wwPDB X-ray Structure Validation Summary Report (i)

Mar 3, 2024 – 11:37 PM EST

PDB ID	:	6OIW
Title	:	Structure of Escherichia coli dGTPase bound to dGTP-1-thiol
Authors	:	Barnes, C.O.; Wu, Y.; Calero, G.
Deposited on	:	2019-04-09
Resolution	:	3.35 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

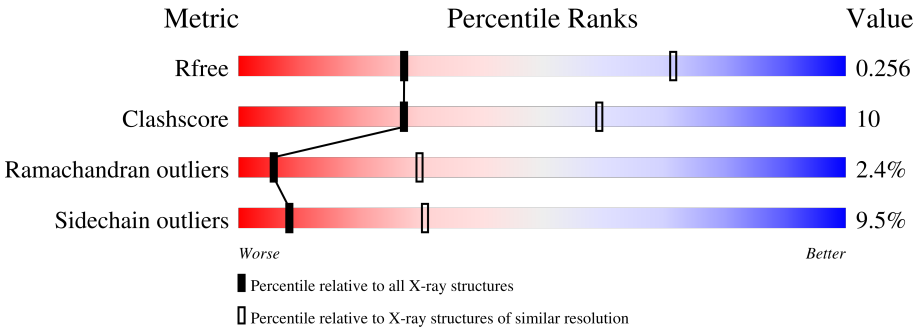
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	505	73% 23% ·
1	B	505	67% 26% 6%
1	C	505	73% 22% ·
1	D	505	73% 23% ·
1	E	505	74% 23% · ·
1	F	505	74% 21% ·

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 25272 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 Deoxyguanosinetriphosphate triphosphohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	0	0	0
			4179	2663	747	753	16			
1	B	503	Total	C	N	O	S	0	0	0
			4174	2661	746	751	16			
1	C	503	Total	C	N	O	S	0	0	0
			4174	2661	746	751	16			
1	D	504	Total	C	N	O	S	0	0	0
			4179	2663	747	753	16			
1	E	503	Total	C	N	O	S	0	0	0
			4174	2661	746	751	16			
1	F	503	Total	C	N	O	S	0	0	0
			4174	2661	746	751	16			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		

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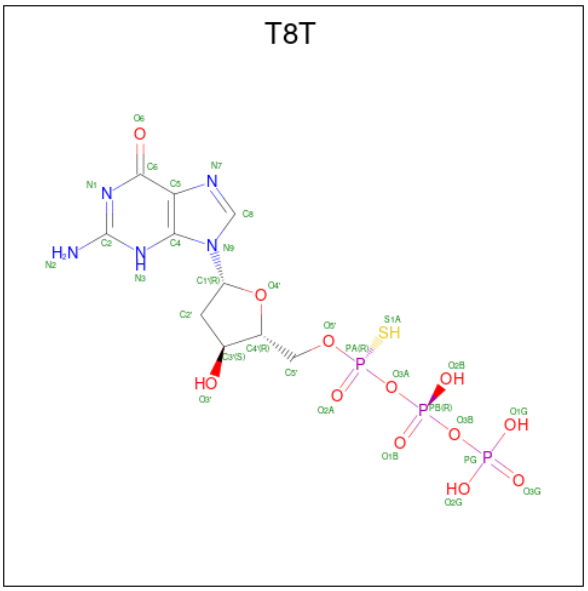
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Mn 1 1	0	0
3	E	1	Total Mn 1 1	0	0
3	F	1	Total Mn 1 1	0	0

- Molecule 4 is 2'-deoxyguanosine-5'-O-(1-thiotriphosphate) (three-letter code: T8T) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P S 31 10 5 12 3 1	0	0
4	B	1	Total C N O P S 31 10 5 12 3 1	0	0
4	C	1	Total C N O P S 31 10 5 12 3 1	0	0
4	D	1	Total C N O P S 31 10 5 12 3 1	0	0
4	E	1	Total C N O P S 31 10 5 12 3 1	0	0
4	F	1	Total C N O P S 31 10 5 12 3 1	0	0

- Molecule 5 is water.

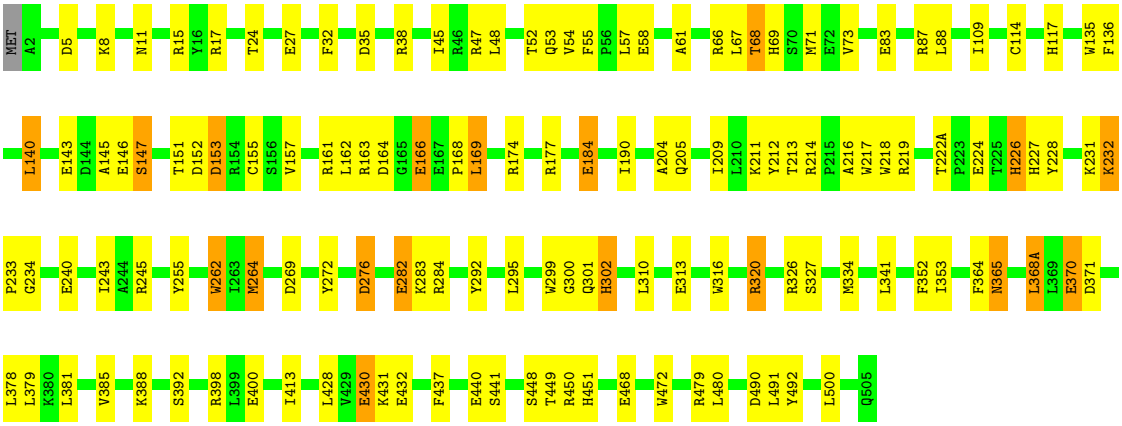
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	5	Total O 5 5	0	0
5	B	4	Total O 4 4	0	0
5	C	2	Total O 2 2	0	0
5	D	5	Total O 5 5	0	0
5	E	4	Total O 4 4	0	0
5	F	3	Total O 3 3	0	0

3 Residue-property plots (i)

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. 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. 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.

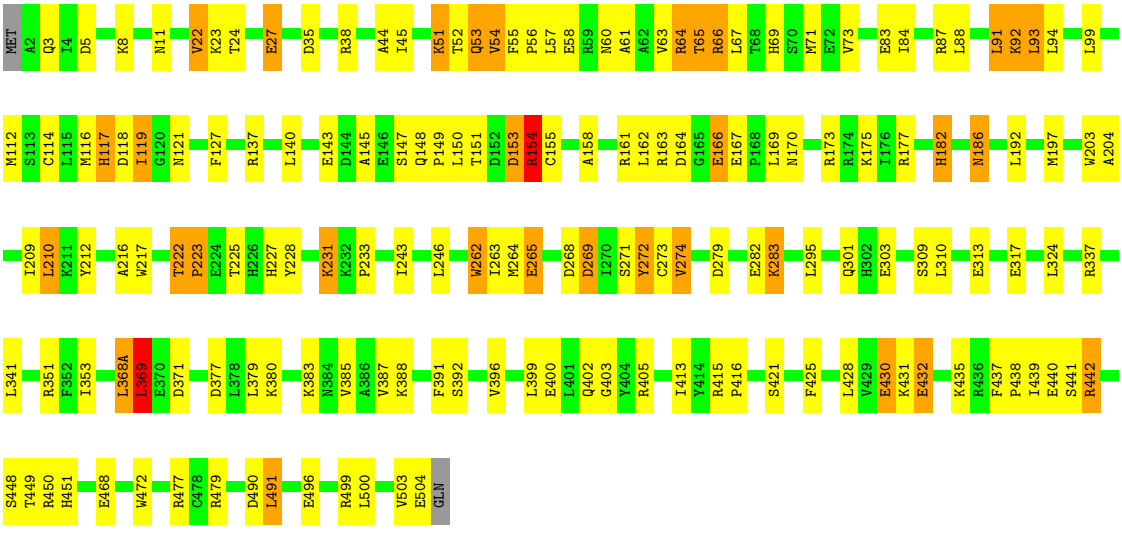
• Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase

Chain A:



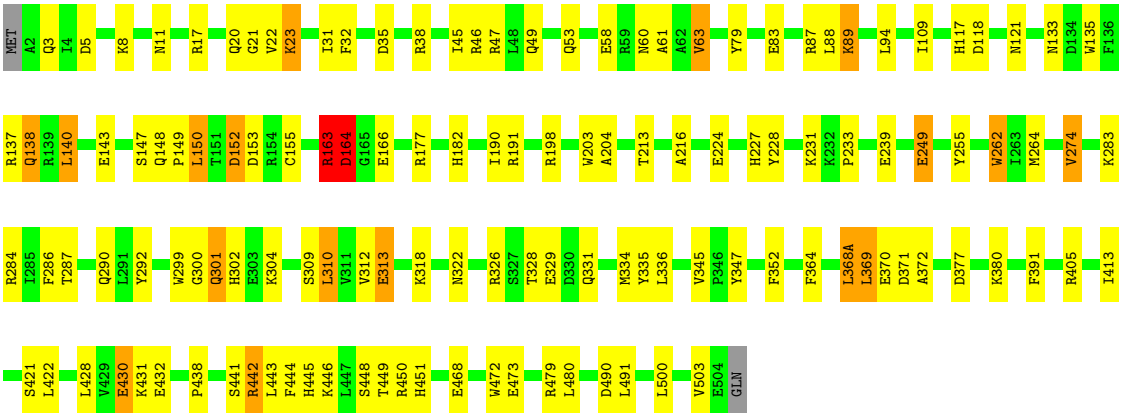
• Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase

Chain B:



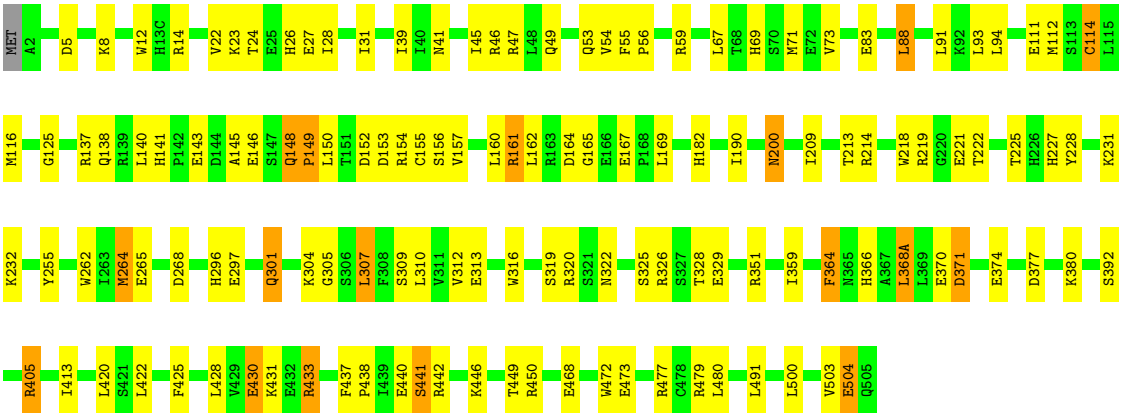
• Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase

Chain C:



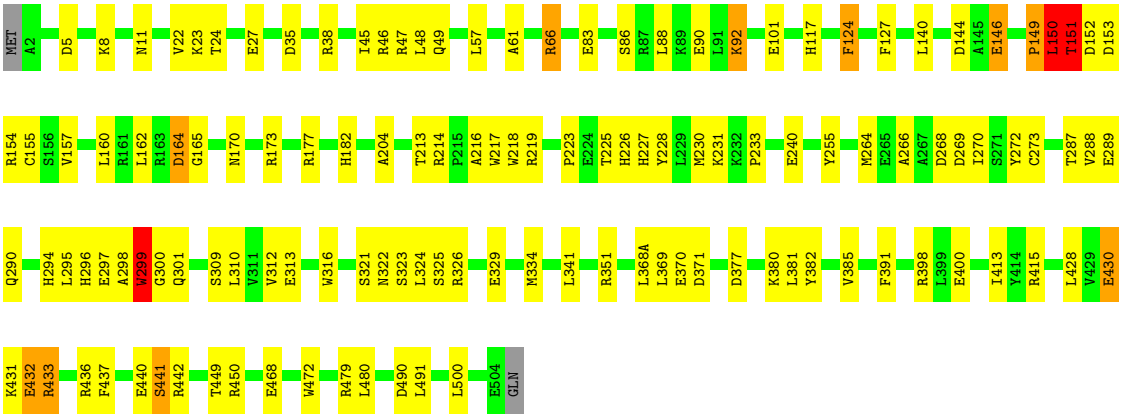
• Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase

Chain D:



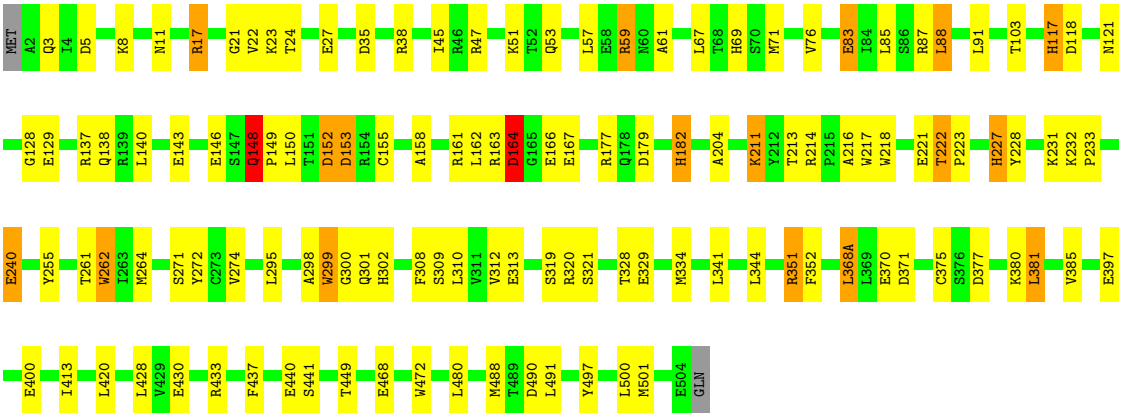
• Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase

Chain E:



• Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase

Chain F:


MET A2 Q3 I4 D5 K8 N11 R17 G21 V22 K23 T24 E27 D35 R38 I45 R46 R47 K51 T52 Q53 L57 E58 R59 N60 A61 L67 T68 H69 S70 M71 V76 E83 I84 L85 S86 R87 L88 L91 T103 H117 D118 N121
G128 E129 R137 Q138 R139 L140 E143 E146 S147 Q148 P149 L150 T151 D152 D153 R154 C155 A158 R161 L162 R163 D164 G165 E166 E167 R177 Q178 D179 H182 A204 K211 Y212 T213 R214 P215 A216 W217 W218 E221 T222 P223 H227 Y228 K231 K232 P233
E240 Y255 T261 W262 I263 M264 S271 Y272 C273 V274 L295 A298 W299 G300 Q301 H302 F308 S309 L310 V311 V312 E313 S319 R320 S321 T328 E329 M334 L341 L344 R351 F352 L368A L369 E370 D371 C375 S376 D377 K380 L381 V385 E397
E400 I413 L420 L428 V429 E430 R433 F437 E440 S441 T449 E468 W472 L480 M488 T489 D490 L491 Y497 L500 M501 E504 GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	191.24Å 191.24Å 298.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.48 – 3.35 48.48 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.48-3.35) 99.8 (48.48-3.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.29	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 3.33Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.178 , 0.212 0.233 , 0.256	Depositor DCC
R_{free} test set	2451 reflections (3.07%)	wwPDB-VP
Wilson B-factor (Å^2)	112.4	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 121.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	25272	wwPDB-VP
Average B, all atoms (Å^2)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MN, T8T

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	0.71	2/4282 (0.0%)	0.80	1/5792 (0.0%)
1	B	0.58	0/4277	0.82	8/5784 (0.1%)
1	C	0.58	0/4277	0.77	3/5784 (0.1%)
1	D	0.51	0/4282	0.73	2/5792 (0.0%)
1	E	0.57	0/4277	0.75	3/5784 (0.1%)
1	F	0.61	0/4277	0.78	1/5784 (0.0%)
All	All	0.60	2/25672 (0.0%)	0.77	18/34720 (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	B	0	1
1	C	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	THR	C-O	-7.03	1.09	1.23
1	A	184	GLU	CD-OE1	-5.59	1.19	1.25

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	154	ARG	N-CA-CB	-11.85	89.28	110.60
1	B	153	ASP	C-N-CA	-7.48	103.01	121.70
1	B	265	GLU	CB-CA-C	-7.27	95.86	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	263	ILE	C-N-CA	6.47	137.88	121.70
1	B	92	LYS	C-N-CA	6.36	137.59	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	64	ARG	Sidechain
1	C	442	ARG	Sidechain

5.2 Too-close contacts (i)

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	4179	0	4129	87	0
1	B	4174	0	4129	153	0
1	C	4174	0	4132	71	0
1	D	4179	0	4129	82	0
1	E	4174	0	4132	76	0
1	F	4174	0	4132	70	0
2	A	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	31	0	13	7	0
4	B	31	0	13	1	0
4	C	31	0	13	4	0
4	D	31	0	13	1	0
4	E	31	0	13	3	0
4	F	31	0	13	4	0
5	A	5	0	0	1	0
5	B	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	2	0	0	0	0
5	D	5	0	0	0	0
5	E	4	0	0	0	0
5	F	3	0	0	0	0
All	All	25272	0	24861	505	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 10.

The worst 5 of 505 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:B:153:ASP:O	1:B:155:CYS:N	1.58	1.32
1:A:53:GLN:NE2	4:A:603:T8T:O3'	1.67	1.25
1:C:53:GLN:NE2	4:C:602:T8T:O3'	1.70	1.24
1:B:147:SER:OG	1:B:148:GLN:OE1	1.55	1.22
1:F:53:GLN:NE2	4:F:603:T8T:O3'	1.74	1.19

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	502/505 (99%)	463 (92%)	29 (6%)	10 (2%)	7 33
1	B	501/505 (99%)	460 (92%)	31 (6%)	10 (2%)	7 33
1	C	501/505 (99%)	457 (91%)	28 (6%)	16 (3%)	4 24
1	D	502/505 (99%)	456 (91%)	36 (7%)	10 (2%)	7 33
1	E	501/505 (99%)	455 (91%)	31 (6%)	15 (3%)	4 26
1	F	501/505 (99%)	452 (90%)	38 (8%)	11 (2%)	6 32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3008/3030 (99%)	2743 (91%)	193 (6%)	72 (2%)	6 30

5 of 72 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	SER
1	A	166	GLU
1	B	22	VAL
1	B	93	LEU
1	B	154	ARG

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	448/450 (100%)	408 (91%)	40 (9%)	9 34
1	B	448/450 (100%)	399 (89%)	49 (11%)	6 25
1	C	448/450 (100%)	405 (90%)	43 (10%)	8 30
1	D	448/450 (100%)	407 (91%)	41 (9%)	9 32
1	E	448/450 (100%)	411 (92%)	37 (8%)	11 37
1	F	448/450 (100%)	403 (90%)	45 (10%)	7 29
All	All	2688/2700 (100%)	2433 (90%)	255 (10%)	8 31

5 of 255 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	313	GLU
1	F	148	GLN
1	D	152	ASP
1	F	143	GLU
1	F	299	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	402	GLN
1	D	322	ASN
1	F	148	GLN
1	C	445	HIS
1	D	148	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 9 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
4	T8T	B	602	-	22,33,33	1.49	5 (22%)	30,52,52	0.81	0
4	T8T	A	603	2	22,33,33	1.83	4 (18%)	30,52,52	1.32	2 (6%)
4	T8T	C	602	-	22,33,33	1.89	4 (18%)	30,52,52	1.33	3 (10%)
4	T8T	E	603	-	22,33,33	1.22	3 (13%)	30,52,52	1.81	5 (16%)
4	T8T	F	603	-	22,33,33	1.27	3 (13%)	30,52,52	0.82	0
4	T8T	D	602	-	22,33,33	1.33	3 (13%)	30,52,52	0.69	0

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
4	T8T	B	602	-	-	3/14/34/34	0/3/3/3
4	T8T	A	603	2	-	5/14/34/34	0/3/3/3
4	T8T	C	602	-	-	6/14/34/34	0/3/3/3
4	T8T	E	603	-	-	1/14/34/34	0/3/3/3
4	T8T	F	603	-	-	2/14/34/34	0/3/3/3
4	T8T	D	602	-	-	4/14/34/34	0/3/3/3

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	T8T	PG-O3G	-6.18	1.30	1.50
4	C	602	T8T	PA-O5'	-5.26	1.49	1.57
4	C	602	T8T	PG-O3G	-4.06	1.37	1.50
4	B	602	T8T	PG-O3G	-3.55	1.39	1.50
4	B	602	T8T	PA-O5'	-3.45	1.52	1.57

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	603	T8T	PB-O3B-PG	-5.44	114.15	132.83
4	E	603	T8T	O5'-PA-O3A	5.12	119.67	101.37
4	A	603	T8T	PA-O5'-C5'	4.85	135.47	120.16
4	E	603	T8T	O5'-PA-O2A	-3.66	100.94	114.42
4	C	602	T8T	PB-O3B-PG	-3.55	120.65	132.83

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	603	T8T	PB-O3B-PG-O1G
4	B	602	T8T	PB-O3B-PG-O1G
4	C	602	T8T	PB-O3B-PG-O2G
4	D	602	T8T	PB-O3B-PG-O2G
4	A	603	T8T	C5'-O5'-PA-O2A

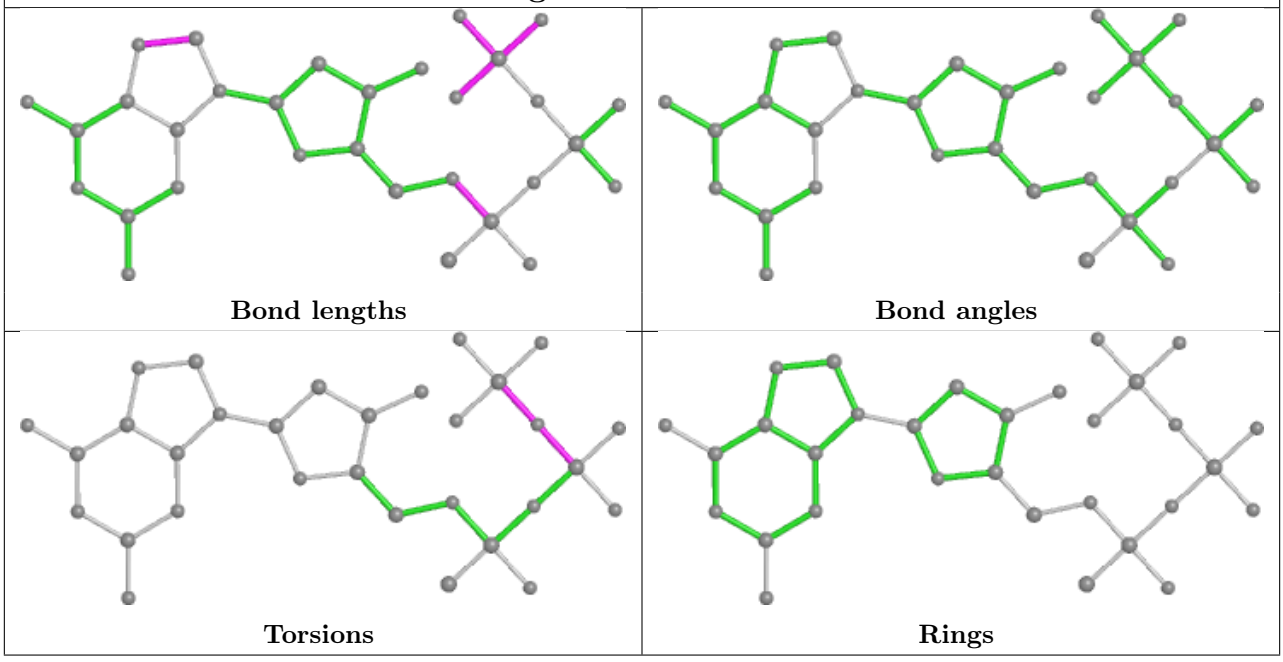
There are no ring outliers.

6 monomers are involved in 20 short contacts:

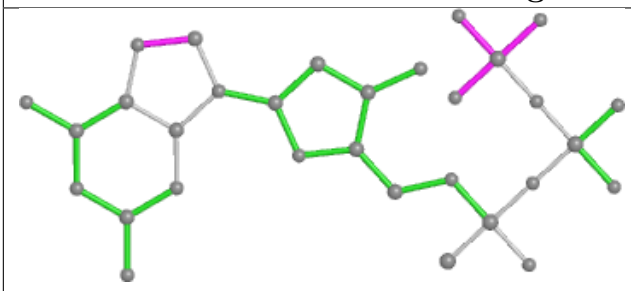
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	602	T8T	1	0
4	A	603	T8T	7	0
4	C	602	T8T	4	0
4	E	603	T8T	3	0
4	F	603	T8T	4	0
4	D	602	T8T	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

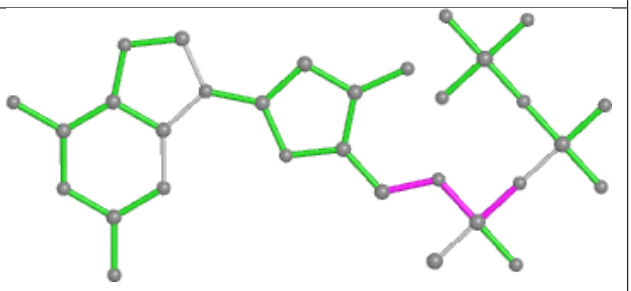
Ligand T8T B 602



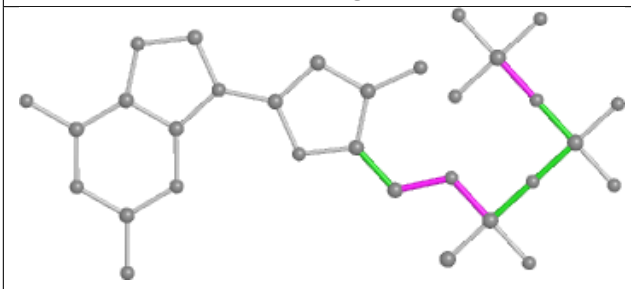
Ligand T8T A 603



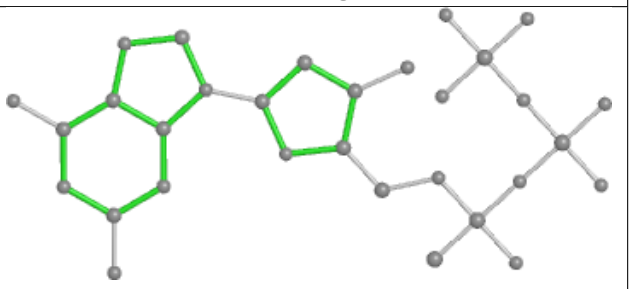
Bond lengths



Bond angles

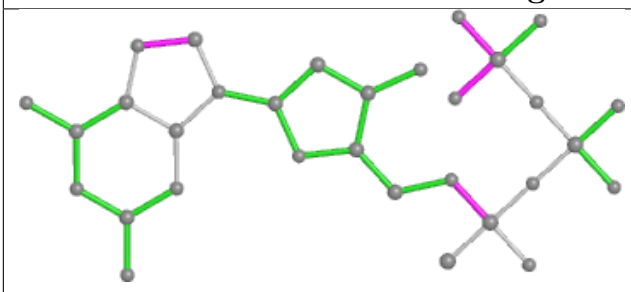


Torsions

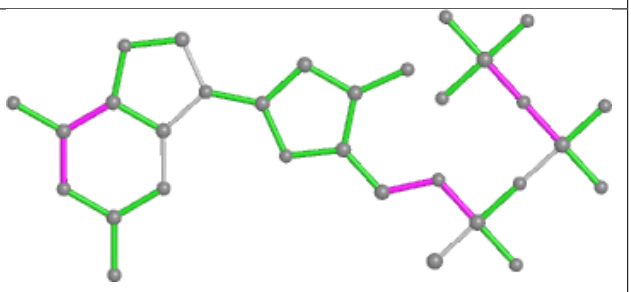


Rings

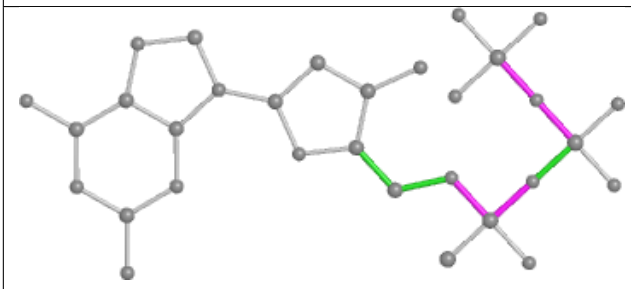
Ligand T8T C 602



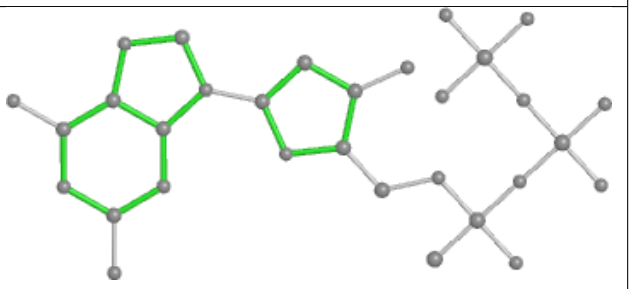
Bond lengths



Bond angles

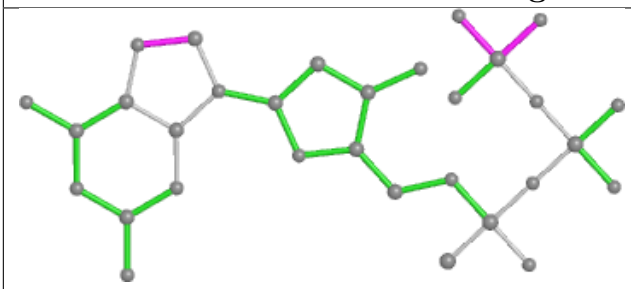


Torsions

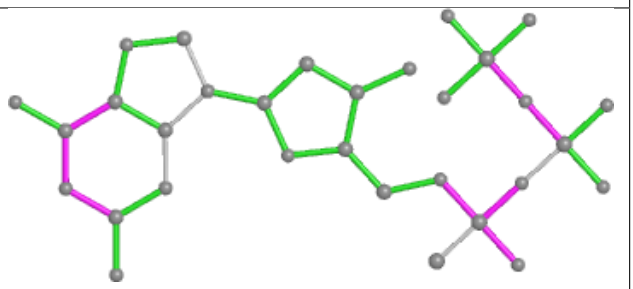


Rings

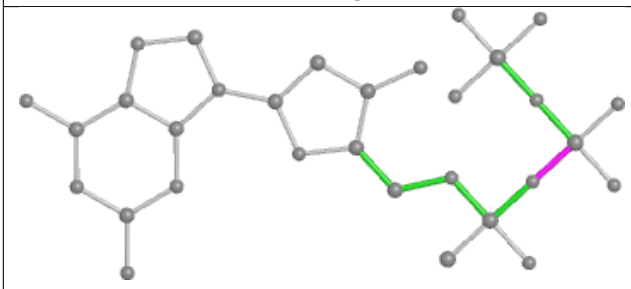
Ligand T8T E 603



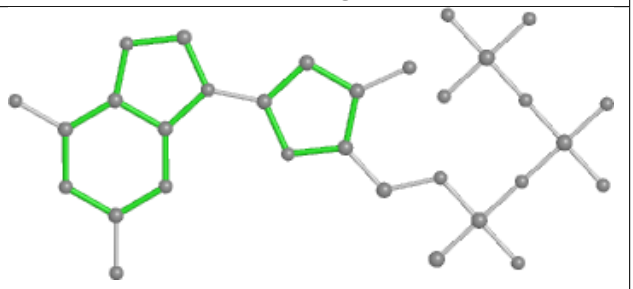
Bond lengths



Bond angles

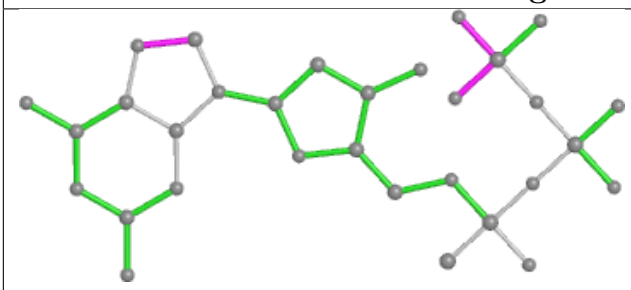


Torsions

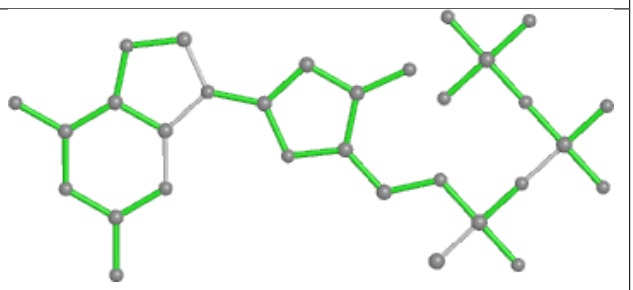


Rings

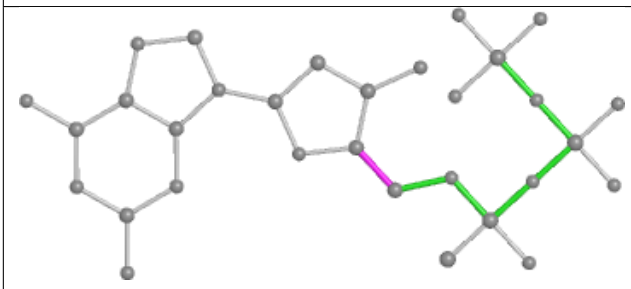
Ligand T8T F 603



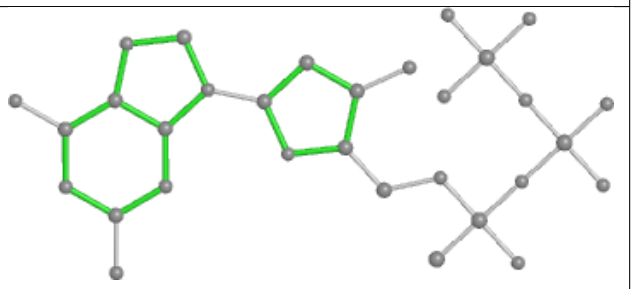
Bond lengths



Bond angles

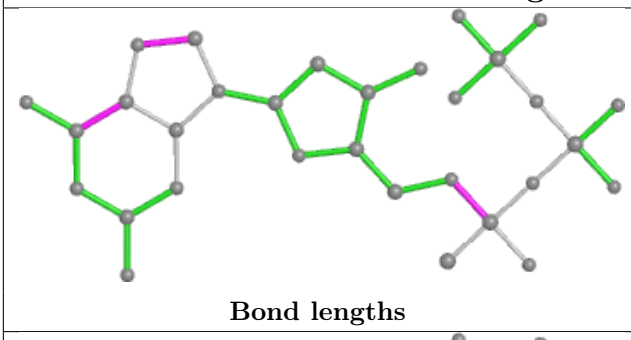


Torsions

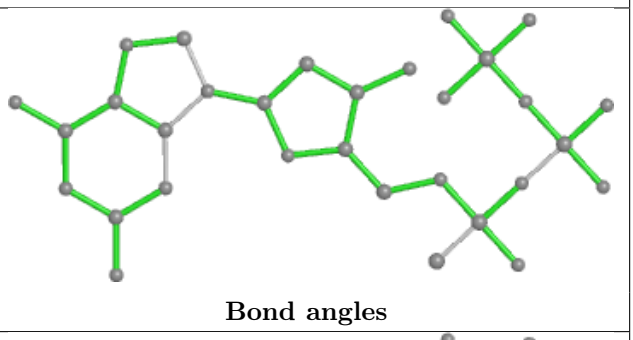


Rings

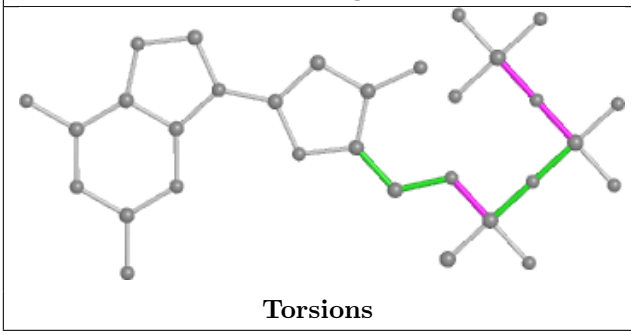
Ligand T8T D 602



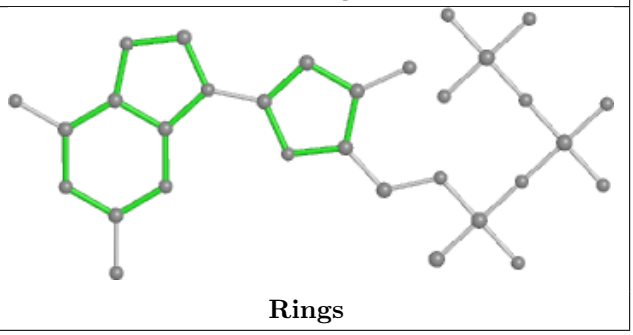
Bond lengths



Bond angles



Torsions



Rings

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

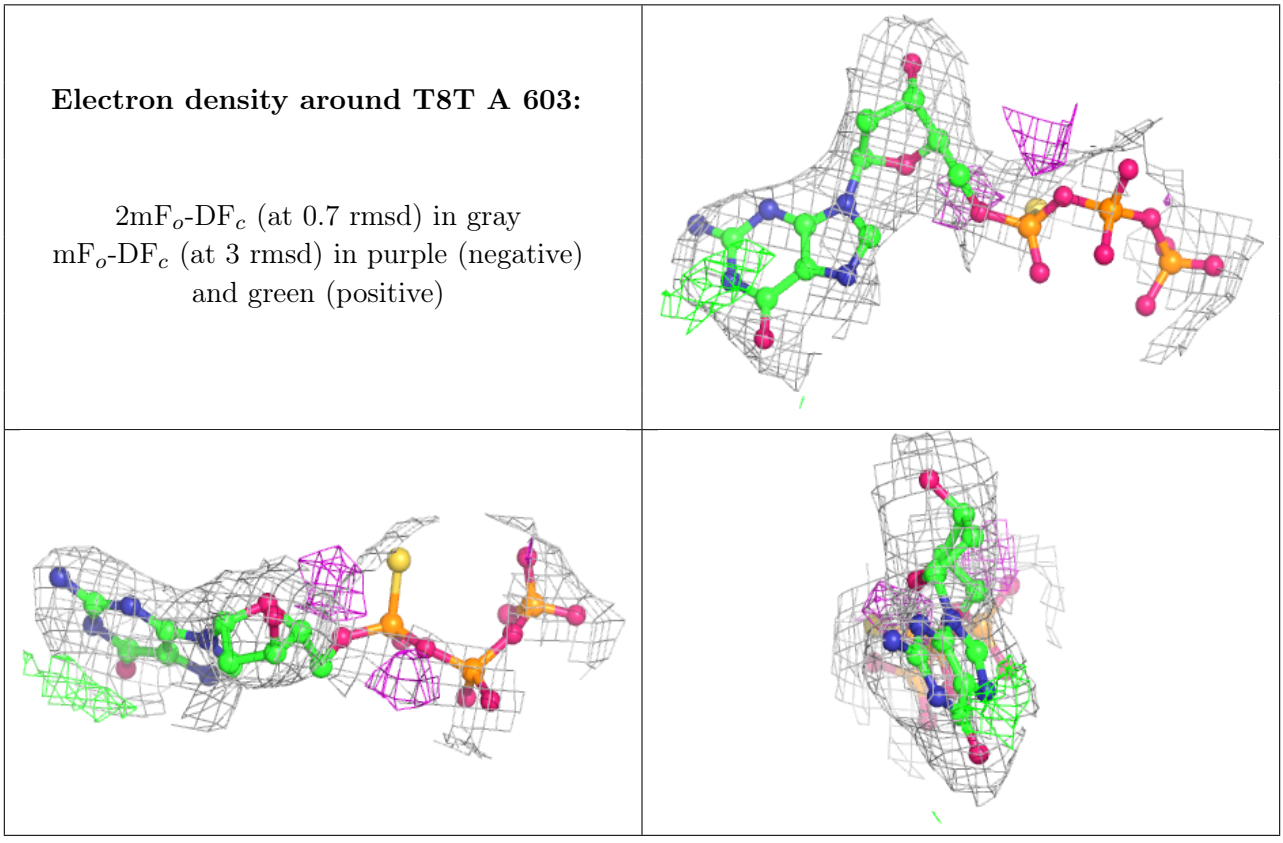
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

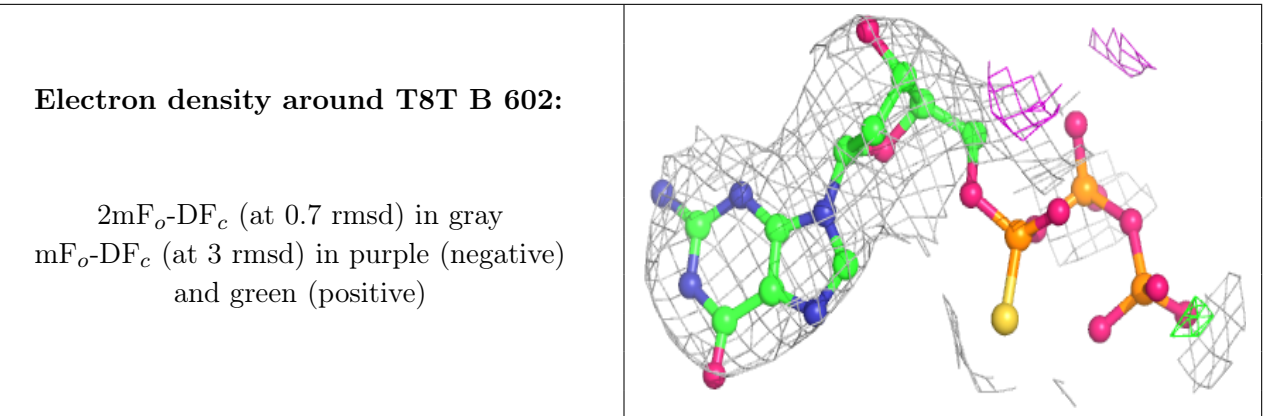
Electron density around T8T A 603:

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



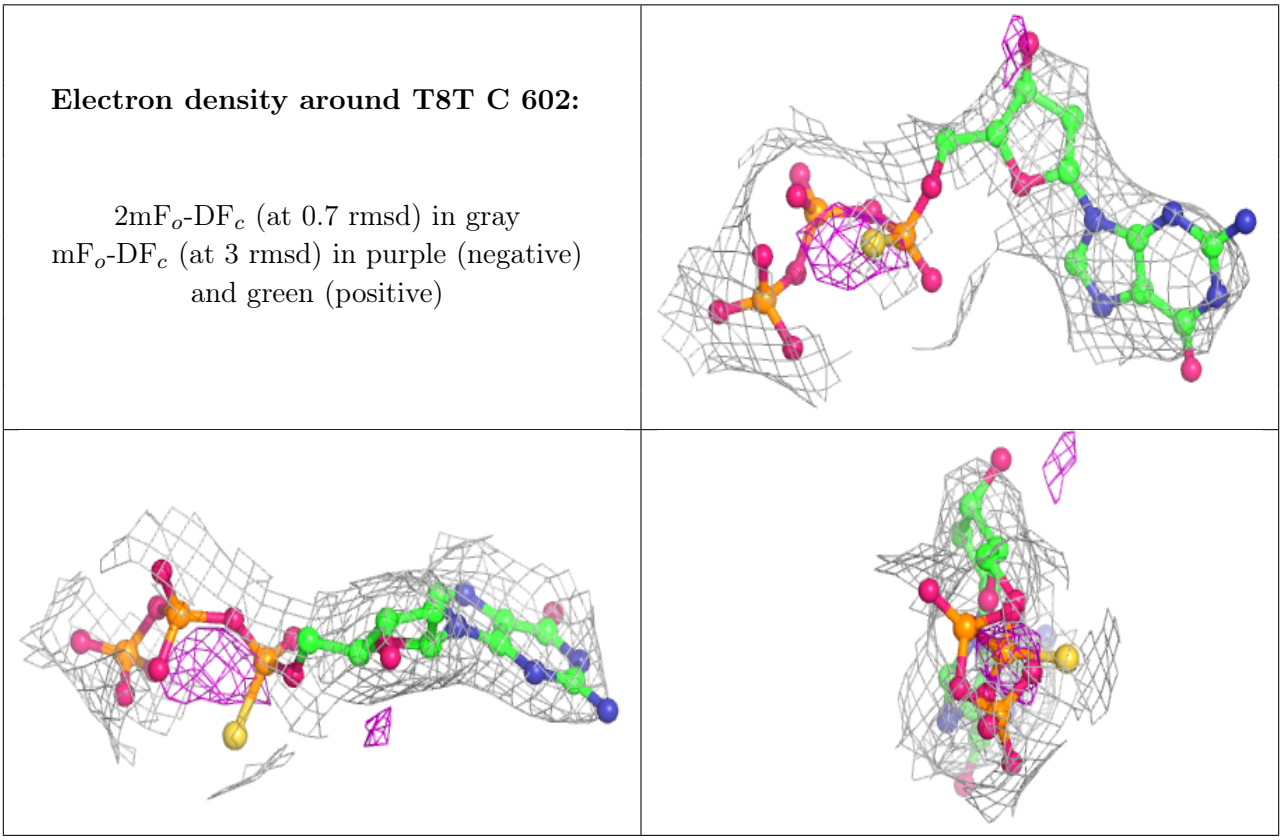
Electron density around T8T B 602:

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



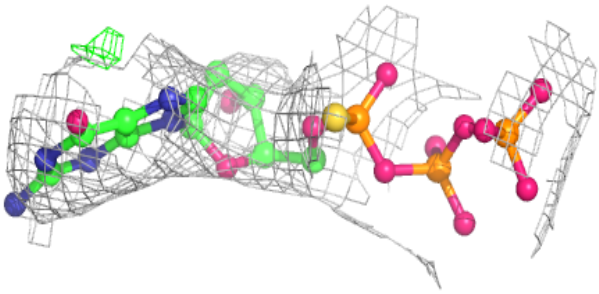
Electron density around T8T C 602:

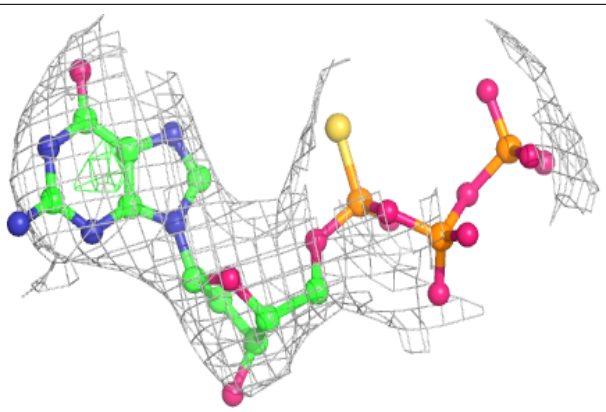
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

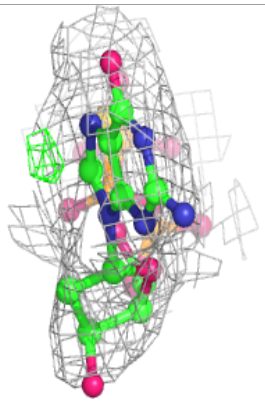


Electron density around T8T D 602:

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

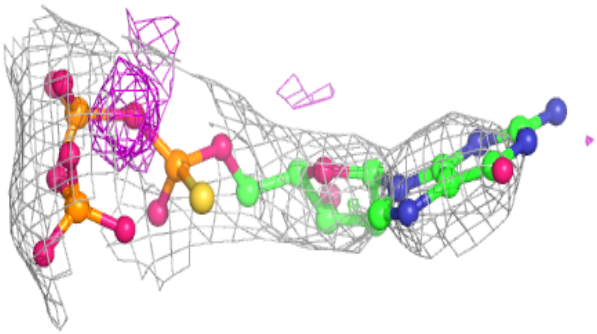


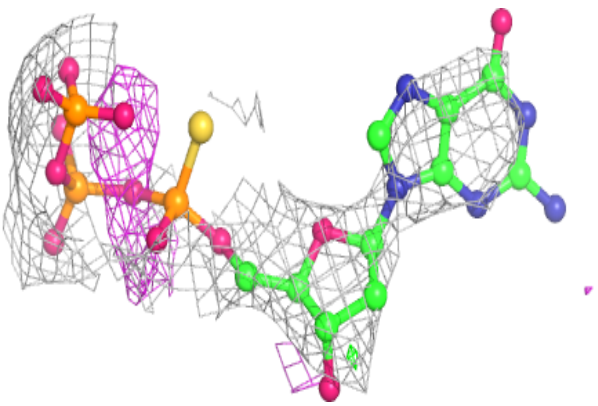


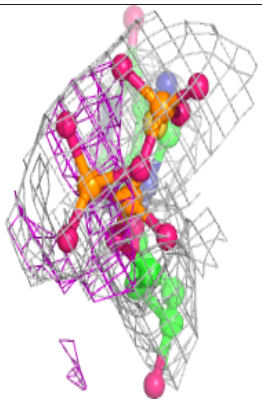


Electron density around T8T E 603:

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

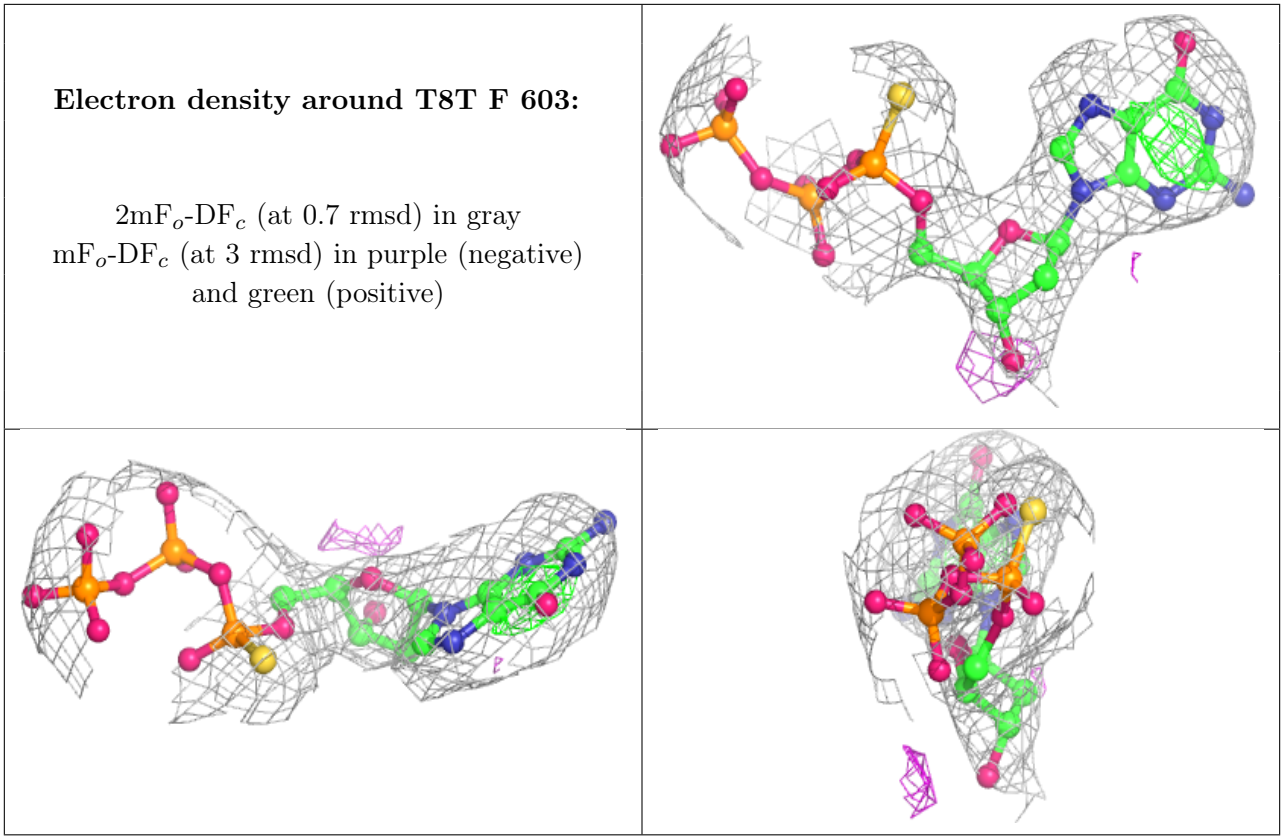






Electron density around T8T F 603:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.