



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:32 PM UTC

PDB ID : 4TNZ / pdb_00004tnz
Title : Structure basis of cellular dNTP regulation, SAMHD1-GTP-dATP-dTTP complex
Authors : Ji, X.; Tang, C.; Zhao, Q.; Wang, W.; Xiong, Y.
Deposited on : 2014-06-05
Resolution : 2.38 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

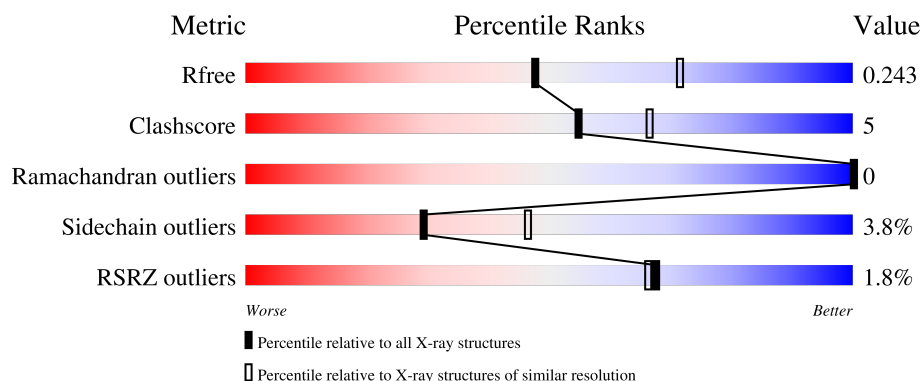
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	% 82% 10% • 7%
1	B	514	5% 82% 11% • 6%
1	C	514	81% 12% • 6%
1	D	514	% 81% 11% • 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16280 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.

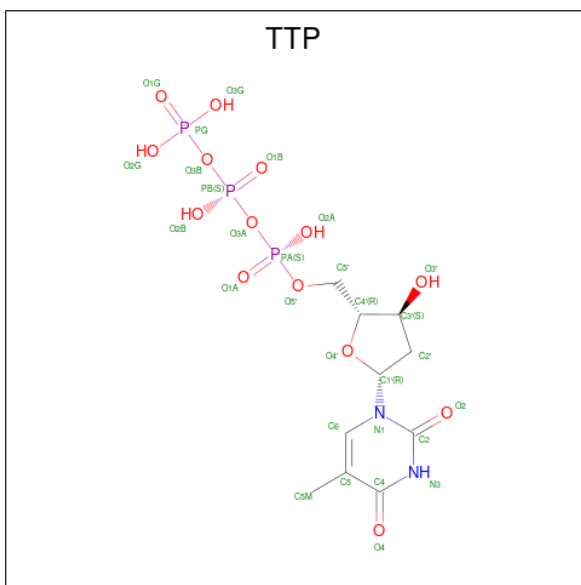
- Molecule 1 is a protein called Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	481	Total	C	N	O	S	0	2	0
			3948	2525	687	715	21			
1	A	480	Total	C	N	O	S	0	2	0
			3940	2521	686	712	21			
1	D	480	Total	C	N	O	S	0	1	0
			3934	2518	684	712	20			
1	B	481	Total	C	N	O	S	0	1	0
			3939	2520	686	712	21			

There are 8 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is THYMIDINE-5'-TRIPHOSPHATE (CCD ID: TTP) (formula: C₁₀H₁₇N₂O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total 29	C 10	N 2	O 14	P 3	0	0
2	A	1	Total 29	C 10	N 2	O 14	P 3	0	0
2	D	1	Total 29	C 10	N 2	O 14	P 3	0	0
2	B	1	Total 29	C 10	N 2	O 14	P 3	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

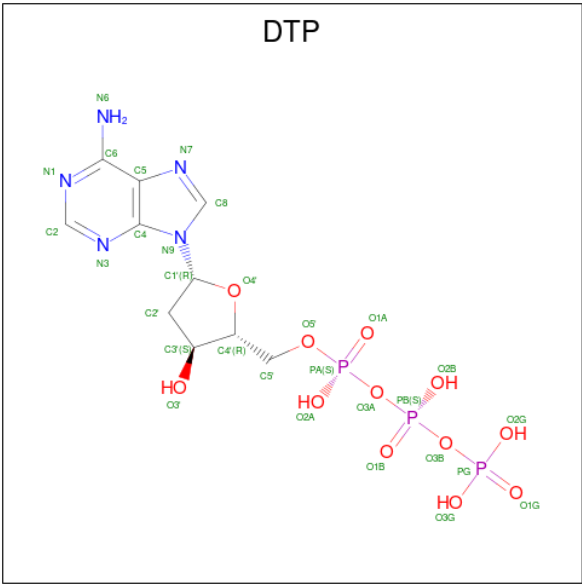
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	2	Total Mg 2 2	0	0
3	A	3	Total Mg 3 3	0	0
3	D	2	Total Mg 2 2	0	0
3	B	1	Total Mg 1 1	0	0

- Molecule 4 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
4	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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



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

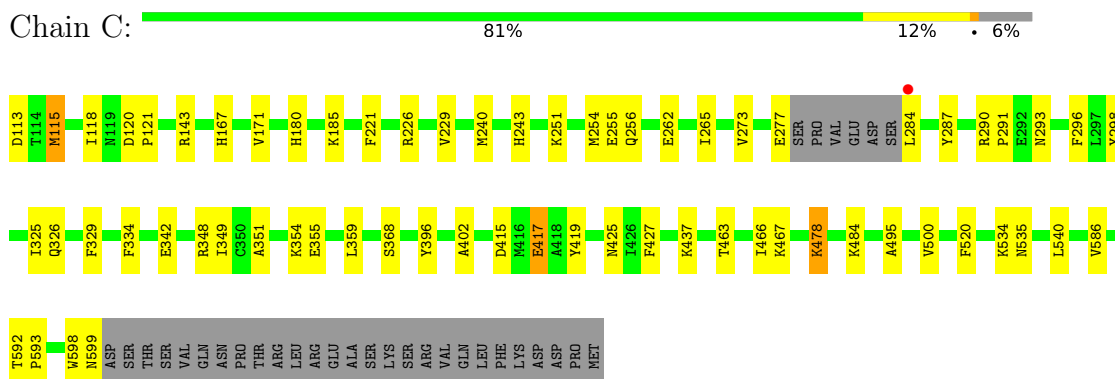
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	53	Total	O	0	0
			53	53		
6	A	47	Total	O	0	0
			47	47		
6	D	32	Total	O	0	0
			32	32		
6	B	15	Total	O	0	0
			15	15		

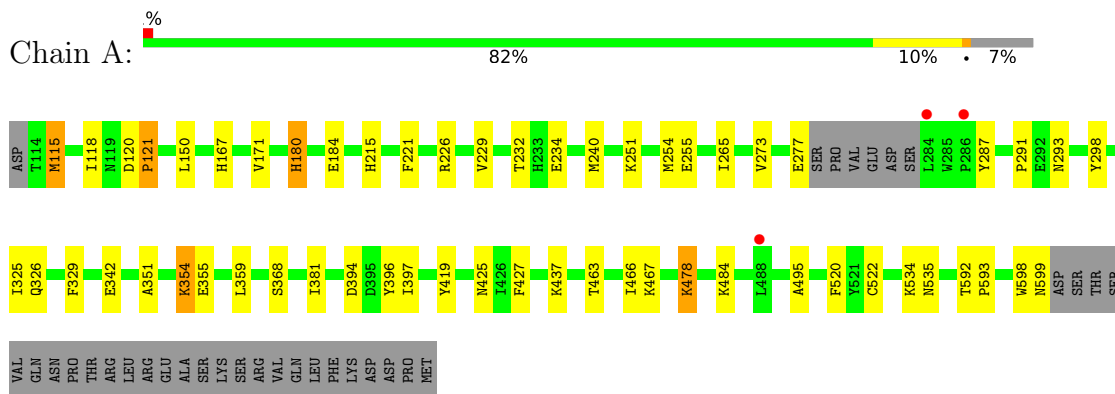
3 Residue-property plots

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.

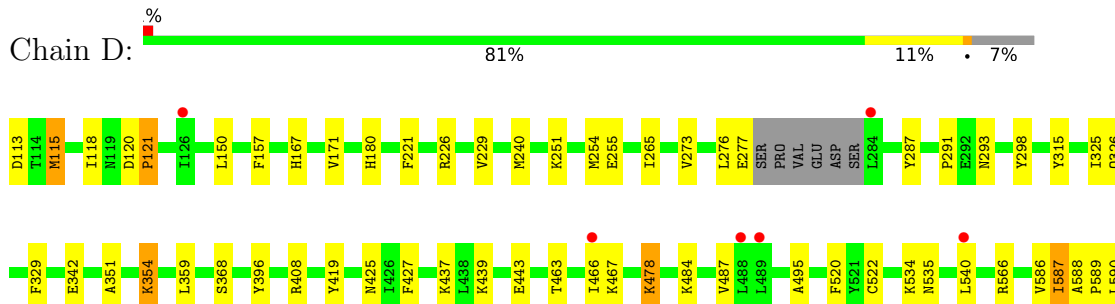
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

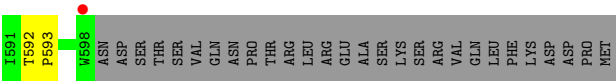


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

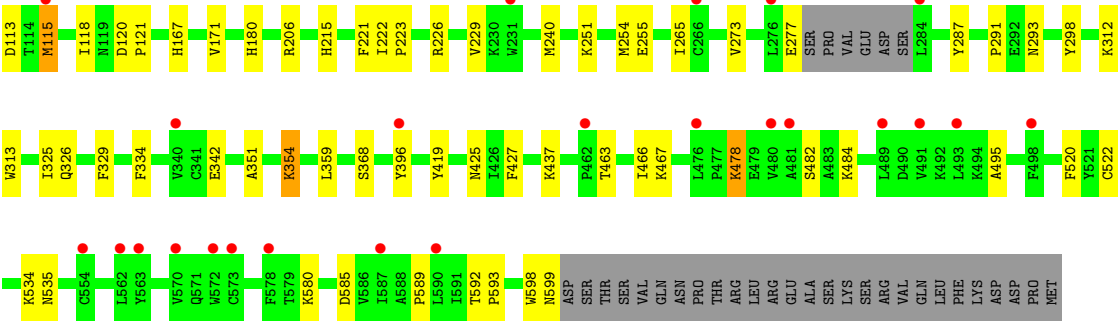
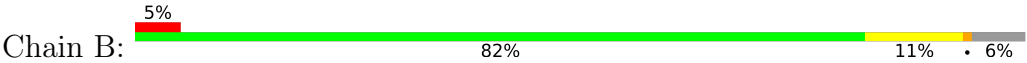


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





● 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	86.13Å 141.75Å 98.47Å 90.00° 116.29° 90.00°	Depositor
Resolution (Å)	88.29 – 2.38 88.29 – 2.38	Depositor EDS
% Data completeness (in resolution range)	98.4 (88.29-2.38) 98.4 (88.29-2.38)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.212 , 0.243 0.212 , 0.243	Depositor DCC
R_{free} test set	4172 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16280	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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: TTP, GTP, DTP, 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	0.79	1/4032 (0.0%)	0.91	2/5442 (0.0%)
1	B	0.73	0/4031	0.89	2/5441 (0.0%)
1	C	0.84	1/4040 (0.0%)	0.91	4/5453 (0.1%)
1	D	0.79	2/4026 (0.0%)	0.91	2/5434 (0.0%)
All	All	0.79	4/16129 (0.0%)	0.90	10/21770 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	121	PRO	C-O	-5.40	1.17	1.24
1	D	157	PHE	C-O	-5.31	1.19	1.24
1	C	500	VAL	C-O	-5.24	1.18	1.24
1	A	121	PRO	C-O	-5.02	1.18	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	221	PHE	N-CA-C	6.13	117.76	111.14
1	B	329	PHE	N-CA-C	6.13	118.51	108.52
1	D	329	PHE	N-CA-C	6.10	118.46	108.52
1	A	221	PHE	N-CA-C	6.09	117.72	111.14
1	C	221	PHE	N-CA-C	5.84	117.45	111.14
1	A	329	PHE	N-CA-C	5.58	117.62	108.52
1	C	329	PHE	N-CA-C	5.27	117.11	108.52
1	D	221	PHE	N-CA-C	5.20	116.75	111.14
1	C	290	ARG	CA-C-N	5.03	125.50	120.52
1	C	290	ARG	C-N-CA	5.03	125.50	120.52

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	3940	0	3926	33	0
1	B	3939	0	3925	37	0
1	C	3948	0	3930	41	0
1	D	3934	0	3920	46	0
2	A	29	0	13	4	0
2	B	29	0	13	8	0
2	C	29	0	13	1	0
2	D	29	0	13	3	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	32	0	12	0	0
4	B	32	0	12	0	0
4	C	32	0	12	1	0
4	D	32	0	12	0	0
5	A	30	0	12	1	0
5	B	30	0	12	1	0
5	C	30	0	12	0	0
5	D	30	0	12	1	0
6	A	47	0	0	3	0
6	B	15	0	0	1	0
6	C	53	0	0	7	0
6	D	32	0	0	2	0
All	All	16280	0	15849	154	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.

All (154) 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:566:ARG:CG	1:D:587:ILE:HD11	1.71	1.20
1:D:566:ARG:HG2	1:D:587:ILE:HD11	1.25	1.12
1:D:566:ARG:CB	1:D:587:ILE:HD11	1.82	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:566:ARG:HB3	1:D:587:ILE:CD1	1.88	1.04
1:D:566:ARG:HB3	1:D:587:ILE:HD11	1.45	0.95
1:D:588:ALA:O	1:D:592:THR:HG23	1.66	0.95
1:C:415:ASP:CG	1:C:417:GLU:HG2	1.97	0.89
1:C:415:ASP:OD2	1:C:417:GLU:HG2	1.73	0.89
1:B:312:LYS:NZ	2:B:702:TTP:O1G	2.06	0.88
1:D:408:ARG:HD2	6:D:831:HOH:O	1.86	0.75
1:D:566:ARG:HG2	1:D:587:ILE:CD1	2.11	0.74
1:D:589:PRO:O	1:D:593:PRO:HD3	1.88	0.73
1:C:415:ASP:OD1	1:C:417:GLU:HG2	1.90	0.70
1:A:355:GLU:OE1	6:A:822:HOH:O	2.09	0.70
1:C:402:ALA:HB2	1:C:417:GLU:HG3	1.72	0.70
1:C:417:GLU:H	1:C:417:GLU:CD	1.97	0.70
1:A:226:ARG:O	1:A:229:VAL:HG12	1.93	0.69
1:D:226:ARG:O	1:D:229:VAL:HG12	1.93	0.68
1:B:226:ARG:O	1:B:229:VAL:HG12	1.93	0.68
1:B:291:PRO:HG2	1:B:293:ASN:OD1	1.94	0.68
1:C:326:GLN:HG2	1:A:326:GLN:HG2	1.76	0.68
1:A:150:LEU:CD2	2:A:703:TTP:H2'1	2.23	0.68
1:C:226:ARG:O	1:C:229:VAL:HG12	1.94	0.67
1:D:326:GLN:HG2	1:B:326:GLN:HG2	1.76	0.67
1:C:291:PRO:HG2	1:C:293:ASN:OD1	1.94	0.66
1:A:291:PRO:HG2	1:A:293:ASN:OD1	1.96	0.66
1:D:291:PRO:HG2	1:D:293:ASN:OD1	1.96	0.66
1:C:120:ASP:OD1	1:C:121:PRO:HD2	1.96	0.65
1:D:590:LEU:O	1:D:593:PRO:HD2	1.95	0.65
1:D:592:THR:N	1:D:593:PRO:CD	2.61	0.64
1:C:415:ASP:OD1	1:C:417:GLU:CG	2.46	0.64
1:B:120:ASP:OD1	1:B:121:PRO:HD2	1.98	0.64
1:D:120:ASP:OD1	1:D:121:PRO:HD2	1.98	0.64
1:B:589:PRO:O	1:B:593:PRO:HD3	1.98	0.64
1:D:566:ARG:CG	1:D:587:ILE:CD1	2.63	0.63
1:A:120:ASP:OD1	1:A:121:PRO:HD2	1.99	0.63
1:C:417:GLU:N	1:C:417:GLU:OE2	2.31	0.62
1:C:586:VAL:HG11	1:A:522[A]:CYS:SG	2.39	0.62
1:B:312:LYS:CE	2:B:702:TTP:O1G	2.48	0.61
1:C:348:ARG:HD3	6:C:835:HOH:O	2.00	0.61
1:C:262:GLU:HG3	6:C:843:HOH:O	2.01	0.60
1:D:566:ARG:HD3	1:D:587:ILE:CG1	2.31	0.60
1:C:425:ASN:OD1	1:B:425:ASN:OD1	2.19	0.59
1:D:566:ARG:HB3	1:D:587:ILE:HD13	1.80	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:GLU:OE1	6:C:849:HOH:O	2.17	0.58
1:A:287:TYR:CD1	1:A:298:TYR:CE1	2.93	0.57
1:B:287:TYR:CD1	1:B:298:TYR:CE1	2.93	0.57
1:B:206:ARG:NH2	2:B:702:TTP:O2B	2.38	0.56
1:C:287:TYR:CD1	1:C:298:TYR:CE1	2.95	0.55
1:B:215:HIS:CE1	2:B:702:TTP:O2A	2.59	0.55
1:D:240:MET:CE	1:D:419:TYR:HD2	2.21	0.53
1:B:313:TRP:CZ2	1:B:334:PHE:HD1	2.27	0.53
1:D:589:PRO:O	1:D:593:PRO:CD	2.55	0.53
1:C:240:MET:CE	1:C:419:TYR:HD2	2.23	0.52
1:C:254:MET:HE1	1:C:265:ILE:HG13	1.90	0.52
1:A:240:MET:CE	1:A:419:TYR:HD2	2.23	0.52
1:C:415:ASP:OD1	1:C:417:GLU:OE1	2.27	0.52
1:D:287:TYR:CD1	1:D:298:TYR:CE1	2.98	0.52
1:C:415:ASP:OD1	1:C:417:GLU:CD	2.52	0.51
1:C:417:GLU:CD	1:C:417:GLU:N	2.67	0.51
1:C:592:THR:N	1:C:593:PRO:CD	2.73	0.51
1:A:167:HIS:O	1:A:171:VAL:HG23	2.10	0.51
1:A:254:MET:HE1	1:A:265:ILE:HG13	1.91	0.51
1:D:167:HIS:O	1:D:171:VAL:HG23	2.10	0.51
1:C:167:HIS:O	1:C:171:VAL:HG23	2.10	0.51
1:A:592:THR:N	1:A:593:PRO:CD	2.73	0.51
1:B:592:THR:N	1:B:593:PRO:CD	2.73	0.51
1:B:240:MET:CE	1:B:419:TYR:HD2	2.24	0.51
1:B:167:HIS:O	1:B:171:VAL:HG23	2.11	0.51
1:A:397:ILE:HB	6:A:832:HOH:O	2.10	0.51
1:B:254:MET:HE1	1:B:265:ILE:HG13	1.91	0.50
1:B:312:LYS:HE3	2:B:702:TTP:O1G	2.11	0.50
1:C:185:LYS:HD2	6:C:839:HOH:O	2.11	0.50
1:D:586:VAL:HG11	1:B:522[A]:CYS:SG	2.51	0.50
1:B:215:HIS:NE2	2:B:702:TTP:O5'	2.40	0.50
1:C:334:PHE:HA	6:C:849:HOH:O	2.12	0.50
1:D:254:MET:HE1	1:D:265:ILE:HG13	1.94	0.49
1:C:256:GLN:HG3	6:C:801:HOH:O	2.12	0.49
1:A:598:TRP:O	1:A:599:ASN:HB2	2.12	0.49
2:B:702:TTP:O3G	2:B:702:TTP:O1B	2.29	0.49
1:A:354:LYS:NZ	5:A:701:DTP:O1A	2.45	0.48
1:D:276:LEU:C	6:D:830:HOH:O	2.56	0.48
1:B:589:PRO:O	1:B:593:PRO:CD	2.61	0.48
1:B:427:PHE:CD1	1:B:427:PHE:C	2.92	0.48
1:B:580:LYS:CE	1:B:585:ASP:OD2	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:ASN:OD1	1:D:425:ASN:OD1	2.30	0.48
1:D:315:TYR:CE2	2:D:702:TTP:H5'1	2.49	0.47
2:D:702:TTP:O2G	2:D:702:TTP:O2B	2.32	0.47
1:B:313:TRP:CZ2	1:B:334:PHE:CD1	3.02	0.47
1:A:396:TYR:CD1	1:A:437:LYS:HD2	2.50	0.47
1:D:354:LYS:NZ	5:D:705:DTP:O1A	2.48	0.47
1:D:427:PHE:C	1:D:427:PHE:CD1	2.93	0.46
1:B:478:LYS:HE2	1:B:495:ALA:HB1	1.98	0.46
1:B:463:THR:O	1:B:466:ILE:HG12	2.15	0.46
1:B:396:TYR:CD1	1:B:437:LYS:HD2	2.50	0.46
1:A:215:HIS:NE2	2:A:703:TTP:O5'	2.49	0.46
1:A:463:THR:O	1:A:466:ILE:HG12	2.16	0.46
1:D:478:LYS:HE2	1:D:495:ALA:HB1	1.98	0.46
1:D:592:THR:N	1:D:593:PRO:HD3	2.30	0.46
1:B:482:SER:C	6:B:814:HOH:O	2.59	0.46
1:A:478:LYS:HE2	1:A:495:ALA:HB1	1.98	0.46
1:D:463:THR:O	1:D:466:ILE:HG12	2.16	0.46
1:A:427:PHE:C	1:A:427:PHE:CD1	2.94	0.46
1:C:251:LYS:O	1:C:255:GLU:HG3	2.16	0.45
1:C:427:PHE:CD1	1:C:427:PHE:C	2.94	0.45
1:D:396:TYR:CD1	1:D:437:LYS:HD2	2.51	0.45
1:C:478:LYS:HE2	1:C:495:ALA:HB1	1.98	0.45
4:C:703:GTP:O1B	4:C:703:GTP:O1A	2.33	0.45
1:A:287:TYR:HB3	1:A:298:TYR:OH	2.17	0.45
1:D:251:LYS:O	1:D:255:GLU:HG3	2.16	0.45
1:B:598:TRP:O	1:B:599:ASN:HB2	2.17	0.45
1:C:396:TYR:CD1	1:C:437:LYS:HD2	2.52	0.45
1:D:566:ARG:HD3	1:D:587:ILE:HG13	1.97	0.45
1:A:251:LYS:O	1:A:255:GLU:HG3	2.17	0.44
1:C:463:THR:O	1:C:466:ILE:HG12	2.17	0.44
1:B:580:LYS:NZ	1:B:585:ASP:OD2	2.50	0.44
1:D:487:VAL:HG22	1:D:590:LEU:CD1	2.48	0.44
1:B:251:LYS:O	1:B:255:GLU:HG3	2.17	0.44
1:B:215:HIS:HE1	2:B:702:TTP:O2A	2.01	0.44
1:D:287:TYR:HB3	1:D:298:TYR:OH	2.18	0.43
1:C:243:HIS:CE1	1:C:417:GLU:OE2	2.71	0.43
1:C:325:ILE:CG2	1:C:326:GLN:N	2.81	0.43
1:D:566:ARG:CB	1:D:587:ILE:CD1	2.57	0.43
1:B:287:TYR:HB3	1:B:298:TYR:OH	2.17	0.43
1:C:287:TYR:HB3	1:C:298:TYR:OH	2.18	0.43
1:A:215:HIS:HE2	2:A:703:TTP:PA	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:598:TRP:O	1:C:599:ASN:HB2	2.18	0.43
1:D:351:ALA:O	1:D:520:PHE:HA	2.18	0.43
1:D:487:VAL:HG22	1:D:590:LEU:HD12	2.01	0.43
1:A:351:ALA:O	1:A:520:PHE:HA	2.19	0.42
2:C:701:TTP:O2G	2:C:701:TTP:O1B	2.36	0.42
1:D:150:LEU:CD2	2:D:702:TTP:H2'1	2.50	0.42
1:B:351:ALA:O	1:B:520:PHE:HA	2.19	0.42
1:C:143:ARG:HD3	6:C:833:HOH:O	2.20	0.42
1:C:115:MET:SD	1:C:115:MET:C	3.02	0.42
1:A:150:LEU:HD22	2:A:703:TTP:H2'1	1.99	0.42
1:B:354:LYS:NZ	5:B:701:DTP:O2A	2.53	0.42
1:A:232:THR:HB	1:A:234:GLU:OE1	2.19	0.42
1:A:381:ILE:HD12	1:A:381:ILE:HA	1.94	0.42
1:D:566:ARG:HD3	1:D:587:ILE:HG12	2.00	0.42
1:A:115:MET:C	1:A:115:MET:SD	3.03	0.41
1:C:326:GLN:CG	1:A:326:GLN:HG2	2.48	0.41
1:C:351:ALA:O	1:C:520:PHE:HA	2.20	0.41
1:D:439:LYS:O	1:D:443:GLU:HG2	2.20	0.41
1:B:222:ILE:HB	1:B:223:PRO:HD3	2.02	0.41
1:D:325:ILE:CG2	1:D:326:GLN:N	2.83	0.41
1:B:115:MET:C	1:B:115:MET:SD	3.04	0.41
1:D:115:MET:C	1:D:115:MET:SD	3.03	0.41
1:A:394:ASP:HA	6:A:832:HOH:O	2.21	0.41
1:A:325:ILE:CG2	1:A:326:GLN:N	2.82	0.40
1:A:180:HIS:O	1:A:184:GLU:HG2	2.20	0.40
1:D:592:THR:OG1	1:D:593:PRO:HD3	2.22	0.40
1:B:325:ILE:CG2	1:B:326:GLN:N	2.82	0.40
1:C:296:PHE:HB2	1:C:349:ILE:HG13	2.04	0.40

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	478/514 (93%)	470 (98%)	8 (2%)	0	100	100
1	B	478/514 (93%)	469 (98%)	9 (2%)	0	100	100
1	C	479/514 (93%)	471 (98%)	8 (2%)	0	100	100
1	D	477/514 (93%)	468 (98%)	9 (2%)	0	100	100
All	All	1912/2056 (93%)	1878 (98%)	34 (2%)	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	428/459 (93%)	414 (97%)	14 (3%)	33	52
1	B	428/459 (93%)	413 (96%)	15 (4%)	32	50
1	C	429/459 (94%)	411 (96%)	18 (4%)	26	42
1	D	427/459 (93%)	409 (96%)	18 (4%)	26	42
All	All	1712/1836 (93%)	1647 (96%)	65 (4%)	29	46

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	113	ASP
1	C	115	MET
1	C	118	ILE
1	C	180	HIS
1	C	273	VAL
1	C	277	GLU
1	C	284	LEU
1	C	342	GLU
1	C	354	LYS
1	C	359	LEU
1	C	368	SER
1	C	417	GLU
1	C	467	LYS

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Mol	Chain	Res	Type
1	C	478	LYS
1	C	484	LYS
1	C	534	LYS
1	C	535	ASN
1	C	540	LEU
1	A	115	MET
1	A	118	ILE
1	A	180	HIS
1	A	273	VAL
1	A	277	GLU
1	A	342	GLU
1	A	354	LYS
1	A	359	LEU
1	A	368	SER
1	A	467	LYS
1	A	478	LYS
1	A	484	LYS
1	A	534	LYS
1	A	535	ASN
1	D	113	ASP
1	D	115	MET
1	D	118	ILE
1	D	180	HIS
1	D	273	VAL
1	D	277	GLU
1	D	342	GLU
1	D	354	LYS
1	D	359	LEU
1	D	368	SER
1	D	467	LYS
1	D	478	LYS
1	D	484	LYS
1	D	522	CYS
1	D	534	LYS
1	D	535	ASN
1	D	540	LEU
1	D	587	ILE
1	B	113	ASP
1	B	115	MET
1	B	118	ILE
1	B	180	HIS
1	B	273	VAL

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Mol	Chain	Res	Type
1	B	277	GLU
1	B	342	GLU
1	B	354	LYS
1	B	359	LEU
1	B	368	SER
1	B	467	LYS
1	B	478	LYS
1	B	484	LYS
1	B	534	LYS
1	B	535	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	140	GLN
1	C	200	GLN
1	C	235	GLN
1	C	243	HIS
1	C	248	ASN
1	C	328	ASN
1	C	364	HIS
1	A	140	GLN
1	A	149	GLN
1	A	200	GLN
1	A	235	GLN
1	A	243	HIS
1	A	248	ASN
1	A	328	ASN
1	A	364	HIS
1	D	140	GLN
1	D	149	GLN
1	D	163	ASN
1	D	200	GLN
1	D	235	GLN
1	D	243	HIS
1	D	248	ASN
1	D	328	ASN
1	D	364	HIS
1	D	517	HIS
1	D	571	GLN
1	D	594	GLN
1	B	140	GLN

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Mol	Chain	Res	Type
1	B	149	GLN
1	B	200	GLN
1	B	235	GLN
1	B	243	HIS
1	B	248	ASN
1	B	328	ASN
1	B	364	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
2	TTP	B	702	3	29,30,30	1.37	4 (13%)	43,47,47	2.02	11 (25%)
4	GTP	A	705	3	33,34,34	1.45	6 (18%)	50,54,54	1.92	20 (40%)
4	GTP	C	703	3	33,34,34	1.33	4 (12%)	50,54,54	1.81	9 (18%)
5	DTP	C	704	3	31,32,32	1.51	6 (19%)	46,50,50	1.62	7 (15%)
2	TTP	A	703	3	29,30,30	1.61	8 (27%)	43,47,47	2.17	8 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DTP	A	701	3	31,32,32	1.56	8 (25%)	46,50,50	1.58	7 (15%)
5	DTP	B	701	3	31,32,32	1.80	8 (25%)	46,50,50	1.45	8 (17%)
4	GTP	D	704	3	33,34,34	1.49	7 (21%)	50,54,54	1.82	13 (26%)
5	DTP	D	705	3	31,32,32	1.82	7 (22%)	46,50,50	1.77	11 (23%)
2	TTP	C	701	3	29,30,30	1.55	5 (17%)	43,47,47	2.03	10 (23%)
4	GTP	B	704	3	33,34,34	1.48	6 (18%)	50,54,54	1.55	10 (20%)
2	TTP	D	702	3	29,30,30	1.40	6 (20%)	43,47,47	1.83	7 (16%)

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	TTP	B	702	3	-	6/22/34/34	0/2/2/2
4	GTP	A	705	3	-	7/22/38/38	0/3/3/3
4	GTP	C	703	3	-	6/22/38/38	0/3/3/3
5	DTP	C	704	3	-	4/22/34/34	0/3/3/3
2	TTP	A	703	3	-	5/22/34/34	0/2/2/2
5	DTP	A	701	3	-	6/22/34/34	0/3/3/3
5	DTP	B	701	3	-	2/22/34/34	0/3/3/3
4	GTP	D	704	3	-	6/22/38/38	0/3/3/3
5	DTP	D	705	3	-	6/22/34/34	0/3/3/3
2	TTP	C	701	3	-	5/22/34/34	0/2/2/2
4	GTP	B	704	3	-	4/22/38/38	0/3/3/3
2	TTP	D	702	3	-	7/22/34/34	0/2/2/2

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	701	DTP	C5-C4	5.38	1.48	1.39
5	D	705	DTP	PA-O3A	5.07	1.65	1.59
5	D	705	DTP	C5-C4	4.64	1.47	1.39
4	A	705	GTP	C5-N7	-3.83	1.31	1.39
4	C	703	GTP	C6-N1	-3.83	1.31	1.38
2	B	702	TTP	C4-C5	3.80	1.51	1.44
2	C	701	TTP	PB-O3B	3.74	1.63	1.59
5	C	704	DTP	C5-C4	3.72	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	701	DTP	PA-O3A	3.58	1.63	1.59
2	A	703	TTP	PB-O3B	3.55	1.63	1.59
2	D	702	TTP	PB-O3B	3.46	1.63	1.59
4	B	704	GTP	C5-N7	-3.42	1.32	1.39
4	D	704	GTP	C6-N1	-3.33	1.32	1.38
5	A	701	DTP	C5-C4	3.33	1.45	1.39
4	A	705	GTP	C4-N9	-3.29	1.29	1.38
2	D	702	TTP	C2-N1	3.22	1.43	1.38
4	B	704	GTP	C4-N9	-3.16	1.30	1.38
5	C	704	DTP	PA-O3A	3.14	1.62	1.59
5	C	704	DTP	C4-N9	-3.08	1.31	1.37
2	A	703	TTP	C4-C5	3.06	1.49	1.44
5	A	701	DTP	O4'-C4'	-3.04	1.38	1.45
4	B	704	GTP	C5-C4	3.00	1.47	1.38
5	B	701	DTP	C4-N9	-2.98	1.31	1.37
5	D	705	DTP	C8-N9	-2.90	1.32	1.37
4	D	704	GTP	C5-C4	2.89	1.46	1.38
5	D	705	DTP	C5-N7	-2.88	1.33	1.39
4	D	704	GTP	PB-O3A	2.84	1.62	1.59
5	D	705	DTP	C8-N7	2.84	1.37	1.31
2	B	702	TTP	C2-N1	2.83	1.42	1.38
5	A	701	DTP	O4'-C1'	2.82	1.48	1.42
5	D	705	DTP	PB-O3A	2.81	1.62	1.59
4	D	704	GTP	PA-O3A	2.80	1.62	1.59
2	C	701	TTP	C4-N3	-2.80	1.33	1.38
2	A	703	TTP	PB-O3A	2.79	1.62	1.59
5	A	701	DTP	C8-N9	-2.79	1.32	1.37
5	A	701	DTP	C4-N9	-2.75	1.32	1.37
4	D	704	GTP	C5-N7	-2.73	1.33	1.39
4	A	705	GTP	PB-O3A	2.73	1.62	1.59
5	B	701	DTP	C5-N7	-2.71	1.34	1.39
5	B	701	DTP	C8-N7	2.71	1.36	1.31
4	C	703	GTP	C5-C4	2.69	1.46	1.38
2	C	701	TTP	C4-C5	2.64	1.49	1.44
4	B	704	GTP	PB-O3A	2.64	1.62	1.59
2	C	701	TTP	PA-O3A	2.61	1.62	1.59
5	C	704	DTP	PB-O3B	2.60	1.62	1.59
4	A	705	GTP	C5-C4	2.58	1.45	1.38
2	C	701	TTP	C6-N1	-2.52	1.33	1.38
4	B	704	GTP	C6-N1	-2.51	1.34	1.38
2	A	703	TTP	C2-N1	2.49	1.42	1.38
2	A	703	TTP	C4-N3	-2.48	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	704	GTP	PA-O3A	2.41	1.62	1.59
2	D	702	TTP	C4-N3	-2.37	1.34	1.38
2	B	702	TTP	C6-C5	2.34	1.38	1.34
4	A	705	GTP	C8-N9	-2.31	1.32	1.37
2	A	703	TTP	C2-N3	-2.30	1.34	1.38
5	D	705	DTP	C5-C6	2.28	1.47	1.41
5	A	701	DTP	C8-N7	2.25	1.36	1.31
5	A	701	DTP	C2-N1	2.23	1.37	1.33
5	C	704	DTP	PB-O3A	2.22	1.61	1.59
4	C	703	GTP	C5-N7	-2.19	1.34	1.39
2	A	703	TTP	PG-O2G	-2.18	1.46	1.54
5	A	701	DTP	PA-O2A	-2.17	1.45	1.55
4	C	703	GTP	PB-O3A	2.17	1.61	1.59
5	B	701	DTP	PG-O2G	-2.16	1.46	1.54
2	B	702	TTP	C4-N3	-2.15	1.34	1.38
2	A	703	TTP	C6-N1	-2.14	1.34	1.38
5	C	704	DTP	C8-N7	2.10	1.35	1.31
5	B	701	DTP	PB-O3A	-2.10	1.57	1.59
5	B	701	DTP	PG-O3G	-2.09	1.47	1.54
4	D	704	GTP	O6-C6	2.08	1.27	1.23
2	D	702	TTP	O2-C2	2.06	1.26	1.23
2	D	702	TTP	PA-O3A	2.06	1.61	1.59
2	D	702	TTP	C6-N1	-2.04	1.34	1.38
4	D	704	GTP	C4-N9	-2.04	1.32	1.38
4	A	705	GTP	PB-O3B	-2.02	1.57	1.59

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	703	TTP	C4-N3-C2	-6.30	119.08	127.34
2	C	701	TTP	C4-N3-C2	-6.06	119.40	127.34
4	C	703	GTP	C5-C4-N3	-5.97	118.89	128.39
2	C	701	TTP	N3-C2-N1	5.91	122.58	114.89
2	B	702	TTP	C4-N3-C2	-5.60	120.00	127.34
4	D	704	GTP	C5-C4-N3	-5.40	119.79	128.39
2	D	702	TTP	C4-N3-C2	-5.39	120.28	127.34
2	A	703	TTP	C5-C4-N3	5.36	119.98	115.32
2	A	703	TTP	N3-C2-N1	5.21	121.68	114.89
5	D	705	DTP	C5-C4-N3	-5.08	119.72	126.72
4	C	703	GTP	C2-N3-C4	5.00	120.91	112.30
2	D	702	TTP	C5-C4-N3	4.87	119.56	115.32
4	A	705	GTP	C5-C4-N3	-4.78	120.79	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	704	GTP	C5-C4-N3	-4.76	120.81	128.39
2	B	702	TTP	N3-C2-N1	4.70	121.01	114.89
2	B	702	TTP	C5-C4-N3	4.69	119.40	115.32
2	A	703	TTP	O4-C4-C5	-4.54	119.72	124.92
2	A	703	TTP	C5-C6-N1	-4.46	118.47	123.31
4	C	703	GTP	N9-C4-N3	4.32	134.59	125.95
2	B	702	TTP	C5-C6-N1	-4.32	118.62	123.31
5	B	701	DTP	C5-C4-N3	-4.29	120.81	126.72
2	D	702	TTP	N3-C2-N1	4.29	120.47	114.89
5	C	704	DTP	C4-N9-C8	4.23	110.18	105.74
5	A	701	DTP	C4-N9-C8	4.21	110.16	105.74
4	D	704	GTP	C2-N3-C4	4.20	119.54	112.30
5	D	705	DTP	N3-C4-N9	4.19	134.29	127.17
2	C	701	TTP	C5-C4-N3	4.15	118.93	115.32
2	D	702	TTP	O4-C4-C5	-3.99	120.36	124.92
2	B	702	TTP	O4-C4-C5	-3.98	120.37	124.92
2	D	702	TTP	C5-C6-N1	-3.96	119.01	123.31
2	C	701	TTP	C5-C6-N1	-3.93	119.05	123.31
2	C	701	TTP	O4-C4-C5	-3.90	120.46	124.92
5	A	701	DTP	N3-C4-N9	3.88	133.76	127.17
5	A	701	DTP	C5-C4-N3	-3.86	121.41	126.72
4	B	704	GTP	C2-N3-C4	3.80	118.84	112.30
5	C	704	DTP	N3-C4-N9	3.72	133.49	127.17
4	C	703	GTP	O3G-PG-O2G	3.63	121.41	107.80
5	C	704	DTP	N3-C2-N1	-3.59	123.15	128.58
5	C	704	DTP	C5-C4-N3	-3.59	121.78	126.72
4	D	704	GTP	C3'-C2'-C1'	3.55	108.18	101.46
4	A	705	GTP	O2G-PG-O3B	3.45	116.19	104.64
4	A	705	GTP	C2-N3-C4	3.41	118.18	112.30
4	D	704	GTP	O2G-PG-O3B	3.41	116.06	104.64
5	B	701	DTP	N3-C4-N9	3.35	132.86	127.17
5	D	705	DTP	C4-C5-N7	-3.34	106.76	110.58
2	B	702	TTP	C5M-C5-C4	3.31	122.32	118.78
5	D	705	DTP	O2A-PA-O3A	3.26	116.07	107.27
2	A	703	TTP	C5M-C5-C4	3.24	122.25	118.78
5	C	704	DTP	C2-N3-C4	3.24	119.73	111.83
4	C	703	GTP	C6-C5-N7	3.21	136.12	130.29
5	D	705	DTP	O3G-PG-O2G	3.14	119.58	107.80
4	B	704	GTP	C6-C5-N7	3.12	135.97	130.29
4	A	705	GTP	N2-C2-N3	-3.09	113.63	119.67
4	D	704	GTP	N9-C4-N3	3.08	132.12	125.95
4	A	705	GTP	O3B-PG-O1G	-3.07	94.89	111.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	705	GTP	O6-C6-C5	-3.07	118.43	126.53
2	A	703	TTP	C5M-C5-C6	-3.06	118.71	122.85
5	B	701	DTP	O4'-C1'-N9	-3.02	102.54	107.96
2	B	702	TTP	C5M-C5-C6	-2.99	118.81	122.85
4	B	704	GTP	N9-C4-N3	2.99	131.93	125.95
4	D	704	GTP	O3B-PG-O1G	-2.98	95.34	111.04
5	D	705	DTP	C4-N9-C8	2.96	108.85	105.74
5	D	705	DTP	C2-N3-C4	2.95	119.04	111.83
4	B	704	GTP	O3G-PG-O2G	2.92	118.76	107.80
4	D	704	GTP	C6-C5-N7	2.90	135.57	130.29
4	D	704	GTP	C4-C5-N7	-2.88	106.11	110.67
4	A	705	GTP	N9-C4-N3	2.87	131.69	125.95
4	A	705	GTP	N2-C2-N1	2.86	122.80	116.76
4	D	704	GTP	O5'-PA-O1A	-2.83	97.71	108.94
5	B	701	DTP	C4-C5-N7	-2.83	107.35	110.58
4	A	705	GTP	O2B-PB-O1B	2.82	125.58	112.44
5	A	701	DTP	O3B-PG-O1G	-2.75	96.57	111.04
4	B	704	GTP	C4-C5-N7	-2.71	106.37	110.67
5	B	701	DTP	O3G-PG-O1G	2.67	121.24	110.83
4	D	704	GTP	O3A-PA-O1A	2.67	118.73	110.70
2	B	702	TTP	O2-C2-N1	-2.66	119.34	122.80
5	A	701	DTP	O3G-PG-O2G	2.63	117.68	107.80
4	A	705	GTP	O3B-PB-O1B	-2.63	102.79	110.70
4	A	705	GTP	C4-C5-N7	-2.60	106.55	110.67
5	A	701	DTP	N6-C6-N1	2.59	124.14	118.38
4	A	705	GTP	O2'-C2'-C1'	-2.57	101.24	110.10
4	A	705	GTP	C6-C5-N7	2.57	134.97	130.29
2	C	701	TTP	O3B-PB-O1B	-2.56	103.01	110.70
4	A	705	GTP	O3A-PB-O1B	-2.55	103.04	110.70
5	D	705	DTP	N3-C2-N1	-2.52	124.77	128.58
4	A	705	GTP	O6-C6-N1	2.50	124.82	120.11
4	A	705	GTP	O2B-PB-O3A	2.48	113.98	107.27
5	A	701	DTP	C2'-C3'-C4'	2.48	107.82	102.80
2	B	702	TTP	O4'-C1'-N1	2.44	112.19	107.86
2	C	701	TTP	O4'-C1'-N1	2.42	112.16	107.86
2	B	702	TTP	O3G-PG-O2G	2.35	116.62	107.80
4	C	703	GTP	C3'-C2'-C1'	2.33	105.87	101.46
5	C	704	DTP	O3G-PG-O1G	2.31	119.85	110.83
5	B	701	DTP	C4-N9-C8	2.31	108.16	105.74
2	D	702	TTP	C5M-C5-C6	-2.29	119.75	122.85
5	B	701	DTP	C2'-C3'-C4'	2.27	107.40	102.80
4	A	705	GTP	O3G-PG-O1G	2.26	119.64	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	705	DTP	C5-N7-C8	2.25	106.98	103.45
4	D	704	GTP	O4'-C4'-C3'	-2.24	100.70	105.15
4	D	704	GTP	O3A-PB-O1B	2.22	117.38	110.70
4	A	705	GTP	O5'-PA-O1A	-2.21	100.17	108.94
4	C	703	GTP	C5-C6-N1	2.21	118.88	113.25
4	B	704	GTP	C3'-C2'-C1'	2.20	105.63	101.46
2	C	701	TTP	O2-C2-N1	-2.20	119.94	122.80
2	D	702	TTP	O3G-PG-O2G	2.19	116.03	107.80
5	D	705	DTP	O2B-PB-O1B	2.19	122.65	112.44
5	D	705	DTP	C2-N1-C6	2.18	122.32	118.73
2	C	701	TTP	O2-C2-N3	-2.17	117.48	121.49
4	C	703	GTP	O2'-C2'-C1'	-2.17	102.63	110.10
4	B	704	GTP	O2A-PA-O1A	2.16	122.49	112.44
5	C	704	DTP	C2-N1-C6	2.15	122.27	118.73
4	D	704	GTP	O4'-C1'-C2'	-2.14	102.03	106.62
4	B	704	GTP	O2'-C2'-C1'	-2.12	102.79	110.10
4	A	705	GTP	C3'-C2'-C1'	2.11	105.46	101.46
4	C	703	GTP	C4-C5-N7	-2.10	107.34	110.67
4	A	705	GTP	O2A-PA-O1A	2.10	122.20	112.44
4	B	704	GTP	O6-C6-C5	-2.10	121.00	126.53
5	B	701	DTP	C2-N3-C4	2.08	116.91	111.83
2	B	702	TTP	O2A-PA-O1A	2.06	122.01	112.44
2	C	701	TTP	O3G-PG-O2G	2.03	115.41	107.80
2	A	703	TTP	O2A-PA-O1A	2.00	121.76	112.44

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	701	TTP	C5'-O5'-PA-O2A
2	C	701	TTP	C5'-O5'-PA-O3A
2	A	703	TTP	C5'-O5'-PA-O1A
2	A	703	TTP	C5'-O5'-PA-O2A
2	A	703	TTP	C5'-O5'-PA-O3A
2	D	702	TTP	PB-O3A-PA-O5'
2	D	702	TTP	C5'-O5'-PA-O2A
2	B	702	TTP	O4'-C1'-N1-C2
2	B	702	TTP	O4'-C1'-N1-C6
4	C	703	GTP	PB-O3B-PG-O3G
4	A	705	GTP	PB-O3B-PG-O2G
4	D	704	GTP	PB-O3B-PG-O2G
4	B	704	GTP	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
5	A	701	DTP	PB-O3B-PG-O3G
5	D	705	DTP	PB-O3B-PG-O2G
5	D	705	DTP	PB-O3B-PG-O3G
2	C	701	TTP	O4'-C4'-C5'-O5'
2	C	701	TTP	C3'-C4'-C5'-O5'
2	D	702	TTP	C4'-C5'-O5'-PA
2	A	703	TTP	PB-O3A-PA-O1A
2	B	702	TTP	C3'-C4'-C5'-O5'
2	D	702	TTP	PG-O3B-PB-O2B
4	C	703	GTP	PG-O3B-PB-O1B
4	A	705	GTP	PG-O3B-PB-O2B
4	B	704	GTP	PG-O3B-PB-O1B
5	C	704	DTP	PG-O3B-PB-O2B
5	A	701	DTP	PG-O3B-PB-O1B
5	B	701	DTP	PG-O3B-PB-O1B
5	B	701	DTP	PB-O3A-PA-O1A
2	B	702	TTP	O4'-C4'-C5'-O5'
2	D	702	TTP	C5'-O5'-PA-O3A
2	C	701	TTP	C4'-C5'-O5'-PA
4	D	704	GTP	PB-O3B-PG-O1G
2	A	703	TTP	PB-O3A-PA-O2A
2	B	702	TTP	PA-O3A-PB-O2B
4	C	703	GTP	PB-O3A-PA-O1A
4	A	705	GTP	PG-O3B-PB-O1B
4	A	705	GTP	PB-O3A-PA-O2A
4	D	704	GTP	PG-O3B-PB-O2B
4	D	704	GTP	PB-O3A-PA-O2A
5	A	701	DTP	PB-O3A-PA-O2A
5	D	705	DTP	PG-O3B-PB-O2B
4	C	703	GTP	C4'-C5'-O5'-PA
4	A	705	GTP	C4'-C5'-O5'-PA
4	B	704	GTP	C4'-C5'-O5'-PA
5	C	704	DTP	PG-O3B-PB-O1B
4	D	704	GTP	C4'-C5'-O5'-PA
5	D	705	DTP	PB-O3B-PG-O1G
5	A	701	DTP	PB-O3B-PG-O2G
2	B	702	TTP	PA-O3A-PB-O1B
4	C	703	GTP	PG-O3B-PB-O2B
4	D	704	GTP	PB-O3A-PA-O1A
5	A	701	DTP	PB-O3A-PA-O1A
5	D	705	DTP	PG-O3B-PB-O1B
5	D	705	DTP	PB-O3A-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	D	702	TTP	C3'-C4'-C5'-O5'
4	A	705	GTP	PB-O3B-PG-O1G
2	D	702	TTP	PG-O3B-PB-O1B
4	C	703	GTP	PB-O3A-PA-O2A
4	A	705	GTP	PB-O3A-PA-O1A
4	B	704	GTP	PB-O3A-PA-O2A
5	C	704	DTP	PB-O3A-PA-O1A
5	C	704	DTP	PB-O3A-PA-O2A
5	A	701	DTP	PG-O3B-PB-O2B

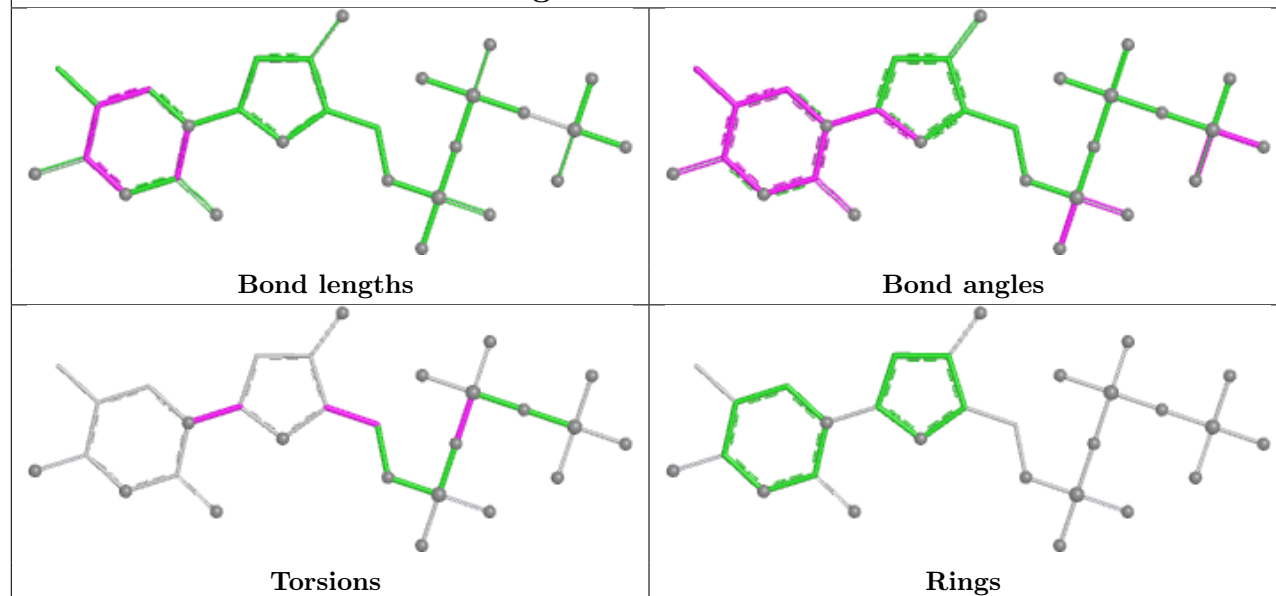
There are no ring outliers.

8 monomers are involved in 20 short contacts:

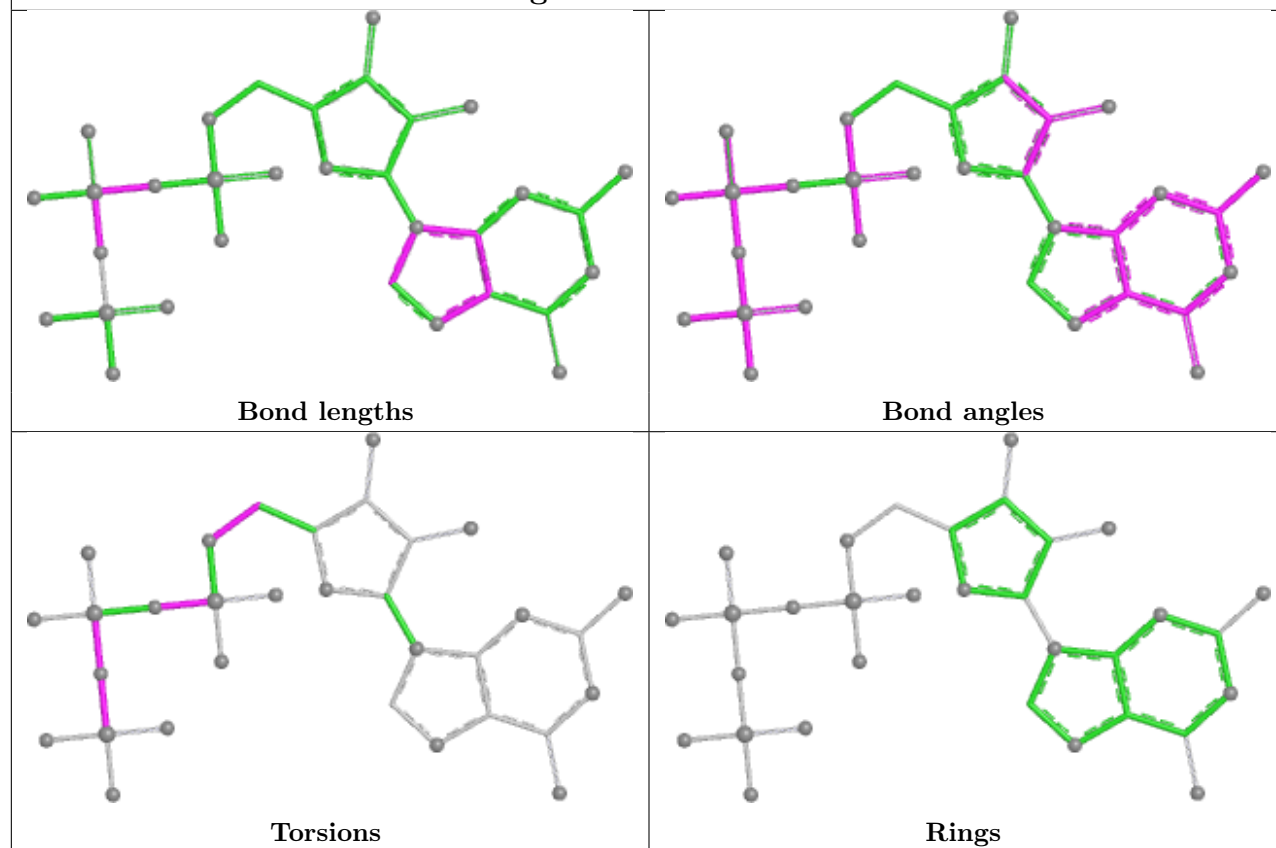
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	702	TTP	8	0
4	C	703	GTP	1	0
2	A	703	TTP	4	0
5	A	701	DTP	1	0
5	B	701	DTP	1	0
5	D	705	DTP	1	0
2	C	701	TTP	1	0
2	D	702	TTP	3	0

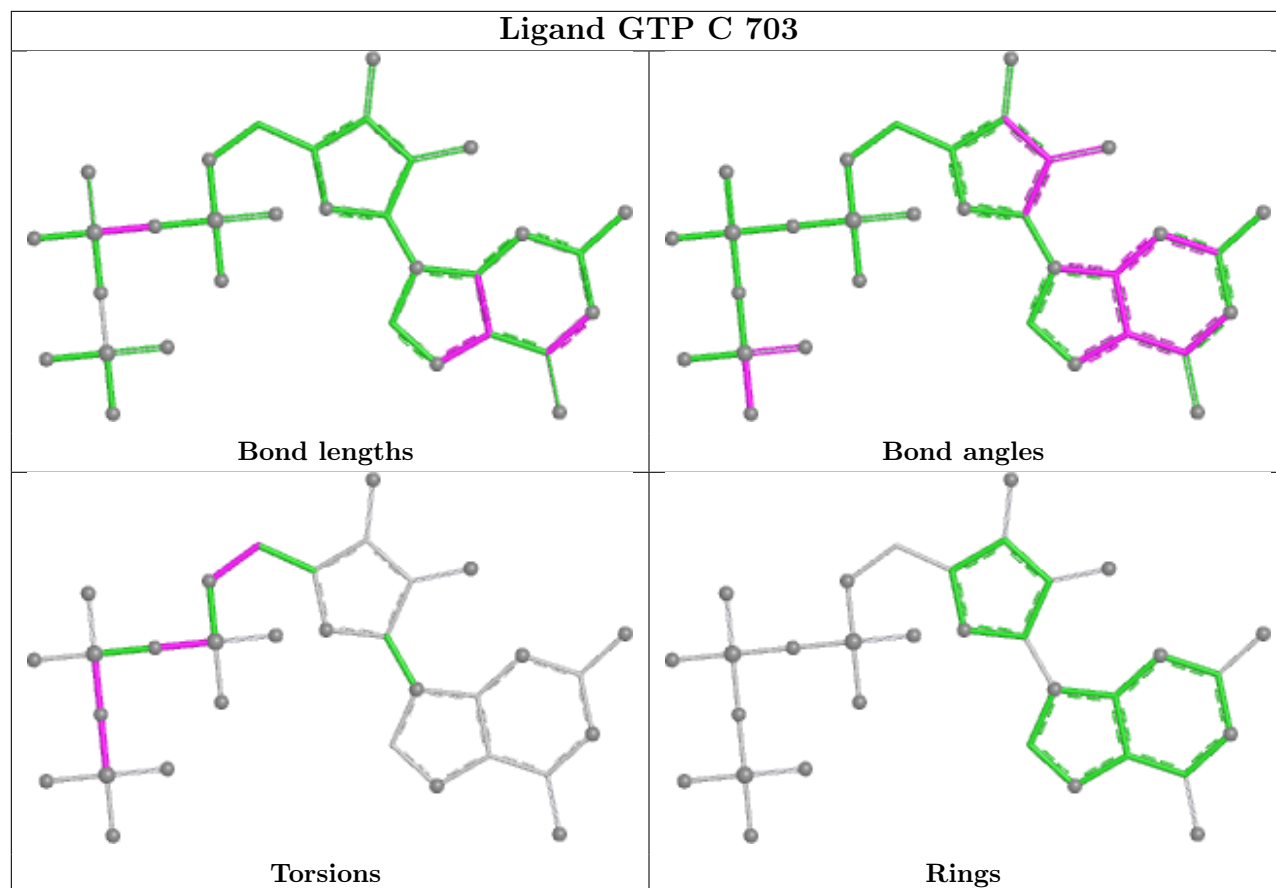
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 TTP B 702

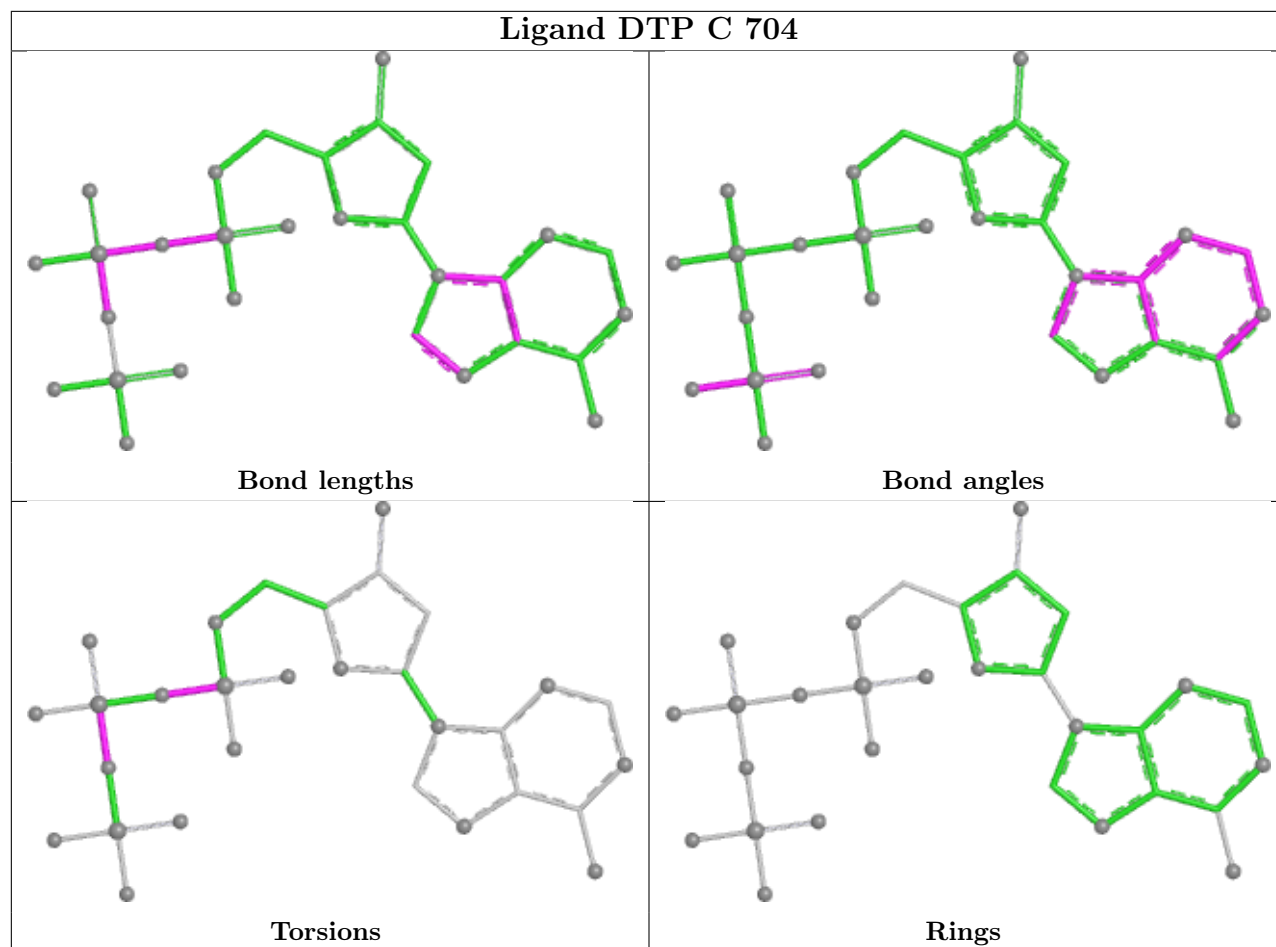


Ligand GTP A 705

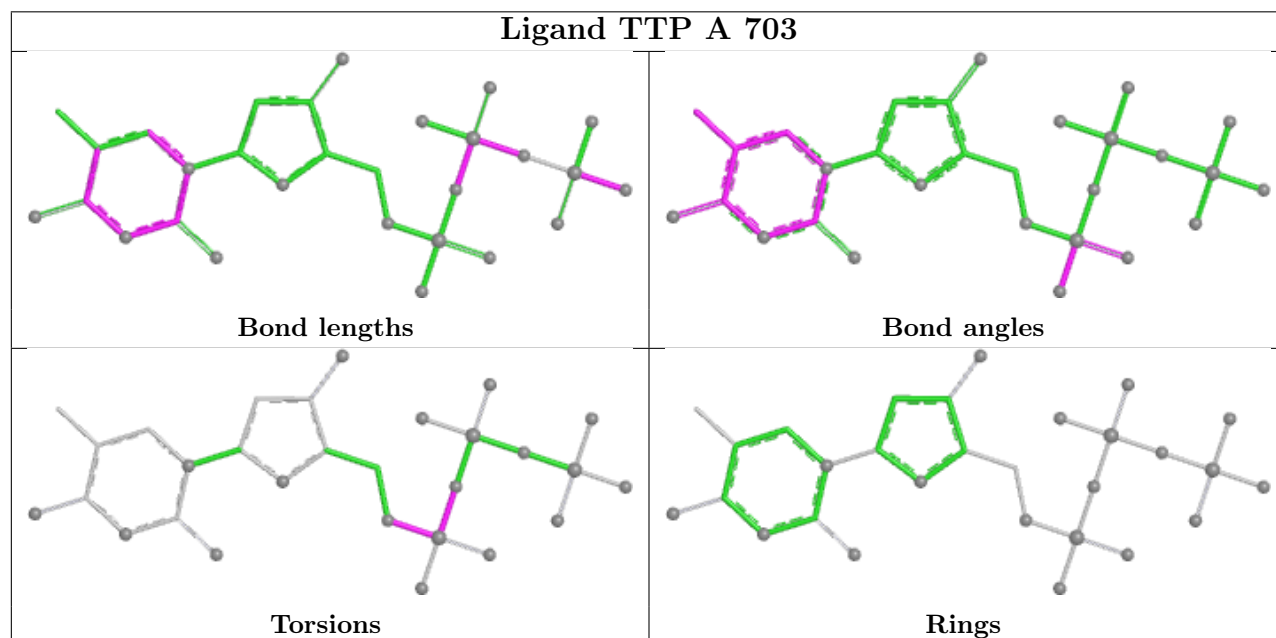


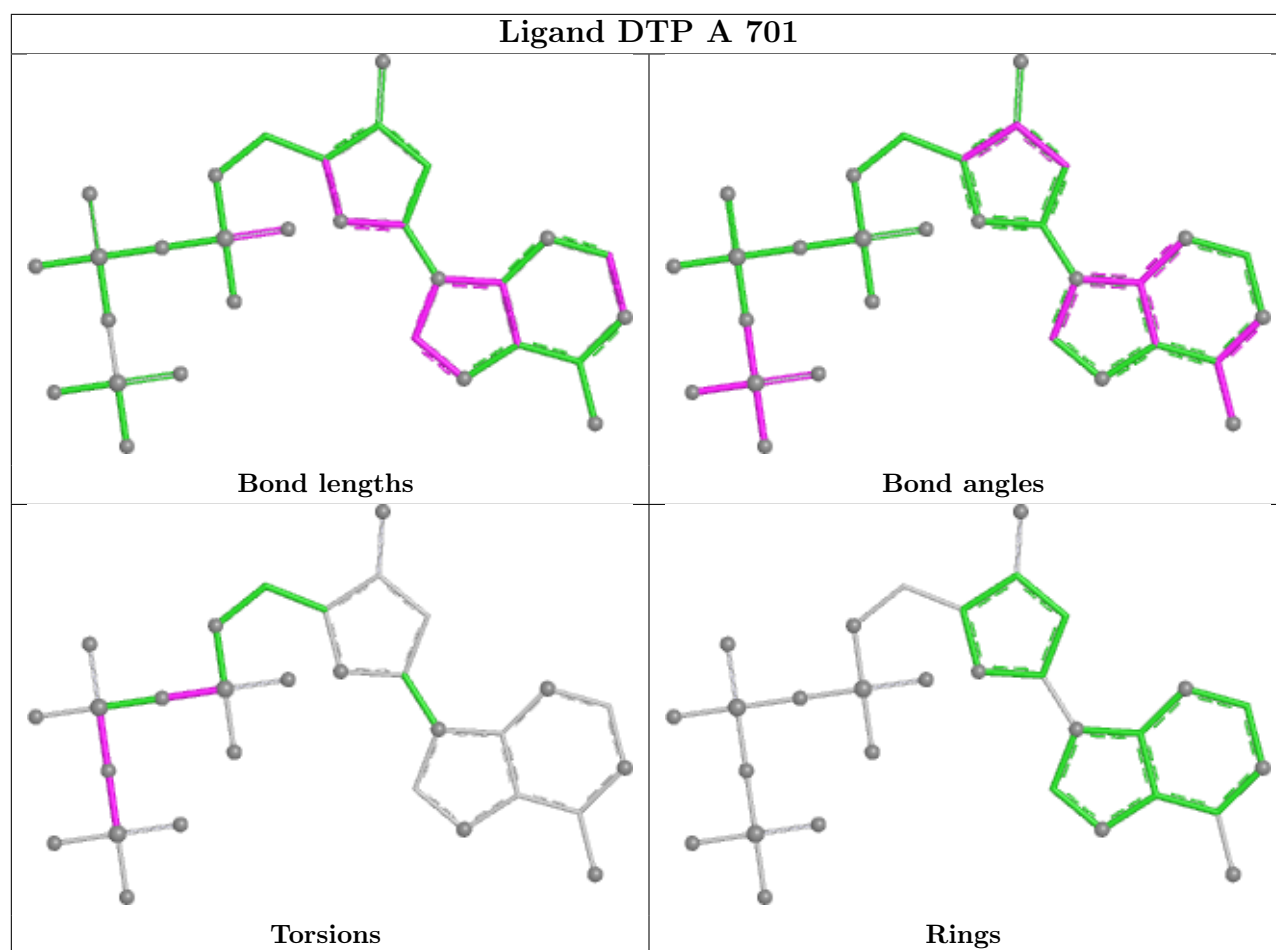


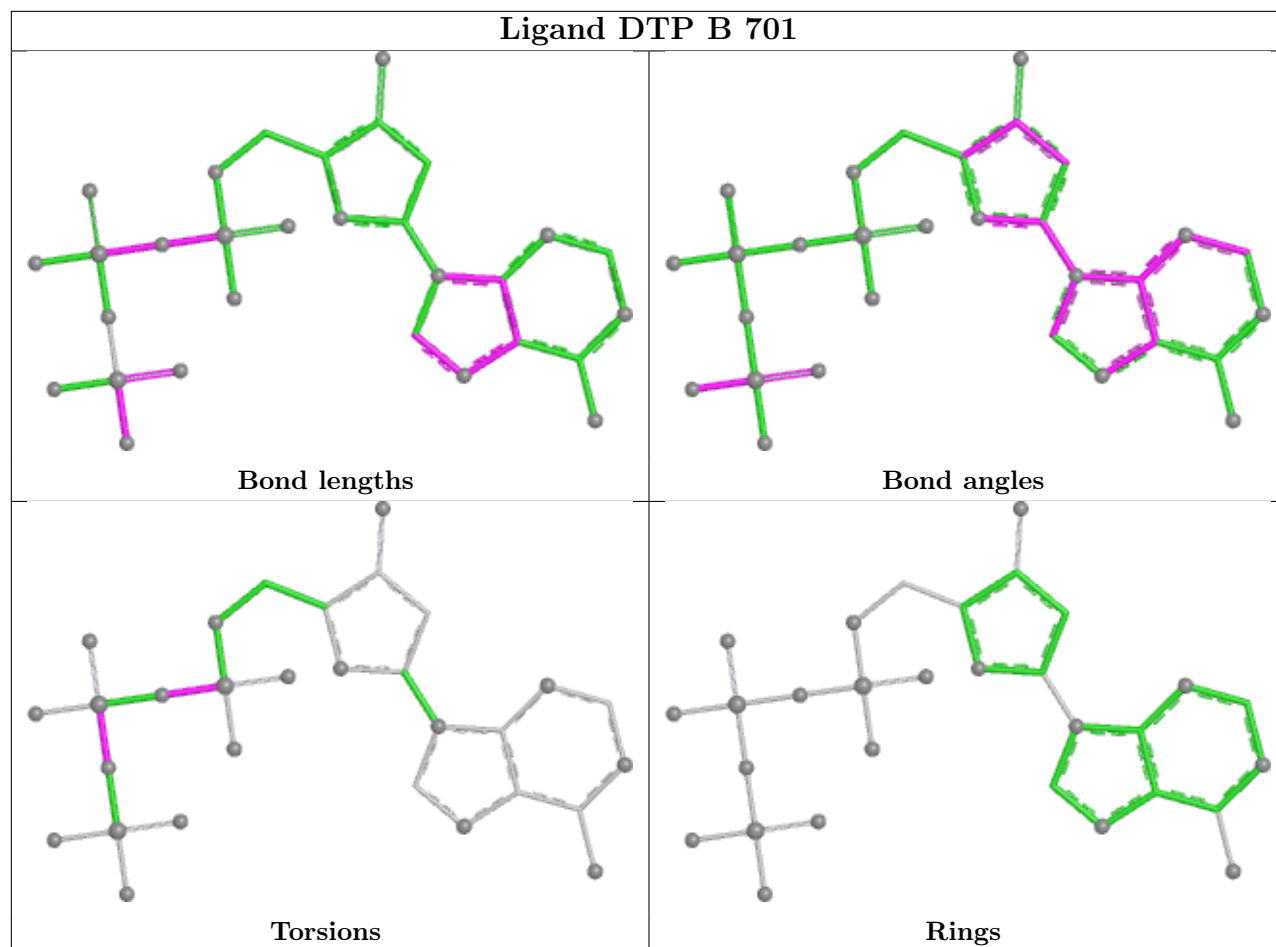
Ligand DTP C 704

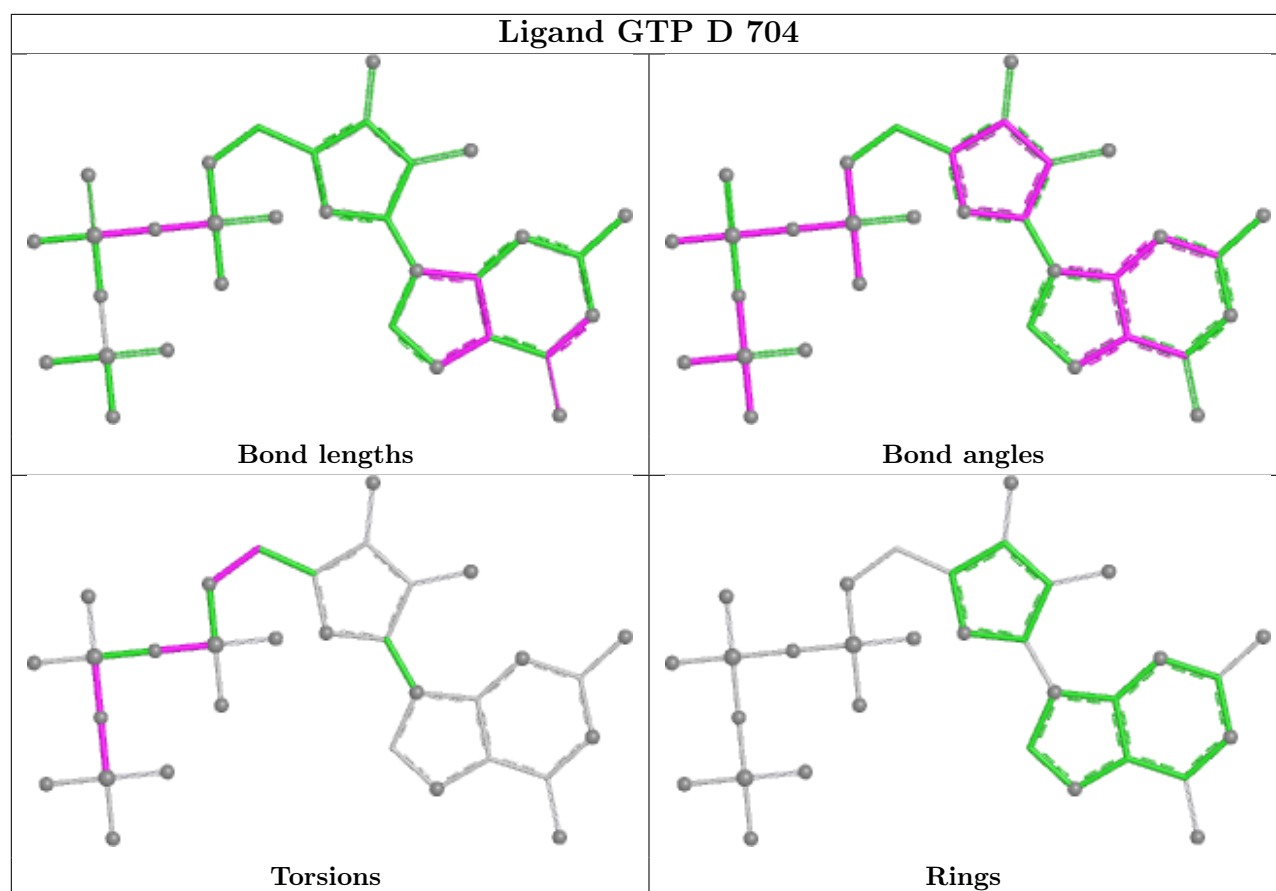


Ligand TTP A 703

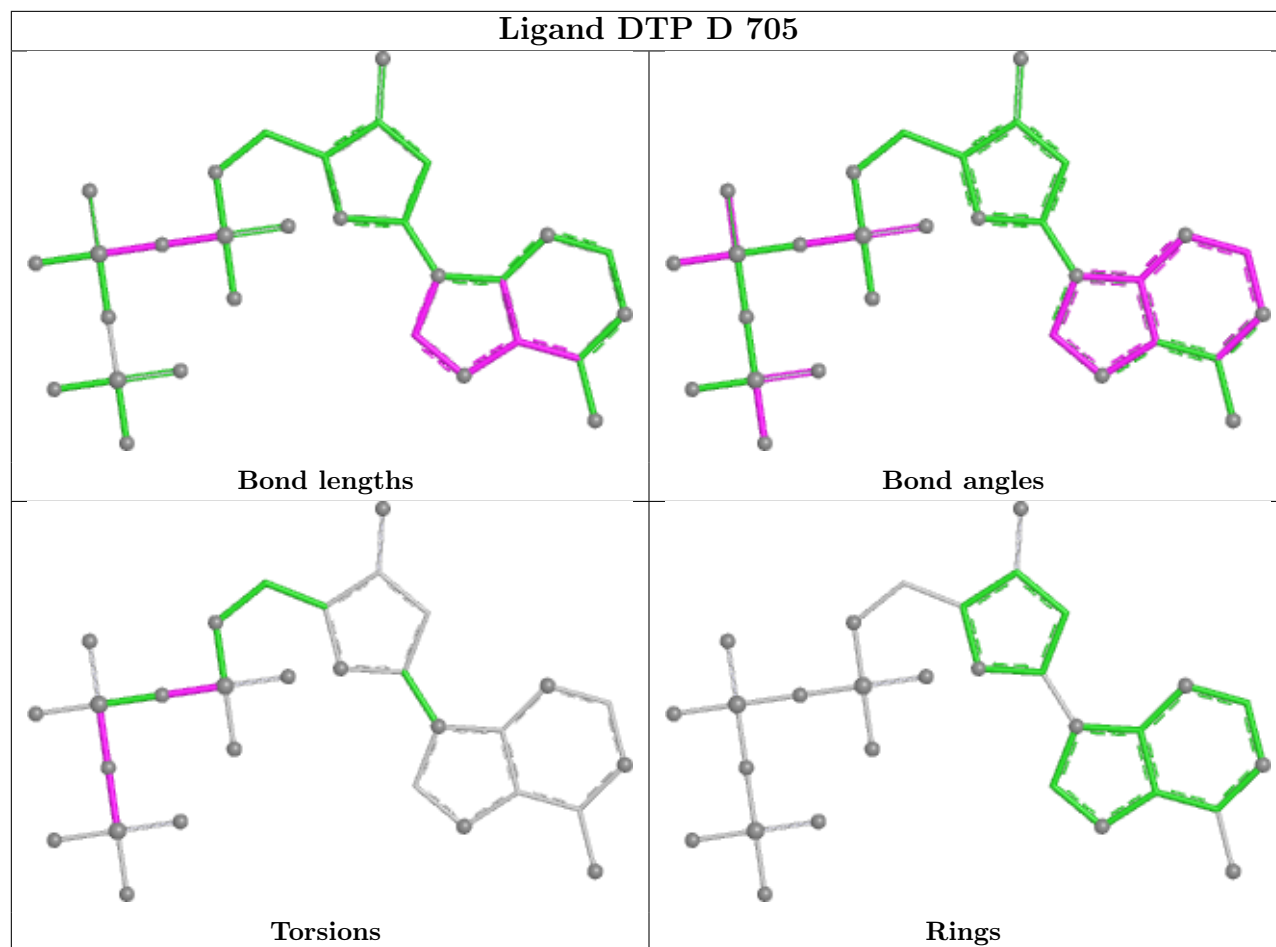




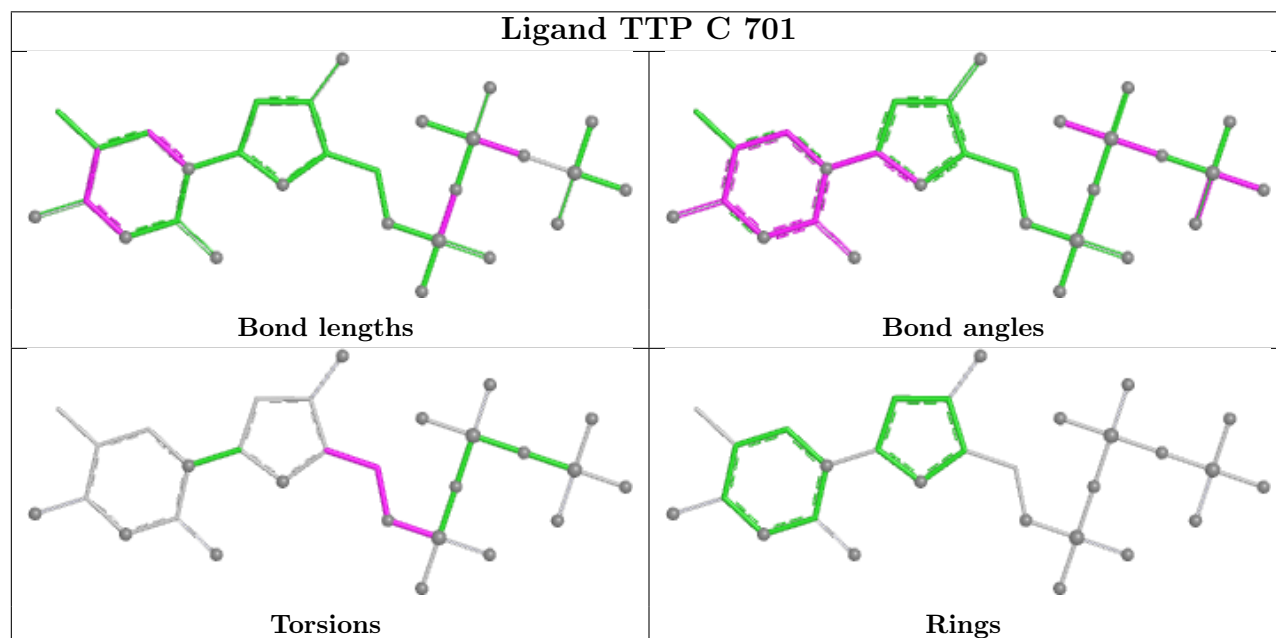


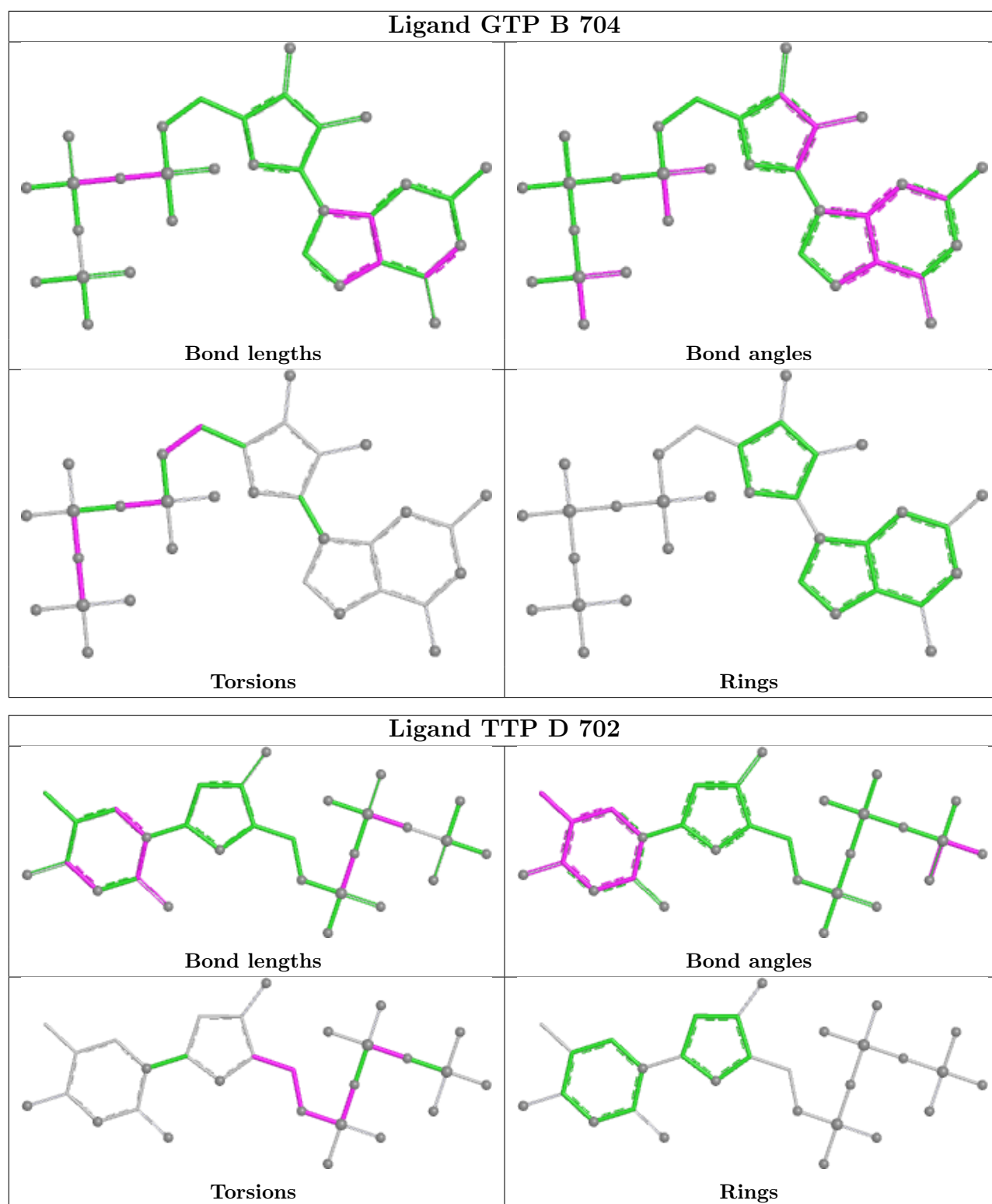


Ligand DTP D 705



Ligand TTP C 701





5.7 Other polymers [i](#)

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(Å ²)	Q<0.9
1	A	480/514 (93%)	0.18	3 (0%) 85 85	26, 73, 120, 159	2 (0%)
1	B	481/514 (93%)	0.64	24 (4%) 34 34	40, 94, 159, 200	1 (0%)
1	C	481/514 (93%)	0.07	1 (0%) 91 90	33, 63, 106, 136	2 (0%)
1	D	480/514 (93%)	0.23	7 (1%) 72 71	34, 74, 119, 155	1 (0%)
All	All	1922/2056 (93%)	0.28	35 (1%) 67 66	26, 75, 134, 200	6 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	284	LEU	4.8
1	B	284	LEU	4.3
1	C	284	LEU	3.7
1	B	480	VAL	3.5
1	B	476	LEU	3.3
1	A	284	LEU	3.3
1	A	488	LEU	3.2
1	B	493	LEU	3.0
1	D	540	LEU	2.9
1	B	590	LEU	2.9
1	B	491	VAL	2.8
1	A	286	PRO	2.7
1	B	572	TRP	2.7
1	B	573	CYS	2.7
1	B	481	ALA	2.7
1	B	498	PHE	2.6
1	B	115	MET	2.6
1	B	563	TYR	2.6
1	D	489	LEU	2.5
1	B	489	LEU	2.5
1	B	562	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	578	PHE	2.5
1	B	276	LEU	2.5
1	B	266	CYS	2.4
1	D	488	LEU	2.4
1	B	554	CYS	2.3
1	B	231	TRP	2.3
1	D	466	ILE	2.3
1	D	598	TRP	2.2
1	B	587	ILE	2.2
1	B	340	VAL	2.1
1	D	126	ILE	2.0
1	B	462	PRO	2.0
1	B	396	TYR	2.0
1	B	570	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
3	MG	C	702	1/1	0.55	0.13	77,77,77,77	0
3	MG	A	704	1/1	0.65	0.12	85,85,85,85	0
3	MG	D	703	1/1	0.75	0.22	85,85,85,85	0
3	MG	B	703	1/1	0.76	0.13	92,92,92,92	0
2	TTP	B	702	29/29	0.83	0.11	77,86,112,129	0
2	TTP	D	702	29/29	0.87	0.10	48,65,100,100	0
2	TTP	C	701	29/29	0.89	0.09	40,56,96,101	0
2	TTP	A	703	29/29	0.90	0.08	50,66,100,108	0
4	GTP	B	704	32/32	0.95	0.06	54,64,80,83	0

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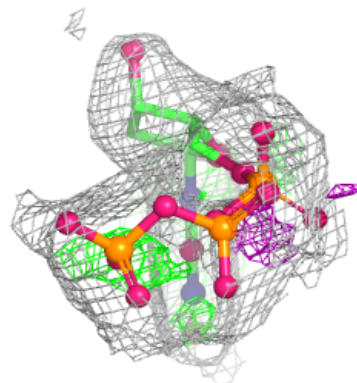
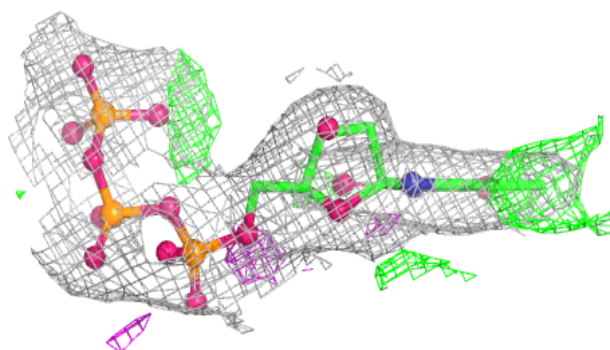
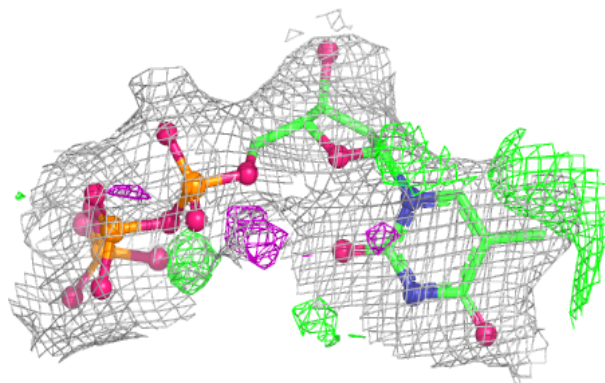
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GTP	D	704	32/32	0.96	0.05	44,54,68,71	0
5	DTP	D	705	30/30	0.97	0.05	49,57,69,74	0
5	DTP	B	701	30/30	0.97	0.05	43,49,60,61	0
3	MG	A	706	1/1	0.98	0.03	76,76,76,76	0
5	DTP	A	701	30/30	0.98	0.04	31,35,41,44	0
4	GTP	A	705	32/32	0.98	0.04	38,45,53,54	0
3	MG	C	705	1/1	0.98	0.03	77,77,77,77	0
5	DTP	C	704	30/30	0.99	0.04	31,42,52,53	0
3	MG	A	702	1/1	0.99	0.03	54,54,54,54	0
3	MG	D	701	1/1	0.99	0.02	52,52,52,52	0
4	GTP	C	703	32/32	0.99	0.04	36,41,47,50	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.

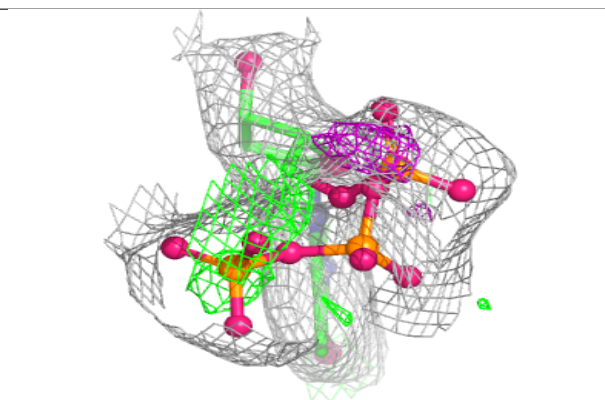
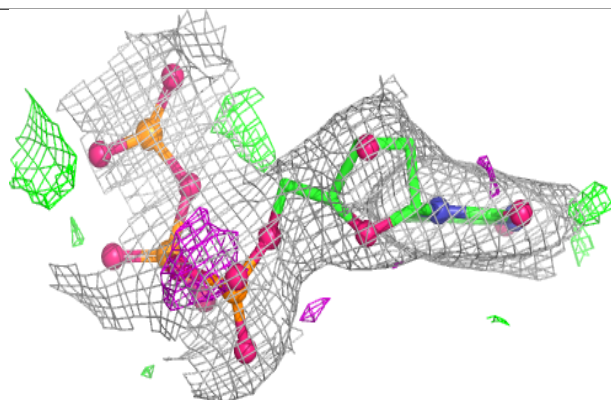
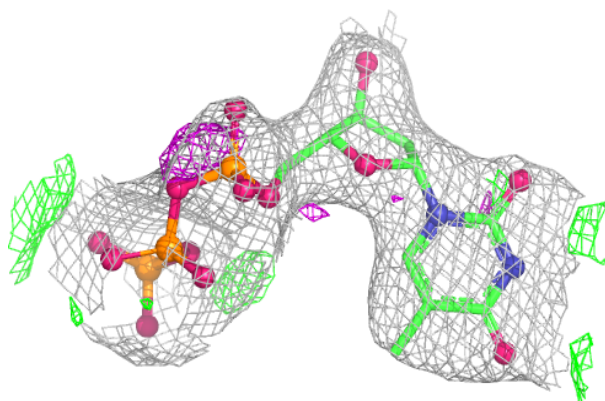
Electron density around TTP B 702:

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

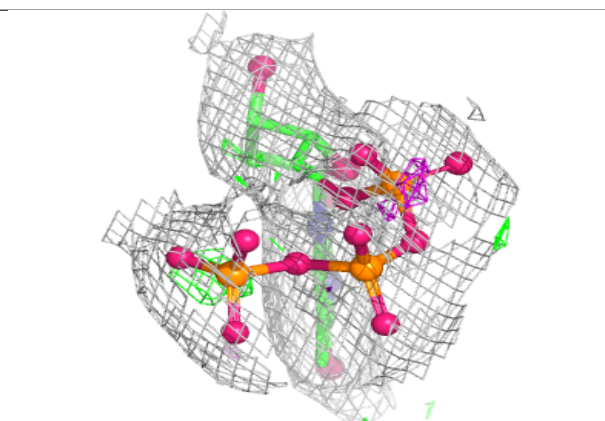
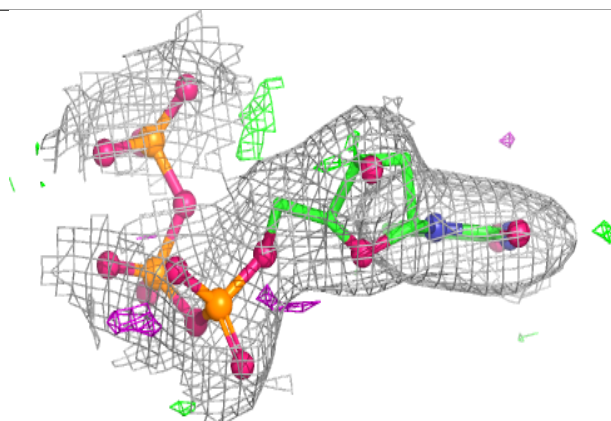
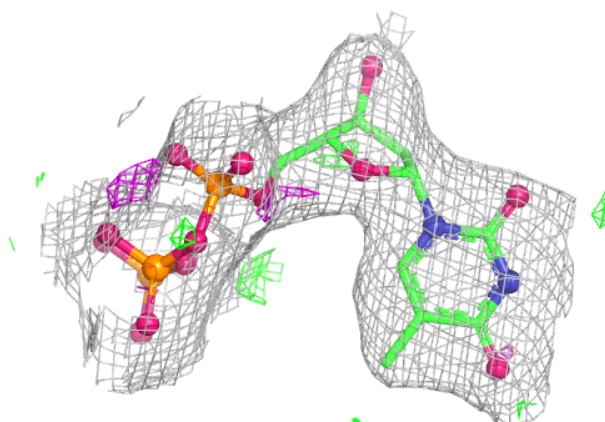


Electron density around TTP D 702:

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

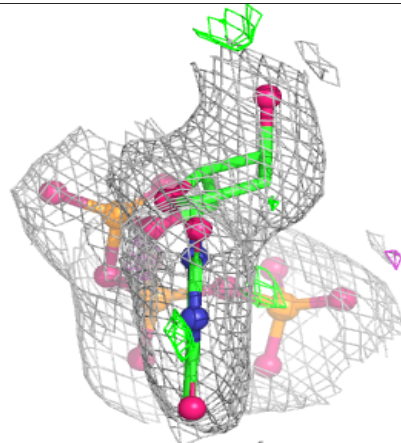
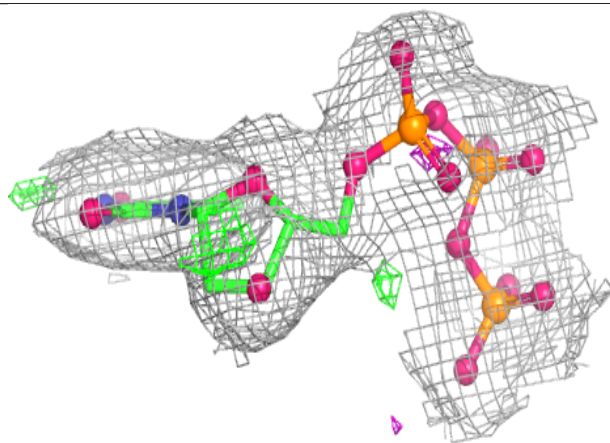
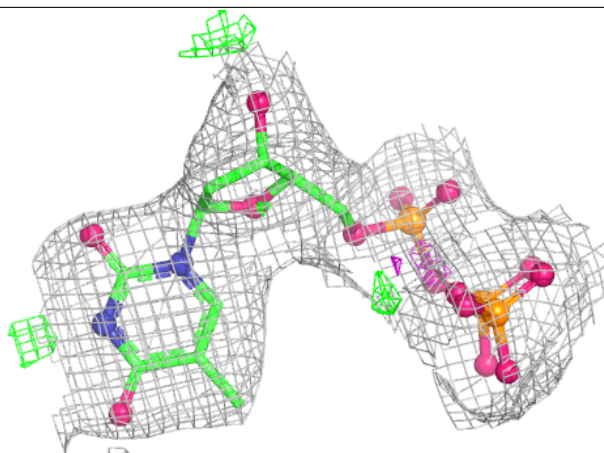
**Electron density around TTP C 701:**

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

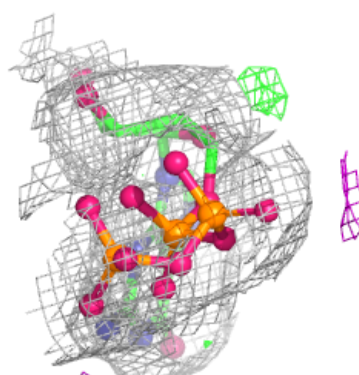
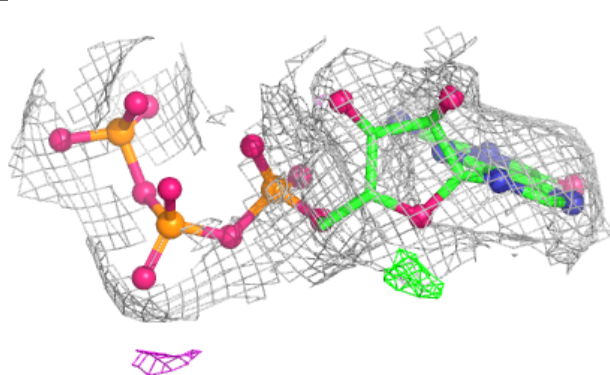
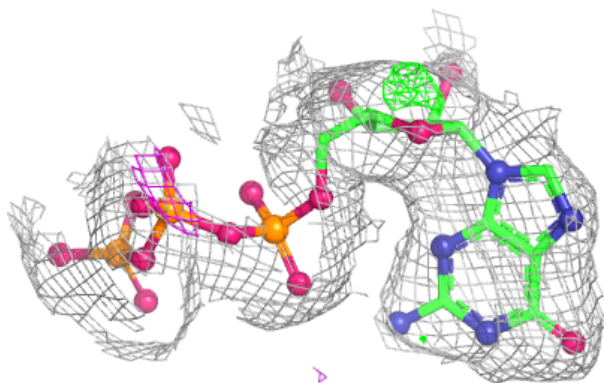


Electron density around TTP A 703:

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

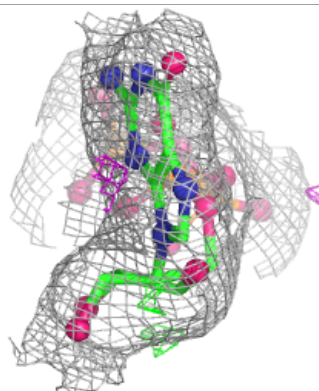
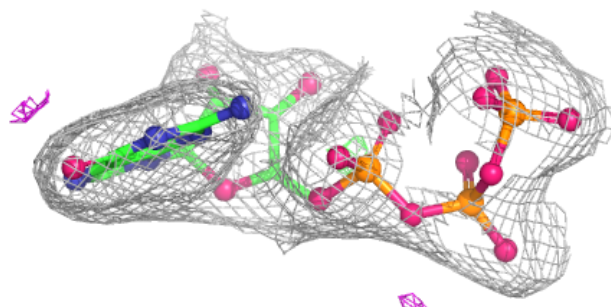
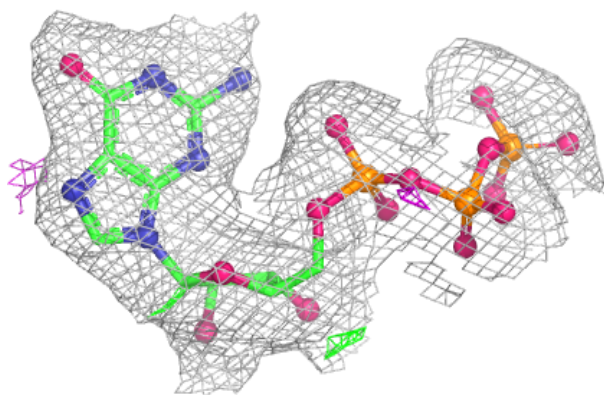
**Electron density around GTP B 704:**

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

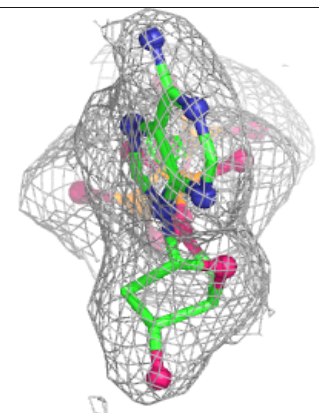
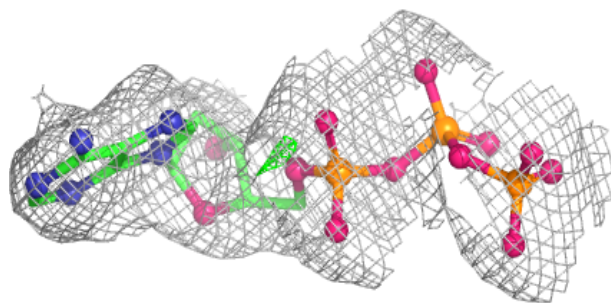
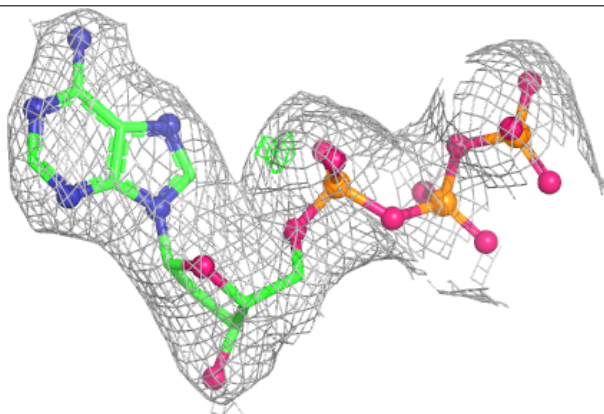


Electron density around GTP D 704:

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

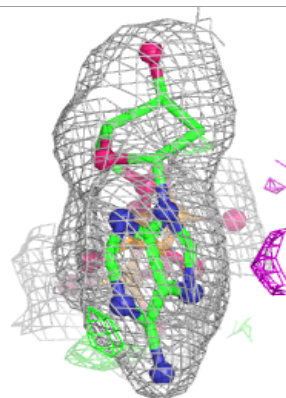
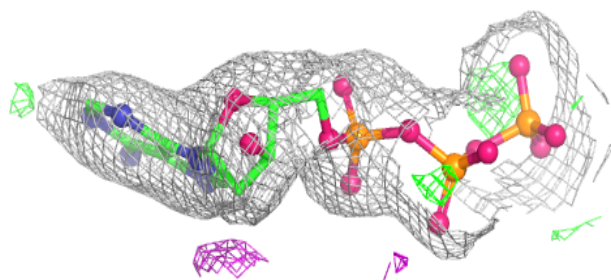
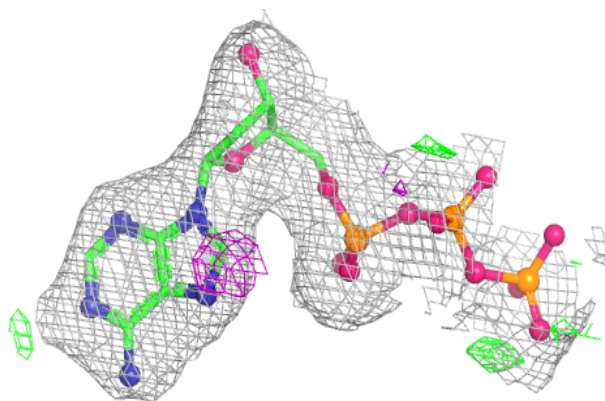
**Electron density around DTP D 705:**

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

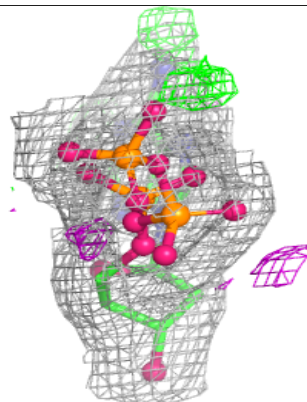
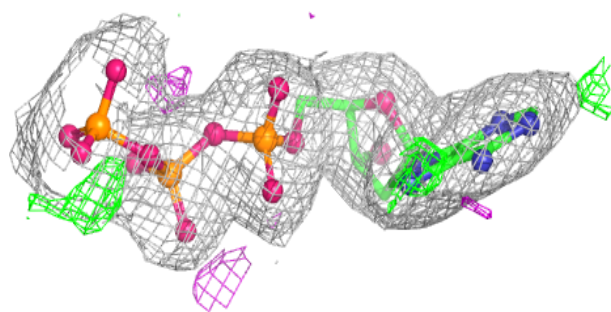
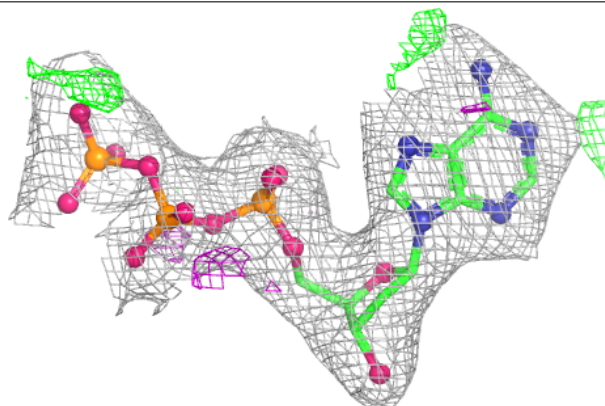


Electron density around DTP B 701:

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

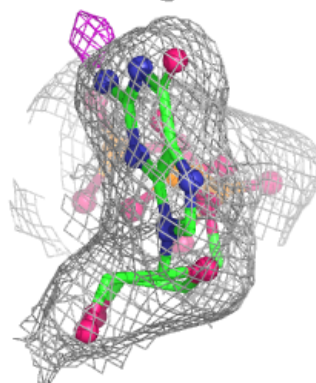
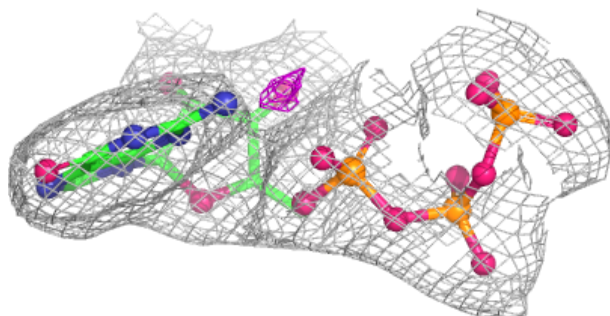
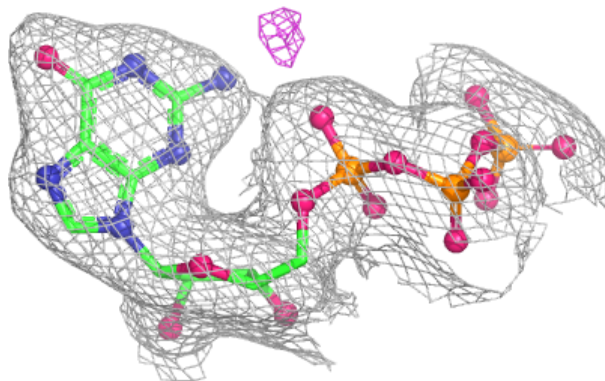
**Electron density around DTP A 701:**

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

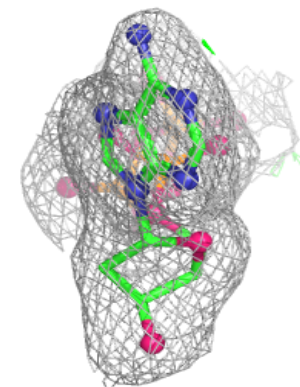
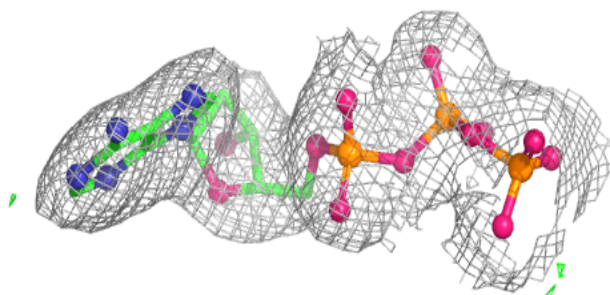
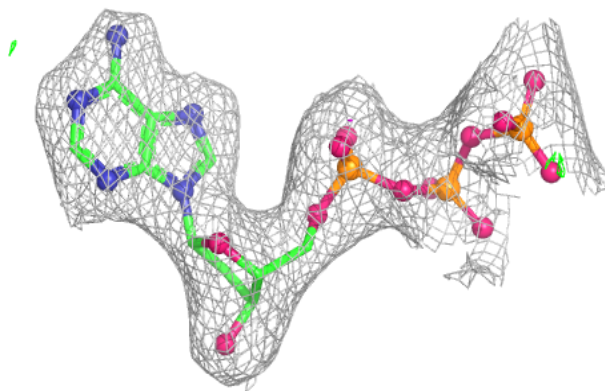


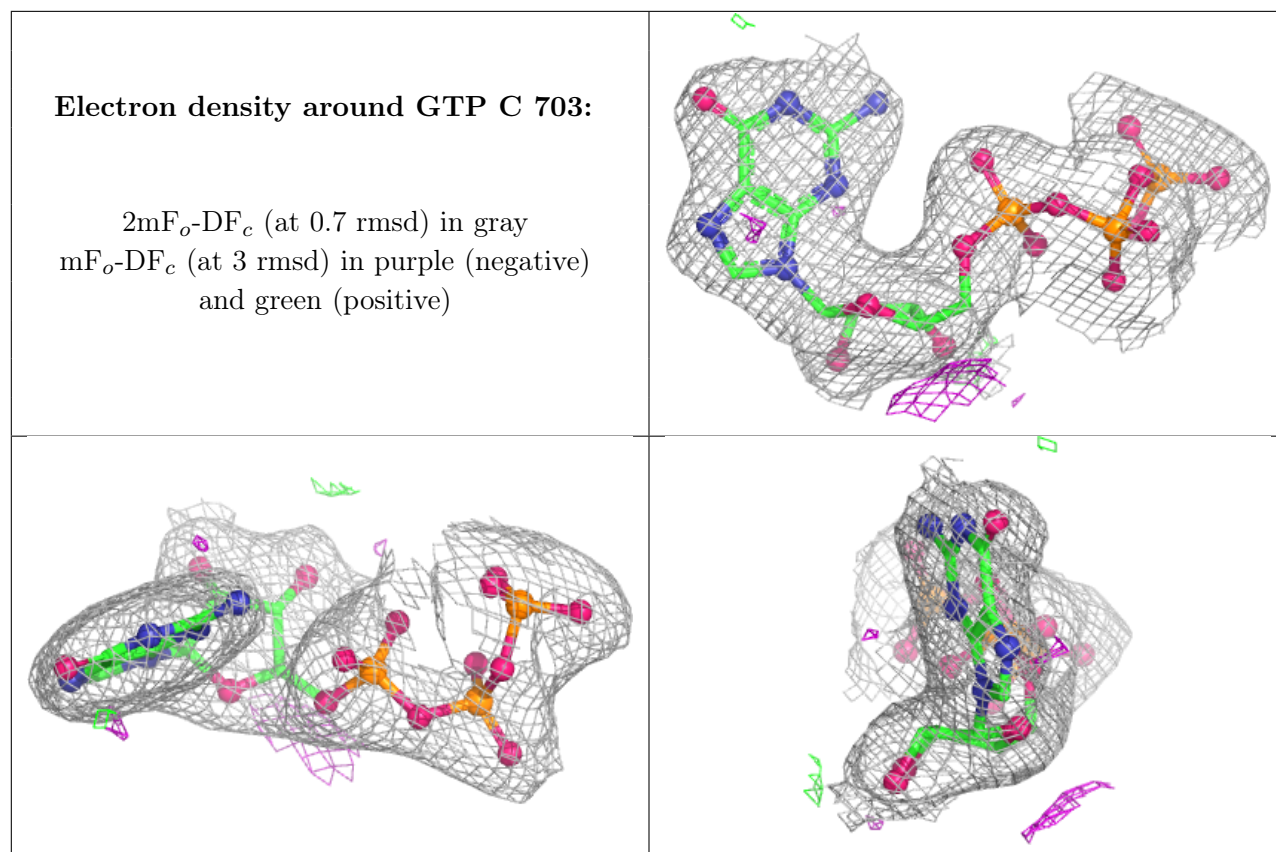
Electron density around GTP A 705:

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

**Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.