



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 04:52 pm BST

PDB ID : 1G2V  
Title : THE STRUCTURAL BASIS OF THE CATALYTIC MECHANISM AND  
REGULATION OF GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE (RMLA). TTP COMPLEX.  
Authors : Blankenfeldt, W.; Asuncion, M.; Lam, J.S.; Naismith, J.H.  
Deposited on : 2000-10-21  
Resolution : 2.60 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

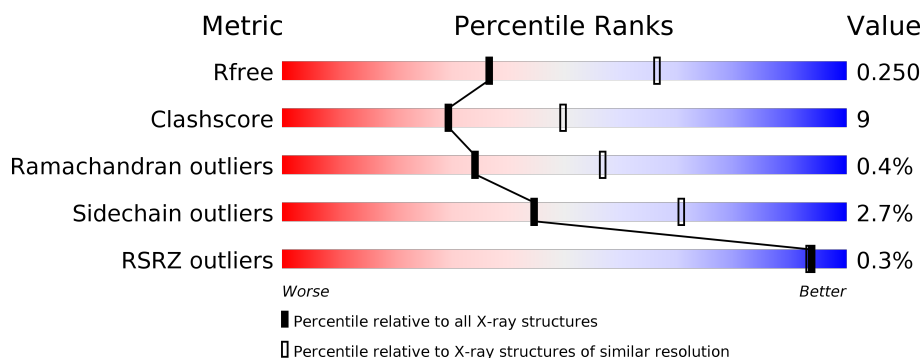
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

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





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	293	<div> <div>80%</div> <div>17%</div> <div>.</div> </div>
1	B	293	<div> <div>77%</div> <div>20%</div> <div>.</div> </div>
1	C	293	<div> <div>%</div> <div>77%</div> <div>20%</div> <div>.</div> </div>
1	D	293	<div> <div>%</div> <div>75%</div> <div>23%</div> <div>.</div> </div>
1	E	293	<div> <div>80%</div> <div>17%</div> <div>.</div> </div>
1	F	293	<div> <div>79%</div> <div>18%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	293	 77% 21% •
1	H	293	 76% 20% •

## 2 Entry composition

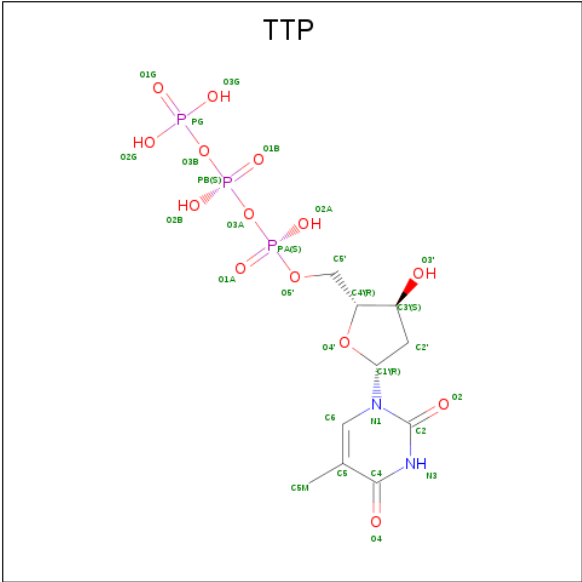
There are 2 unique types of molecules in this entry. The entry contains 18744 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	0
			2285	1462	385	434	4			
1	B	292	Total	C	N	O	S	0	0	0
			2285	1462	385	434	4			
1	C	292	Total	C	N	O	S	0	0	0
			2285	1462	385	434	4			
1	D	292	Total	C	N	O	S	0	0	0
			2285	1462	385	434	4			
1	E	292	Total	C	N	O	S	0	0	0
			2285	1462	385	434	4			
1	F	292	Total	C	N	O	S	0	0	0
			2285	1462	385	434	4			
1	G	292	Total	C	N	O	S	0	0	0
			2285	1462	385	434	4			
1	H	292	Total	C	N	O	S	0	0	0
			2285	1462	385	434	4			

- Molecule 2 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>2</sub>O<sub>14</sub>P<sub>3</sub>).



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

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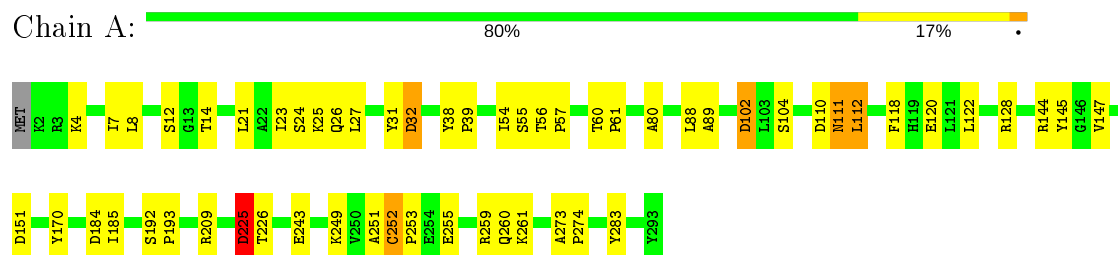
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	H	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

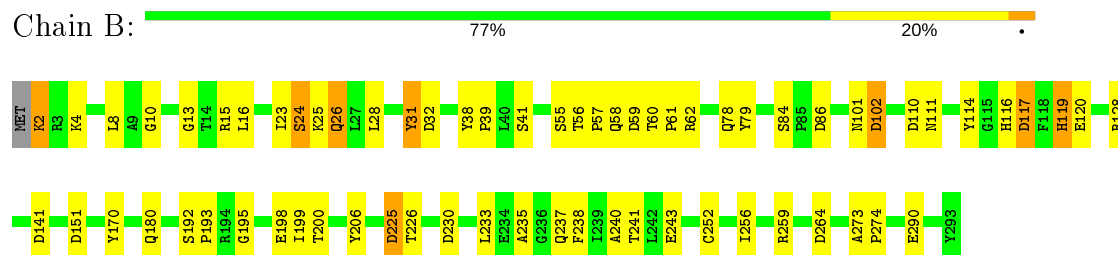
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

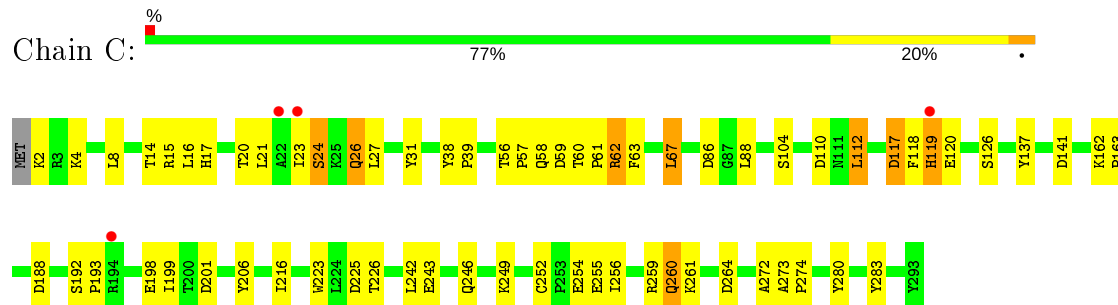
#### • Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLTRANSFERASE



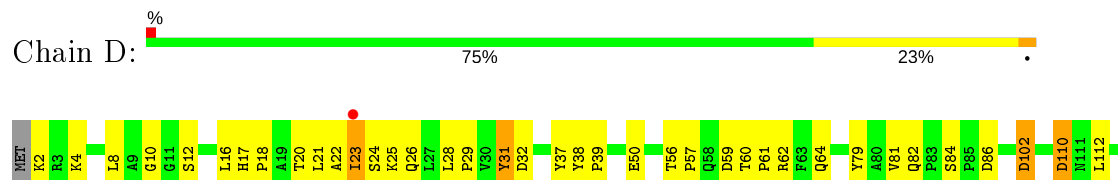
#### • Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLTRANSFERASE

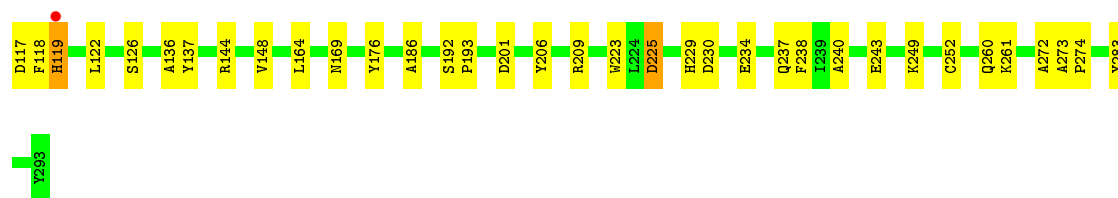


#### • Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLTRANSFERASE



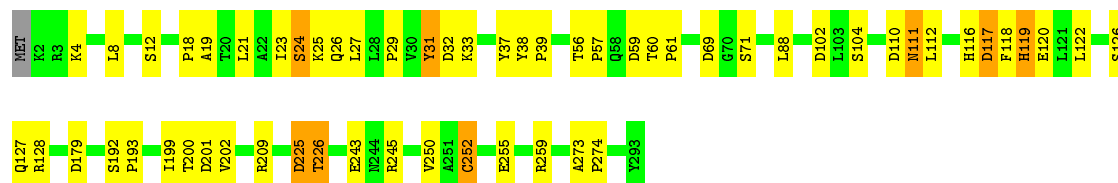
#### • Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLTRANSFERASE





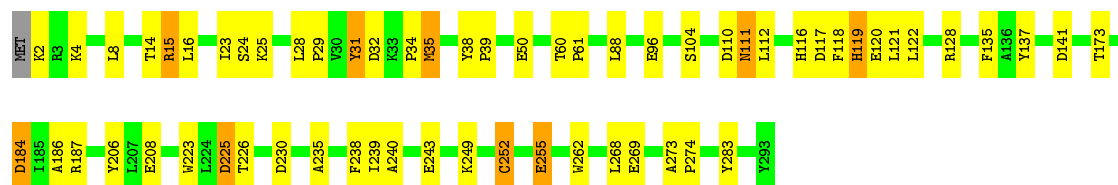
• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

Chain E: 80% 17%



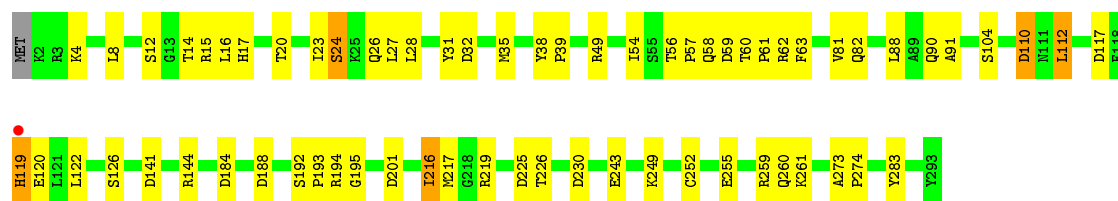
• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

Chain F: 79% 18%



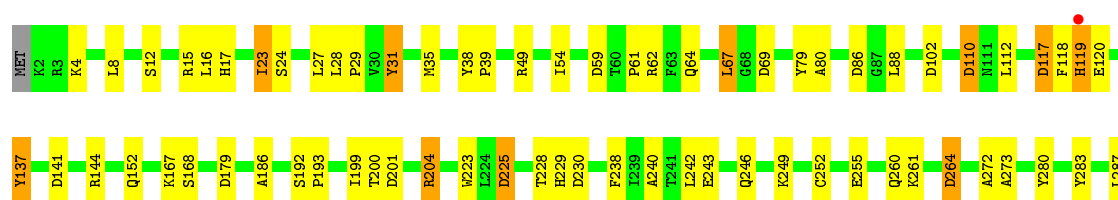
• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

Chain G: 77% 21%



• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

Chain H: 76% 20%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.02Å 134.36Å 140.90Å 90.00° 98.22° 90.00°	Depositor
Resolution (Å)	100.00 – 2.60 50.26 – 2.60	Depositor EDS
% Data completeness (in resolution range)	91.4 (100.00-2.60) 91.4 (50.26-2.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.33 (at 2.61Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.215 , 0.242 0.225 , 0.250	Depositor DCC
$R_{free}$ test set	3797 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.6	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 26.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	18744	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.28 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.6250e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	1.24	6/2335 (0.3%)	1.16	10/3168 (0.3%)
1	B	1.31	10/2335 (0.4%)	1.20	14/3168 (0.4%)
1	C	1.24	2/2335 (0.1%)	1.17	16/3168 (0.5%)
1	D	1.26	6/2335 (0.3%)	1.18	9/3168 (0.3%)
1	E	1.29	4/2335 (0.2%)	1.15	10/3168 (0.3%)
1	F	1.39	11/2335 (0.5%)	1.19	7/3168 (0.2%)
1	G	1.24	1/2335 (0.0%)	1.19	14/3168 (0.4%)
1	H	1.24	5/2335 (0.2%)	1.21	17/3168 (0.5%)
All	All	1.28	45/18680 (0.2%)	1.18	97/25344 (0.4%)

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	35	MET	SD-CE	-14.80	0.94	1.77
1	F	35	MET	CG-SD	-7.64	1.61	1.81
1	B	206	TYR	CD2-CE2	-7.53	1.28	1.39
1	H	280	TYR	CD2-CE2	-7.50	1.28	1.39
1	D	37	TYR	CD2-CE2	-7.20	1.28	1.39

The worst 5 of 97 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	15	ARG	NE-CZ-NH1	11.07	125.84	120.30
1	H	86	ASP	CB-CG-OD2	10.98	128.18	118.30
1	H	110	ASP	CB-CG-OD2	10.30	127.57	118.30
1	B	230	ASP	CB-CG-OD2	8.38	125.84	118.30
1	C	201	ASP	CB-CG-OD2	8.33	125.80	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2285	0	2272	37	0
1	B	2285	0	2272	40	0
1	C	2285	0	2272	50	0
1	D	2285	0	2272	54	0
1	E	2285	0	2272	34	1
1	F	2285	0	2272	59	0
1	G	2285	0	2272	47	0
1	H	2285	0	2272	46	1
2	A	58	0	26	3	0
2	B	58	0	26	4	0
2	C	58	0	26	3	0
2	D	58	0	26	3	0
2	E	58	0	26	2	0
2	F	58	0	26	3	0
2	G	58	0	26	3	0
2	H	58	0	26	3	0
All	All	18744	0	18384	352	1

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 9.

The worst 5 of 352 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:F:35:MET:CG	1:F:35:MET:CE	1.98	1.40
1:F:35:MET:CG	1:F:35:MET:HE2	1.66	1.14
1:F:35:MET:SD	1:F:35:MET:CE	0.95	1.04
1:F:23:ILE:CG2	1:F:28:LEU:HD21	1.87	1.03
1:F:35:MET:SD	1:F:35:MET:HE2	1.56	0.97

All (1) 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:E:127:GLN:OE1	1:H:167:LYS:NZ[2_647]	2.19	0.01

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	290/293 (99%)	285 (98%)	4 (1%)	1 (0%)	41	64
1	B	290/293 (99%)	282 (97%)	7 (2%)	1 (0%)	41	64
1	C	290/293 (99%)	280 (97%)	9 (3%)	1 (0%)	41	64
1	D	290/293 (99%)	283 (98%)	5 (2%)	2 (1%)	22	43
1	E	290/293 (99%)	282 (97%)	7 (2%)	1 (0%)	41	64
1	F	290/293 (99%)	284 (98%)	5 (2%)	1 (0%)	41	64
1	G	290/293 (99%)	281 (97%)	8 (3%)	1 (0%)	41	64
1	H	290/293 (99%)	283 (98%)	5 (2%)	2 (1%)	22	43
All	All	2320/2344 (99%)	2260 (97%)	50 (2%)	10 (0%)	34	57

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	23	ILE
1	C	31	TYR
1	A	31	TYR
1	B	31	TYR
1	D	31	TYR

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	239/240 (100%)	234 (98%)	5 (2%)	53	77
1	B	239/240 (100%)	234 (98%)	5 (2%)	53	77
1	C	239/240 (100%)	231 (97%)	8 (3%)	38	64
1	D	239/240 (100%)	231 (97%)	8 (3%)	38	64
1	E	239/240 (100%)	230 (96%)	9 (4%)	33	59
1	F	239/240 (100%)	234 (98%)	5 (2%)	53	77
1	G	239/240 (100%)	231 (97%)	8 (3%)	38	64
1	H	239/240 (100%)	235 (98%)	4 (2%)	60	81
All	All	1912/1920 (100%)	1860 (97%)	52 (3%)	44	71

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	209	ARG
1	E	117	ASP
1	H	12	SER
1	D	225	ASP
1	E	12	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	119	HIS
1	E	26	GLN
1	G	17	HIS
1	D	26	GLN
1	G	119	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

16 ligands are modelled in this entry.

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	E	3508	-	23,30,30	2.26	7 (30%)	29,47,47	2.16	10 (34%)
2	TTP	D	3506	-	23,30,30	2.33	7 (30%)	29,47,47	1.98	9 (31%)
2	TTP	G	3513	-	23,30,30	2.42	8 (34%)	29,47,47	3.56	9 (31%)
2	TTP	B	3502	-	23,30,30	2.48	9 (39%)	29,47,47	2.39	7 (24%)
2	TTP	F	3511	-	23,30,30	2.45	8 (34%)	29,47,47	2.96	11 (37%)
2	TTP	H	3515	-	23,30,30	2.39	9 (39%)	29,47,47	2.29	10 (34%)
2	TTP	B	3503	-	23,30,30	2.54	6 (26%)	29,47,47	2.03	8 (27%)
2	TTP	A	3501	-	23,30,30	2.35	7 (30%)	29,47,47	2.08	12 (41%)
2	TTP	C	3504	-	23,30,30	2.24	7 (30%)	29,47,47	2.28	10 (34%)
2	TTP	G	3512	-	23,30,30	2.24	6 (26%)	29,47,47	2.03	8 (27%)
2	TTP	F	3510	-	23,30,30	2.33	6 (26%)	29,47,47	2.61	12 (41%)
2	TTP	D	3507	-	23,30,30	2.44	8 (34%)	29,47,47	2.99	9 (31%)
2	TTP	A	3500	-	23,30,30	2.42	6 (26%)	29,47,47	2.04	9 (31%)
2	TTP	C	3505	-	23,30,30	2.64	8 (34%)	29,47,47	2.65	8 (27%)
2	TTP	E	3509	-	23,30,30	2.34	7 (30%)	29,47,47	2.17	10 (34%)
2	TTP	H	3514	-	23,30,30	2.32	9 (39%)	29,47,47	2.06	10 (34%)

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	E	3508	-	-	5/19/34/34	0/2/2/2
2	TTP	D	3506	-	-	2/19/34/34	0/2/2/2
2	TTP	G	3513	-	-	2/19/34/34	0/2/2/2
2	TTP	B	3502	-	-	4/19/34/34	0/2/2/2
2	TTP	F	3511	-	-	5/19/34/34	0/2/2/2
2	TTP	H	3515	-	-	9/19/34/34	0/2/2/2
2	TTP	B	3503	-	-	2/19/34/34	0/2/2/2
2	TTP	A	3501	-	-	2/19/34/34	0/2/2/2
2	TTP	C	3504	-	-	6/19/34/34	0/2/2/2
2	TTP	G	3512	-	-	5/19/34/34	0/2/2/2
2	TTP	F	3510	-	-	5/19/34/34	0/2/2/2
2	TTP	D	3507	-	-	7/19/34/34	0/2/2/2
2	TTP	A	3500	-	-	4/19/34/34	0/2/2/2
2	TTP	C	3505	-	-	4/19/34/34	0/2/2/2
2	TTP	E	3509	-	-	1/19/34/34	0/2/2/2
2	TTP	H	3514	-	-	4/19/34/34	0/2/2/2

The worst 5 of 118 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3505	TTP	C3'-C4'	-6.01	1.36	1.53
2	F	3510	TTP	C3'-C4'	-5.86	1.36	1.53
2	F	3511	TTP	C3'-C4'	-5.76	1.37	1.53
2	D	3507	TTP	C3'-C4'	-5.60	1.37	1.53
2	B	3503	TTP	C3'-C4'	-5.55	1.37	1.53

The worst 5 of 152 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	3513	TTP	C5-C6-N1	-13.54	107.60	122.19
2	F	3511	TTP	C5-C6-N1	-11.41	109.90	122.19
2	D	3507	TTP	C5-C6-N1	-10.46	110.92	122.19
2	B	3502	TTP	C4-N3-C2	9.88	123.49	115.14
2	F	3510	TTP	C5-C6-N1	-9.43	112.03	122.19

There are no chirality outliers.

5 of 67 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	3508	TTP	C5'-O5'-PA-O1A
2	E	3508	TTP	C5'-O5'-PA-O3A
2	D	3506	TTP	C5'-O5'-PA-O1A
2	G	3513	TTP	O4'-C1'-N1-C6
2	B	3502	TTP	PB-O3A-PA-O5'

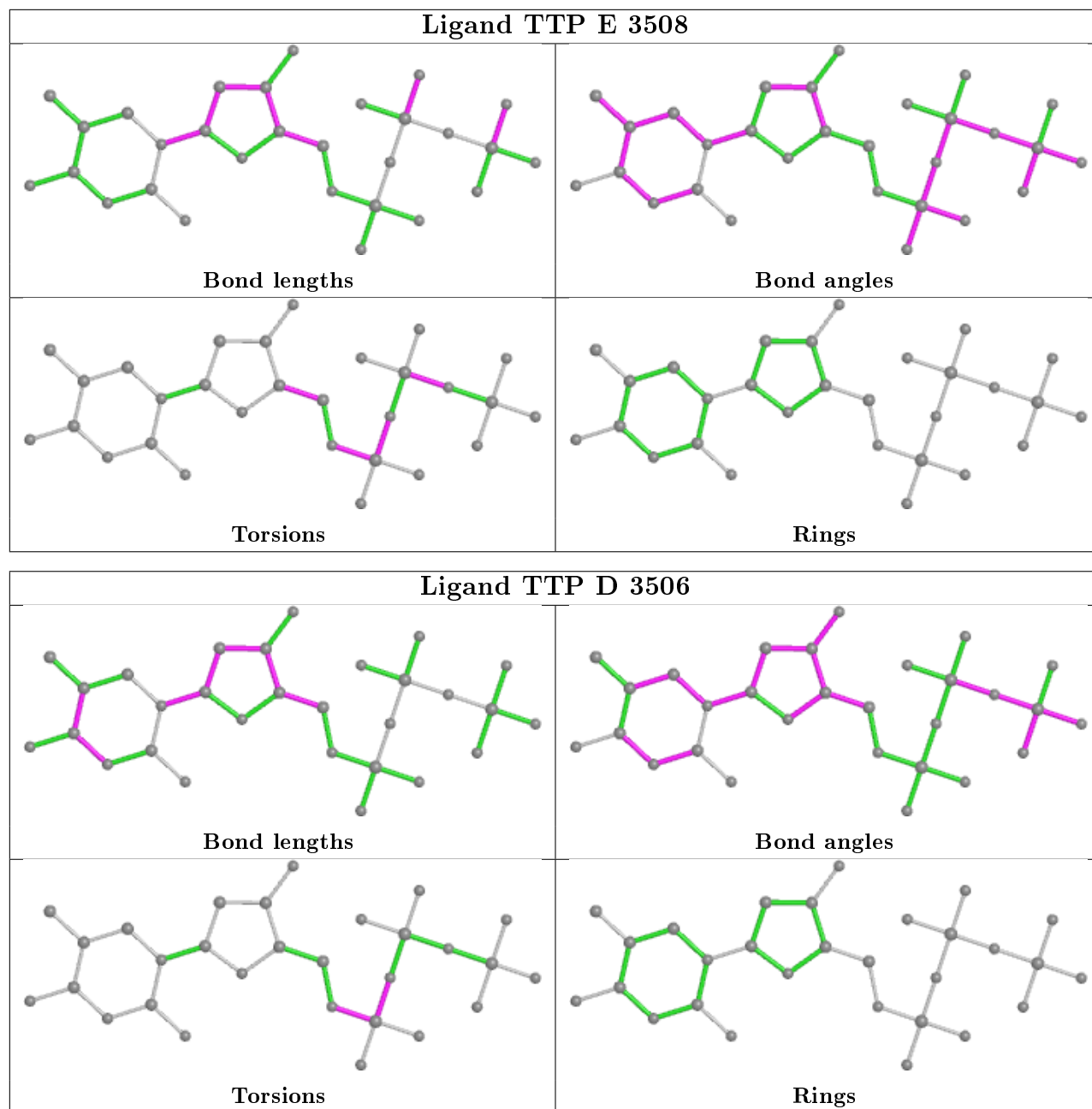
There are no ring outliers.

8 monomers are involved in 24 short contacts:

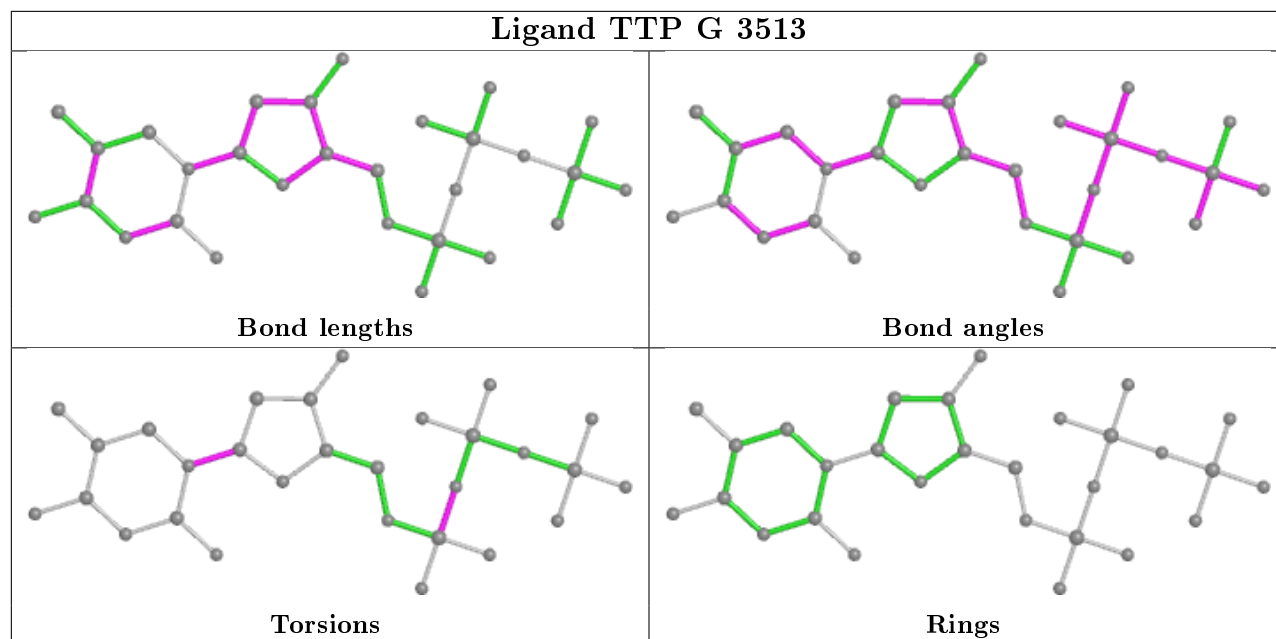
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	3508	TTP	2	0
2	D	3506	TTP	3	0
2	B	3502	TTP	4	0
2	C	3504	TTP	3	0
2	G	3512	TTP	3	0
2	F	3510	TTP	3	0
2	A	3500	TTP	3	0
2	H	3514	TTP	3	0

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.

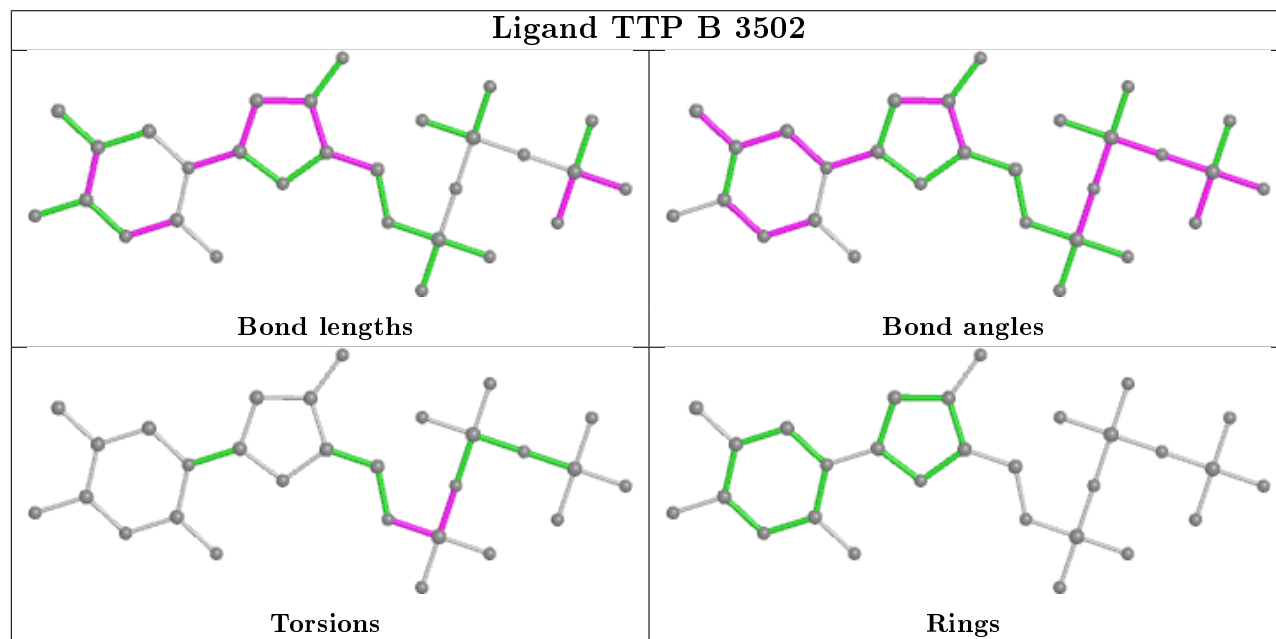


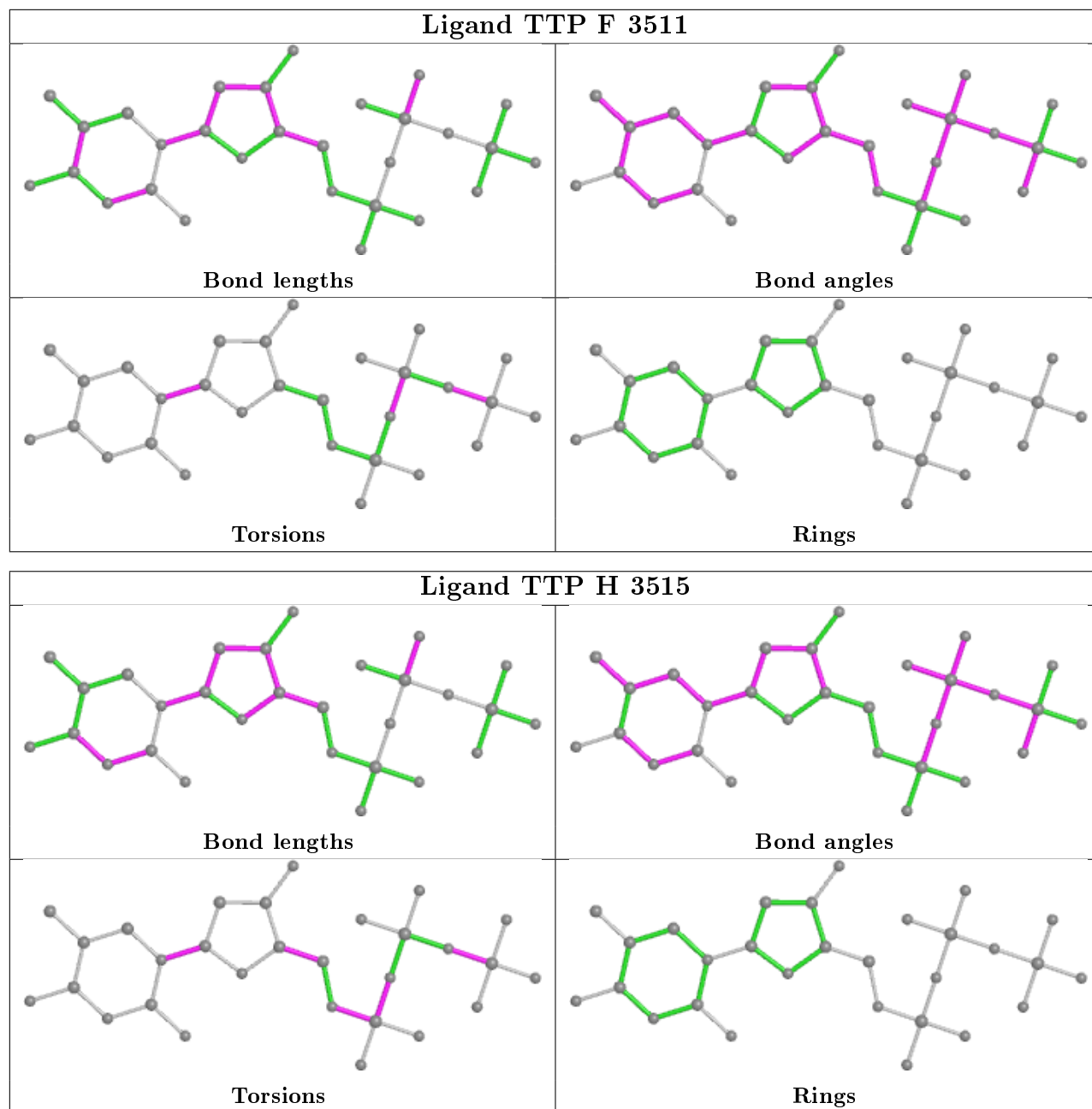


## Ligand TTP G 3513

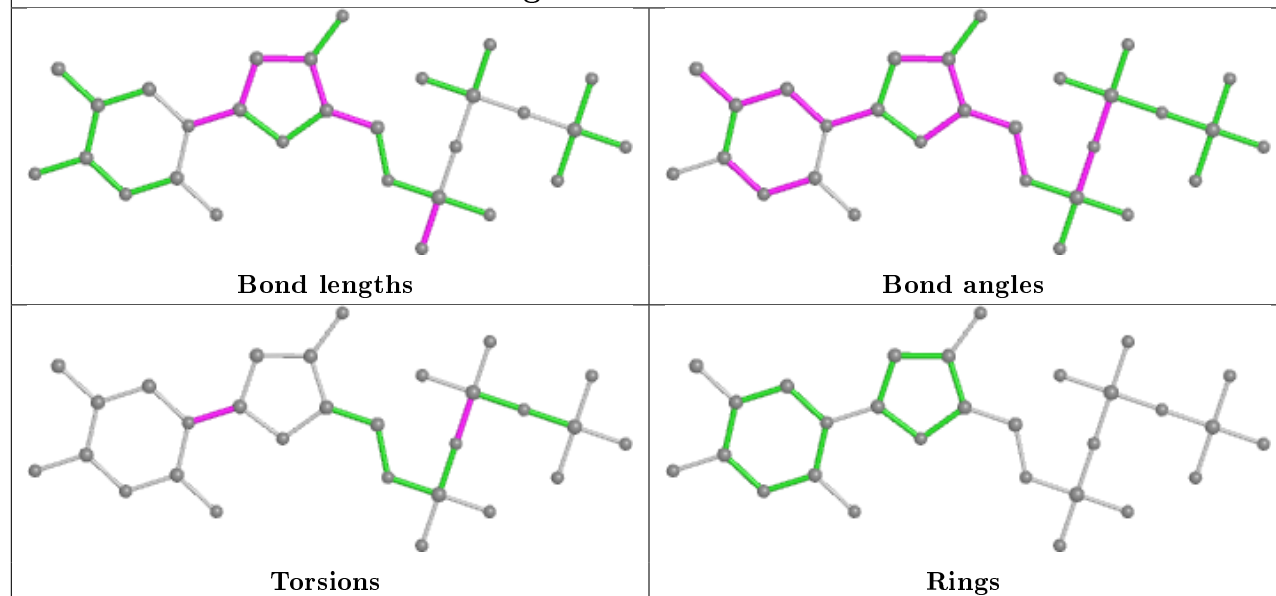


## Ligand TTP B 3502

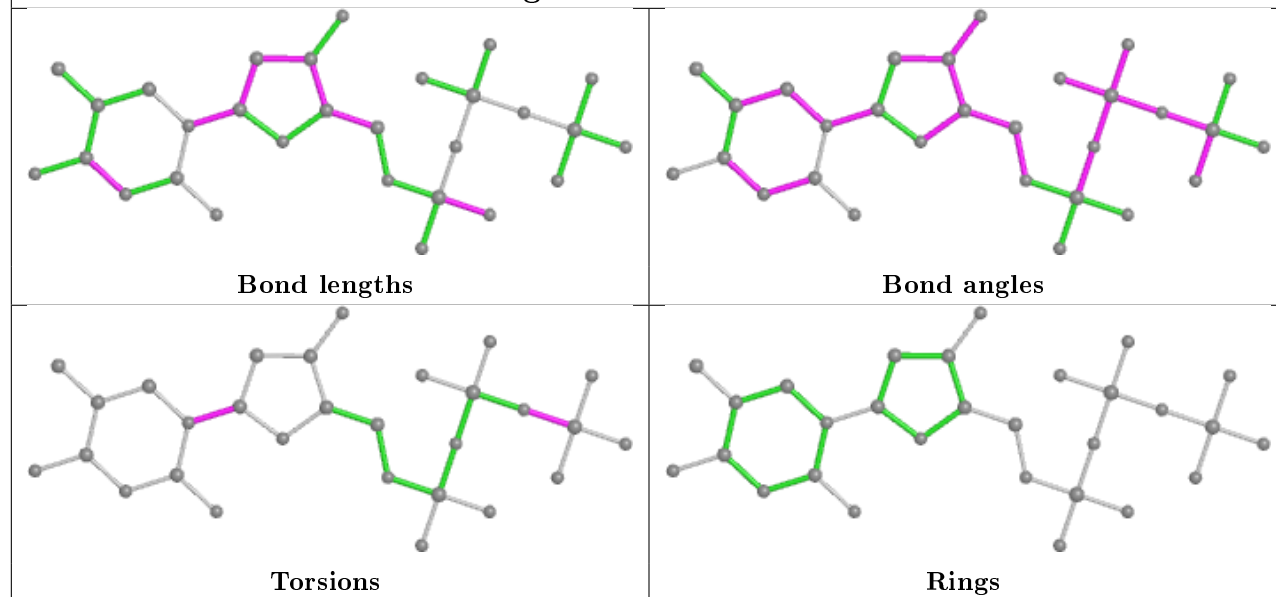




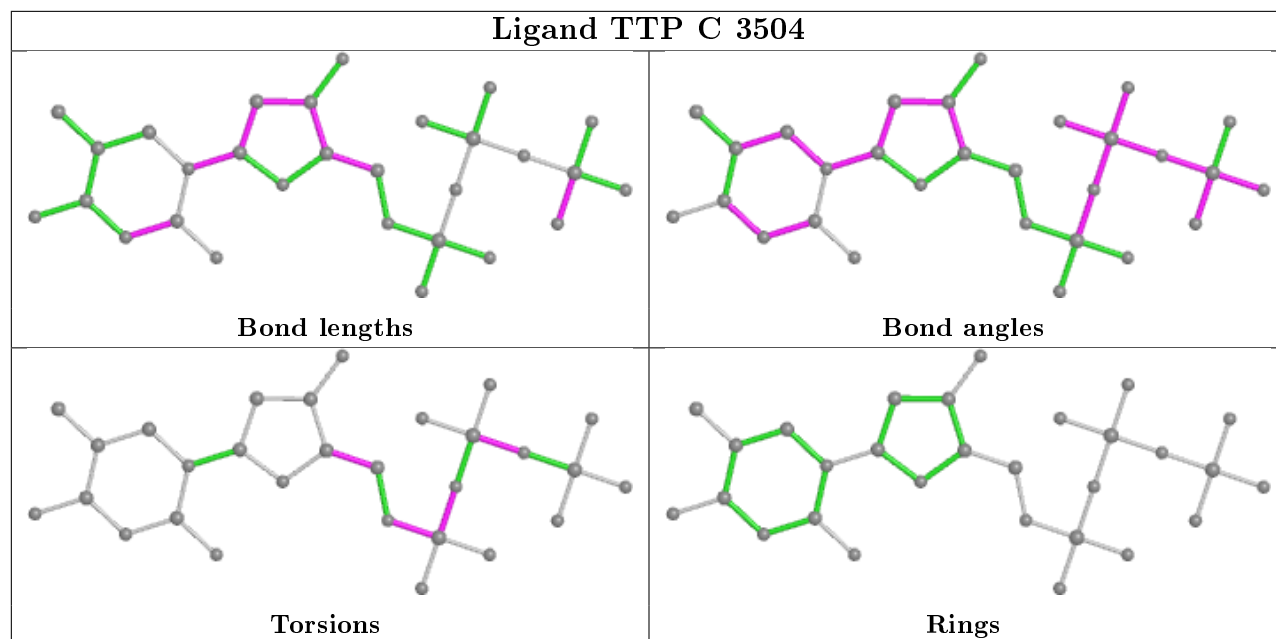
## Ligand TTP B 3503



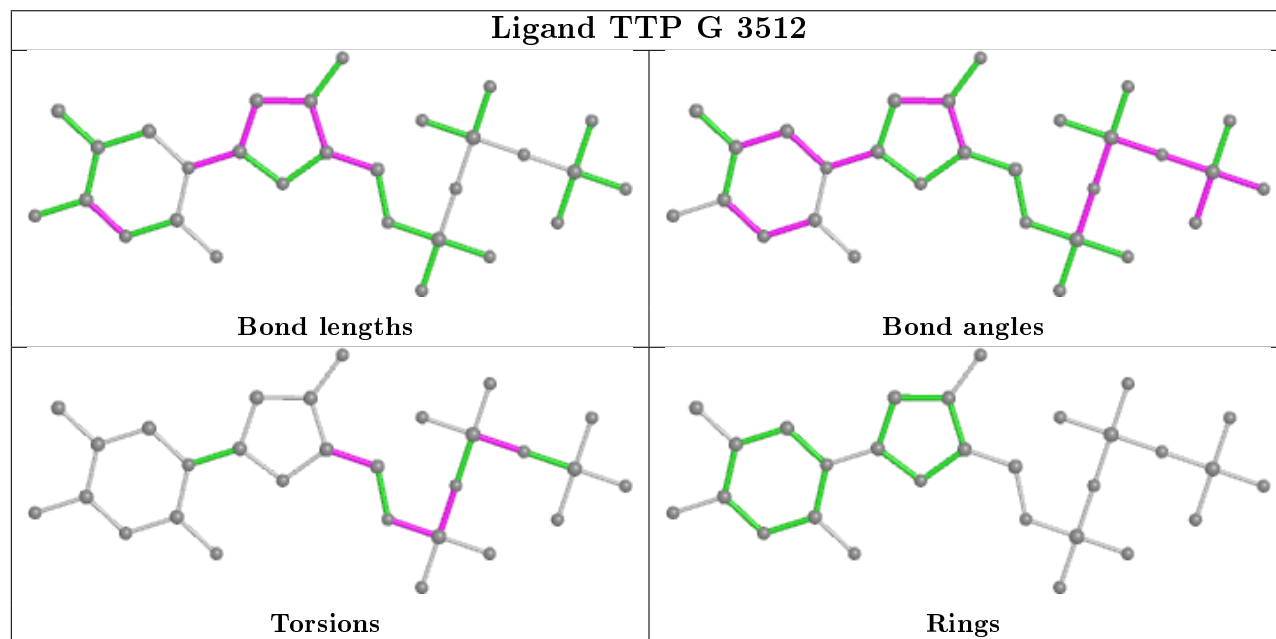
## Ligand TTP A 3501

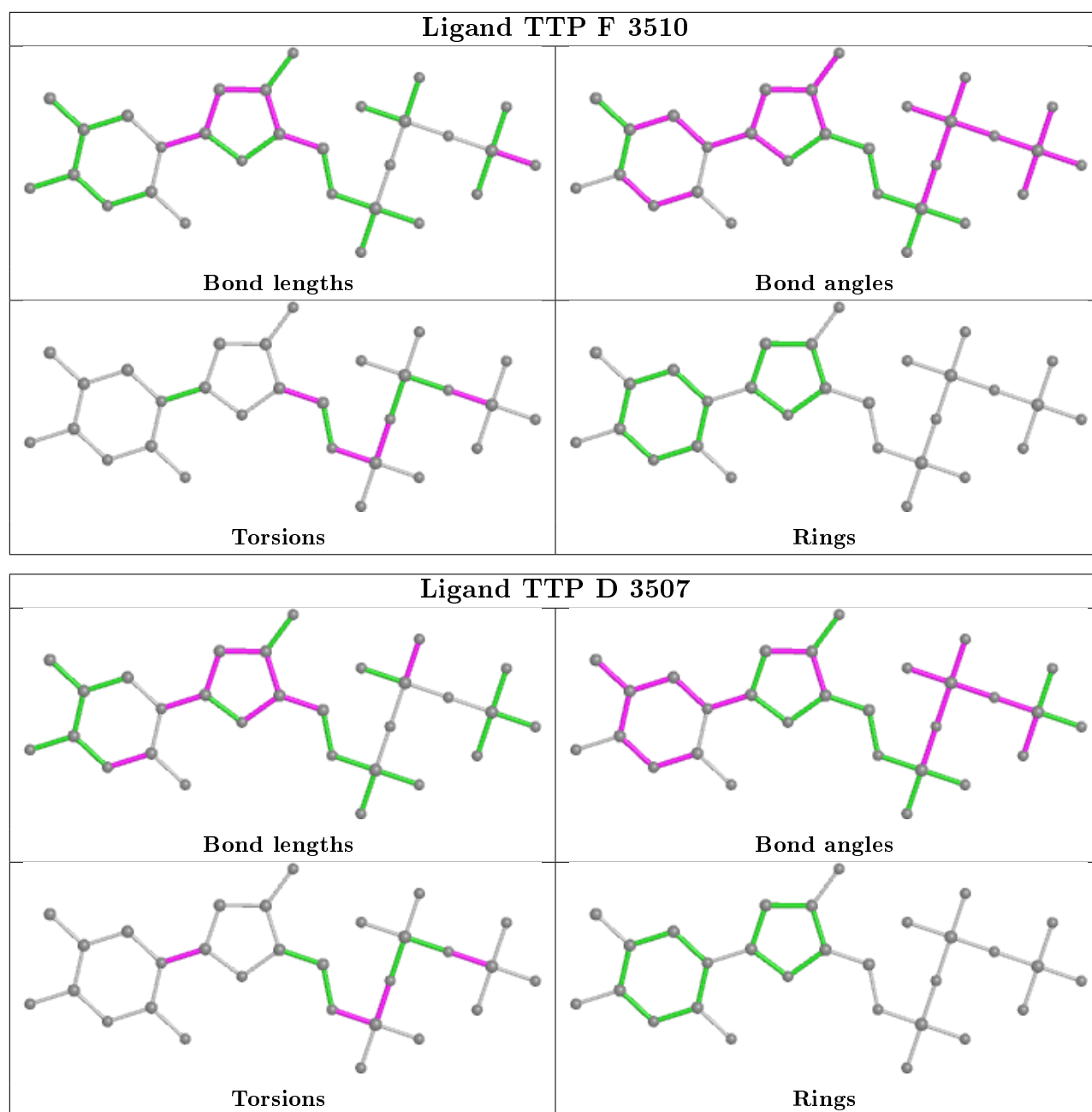


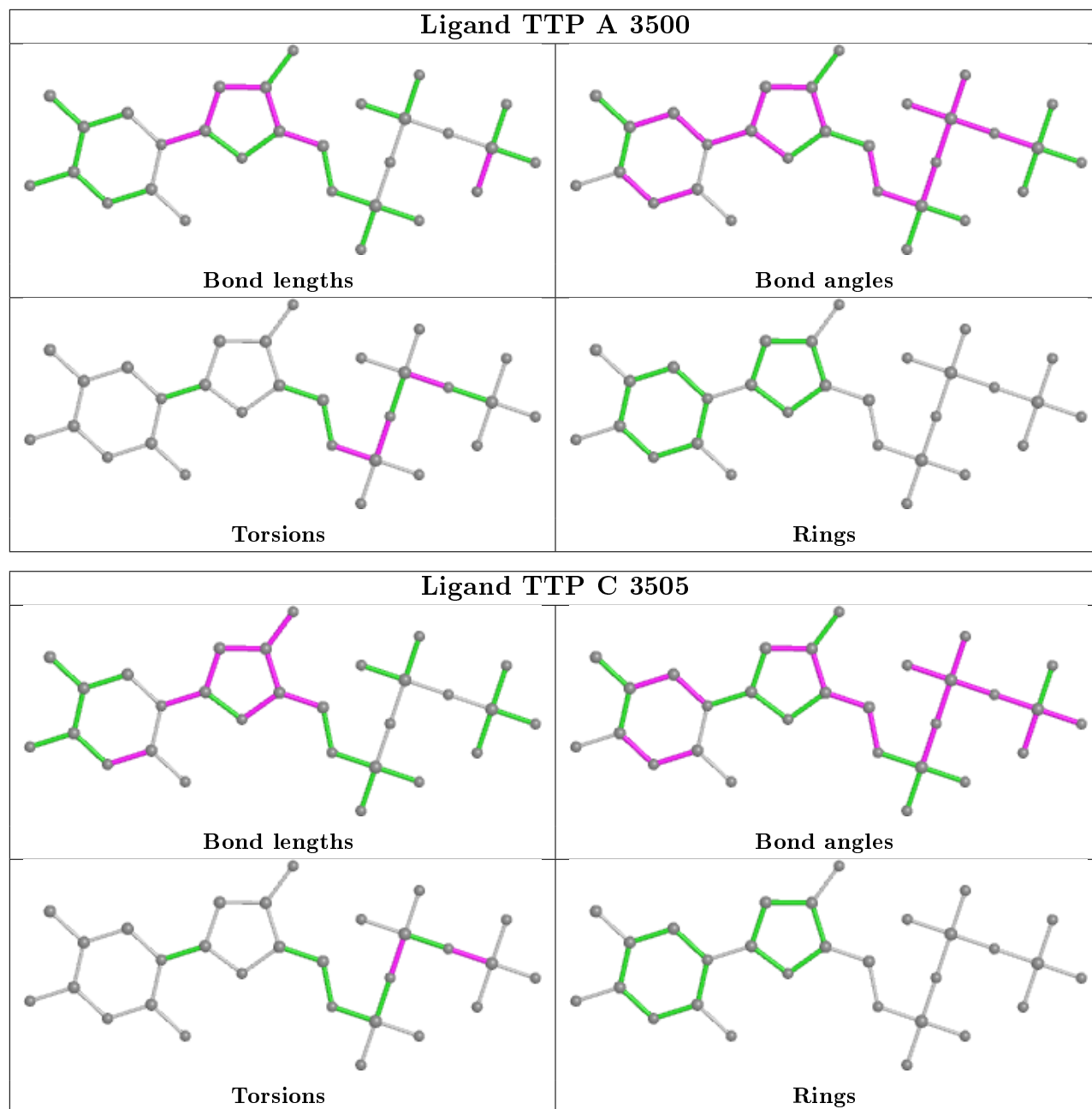
## Ligand TTP C 3504

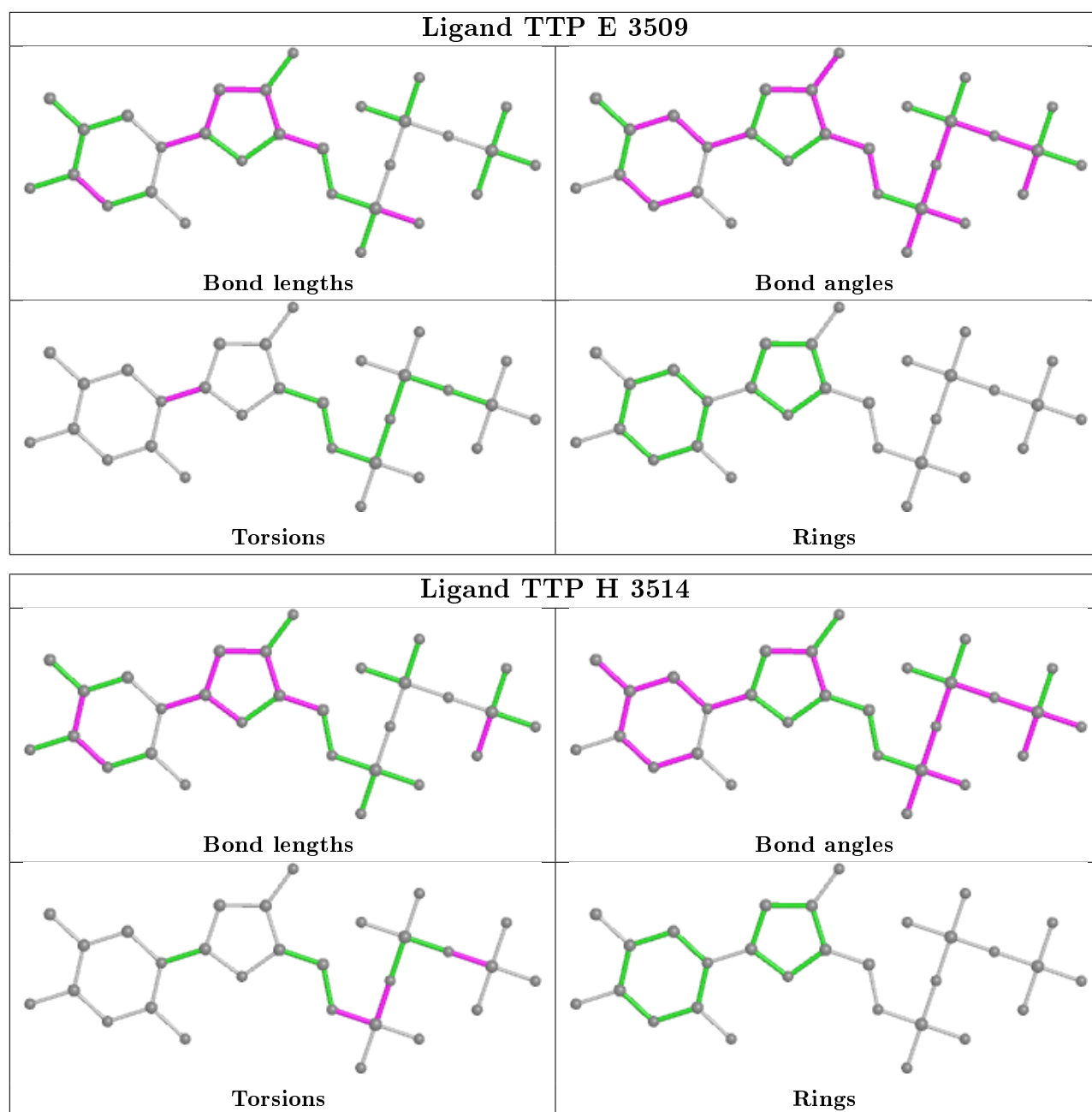


## Ligand TTP G 3512









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	292/293 (99%)	-0.51	0 100 100	6, 12, 23, 33	0
1	B	292/293 (99%)	-0.43	0 100 100	6, 12, 23, 33	0
1	C	292/293 (99%)	-0.35	4 (1%) 75 71	5, 12, 23, 39	0
1	D	292/293 (99%)	-0.31	2 (0%) 87 86	5, 12, 24, 33	0
1	E	292/293 (99%)	-0.49	0 100 100	5, 12, 23, 35	0
1	F	292/293 (99%)	-0.47	0 100 100	5, 12, 24, 34	0
1	G	292/293 (99%)	-0.37	1 (0%) 94 93	6, 12, 23, 33	0
1	H	292/293 (99%)	-0.39	1 (0%) 94 93	6, 12, 25, 32	0
All	All	2336/2344 (99%)	-0.42	8 (0%) 94 93	5, 12, 24, 39	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	22	ALA	4.2
1	D	119	HIS	3.0
1	H	119	HIS	2.8
1	C	23	ILE	2.7
1	C	119	HIS	2.7

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

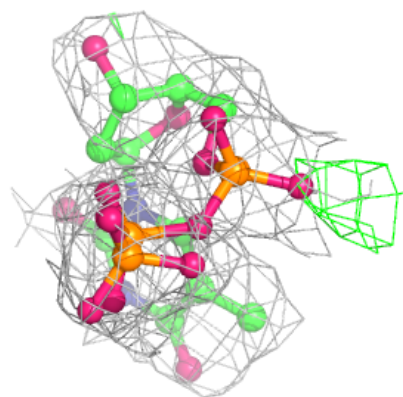
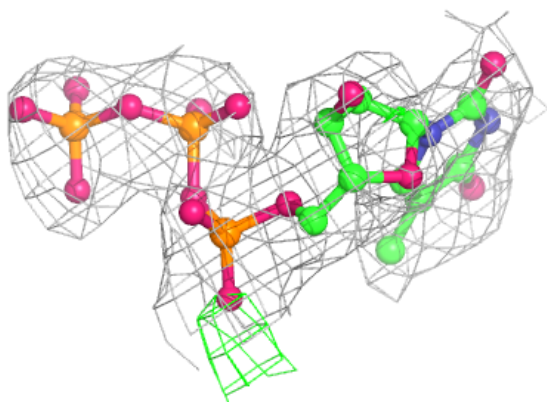
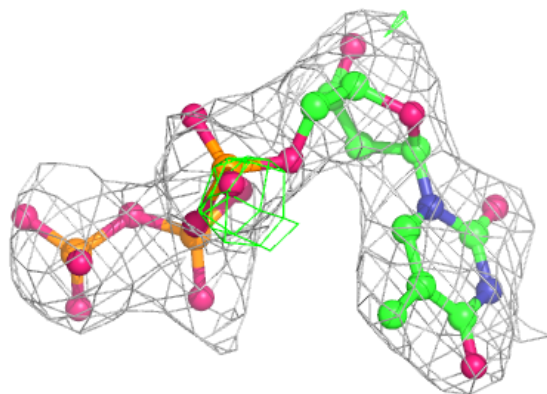
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	TTP	D	3506	29/29	0.89	0.20	25,33,45,49	0
2	TTP	G	3513	29/29	0.93	0.14	9,24,41,47	0
2	TTP	B	3502	29/29	0.93	0.16	18,30,43,46	0
2	TTP	F	3511	29/29	0.93	0.17	8,22,39,41	0
2	TTP	G	3512	29/29	0.93	0.15	13,29,40,44	0
2	TTP	A	3501	29/29	0.93	0.16	12,20,43,46	0
2	TTP	H	3514	29/29	0.93	0.15	26,31,38,43	0
2	TTP	H	3515	29/29	0.94	0.15	10,22,42,47	0
2	TTP	C	3505	29/29	0.94	0.15	11,26,46,47	0
2	TTP	F	3510	29/29	0.94	0.15	15,29,38,41	0
2	TTP	D	3507	29/29	0.94	0.15	11,21,43,45	0
2	TTP	A	3500	29/29	0.94	0.16	20,30,41,42	0
2	TTP	E	3509	29/29	0.94	0.15	10,20,40,42	0
2	TTP	B	3503	29/29	0.94	0.16	6,20,29,33	0
2	TTP	E	3508	29/29	0.95	0.15	19,27,36,43	0
2	TTP	C	3504	29/29	0.95	0.15	22,30,37,41	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.

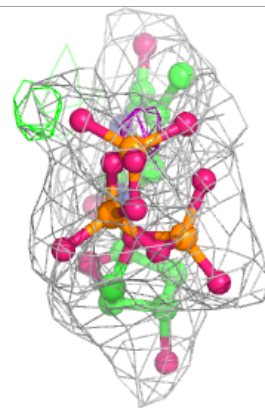
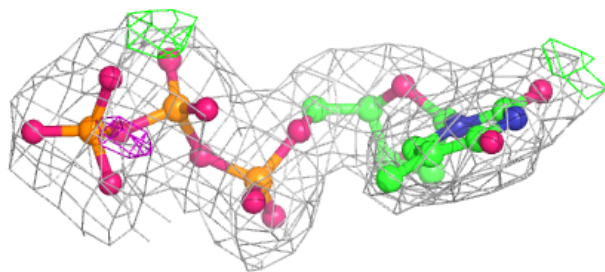
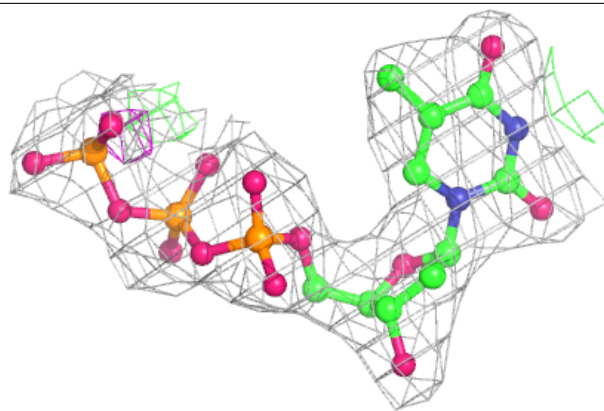
**Electron density around TTP D 3506:**

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



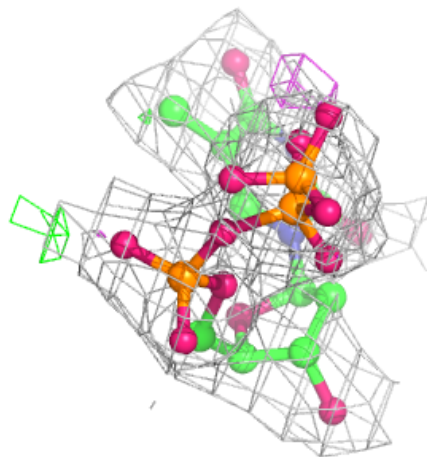
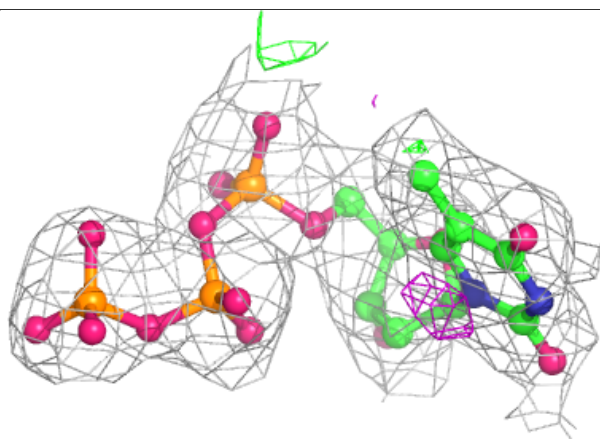
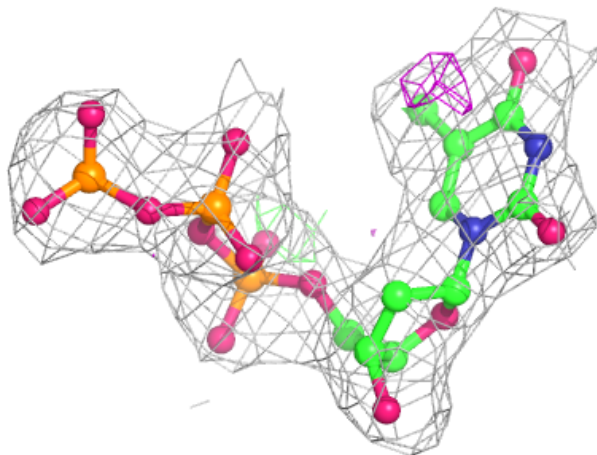
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and green (positive)



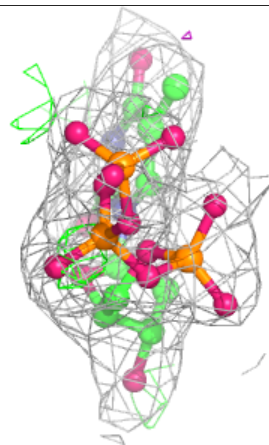
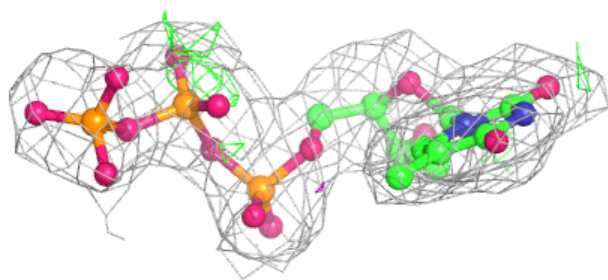
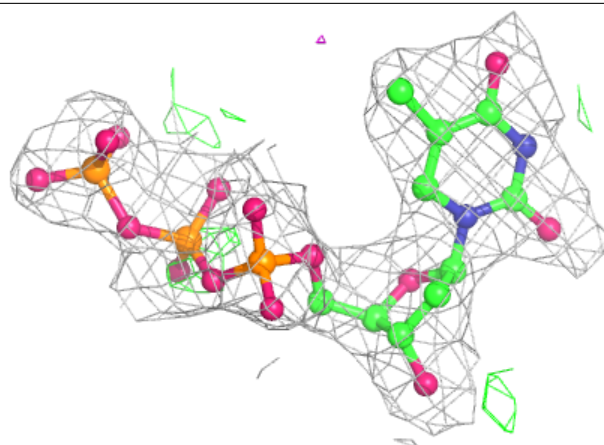
**Electron density around TTP B 3502:**

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



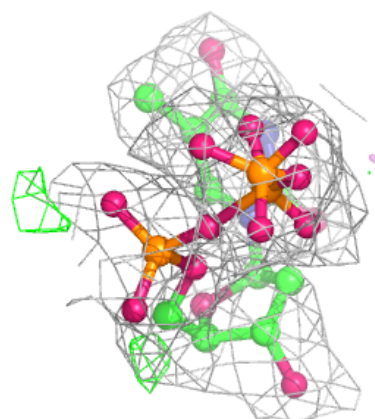
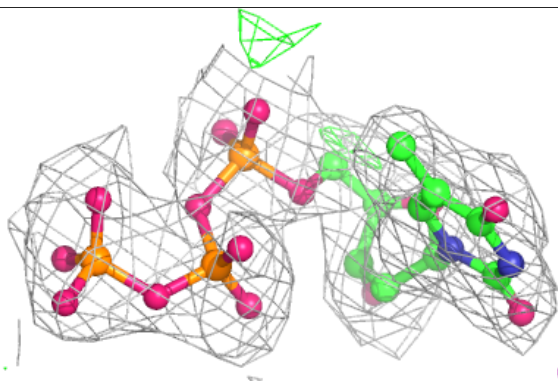
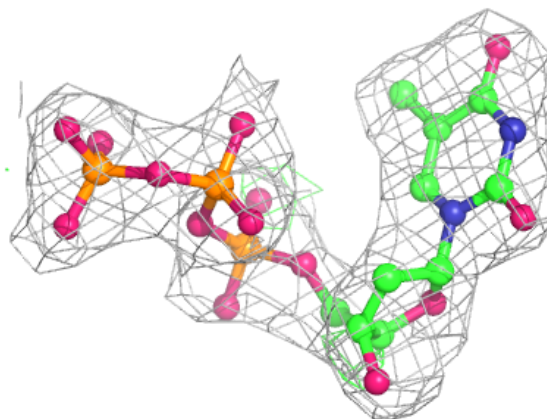
**Electron density around TTP F 3511:**

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and green (positive)

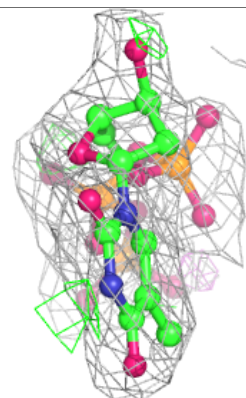
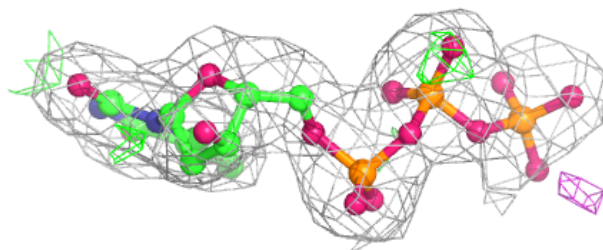
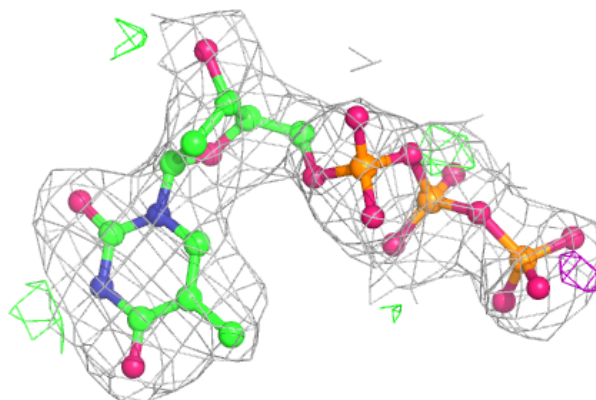


**Electron density around TTP G 3512:**

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and green (positive)

**Electron density around TTP A 3501:**

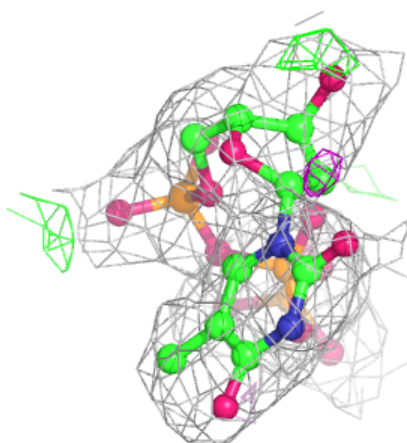
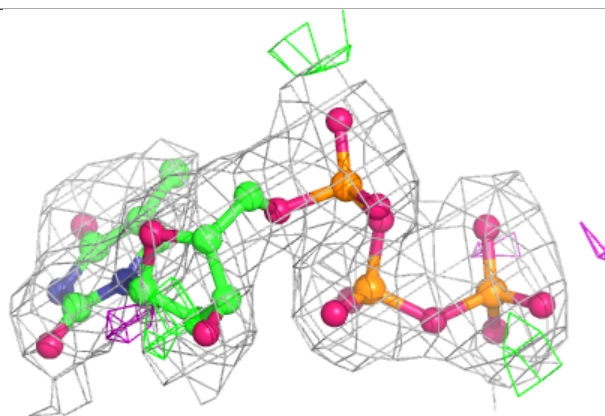
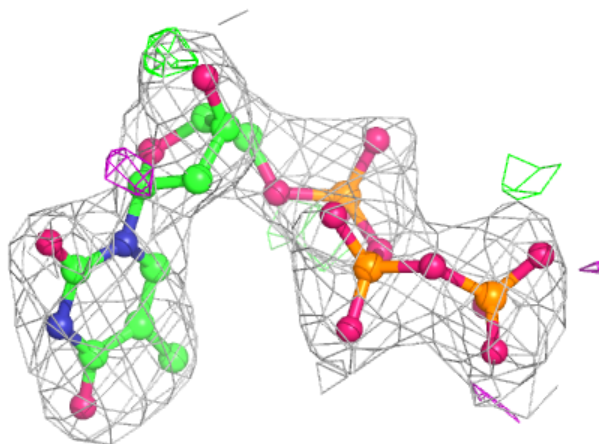
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and green (positive)





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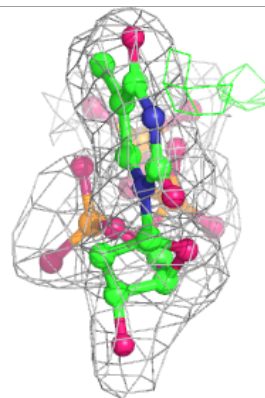
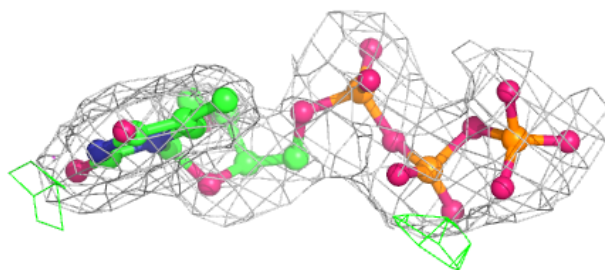
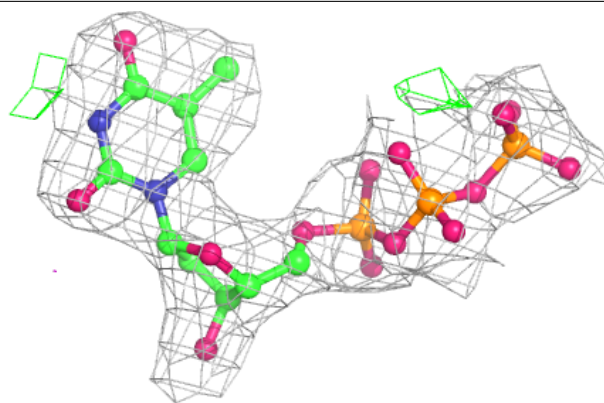
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and green (positive)



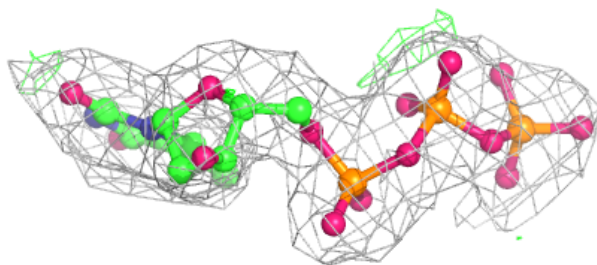
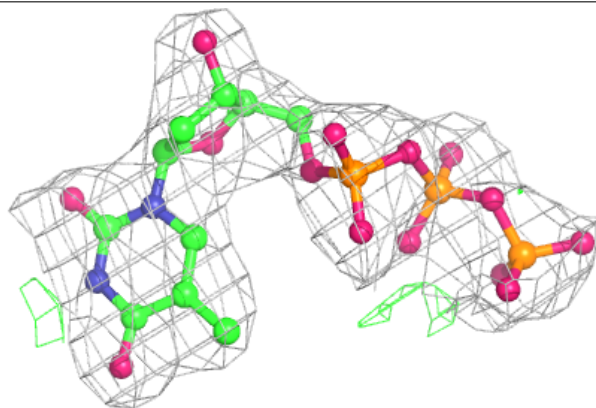


**Electron density around TTP H 3515:**

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and green (positive)

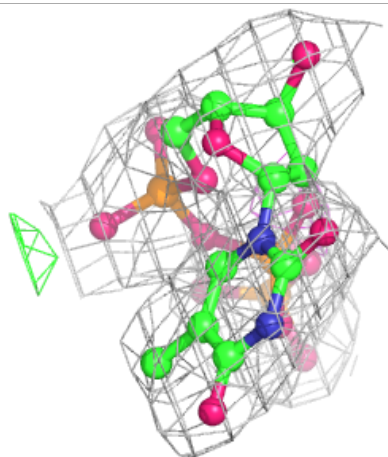
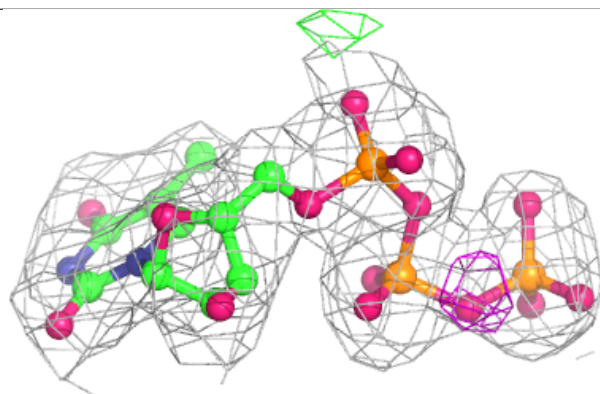
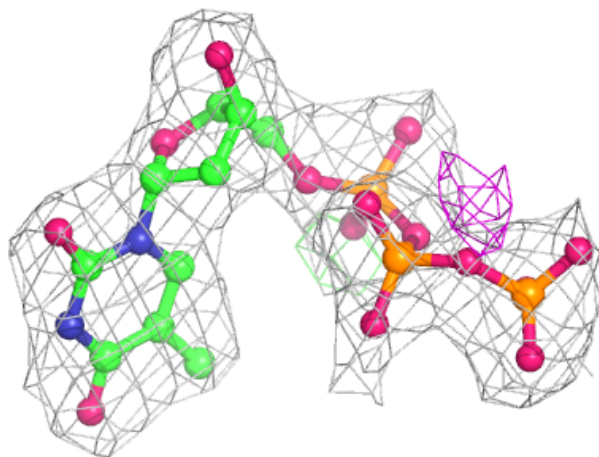
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and green (positive)



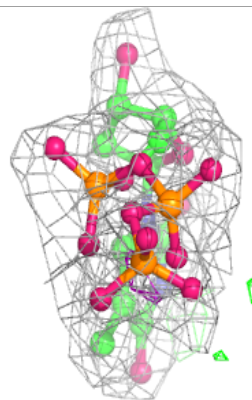
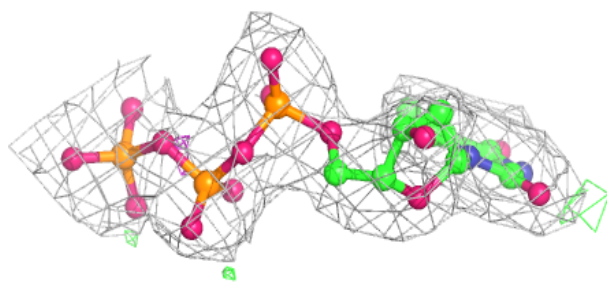
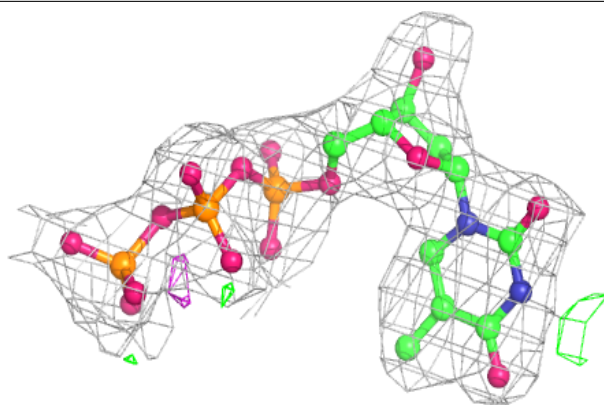
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and green (positive)



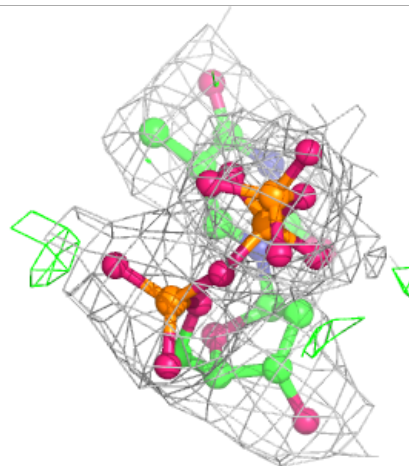
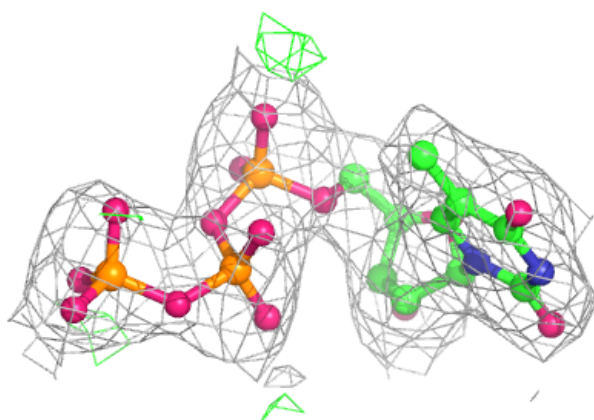
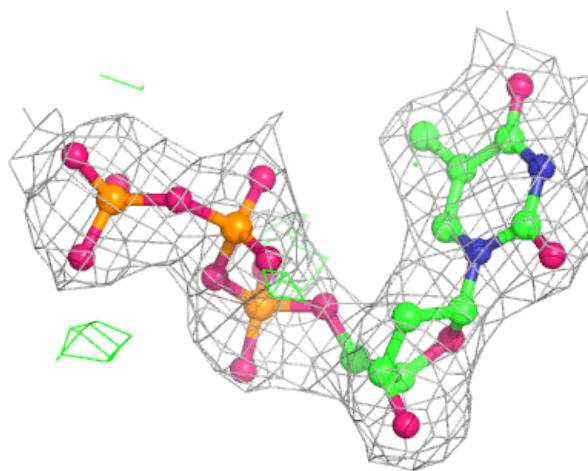
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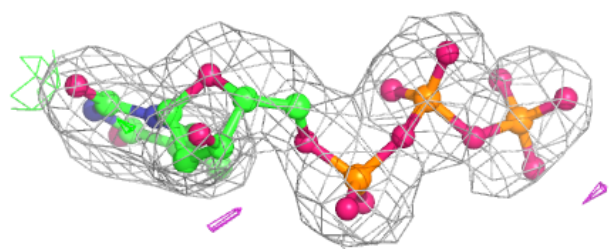
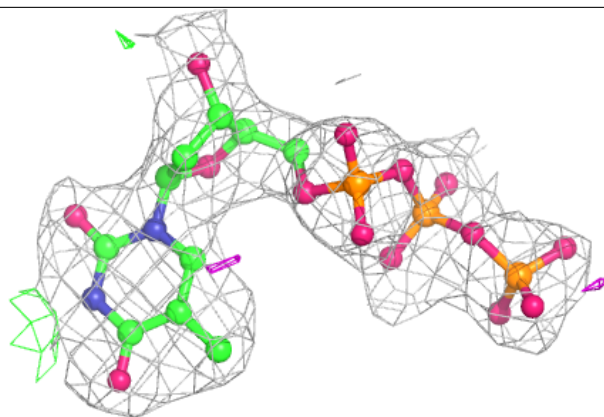
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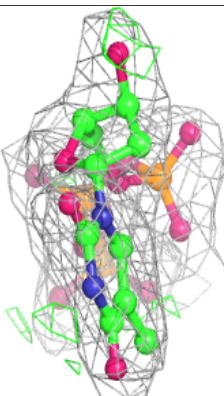
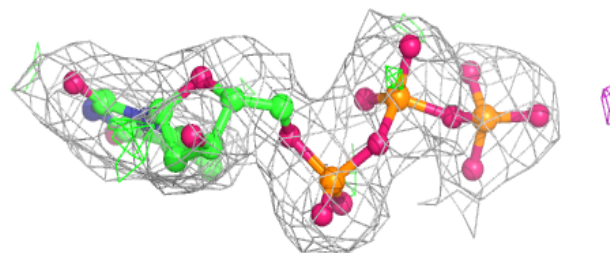
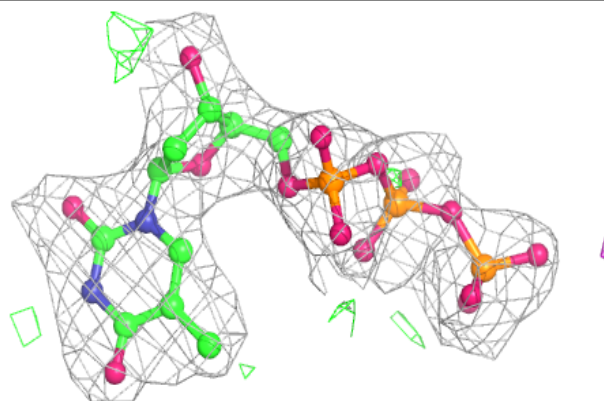


**Electron density around TTP E 3509:**

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and green (positive)

**Electron density around TTP B 3503:**

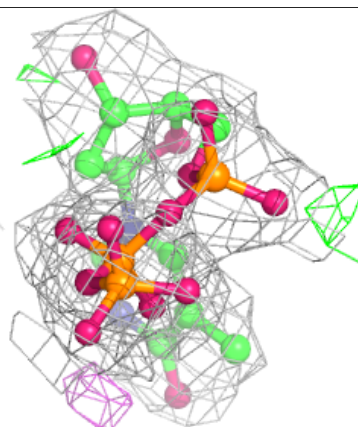
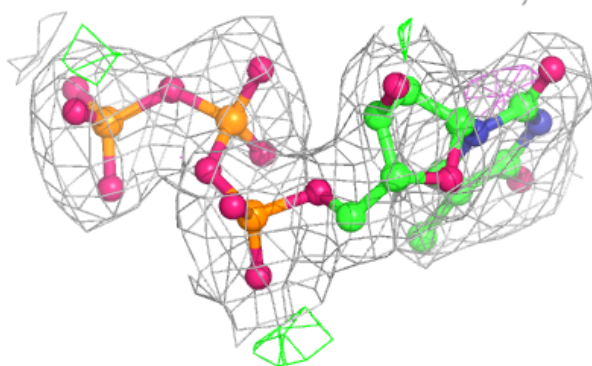
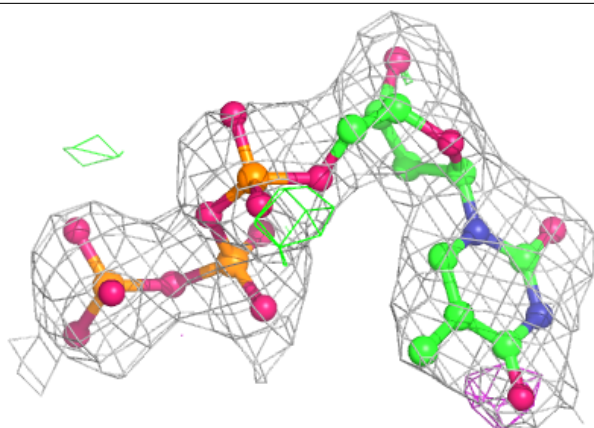
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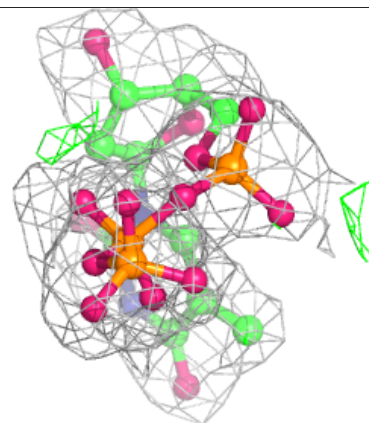
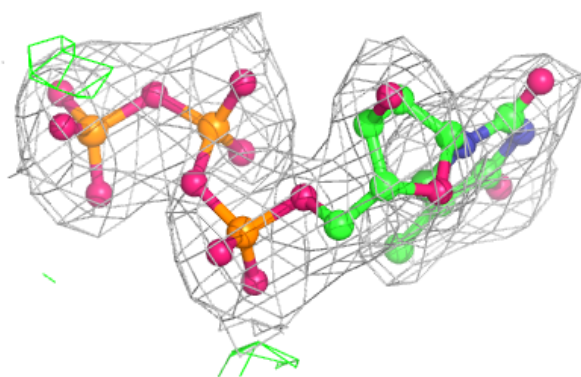
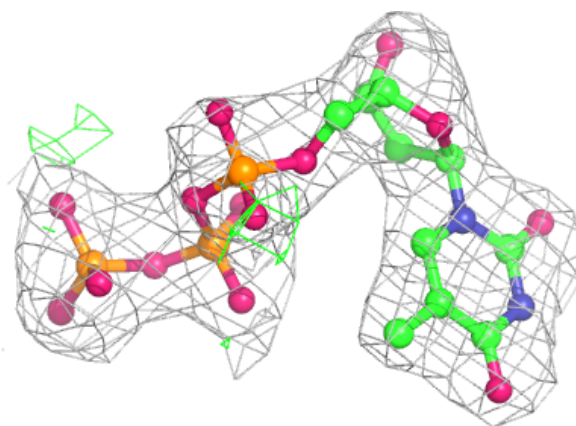
**Electron density around TTP E 3508:**

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



**Electron density around TTP C 3504:**

$2mF_o-DF_c$  (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.