



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 06:01 am BST

PDB ID : 4QFZ  
Title : Crystal structure of the tetrameric dGTP/dTTP-bound SAMHD1 (RN206) mutant catalytic core  
Authors : Koharudin, L.M.I.; Wu, Y.; DeLucia, M.; Mehrens, J.; Gronenborn, A.M.; Ahn, J.  
Deposited on : 2014-05-22  
Resolution : 2.30 Å(reported)

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

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

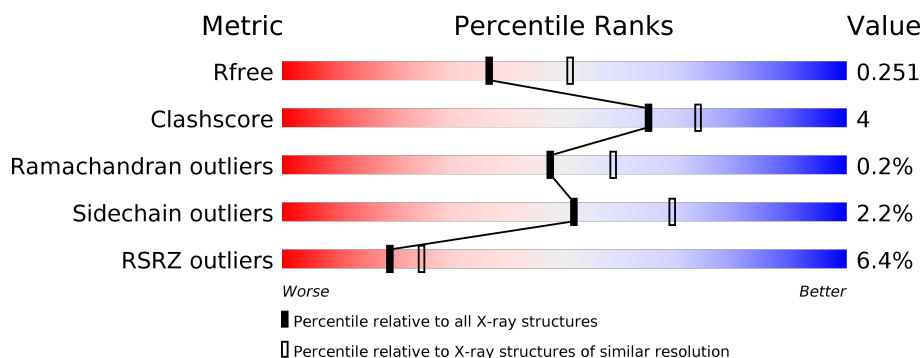
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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	550	<div> <div>7%</div> <div> <div></div> <div>79%</div> <div>8%</div> <div>13%</div> </div> </div>
1	B	550	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>9%</div> <div>13%</div> </div> </div>
1	C	550	<div> <div>7%</div> <div> <div></div> <div>74%</div> <div>12%</div> <div>13%</div> </div> </div>
1	D	550	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>8%</div> <div>13%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16390 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	1	0
			3938	2520	686	712	20			
1	B	481	Total	C	N	O	S	0	3	0
			3957	2531	691	715	20			
1	C	481	Total	C	N	O	S	0	0	0
			3933	2517	685	711	20			
1	D	481	Total	C	N	O	S	0	5	0
			3970	2541	694	715	20			

There are 152 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
A	97	MET	-	EXPRESSION TAG	UNP Q9Y3Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
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
A	206	ARG	HIS	ENGINEERED MUTATION	UNP Q9Y3Z3
A	207	ASN	ASP	ENGINEERED MUTATION	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	102	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
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
B	206	ARG	HIS	ENGINEERED MUTATION	UNP Q9Y3Z3
B	207	ASN	ASP	ENGINEERED MUTATION	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

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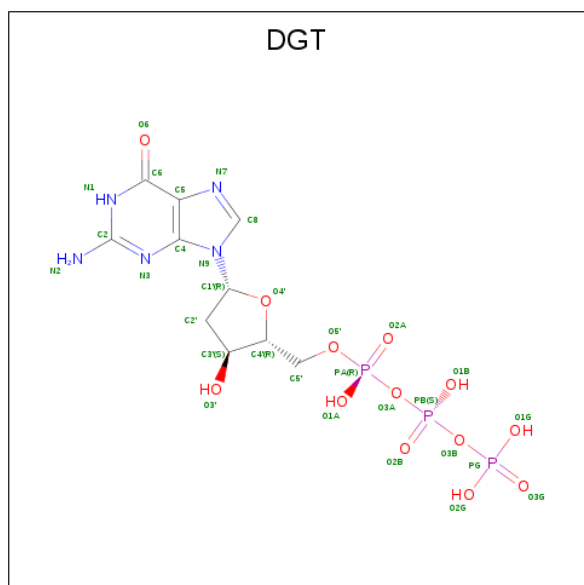
Chain	Residue	Modelled	Actual	Comment	Reference
C	106	MET	-	EXPRESSION TAG	UNP Q9Y3Z3
C	107	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
C	108	ARG	-	EXPRESSION TAG	UNP Q9Y3Z3
C	109	ASP	-	EXPRESSION TAG	UNP Q9Y3Z3
C	110	PRO	-	EXPRESSION TAG	UNP Q9Y3Z3
C	111	ASN	-	EXPRESSION TAG	UNP Q9Y3Z3
C	112	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
C	206	ARG	HIS	ENGINEERED MUTATION	UNP Q9Y3Z3
C	207	ASN	ASP	ENGINEERED MUTATION	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

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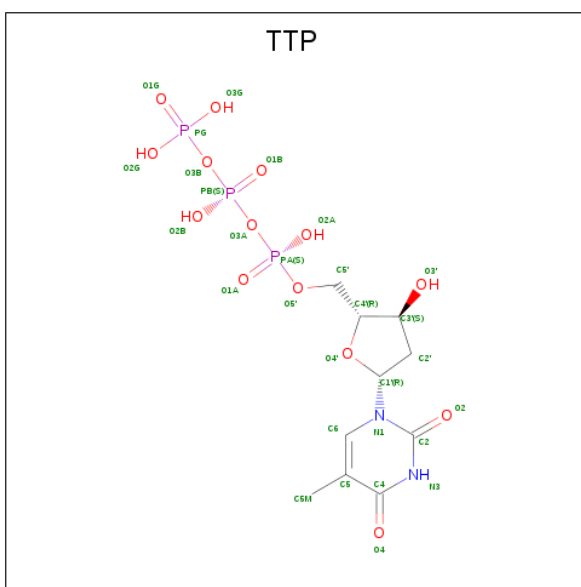
Chain	Residue	Modelled	Actual	Comment	Reference
D	110	PRO	-	EXPRESSION TAG	UNP Q9Y3Z3
D	111	ASN	-	EXPRESSION TAG	UNP Q9Y3Z3
D	112	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
D	206	ARG	HIS	ENGINEERED MUTATION	UNP Q9Y3Z3
D	207	ASN	ASP	ENGINEERED MUTATION	UNP Q9Y3Z3

- Molecule 2 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula:  $C_{10}H_{17}N_2O_{14}P_3$ ).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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



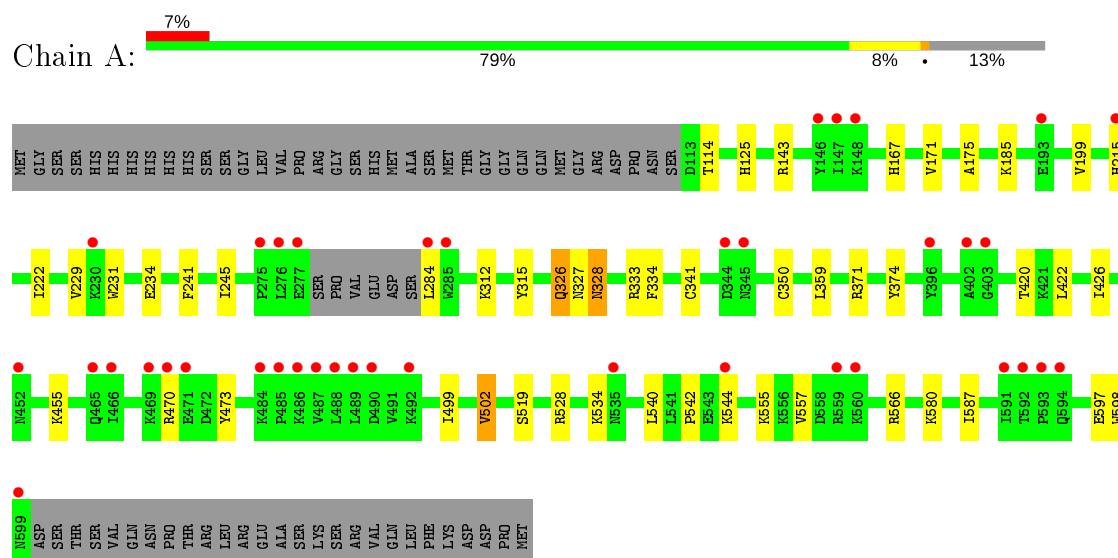
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	40	Total 40	O 40	0	0
5	B	62	Total 62	O 62	0	0
5	C	52	Total 52	O 52	0	0
5	D	73	Total 73	O 73	0	0

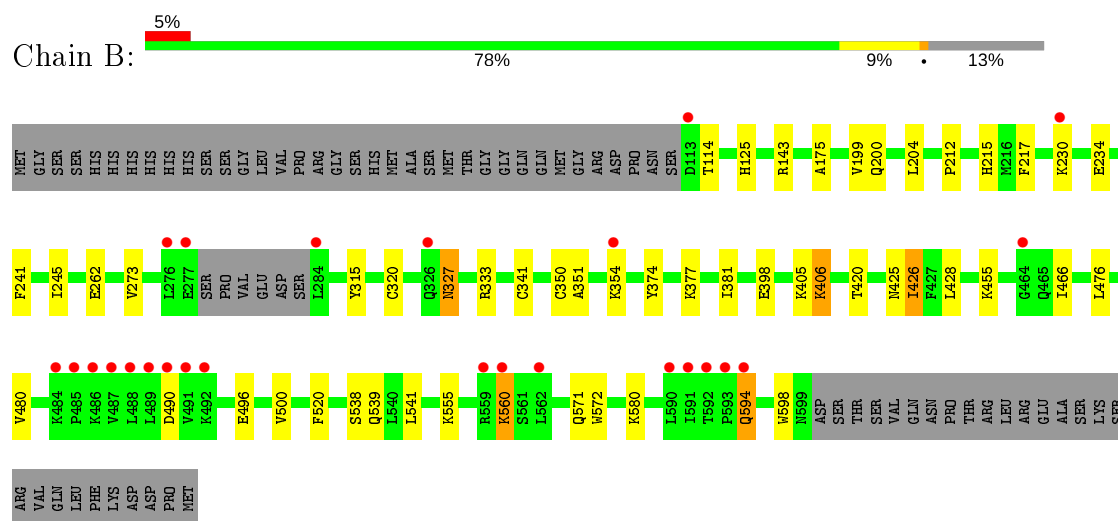
### 3 Residue-property plots [i](#)

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: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

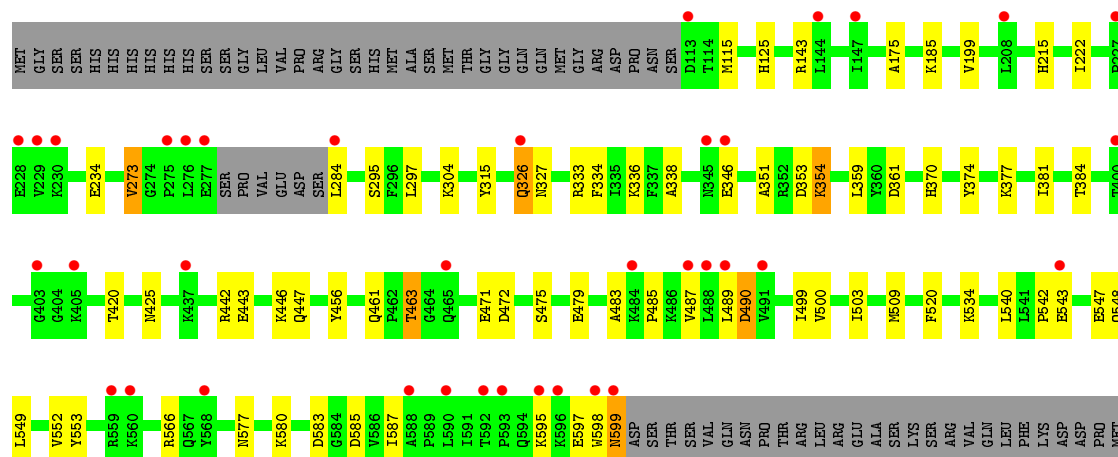


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

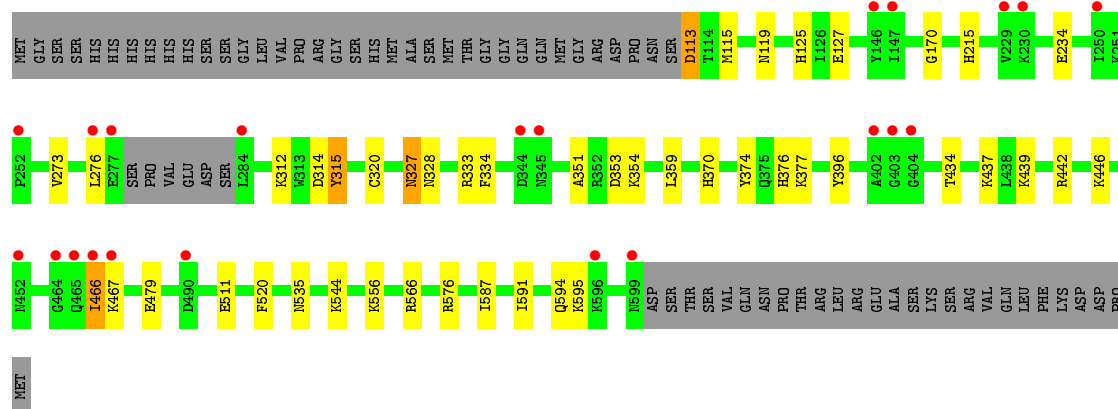
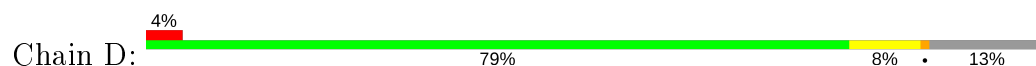


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.83Å 146.74Å 98.94Å 90.00° 114.29° 90.00°	Depositor
Resolution (Å)	33.98 – 2.30 33.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (33.98-2.30) 99.8 (33.98-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.209 , 0.250 0.210 , 0.251	Depositor DCC
$R_{free}$ test set	2013 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.4	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.20 , 34.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.003 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16390	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: MG, TTP, DGT

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	0.29	0/4033	0.47	0/5444
1	B	0.31	0/4053	0.48	0/5471
1	C	0.29	0/4025	0.46	0/5433
1	D	0.31	0/4072	0.48	0/5496
All	All	0.30	0/16183	0.47	0/21844

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	3938	0	3927	36	0
1	B	3957	0	3941	33	0
1	C	3933	0	3921	48	0
1	D	3970	0	3965	27	0
2	A	31	0	12	0	0
2	C	62	0	24	0	0
2	D	31	0	12	0	0
3	A	58	0	26	3	0
3	B	58	0	26	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	58	0	26	4	0
3	D	58	0	26	3	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	3	0	0	0	0
5	A	40	0	0	0	0
5	B	62	0	0	0	0
5	C	52	0	0	0	0
5	D	73	0	0	0	0
All	All	16390	0	15906	131	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 4.

All (131) 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:C:566:ARG:HD3	1:C:587:ILE:HB	1.70	0.73
1:A:215:HIS:NE2	3:A:702:TTP:O1A	2.20	0.72
1:B:320:CYS:SG	1:B:327[B]:ASN:HB2	2.32	0.69
1:B:425:ASN:ND2	1:C:425:ASN:OD1	2.27	0.68
1:B:490:ASP:OD2	1:B:560:LYS:NZ	2.26	0.67
1:D:113:ASP:OD1	1:D:113:ASP:N	2.28	0.66
1:A:371:ARG:NH2	1:C:361:ASP:OD1	2.29	0.64
1:B:476:LEU:HD23	1:B:500:VAL:HG11	1.78	0.64
1:C:490:ASP:N	1:C:490:ASP:OD1	2.24	0.64
1:C:215:HIS:NE2	3:C:704:TTP:O2A	2.28	0.62
1:B:398:GLU:OE1	1:B:406:LYS:NZ	2.33	0.61
1:A:534:LYS:NZ	1:A:542:PRO:O	2.24	0.61
1:C:185:LYS:NZ	1:C:338:ALA:O	2.23	0.60
3:C:701:TTP:H6	1:D:119:ASN:HD22	1.50	0.59
1:B:354:LYS:NZ	3:B:702:TTP:O3B	2.36	0.59
1:B:215[A]:HIS:HE2	3:B:701:TTP:PA	2.26	0.58
1:B:215[A]:HIS:NE2	3:B:701:TTP:O2A	2.37	0.57
1:D:320:CYS:SG	1:D:327:ASN:HB2	2.45	0.57
1:A:528:ARG:NH1	1:C:585:ASP:O	2.37	0.56
1:C:234:GLU:N	1:C:234:GLU:OE1	2.34	0.55
1:D:566:ARG:HD3	1:D:587:ILE:HB	1.88	0.55
1:C:534:LYS:NZ	1:C:543:GLU:OE2	2.39	0.54
1:C:374:TYR:O	3:C:704:TTP:HM52	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215[A]:HIS:HE2	3:D:703:TTP:PA	2.31	0.53
1:B:374:TYR:O	3:B:701:TTP:HM52	2.09	0.53
1:C:336:LYS:HE3	1:D:127:GLU:HG3	1.90	0.53
1:A:566:ARG:HD3	1:A:587:ILE:HB	1.91	0.52
1:A:312:LYS:HA	1:A:315:TYR:CE2	2.45	0.52
1:B:580:LYS:HB2	1:B:598:TRP:CD2	2.45	0.51
1:D:479:GLU:OE1	1:D:576:ARG:NH1	2.43	0.51
1:D:374:TYR:O	3:D:703:TTP:HM52	2.10	0.51
1:D:591:ILE:O	1:D:594:GLN:HG2	2.11	0.51
1:C:125:HIS:CE1	1:D:333:ARG:HB2	2.46	0.51
1:C:334:PHE:CE2	1:C:359:LEU:HD21	2.45	0.51
1:A:125:HIS:CE1	1:B:333:ARG:HB2	2.45	0.51
1:C:461:GLN:NE2	1:C:547:GLU:OE1	2.44	0.51
1:A:341:CYS:HB2	1:A:350:CYS:SG	2.51	0.50
1:C:215:HIS:HE2	3:C:704:TTP:PA	2.35	0.50
1:B:538:SER:HB3	1:B:541:LEU:HG	1.94	0.50
1:B:539:GLN:HG2	1:D:544:LYS:NZ	2.27	0.49
1:B:466:ILE:HD12	1:B:466:ILE:H	1.76	0.49
1:D:466:ILE:HG13	1:D:467:LYS:N	2.28	0.49
1:A:333:ARG:HB2	1:B:125:HIS:CE1	2.47	0.49
1:C:483:ALA:O	1:C:485:PRO:HD3	2.13	0.48
1:B:455:LYS:HA	1:B:455:LYS:HE2	1.94	0.48
1:C:463:THR:OG1	1:C:577:ASN:O	2.28	0.48
1:C:475:SER:O	1:C:479:GLU:HG3	2.14	0.48
1:A:215:HIS:HE2	3:A:702:TTP:PA	2.37	0.48
1:D:594:GLN:HG3	1:D:595:LYS:N	2.28	0.47
1:A:455:LYS:HG2	1:A:557:VAL:HG12	1.96	0.47
1:C:175:ALA:HB1	1:C:199:VAL:HG12	1.95	0.47
1:A:422:LEU:HD11	1:A:426:ILE:HD11	1.97	0.47
1:C:500:VAL:HG22	1:C:552:VAL:HG22	1.96	0.47
1:A:222:ILE:HG21	1:A:231:TRP:HB3	1.96	0.47
1:C:333:ARG:HB2	1:D:125:HIS:CE1	2.50	0.47
1:C:442:ARG:HG2	1:C:446:LYS:HE2	1.95	0.47
1:C:599:ASN:ND2	1:C:599:ASN:O	2.46	0.46
1:C:353:ASP:OD1	1:C:354:LYS:N	2.47	0.46
1:D:234:GLU:HB3	1:D:273:VAL:HG23	1.97	0.46
1:A:374:TYR:O	3:A:702:TTP:HM52	2.16	0.45
1:B:341:CYS:HB2	1:B:350:CYS:SG	2.57	0.45
1:B:351:ALA:O	1:B:520:PHE:HA	2.16	0.45
1:C:359:LEU:HD23	1:C:359:LEU:HA	1.74	0.45
1:D:170:GLY:HA3	1:D:314:ASP:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:PRO:HB2	1:A:544:LYS:O	2.17	0.45
1:C:503:ILE:HB	1:C:549:LEU:HB2	1.99	0.45
1:C:580:LYS:HB2	1:C:598:TRP:CD2	2.52	0.44
1:B:143:ARG:HD2	1:B:420:THR:HA	1.99	0.44
1:A:422:LEU:CD1	1:A:426:ILE:HD11	2.47	0.44
1:B:381:ILE:HA	1:B:381:ILE:HD12	1.79	0.44
1:C:461:GLN:HG2	1:C:548:GLN:O	2.17	0.44
1:A:470:ARG:HG3	1:A:473:TYR:CE2	2.53	0.44
1:D:215[A]:HIS:NE2	3:D:703:TTP:O2A	2.50	0.44
1:B:571:GLN:HE22	1:B:594:GLN:HE22	1.65	0.44
1:D:353:ASP:OD1	1:D:354:LYS:N	2.48	0.44
1:A:542:PRO:HB3	1:C:540:LEU:O	2.18	0.44
1:A:167:HIS:O	1:A:171:VAL:HG23	2.18	0.43
1:A:175:ALA:HB1	1:A:199:VAL:HG12	1.99	0.43
1:A:185:LYS:HD3	1:A:185:LYS:HA	1.80	0.43
1:A:326:GLN:HG2	1:C:327:ASN:O	2.17	0.43
1:C:234:GLU:HB3	1:C:273:VAL:HG23	1.99	0.43
1:A:326:GLN:CD	1:C:326:GLN:HG2	2.39	0.43
1:A:234:GLU:N	1:A:234:GLU:OE1	2.48	0.43
1:A:326:GLN:HG3	1:A:327:ASN:N	2.31	0.43
1:B:175:ALA:HB1	1:B:199:VAL:HG12	2.00	0.43
1:D:442:ARG:HG2	1:D:446:LYS:HE2	2.00	0.43
1:B:496:GLU:O	1:B:555:LYS:HD2	2.19	0.43
1:C:351:ALA:O	1:C:520:PHE:HA	2.19	0.43
1:A:359:LEU:HD23	1:A:359:LEU:HA	1.87	0.43
1:A:540:LEU:O	1:C:542:PRO:HB3	2.18	0.43
1:B:200:GLN:O	1:B:204:LEU:HB2	2.19	0.43
1:C:295:SER:OG	1:C:346:GLU:OE1	2.33	0.43
1:C:370:HIS:HA	1:C:374:TYR:HB2	2.01	0.43
1:C:384:THR:HG21	1:C:499:ILE:HD13	2.01	0.43
1:D:396:TYR:CE1	1:D:437:LYS:HE2	2.53	0.43
1:A:580:LYS:HD2	1:A:598:TRP:HB3	2.01	0.42
1:B:405:LYS:HD2	1:B:406:LYS:H	1.84	0.42
1:B:480:VAL:HG22	1:B:572:TRP:CD2	2.55	0.42
1:A:143:ARG:HD2	1:A:420:THR:HA	2.01	0.42
1:C:143:ARG:HD2	1:C:420:THR:HA	2.02	0.42
1:C:509:MET:HB3	1:C:509:MET:HE2	1.72	0.42
1:B:241:PHE:O	1:B:245:ILE:HG12	2.19	0.42
1:C:381:ILE:HD13	1:C:553:TYR:CD1	2.54	0.42
1:C:297:LEU:HD23	1:C:297:LEU:HA	1.88	0.42
1:D:334:PHE:CE2	1:D:359:LEU:HD11	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:351:ALA:O	1:D:520:PHE:HA	2.20	0.42
1:A:241:PHE:CZ	1:A:245:ILE:HD11	2.54	0.41
1:C:443:GLU:O	1:C:447:GLN:HG2	2.19	0.41
1:C:471:GLU:HG2	1:C:472:ASP:OD1	2.20	0.41
1:B:212:PRO:HB3	1:B:426:ILE:HD11	2.01	0.41
1:D:312:LYS:HA	1:D:315:TYR:CE2	2.55	0.41
1:C:377:LYS:HD2	1:C:456:TYR:CG	2.55	0.41
1:B:426:ILE:HG13	1:B:426:ILE:H	1.55	0.41
1:D:556:LYS:HD3	1:D:556:LYS:HA	1.85	0.41
1:B:212:PRO:HD2	1:B:217:PHE:CD1	2.56	0.41
1:A:350:CYS:SG	1:A:519:SER:HB2	2.61	0.41
1:B:320:CYS:SG	1:B:327[A]:ASN:HB2	2.61	0.41
1:D:370:HIS:HA	1:D:374:TYR:HB2	2.02	0.41
1:B:428:LEU:HD13	1:C:425:ASN:HB2	2.03	0.41
1:A:473:TYR:CE1	1:A:502:VAL:HG11	2.56	0.41
3:B:702:TTP:O2A	1:D:376:HIS:NE2	2.49	0.41
1:C:222:ILE:HD13	1:C:222:ILE:HA	1.92	0.41
1:A:499:ILE:HD11	1:A:555:LYS:HE2	2.03	0.40
1:C:185:LYS:HE3	1:C:185:LYS:HB2	1.82	0.40
1:A:334:PHE:CE2	1:A:359:LEU:HD21	2.56	0.40
1:C:583:ASP:OD1	1:C:583:ASP:N	2.53	0.40
1:A:597:GLU:OE1	1:A:597:GLU:N	2.40	0.40
1:B:234:GLU:HB3	1:B:273:VAL:HG23	2.03	0.40
3:B:702:TTP:H2'2	3:B:702:TTP:O2	2.22	0.40

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	478/550 (87%)	463 (97%)	15 (3%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	480/550 (87%)	464 (97%)	14 (3%)	2 (0%)	34	42
1	C	477/550 (87%)	447 (94%)	29 (6%)	1 (0%)	47	58
1	D	482/550 (88%)	461 (96%)	20 (4%)	1 (0%)	47	58
All	All	1917/2200 (87%)	1835 (96%)	78 (4%)	4 (0%)	47	58

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	327	ASN
1	B	327[A]	ASN
1	B	327[B]	ASN
1	C	595	LYS

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	428/488 (88%)	421 (98%)	7 (2%)	62	78
1	B	430/488 (88%)	421 (98%)	9 (2%)	53	70
1	C	427/488 (88%)	414 (97%)	13 (3%)	41	57
1	D	432/488 (88%)	422 (98%)	10 (2%)	50	67
All	All	1717/1952 (88%)	1678 (98%)	39 (2%)	52	67

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	THR
1	A	229	VAL
1	A	284	LEU
1	A	326	GLN
1	A	328[A]	ASN
1	A	328[B]	ASN
1	A	502	VAL

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Mol	Chain	Res	Type
1	B	114	THR
1	B	230	LYS
1	B	262	GLU
1	B	315	TYR
1	B	377	LYS
1	B	406	LYS
1	B	426	ILE
1	B	560	LYS
1	B	594	GLN
1	C	115	MET
1	C	273	VAL
1	C	284	LEU
1	C	304	LYS
1	C	315	TYR
1	C	326	GLN
1	C	354	LYS
1	C	463	THR
1	C	487	VAL
1	C	489	LEU
1	C	490	ASP
1	C	597	GLU
1	C	599	ASN
1	D	113	ASP
1	D	115	MET
1	D	276	LEU
1	D	315	TYR
1	D	377	LYS
1	D	434	THR
1	D	439	LYS
1	D	466	ILE
1	D	511	GLU
1	D	535	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	246	ASN
1	A	322	HIS
1	B	149	GLN
1	B	425	ASN
1	B	571	GLN
1	C	243	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 ⓘ

Of 21 ligands modelled in this entry, 9 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	TTP	C	701	4	23,30,30	1.87	5 (21%)	29,47,47	1.93	5 (17%)
3	TTP	D	703	4	23,30,30	1.83	4 (17%)	29,47,47	1.88	5 (17%)
2	DGT	C	703	4	26,33,33	1.58	5 (19%)	32,52,52	1.79	9 (28%)
3	TTP	A	703	4	23,30,30	1.86	5 (21%)	29,47,47	1.91	7 (24%)
2	DGT	D	702	4	26,33,33	1.58	5 (19%)	32,52,52	1.82	8 (25%)
2	DGT	C	702	4	26,33,33	1.60	6 (23%)	32,52,52	1.82	9 (28%)
3	TTP	A	702	4	23,30,30	1.90	5 (21%)	29,47,47	1.92	5 (17%)
3	TTP	B	702	4	23,30,30	1.87	5 (21%)	29,47,47	2.03	6 (20%)
2	DGT	A	701	4	26,33,33	1.62	6 (23%)	32,52,52	1.74	8 (25%)
3	TTP	D	701	4	23,30,30	1.90	5 (21%)	29,47,47	1.92	6 (20%)
3	TTP	B	701	4	23,30,30	1.91	5 (21%)	29,47,47	1.96	6 (20%)
3	TTP	C	704	4	23,30,30	1.89	5 (21%)	29,47,47	1.96	5 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.  
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TTP	C	701	4	-	3/19/34/34	0/2/2/2
3	TTP	D	703	4	-	4/19/34/34	0/2/2/2
2	DGT	C	703	4	-	4/18/34/34	0/3/3/3
3	TTP	A	703	4	-	2/19/34/34	0/2/2/2
2	DGT	D	702	4	-	2/18/34/34	0/3/3/3
2	DGT	C	702	4	-	6/18/34/34	0/3/3/3
3	TTP	A	702	4	-	6/19/34/34	0/2/2/2
3	TTP	B	702	4	-	5/19/34/34	0/2/2/2
2	DGT	A	701	4	-	2/18/34/34	0/3/3/3
3	TTP	D	701	4	-	2/19/34/34	0/2/2/2
3	TTP	B	701	4	-	7/19/34/34	0/2/2/2
3	TTP	C	704	4	-	4/19/34/34	0/2/2/2

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	TTP	O4-C4	5.10	1.37	1.24
3	C	701	TTP	O4-C4	5.02	1.37	1.24
3	D	703	TTP	O4-C4	5.01	1.37	1.24
3	B	701	TTP	O4-C4	5.01	1.37	1.24
3	A	703	TTP	O4-C4	5.01	1.37	1.24
3	D	701	TTP	O4-C4	4.98	1.37	1.24
3	A	702	TTP	O4-C4	4.93	1.36	1.24
3	C	704	TTP	O4-C4	4.93	1.36	1.24
3	D	701	TTP	C3'-C4'	-4.42	1.40	1.53
3	A	702	TTP	C3'-C4'	-4.42	1.40	1.53
3	B	701	TTP	C3'-C4'	-4.38	1.41	1.53
3	C	704	TTP	C3'-C4'	-4.33	1.41	1.53
3	C	701	TTP	C3'-C4'	-4.28	1.41	1.53
3	A	703	TTP	C3'-C4'	-4.25	1.41	1.53
2	C	702	DGT	O6-C6	4.18	1.35	1.24
3	D	703	TTP	C3'-C4'	-4.14	1.41	1.53
2	A	701	DGT	O6-C6	4.13	1.34	1.24
2	D	702	DGT	O6-C6	4.09	1.34	1.24
3	B	702	TTP	C3'-C4'	-4.08	1.41	1.53
2	C	703	DGT	O6-C6	4.02	1.34	1.24
3	D	701	TTP	C2'-C1'	-3.90	1.41	1.52
3	C	704	TTP	C2'-C1'	-3.89	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	TTP	C2'-C1'	-3.88	1.41	1.52
3	B	702	TTP	C2'-C1'	-3.88	1.41	1.52
2	A	701	DGT	C2-N2	3.83	1.41	1.33
3	B	701	TTP	C2'-C1'	-3.80	1.41	1.52
3	C	701	TTP	C2'-C1'	-3.77	1.41	1.52
3	A	703	TTP	C2'-C1'	-3.77	1.41	1.52
2	C	703	DGT	C2-N2	3.75	1.41	1.33
3	D	703	TTP	C2'-C1'	-3.73	1.41	1.52
2	C	702	DGT	C2-N2	3.66	1.41	1.33
2	D	702	DGT	C2-N2	3.65	1.41	1.33
2	C	702	DGT	O3'-C3'	-3.06	1.36	1.43
2	D	702	DGT	O3'-C3'	-3.06	1.36	1.43
2	A	701	DGT	O3'-C3'	-3.00	1.37	1.43
2	C	703	DGT	O3'-C3'	-2.92	1.37	1.43
2	C	703	DGT	C5'-C4'	-2.52	1.43	1.51
2	A	701	DGT	C5'-C4'	-2.49	1.43	1.51
2	C	702	DGT	C5'-C4'	-2.45	1.44	1.51
3	C	704	TTP	C2'-C3'	-2.33	1.46	1.52
2	D	702	DGT	C5'-C4'	-2.28	1.44	1.51
3	B	702	TTP	O4'-C4'	-2.28	1.39	1.45
3	B	701	TTP	O4'-C4'	-2.27	1.39	1.45
2	A	701	DGT	C2'-C3'	-2.25	1.46	1.52
3	A	702	TTP	O4'-C4'	-2.22	1.40	1.45
3	A	702	TTP	C2'-C3'	-2.22	1.47	1.52
3	D	703	TTP	C2'-C3'	-2.17	1.47	1.52
3	D	701	TTP	O4'-C4'	-2.16	1.40	1.45
2	C	703	DGT	C2'-C3'	-2.16	1.47	1.52
3	B	701	TTP	C2'-C3'	-2.15	1.47	1.52
3	C	704	TTP	O4'-C4'	-2.14	1.40	1.45
2	D	702	DGT	C2'-C3'	-2.13	1.47	1.52
3	C	701	TTP	O4'-C4'	-2.13	1.40	1.45
2	C	702	DGT	C3'-C4'	-2.12	1.47	1.53
2	A	701	DGT	C3'-C4'	-2.11	1.47	1.53
2	C	702	DGT	C2'-C3'	-2.10	1.47	1.52
3	A	703	TTP	O4'-C4'	-2.10	1.40	1.45
3	A	703	TTP	C2'-C3'	-2.08	1.47	1.52
3	D	701	TTP	C2-N3	-2.07	1.34	1.38
3	C	701	TTP	C2'-C3'	-2.06	1.47	1.52
3	B	702	TTP	C2-N3	-2.03	1.34	1.38

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	704	TTP	C4-N3-C2	7.80	121.73	115.14
3	B	702	TTP	C4-N3-C2	7.76	121.69	115.14
3	C	701	TTP	C4-N3-C2	7.71	121.65	115.14
3	B	701	TTP	C4-N3-C2	7.68	121.62	115.14
3	A	703	TTP	C4-N3-C2	7.66	121.61	115.14
3	D	701	TTP	C4-N3-C2	7.63	121.58	115.14
3	A	702	TTP	C4-N3-C2	7.47	121.45	115.14
3	D	703	TTP	C4-N3-C2	7.24	121.26	115.14
2	C	702	DGT	C2-N3-C4	4.48	120.48	115.36
2	C	703	DGT	C2-N3-C4	4.44	120.42	115.36
2	A	701	DGT	C2-N3-C4	4.36	120.33	115.36
2	D	702	DGT	C2-N3-C4	4.25	120.21	115.36
2	D	702	DGT	N3-C2-N1	-4.25	121.55	127.22
2	A	701	DGT	N3-C2-N1	-4.04	121.84	127.22
2	C	702	DGT	N3-C2-N1	-4.01	121.88	127.22
2	C	703	DGT	N3-C2-N1	-3.97	121.93	127.22
3	B	702	TTP	C5-C6-N1	-3.80	118.10	122.19
3	C	704	TTP	PB-O3A-PA	-3.77	119.88	132.83
3	B	701	TTP	PB-O3A-PA	-3.59	120.49	132.83
3	A	702	TTP	PB-O3A-PA	-3.59	120.51	132.83
3	D	701	TTP	C5-C6-N1	-3.59	118.33	122.19
3	B	701	TTP	C5-C6-N1	-3.58	118.33	122.19
3	A	703	TTP	C5-C6-N1	-3.52	118.40	122.19
3	C	704	TTP	C5-C6-N1	-3.44	118.48	122.19
3	D	703	TTP	C5-C6-N1	-3.42	118.50	122.19
3	A	702	TTP	C5-C6-N1	-3.41	118.52	122.19
3	D	703	TTP	PB-O3A-PA	-3.37	121.25	132.83
3	C	701	TTP	C5-C6-N1	-3.31	118.63	122.19
3	B	702	TTP	O5'-C5'-C4'	3.23	120.12	108.99
2	C	702	DGT	C4-C5-N7	-3.19	106.08	109.40
2	D	702	DGT	C6-C5-C4	-3.11	117.82	120.80
2	A	701	DGT	PA-O3A-PB	-3.11	122.16	132.83
3	C	701	TTP	C2'-C1'-N1	3.10	121.42	114.27
2	D	702	DGT	C6-N1-C2	3.00	120.70	115.93
2	D	702	DGT	PA-O3A-PB	-2.98	122.61	132.83
2	D	702	DGT	O5'-C5'-C4'	2.98	119.24	108.99
2	C	703	DGT	O2G-PG-O3B	2.94	114.50	104.64
2	C	702	DGT	O2G-PG-O3B	2.94	114.49	104.64
3	B	702	TTP	PB-O3A-PA	-2.93	122.75	132.83
2	A	701	DGT	C4-C5-N7	-2.89	106.38	109.40
2	D	702	DGT	C4-C5-N7	-2.89	106.39	109.40
2	C	703	DGT	PA-O3A-PB	-2.89	122.92	132.83
2	A	701	DGT	C6-C5-C4	-2.88	118.05	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	702	DGT	C6-C5-C4	-2.82	118.10	120.80
2	C	703	DGT	C4-C5-N7	-2.78	106.50	109.40
2	C	703	DGT	C6-C5-C4	-2.75	118.17	120.80
3	D	701	TTP	PB-O3B-PG	-2.74	123.41	132.83
2	D	702	DGT	C5-C6-N1	-2.73	119.70	123.43
2	C	702	DGT	O5'-C5'-C4'	2.71	118.30	108.99
2	C	703	DGT	O5'-C5'-C4'	2.69	118.26	108.99
2	A	701	DGT	C6-N1-C2	2.69	120.20	115.93
3	D	701	TTP	C2'-C1'-N1	2.68	120.45	114.27
3	A	703	TTP	PB-O3A-PA	-2.65	123.74	132.83
3	D	703	TTP	PB-O3B-PG	-2.60	123.89	132.83
2	C	702	DGT	C6-N1-C2	2.58	120.03	115.93
2	A	701	DGT	O5'-C5'-C4'	2.57	117.85	108.99
2	C	702	DGT	C5-C6-N1	-2.52	119.99	123.43
2	C	703	DGT	C6-N1-C2	2.50	119.90	115.93
3	C	701	TTP	PB-O3A-PA	-2.48	124.31	132.83
2	A	701	DGT	C5-C6-N1	-2.47	120.05	123.43
3	B	702	TTP	C2'-C1'-N1	2.47	119.96	114.27
2	C	702	DGT	PA-O3A-PB	-2.47	124.37	132.83
3	A	702	TTP	PB-O3B-PG	-2.46	124.40	132.83
3	C	701	TTP	PB-O3B-PG	-2.44	124.46	132.83
2	C	703	DGT	C5-C6-N1	-2.35	120.22	123.43
3	A	702	TTP	O5'-C5'-C4'	2.34	117.03	108.99
3	B	701	TTP	PB-O3B-PG	-2.27	125.05	132.83
3	A	703	TTP	PB-O3B-PG	-2.25	125.10	132.83
3	C	704	TTP	O5'-C5'-C4'	2.24	116.70	108.99
3	D	703	TTP	O5'-C5'-C4'	2.22	116.64	108.99
3	B	702	TTP	PB-O3B-PG	-2.20	125.28	132.83
3	A	703	TTP	C2'-C1'-N1	2.18	119.29	114.27
3	C	704	TTP	PB-O3B-PG	-2.16	125.41	132.83
3	B	701	TTP	O5'-C5'-C4'	2.15	116.39	108.99
3	A	703	TTP	O3G-PG-O3B	2.07	111.56	104.64
3	B	701	TTP	O2G-PG-O3B	2.06	111.56	104.64
3	A	703	TTP	C2'-C3'-C4'	2.06	107.06	102.76
3	D	701	TTP	PB-O3A-PA	-2.04	125.83	132.83
3	D	701	TTP	O2G-PG-O3B	2.04	111.47	104.64

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	701	TTP	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
3	D	703	TTP	PB-O3A-PA-O5'
2	C	703	DGT	PB-O3B-PG-O2G
3	A	703	TTP	O4'-C1'-N1-C6
2	C	702	DGT	PB-O3B-PG-O2G
3	A	702	TTP	C5'-O5'-PA-O1A
3	A	702	TTP	C3'-C4'-C5'-O5'
3	B	702	TTP	O4'-C4'-C5'-O5'
3	B	702	TTP	O4'-C1'-N1-C6
3	D	701	TTP	O4'-C1'-N1-C6
3	B	701	TTP	C5'-O5'-PA-O1A
3	B	701	TTP	C5'-O5'-PA-O2A
3	B	702	TTP	C3'-C4'-C5'-O5'
3	C	704	TTP	C3'-C4'-C5'-O5'
3	A	702	TTP	O4'-C4'-C5'-O5'
3	B	701	TTP	C3'-C4'-C5'-O5'
3	D	703	TTP	C3'-C4'-C5'-O5'
3	C	701	TTP	PB-O3A-PA-O1A
2	C	702	DGT	PG-O3B-PB-O2B
3	D	703	TTP	C4'-C5'-O5'-PA
2	A	701	DGT	PB-O3B-PG-O2G
3	A	702	TTP	C5'-O5'-PA-O3A
3	B	701	TTP	C5'-O5'-PA-O3A
3	A	702	TTP	PB-O3A-PA-O1A
3	B	701	TTP	PB-O3A-PA-O2A
3	A	702	TTP	C5'-O5'-PA-O2A
3	D	703	TTP	O4'-C4'-C5'-O5'
2	C	703	DGT	PG-O3B-PB-O2B
2	C	702	DGT	PB-O3A-PA-O1A
3	B	702	TTP	PA-O3A-PB-O2B
3	B	701	TTP	C4'-C5'-O5'-PA
3	A	703	TTP	PA-O3A-PB-O1B
3	D	701	TTP	PA-O3A-PB-O2B
3	C	704	TTP	O4'-C4'-C5'-O5'
3	B	701	TTP	O4'-C4'-C5'-O5'
2	D	702	DGT	PB-O3B-PG-O2G
2	C	702	DGT	PB-O3B-PG-O1G
3	C	701	TTP	PB-O3A-PA-O2A
2	C	703	DGT	PG-O3B-PB-O1B
2	D	702	DGT	PG-O3B-PB-O1B
2	C	702	DGT	PB-O3A-PA-O2A
3	B	702	TTP	PA-O3A-PB-O1B
2	A	701	DGT	PG-O3B-PB-O1B

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Mol	Chain	Res	Type	Atoms
3	C	704	TTP	PB-O3A-PA-O2A
2	C	702	DGT	C5'-O5'-PA-O2A
3	C	704	TTP	C5'-O5'-PA-O1A
2	C	703	DGT	PB-O3B-PG-O3G

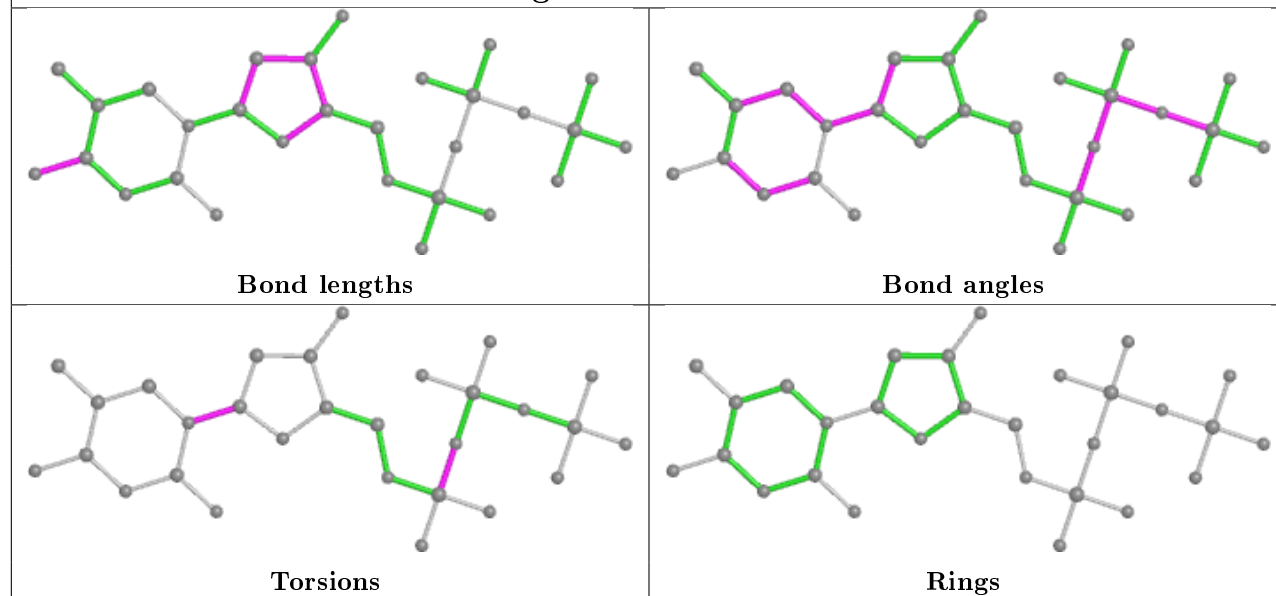
There are no ring outliers.

6 monomers are involved in 16 short contacts:

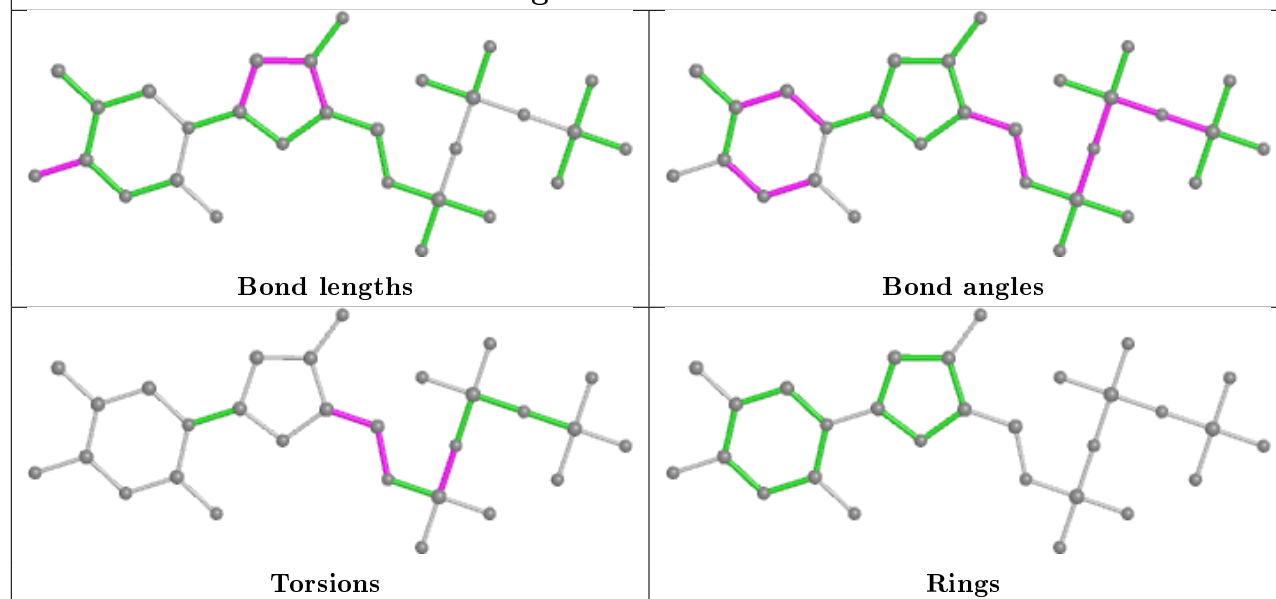
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	701	TTP	1	0
3	D	703	TTP	3	0
3	A	702	TTP	3	0
3	B	702	TTP	3	0
3	B	701	TTP	3	0
3	C	704	TTP	3	0

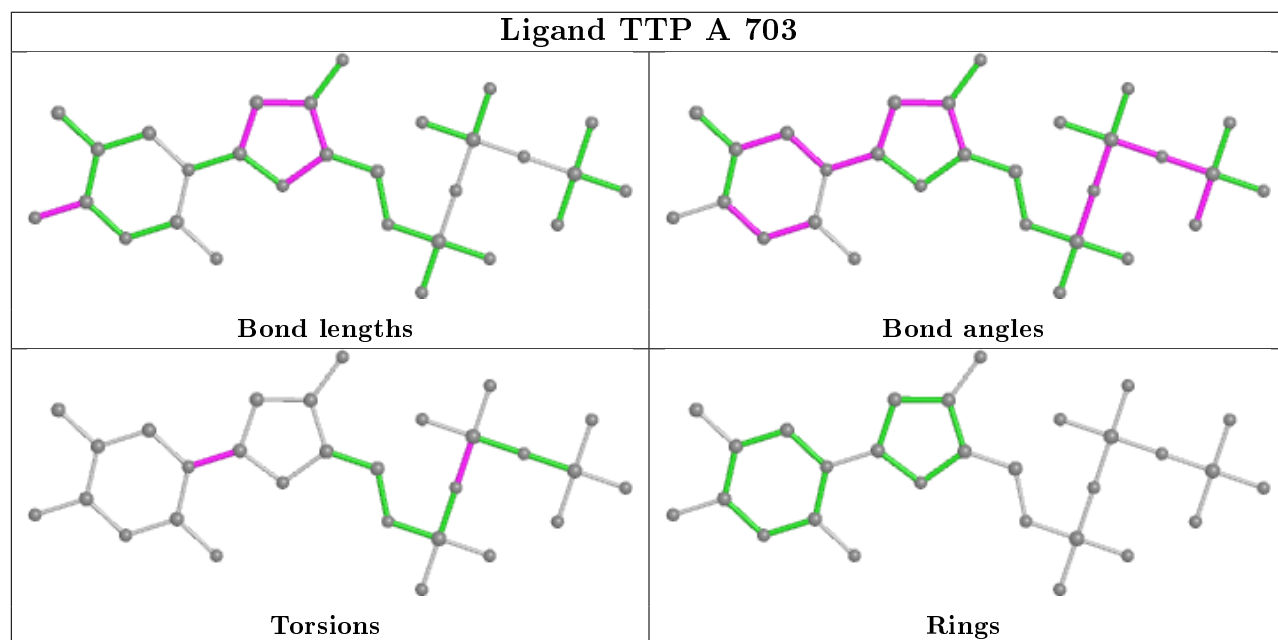
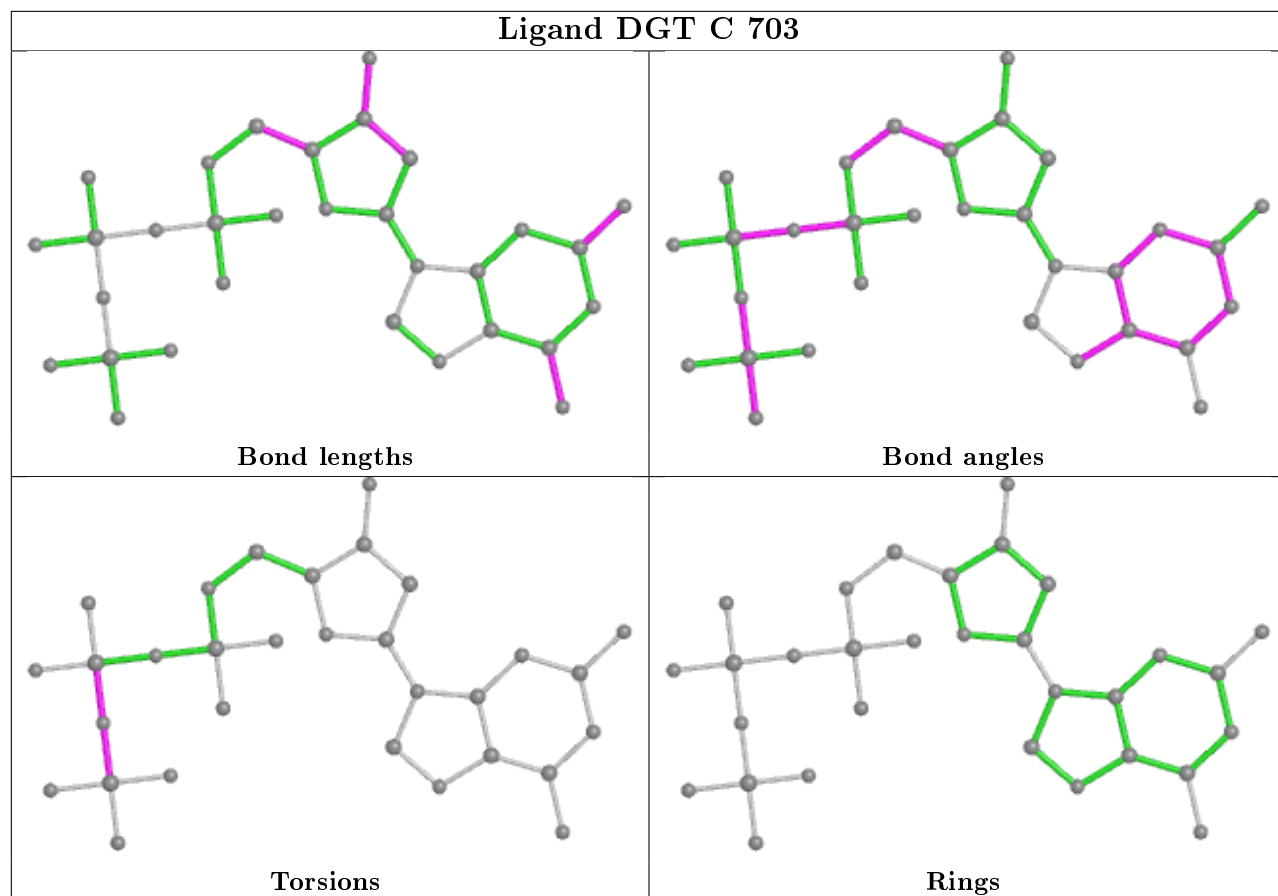
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

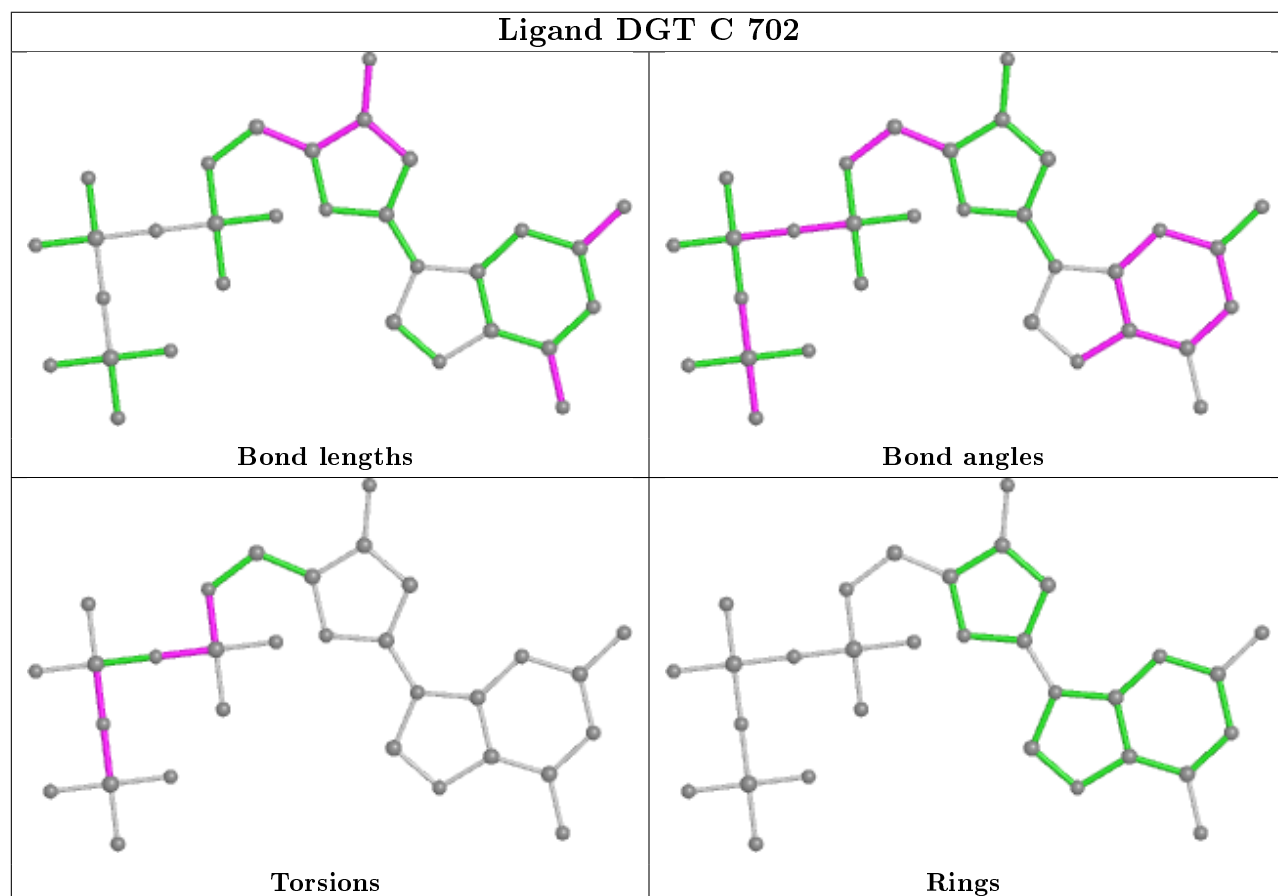
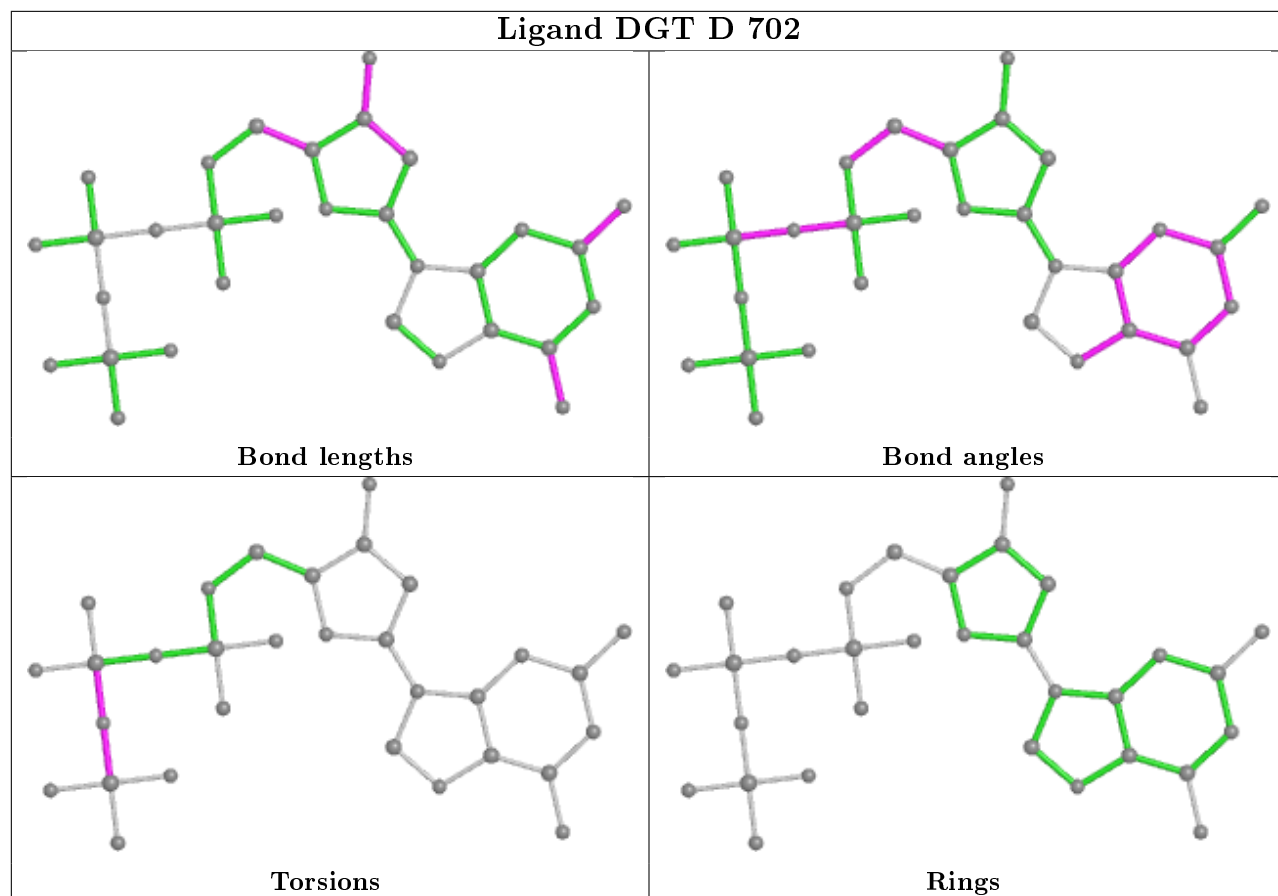
## Ligand TTP C 701



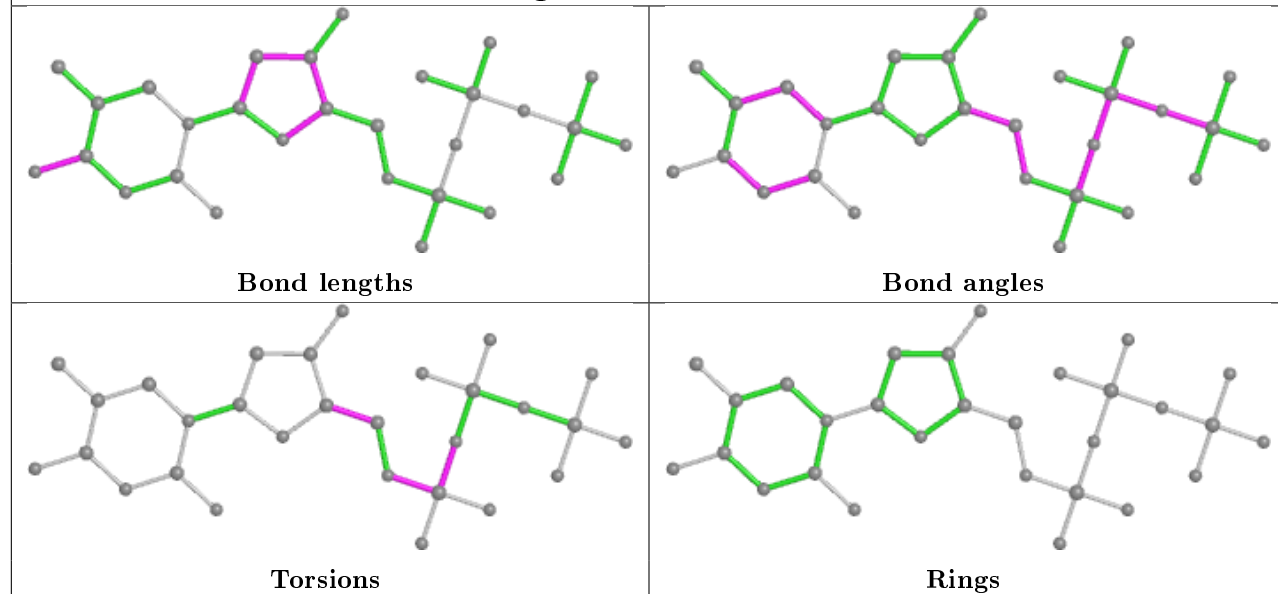
## Ligand TTP D 703



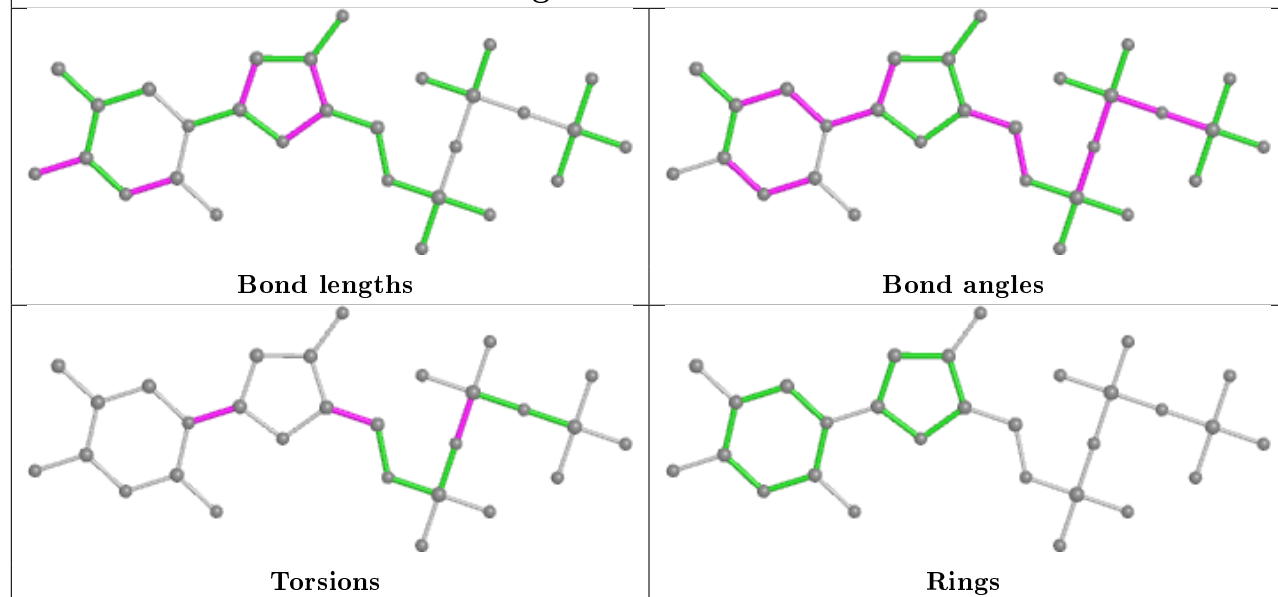


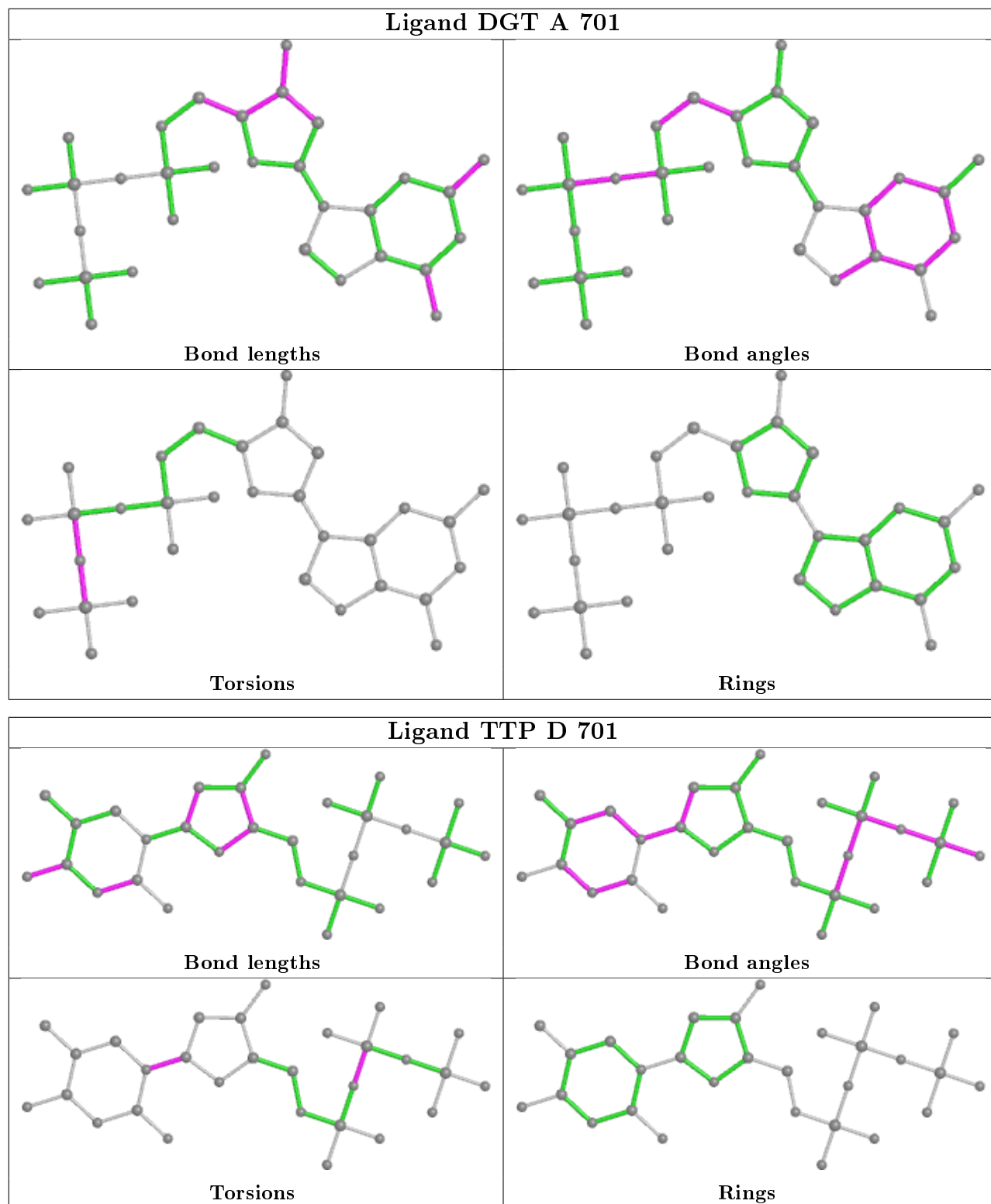


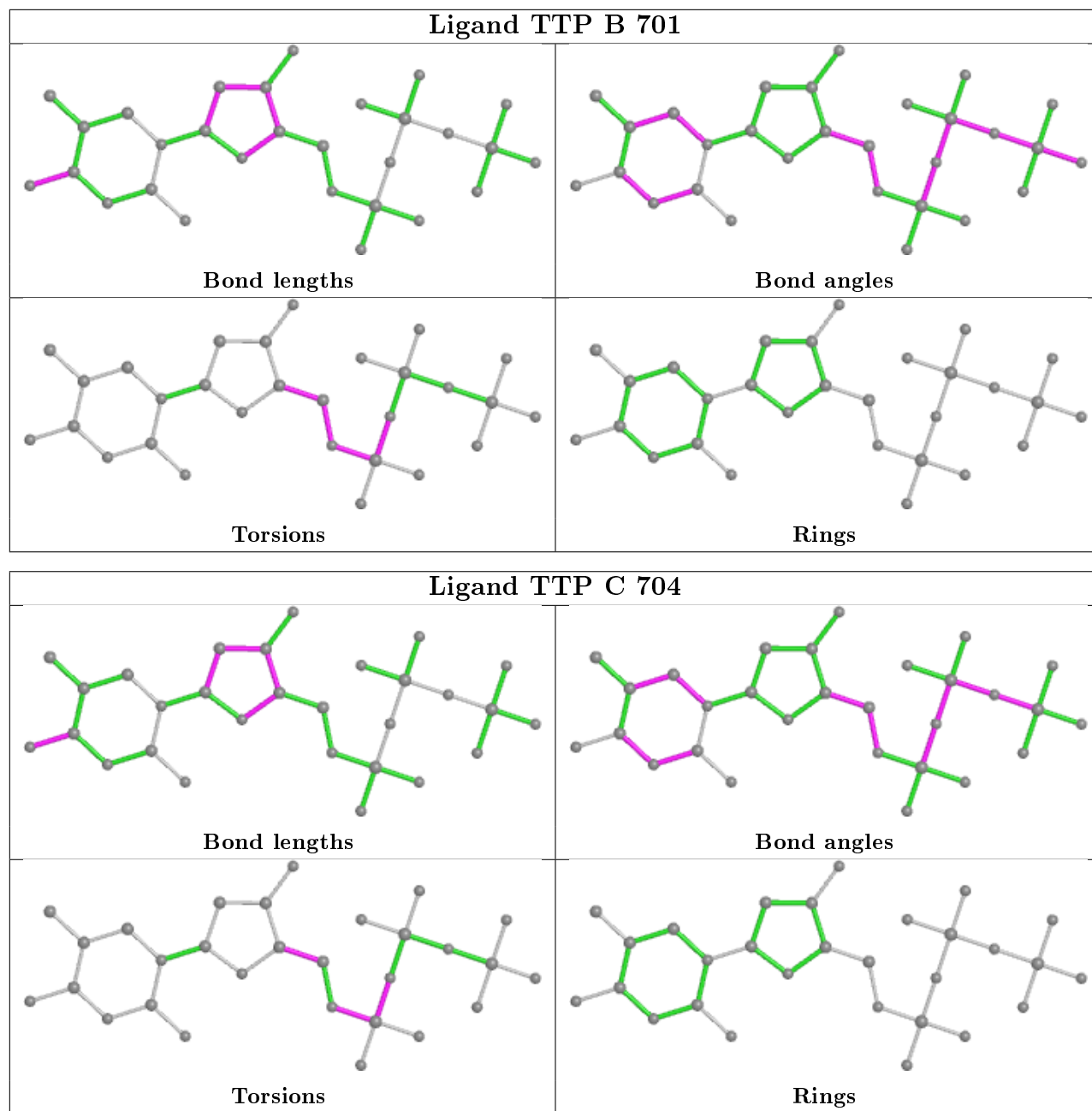
## Ligand TTP A 702



## Ligand TTP B 702







## 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	481/550 (87%)	0.43	39 (8%) 12 16	28, 50, 76, 90	481 (100%)
1	B	481/550 (87%)	0.30	25 (5%) 27 34	31, 44, 71, 91	479 (99%)
1	C	481/550 (87%)	0.46	37 (7%) 13 17	31, 51, 82, 113	481 (100%)
1	D	481/550 (87%)	0.13	22 (4%) 32 39	26, 43, 62, 82	479 (99%)
All	All	1924/2200 (87%)	0.33	123 (6%) 19 25	26, 47, 75, 113	1920 (99%)

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	489	LEU	10.2
1	B	488	LEU	7.6
1	C	488	LEU	7.2
1	C	276	LEU	6.6
1	C	284	LEU	6.5
1	B	590	LEU	6.0
1	C	590	LEU	6.0
1	D	284	LEU	5.7
1	A	277	GLU	5.7
1	B	487	VAL	5.6
1	A	488	LEU	5.5
1	A	147	ILE	5.1
1	C	277	GLU	5.1
1	B	284	LEU	5.0
1	A	284	LEU	4.9
1	C	592	THR	4.6
1	B	490	ASP	4.4
1	B	560	LYS	4.4
1	C	230	LYS	4.4
1	C	491	VAL	4.2
1	B	591	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	598	TRP	4.0
1	D	404	GLY	4.0
1	A	487	VAL	4.0
1	D	466	ILE	4.0
1	B	113	ASP	4.0
1	B	276	LEU	4.0
1	C	596	LYS	4.0
1	D	276	LEU	3.9
1	C	599	ASN	3.9
1	A	486	LYS	3.8
1	C	543	GLU	3.8
1	B	559	ARG	3.8
1	A	344	ASP	3.7
1	A	599	ASN	3.7
1	C	229	VAL	3.6
1	A	465	GLN	3.6
1	B	593	PRO	3.4
1	D	465	GLN	3.4
1	B	326[A]	GLN	3.3
1	A	485	PRO	3.3
1	A	593	PRO	3.3
1	C	595	LYS	3.3
1	B	464	GLY	3.2
1	D	599	ASN	3.2
1	B	277	GLU	3.2
1	B	486	LYS	3.2
1	A	403	GLY	3.2
1	D	490	ASP	3.2
1	C	465	GLN	3.1
1	A	489	LEU	3.1
1	C	228	GLU	3.0
1	A	535	ASN	3.0
1	C	227	PRO	3.0
1	C	275	PRO	3.0
1	C	560	LYS	3.0
1	A	591	ILE	3.0
1	A	276	LEU	2.9
1	A	471	GLU	2.9
1	A	345	ASN	2.9
1	C	588	ALA	2.9
1	A	490	ASP	2.9
1	D	344	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	596	LYS	2.8
1	B	592	THR	2.8
1	A	559	ARG	2.8
1	A	146	TYR	2.8
1	C	403	GLY	2.7
1	C	593	PRO	2.7
1	D	230	LYS	2.7
1	C	147	ILE	2.7
1	A	469	LYS	2.6
1	D	402	ALA	2.6
1	C	484	LYS	2.6
1	C	345	ASN	2.6
1	B	354	LYS	2.6
1	D	229	VAL	2.6
1	C	559	ARG	2.5
1	B	594	GLN	2.5
1	A	466	ILE	2.5
1	D	464	GLY	2.5
1	C	405	LYS	2.5
1	A	396	TYR	2.5
1	B	485	PRO	2.5
1	A	470	ARG	2.4
1	A	148	LYS	2.4
1	C	487	VAL	2.4
1	A	452	ASN	2.4
1	D	252	PRO	2.4
1	B	484	LYS	2.3
1	B	491	VAL	2.3
1	B	562	LEU	2.3
1	C	489	LEU	2.3
1	B	492	LYS	2.3
1	C	437	LYS	2.3
1	A	484	LYS	2.2
1	A	560	LYS	2.2
1	D	452	ASN	2.2
1	D	277	GLU	2.2
1	A	230	LYS	2.2
1	A	193	GLU	2.2
1	A	592	THR	2.2
1	A	594	GLN	2.2
1	D	147	ILE	2.2
1	C	568	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	345	ASN	2.1
1	A	285	TRP	2.1
1	D	403	GLY	2.1
1	A	402	ALA	2.1
1	C	144	LEU	2.1
1	A	215	HIS	2.1
1	B	230	LYS	2.1
1	D	467	LYS	2.1
1	A	544	LYS	2.1
1	C	113	ASP	2.1
1	A	275	PRO	2.1
1	C	346	GLU	2.0
1	C	400	THR	2.0
1	D	250	ILE	2.0
1	A	492	LYS	2.0
1	D	146	TYR	2.0
1	C	208	LEU	2.0
1	C	326	GLN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 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.

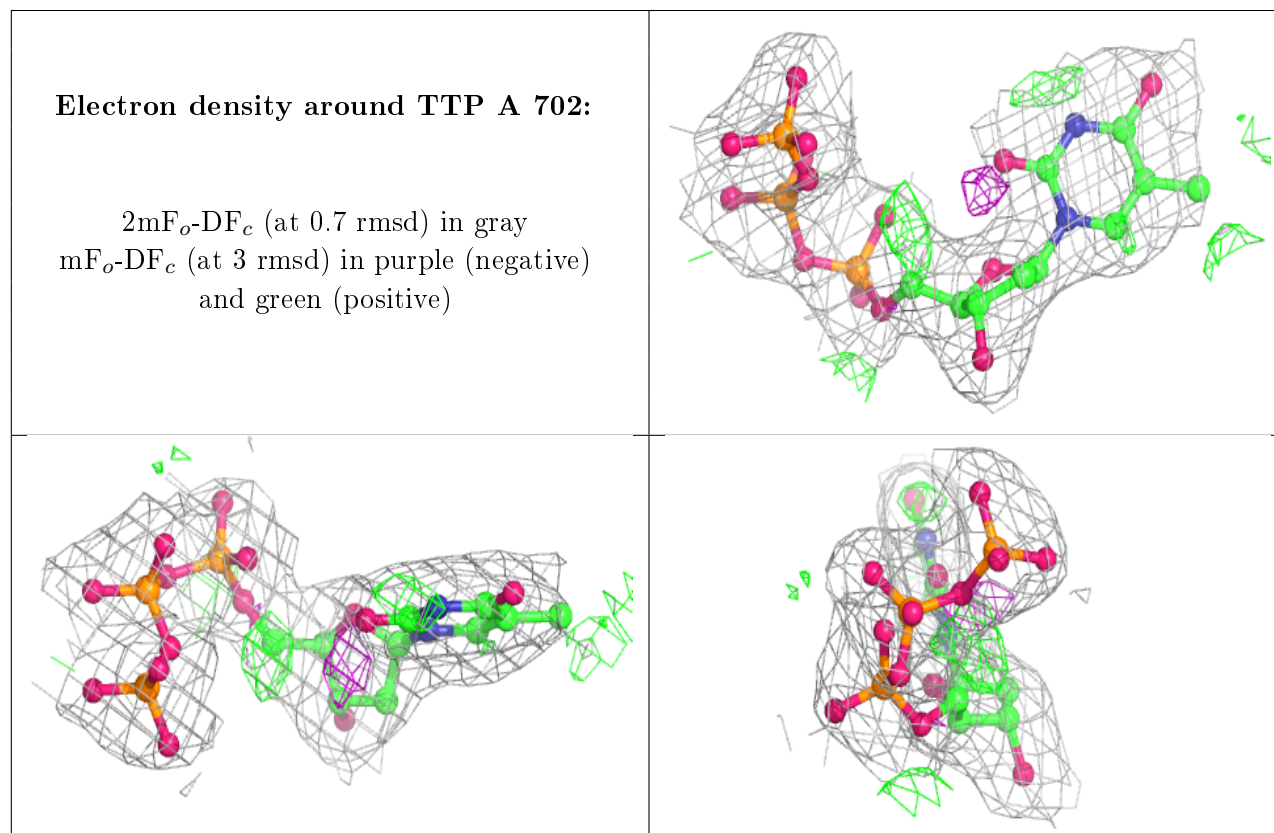
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	MG	A	704	1/1	0.81	0.09	32,32,32,32	1
4	MG	B	703	1/1	0.85	0.13	44,44,44,44	1
4	MG	B	704	1/1	0.88	0.12	55,55,55,55	1
4	MG	C	705	1/1	0.89	0.07	35,35,35,35	1
4	MG	D	705	1/1	0.90	0.23	76,76,76,76	1

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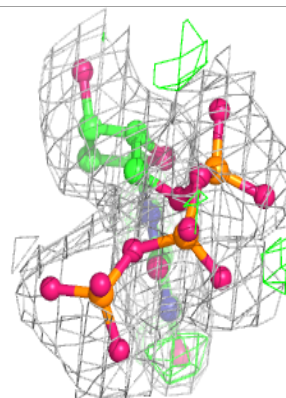
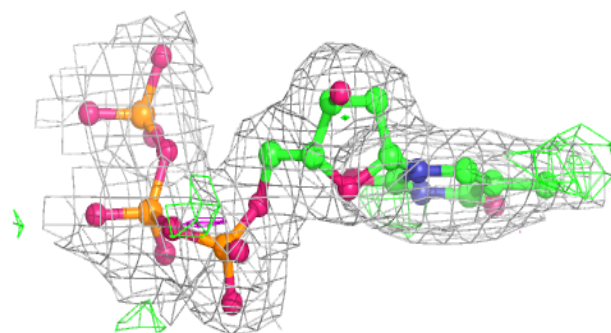
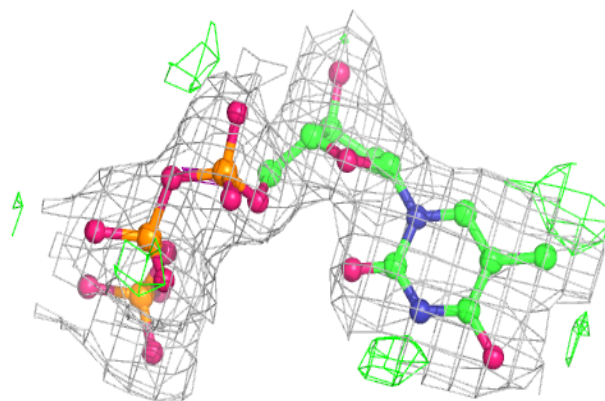
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	A	705	1/1	0.90	0.17	60,60,60,60	1
4	MG	D	704	1/1	0.92	0.06	48,48,48,48	1
4	MG	D	706	1/1	0.94	0.09	43,43,43,43	1
3	TTP	A	702	29/29	0.94	0.17	36,46,54,55	29
3	TTP	D	703	29/29	0.94	0.13	27,40,45,48	29
4	MG	C	706	1/1	0.94	0.15	60,60,60,60	1
3	TTP	B	702	29/29	0.95	0.13	30,34,41,42	29
3	TTP	C	704	29/29	0.95	0.17	40,48,54,57	29
3	TTP	B	701	29/29	0.96	0.14	33,40,47,49	29
2	DGT	C	702	31/31	0.96	0.16	30,34,40,42	31
3	TTP	C	701	29/29	0.96	0.14	32,37,44,47	29
2	DGT	C	703	31/31	0.97	0.17	31,38,47,50	31
3	TTP	A	703	29/29	0.97	0.13	36,41,46,50	29
3	TTP	D	701	29/29	0.97	0.14	33,36,41,45	29
2	DGT	D	702	31/31	0.98	0.14	26,31,34,35	31
2	DGT	A	701	31/31	0.98	0.15	32,36,39,41	31

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.

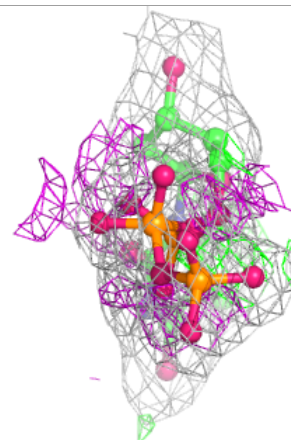
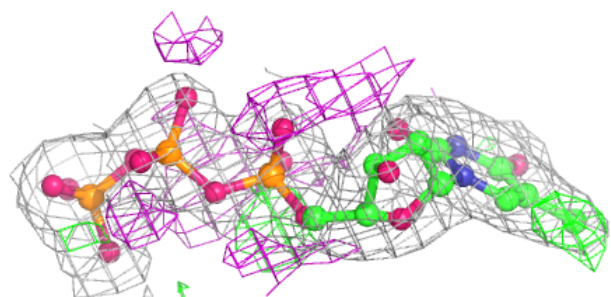
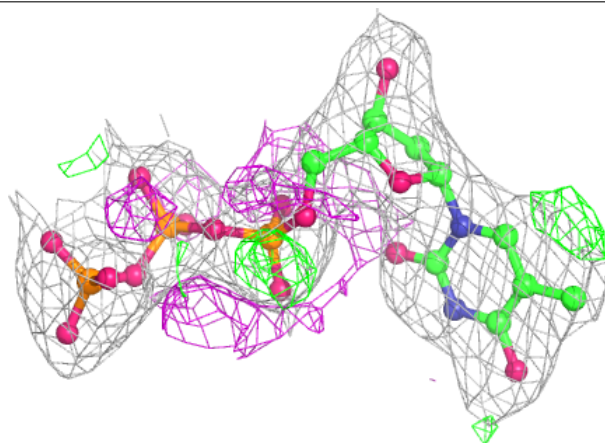


**Electron density around TTP D 703:**

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

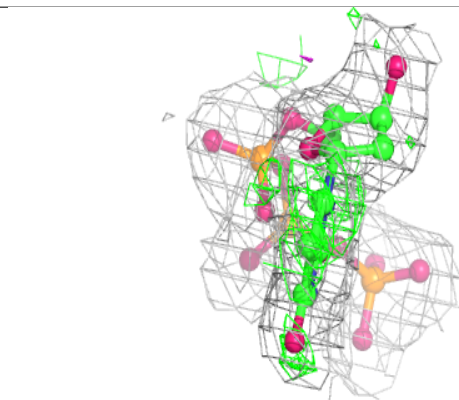
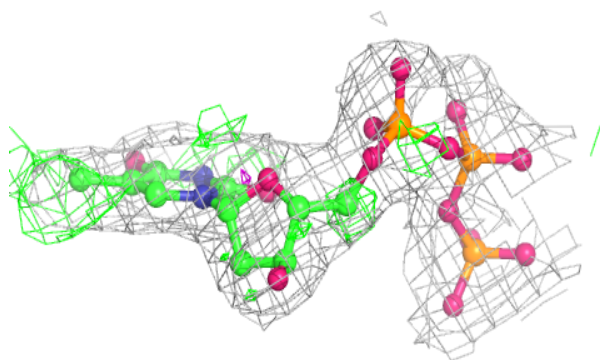
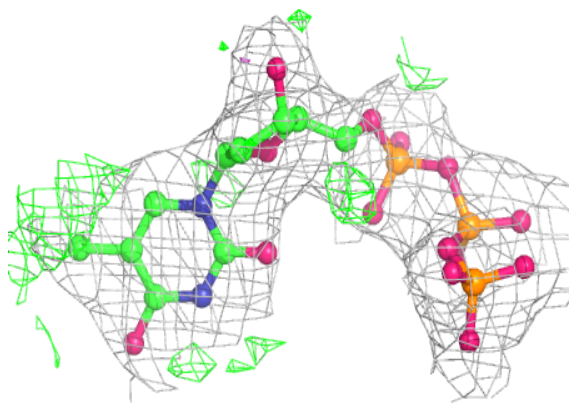
**Electron density around TTP B 702:**

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

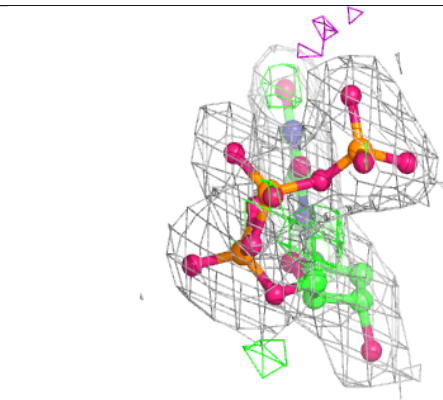
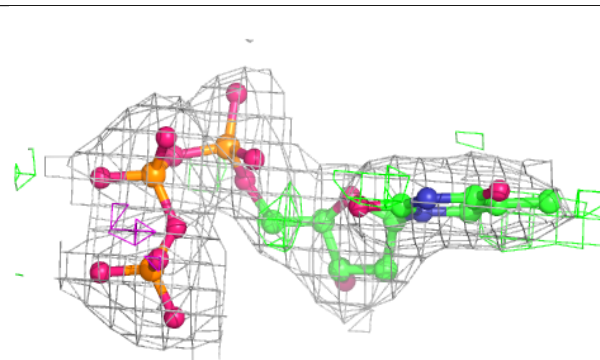
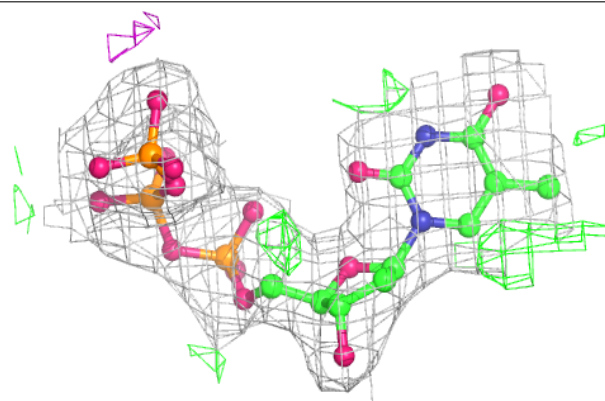


**Electron density around TTP C 704:**

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

**Electron density around TTP B 701:**

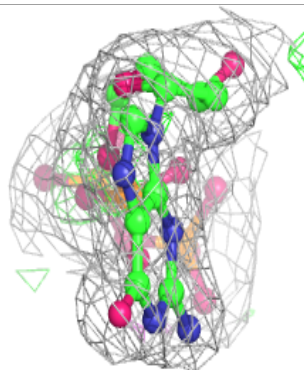
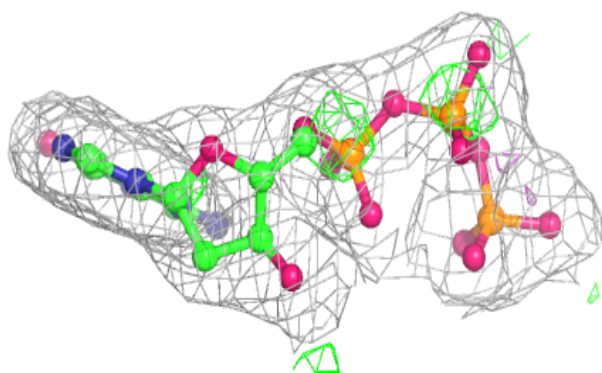
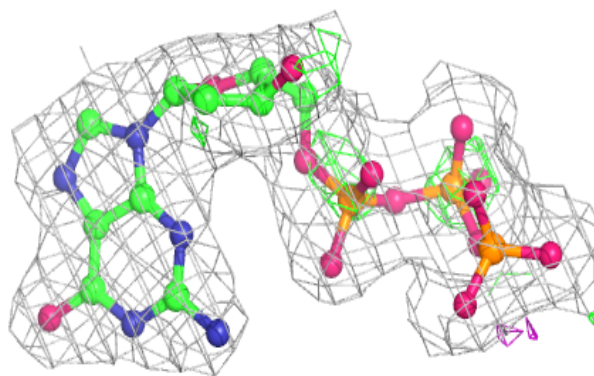
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



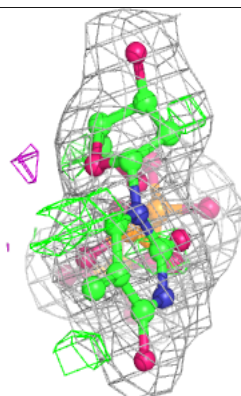
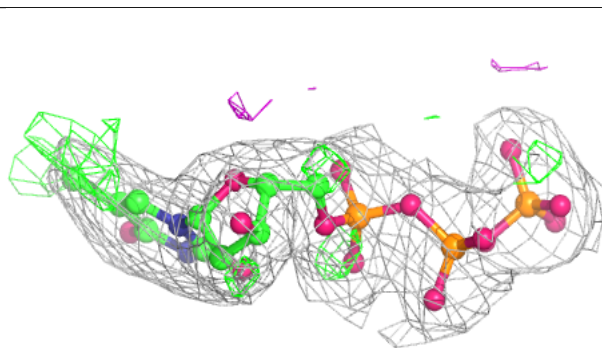
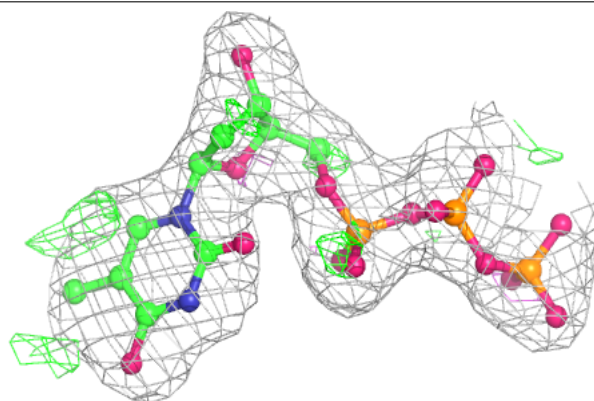


**Electron density around DGT C 702:**

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

**Electron density around TTP C 701:**

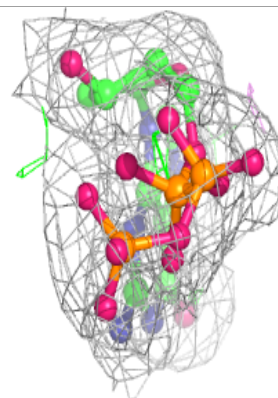
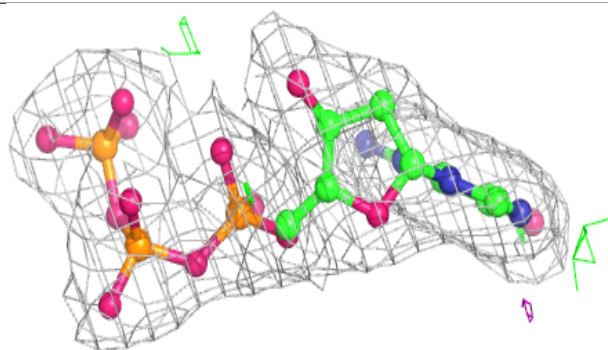
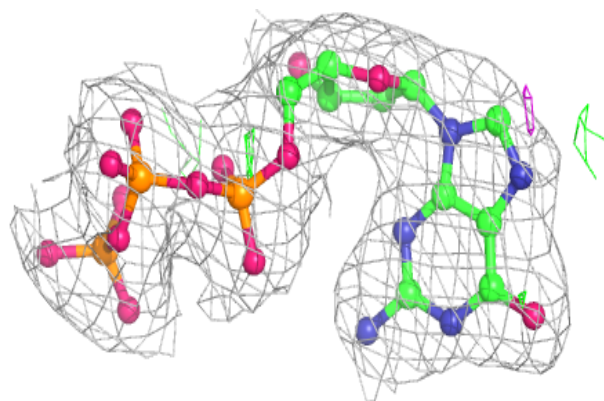
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



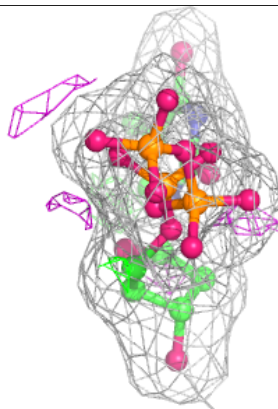
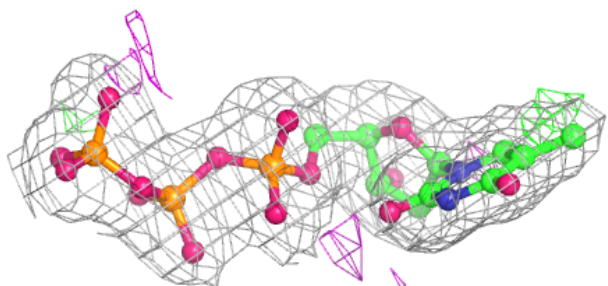
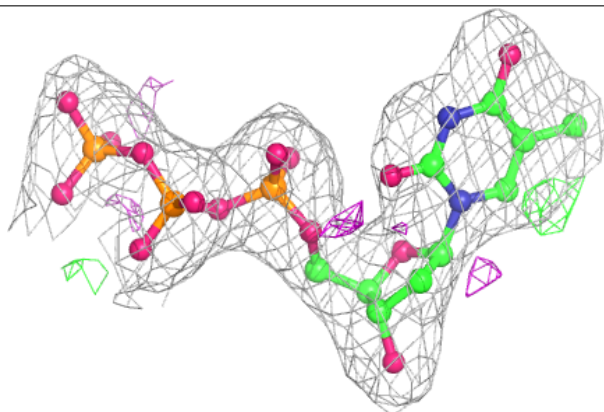


**Electron density around DGT C 703:**

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

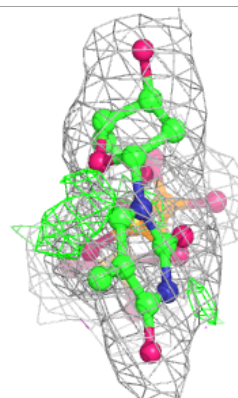
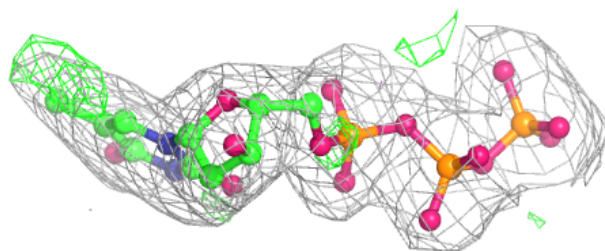
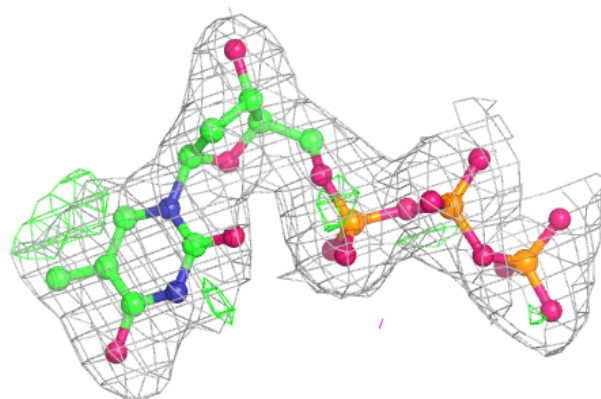
**Electron density around TTP A 703:**

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

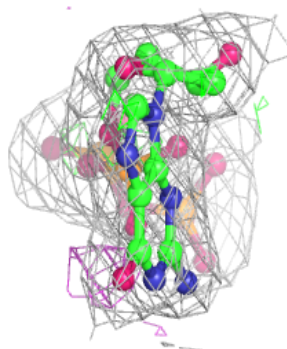
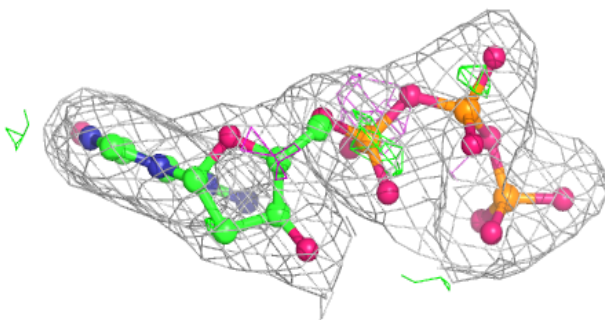
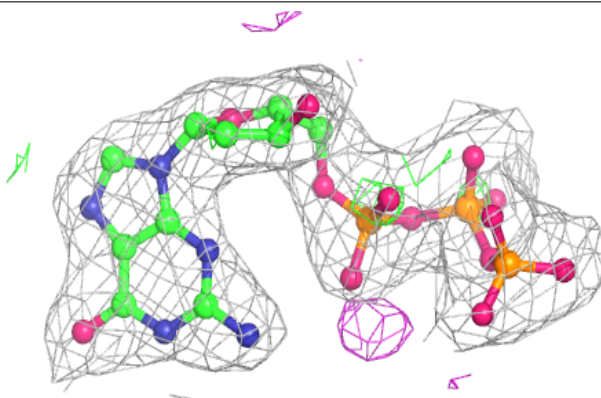


**Electron density around TTP D 701:**

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

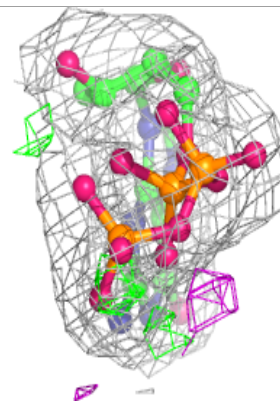
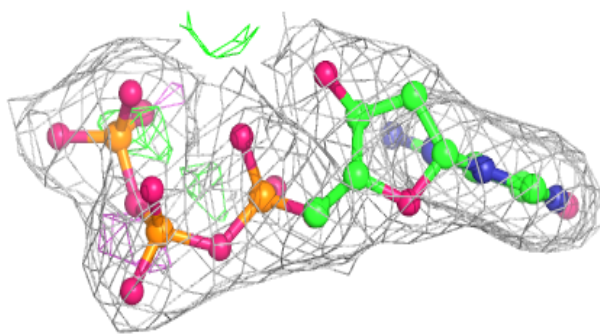
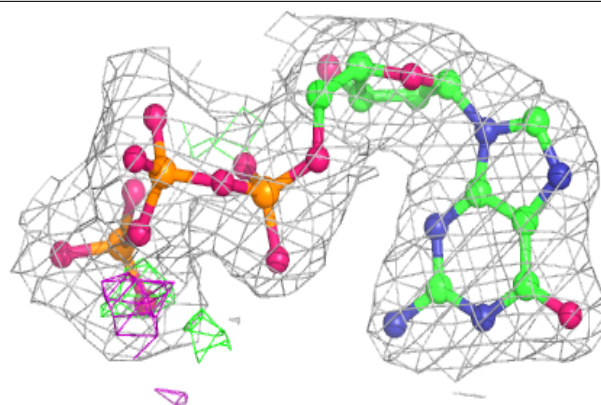
**Electron density around DGT D 702:**

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



**Electron density around DGT A 701:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.