2.93	0.56
1:A:287:TYR:CD1	1:A:298:TYR:CE1	2.93	0.56
1:C:254:MET:HE1	1:C:265:ILE:HG13	1.86	0.56
1:D:287:TYR:CD1	1:D:298:TYR:CE1	2.94	0.56
1:A:226:ARG:O	1:A:229:VAL:HG12	2.05	0.56
1:D:226:ARG:O	1:D:229:VAL:HG12	2.06	0.55
1:C:226:ARG:O	1:C:229:VAL:HG12	2.05	0.55
1:B:120:ASP:OD1	1:B:121:PRO:HD2	2.05	0.55
1:A:120:ASP:OD1	1:A:121:PRO:HD2	2.07	0.55
1:C:120:ASP:OD1	1:C:121:PRO:HD2	2.06	0.54
1:D:321:HIS:CE1	1:A:321:HIS:CE1	2.96	0.54
1:C:586:VAL:HG22	1:A:528:ARG:HD3	1.91	0.52
1:C:287:TYR:CD1	1:C:298:TYR:CE1	2.96	0.52
1:D:377:LYS:NZ	2:B:701:DTP:O2B	2.43	0.52
2:C:704:DTP:N6	1:A:372:ARG:HG2	2.26	0.51
1:A:167:HIS:O	1:A:171:VAL:HG23	2.10	0.51
1:C:586:VAL:HG11	1:A:522[A]:CYS:SG	2.50	0.51
1:A:463:THR:O	1:A:466:ILE:HG12	2.11	0.51
1:D:127:GLU:HG3	1:C:336:LYS:HE3	1.93	0.50
1:B:167:HIS:O	1:B:171:VAL:HG23	2.11	0.50
1:C:167:HIS:O	1:C:171:VAL:HG23	2.10	0.50
1:C:543:GLU:HG3	1:A:543:GLU:HG3	1.93	0.50
1:C:326:GLN:HG2	1:A:326:GLN:CG	2.39	0.50
1:B:463:THR:O	1:B:466:ILE:HG12	2.12	0.50
1:D:463:THR:O	1:D:466:ILE:HG12	2.11	0.49
1:C:326:GLN:CG	1:A:326:GLN:HG2	2.39	0.49
1:C:463:THR:O	1:C:466:ILE:HG12	2.12	0.49
1:D:167:HIS:O	1:D:171:VAL:HG23	2.13	0.48
1:C:116:LYS:HE3	3:C:703:GTP:O1A	2.14	0.48
1:C:592:THR:N	1:C:593:PRO:CD	2.77	0.48
1:C:251:LYS:O	1:C:255:GLU:HG3	2.14	0.47
1:B:336:LYS:HE3	1:A:127:GLU:HG3	1.97	0.47
1:D:592:THR:N	1:D:593:PRO:CD	2.78	0.47
1:A:592:THR:N	1:A:593:PRO:CD	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:LYS:O	1:D:255:GLU:HG3	2.14	0.47
1:D:320:CYS:HB3	1:D:325:ILE:O	2.15	0.47
1:B:592:THR:N	1:B:593:PRO:CD	2.78	0.47
1:A:251:LYS:O	1:A:255:GLU:HG3	2.16	0.46
1:C:351:ALA:O	1:C:520:PHE:HA	2.16	0.46
1:B:232:THR:HB	1:B:234:GLU:OE1	2.16	0.46
1:D:326:GLN:HG2	1:B:326:GLN:CG	2.42	0.46
1:D:478:LYS:HE2	1:D:495:ALA:HB1	1.98	0.46
1:B:240:MET:CE	1:B:419:TYR:HD2	2.28	0.46
1:A:478:LYS:HE2	1:A:495:ALA:HB1	1.98	0.46
1:B:251:LYS:O	1:B:255:GLU:HG3	2.16	0.45
1:A:396:TYR:CD1	1:A:437:LYS:HD2	2.50	0.45
1:B:396:TYR:CD1	1:B:437:LYS:HD2	2.52	0.45
3:D:702:GTP:O2G	1:A:116:LYS:NZ	2.29	0.45
1:C:478:LYS:HE2	1:C:495:ALA:HB1	1.98	0.45
1:C:522[A]:CYS:SG	1:A:586:VAL:HG11	2.56	0.45
1:D:396:TYR:CD1	1:D:437:LYS:HD2	2.52	0.45
1:D:543:GLU:CG	1:B:543:GLU:CG	2.95	0.44
1:C:240:MET:CE	1:C:419:TYR:HD2	2.31	0.44
1:A:351:ALA:O	1:A:520:PHE:HA	2.17	0.44
1:C:320:CYS:HB3	1:C:325:ILE:O	2.17	0.44
1:D:171:VAL:HG13	1:D:310:VAL:HG23	2.00	0.44
1:B:478:LYS:HE2	1:B:495:ALA:HB1	1.98	0.44
1:D:543:GLU:HG2	1:B:543:GLU:HG2	2.00	0.44
1:D:240:MET:CE	1:D:419:TYR:HD2	2.30	0.44
1:C:396:TYR:CD1	1:C:437:LYS:HD2	2.53	0.44
1:C:156:VAL:O	2:A:702:DTP:O3'	2.32	0.43
1:A:427:PHE:CD1	1:A:427:PHE:C	2.96	0.43
1:D:351:ALA:O	1:D:520:PHE:HA	2.17	0.43
1:A:240:MET:CE	1:A:419:TYR:HD2	2.30	0.43
1:C:171:VAL:HG13	1:C:310:VAL:HG23	2.01	0.43
3:D:702:GTP:PA	3:D:702:GTP:H3'	2.58	0.43
1:B:351:ALA:O	1:B:520:PHE:HA	2.18	0.43
1:B:598:TRP:O	1:B:599:ASN:HB2	2.19	0.43
1:C:427:PHE:CD1	1:C:427:PHE:C	2.97	0.43
1:D:427:PHE:C	1:D:427:PHE:CD1	2.97	0.43
1:C:215:HIS:NE2	2:C:701:DTP:H8	2.34	0.43
1:A:171:VAL:HG13	1:A:310:VAL:HG23	2.01	0.43
1:D:598:TRP:O	1:D:599:ASN:HB2	2.19	0.43
1:B:427:PHE:CD1	1:B:427:PHE:C	2.97	0.43
1:C:598:TRP:O	1:C:599:ASN:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:TRP:O	1:A:599:ASN:HB2	2.18	0.42
1:C:381:ILE:HD12	1:C:381:ILE:HA	1.91	0.42
1:C:586:VAL:HG11	1:A:525:ALA:HB3	2.01	0.42
1:A:320:CYS:HB3	1:A:325:ILE:O	2.18	0.42
1:D:428:LEU:HD12	1:A:425:ASN:HB2	2.01	0.42
1:B:513:ASN:OD1	1:B:513:ASN:C	2.63	0.42
1:D:428:LEU:CD1	1:A:425:ASN:HB2	2.50	0.42
1:B:215:HIS:HE1	2:B:704:DTP:O2B	2.03	0.42
1:D:175:ALA:HB1	1:D:199:VAL:HG12	2.02	0.41
1:B:251:LYS:N	1:B:252:PRO:HD2	2.35	0.41
1:A:175:ALA:HB1	1:A:199:VAL:HG12	2.02	0.41
1:D:425:ASN:HB2	1:A:428:LEU:CD1	2.51	0.41
1:C:321:HIS:CE1	1:B:321:HIS:CE1	3.09	0.41
1:C:175:ALA:HB1	1:C:199:VAL:HG12	2.03	0.41
1:B:320:CYS:HB3	1:B:325:ILE:O	2.20	0.41
1:B:354:LYS:NZ	2:B:701:DTP:O1A	2.54	0.41
1:C:150:LEU:CD2	2:C:701:DTP:H2'1	2.51	0.41
1:C:232:THR:HB	1:C:234:GLU:OE1	2.21	0.41
1:B:287:TYR:HB3	1:B:298:TYR:OH	2.21	0.40
1:B:171:VAL:HG13	1:B:310:VAL:HG23	2.02	0.40
1:C:126:ILE:HD13	1:C:126:ILE:HG21	1.89	0.40
1:B:240:MET:HE1	1:B:419:TYR:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	479/514 (93%)	474 (99%)	5 (1%)	0	100	100
1	B	479/514 (93%)	475 (99%)	4 (1%)	0	100	100
1	C	479/514 (93%)	474 (99%)	5 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	479/514 (93%)	473 (99%)	6 (1%)	0	100	100
All	All	1916/2056 (93%)	1896 (99%)	20 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	429/459 (94%)	409 (95%)	20 (5%)	23	45
1	B	429/459 (94%)	409 (95%)	20 (5%)	23	45
1	C	429/459 (94%)	409 (95%)	20 (5%)	23	45
1	D	429/459 (94%)	409 (95%)	20 (5%)	23	45
All	All	1716/1836 (94%)	1636 (95%)	80 (5%)	23	45

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	113	ASP
1	D	115	MET
1	D	118	ILE
1	D	180	HIS
1	D	190	GLN
1	D	193	GLU
1	D	277	GLU
1	D	284	LEU
1	D	342	GLU
1	D	359	LEU
1	D	368	SER
1	D	467	LYS
1	D	469	LYS
1	D	478	LYS
1	D	484	LYS
1	D	486	LYS

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Mol	Chain	Res	Type
1	D	496	GLU
1	D	534	LYS
1	D	535	ASN
1	D	539	GLN
1	C	113	ASP
1	C	115	MET
1	C	118	ILE
1	C	180	HIS
1	C	190	GLN
1	C	193	GLU
1	C	277	GLU
1	C	284	LEU
1	C	342	GLU
1	C	359	LEU
1	C	368	SER
1	C	467	LYS
1	C	469	LYS
1	C	478	LYS
1	C	484	LYS
1	C	486	LYS
1	C	496	GLU
1	C	534	LYS
1	C	535	ASN
1	C	539	GLN
1	B	113	ASP
1	B	115	MET
1	B	118	ILE
1	B	180	HIS
1	B	190	GLN
1	B	193	GLU
1	B	277	GLU
1	B	284	LEU
1	B	342	GLU
1	B	359	LEU
1	B	368	SER
1	B	467	LYS
1	B	469	LYS
1	B	478	LYS
1	B	484	LYS
1	B	486	LYS
1	B	496	GLU
1	B	534	LYS

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Mol	Chain	Res	Type
1	B	535	ASN
1	B	539	GLN
1	A	113	ASP
1	A	115	MET
1	A	118	ILE
1	A	180	HIS
1	A	190	GLN
1	A	193	GLU
1	A	277	GLU
1	A	284	LEU
1	A	342	GLU
1	A	359	LEU
1	A	368	SER
1	A	467	LYS
1	A	469	LYS
1	A	478	LYS
1	A	484	LYS
1	A	486	LYS
1	A	496	GLU
1	A	534	LYS
1	A	535	ASN
1	A	539	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	149	GLN
1	D	200	GLN
1	D	235	GLN
1	D	243	HIS
1	D	375	GLN
1	D	380	ASN
1	D	447	GLN
1	D	567	GLN
1	C	149	GLN
1	C	163	ASN
1	C	200	GLN
1	C	235	GLN
1	C	243	HIS
1	C	567	GLN
1	B	149	GLN
1	B	200	GLN

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Mol	Chain	Res	Type
1	B	235	GLN
1	B	243	HIS
1	B	364	HIS
1	B	375	GLN
1	B	380	ASN
1	B	567	GLN
1	A	149	GLN
1	A	200	GLN
1	A	235	GLN
1	A	243	HIS
1	A	364	HIS
1	A	567	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DTP	D	703	4	31,32,32	1.73	9 (29%)	46,50,50	2.10	16 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GTP	B	703	4	33,34,34	1.40	6 (18%)	50,54,54	1.54	7 (14%)
2	DTP	C	701	-	31,32,32	1.96	6 (19%)	46,50,50	1.98	12 (26%)
2	DTP	B	701	4	31,32,32	1.61	8 (25%)	46,50,50	1.96	11 (23%)
2	DTP	B	704	-	31,32,32	1.83	6 (19%)	46,50,50	1.86	11 (23%)
2	DTP	A	702	4	31,32,32	1.86	7 (22%)	46,50,50	1.99	12 (26%)
3	GTP	A	703	4	33,34,34	1.27	4 (12%)	50,54,54	1.68	11 (22%)
3	GTP	C	703	4	33,34,34	1.35	4 (12%)	50,54,54	1.84	11 (22%)
3	GTP	D	702	4	33,34,34	1.26	3 (9%)	50,54,54	1.81	10 (20%)
2	DTP	C	704	4	31,32,32	1.62	6 (19%)	46,50,50	1.95	13 (28%)
2	DTP	D	701	-	31,32,32	2.28	7 (22%)	46,50,50	1.75	9 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DTP	D	703	4	-	0/22/34/34	0/3/3/3
3	GTP	B	703	4	-	3/22/38/38	0/3/3/3
2	DTP	C	701	-	-	2/22/34/34	0/3/3/3
2	DTP	B	701	4	-	2/22/34/34	0/3/3/3
2	DTP	B	704	-	-	2/22/34/34	0/3/3/3
2	DTP	A	702	4	-	0/22/34/34	0/3/3/3
3	GTP	A	703	4	-	5/22/38/38	0/3/3/3
3	GTP	C	703	4	-	4/22/38/38	0/3/3/3
3	GTP	D	702	4	-	5/22/38/38	0/3/3/3
2	DTP	C	704	4	-	5/22/34/34	0/3/3/3
2	DTP	D	701	-	-	2/22/34/34	0/3/3/3

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	DTP	C5-C4	5.86	1.49	1.39
2	B	704	DTP	C5-C4	5.73	1.49	1.39
2	D	701	DTP	PB-O3A	5.30	1.65	1.59
2	D	701	DTP	PA-O3A	5.24	1.65	1.59
2	C	701	DTP	C5-C4	5.19	1.48	1.39
2	A	702	DTP	C5-C4	4.91	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	DTP	PB-O3B	4.74	1.64	1.59
2	A	702	DTP	PB-O3B	4.44	1.64	1.59
2	C	704	DTP	C5-C4	4.29	1.46	1.39
2	B	701	DTP	C5-C4	4.21	1.46	1.39
2	C	701	DTP	PA-O3A	4.19	1.64	1.59
2	C	701	DTP	PB-O3B	4.19	1.64	1.59
2	D	703	DTP	C5-C4	4.12	1.46	1.39
2	C	701	DTP	PB-O3A	3.86	1.63	1.59
3	B	703	GTP	PA-O3A	3.81	1.63	1.59
2	D	701	DTP	C5-C6	3.68	1.51	1.41
2	B	704	DTP	C5-C6	3.52	1.50	1.41
3	C	703	GTP	C5-N7	-3.48	1.32	1.39
2	B	704	DTP	PB-O3B	3.46	1.63	1.59
2	A	702	DTP	C5-C6	3.43	1.50	1.41
3	A	703	GTP	C5-C4	3.39	1.48	1.38
3	D	702	GTP	C5-C4	3.33	1.47	1.38
3	C	703	GTP	C6-N1	-3.25	1.32	1.38
2	C	701	DTP	C5-C6	3.21	1.49	1.41
2	D	703	DTP	PA-O3A	3.15	1.62	1.59
2	B	701	DTP	PB-O3B	3.14	1.62	1.59
2	B	704	DTP	C8-N7	3.13	1.37	1.31
3	D	702	GTP	C6-N1	-3.11	1.33	1.38
3	A	703	GTP	C5-N7	-3.09	1.32	1.39
2	D	701	DTP	C8-N7	3.09	1.37	1.31
3	C	703	GTP	C4-N9	-3.05	1.30	1.38
2	D	703	DTP	PB-O3A	3.00	1.62	1.59
2	C	704	DTP	C8-N9	-2.99	1.32	1.37
2	B	704	DTP	PB-O3A	2.97	1.62	1.59
2	A	702	DTP	C8-N9	-2.94	1.32	1.37
2	C	704	DTP	C5-C6	2.91	1.49	1.41
3	A	703	GTP	C4-N9	-2.87	1.30	1.38
3	B	703	GTP	C5-C4	2.85	1.46	1.38
2	B	704	DTP	PA-O3A	2.80	1.62	1.59
2	D	703	DTP	C8-N9	-2.79	1.32	1.37
2	B	701	DTP	C5-C6	2.78	1.48	1.41
2	D	703	DTP	C8-N7	2.69	1.36	1.31
3	B	703	GTP	PB-O3A	2.69	1.62	1.59
2	C	701	DTP	C8-N7	2.67	1.36	1.31
3	C	703	GTP	C5-C4	2.66	1.46	1.38
2	A	702	DTP	C5-N7	-2.65	1.34	1.39
2	D	703	DTP	O4'-C4'	-2.61	1.39	1.45
2	C	704	DTP	PA-O3A	2.60	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	704	DTP	C8-N7	2.57	1.36	1.31
3	B	703	GTP	C4-N9	-2.53	1.31	1.38
3	B	703	GTP	C5-N7	-2.47	1.34	1.39
2	D	701	DTP	C1'-N9	2.47	1.51	1.46
2	D	703	DTP	C5-N7	-2.45	1.34	1.39
3	D	702	GTP	C4-N9	-2.30	1.32	1.38
2	B	701	DTP	O4'-C1'	2.27	1.47	1.42
2	B	701	DTP	C8-N7	2.24	1.36	1.31
3	A	703	GTP	PB-O3B	2.24	1.61	1.59
2	A	702	DTP	C4-N9	-2.23	1.33	1.37
2	B	701	DTP	C5-N7	-2.22	1.35	1.39
2	A	702	DTP	PG-O2G	-2.11	1.47	1.54
3	B	703	GTP	C6-N1	-2.11	1.34	1.38
2	D	703	DTP	PB-O3B	2.07	1.61	1.59
2	C	704	DTP	C5-N7	-2.04	1.35	1.39
2	D	703	DTP	C5-C6	2.04	1.46	1.41
2	B	701	DTP	PB-O2B	-2.02	1.46	1.55
2	B	701	DTP	C4-N9	-2.01	1.33	1.37

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	704	DTP	C5-C4-N3	-6.04	118.40	126.72
3	C	703	GTP	C5-C4-N3	-5.98	118.88	128.39
2	B	701	DTP	C5-C4-N3	-5.68	118.90	126.72
3	D	702	GTP	C5-C4-N3	-5.61	119.46	128.39
2	C	701	DTP	C5-C4-N3	-5.59	119.02	126.72
2	C	704	DTP	C5-C4-N3	-5.55	119.08	126.72
2	D	701	DTP	C5-C4-N3	-5.36	119.34	126.72
3	C	703	GTP	C2-N3-C4	5.21	121.28	112.30
2	A	702	DTP	C4-C5-N7	-5.04	104.82	110.58
2	A	702	DTP	C5-C4-N3	-5.02	119.80	126.72
3	A	703	GTP	C2-N3-C4	4.90	120.73	112.30
3	D	702	GTP	C2-N3-C4	4.87	120.69	112.30
2	B	704	DTP	N3-C4-N9	4.87	135.44	127.17
3	A	703	GTP	C5-C4-N3	-4.83	120.71	128.39
2	D	703	DTP	N3-C2-N1	-4.80	121.32	128.58
2	B	701	DTP	N3-C4-N9	4.79	135.32	127.17
2	C	701	DTP	N3-C4-N9	4.77	135.28	127.17
3	B	703	GTP	C5-C4-N3	-4.57	121.11	128.39
3	B	703	GTP	C2-N3-C4	4.57	120.17	112.30
2	C	704	DTP	N3-C4-N9	4.53	134.87	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	703	DTP	C5-C4-N3	-4.43	120.62	126.72
2	C	704	DTP	C4-C5-N7	-4.33	105.63	110.58
3	D	702	GTP	C3'-C2'-C1'	4.18	109.37	101.46
3	B	703	GTP	N9-C4-N3	4.08	134.12	125.95
3	D	702	GTP	N9-C4-N3	4.04	134.03	125.95
2	B	704	DTP	C2-N3-C4	4.02	121.64	111.83
2	A	702	DTP	N3-C4-N9	4.01	133.99	127.17
2	D	701	DTP	N3-C4-N9	4.00	133.96	127.17
2	C	701	DTP	C2-N3-C4	3.96	121.50	111.83
2	C	701	DTP	N3-C2-N1	-3.95	122.60	128.58
2	D	703	DTP	C2-N1-C6	3.84	125.04	118.73
2	D	703	DTP	N3-C4-N9	3.84	133.70	127.17
2	A	702	DTP	C4-N9-C8	3.82	109.74	105.74
2	B	701	DTP	C4-N9-C8	3.80	109.73	105.74
2	C	704	DTP	C4-N9-C8	3.77	109.70	105.74
2	D	701	DTP	C4-C5-N7	-3.77	106.27	110.58
3	C	703	GTP	N9-C4-N3	3.77	133.49	125.95
2	D	701	DTP	C2-N3-C4	3.69	120.85	111.83
2	B	704	DTP	N3-C2-N1	-3.68	123.01	128.58
2	A	702	DTP	C5-N7-C8	3.68	109.23	103.45
2	B	704	DTP	C4-C5-N7	-3.68	106.38	110.58
2	D	703	DTP	C2-N3-C4	3.63	120.71	111.83
2	D	703	DTP	C6-C5-N7	3.62	139.07	132.09
2	D	703	DTP	C4-N9-C8	3.57	109.49	105.74
2	C	701	DTP	C4-N9-C8	3.53	109.45	105.74
2	B	701	DTP	C4-C5-N7	-3.53	106.54	110.58
2	C	704	DTP	O3A-PA-O1A	-3.52	100.13	110.70
3	C	703	GTP	C6-C5-N7	3.50	136.65	130.29
2	C	701	DTP	C4-C5-N7	-3.44	106.65	110.58
2	D	703	DTP	O2G-PG-O1G	3.44	124.23	110.83
3	A	703	GTP	N9-C4-N3	3.41	132.77	125.95
2	B	701	DTP	C2-N3-C4	3.41	120.15	111.83
2	A	702	DTP	C2'-C3'-C4'	3.32	109.54	102.80
2	D	701	DTP	N3-C2-N1	-3.31	123.57	128.58
2	D	703	DTP	C4-C5-N7	-3.26	106.85	110.58
2	D	703	DTP	C2'-C3'-C4'	3.26	109.41	102.80
2	A	702	DTP	N3-C2-N1	-3.24	123.68	128.58
2	C	704	DTP	C5-N7-C8	3.23	108.53	103.45
2	C	704	DTP	C2-N3-C4	3.14	119.49	111.83
3	A	703	GTP	O6-C6-C5	-3.12	118.30	126.53
2	A	702	DTP	C2-N3-C4	3.10	119.41	111.83
3	D	702	GTP	O3B-PB-O1B	-3.00	101.68	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	DTP	C5-N7-C8	2.96	108.11	103.45
2	B	704	DTP	C4-N9-C8	2.95	108.84	105.74
2	B	701	DTP	C5-N7-C8	2.87	107.95	103.45
3	C	703	GTP	C3'-C2'-C1'	2.86	106.87	101.46
2	B	701	DTP	O2G-PG-O1G	2.85	121.96	110.83
3	D	702	GTP	O2G-PG-O1G	2.85	121.95	110.83
2	B	701	DTP	N9-C8-N7	-2.81	109.96	113.94
2	D	703	DTP	O3G-PG-O3B	2.80	114.02	104.64
2	A	702	DTP	N9-C8-N7	-2.79	109.98	113.94
2	C	704	DTP	N9-C8-N7	-2.71	110.09	113.94
2	C	701	DTP	N9-C8-N7	-2.70	110.10	113.94
2	A	702	DTP	C2-N1-C6	2.70	123.17	118.73
2	B	704	DTP	C5-N7-C8	2.70	107.70	103.45
2	A	702	DTP	C6-C5-N7	2.69	137.27	132.09
2	C	701	DTP	C6-C5-N7	2.64	137.18	132.09
3	B	703	GTP	O2A-PA-O3A	2.63	114.39	107.27
2	D	701	DTP	C4-N9-C8	2.59	108.45	105.74
3	D	702	GTP	C6-C5-N7	2.58	134.99	130.29
2	D	701	DTP	C6-C5-N7	2.58	137.07	132.09
3	B	703	GTP	O6-C6-C5	-2.57	119.75	126.53
2	D	701	DTP	C5-N7-C8	2.55	107.46	103.45
2	C	704	DTP	C2'-C3'-C4'	2.55	107.98	102.80
2	D	703	DTP	O3A-PB-O1B	-2.53	103.10	110.70
2	D	703	DTP	C5-N7-C8	2.47	107.33	103.45
2	B	704	DTP	C6-C5-N7	2.44	136.80	132.09
2	C	704	DTP	C6-C5-N7	2.44	136.80	132.09
3	C	703	GTP	C4-C5-N7	-2.43	106.81	110.67
2	B	701	DTP	O2G-PG-O3B	-2.43	96.49	104.64
3	A	703	GTP	O3A-PB-O1B	-2.42	103.44	110.70
2	B	701	DTP	O2B-PB-O3A	2.40	113.76	107.27
3	A	703	GTP	O2B-PB-O3B	2.40	113.75	107.27
3	D	702	GTP	O3B-PG-O1G	-2.37	98.55	111.04
3	A	703	GTP	N2-C2-N1	2.37	121.77	116.76
2	D	703	DTP	O2G-PG-O3B	-2.37	96.68	104.64
3	D	702	GTP	O2'-C2'-C1'	-2.37	101.95	110.10
2	C	704	DTP	N3-C2-N1	-2.34	125.05	128.58
3	C	703	GTP	O5'-PA-O1A	-2.33	99.68	108.94
2	D	703	DTP	N9-C8-N7	-2.33	110.64	113.94
2	C	701	DTP	O2A-PA-O1A	2.33	123.26	112.44
2	B	701	DTP	N3-C2-N1	-2.32	125.06	128.58
2	C	701	DTP	C2'-C3'-C4'	2.32	107.51	102.80
3	A	703	GTP	O3B-PG-O1G	-2.32	98.83	111.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	704	DTP	O3G-PG-O2G	2.30	116.42	107.80
2	B	704	DTP	C2-N1-C6	2.30	122.50	118.73
3	A	703	GTP	C6-C5-N7	2.29	134.45	130.29
2	D	703	DTP	C6-C5-C4	-2.28	114.06	117.18
3	C	703	GTP	C5-C6-N1	2.24	118.94	113.25
2	C	704	DTP	O2B-PB-O1B	2.23	122.80	112.44
3	A	703	GTP	O2B-PB-O3A	2.21	113.24	107.27
2	C	704	DTP	C2-N1-C6	2.15	122.27	118.73
3	B	703	GTP	C6-C5-N7	2.12	134.15	130.29
2	B	704	DTP	N9-C8-N7	-2.12	110.94	113.94
3	C	703	GTP	O4'-C1'-N9	2.11	113.14	108.36
2	D	701	DTP	C2-N1-C6	2.09	122.16	118.73
3	C	703	GTP	O2'-C2'-C1'	-2.08	102.94	110.10
3	C	703	GTP	O2G-PG-O1G	2.07	118.88	110.83
3	D	702	GTP	O2A-PA-O3A	2.06	112.85	107.27
2	A	702	DTP	O4'-C1'-N9	2.05	111.65	107.96
3	B	703	GTP	N2-C2-N1	2.02	121.03	116.76
2	C	701	DTP	C2'-C1'-N9	-2.02	109.88	114.63
3	A	703	GTP	O6-C6-N1	2.01	123.89	120.11

There are no chirality outliers.

All (30) torsion outliers are listed below:

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

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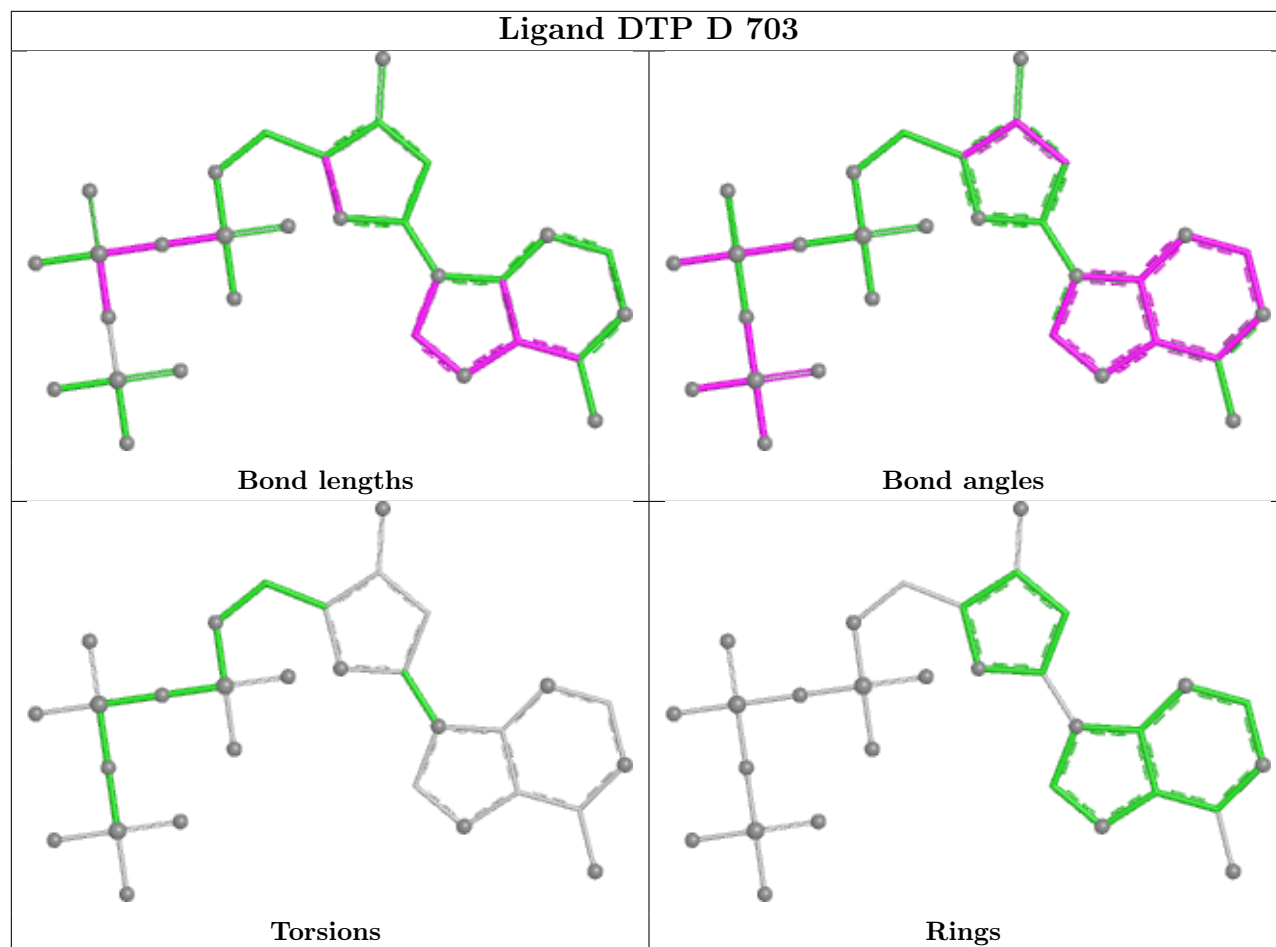
Mol	Chain	Res	Type	Atoms
3	B	703	GTP	C4'-C5'-O5'-PA
3	C	703	GTP	PB-O3B-PG-O2G
2	C	704	DTP	PG-O3B-PB-O2B
2	C	704	DTP	PB-O3A-PA-O1A
2	B	704	DTP	PG-O3B-PB-O1B
3	D	702	GTP	PG-O3B-PB-O1B
3	D	702	GTP	PB-O3A-PA-O2A
3	C	703	GTP	PB-O3A-PA-O1A
3	B	703	GTP	PB-O3A-PA-O2A
3	A	703	GTP	PG-O3B-PB-O1B
2	C	701	DTP	PG-O3B-PB-O2B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

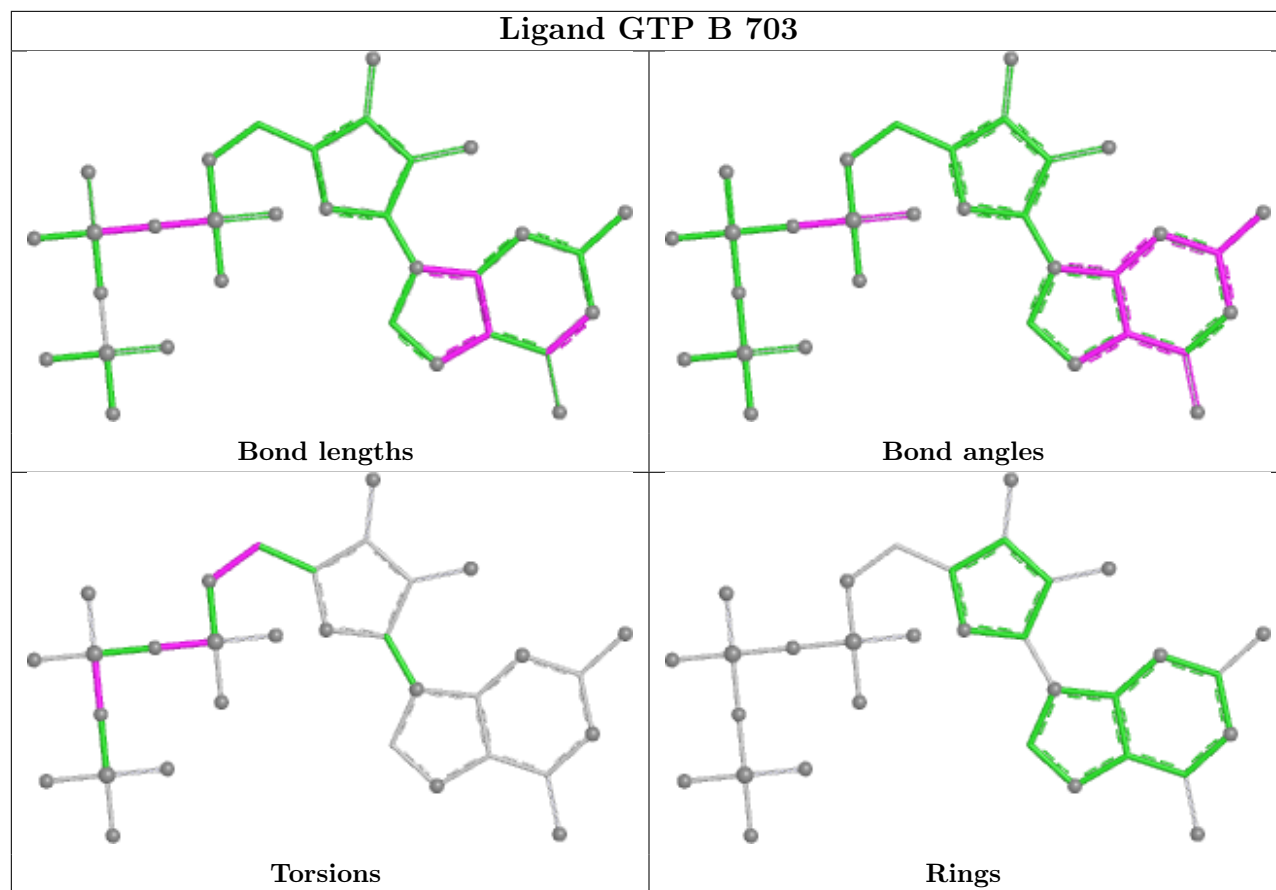
There are no ring outliers.

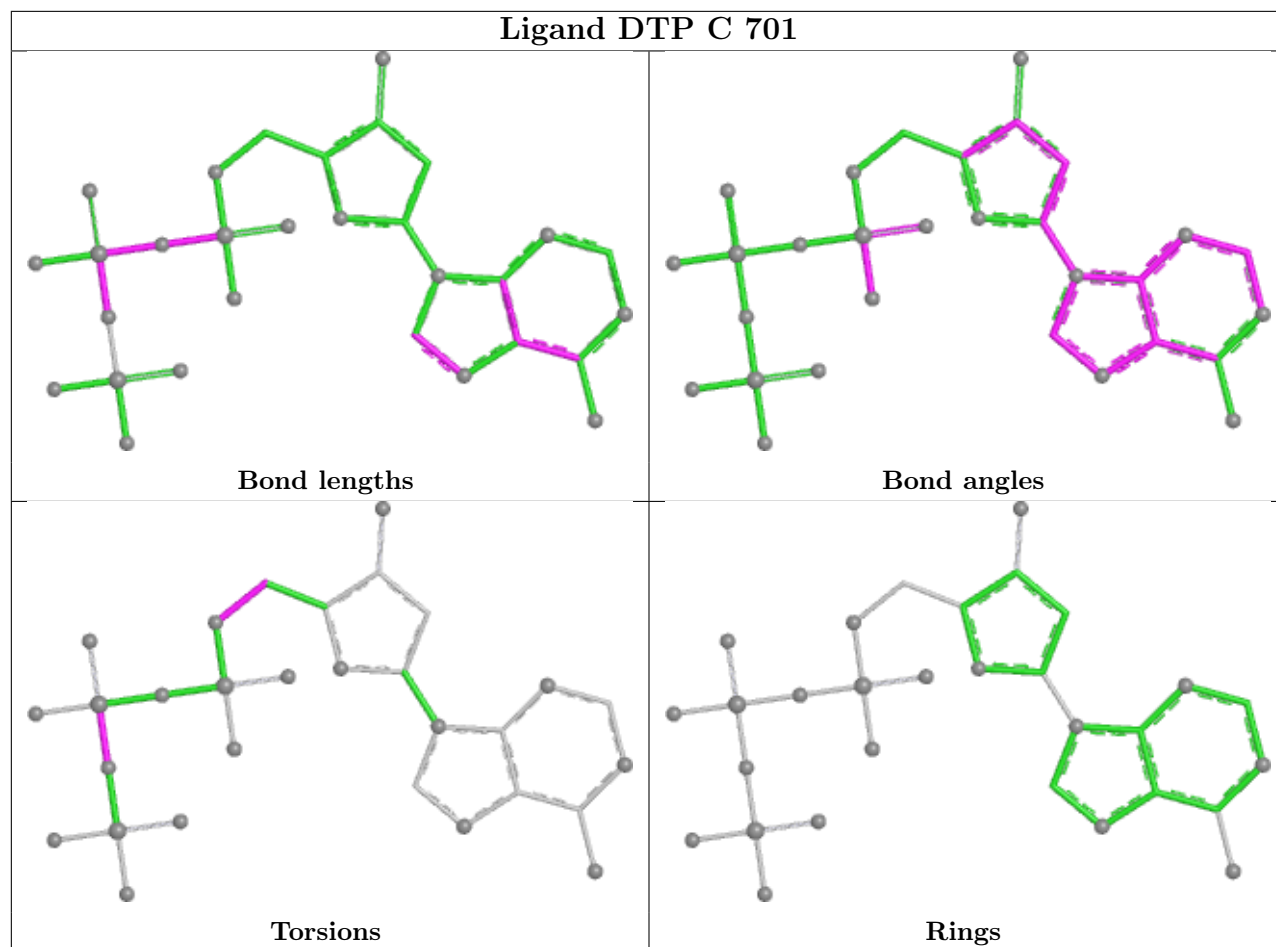
9 monomers are involved in 16 short contacts:

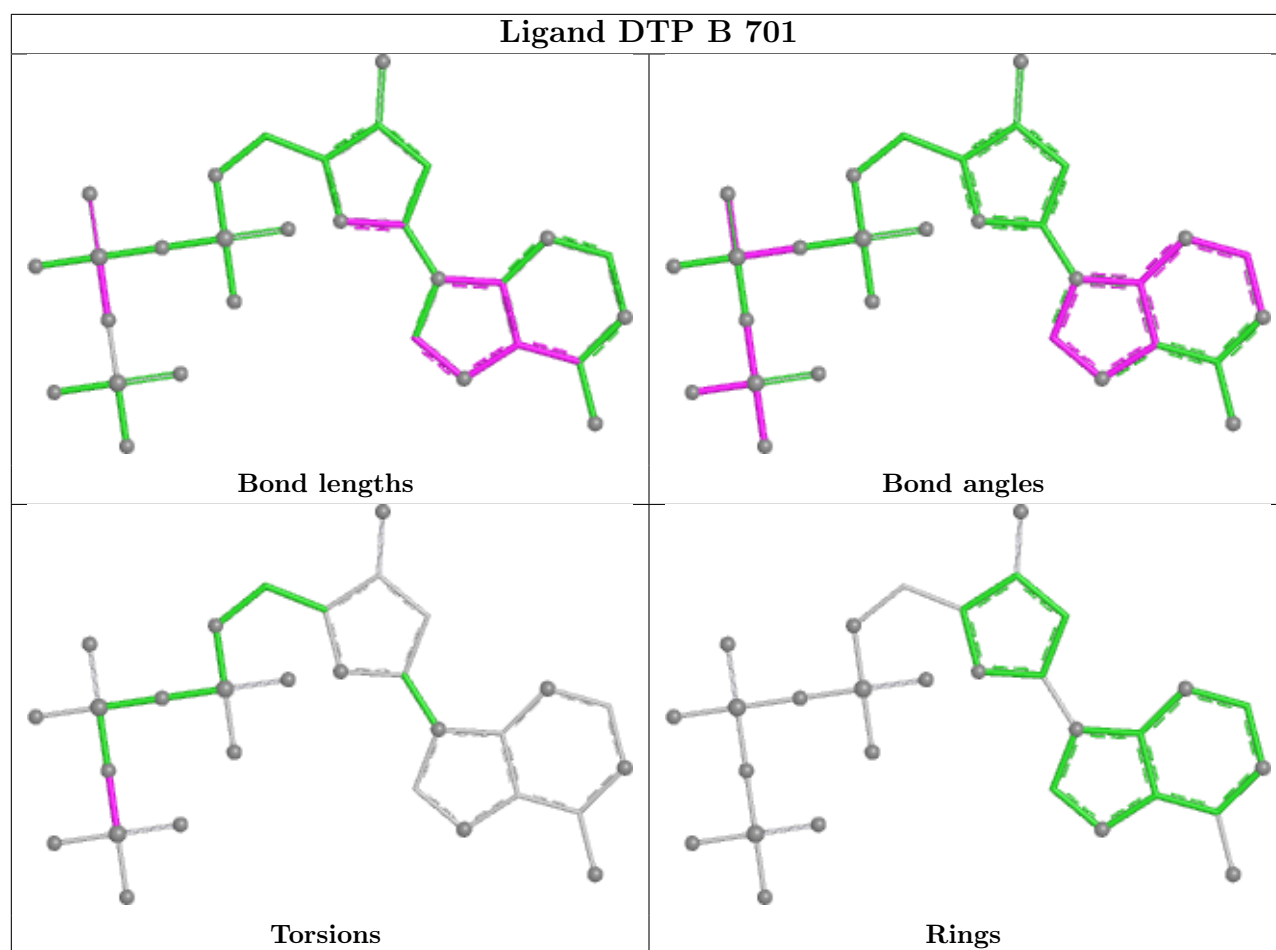
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	703	DTP	1	0
2	C	701	DTP	3	0
2	B	701	DTP	2	0
2	B	704	DTP	3	0
2	A	702	DTP	2	0
3	C	703	GTP	1	0
3	D	702	GTP	2	0
2	C	704	DTP	1	0
2	D	701	DTP	1	0

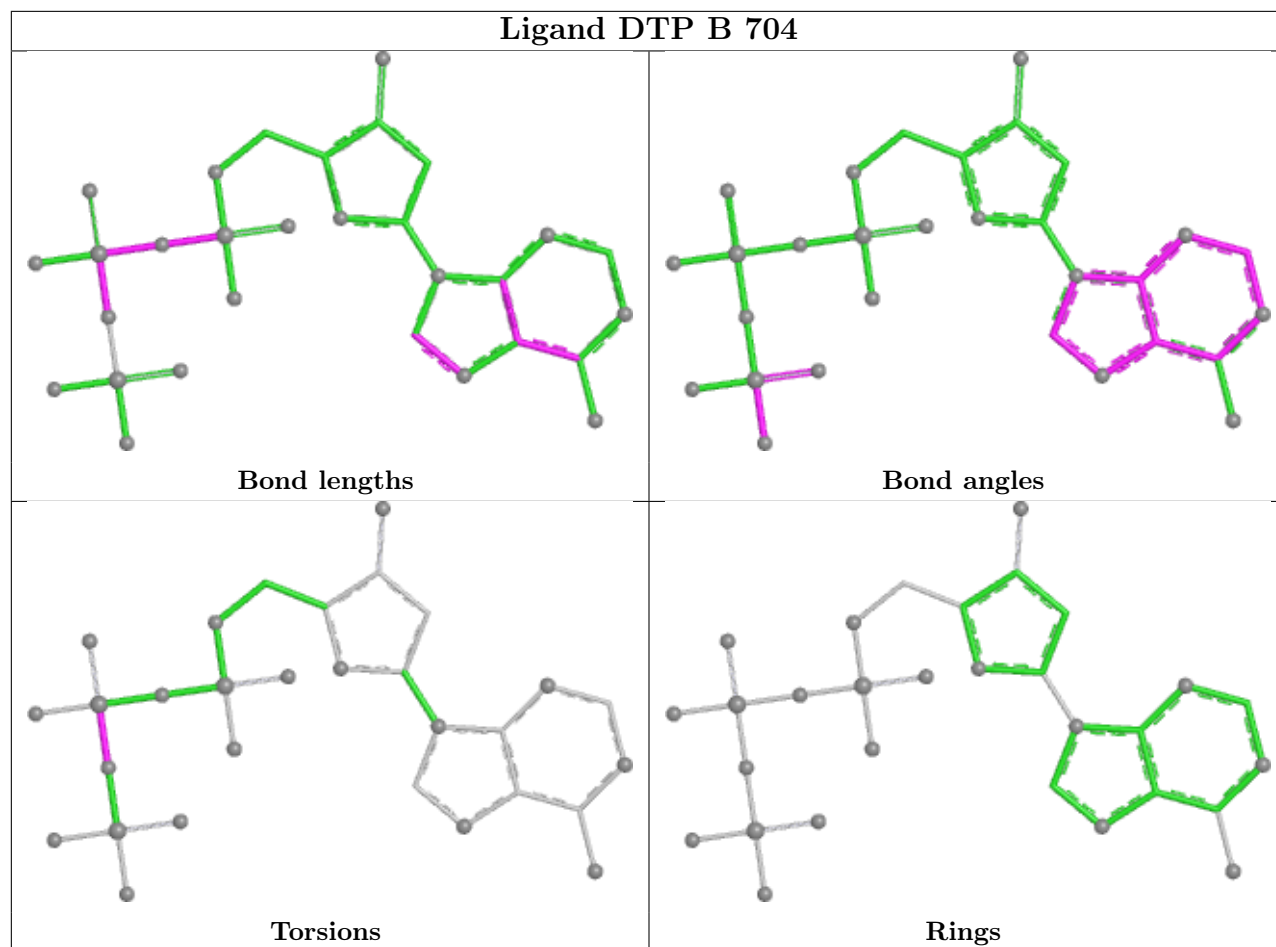
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

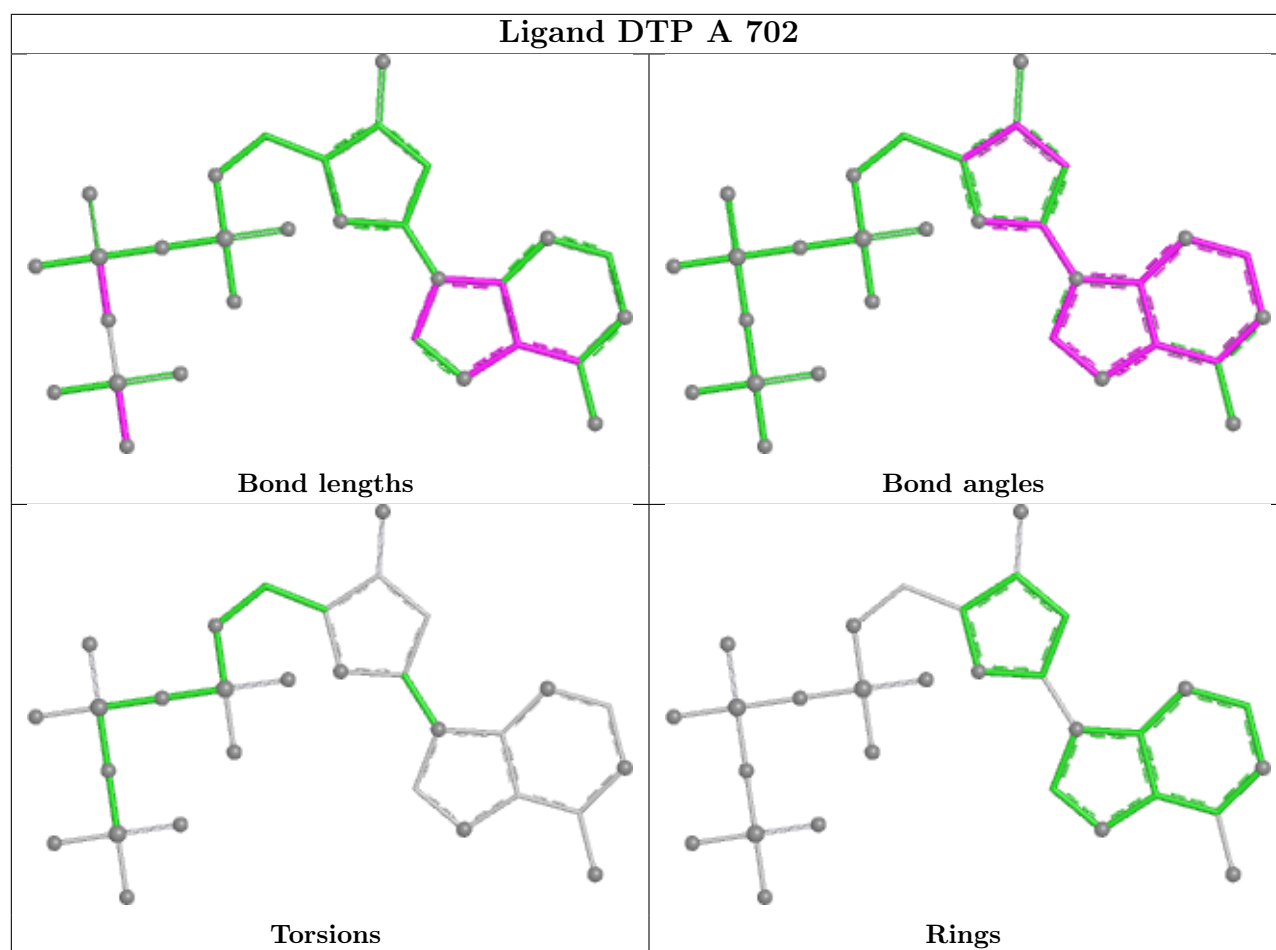




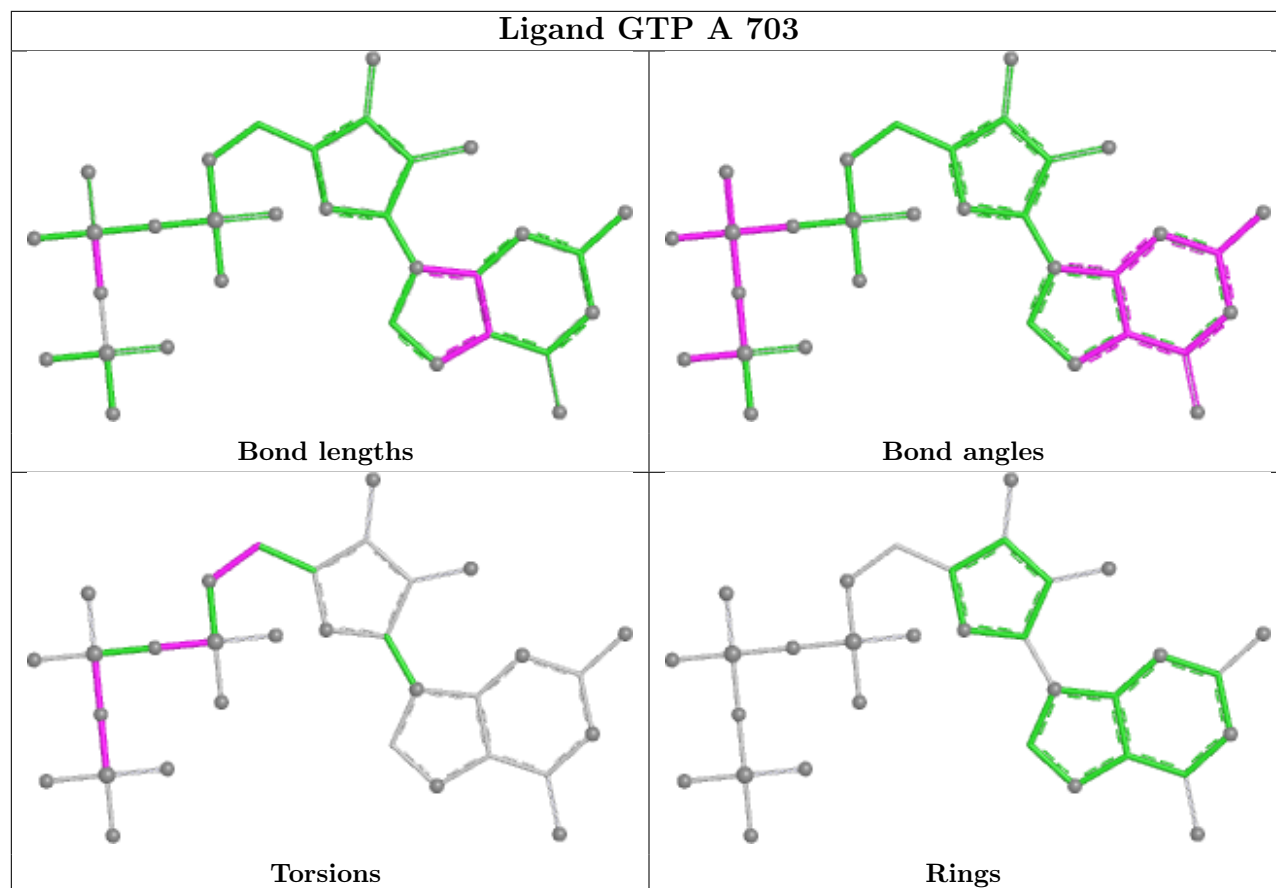




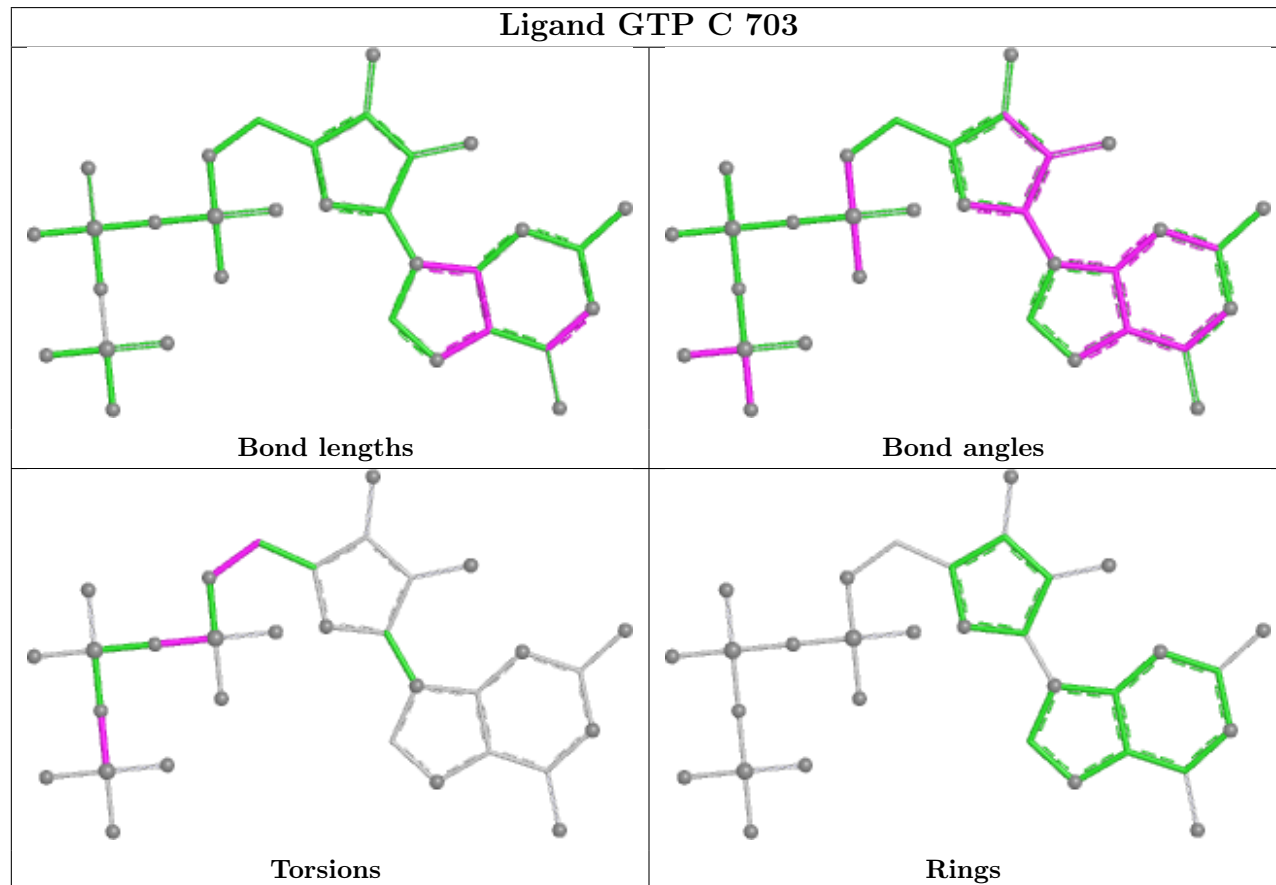


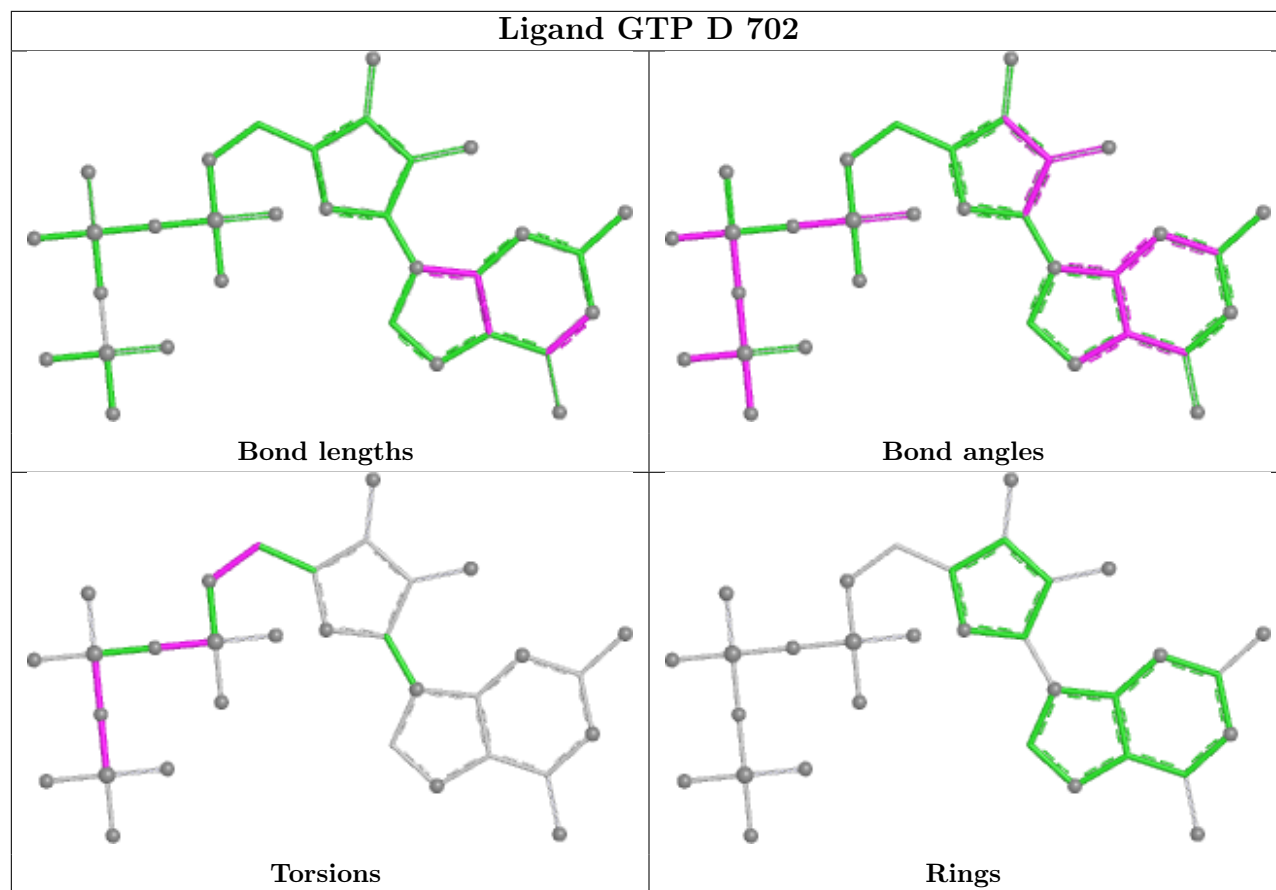


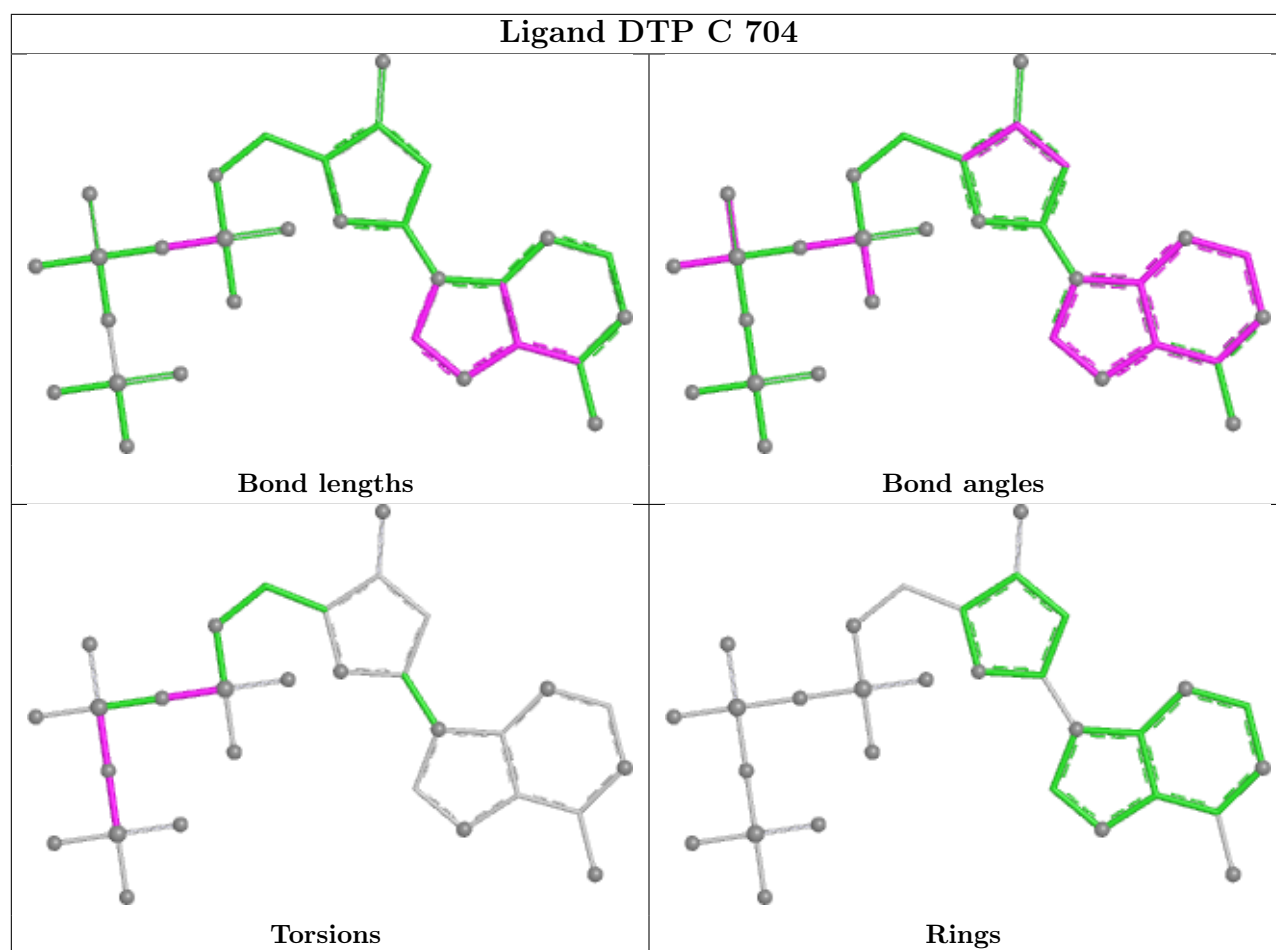
Ligand GTP A 703

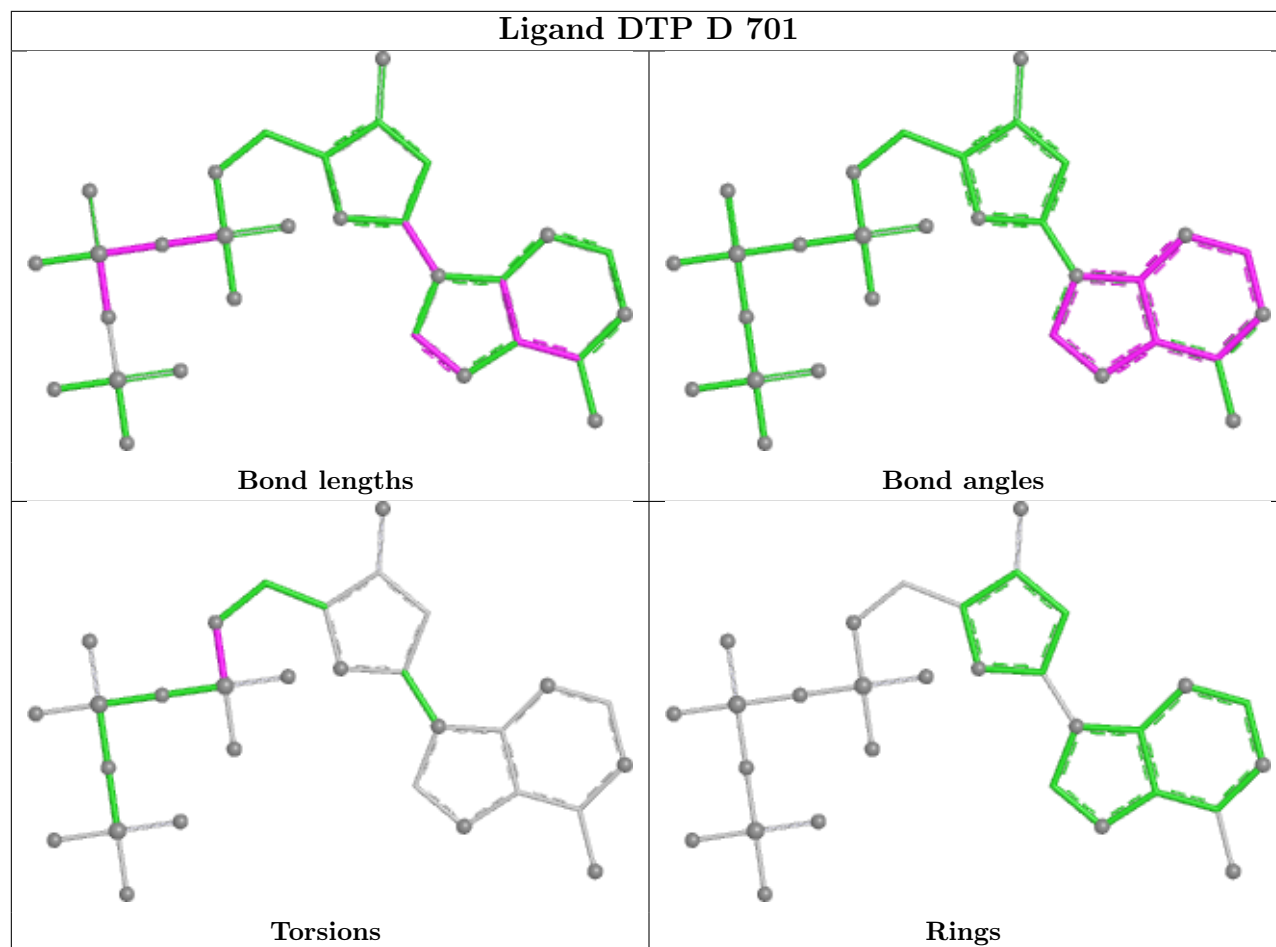


Ligand GTP C 703









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	481/514 (93%)	0.74	37 (7%) 19 19	43, 113, 190, 223	2 (0%)
1	B	481/514 (93%)	0.28	3 (0%) 85 86	29, 91, 150, 190	2 (0%)
1	C	481/514 (93%)	0.47	22 (4%) 37 36	37, 87, 161, 200	2 (0%)
1	D	481/514 (93%)	0.23	6 (1%) 76 76	37, 73, 115, 162	2 (0%)
All	All	1924/2056 (93%)	0.43	68 (3%) 47 44	29, 89, 164, 223	8 (0%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	341	CYS	3.6
1	C	488	LEU	3.6
1	A	284	LEU	3.6
1	C	572	TRP	3.4
1	A	476	LEU	3.3
1	A	457	VAL	3.3
1	C	480	VAL	3.3
1	A	562	LEU	3.2
1	C	498	PHE	3.2
1	C	284	LEU	2.9
1	A	572	TRP	2.9
1	A	502	VAL	2.9
1	C	557	VAL	2.8
1	C	511[A]	GLU	2.8
1	C	482	SER	2.8
1	D	284	LEU	2.8
1	C	493	LEU	2.8
1	B	488	LEU	2.8
1	A	545	PHE	2.8
1	A	468	ILE	2.7
1	A	349	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	584	GLY	2.7
1	A	480	VAL	2.7
1	C	573	CYS	2.6
1	D	205	CYS	2.5
1	A	185	LYS	2.5
1	C	489	LEU	2.5
1	B	284	LEU	2.5
1	A	350	CYS	2.5
1	A	563	TYR	2.4
1	A	441	ALA	2.4
1	A	224	LEU	2.4
1	A	466	ILE	2.4
1	A	493	LEU	2.4
1	A	573	CYS	2.4
1	A	500	VAL	2.4
1	C	492	LYS	2.3
1	A	492	LYS	2.3
1	C	485	PRO	2.3
1	A	229	VAL	2.3
1	C	483	ALA	2.3
1	A	525	ALA	2.3
1	C	476	LEU	2.3
1	A	554	CYS	2.3
1	A	569	PHE	2.3
1	C	490	ASP	2.3
1	A	276	LEU	2.2
1	A	262	GLU	2.2
1	C	491	VAL	2.2
1	A	530	ILE	2.2
1	D	510	GLN	2.2
1	D	491	VAL	2.2
1	A	487	VAL	2.2
1	C	564	ALA	2.1
1	A	418	ALA	2.1
1	A	302	SER	2.1
1	C	462	PRO	2.1
1	D	490	ASP	2.1
1	A	383	ASP	2.1
1	C	587	ILE	2.1
1	C	500	VAL	2.1
1	A	546	ALA	2.0
1	A	431	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	466	ILE	2.0
1	A	475	SER	2.0
1	D	403	GLY	2.0
1	A	191	ILE	2.0
1	A	273	VAL	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 oligosaccharides in this entry.

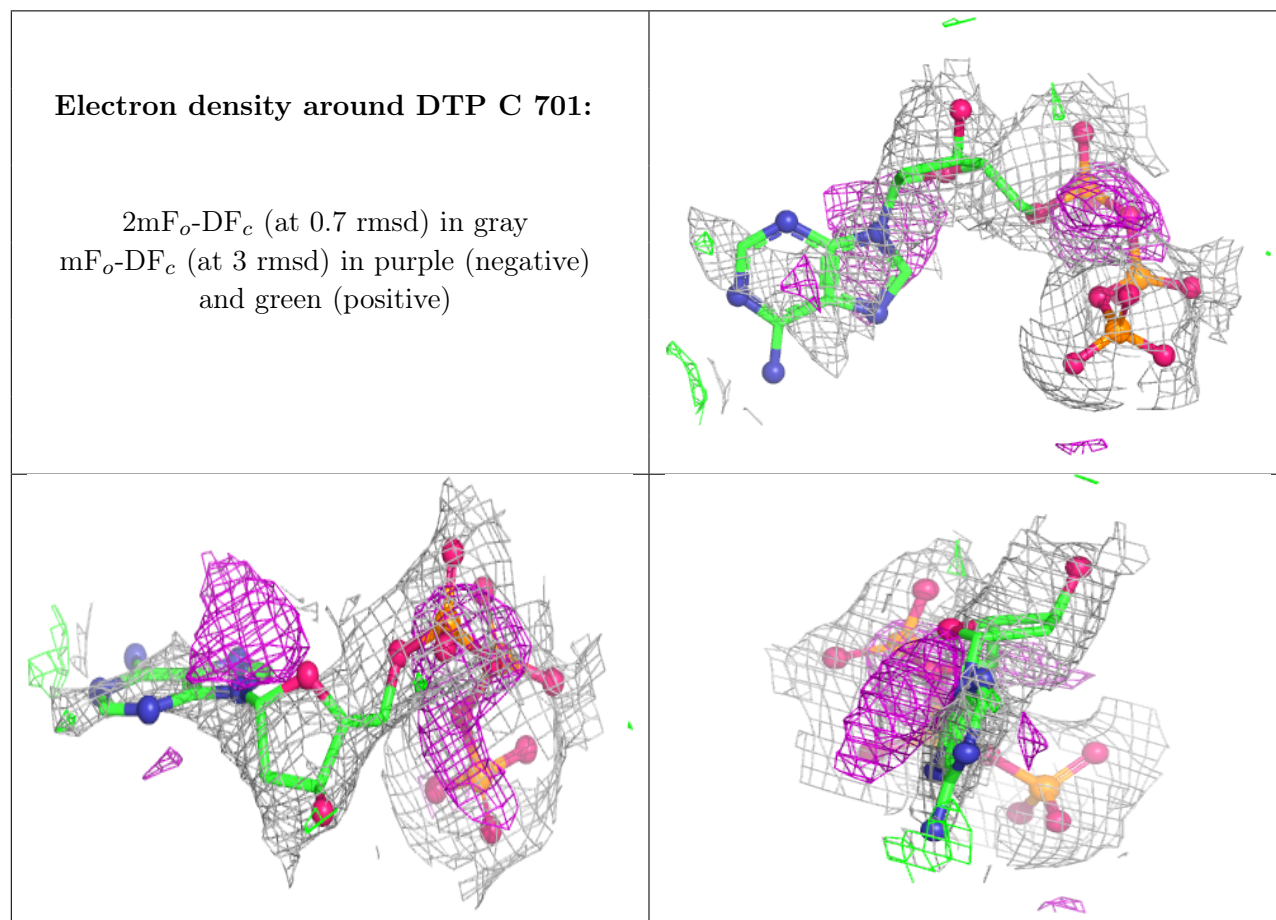
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
2	DTP	C	701	30/30	0.75	0.15	84,115,131,132	0
2	DTP	B	704	30/30	0.76	0.16	81,126,144,148	0
2	DTP	D	701	30/30	0.83	0.13	56,84,110,114	0
3	GTP	A	703	32/32	0.94	0.08	63,72,89,93	0
3	GTP	B	703	32/32	0.95	0.07	63,73,91,94	0
2	DTP	A	702	30/30	0.95	0.08	60,67,89,90	0
3	GTP	C	703	32/32	0.96	0.06	39,43,54,57	0
2	DTP	C	704	30/30	0.97	0.06	52,60,75,79	0
4	MG	B	702	1/1	0.97	0.05	88,88,88,88	0
2	DTP	B	701	30/30	0.98	0.05	41,42,45,46	0
3	GTP	D	702	32/32	0.98	0.05	37,41,45,46	0
4	MG	D	704	1/1	0.98	0.04	72,72,72,72	0
4	MG	C	702	1/1	0.98	0.05	46,46,46,46	0
2	DTP	D	703	30/30	0.98	0.05	42,48,61,63	0
4	MG	A	701	1/1	0.98	0.05	46,46,46,46	0

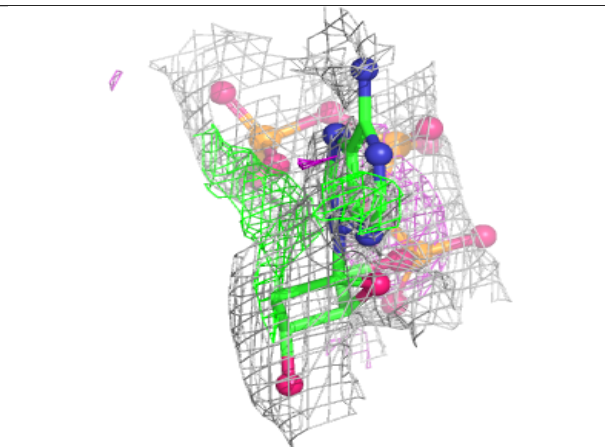
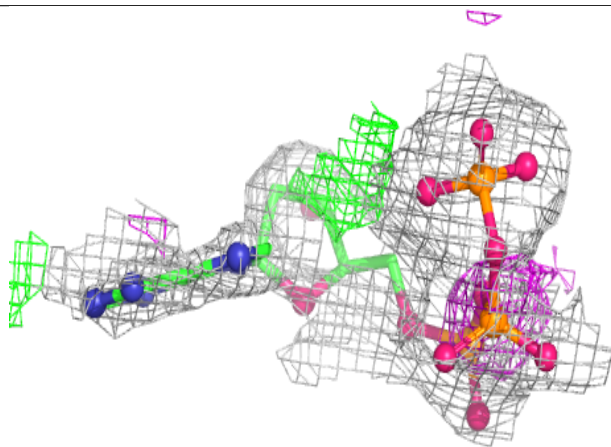
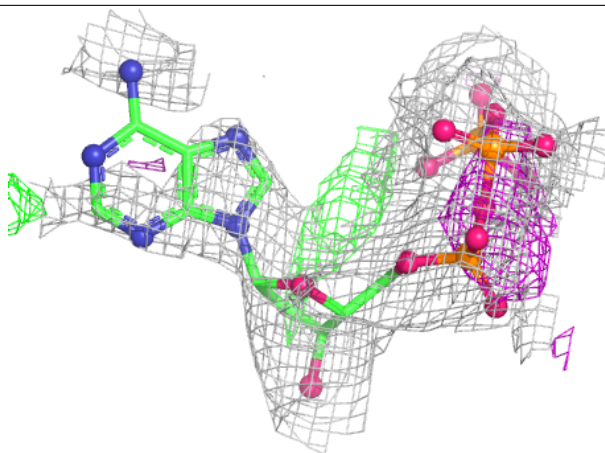
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

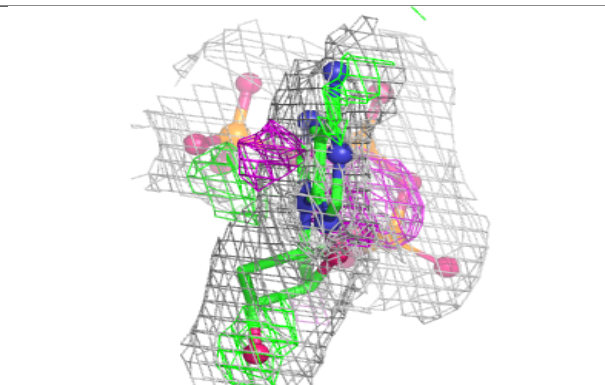
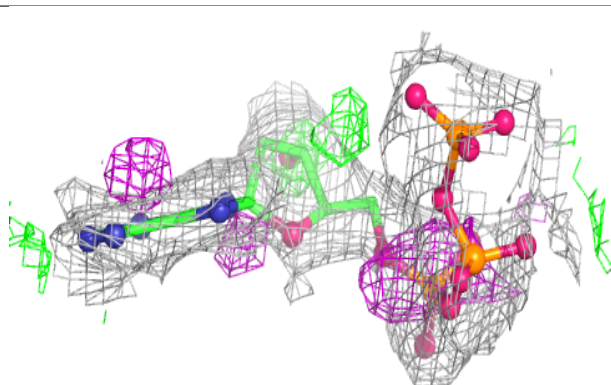
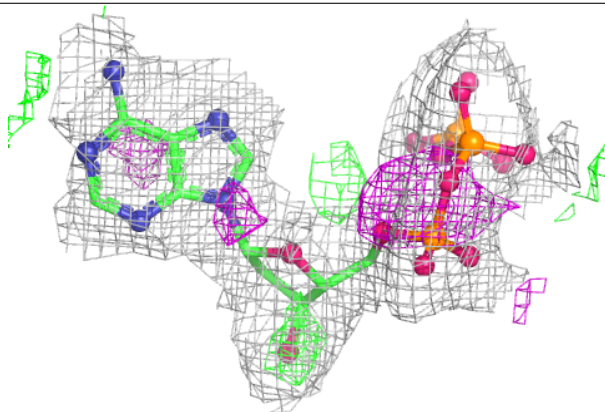


Electron density around DTP B 704:

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

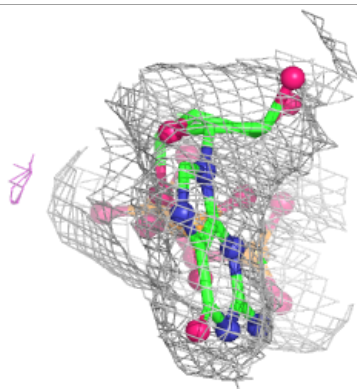
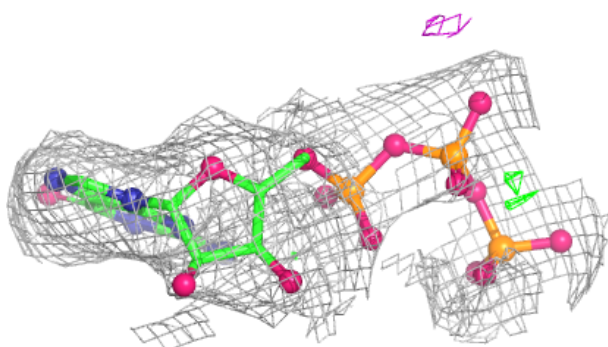
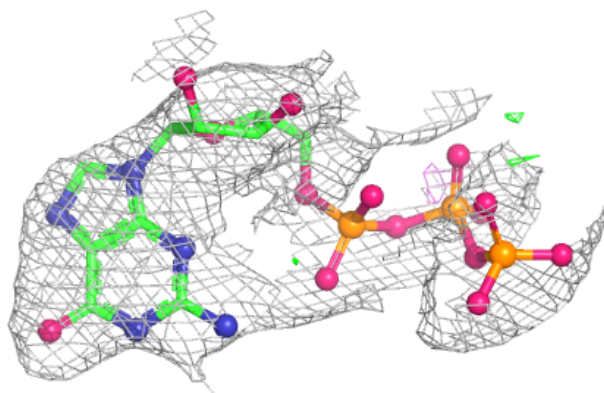
**Electron density around DTP D 701:**

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

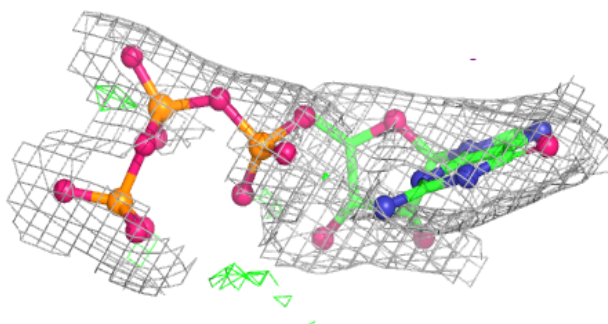
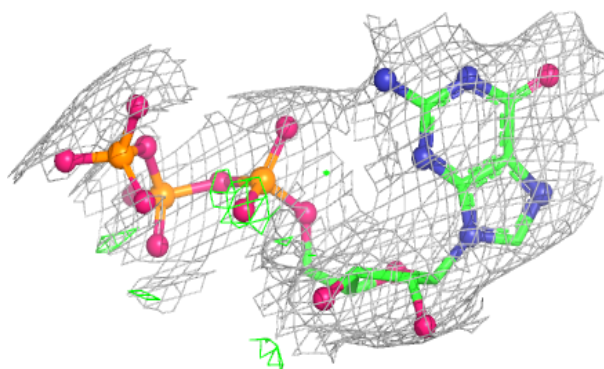


Electron density around GTP A 703:

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

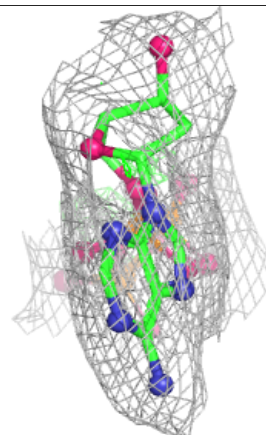
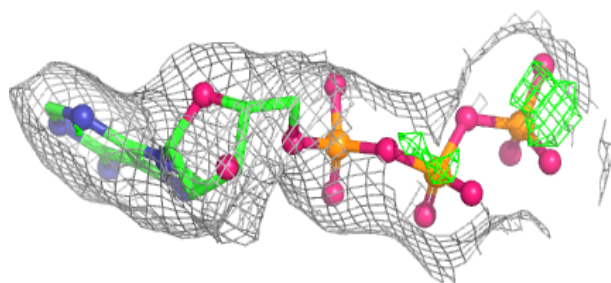
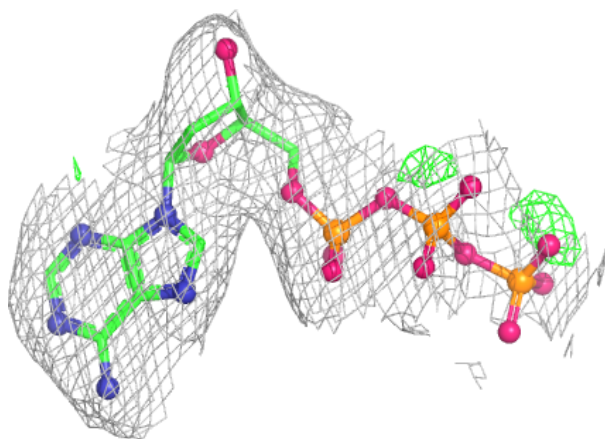
**Electron density around GTP B 703:**

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

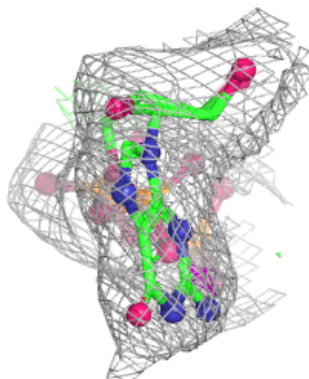
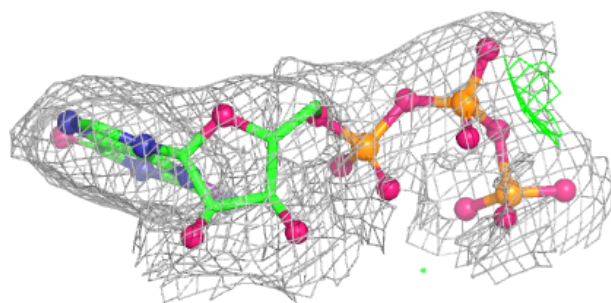
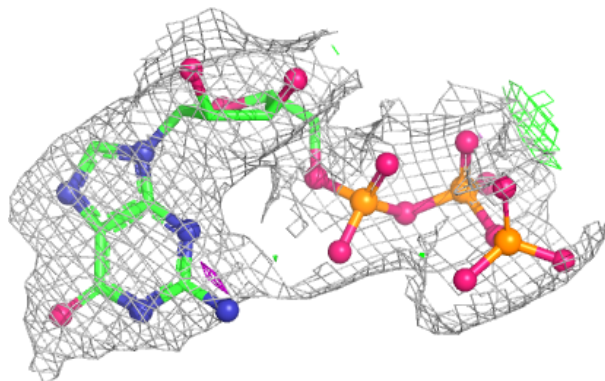


Electron density around DTP A 702:

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

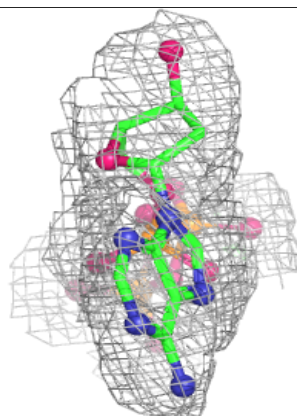
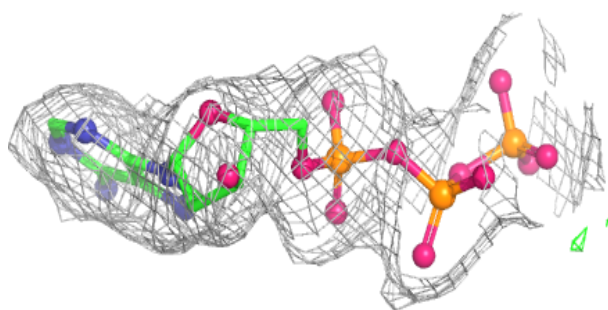
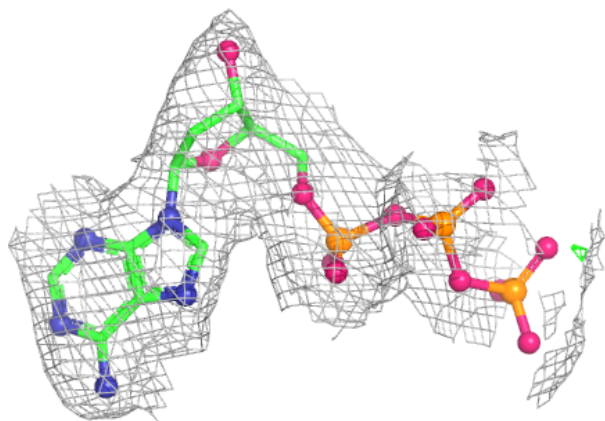
**Electron density around GTP C 703:**

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



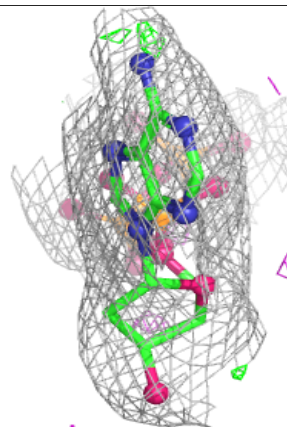
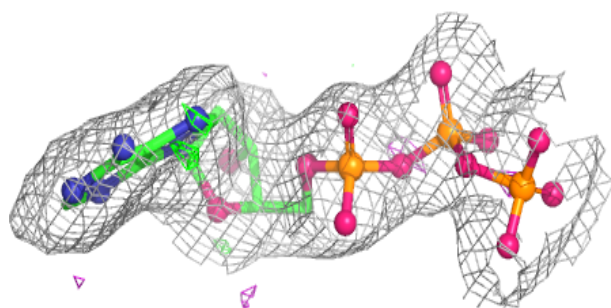
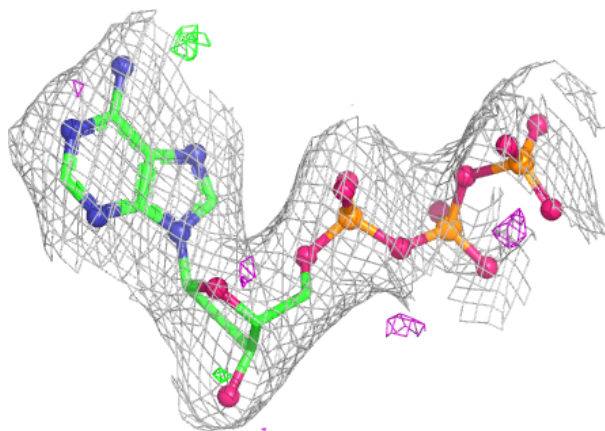
Electron density around DTP C 704:

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

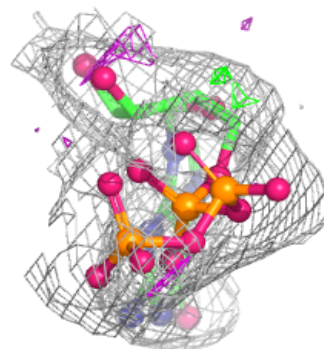
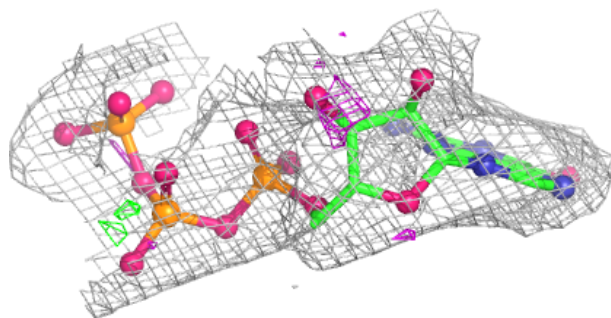
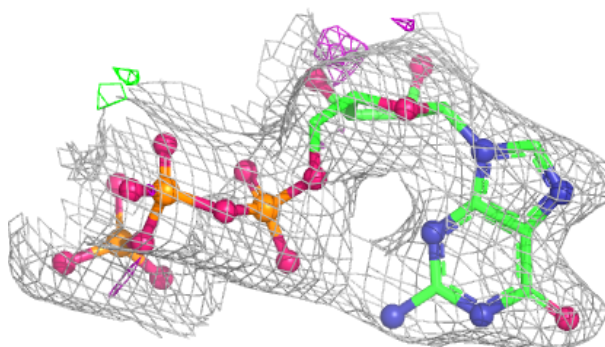


Electron density around DTP B 701:

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

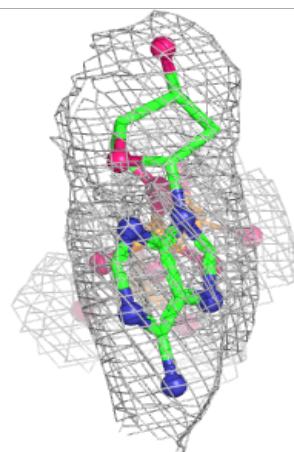
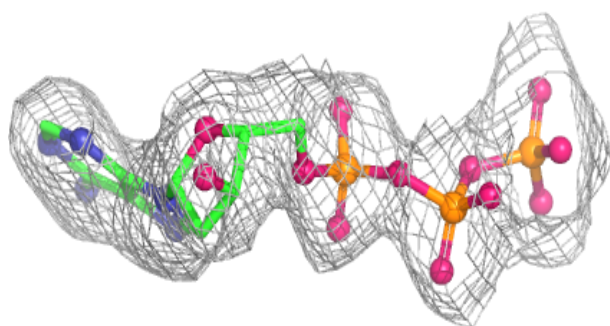
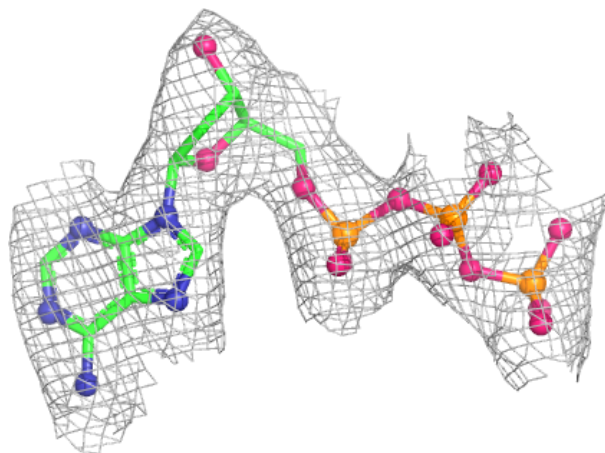
**Electron density around GTP D 702:**

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



Electron density around DTP D 703:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.