



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:50 AM UTC

PDB ID : 4TNQ / pdb_00004tnq
Title : Structural basis of cellular dNTP regulation, SAMHD1-GTP-dTTP-dTTP complex
Authors : Ji, X.; Tang, C.; Zhao, Q.; Wang, W.; Xiong, Y.
Deposited on : 2014-06-04
Resolution : 2.55 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

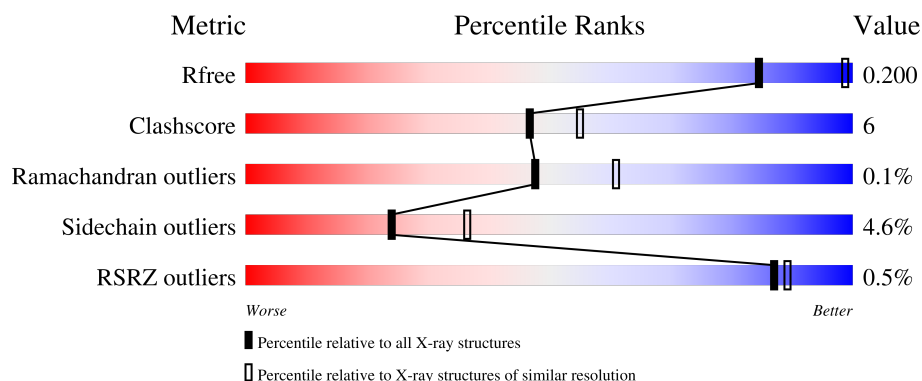
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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% 9% • • 7%
1	B	514	 81% 11% • 7%
1	C	514	 82% 10% • 7%
1	D	514	 81% 10% • 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16302 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

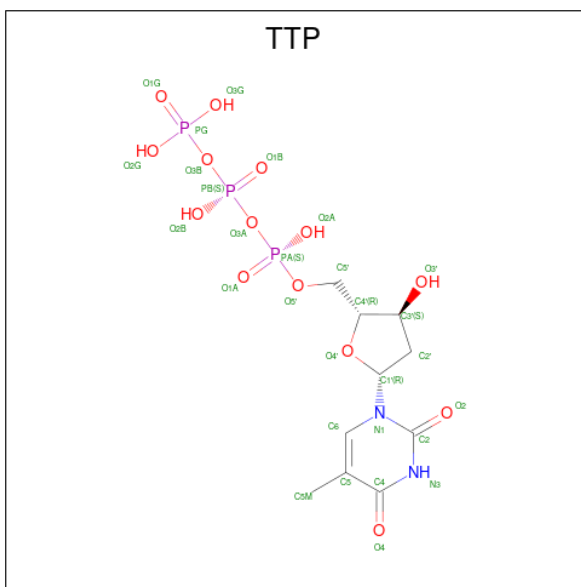
- Molecule 1 is a protein called Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	0	0
			3923	2512	683	708	20			
1	C	479	Total	C	N	O	S	0	1	0
			3922	2511	684	706	21			
1	D	480	Total	C	N	O	S	0	1	0
			3930	2515	685	709	21			
1	B	480	Total	C	N	O	S	0	0	0
			3925	2513	684	708	20			

There are 8 discrepancies between the modelled and reference sequences:

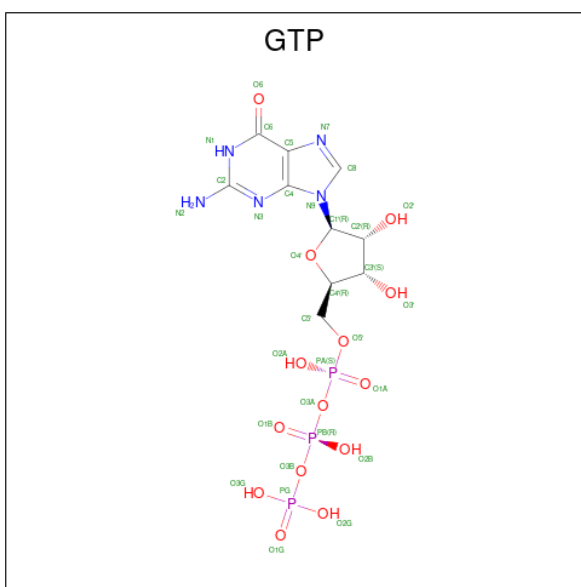
Chain	Residue	Modelled	Actual	Comment	Reference
A	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
A	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
C	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
C	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
D	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
D	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
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	A	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	C	1	Total 29	C 10	N 2	O 14	P 3	0	0
2	C	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	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
2	B	1	Total 29	C 10	N 2	O 14	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	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	D	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	B	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	C	2	Total	Mg	0	0
			2	2		
4	B	2	Total	Mg	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	69	Total	O	0	0
			69	69		
5	C	44	Total	O	0	0
			44	44		
5	D	81	Total	O	0	0
			81	81		

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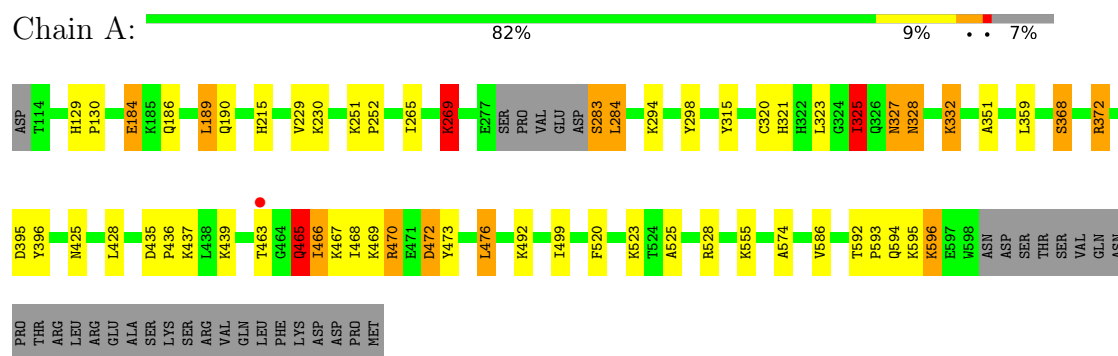
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	44	Total	O	0	0
			44	44		

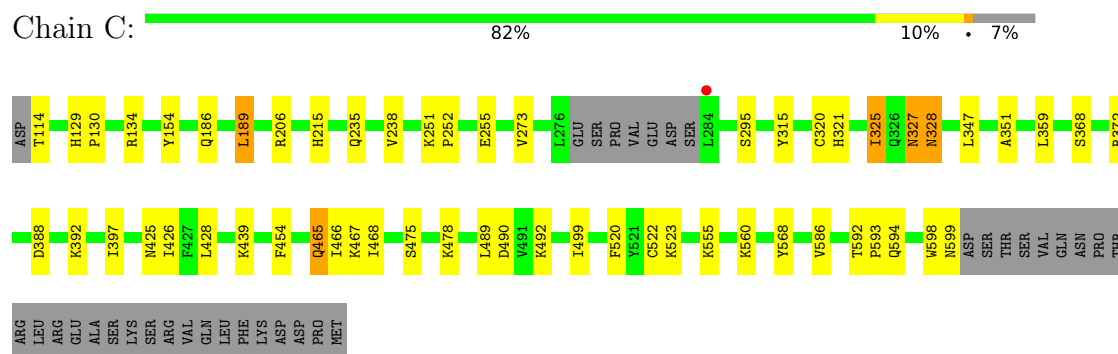
3 Residue-property plots

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.

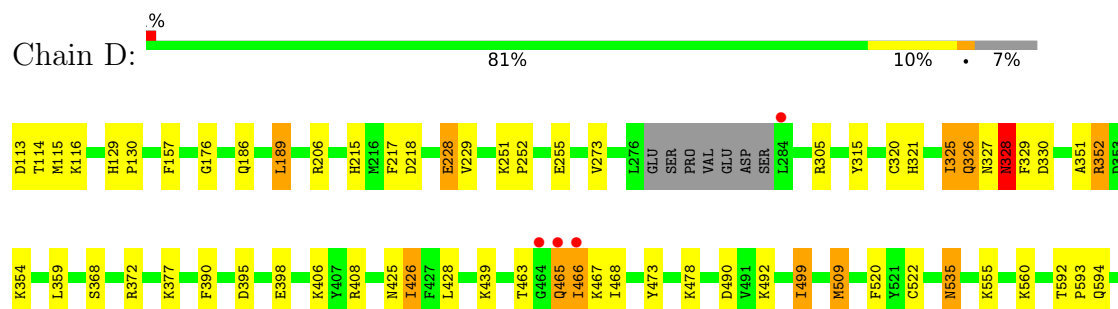
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



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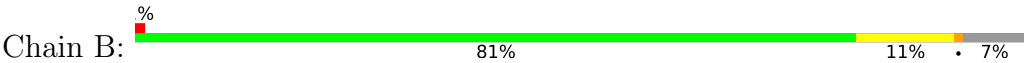


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.16Å 140.29Å 97.27Å 90.00° 114.56° 90.00°	Depositor
Resolution (Å)	50.00 – 2.55 50.00 – 2.55	Depositor EDS
% Data completeness (in resolution range)	95.1 (50.00-2.55) 95.1 (50.00-2.55)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.161 , 0.198 0.166 , 0.200	Depositor DCC
R_{free} test set	2966 reflections (2.98%)	wwPDB-VP
Wilson B-factor (Å ²)	50.4	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16302	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

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

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: TTP, GTP, 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	0.90	1/4015 (0.0%)	0.94	6/5419 (0.1%)
1	B	0.81	1/4017 (0.0%)	0.93	3/5422 (0.1%)
1	C	0.84	1/4014 (0.0%)	0.91	2/5418 (0.0%)
1	D	0.93	1/4022 (0.0%)	0.95	6/5429 (0.1%)
All	All	0.87	4/16068 (0.0%)	0.93	17/21688 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	218	ASP	CB-CG	-5.83	1.37	1.52
1	A	325	ILE	C-O	-5.16	1.18	1.24
1	B	405	LYS	N-CA	-5.12	1.39	1.45
1	C	465	GLN	CA-C	5.05	1.59	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	483	ALA	N-CA-C	12.40	126.00	111.11
1	D	218	ASP	N-CA-CB	-7.88	98.59	110.01
1	B	352	ARG	CG-CD-NE	-7.02	96.55	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	476	LEU	CD1-CG-CD2	-6.74	95.96	110.80
1	D	352	ARG	CG-CD-NE	-6.27	98.20	112.00
1	D	217	PHE	CA-C-N	6.17	128.46	120.44
1	D	217	PHE	C-N-CA	6.17	128.46	120.44
1	A	465	GLN	CB-CA-C	-6.17	100.19	110.68
1	B	405	LYS	N-CA-CB	-5.94	100.94	110.63
1	A	269	LYS	CB-CG-CD	5.71	124.44	111.30
1	D	509	MET	CB-CA-C	-5.59	101.73	111.35
1	C	466	ILE	N-CA-C	5.49	116.66	109.58
1	A	372	ARG	NE-CZ-NH1	-5.22	116.28	121.50
1	C	328	ASN	N-CA-C	5.15	116.03	107.73
1	D	228	GLU	CB-CA-C	-5.14	102.25	110.79
1	A	184	GLU	CB-CA-C	-5.01	103.01	110.88
1	A	528	ARG	CA-CB-CG	-5.01	104.08	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	465	GLN	Peptide
1	B	276	LEU	Peptide

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	3923	0	3916	58	2
1	B	3925	0	3917	51	2
1	C	3922	0	3915	32	1
1	D	3930	0	3919	45	1
2	A	58	0	26	5	0
2	B	58	0	26	5	0
2	C	58	0	26	4	0
2	D	58	0	26	6	0
3	A	32	0	12	0	0
3	B	64	0	24	1	0
3	D	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2	0	0	0	0
4	C	2	0	0	0	0
5	A	69	0	0	4	0
5	B	44	0	0	2	0
5	C	44	0	0	3	0
5	D	81	0	0	5	0
All	All	16302	0	15819	183	3

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 6.

All (183) 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:A:574:ALA:O	1:A:595:LYS:NZ	1.61	1.33
1:B:422:LEU:HD12	1:B:426:ILE:CD1	1.65	1.26
1:A:463:THR:O	1:A:466:ILE:HD13	1.42	1.15
1:A:283:SER:HB2	1:A:284:LEU:HA	1.17	1.15
1:B:226:ARG:HG2	1:B:226:ARG:HH21	1.11	1.14
1:D:390:PHE:CZ	1:D:426:ILE:HD11	1.82	1.13
1:B:422:LEU:HD12	1:B:426:ILE:HD11	1.14	1.12
2:A:701:TTP:O1A	5:A:824:HOH:O	1.70	1.08
2:D:701:TTP:O1G	5:D:836:HOH:O	1.72	1.06
1:A:283:SER:HB2	1:A:284:LEU:CA	1.87	1.03
1:B:228:GLU:CD	1:B:229:VAL:HG23	1.85	1.00
1:D:328:ASN:HD22	1:D:328:ASN:C	1.69	0.99
1:D:390:PHE:CE2	1:D:426:ILE:HD11	1.96	0.99
1:A:283:SER:CB	1:A:284:LEU:HA	1.94	0.98
1:B:422:LEU:CD1	1:B:426:ILE:CD1	2.43	0.96
1:B:422:LEU:CD1	1:B:426:ILE:HD11	1.97	0.95
1:A:463:THR:O	1:A:466:ILE:CD1	2.18	0.91
1:B:298:TYR:O	5:B:814:HOH:O	1.89	0.88
1:B:228:GLU:OE2	1:B:229:VAL:HG23	1.71	0.88
1:B:327:ASN:HD22	1:B:328:ASN:H	1.23	0.85
1:D:390:PHE:CZ	1:D:426:ILE:CD1	2.63	0.82
1:B:466:ILE:N	1:B:466:ILE:HD13	1.96	0.81
1:B:228:GLU:OE2	1:B:229:VAL:CG2	2.30	0.79
1:A:470:ARG:CZ	1:A:470:ARG:HB2	2.12	0.78
1:D:398:GLU:OE2	1:D:406:LYS:HD3	1.83	0.78
1:B:422:LEU:CD1	1:B:426:ILE:HD13	2.13	0.77
1:A:472:ASP:O	1:A:476:LEU:HD12	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:ARG:HG2	1:B:226:ARG:NH2	1.90	0.77
1:A:466:ILE:H	1:A:466:ILE:HD12	1.51	0.76
1:A:328:ASN:HD22	1:A:328:ASN:C	1.94	0.75
1:A:466:ILE:HD12	1:A:466:ILE:N	2.02	0.75
1:A:473:TYR:HA	1:A:476:LEU:HD13	1.67	0.74
1:A:298:TYR:O	5:A:851:HOH:O	2.06	0.74
1:D:327:ASN:O	1:D:328:ASN:HB3	1.88	0.73
1:D:328:ASN:C	1:D:328:ASN:ND2	2.43	0.73
1:D:466:ILE:HD13	1:D:466:ILE:N	2.03	0.73
1:C:328:ASN:O	5:C:832:HOH:O	2.10	0.69
1:A:473:TYR:HA	1:A:476:LEU:CD1	2.21	0.69
1:A:574:ALA:C	1:A:595:LYS:NZ	2.50	0.68
1:D:327:ASN:O	1:D:328:ASN:CB	2.42	0.68
1:B:422:LEU:HD12	1:B:426:ILE:HD13	1.69	0.67
1:A:320:CYS:SG	1:A:327:ASN:O	2.53	0.66
1:B:327:ASN:HD22	1:B:328:ASN:N	1.93	0.66
1:A:470:ARG:HA	1:A:473:TYR:CE2	2.31	0.66
1:B:463:THR:O	1:B:466:ILE:HG12	1.96	0.65
1:D:115:MET:C	1:D:115:MET:SD	2.79	0.65
1:A:596:LYS:HD3	1:A:596:LYS:H	1.61	0.65
1:A:466:ILE:CD1	1:A:466:ILE:H	2.10	0.65
1:B:326:GLN:O	1:B:326:GLN:HG3	1.96	0.65
2:D:703:TTP:O1B	1:B:377:LYS:NZ	2.30	0.65
1:A:472:ASP:O	1:A:476:LEU:CD1	2.46	0.64
1:A:372:ARG:HD2	2:C:701:TTP:O4	1.99	0.63
1:B:466:ILE:N	1:B:466:ILE:CD1	2.61	0.63
1:B:327:ASN:ND2	1:B:328:ASN:H	1.96	0.63
1:A:596:LYS:HD3	1:A:596:LYS:N	2.15	0.61
1:C:397:ILE:HG21	1:C:426:ILE:HD11	1.82	0.61
1:A:470:ARG:HB2	1:A:470:ARG:NH1	2.15	0.61
2:C:703:TTP:PA	2:C:703:TTP:O1G	2.60	0.59
1:C:215:HIS:CD2	2:C:703:TTP:C6	2.91	0.59
1:B:422:LEU:HD11	1:B:426:ILE:HD13	1.85	0.58
1:B:466:ILE:HD13	1:B:466:ILE:H	1.68	0.58
1:A:190:GLN:O	1:A:294:LYS:NZ	2.37	0.58
1:C:490:ASP:OD2	1:C:560:LYS:HE2	2.04	0.57
1:B:226:ARG:NH2	1:B:229:VAL:HG21	2.19	0.57
1:D:535:ASN:OD1	1:D:535:ASN:N	2.27	0.56
1:A:596:LYS:N	1:A:596:LYS:CD	2.69	0.56
1:B:228:GLU:CD	1:B:229:VAL:CG2	2.70	0.56
1:D:473:TYR:OH	5:D:865:HOH:O	2.16	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:HIS:CE1	1:D:321:HIS:CE1	2.93	0.56
1:C:206:ARG:NH1	2:C:703:TTP:O2B	2.38	0.56
1:B:354:LYS:NZ	5:B:842:HOH:O	2.39	0.56
1:A:396:TYR:CE2	1:A:437:LYS:HB3	2.41	0.55
1:A:574:ALA:C	1:A:595:LYS:HZ2	2.13	0.55
1:D:465:GLN:HA	1:D:465:GLN:OE1	2.06	0.55
1:D:390:PHE:CE1	1:D:426:ILE:CD1	2.91	0.54
1:A:283:SER:HB2	1:A:284:LEU:C	2.33	0.53
1:C:235:GLN:O	1:C:238:VAL:HG22	2.09	0.53
1:D:395:ASP:OD1	1:D:408:ARG:NH1	2.38	0.53
1:D:113:ASP:HB3	1:D:130:PRO:HB3	1.91	0.53
1:D:466:ILE:N	1:D:466:ILE:CD1	2.71	0.53
1:C:154:TYR:O	5:C:839:HOH:O	2.18	0.53
1:C:388:ASP:OD2	1:C:392:LYS:HE3	2.10	0.51
1:D:522[A]:CYS:SG	1:B:586:VAL:HG11	2.50	0.51
2:D:703:TTP:H2'1	1:B:157:PHE:CE1	2.45	0.51
1:D:390:PHE:CE1	1:D:426:ILE:HD11	2.40	0.51
1:D:592:THR:OG1	1:D:593:PRO:HD3	2.11	0.51
1:C:327:ASN:O	1:C:328:ASN:HB2	2.11	0.51
1:A:425:ASN:HB2	1:D:428:LEU:HD13	1.93	0.50
1:B:467:LYS:HG3	1:B:468:ILE:N	2.27	0.50
1:C:592:THR:OG1	1:C:593:PRO:HD3	2.12	0.50
1:D:466:ILE:HD13	1:D:466:ILE:H	1.77	0.50
1:B:215:HIS:CD2	2:B:705:TTP:C6	2.99	0.50
1:A:396:TYR:CZ	1:A:437:LYS:HB3	2.47	0.50
1:C:295:SER:HB2	5:C:831:HOH:O	2.12	0.50
1:D:467:LYS:HG3	1:D:468:ILE:N	2.26	0.50
1:A:470:ARG:CZ	1:A:470:ARG:CB	2.87	0.49
2:A:701:TTP:O5'	2:A:701:TTP:O1B	2.29	0.49
1:D:499:ILE:HD11	1:D:555:LYS:HE2	1.94	0.49
1:A:315:TYR:CE2	2:A:701:TTP:H5'1	2.47	0.49
1:D:305:ARG:NH2	1:D:305:ARG:HG2	2.27	0.49
1:B:592:THR:OG1	1:B:593:PRO:HD3	2.12	0.49
1:C:186:GLN:HB2	1:C:189:LEU:HD22	1.95	0.49
1:D:186:GLN:HB2	1:D:189:LEU:HD22	1.94	0.49
1:D:351:ALA:O	1:D:520:PHE:HA	2.13	0.49
1:A:215:HIS:CE1	2:A:701:TTP:O2A	2.66	0.49
1:D:305:ARG:HG2	1:D:305:ARG:HH21	1.79	0.48
1:A:186:GLN:HB2	1:A:189:LEU:HD22	1.96	0.48
1:C:499:ILE:HD11	1:C:555:LYS:HE2	1.96	0.48
1:A:592:THR:OG1	1:A:593:PRO:HD3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:GLN:HB2	1:B:189:LEU:HD22	1.95	0.48
1:A:323:LEU:HB3	1:A:325:ILE:HD12	1.96	0.47
1:A:351:ALA:O	1:A:520:PHE:HA	2.14	0.47
1:A:499:ILE:HD11	1:A:555:LYS:HE2	1.96	0.47
1:C:467:LYS:HG3	1:C:468:ILE:N	2.29	0.47
1:A:368:SER:O	1:A:372:ARG:HG3	2.15	0.47
1:D:490:ASP:OD2	1:D:560:LYS:HD3	2.15	0.47
1:A:332:LYS:HG2	5:A:847:HOH:O	2.14	0.47
1:A:586:VAL:HG11	1:C:522[A]:CYS:SG	2.55	0.47
1:D:327:ASN:ND2	1:D:328:ASN:H	2.12	0.47
1:A:328:ASN:C	1:A:328:ASN:ND2	2.65	0.47
1:B:351:ALA:O	1:B:520:PHE:HA	2.15	0.47
1:C:351:ALA:O	1:C:520:PHE:HA	2.14	0.47
1:D:215:HIS:CD2	2:D:701:TTP:C6	3.03	0.47
1:D:251:LYS:HB2	1:D:252:PRO:HD3	1.97	0.47
1:D:315:TYR:CE2	2:D:701:TTP:H5'1	2.51	0.46
2:B:705:TTP:O2G	2:B:705:TTP:O2B	2.33	0.46
1:B:327:ASN:ND2	1:B:328:ASN:N	2.61	0.46
1:D:329:PHE:HA	5:D:870:HOH:O	2.14	0.46
1:A:320:CYS:HB3	1:A:325:ILE:O	2.15	0.46
1:A:428:LEU:HD13	1:D:425:ASN:HB2	1.97	0.46
5:A:858:HOH:O	1:C:372:ARG:HD2	2.14	0.46
1:A:467:LYS:HG3	1:A:468:ILE:N	2.30	0.46
1:A:473:TYR:CA	1:A:476:LEU:CD1	2.92	0.45
1:C:251:LYS:HB2	1:C:252:PRO:HD3	1.98	0.45
1:D:352:ARG:HG3	1:D:354:LYS:HG2	1.98	0.45
1:B:499:ILE:HD11	1:B:555:LYS:HE2	1.98	0.45
1:D:320:CYS:HB3	1:D:325:ILE:O	2.16	0.45
1:A:251:LYS:HB2	1:A:252:PRO:HD3	1.99	0.45
1:C:592:THR:N	1:C:593:PRO:CD	2.80	0.45
1:B:352:ARG:HG3	1:B:354:LYS:HG2	1.99	0.44
1:D:330:ASP:N	5:D:870:HOH:O	1.99	0.44
1:C:489:LEU:CD1	1:C:568:TYR:HE2	2.30	0.44
3:B:706:GTP:O3G	3:B:706:GTP:O1B	2.35	0.44
1:D:129:HIS:CG	1:D:130:PRO:HD2	2.53	0.44
1:A:470:ARG:HA	1:A:473:TYR:CD2	2.52	0.44
1:B:592:THR:N	1:B:593:PRO:CD	2.81	0.44
1:A:265:ILE:O	1:A:269:LYS:HG3	2.18	0.44
1:B:251:LYS:HB2	1:B:252:PRO:HD3	1.99	0.44
1:D:176:GLY:HA3	5:D:849:HOH:O	2.18	0.43
2:B:705:TTP:O1B	2:B:705:TTP:O2A	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:372:ARG:HD3	1:B:358:ASN:OD1	2.18	0.43
1:D:157:PHE:CE1	2:B:703:TTP:H2'1	2.53	0.43
1:C:129:HIS:CG	1:C:130:PRO:HD2	2.54	0.43
1:A:129:HIS:CG	1:A:130:PRO:HD2	2.53	0.43
1:C:295:SER:OG	1:C:347:LEU:O	2.36	0.43
2:A:703:TTP:O4	1:C:372:ARG:HG2	2.19	0.43
1:C:321:HIS:CE1	1:B:321:HIS:CE1	3.07	0.43
1:B:226:ARG:NH2	1:B:228:GLU:OE2	2.51	0.43
1:A:466:ILE:CD1	1:A:466:ILE:N	2.68	0.42
1:A:396:TYR:CE2	1:A:437:LYS:O	2.72	0.42
1:B:129:HIS:CG	1:B:130:PRO:HD2	2.55	0.42
1:B:598:TRP:O	1:B:599:ASN:CB	2.68	0.42
1:B:320:CYS:HB3	1:B:325:ILE:O	2.19	0.42
1:B:454:PHE:CD2	1:B:499:ILE:CD1	3.03	0.42
1:C:598:TRP:O	1:C:599:ASN:HB2	2.20	0.42
1:C:598:TRP:O	1:C:599:ASN:CB	2.66	0.41
1:B:315:TYR:OH	2:B:705:TTP:O3G	2.19	0.41
1:A:469:LYS:HA	1:A:469:LYS:HD3	1.86	0.41
1:C:454:PHE:CD2	1:C:499:ILE:CD1	3.02	0.41
1:D:326:GLN:O	1:D:327:ASN:HB2	2.19	0.41
1:C:475:SER:O	1:C:478:LYS:HB3	2.21	0.41
1:A:525:ALA:HB3	1:C:586:VAL:HG11	2.02	0.41
1:B:226:ARG:NH2	1:B:229:VAL:CG2	2.83	0.41
1:D:390:PHE:CE1	1:D:426:ILE:HD12	2.56	0.41
1:B:480:VAL:HG22	1:B:572:TRP:CD2	2.56	0.41
1:A:435:ASP:HA	1:A:436:PRO:HD3	1.95	0.41
1:C:320:CYS:HB3	1:C:325:ILE:O	2.21	0.41
1:A:592:THR:N	1:A:593:PRO:CD	2.84	0.40
2:D:703:TTP:H2'1	1:B:157:PHE:CZ	2.56	0.40
1:C:428:LEU:HD13	1:B:425:ASN:HB2	2.02	0.40
1:C:425:ASN:HB2	1:B:428:LEU:HD13	2.03	0.40
1:B:509:MET:HE1	1:B:517:HIS:CD2	2.56	0.40
1:A:476:LEU:HD12	1:A:476:LEU:H	1.86	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:478:LYS:CE	1:D:395:ASP:O[1_454]	2.01	0.19
1:A:395:ASP:OD2	1:B:407:TYR:OH[1_556]	2.13	0.07
1:A:465:GLN:OE1	1:B:543:GLU:OE2[1_455]	2.18	0.02

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	476/514 (93%)	471 (99%)	5 (1%)	0	100	100
1	B	476/514 (93%)	468 (98%)	8 (2%)	0	100	100
1	C	476/514 (93%)	468 (98%)	8 (2%)	0	100	100
1	D	477/514 (93%)	469 (98%)	7 (2%)	1 (0%)	43	56
All	All	1905/2056 (93%)	1876 (98%)	28 (2%)	1 (0%)	48	61

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	328	ASN

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	426/459 (93%)	404 (95%)	22 (5%)	21	32
1	B	426/459 (93%)	409 (96%)	17 (4%)	28	42
1	C	426/459 (93%)	411 (96%)	15 (4%)	32	48
1	D	427/459 (93%)	402 (94%)	25 (6%)	18	27
All	All	1705/1836 (93%)	1626 (95%)	79 (5%)	24	36

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	184	GLU
1	A	189	LEU
1	A	229	VAL
1	A	230	LYS
1	A	269	LYS
1	A	283	SER
1	A	284	LEU
1	A	325	ILE
1	A	327	ASN
1	A	328	ASN
1	A	332	LYS
1	A	359	LEU
1	A	368	SER
1	A	439	LYS
1	A	465	GLN
1	A	466	ILE
1	A	470	ARG
1	A	472	ASP
1	A	492	LYS
1	A	523	LYS
1	A	594	GLN
1	A	596	LYS
1	C	114	THR
1	C	134	ARG
1	C	189	LEU
1	C	255	GLU
1	C	273	VAL
1	C	315	TYR
1	C	325	ILE
1	C	327	ASN
1	C	359	LEU
1	C	368	SER
1	C	439	LYS
1	C	465	GLN
1	C	492	LYS
1	C	523	LYS
1	C	594	GLN
1	D	114	THR
1	D	116	LYS
1	D	189	LEU
1	D	206	ARG
1	D	228	GLU
1	D	229	VAL

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Mol	Chain	Res	Type
1	D	255	GLU
1	D	273	VAL
1	D	325	ILE
1	D	326	GLN
1	D	328	ASN
1	D	359	LEU
1	D	368	SER
1	D	377	LYS
1	D	426	ILE
1	D	439	LYS
1	D	463	THR
1	D	465	GLN
1	D	466	ILE
1	D	478	LYS
1	D	492	LYS
1	D	499	ILE
1	D	509	MET
1	D	535	ASN
1	D	594	GLN
1	B	115	MET
1	B	189	LEU
1	B	226	ARG
1	B	273	VAL
1	B	277	GLU
1	B	326	GLN
1	B	332	LYS
1	B	345	ASN
1	B	359	LEU
1	B	368	SER
1	B	426	ILE
1	B	439	LYS
1	B	466	ILE
1	B	492	LYS
1	B	511	GLU
1	B	528	ARG
1	B	594	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	GLN
1	A	215	HIS

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Mol	Chain	Res	Type
1	A	243	HIS
1	A	327	ASN
1	A	328	ASN
1	A	364	HIS
1	A	380	ASN
1	A	425	ASN
1	A	517	HIS
1	A	571	GLN
1	A	594	GLN
1	C	149	GLN
1	C	190	GLN
1	C	200	GLN
1	C	243	HIS
1	C	326	GLN
1	C	364	HIS
1	C	425	ASN
1	C	517	HIS
1	C	571	GLN
1	C	594	GLN
1	D	149	GLN
1	D	190	GLN
1	D	200	GLN
1	D	243	HIS
1	D	326	GLN
1	D	327	ASN
1	D	328	ASN
1	D	425	ASN
1	D	571	GLN
1	D	594	GLN
1	B	163	ASN
1	B	190	GLN
1	B	200	GLN
1	B	210	HIS
1	B	233	HIS
1	B	243	HIS
1	B	327	ASN
1	B	517	HIS
1	B	571	GLN
1	B	594	GLN

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 16 ligands modelled in this entry, 4 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
3	GTP	B	702	4	33,34,34	1.57	7 (21%)	50,54,54	1.69	8 (16%)
2	TTP	D	701	-	29,30,30	1.54	6 (20%)	43,47,47	1.97	8 (18%)
3	GTP	A	702	4	33,34,34	1.46	6 (18%)	50,54,54	1.93	12 (24%)
3	GTP	B	706	4	33,34,34	1.37	6 (18%)	50,54,54	1.62	10 (20%)
2	TTP	B	705	-	29,30,30	1.62	8 (27%)	43,47,47	2.01	10 (23%)
2	TTP	C	701	4	29,30,30	1.86	6 (20%)	43,47,47	1.74	8 (18%)
2	TTP	B	703	4	29,30,30	1.50	5 (17%)	43,47,47	2.02	12 (27%)
2	TTP	C	703	-	29,30,30	1.68	6 (20%)	43,47,47	1.65	6 (13%)
2	TTP	A	701	-	29,30,30	1.47	5 (17%)	43,47,47	1.85	6 (13%)
3	GTP	D	702	4	33,34,34	2.04	6 (18%)	50,54,54	1.60	7 (14%)
2	TTP	D	703	4	29,30,30	1.66	7 (24%)	43,47,47	1.50	6 (13%)
2	TTP	A	703	4	29,30,30	2.07	6 (20%)	43,47,47	1.90	10 (23%)

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
3	GTP	B	702	4	-	7/22/38/38	0/3/3/3
2	TTP	D	701	-	-	8/22/34/34	0/2/2/2
3	GTP	A	702	4	-	5/22/38/38	0/3/3/3
3	GTP	B	706	4	-	6/22/38/38	0/3/3/3
2	TTP	B	705	-	-	7/22/34/34	0/2/2/2
2	TTP	C	701	4	-	3/22/34/34	0/2/2/2
2	TTP	B	703	4	-	5/22/34/34	0/2/2/2
2	TTP	C	703	-	-	9/22/34/34	0/2/2/2
2	TTP	A	701	-	-	7/22/34/34	0/2/2/2
3	GTP	D	702	4	-	4/22/38/38	0/3/3/3
2	TTP	D	703	4	-	5/22/34/34	0/2/2/2
2	TTP	A	703	4	-	3/22/34/34	0/2/2/2

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	703	TTP	PB-O3B	6.30	1.66	1.59
3	D	702	GTP	PB-O3B	6.16	1.66	1.59
3	D	702	GTP	PA-O3A	5.89	1.65	1.59
2	C	703	TTP	PA-O3A	4.65	1.64	1.59
2	C	701	TTP	PA-O3A	4.61	1.64	1.59
2	A	701	TTP	PB-O3B	4.24	1.64	1.59
2	C	703	TTP	PB-O3A	4.22	1.64	1.59
2	B	703	TTP	C6-N1	-3.93	1.31	1.38
3	A	702	GTP	C5-N7	-3.87	1.31	1.39
3	B	702	GTP	PA-O3A	3.85	1.63	1.59
2	C	701	TTP	C6-N1	-3.81	1.31	1.38
2	A	703	TTP	C6-N1	-3.80	1.31	1.38
2	A	703	TTP	C2-N3	-3.68	1.31	1.38
3	D	702	GTP	C5-C4	3.66	1.48	1.38
2	D	703	TTP	C4-N3	-3.63	1.32	1.38
2	A	703	TTP	C6-C5	3.59	1.40	1.34
2	A	703	TTP	C4-N3	-3.56	1.32	1.38
2	B	705	TTP	PB-O3B	3.55	1.63	1.59
3	B	702	GTP	C5-C4	3.53	1.48	1.38
3	B	706	GTP	C5-C4	3.47	1.48	1.38
2	D	701	TTP	PA-O3A	3.39	1.63	1.59
2	B	705	TTP	PB-O3A	3.33	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	GTP	C5-N7	-3.27	1.32	1.39
3	B	702	GTP	PB-O3B	3.27	1.63	1.59
2	D	701	TTP	C6-C5	3.25	1.39	1.34
2	B	703	TTP	C6-C5	3.22	1.39	1.34
2	D	703	TTP	PB-O3B	3.22	1.63	1.59
2	D	701	TTP	PB-O3A	3.16	1.62	1.59
2	A	701	TTP	C6-C5	3.15	1.39	1.34
2	C	701	TTP	C4-N3	-3.11	1.33	1.38
3	B	706	GTP	C5-N7	-3.09	1.32	1.39
2	D	703	TTP	C6-C5	3.03	1.39	1.34
3	A	702	GTP	C6-N1	-2.97	1.33	1.38
2	C	701	TTP	PB-O3B	2.94	1.62	1.59
3	D	702	GTP	C4-N9	-2.92	1.30	1.38
3	D	702	GTP	C6-N1	-2.88	1.33	1.38
2	D	701	TTP	PB-O3B	2.87	1.62	1.59
2	D	703	TTP	C2-N3	-2.83	1.33	1.38
2	B	703	TTP	PB-O3B	2.83	1.62	1.59
3	A	702	GTP	C5-C4	2.79	1.46	1.38
2	B	705	TTP	C4-C5	2.70	1.49	1.44
2	B	705	TTP	C6-C5	2.67	1.39	1.34
2	D	703	TTP	PA-O3A	2.66	1.62	1.59
3	A	702	GTP	PB-O3A	2.62	1.62	1.59
2	C	703	TTP	C6-C5	2.51	1.38	1.34
3	D	702	GTP	C5-N7	-2.49	1.34	1.39
2	C	703	TTP	C4-N3	-2.47	1.34	1.38
2	A	701	TTP	C4-N3	-2.45	1.34	1.38
2	D	703	TTP	C2-N1	2.44	1.42	1.38
3	B	706	GTP	PB-O3A	2.42	1.62	1.59
2	B	705	TTP	C4-N3	-2.41	1.34	1.38
2	B	703	TTP	C2-N1	2.41	1.42	1.38
2	C	701	TTP	O4'-C1'	2.37	1.47	1.42
2	B	705	TTP	PA-O3A	2.34	1.62	1.59
3	B	702	GTP	C4-N9	-2.33	1.32	1.38
2	A	701	TTP	C2-N3	-2.28	1.34	1.38
2	D	701	TTP	C4-C5	2.27	1.48	1.44
3	A	702	GTP	PA-O3A	2.25	1.61	1.59
2	C	703	TTP	C2-N3	-2.25	1.34	1.38
3	B	706	GTP	C4-N9	-2.24	1.32	1.38
3	B	702	GTP	O4'-C1'	2.24	1.47	1.42
2	C	703	TTP	O4'-C4'	-2.23	1.40	1.45
2	D	703	TTP	C6-N1	-2.21	1.34	1.38
2	B	703	TTP	O4'-C4'	-2.19	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	TTP	C6-N1	-2.18	1.34	1.38
2	B	705	TTP	O4'-C4'	-2.16	1.40	1.45
2	A	703	TTP	PG-O2G	-2.15	1.46	1.54
2	D	701	TTP	C2-N1	2.15	1.41	1.38
3	B	702	GTP	C6-N1	-2.10	1.34	1.38
3	B	706	GTP	PA-O3A	2.07	1.61	1.59
3	B	706	GTP	O6-C6	2.07	1.27	1.23
2	B	705	TTP	C2-N1	2.07	1.41	1.38
2	C	701	TTP	O2-C2	2.03	1.26	1.23
3	A	702	GTP	C8-N9	-2.01	1.33	1.37

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	GTP	C5-C4-N3	-6.59	117.90	128.39
2	B	703	TTP	C4-N3-C2	-5.86	119.66	127.34
2	B	705	TTP	C5-C4-N3	5.65	120.23	115.32
2	B	705	TTP	C4-N3-C2	-5.63	119.96	127.34
2	A	701	TTP	N3-C2-N1	5.63	122.22	114.89
2	A	703	TTP	N3-C2-N1	5.60	122.18	114.89
3	A	702	GTP	C2-N3-C4	5.50	121.77	112.30
2	D	701	TTP	C4-N3-C2	-5.49	120.14	127.34
2	B	703	TTP	N3-C2-N1	5.46	122.00	114.89
2	D	701	TTP	C5-C4-N3	5.45	120.06	115.32
2	D	701	TTP	O4-C4-C5	-5.38	118.76	124.92
3	B	702	GTP	C5-C4-N3	-5.28	119.98	128.39
2	A	701	TTP	C4-N3-C2	-5.25	120.46	127.34
3	D	702	GTP	C5-C4-N3	-5.06	120.33	128.39
2	D	701	TTP	N3-C2-N1	5.04	121.45	114.89
3	B	706	GTP	C5-C4-N3	-4.98	120.46	128.39
2	B	705	TTP	N3-C2-N1	4.94	121.33	114.89
2	C	701	TTP	C4-N3-C2	-4.87	120.95	127.34
3	A	702	GTP	N9-C4-N3	4.79	135.53	125.95
3	B	706	GTP	C2-N3-C4	4.78	120.53	112.30
2	B	705	TTP	O4-C4-C5	-4.74	119.50	124.92
2	C	703	TTP	N3-C2-N1	4.60	120.88	114.89
2	B	703	TTP	O4-C4-C5	-4.50	119.77	124.92
2	A	703	TTP	C4-N3-C2	-4.50	121.45	127.34
3	B	702	GTP	C2-N3-C4	4.47	120.00	112.30
2	D	703	TTP	C5-C6-N1	-4.39	118.54	123.31
2	A	701	TTP	O4-C4-C5	-4.33	119.97	124.92
2	A	703	TTP	C5-C6-N1	-4.30	118.64	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	TTP	N3-C2-N1	4.28	120.46	114.89
3	B	702	GTP	N9-C4-N3	4.22	134.39	125.95
3	D	702	GTP	N9-C4-N3	4.16	134.27	125.95
3	D	702	GTP	C2-N3-C4	4.13	119.42	112.30
2	D	703	TTP	C5-C4-N3	4.13	118.91	115.32
2	C	703	TTP	C5-C4-N3	4.00	118.80	115.32
2	A	701	TTP	C5-C4-N3	3.97	118.77	115.32
2	C	703	TTP	C4-N3-C2	-3.93	122.19	127.34
2	B	705	TTP	C5-C6-N1	-3.81	119.18	123.31
2	A	701	TTP	C5-C6-N1	-3.76	119.23	123.31
3	D	702	GTP	O2B-PB-O3B	3.63	117.08	107.27
2	D	703	TTP	C4-N3-C2	-3.60	122.62	127.34
2	D	703	TTP	N3-C2-N1	3.59	119.56	114.89
2	C	701	TTP	O3A-PA-O1A	-3.57	99.96	110.70
3	B	706	GTP	N9-C4-N3	3.54	133.04	125.95
2	C	701	TTP	C5-C6-N1	-3.49	119.52	123.31
2	D	701	TTP	C5-C6-N1	-3.43	119.58	123.31
3	A	702	GTP	C3'-C2'-C1'	3.43	107.95	101.46
2	B	703	TTP	C5-C4-N3	3.43	118.31	115.32
2	C	701	TTP	C5-C4-N3	3.42	118.30	115.32
3	D	702	GTP	C3'-C2'-C1'	3.30	107.71	101.46
2	A	703	TTP	C2'-C3'-C4'	3.16	109.20	102.80
3	A	702	GTP	C6-C5-N7	3.14	136.01	130.29
2	C	703	TTP	O4-C4-C5	-3.10	121.38	124.92
2	A	703	TTP	C5-C4-N3	3.05	117.98	115.32
2	C	701	TTP	O4-C4-C5	-2.96	121.53	124.92
2	C	701	TTP	O2A-PA-O1A	2.93	126.07	112.44
3	B	706	GTP	C6-C5-N7	2.92	135.61	130.29
3	B	706	GTP	N2-C2-N1	2.87	122.82	116.76
2	B	703	TTP	C5M-C5-C6	-2.86	118.98	122.85
2	A	703	TTP	O3G-PG-O2G	2.86	118.52	107.80
2	B	703	TTP	C5-C6-N1	-2.84	120.23	123.31
2	B	705	TTP	O2-C2-N1	-2.83	119.11	122.80
2	D	701	TTP	O2B-PB-O3A	2.83	114.93	107.27
3	B	702	GTP	C6-C5-N7	2.74	135.28	130.29
3	A	702	GTP	O2G-PG-O3B	-2.67	95.69	104.64
3	B	706	GTP	C3'-C2'-C1'	2.67	106.51	101.46
2	B	703	TTP	O3G-PG-O2G	2.66	117.77	107.80
3	B	702	GTP	O2B-PB-O3A	2.60	114.31	107.27
3	A	702	GTP	C4-C5-N7	-2.56	106.61	110.67
3	D	702	GTP	O2'-C2'-C1'	-2.56	101.31	110.10
3	A	702	GTP	O2G-PG-O1G	2.44	120.35	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	706	GTP	O6-C6-C5	-2.44	120.10	126.53
2	A	703	TTP	O2-C2-N3	-2.43	117.01	121.49
2	A	701	TTP	O2-C2-N1	-2.41	119.66	122.80
2	A	703	TTP	O2A-PA-O3A	2.41	113.78	107.27
2	A	703	TTP	O2B-PB-O1B	2.40	123.62	112.44
3	A	702	GTP	O2'-C2'-C1'	-2.38	101.92	110.10
2	B	705	TTP	C2'-C3'-C4'	2.33	107.52	102.80
2	B	705	TTP	O3G-PG-O1G	2.31	119.85	110.83
3	B	702	GTP	O3B-PB-O1B	-2.27	103.87	110.70
3	D	702	GTP	C6-C5-N7	2.27	134.42	130.29
2	C	701	TTP	O3G-PG-O2G	2.26	116.28	107.80
2	D	703	TTP	O2-C2-N3	-2.25	117.33	121.49
3	B	706	GTP	O2G-PG-O1G	2.24	119.56	110.83
2	B	703	TTP	O2-C2-N3	-2.23	117.38	121.49
3	B	702	GTP	C4-C5-N7	-2.23	107.14	110.67
2	B	703	TTP	C5M-C5-C4	2.21	121.14	118.78
2	A	703	TTP	C5M-C5-C4	2.17	121.09	118.78
2	B	703	TTP	C2'-C3'-C4'	2.16	107.18	102.80
2	C	703	TTP	C5M-C5-C4	2.14	121.07	118.78
2	B	703	TTP	C6-C5-C4	2.14	119.78	118.02
2	B	703	TTP	C1'-N1-C2	2.11	121.78	117.66
2	B	705	TTP	O3G-PG-O2G	2.09	115.64	107.80
3	A	702	GTP	N2-C2-N1	2.08	121.15	116.76
3	B	702	GTP	O6-C6-C5	-2.07	121.07	126.53
3	A	702	GTP	O2A-PA-O1A	2.07	122.06	112.44
2	D	701	TTP	O4'-C1'-N1	2.06	111.53	107.86
2	B	705	TTP	O2B-PB-O3B	2.06	112.85	107.27
2	D	703	TTP	O2G-PG-O1G	2.05	118.81	110.83
3	B	706	GTP	C4-C5-N7	-2.04	107.43	110.67
3	A	702	GTP	O6-C6-C5	-2.03	121.18	126.53
2	D	701	TTP	O2-C2-N1	-2.03	120.16	122.80
2	C	703	TTP	O4'-C1'-N1	2.03	111.46	107.86
3	B	706	GTP	N2-C2-N3	-2.01	115.74	119.67

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	TTP	C5'-O5'-PA-O1A
2	A	701	TTP	C5'-O5'-PA-O2A
2	A	701	TTP	C5'-O5'-PA-O3A
2	C	703	TTP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
2	C	703	TTP	O4'-C4'-C5'-O5'
2	D	701	TTP	C5'-O5'-PA-O3A
2	B	705	TTP	C5'-O5'-PA-O1A
2	B	705	TTP	PB-O3B-PG-O2G
2	B	705	TTP	PB-O3B-PG-O3G
3	B	706	GTP	PB-O3B-PG-O3G
2	C	703	TTP	C3'-C4'-C5'-O5'
2	B	705	TTP	O4'-C4'-C5'-O5'
2	B	705	TTP	C3'-C4'-C5'-O5'
2	A	701	TTP	C4'-C5'-O5'-PA
3	B	706	GTP	PB-O3B-PG-O1G
2	A	703	TTP	PB-O3A-PA-O1A
2	C	701	TTP	PA-O3A-PB-O1B
2	D	701	TTP	O4'-C4'-C5'-O5'
2	A	701	TTP	PB-O3A-PA-O5'
2	D	701	TTP	C3'-C4'-C5'-O5'
2	A	703	TTP	PB-O3B-PG-O3G
2	C	703	TTP	PB-O3B-PG-O2G
2	D	703	TTP	PB-O3B-PG-O2G
3	B	702	GTP	PB-O3B-PG-O2G
3	B	702	GTP	PB-O3B-PG-O3G
2	A	701	TTP	C3'-C4'-C5'-O5'
2	D	701	TTP	PB-O3A-PA-O2A
2	D	703	TTP	PG-O3B-PB-O2B
2	B	703	TTP	PB-O3A-PA-O2A
3	A	702	GTP	PG-O3B-PB-O1B
3	B	702	GTP	PG-O3B-PB-O2B
3	B	706	GTP	PG-O3B-PB-O1B
2	C	703	TTP	C5'-O5'-PA-O1A
2	D	701	TTP	C5'-O5'-PA-O1A
2	B	703	TTP	C5'-O5'-PA-O1A
2	A	703	TTP	PB-O3A-PA-O2A
2	C	701	TTP	PA-O3A-PB-O2B
2	B	703	TTP	PG-O3B-PB-O1B
2	B	703	TTP	PG-O3B-PB-O2B
2	B	705	TTP	PB-O3A-PA-O1A
3	D	702	GTP	PB-O3A-PA-O2A
2	D	701	TTP	C4'-C5'-O5'-PA
2	C	703	TTP	PA-O3A-PB-O1B
2	D	703	TTP	PB-O3A-PA-O1A
2	B	703	TTP	PB-O3A-PA-O1A
3	D	702	GTP	PG-O3B-PB-O1B

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Mol	Chain	Res	Type	Atoms
3	B	702	GTP	C4'-C5'-O5'-PA
2	A	701	TTP	O4'-C4'-C5'-O5'
3	D	702	GTP	C4'-C5'-O5'-PA
3	B	706	GTP	C4'-C5'-O5'-PA
2	C	703	TTP	PB-O3B-PG-O3G
3	A	702	GTP	C4'-C5'-O5'-PA
2	D	701	TTP	PB-O3A-PA-O1A
2	D	703	TTP	PG-O3B-PB-O1B
2	B	705	TTP	PB-O3A-PA-O2A
3	A	702	GTP	PG-O3B-PB-O2B
3	A	702	GTP	PB-O3A-PA-O2A
3	B	702	GTP	PG-O3B-PB-O1B
3	B	702	GTP	PB-O3A-PA-O1A
3	B	702	GTP	PB-O3A-PA-O2A
3	B	706	GTP	PG-O3B-PB-O2B
2	C	701	TTP	PB-O3A-PA-O2A
2	C	703	TTP	PA-O3A-PB-O2B
2	C	703	TTP	PG-O3B-PB-O2B
2	D	701	TTP	PG-O3B-PB-O2B
2	D	703	TTP	PB-O3A-PA-O2A
3	A	702	GTP	PB-O3A-PA-O1A
3	D	702	GTP	PG-O3B-PB-O2B
3	B	706	GTP	PB-O3A-PA-O2A

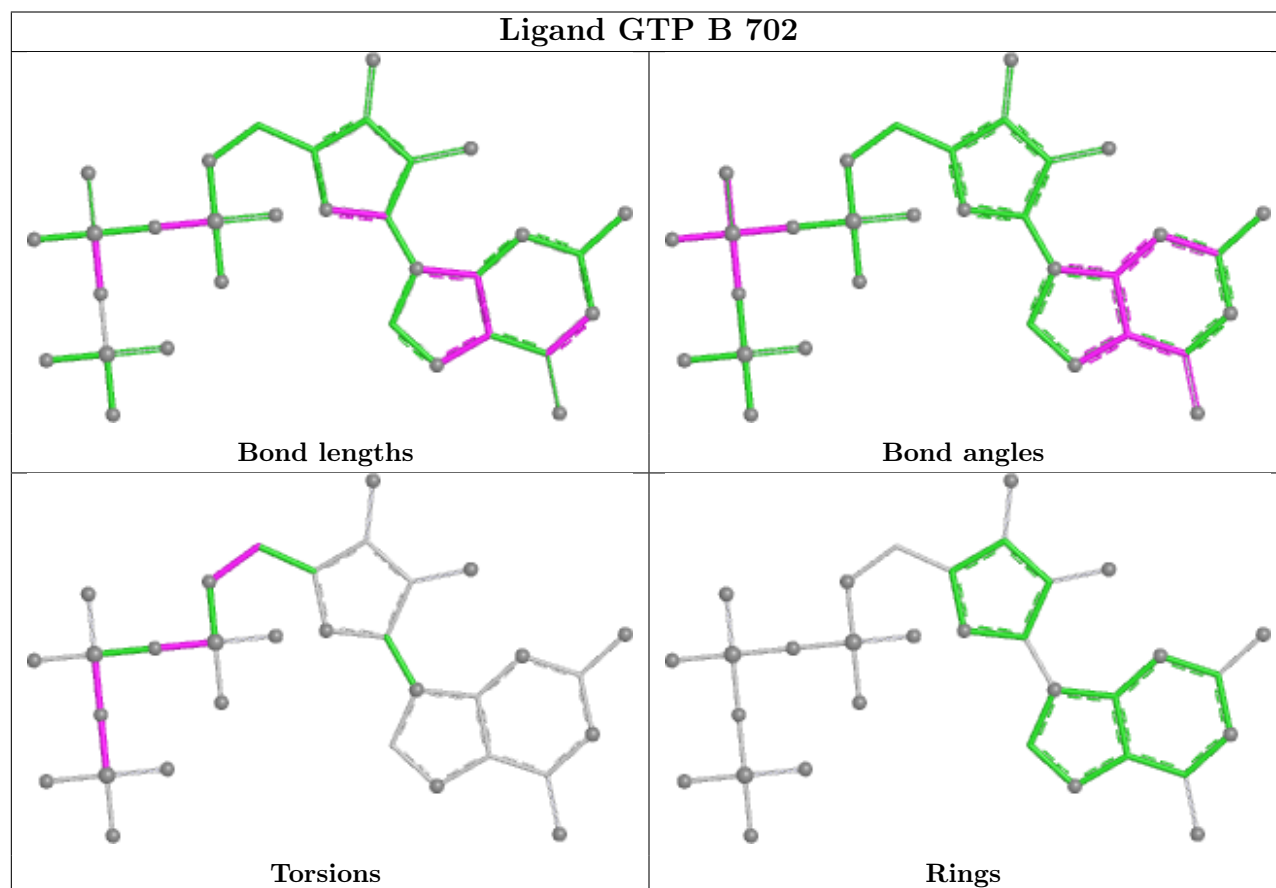
There are no ring outliers.

9 monomers are involved in 21 short contacts:

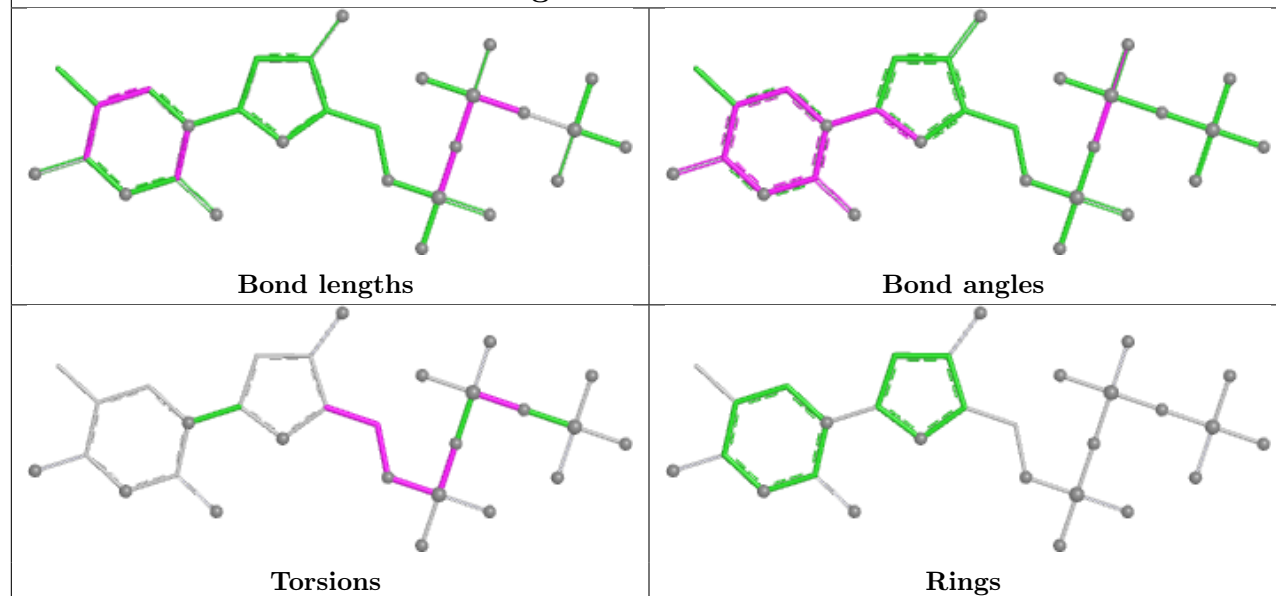
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	701	TTP	3	0
3	B	706	GTP	1	0
2	B	705	TTP	4	0
2	C	701	TTP	1	0
2	B	703	TTP	1	0
2	C	703	TTP	3	0
2	A	701	TTP	4	0
2	D	703	TTP	3	0
2	A	703	TTP	1	0

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

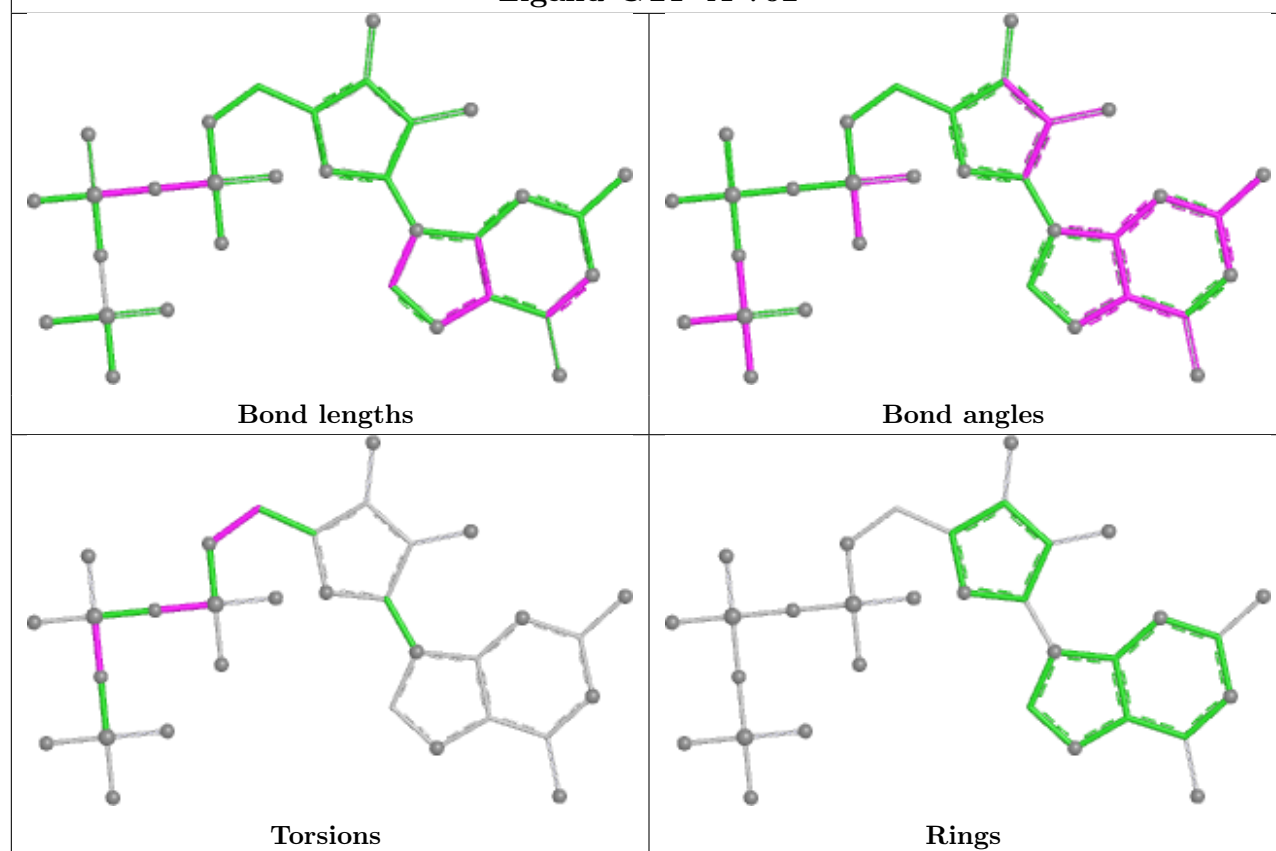
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.



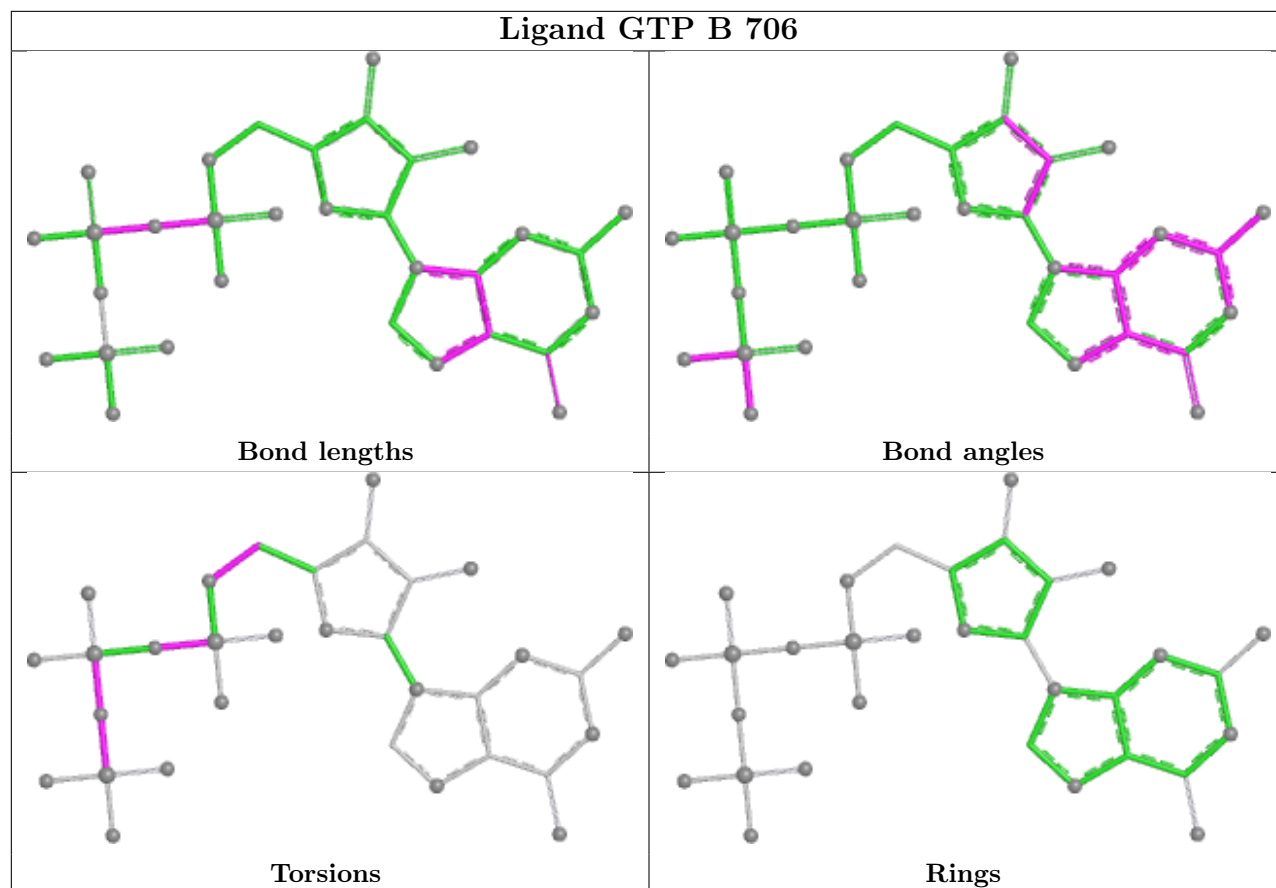
Ligand TTP D 701



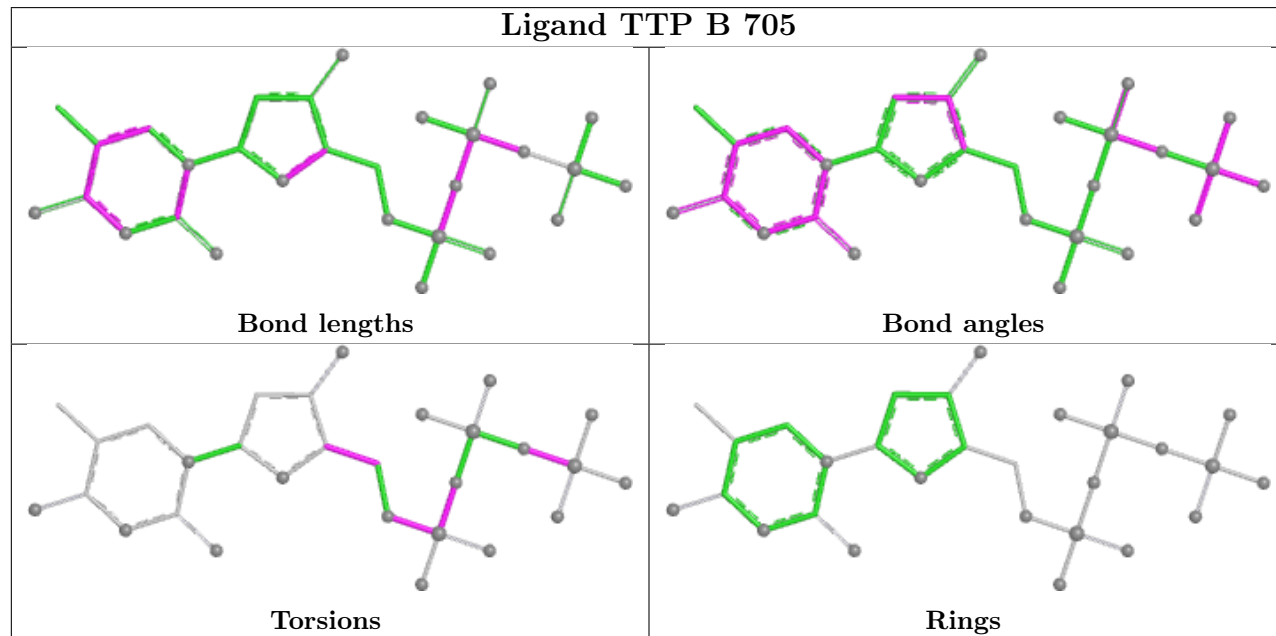
Ligand GTP A 702



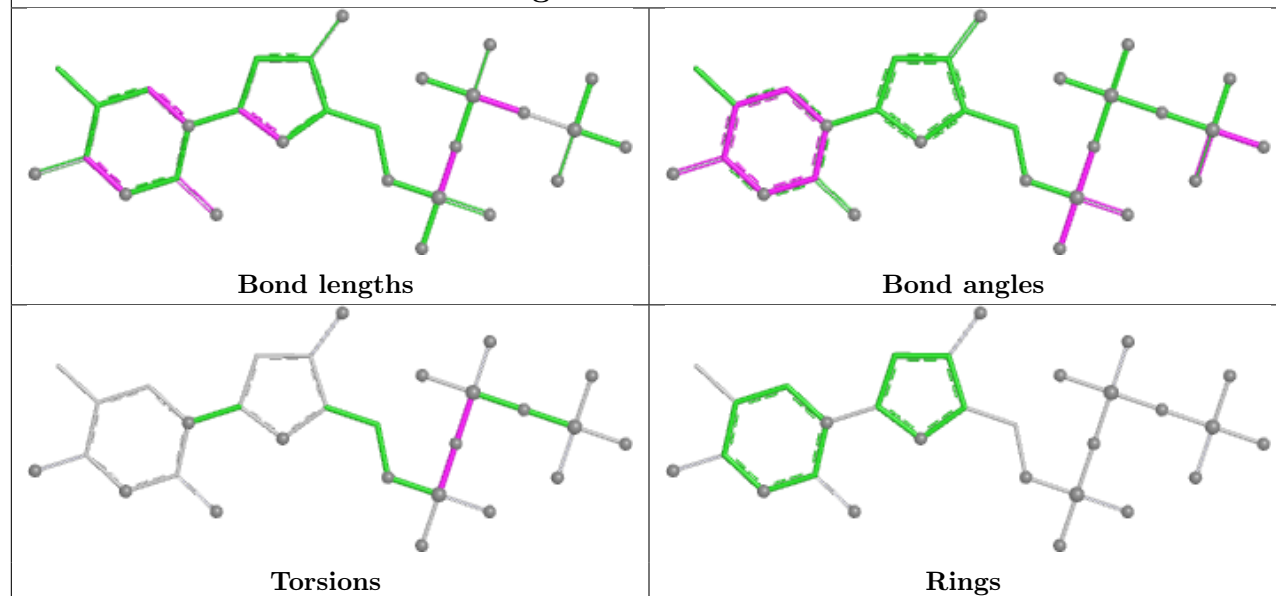
Ligand GTP B 706



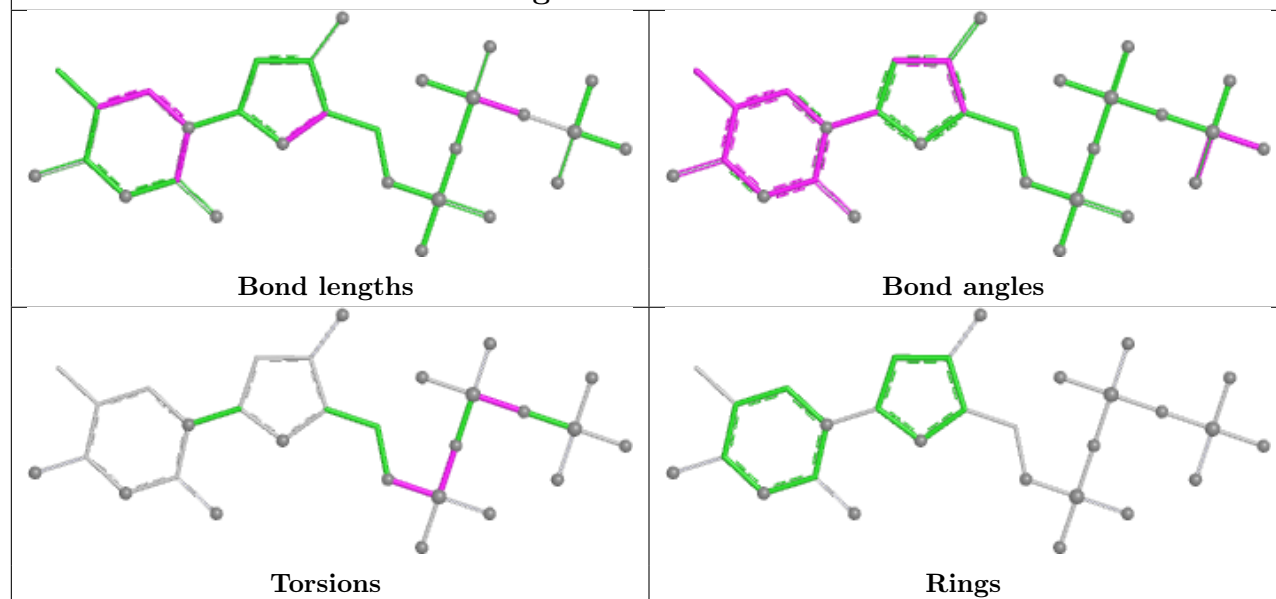
Ligand TTP B 705



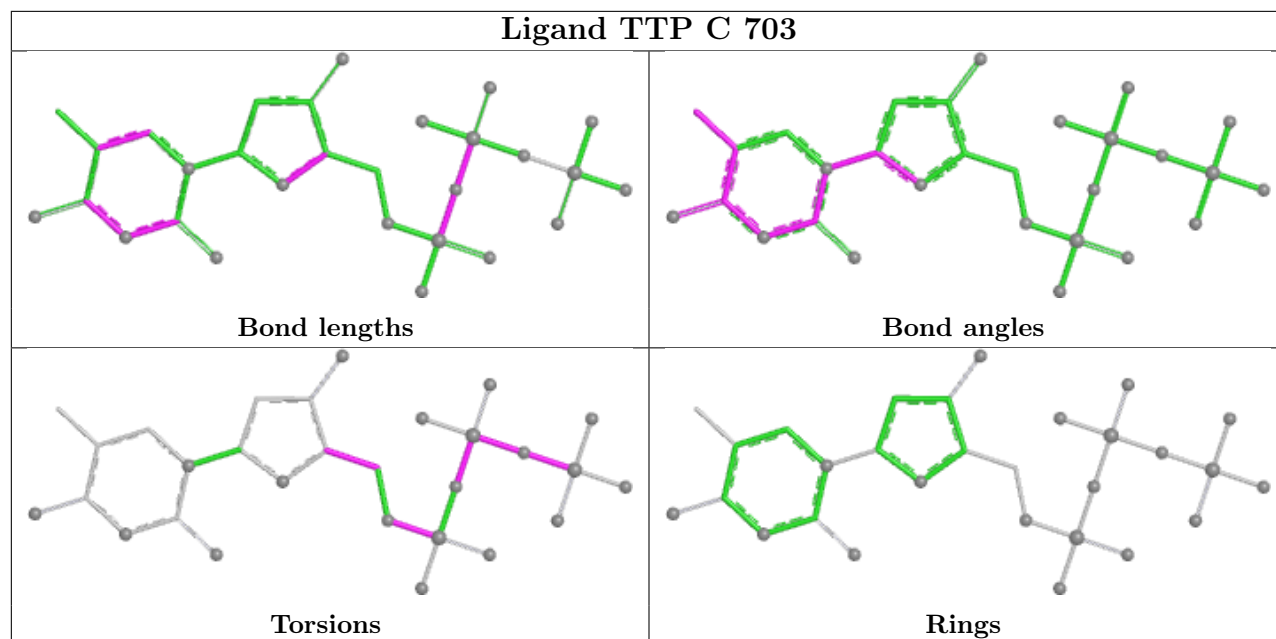
Ligand TTP C 701



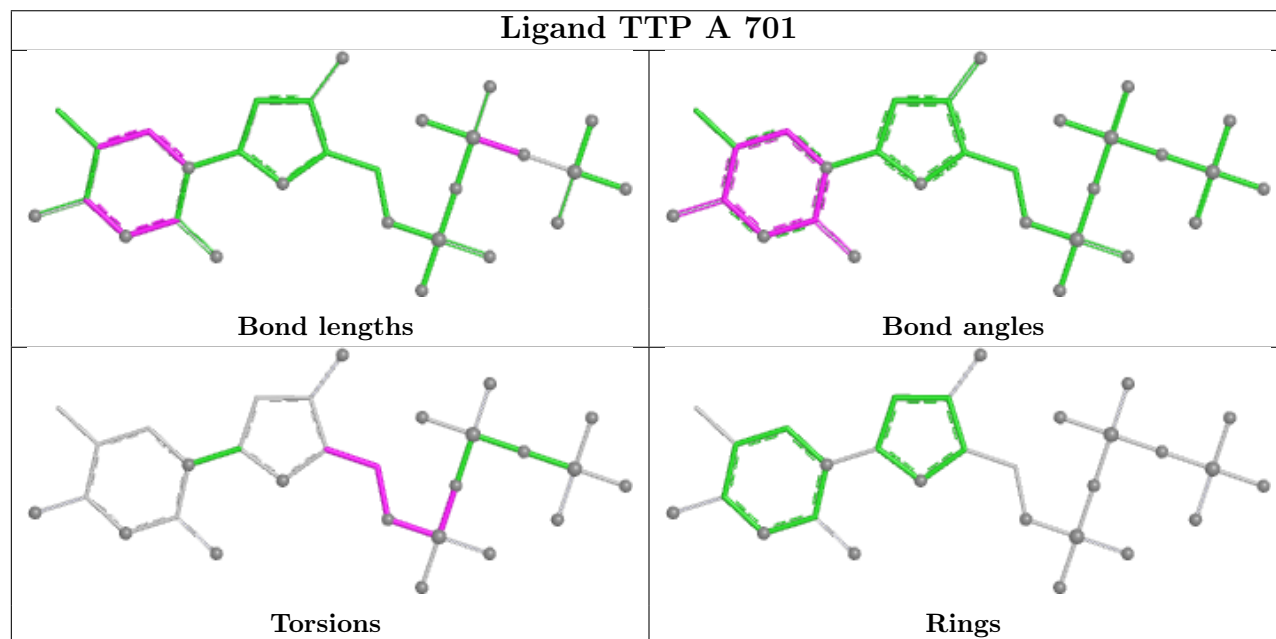
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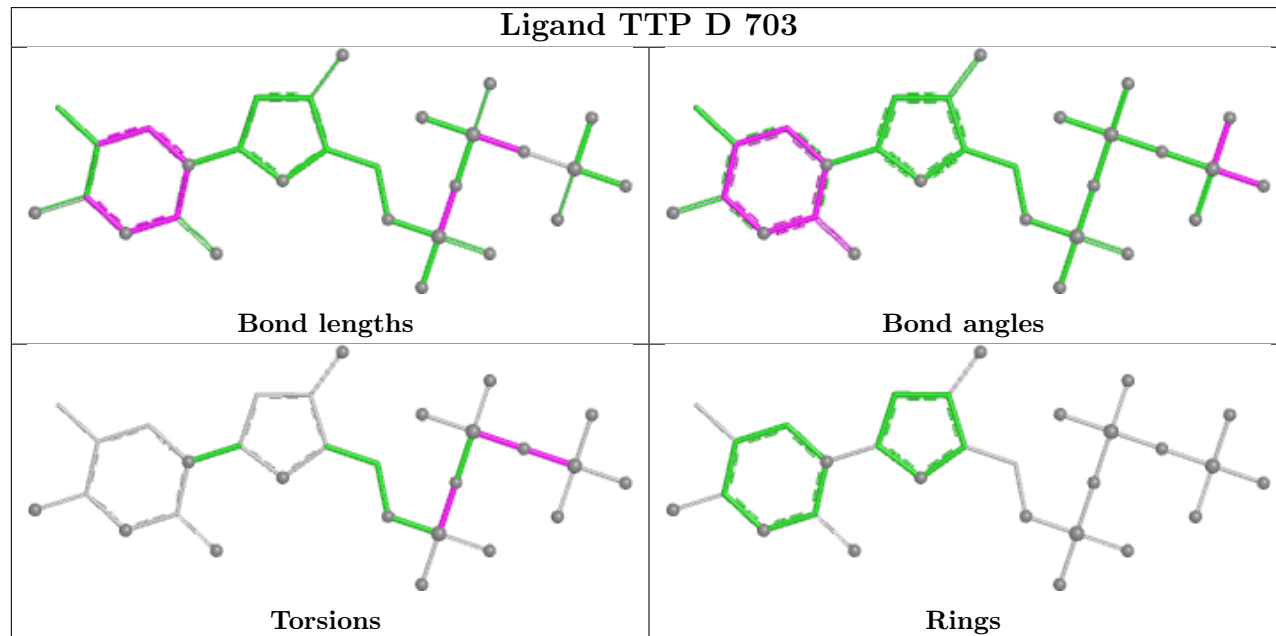
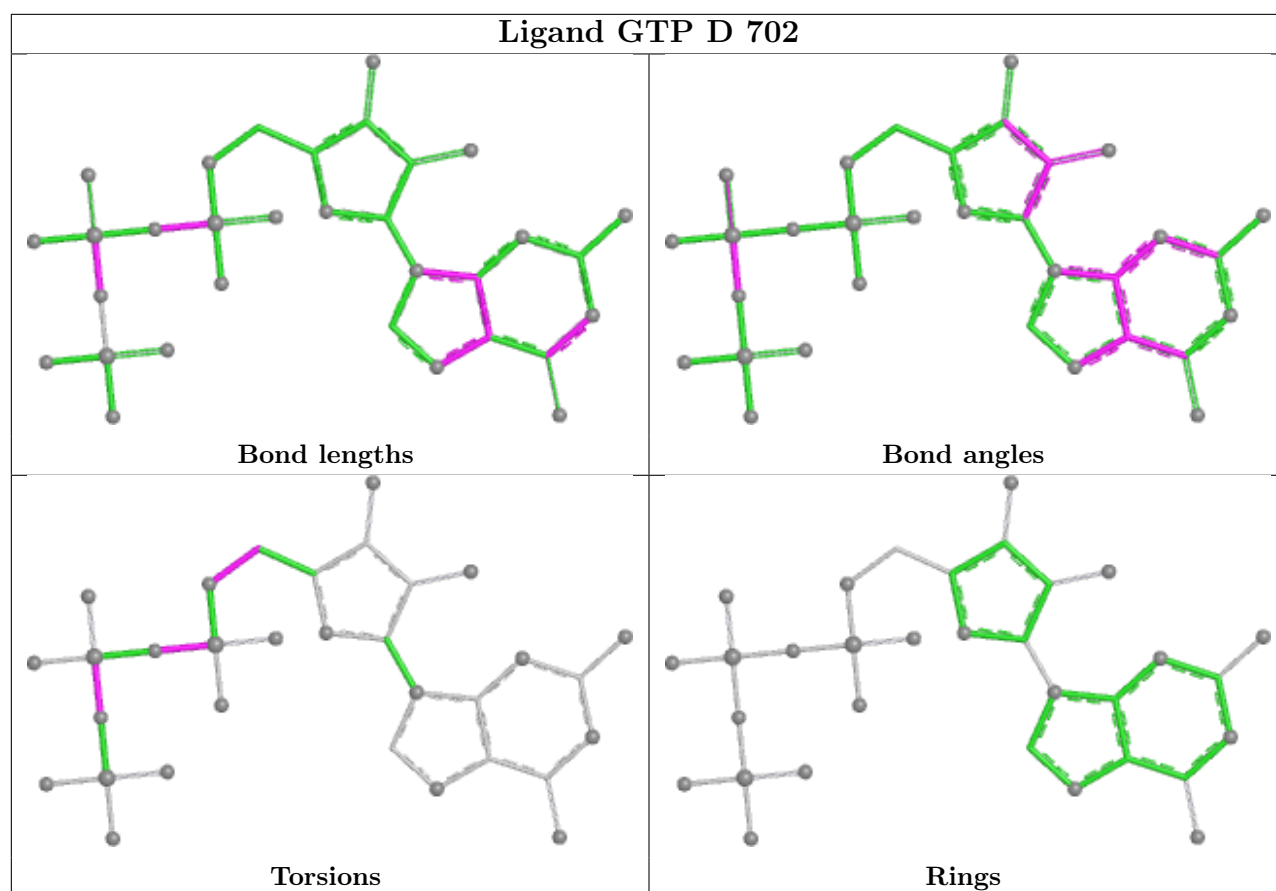


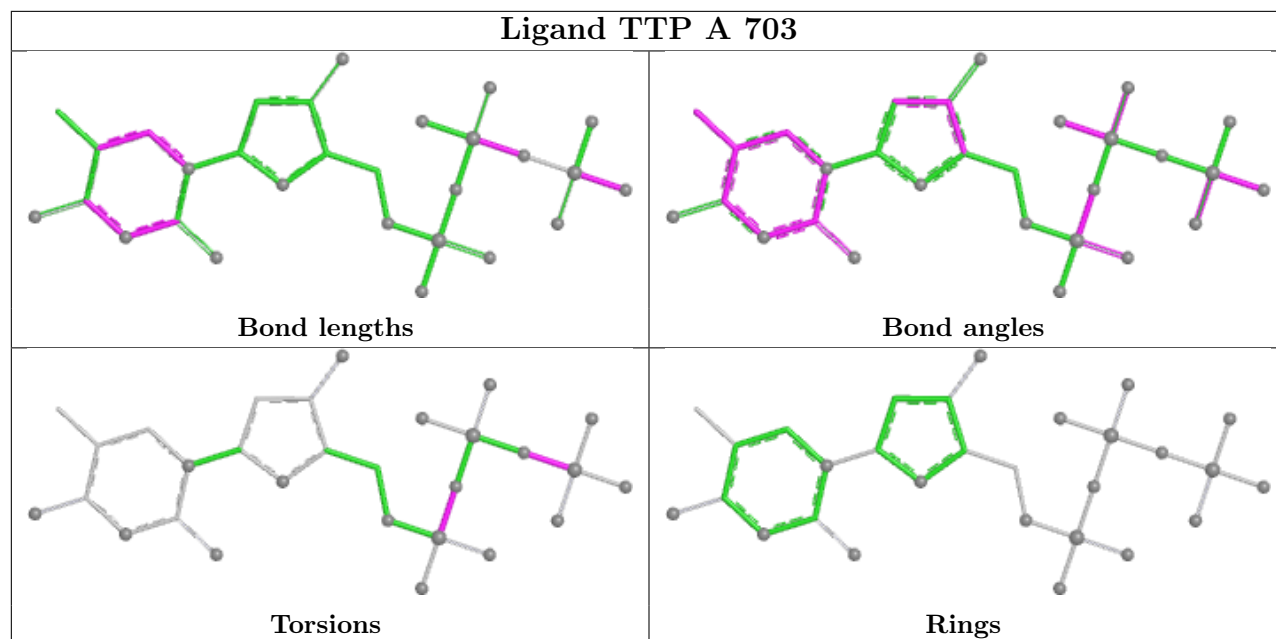
Ligand TTP C 703



Ligand TTP A 701







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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.29	1 (0%) 91 93	27, 51, 102, 144	0
1	B	480/514 (93%)	-0.19	4 (0%) 82 84	32, 60, 103, 130	0
1	C	479/514 (93%)	-0.26	1 (0%) 91 93	27, 59, 92, 122	1 (0%)
1	D	480/514 (93%)	-0.37	4 (0%) 82 84	27, 48, 82, 116	1 (0%)
All	All	1919/2056 (93%)	-0.28	10 (0%) 87 89	27, 55, 94, 144	2 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	284	LEU	3.9
1	D	284	LEU	3.4
1	B	466	ILE	3.4
1	D	464	GLY	3.1
1	B	284	LEU	2.5
1	B	327	ASN	2.4
1	D	466	ILE	2.3
1	A	463	THR	2.2
1	D	465	GLN	2.1
1	B	328	ASN	2.1

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 ⓘ

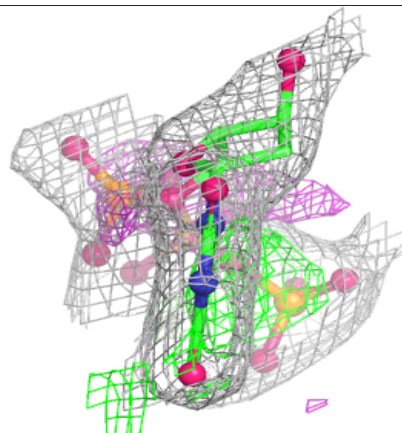
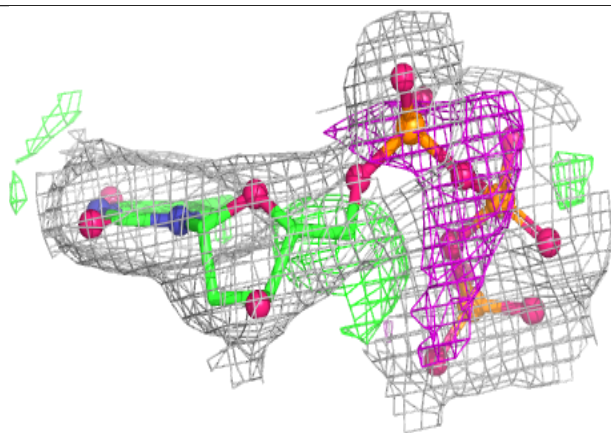
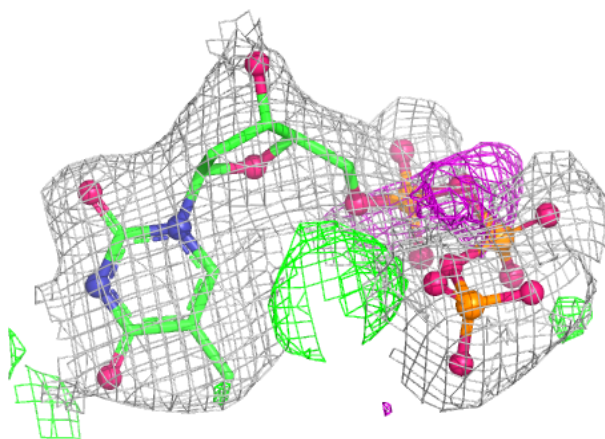
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	TTP	B	705	29/29	0.83	0.11	49,62,110,118	0
2	TTP	C	703	29/29	0.85	0.10	45,68,95,99	0
2	TTP	A	701	29/29	0.89	0.09	41,59,95,101	0
2	TTP	D	701	29/29	0.92	0.08	38,53,85,109	0
4	MG	C	704	1/1	0.93	0.06	59,59,59,59	0
2	TTP	D	703	29/29	0.98	0.04	38,45,49,50	0
2	TTP	B	703	29/29	0.98	0.04	29,34,40,41	0
2	TTP	A	703	29/29	0.98	0.05	34,38,40,49	0
3	GTP	A	702	32/32	0.98	0.04	31,32,41,42	0
3	GTP	D	702	32/32	0.98	0.04	28,33,42,49	0
3	GTP	B	702	32/32	0.98	0.05	35,39,47,49	0
3	GTP	B	706	32/32	0.98	0.04	36,43,56,57	0
2	TTP	C	701	29/29	0.98	0.04	32,36,44,46	0
4	MG	C	702	1/1	0.99	0.04	41,41,41,41	0
4	MG	B	701	1/1	1.00	0.03	40,40,40,40	0
4	MG	B	704	1/1	1.00	0.03	49,49,49,49	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.

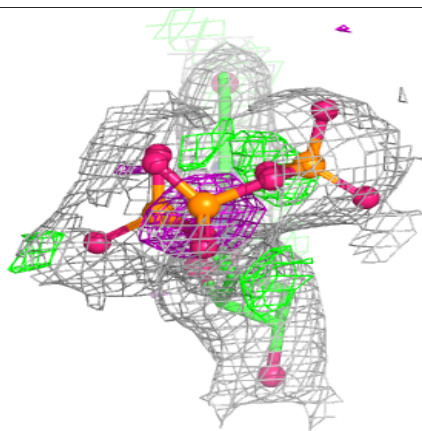
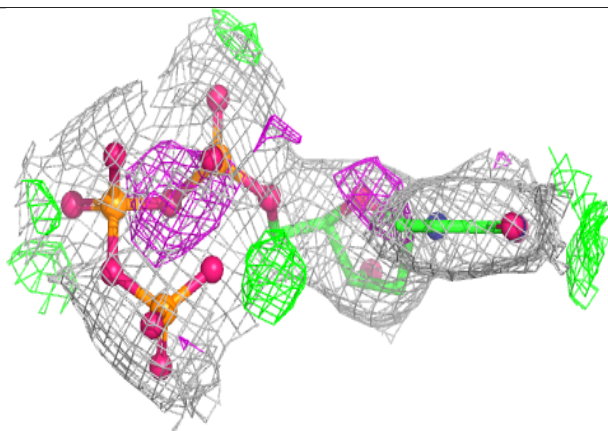
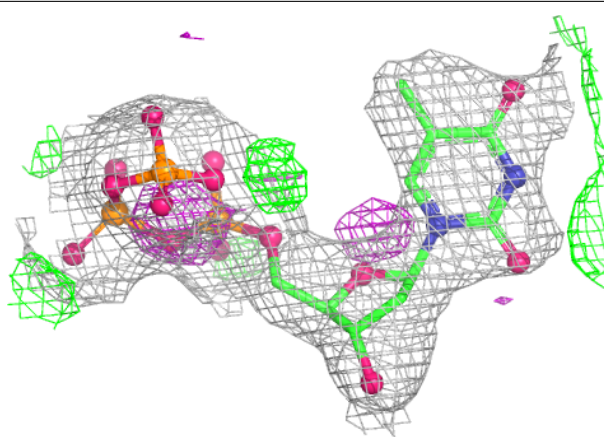
Electron density around TTP B 705:

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



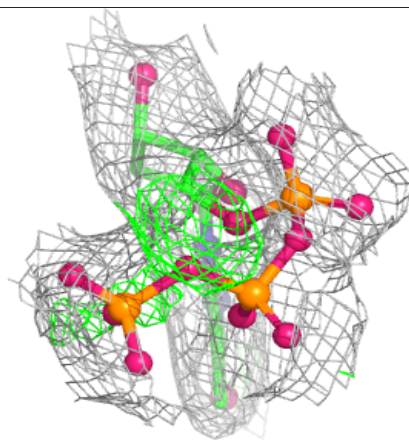
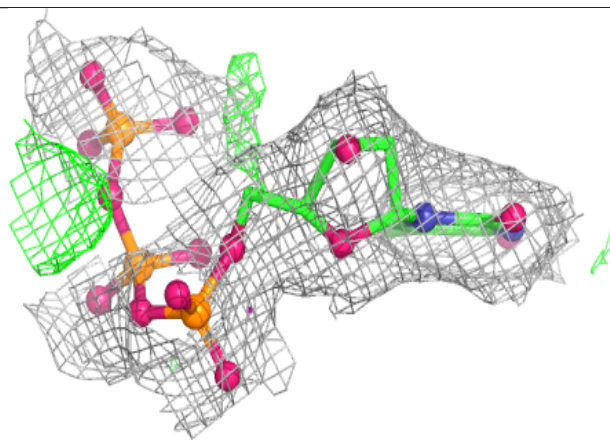
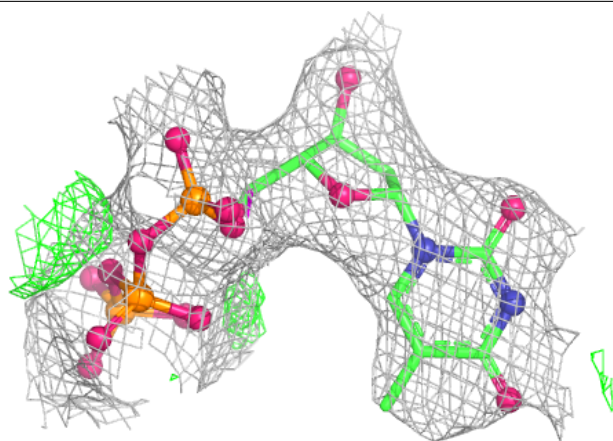
Electron density around TTP C 703:

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



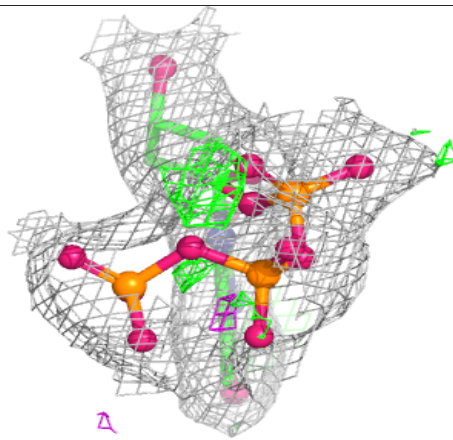
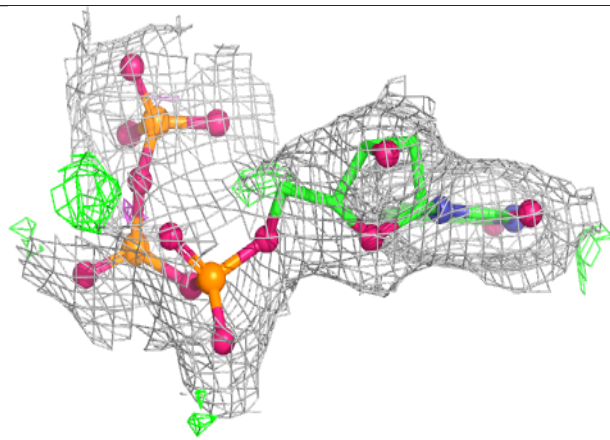
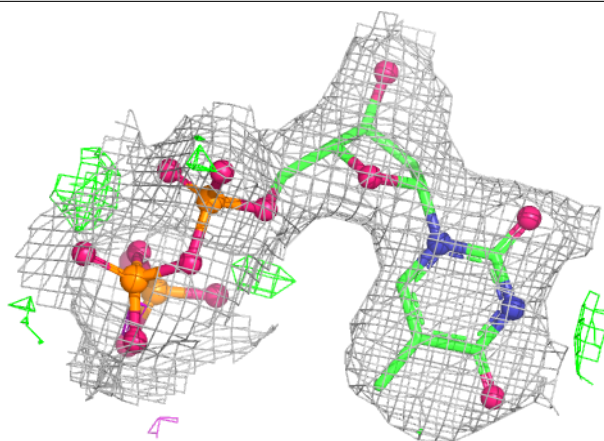
Electron density around TTP A 701:

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



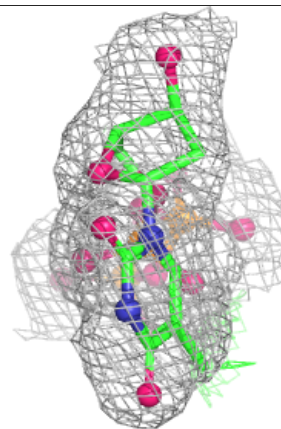
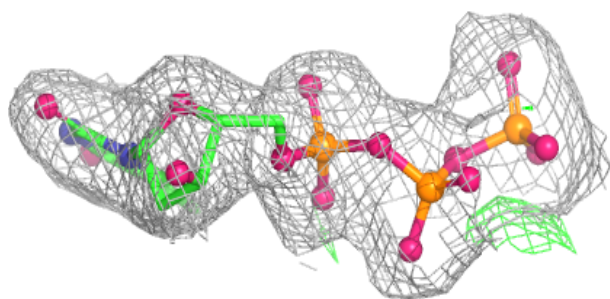
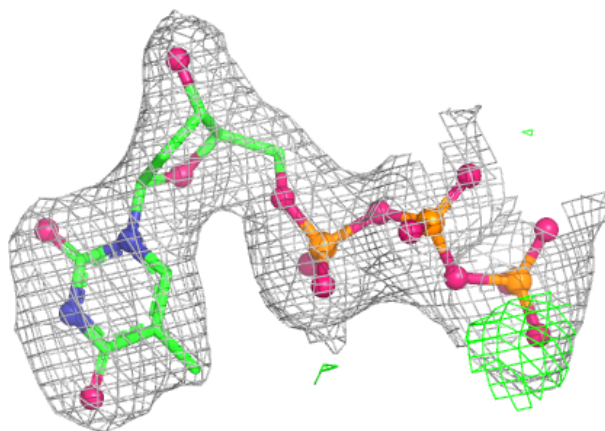
Electron density around TTP D 701:

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



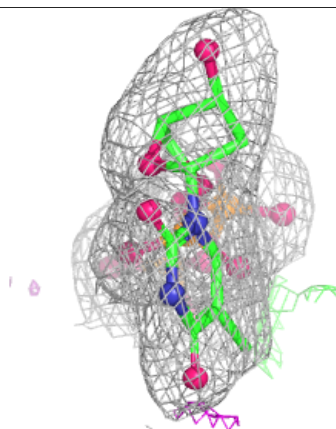
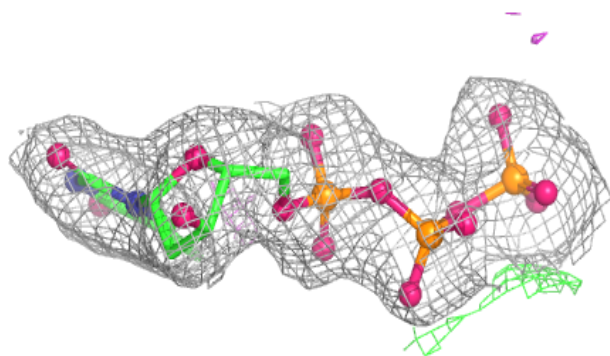
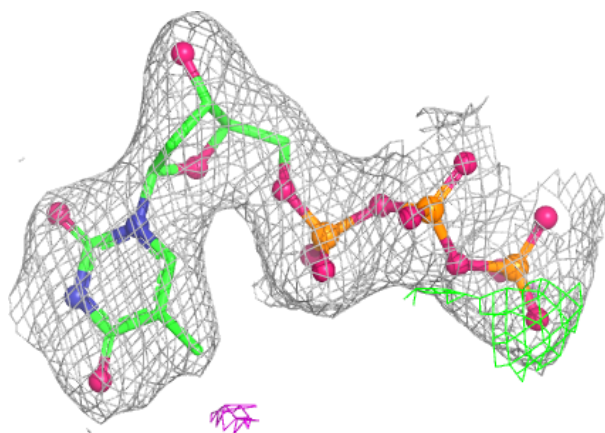
Electron density around TTP D 703:

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



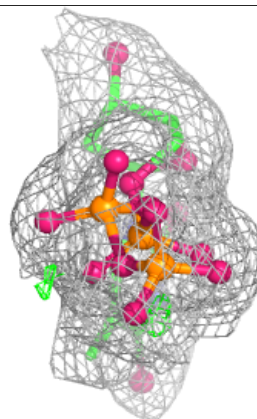
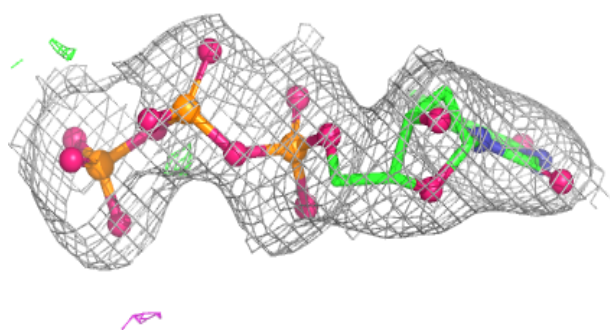
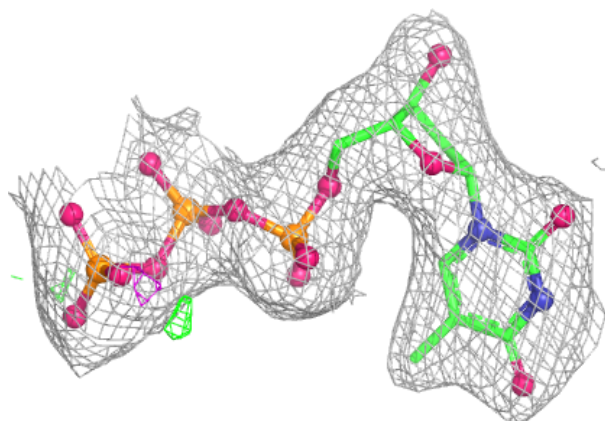
Electron density around TTP B 703:

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

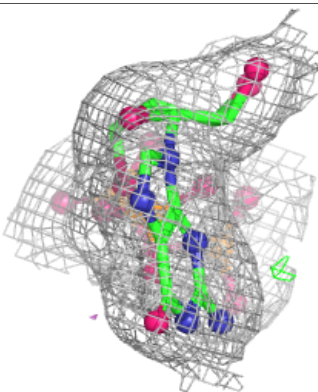
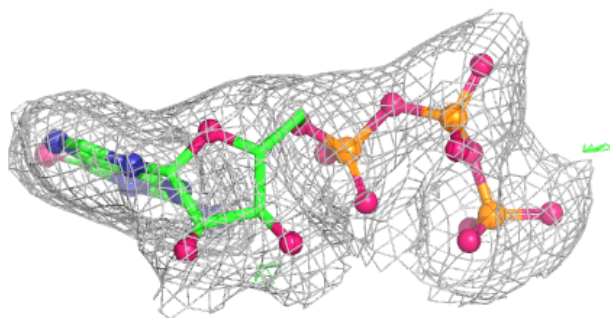
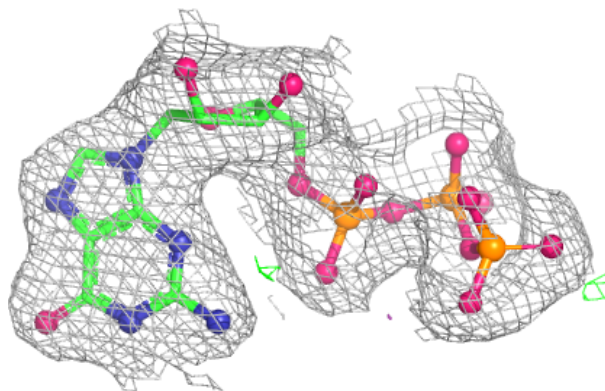


Electron density around TTP A 703:

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

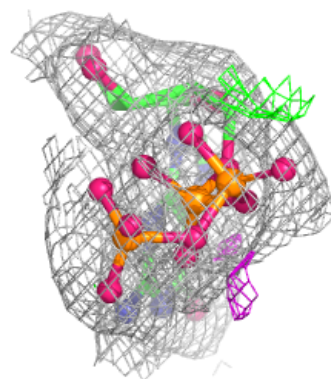
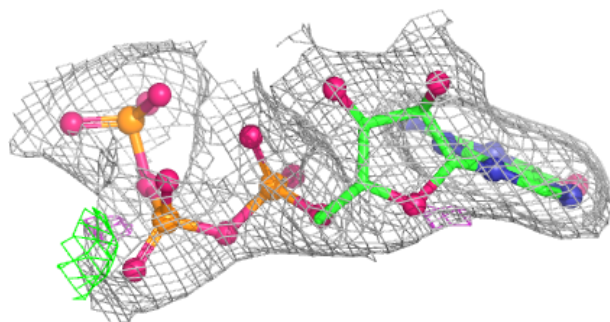
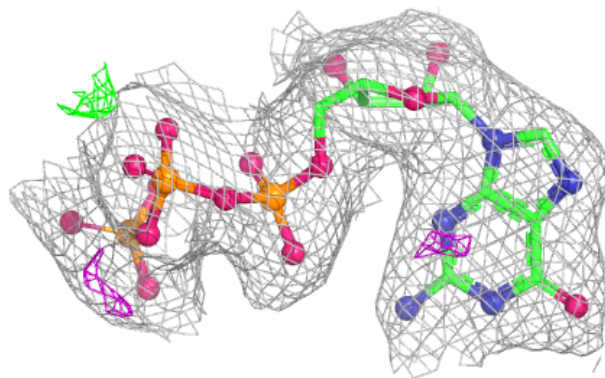
**Electron density around GTP A 702:**

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

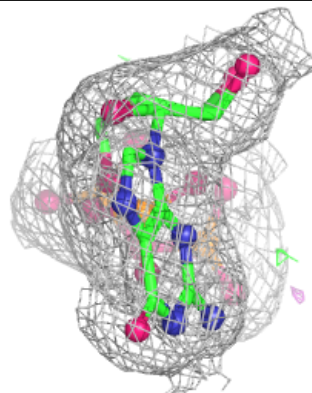
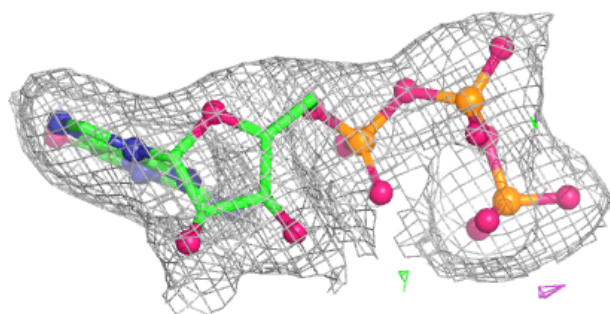
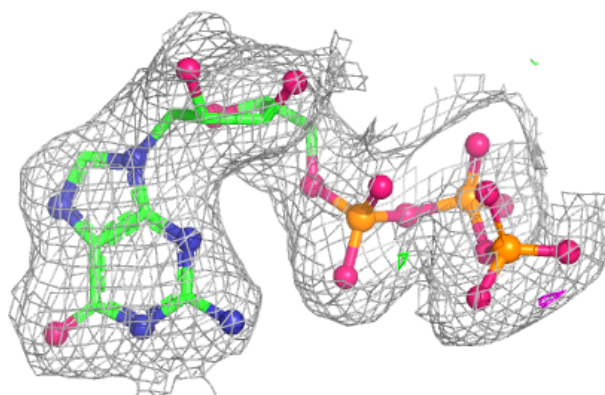


Electron density around GTP D 702:

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

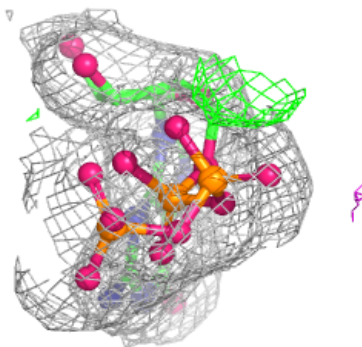
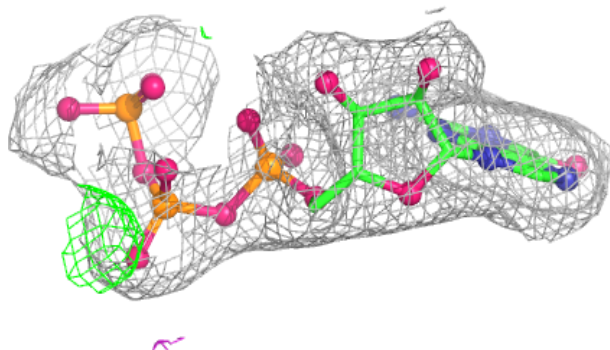
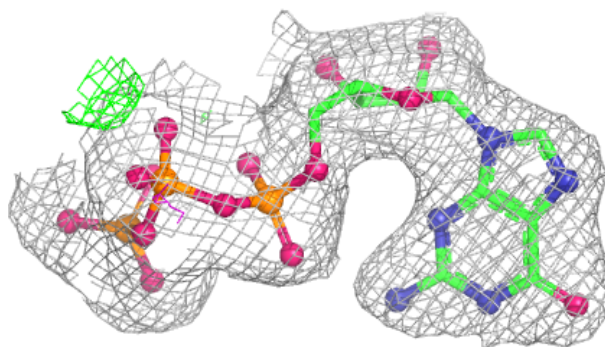
**Electron density around GTP B 702:**

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

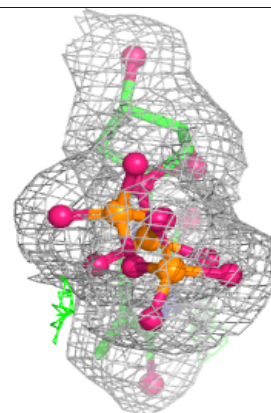
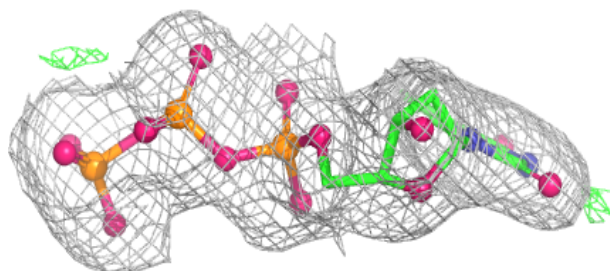
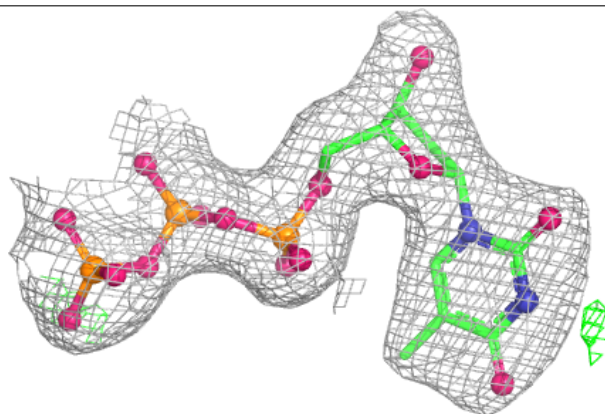


Electron density around GTP B 706:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.