



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 01:45 AM UTC

PDB ID : 4BZC / pdb_00004bzc
Title : Crystal structure of the tetrameric dGTP-bound wild type SAMHD1 catalytic core
Authors : Ji, X.; Yang, H.; Wu, Y.; Yan, J.; Mehrens, J.; DeLucia, M.; Hao, C.; Gronenborn, A.M.; Skowronski, J.; Ahn, J.; Xiong, Y.
Deposited on : 2013-07-25
Resolution : 2.88 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 ⓘ 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

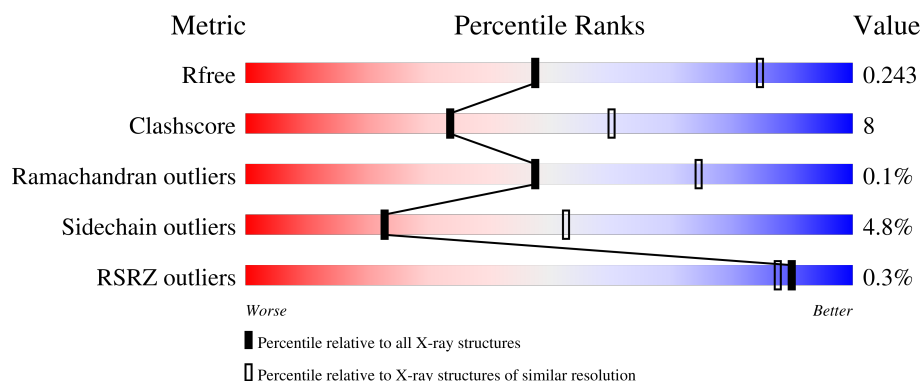
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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	550	
1	B	550	
1	C	550	
1	D	550	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 15954 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 TRIPHOSPHO-HYDROLASE SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	0	0	0
			3880	2483	672	705	20			
1	B	477	Total	C	N	O	S	0	0	0
			3887	2489	678	700	20			
1	C	481	Total	C	N	O	S	0	0	0
			3932	2517	683	712	20			
1	D	470	Total	C	N	O	S	0	0	0
			3841	2462	666	693	20			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	MET	-	expression tag	UNP Q9Y3Z3
A	78	GLY	-	expression tag	UNP Q9Y3Z3
A	79	SER	-	expression tag	UNP Q9Y3Z3
A	80	SER	-	expression tag	UNP Q9Y3Z3
A	81	HIS	-	expression tag	UNP Q9Y3Z3
A	82	HIS	-	expression tag	UNP Q9Y3Z3
A	83	HIS	-	expression tag	UNP Q9Y3Z3
A	84	HIS	-	expression tag	UNP Q9Y3Z3
A	85	HIS	-	expression tag	UNP Q9Y3Z3
A	86	HIS	-	expression tag	UNP Q9Y3Z3
A	87	SER	-	expression tag	UNP Q9Y3Z3
A	88	SER	-	expression tag	UNP Q9Y3Z3
A	89	GLY	-	expression tag	UNP Q9Y3Z3
A	90	LEU	-	expression tag	UNP Q9Y3Z3
A	91	VAL	-	expression tag	UNP Q9Y3Z3
A	92	PRO	-	expression tag	UNP Q9Y3Z3
A	93	ARG	-	expression tag	UNP Q9Y3Z3
A	94	GLY	-	expression tag	UNP Q9Y3Z3
A	95	SER	-	expression tag	UNP Q9Y3Z3
A	96	HIS	-	expression tag	UNP Q9Y3Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	97	MET	-	expression tag	UNP Q9Y3Z3
A	98	ALA	-	expression tag	UNP Q9Y3Z3
A	99	SER	-	expression tag	UNP Q9Y3Z3
A	100	MET	-	expression tag	UNP Q9Y3Z3
A	101	THR	-	expression tag	UNP Q9Y3Z3
A	102	GLY	-	expression tag	UNP Q9Y3Z3
A	103	GLY	-	expression tag	UNP Q9Y3Z3
A	104	GLN	-	expression tag	UNP Q9Y3Z3
A	105	GLN	-	expression tag	UNP Q9Y3Z3
A	106	MET	-	expression tag	UNP Q9Y3Z3
A	107	GLY	-	expression tag	UNP Q9Y3Z3
A	108	ARG	-	expression tag	UNP Q9Y3Z3
A	109	ASP	-	expression tag	UNP Q9Y3Z3
A	110	PRO	-	expression tag	UNP Q9Y3Z3
A	111	ASN	-	expression tag	UNP Q9Y3Z3
A	112	SER	-	expression tag	UNP Q9Y3Z3
B	77	MET	-	expression tag	UNP Q9Y3Z3
B	78	GLY	-	expression tag	UNP Q9Y3Z3
B	79	SER	-	expression tag	UNP Q9Y3Z3
B	80	SER	-	expression tag	UNP Q9Y3Z3
B	81	HIS	-	expression tag	UNP Q9Y3Z3
B	82	HIS	-	expression tag	UNP Q9Y3Z3
B	83	HIS	-	expression tag	UNP Q9Y3Z3
B	84	HIS	-	expression tag	UNP Q9Y3Z3
B	85	HIS	-	expression tag	UNP Q9Y3Z3
B	86	HIS	-	expression tag	UNP Q9Y3Z3
B	87	SER	-	expression tag	UNP Q9Y3Z3
B	88	SER	-	expression tag	UNP Q9Y3Z3
B	89	GLY	-	expression tag	UNP Q9Y3Z3
B	90	LEU	-	expression tag	UNP Q9Y3Z3
B	91	VAL	-	expression tag	UNP Q9Y3Z3
B	92	PRO	-	expression tag	UNP Q9Y3Z3
B	93	ARG	-	expression tag	UNP Q9Y3Z3
B	94	GLY	-	expression tag	UNP Q9Y3Z3
B	95	SER	-	expression tag	UNP Q9Y3Z3
B	96	HIS	-	expression tag	UNP Q9Y3Z3
B	97	MET	-	expression tag	UNP Q9Y3Z3
B	98	ALA	-	expression tag	UNP Q9Y3Z3
B	99	SER	-	expression tag	UNP Q9Y3Z3
B	100	MET	-	expression tag	UNP Q9Y3Z3
B	101	THR	-	expression tag	UNP Q9Y3Z3
B	102	GLY	-	expression tag	UNP Q9Y3Z3

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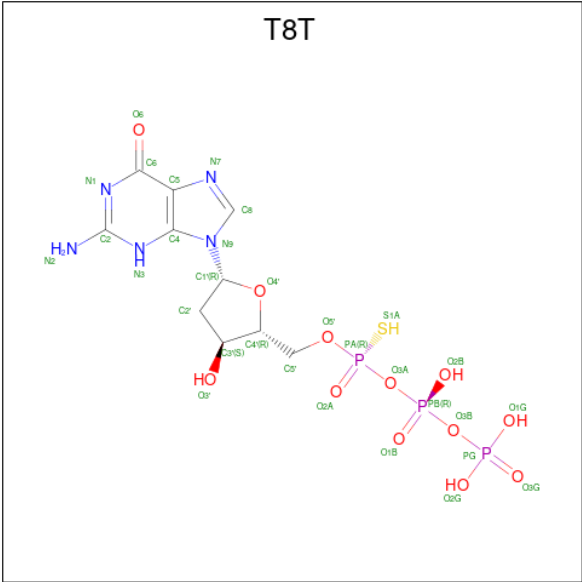
Chain	Residue	Modelled	Actual	Comment	Reference
B	103	GLY	-	expression tag	UNP Q9Y3Z3
B	104	GLN	-	expression tag	UNP Q9Y3Z3
B	105	GLN	-	expression tag	UNP Q9Y3Z3
B	106	MET	-	expression tag	UNP Q9Y3Z3
B	107	GLY	-	expression tag	UNP Q9Y3Z3
B	108	ARG	-	expression tag	UNP Q9Y3Z3
B	109	ASP	-	expression tag	UNP Q9Y3Z3
B	110	PRO	-	expression tag	UNP Q9Y3Z3
B	111	ASN	-	expression tag	UNP Q9Y3Z3
B	112	SER	-	expression tag	UNP Q9Y3Z3
C	77	MET	-	expression tag	UNP Q9Y3Z3
C	78	GLY	-	expression tag	UNP Q9Y3Z3
C	79	SER	-	expression tag	UNP Q9Y3Z3
C	80	SER	-	expression tag	UNP Q9Y3Z3
C	81	HIS	-	expression tag	UNP Q9Y3Z3
C	82	HIS	-	expression tag	UNP Q9Y3Z3
C	83	HIS	-	expression tag	UNP Q9Y3Z3
C	84	HIS	-	expression tag	UNP Q9Y3Z3
C	85	HIS	-	expression tag	UNP Q9Y3Z3
C	86	HIS	-	expression tag	UNP Q9Y3Z3
C	87	SER	-	expression tag	UNP Q9Y3Z3
C	88	SER	-	expression tag	UNP Q9Y3Z3
C	89	GLY	-	expression tag	UNP Q9Y3Z3
C	90	LEU	-	expression tag	UNP Q9Y3Z3
C	91	VAL	-	expression tag	UNP Q9Y3Z3
C	92	PRO	-	expression tag	UNP Q9Y3Z3
C	93	ARG	-	expression tag	UNP Q9Y3Z3
C	94	GLY	-	expression tag	UNP Q9Y3Z3
C	95	SER	-	expression tag	UNP Q9Y3Z3
C	96	HIS	-	expression tag	UNP Q9Y3Z3
C	97	MET	-	expression tag	UNP Q9Y3Z3
C	98	ALA	-	expression tag	UNP Q9Y3Z3
C	99	SER	-	expression tag	UNP Q9Y3Z3
C	100	MET	-	expression tag	UNP Q9Y3Z3
C	101	THR	-	expression tag	UNP Q9Y3Z3
C	102	GLY	-	expression tag	UNP Q9Y3Z3
C	103	GLY	-	expression tag	UNP Q9Y3Z3
C	104	GLN	-	expression tag	UNP Q9Y3Z3
C	105	GLN	-	expression tag	UNP Q9Y3Z3
C	106	MET	-	expression tag	UNP Q9Y3Z3
C	107	GLY	-	expression tag	UNP Q9Y3Z3
C	108	ARG	-	expression tag	UNP Q9Y3Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	109	ASP	-	expression tag	UNP Q9Y3Z3
C	110	PRO	-	expression tag	UNP Q9Y3Z3
C	111	ASN	-	expression tag	UNP Q9Y3Z3
C	112	SER	-	expression tag	UNP Q9Y3Z3
D	77	MET	-	expression tag	UNP Q9Y3Z3
D	78	GLY	-	expression tag	UNP Q9Y3Z3
D	79	SER	-	expression tag	UNP Q9Y3Z3
D	80	SER	-	expression tag	UNP Q9Y3Z3
D	81	HIS	-	expression tag	UNP Q9Y3Z3
D	82	HIS	-	expression tag	UNP Q9Y3Z3
D	83	HIS	-	expression tag	UNP Q9Y3Z3
D	84	HIS	-	expression tag	UNP Q9Y3Z3
D	85	HIS	-	expression tag	UNP Q9Y3Z3
D	86	HIS	-	expression tag	UNP Q9Y3Z3
D	87	SER	-	expression tag	UNP Q9Y3Z3
D	88	SER	-	expression tag	UNP Q9Y3Z3
D	89	GLY	-	expression tag	UNP Q9Y3Z3
D	90	LEU	-	expression tag	UNP Q9Y3Z3
D	91	VAL	-	expression tag	UNP Q9Y3Z3
D	92	PRO	-	expression tag	UNP Q9Y3Z3
D	93	ARG	-	expression tag	UNP Q9Y3Z3
D	94	GLY	-	expression tag	UNP Q9Y3Z3
D	95	SER	-	expression tag	UNP Q9Y3Z3
D	96	HIS	-	expression tag	UNP Q9Y3Z3
D	97	MET	-	expression tag	UNP Q9Y3Z3
D	98	ALA	-	expression tag	UNP Q9Y3Z3
D	99	SER	-	expression tag	UNP Q9Y3Z3
D	100	MET	-	expression tag	UNP Q9Y3Z3
D	101	THR	-	expression tag	UNP Q9Y3Z3
D	102	GLY	-	expression tag	UNP Q9Y3Z3
D	103	GLY	-	expression tag	UNP Q9Y3Z3
D	104	GLN	-	expression tag	UNP Q9Y3Z3
D	105	GLN	-	expression tag	UNP Q9Y3Z3
D	106	MET	-	expression tag	UNP Q9Y3Z3
D	107	GLY	-	expression tag	UNP Q9Y3Z3
D	108	ARG	-	expression tag	UNP Q9Y3Z3
D	109	ASP	-	expression tag	UNP Q9Y3Z3
D	110	PRO	-	expression tag	UNP Q9Y3Z3
D	111	ASN	-	expression tag	UNP Q9Y3Z3
D	112	SER	-	expression tag	UNP Q9Y3Z3

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



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

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

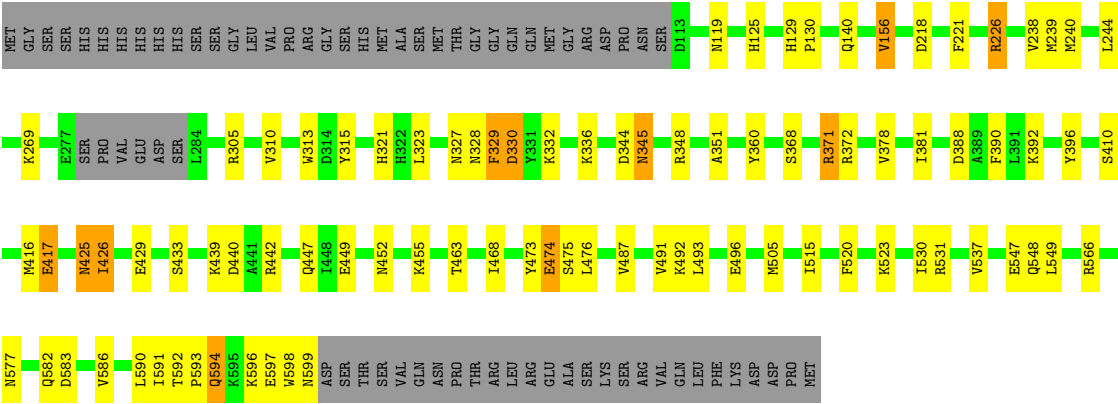
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Mn 1	0	0
3	B	1	Total 1	Mn 1	0	0
3	C	1	Total 1	Mn 1	0	0
3	D	1	Total 1	Mn 1	0	0

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

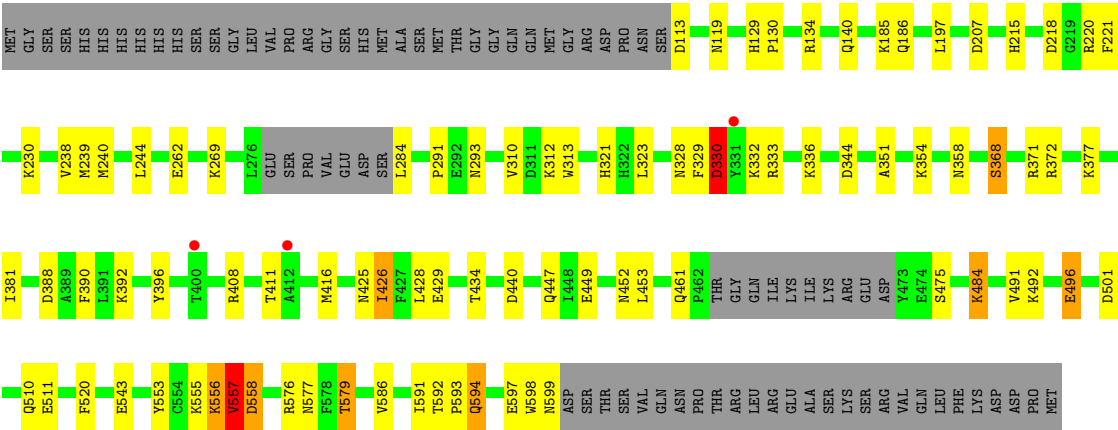
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Mg 1	0	0
4	B	1	Total 1	Mg 1	0	0
4	C	1	Total 1	Mg 1	0	0
4	D	1	Total 1	Mg 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	14	Total 14	O 14	0	0
5	B	9	Total 9	O 9	0	0
5	C	7	Total 7	O 7	0	0
5	D	4	Total 4	O 4	0	0



● Molecule 1: DEOXYNUCLEOSIDE TRIPHOSPHATE TRIPHOSPHOHYDROLASE SAMHD1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.00Å 138.73Å 93.72Å 90.00° 113.56° 90.00°	Depositor
Resolution (Å)	49.71 – 2.88 49.71 – 2.88	Depositor EDS
% Data completeness (in resolution range)	77.5 (49.71-2.88) 77.8 (49.71-2.88)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.80 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.190 , 0.245 0.193 , 0.243	Depositor DCC
R_{free} test set	1668 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	48.8	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 68.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.030 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15954	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.85	0/3972	0.98	9/5364 (0.2%)
1	B	0.79	1/3978 (0.0%)	0.97	9/5369 (0.2%)
1	C	0.85	0/4025	0.95	3/5434 (0.1%)
1	D	0.80	1/3933 (0.0%)	0.94	4/5311 (0.1%)
All	All	0.82	2/15908 (0.0%)	0.96	25/21478 (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	D	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	453	LEU	C-O	-5.36	1.16	1.23
1	B	229	VAL	CA-CB	5.09	1.60	1.54

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	226	ARG	CG-CD-NE	7.79	129.14	112.00
1	B	325	ILE	CB-CA-C	-7.58	100.80	111.19
1	A	434	THR	N-CA-C	-7.50	102.47	111.69
1	A	325	ILE	CB-CA-C	-7.22	101.30	111.19
1	A	440	ASP	N-CA-CB	6.82	120.25	110.16

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	330	ASP	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	3880	0	3844	81	0
1	B	3887	0	3872	57	0
1	C	3932	0	3913	65	2
1	D	3841	0	3817	72	2
2	A	93	0	39	3	0
2	B	93	0	39	4	0
2	C	93	0	39	11	0
2	D	93	0	39	6	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
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	14	0	0	1	0
5	B	9	0	0	1	0
5	C	7	0	0	0	0
5	D	4	0	0	0	0
All	All	15954	0	15602	241	2

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 8.

The worst 5 of 241 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:556:LYS:O	1:D:557:VAL:HG22	1.44	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:HIS:NE2	2:D:700:T8T:O2A	1.84	1.09
1:A:325:ILE:C	1:C:328:ASN:HB2	1.77	1.09
1:B:402:ALA:O	1:B:405:LYS:HD2	1.60	0.99
1:D:368:SER:OG	1:D:372:ARG:NH1	1.97	0.97

All (2) 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:396:TYR:OH	1:D:230:LYS:NZ[1_454]	2.10	0.10
1:C:493:LEU:O	1:D:396:TYR:OH[1_454]	2.10	0.10

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	470/550 (86%)	464 (99%)	6 (1%)	0	100	100
1	B	471/550 (86%)	466 (99%)	5 (1%)	0	100	100
1	C	477/550 (87%)	471 (99%)	6 (1%)	0	100	100
1	D	464/550 (84%)	458 (99%)	5 (1%)	1 (0%)	43	70
All	All	1882/2200 (86%)	1859 (99%)	22 (1%)	1 (0%)	48	74

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	557	VAL

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	421/488 (86%)	401 (95%)	20 (5%)	23	53
1	B	421/488 (86%)	401 (95%)	20 (5%)	23	53
1	C	427/488 (88%)	405 (95%)	22 (5%)	21	50
1	D	417/488 (86%)	398 (95%)	19 (5%)	24	55
All	All	1686/1952 (86%)	1605 (95%)	81 (5%)	23	53

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	492	LYS
1	D	475	SER
1	C	531	ARG
1	D	377	LYS
1	D	510	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	243	HIS
1	C	567	GLN
1	C	461	GLN
1	D	233	HIS
1	B	125	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	T8T	A	800	4	29,33,33	2.36	6 (20%)	36,52,52	1.91	7 (19%)
2	T8T	A	700	-	29,33,33	1.88	5 (17%)	36,52,52	1.74	8 (22%)
2	T8T	C	900	4	29,33,33	2.17	6 (20%)	36,52,52	1.39	6 (16%)
2	T8T	B	800	4	29,33,33	1.91	5 (17%)	36,52,52	1.90	8 (22%)
2	T8T	D	800	4	29,33,33	2.16	5 (17%)	36,52,52	1.53	7 (19%)
2	T8T	B	700	-	29,33,33	2.06	7 (24%)	36,52,52	1.71	9 (25%)
2	T8T	C	700	-	29,33,33	2.00	7 (24%)	36,52,52	1.38	6 (16%)
2	T8T	D	700	-	29,33,33	1.99	4 (13%)	36,52,52	1.01	1 (2%)
2	T8T	B	900	4	29,33,33	1.92	5 (17%)	36,52,52	1.34	3 (8%)
2	T8T	D	900	4	29,33,33	1.93	4 (13%)	36,52,52	1.53	5 (13%)
2	T8T	A	900	4	29,33,33	1.64	4 (13%)	36,52,52	1.47	7 (19%)
2	T8T	C	800	4	29,33,33	1.91	5 (17%)	36,52,52	1.54	7 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	T8T	A	800	4	-	4/19/34/34	0/3/3/3
2	T8T	A	700	-	-	5/19/34/34	0/3/3/3
2	T8T	C	900	4	-	7/19/34/34	0/3/3/3
2	T8T	B	800	4	-	3/19/34/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	T8T	D	800	4	-	1/19/34/34	0/3/3/3
2	T8T	B	700	-	-	6/19/34/34	0/3/3/3
2	T8T	C	700	-	-	3/19/34/34	0/3/3/3
2	T8T	D	700	-	-	5/19/34/34	0/3/3/3
2	T8T	B	900	4	-	3/19/34/34	0/3/3/3
2	T8T	D	900	4	-	4/19/34/34	0/3/3/3
2	T8T	A	900	4	-	5/19/34/34	0/3/3/3
2	T8T	C	800	4	-	2/19/34/34	0/3/3/3

The worst 5 of 63 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	T8T	C4-N9	-9.42	1.27	1.37
2	D	800	T8T	C4-N9	-8.09	1.28	1.37
2	C	900	T8T	C4-N9	-7.90	1.29	1.37
2	C	700	T8T	C4-N9	-7.49	1.29	1.37
2	D	700	T8T	C4-N9	-7.20	1.29	1.37

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	T8T	C5-C4-N9	6.35	109.19	106.25
2	A	700	T8T	C5-C4-N9	-4.81	104.02	106.25
2	A	800	T8T	O6-C6-N1	4.76	128.29	120.27
2	D	800	T8T	C5-C4-N9	4.58	108.36	106.25
2	A	800	T8T	C5-C4-N9	4.42	108.29	106.25

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

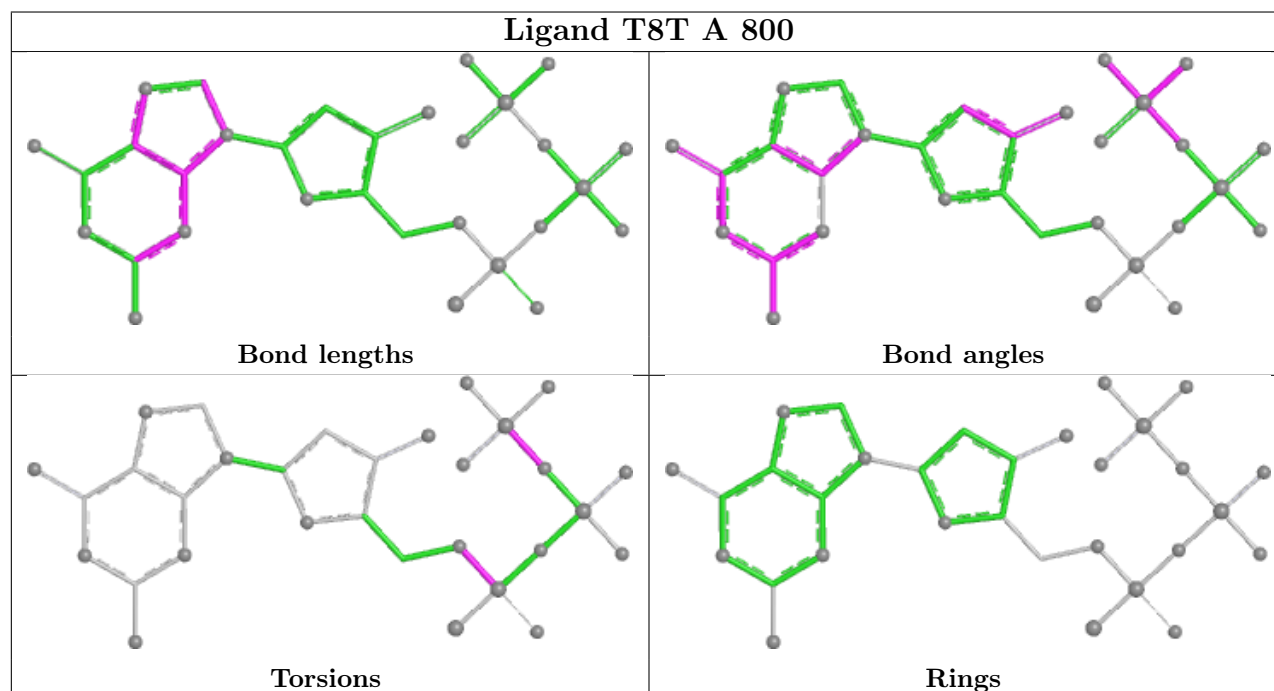
Mol	Chain	Res	Type	Atoms
2	B	700	T8T	O4'-C4'-C5'-O5'
2	B	700	T8T	C4'-C5'-O5'-PA
2	C	900	T8T	PB-O3B-PG-O1G
2	C	900	T8T	PB-O3B-PG-O2G
2	D	700	T8T	C5'-O5'-PA-O3A

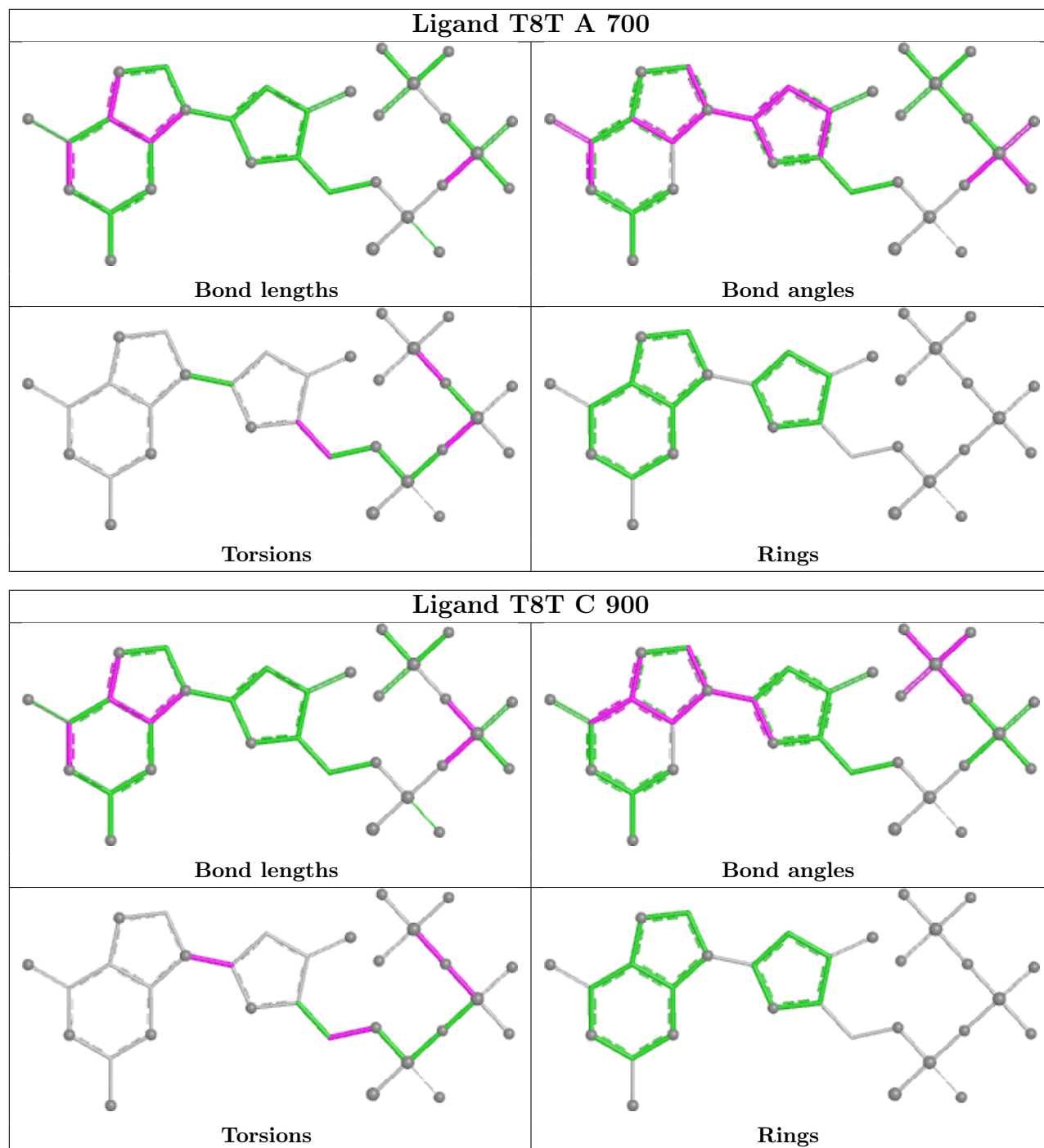
There are no ring outliers.

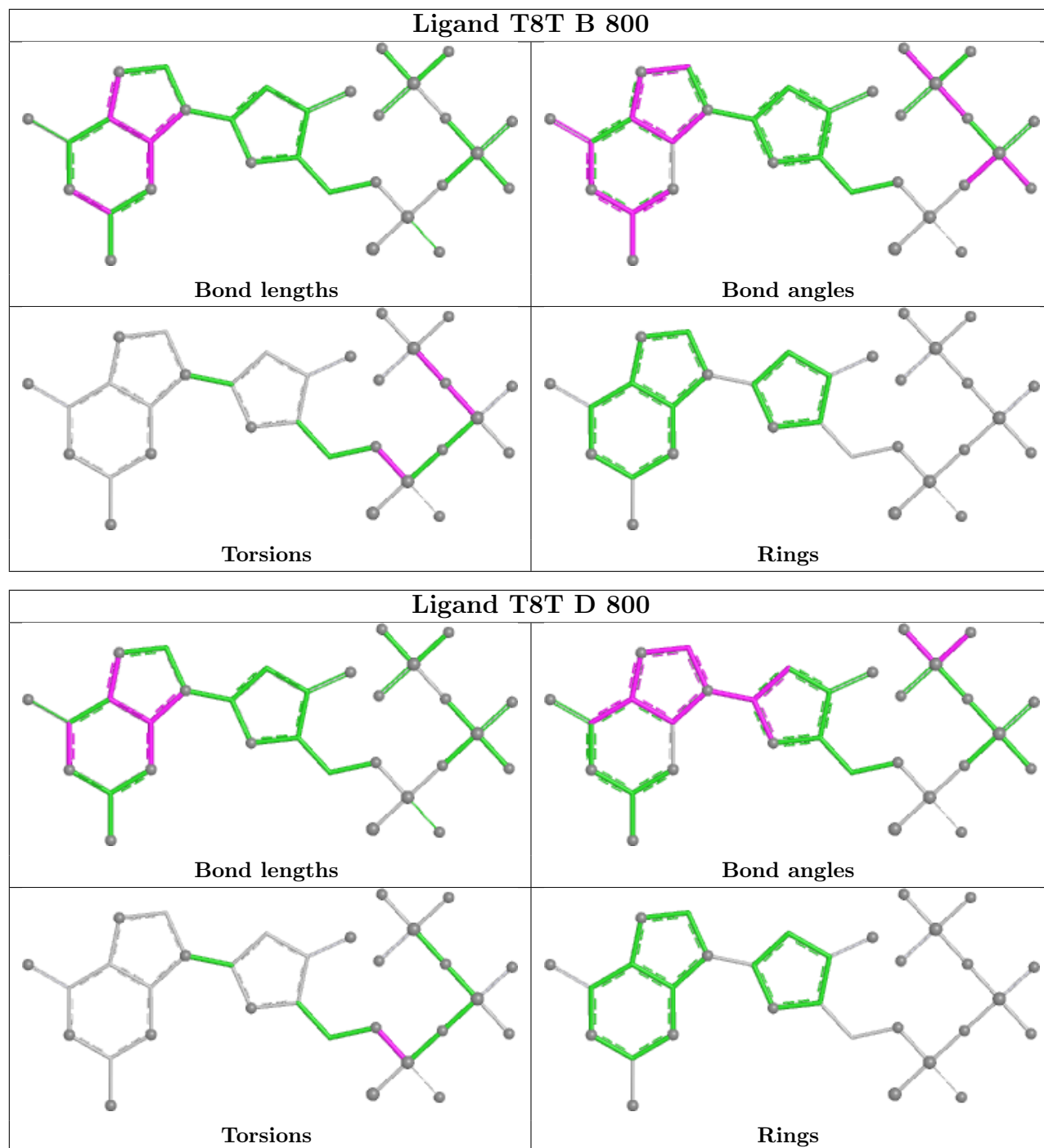
11 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	700	T8T	2	0
2	C	900	T8T	5	0
2	B	800	T8T	3	0
2	D	800	T8T	2	0
2	B	700	T8T	1	0
2	C	700	T8T	3	0
2	D	700	T8T	4	0
2	B	900	T8T	1	0
2	D	900	T8T	1	0
2	A	900	T8T	1	0
2	C	800	T8T	4	0

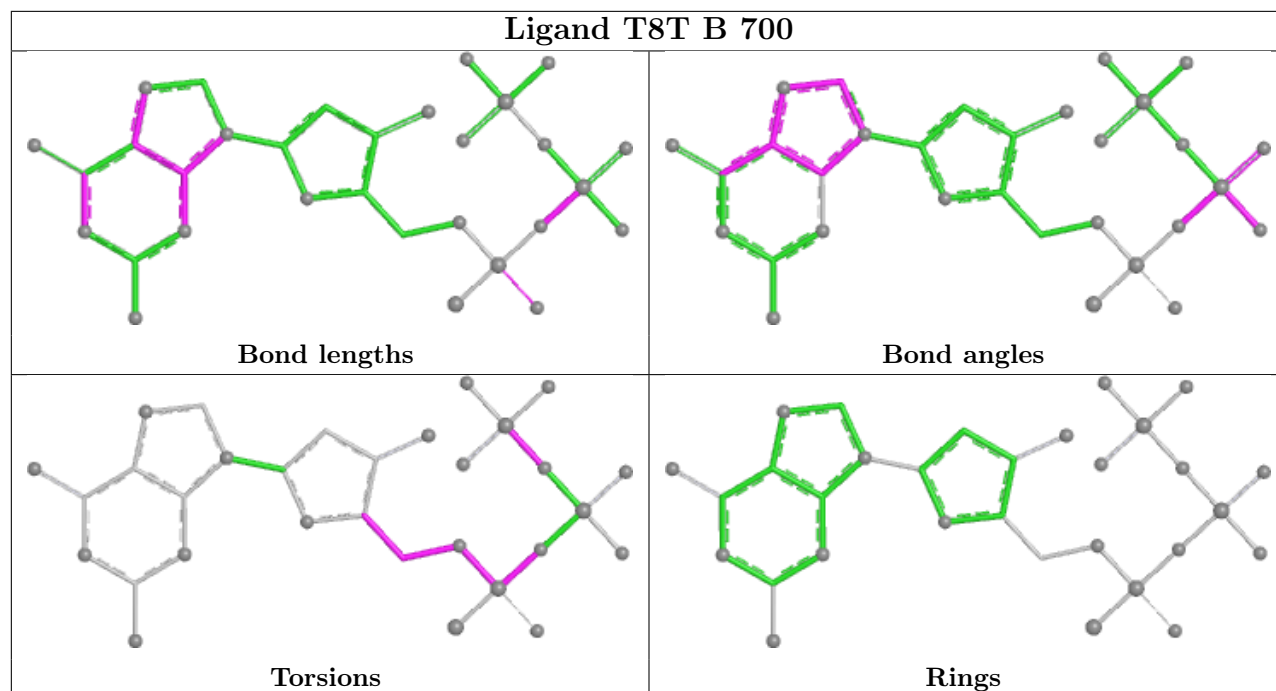
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



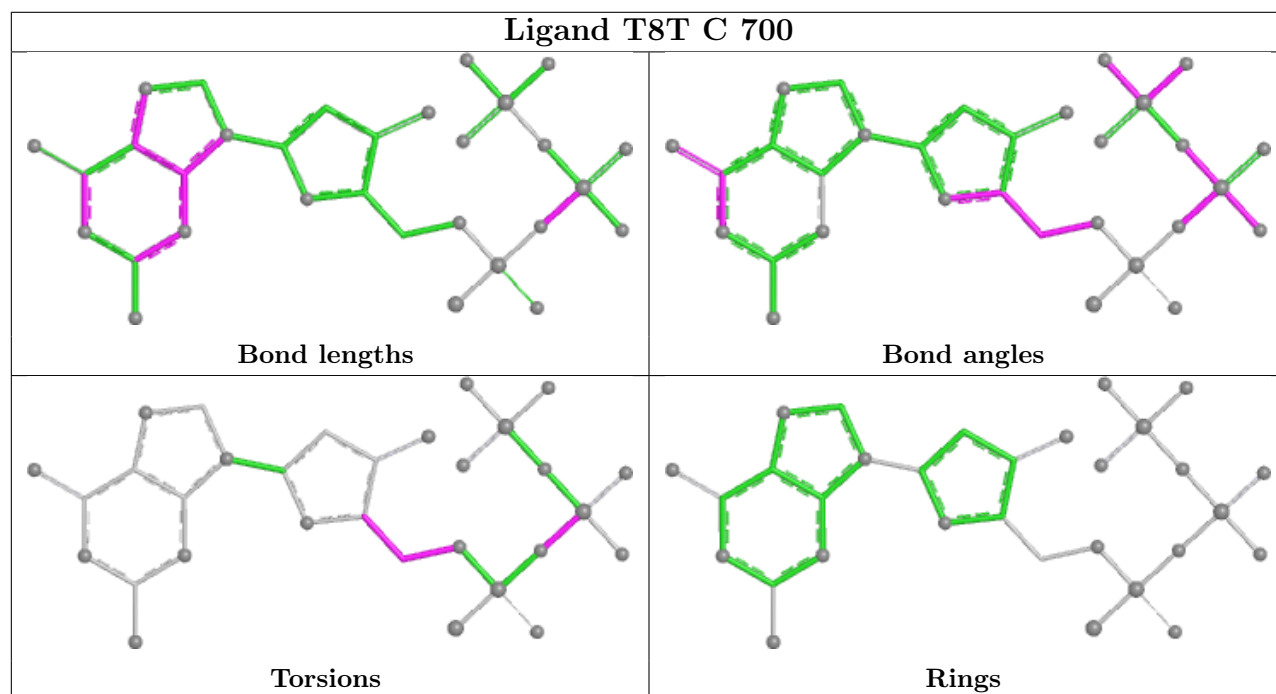




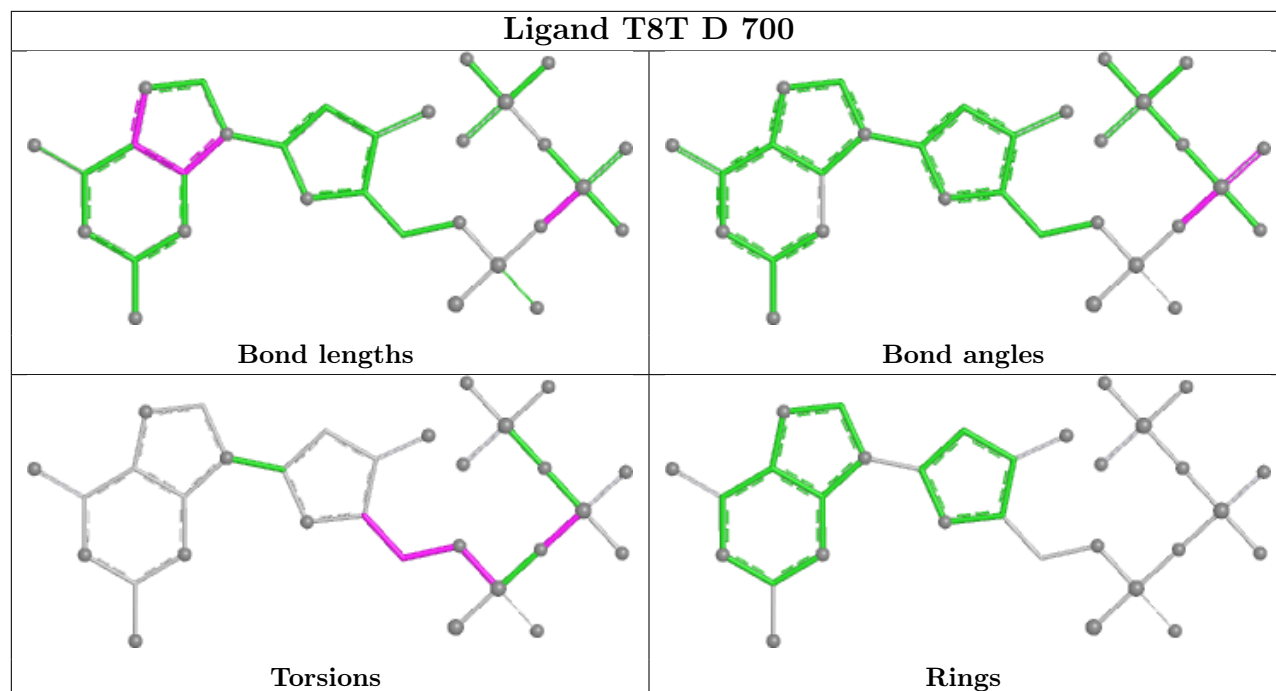
Ligand T8T B 700



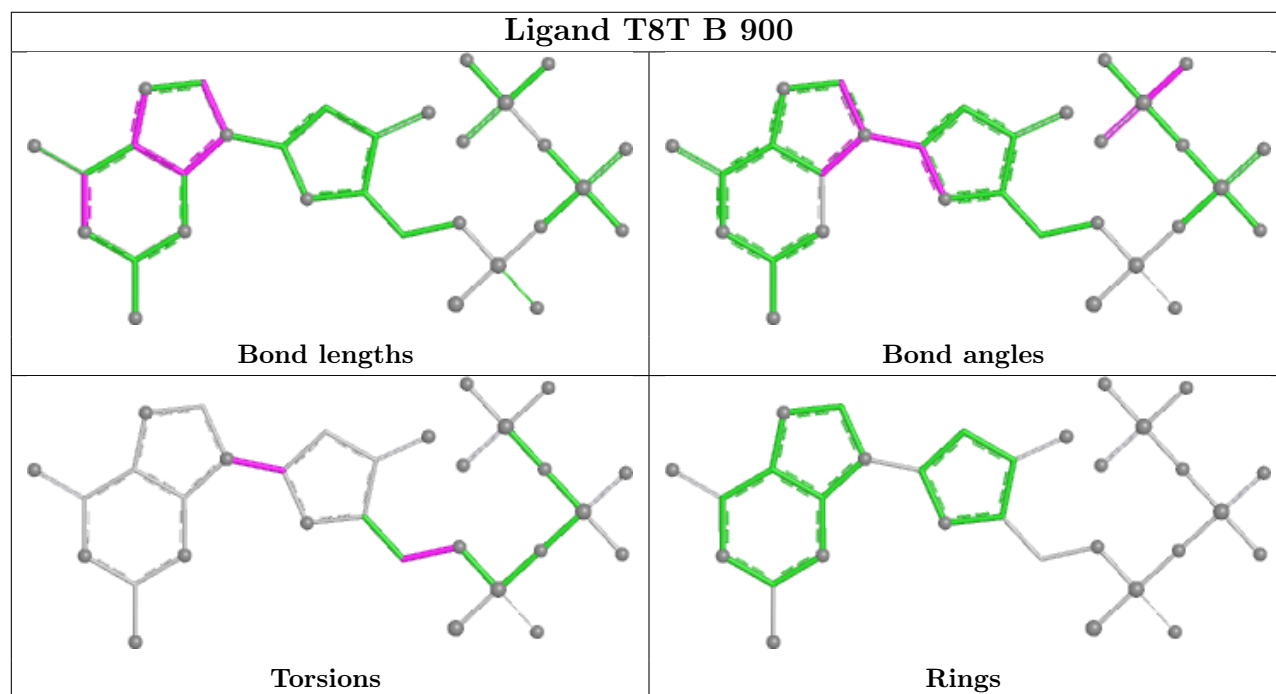
Ligand T8T C 700



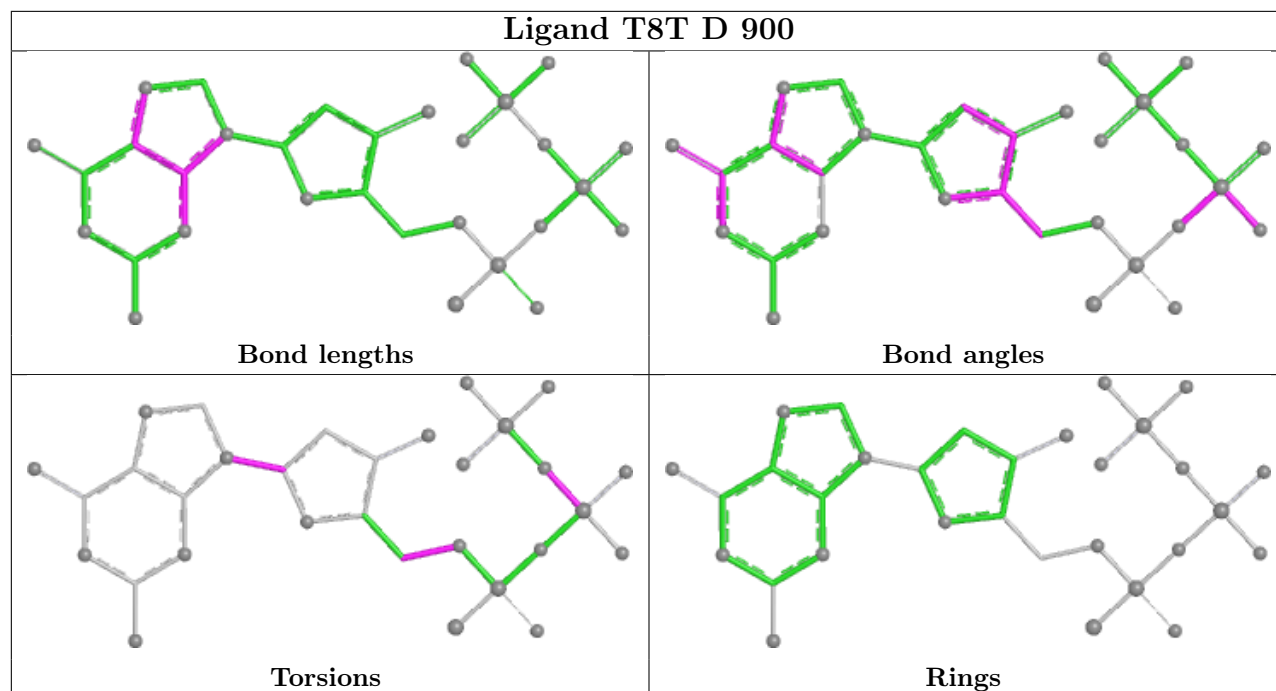
Ligand T8T D 700



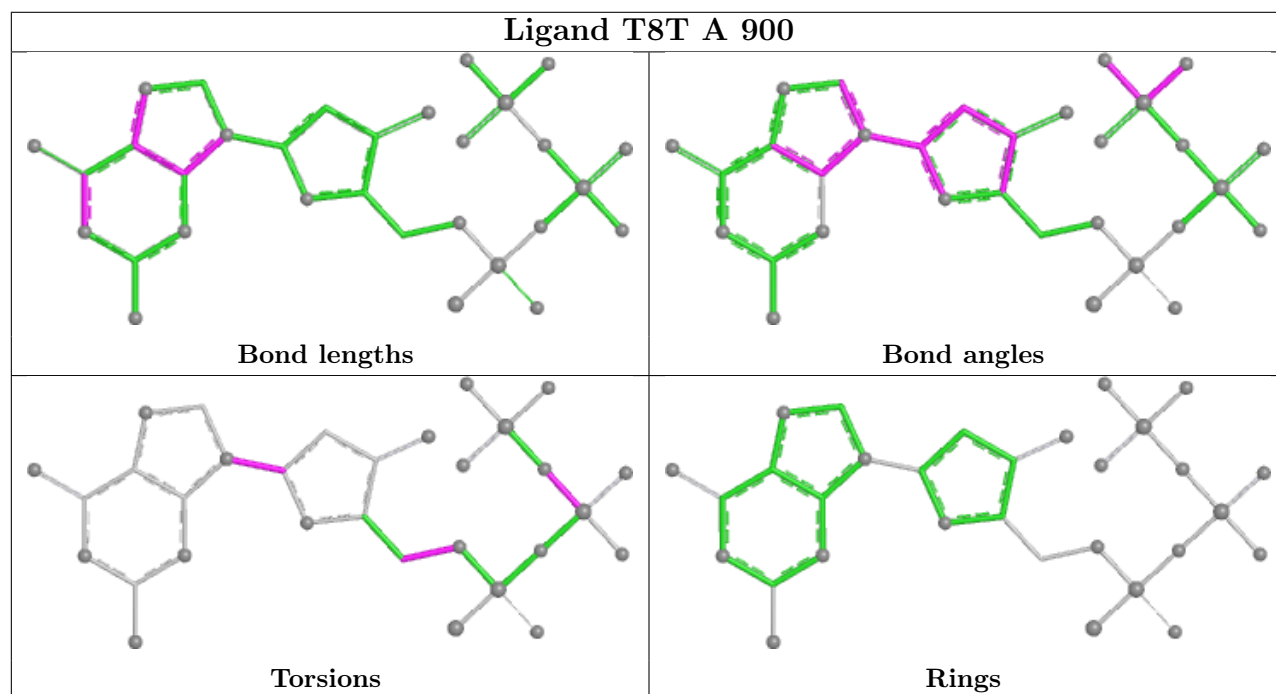
Ligand T8T B 900

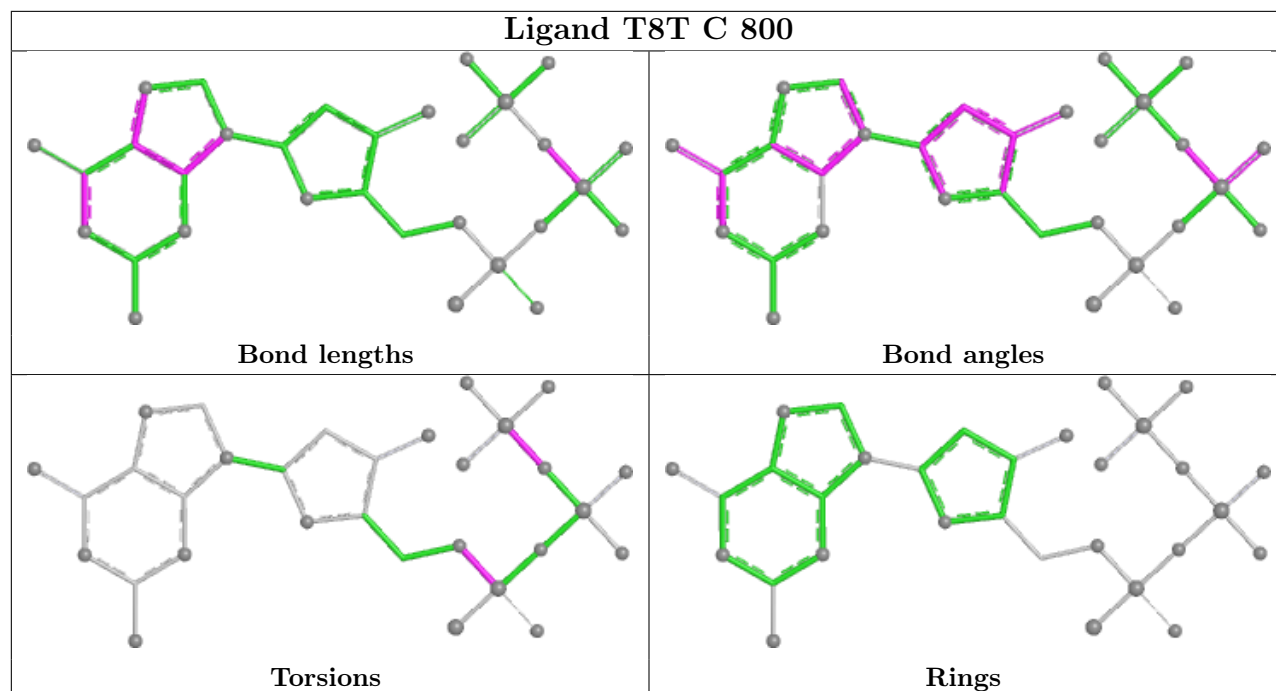


Ligand T8T D 900



Ligand T8T A 900





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	476/550 (86%)	-0.07	0 100 100	29, 53, 94, 127	0
1	B	477/550 (86%)	0.05	3 (0%) 85 81	40, 76, 117, 137	0
1	C	481/550 (87%)	-0.17	0 100 100	28, 56, 102, 140	0
1	D	470/550 (85%)	0.04	3 (0%) 85 81	39, 73, 108, 140	0
All	All	1904/2200 (86%)	-0.04	6 (0%) 90 87	28, 65, 107, 140	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	412	ALA	2.8
1	D	400	THR	2.6
1	D	331	TYR	2.3
1	B	575	ASP	2.2
1	B	414	ASP	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 [i](#)

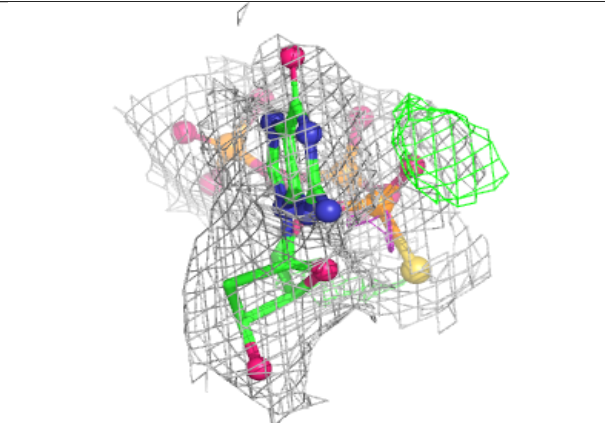
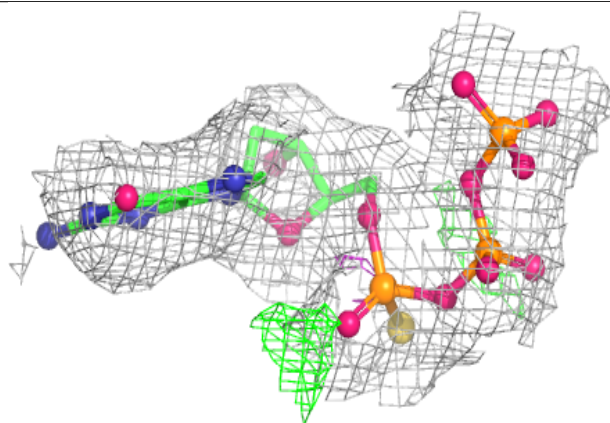
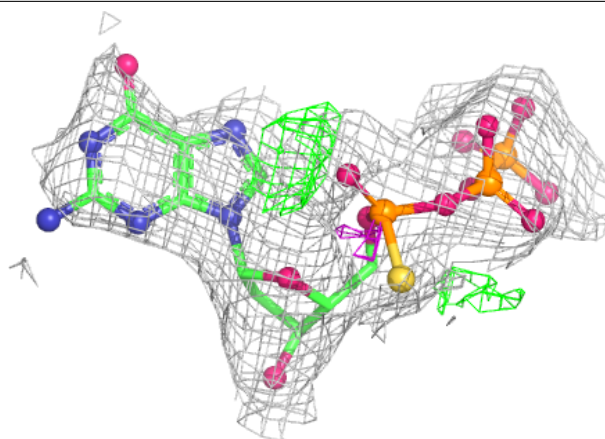
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	T8T	B	700	31/31	0.90	0.08	59,69,80,85	0
2	T8T	A	700	31/31	0.94	0.06	36,41,62,73	0
2	T8T	D	700	31/31	0.94	0.08	63,72,80,88	0
2	T8T	C	700	31/31	0.96	0.06	42,46,51,59	0
2	T8T	D	800	31/31	0.97	0.05	39,43,49,55	0
2	T8T	A	900	31/31	0.98	0.04	27,29,31,31	0
2	T8T	C	900	31/31	0.98	0.04	36,39,41,42	0
2	T8T	B	800	31/31	0.98	0.04	37,40,48,48	0
2	T8T	B	900	31/31	0.98	0.05	36,40,46,47	0
2	T8T	D	900	31/31	0.98	0.04	36,38,42,43	0
4	MG	B	950	1/1	0.98	0.07	36,36,36,36	0
4	MG	C	950	1/1	0.98	0.04	28,28,28,28	0
3	MN	B	750	1/1	0.99	0.02	51,51,51,51	0
2	T8T	A	800	31/31	0.99	0.04	23,24,25,26	0
2	T8T	C	800	31/31	0.99	0.04	30,32,36,37	0
4	MG	D	950	1/1	0.99	0.02	34,34,34,34	0
4	MG	A	950	1/1	1.00	0.01	25,25,25,25	0
3	MN	A	750	1/1	1.00	0.05	25,25,25,25	0
3	MN	C	750	1/1	1.00	0.03	25,25,25,25	0
3	MN	D	750	1/1	1.00	0.04	43,43,43,43	0

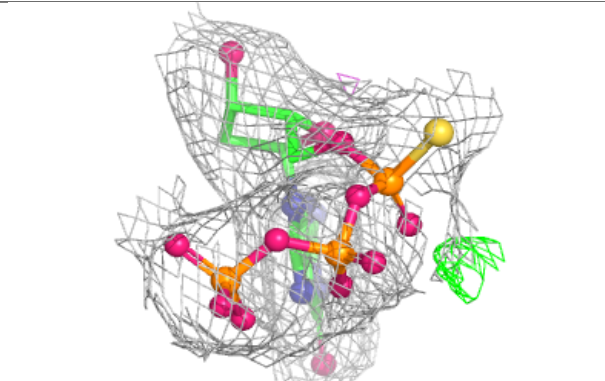
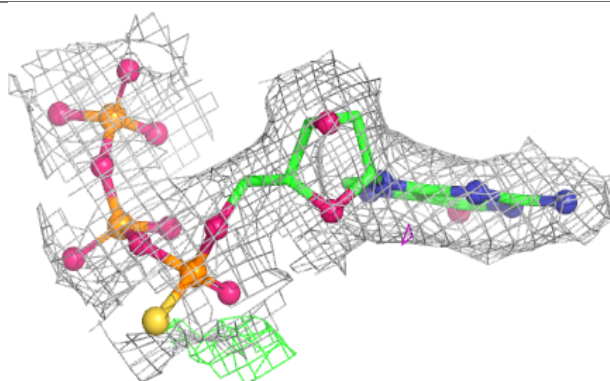
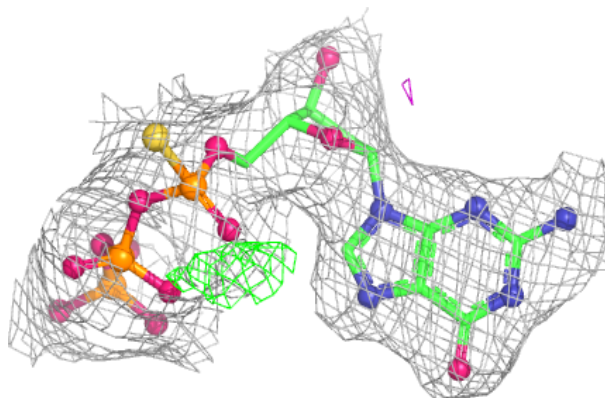
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around T8T B 700:

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

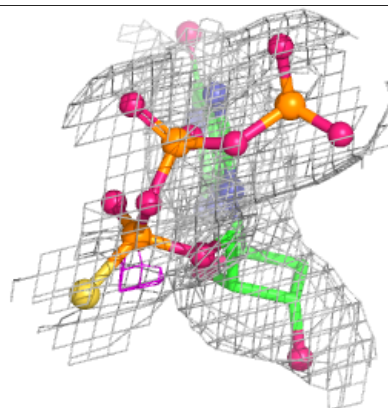
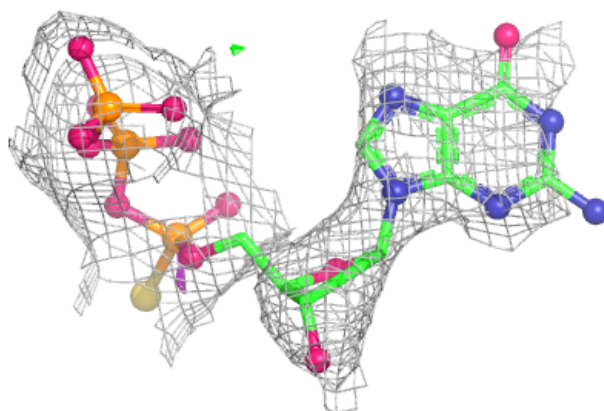
**Electron density around T8T A 700:**

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and green (positive)

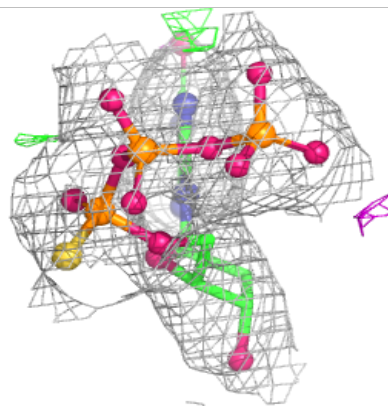
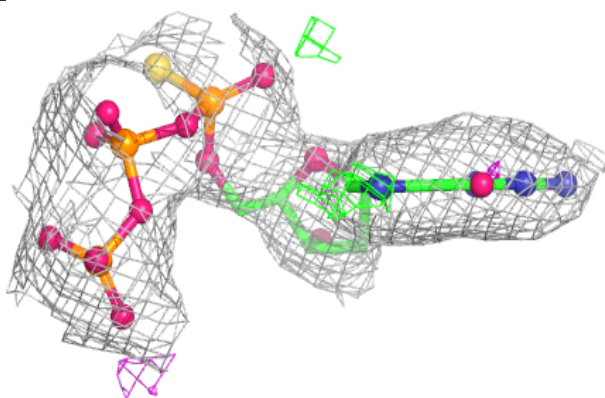
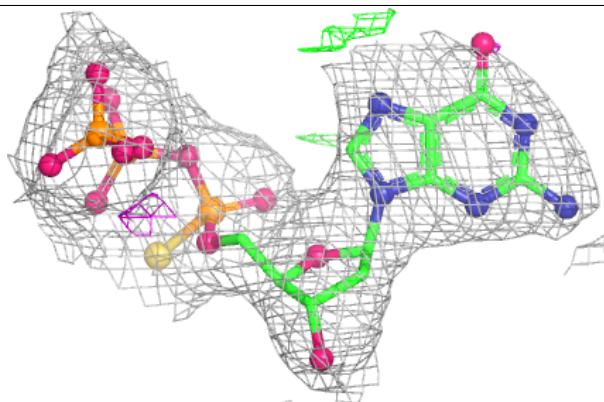


Electron density around T8T D 700:

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

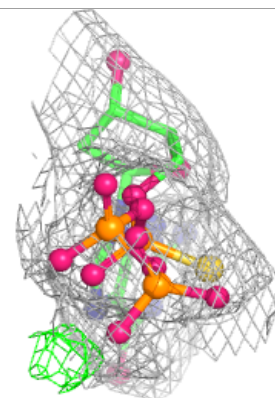
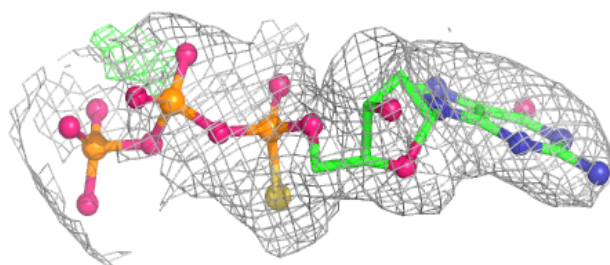
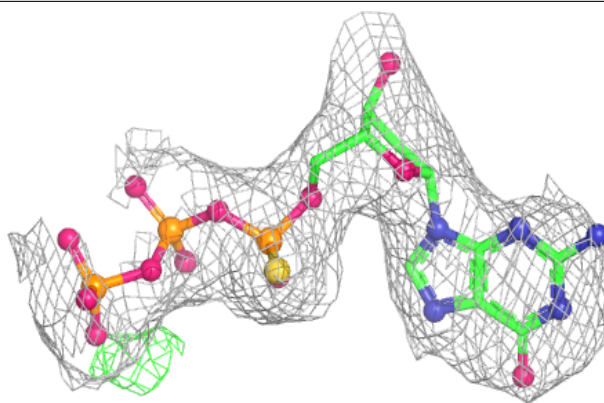
**Electron density around T8T C 700:**

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and green (positive)

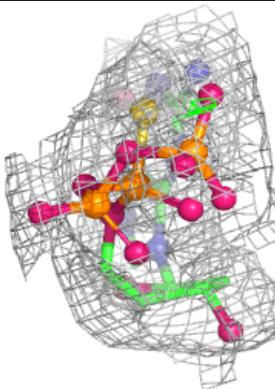
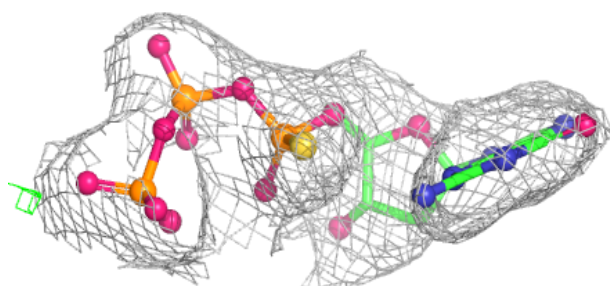
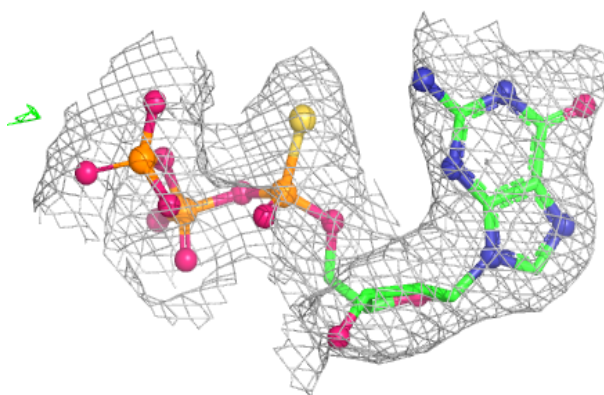


Electron density around T8T D 800:

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and green (positive)

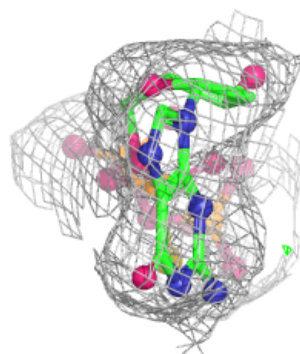
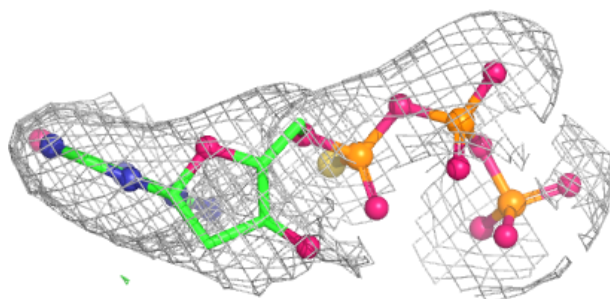
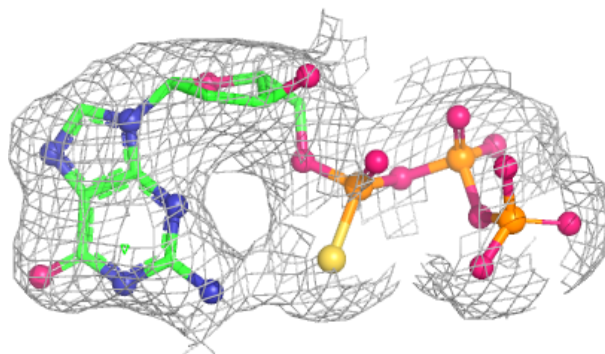
**Electron density around T8T A 900:**

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and green (positive)

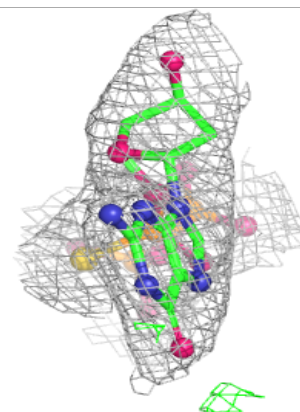
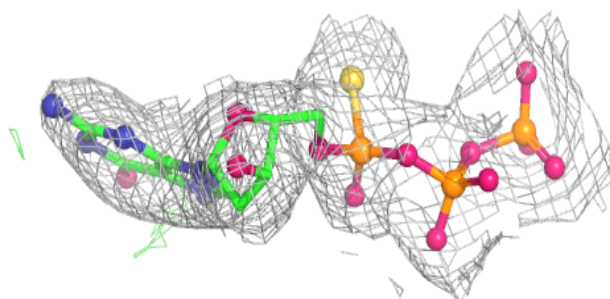
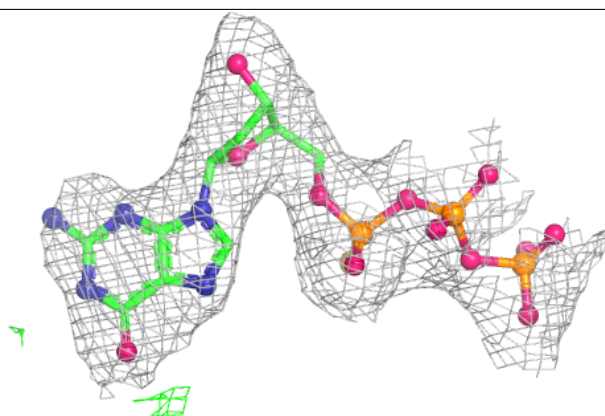


Electron density around T8T C 900:

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and green (positive)

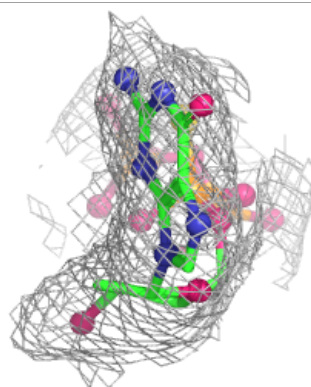
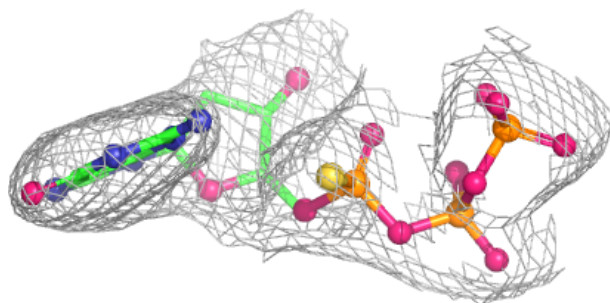
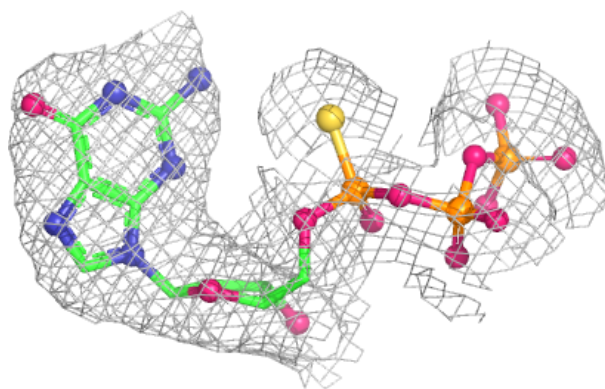
**Electron density around T8T B 800:**

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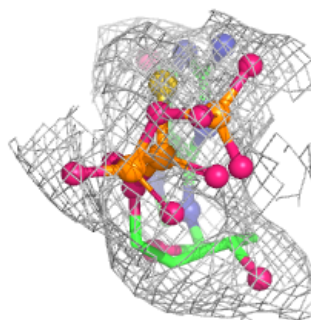
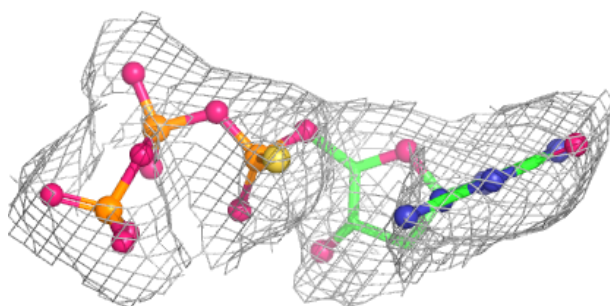
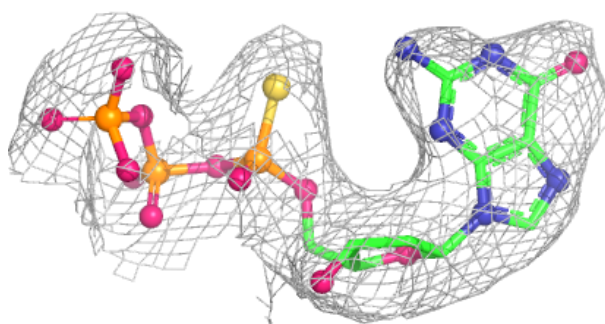


Electron density around T8T B 900:

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

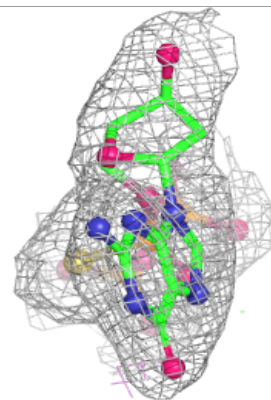
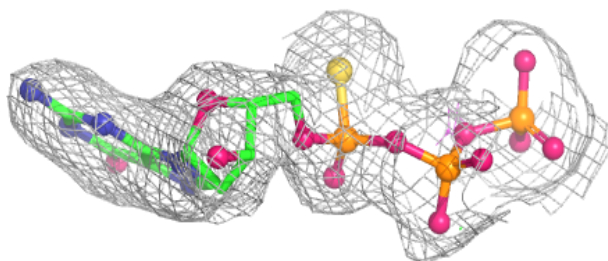
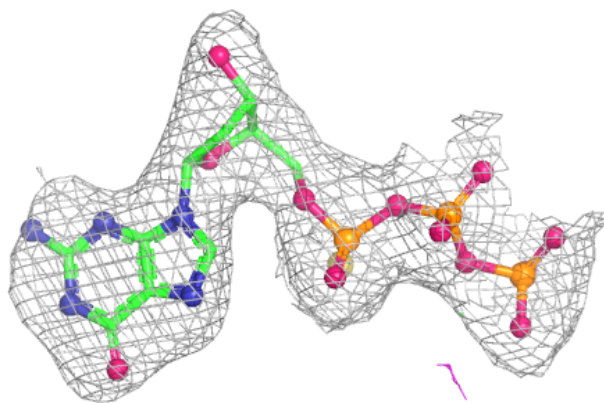
**Electron density around T8T D 900:**

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

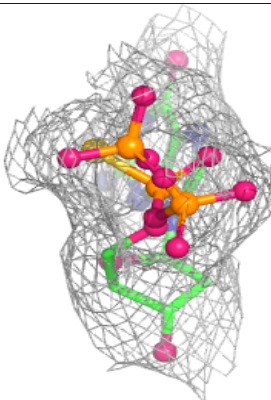
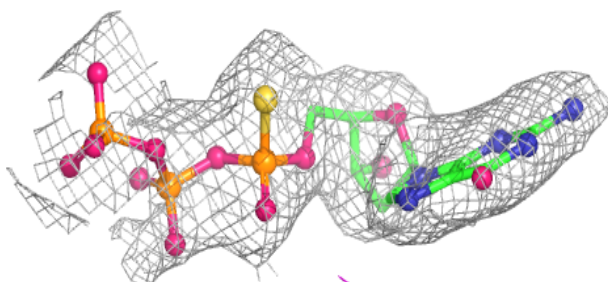
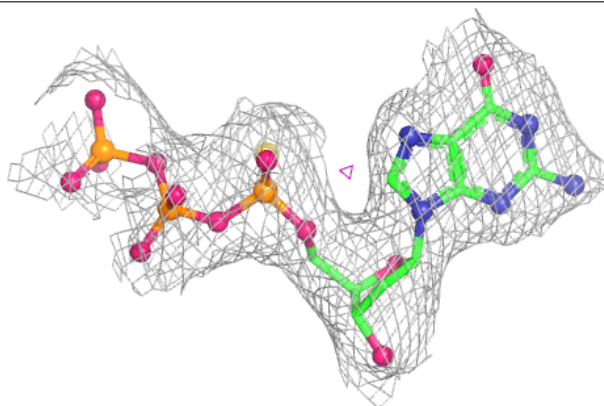


Electron density around T8T A 800:

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

**Electron density around T8T C 800:**

$2mF_o-DF_c$ (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.