



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 27, 2020 – 10:05 AM EDT

PDB ID : 6WPF  
Title : Structure of HIV-1 Reverse Transcriptase (RT) in complex with dsDNA and d4T  
Authors : Bertoletti, N.; Anderson, K.S.  
Deposited on : 2020-04-27  
Resolution : 2.53 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 : 2.14.6  
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) : 2.14.6

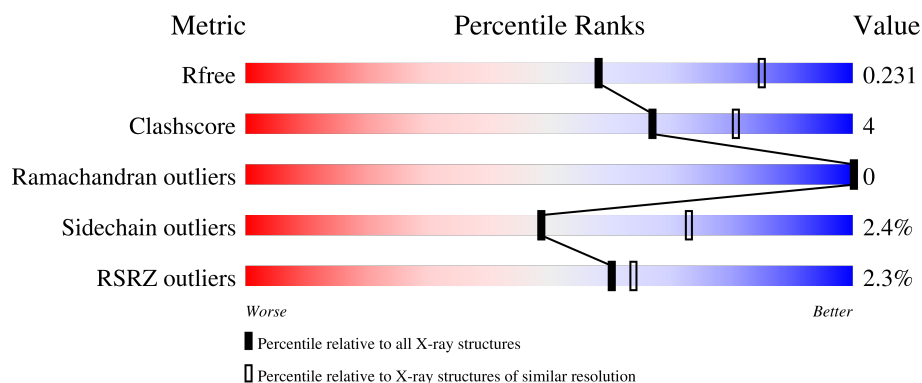
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.53 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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	P	21	<div> <div></div> <div>76%10%14%</div> </div>
2	T	27	<div> <div>4%</div> <div>78%7%15%</div> </div>
3	A	561	<div> <div>2%</div> <div>87%11%..</div> </div>
4	B	452	<div> <div>2%</div> <div>76%10%13%</div> </div>

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 8601 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 DNA chain called DNA Primer 21-mer.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	P	18	Total	C	N	O	P	S	0	0	0
			367	175	64	110	17	1			

- Molecule 2 is a DNA chain called DNA template 27-mer.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	T	23	Total	C	N	O	P		0	0	0
			478	223	98	134	23				

- Molecule 3 is a protein called Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	A	555	Total	C	N	O	S		0	0	0
			4427	2865	743	811	8				

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP P04585
A	258	CYS	GLN	engineered mutation	UNP P04585
A	280	SER	CYS	engineered mutation	UNP P04585

- Molecule 4 is a protein called p51 RT.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	B	394	Total	C	N	O	S		0	0	0
			3114	2026	514	569	5				

There are 13 discrepancies between the modelled and reference sequences:

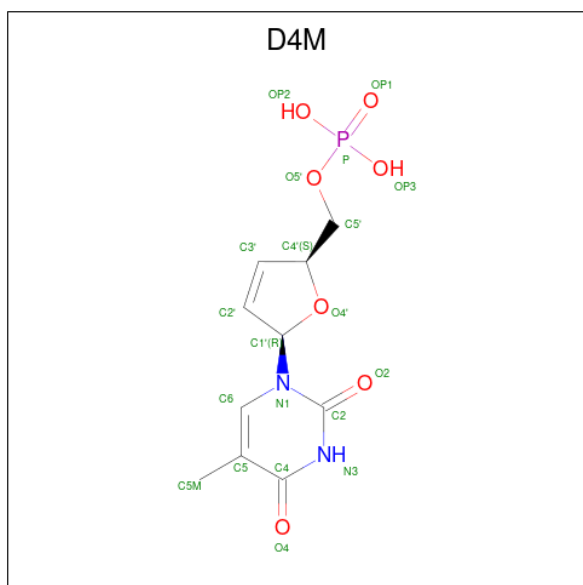
Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	MET	-	expression tag	UNP P04585

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	GLY	-	expression tag	UNP P04585
B	-9	SER	-	expression tag	UNP P04585
B	-8	SER	-	expression tag	UNP P04585
B	-7	HIS	-	expression tag	UNP P04585
B	-6	HIS	-	expression tag	UNP P04585
B	-5	HIS	-	expression tag	UNP P04585
B	-4	HIS	-	expression tag	UNP P04585
B	-3	HIS	-	expression tag	UNP P04585
B	-2	HIS	-	expression tag	UNP P04585
B	-1	SER	-	expression tag	UNP P04585
B	0	SER	-	expression tag	UNP P04585
B	280	SER	CYS	engineered mutation	UNP P04585

- Molecule 5 is [(5R)-5-(5-METHYL-2,4-DIOXO-3,4-DIHYDROPYRIMIDIN-1(2H)-YL)-2,5-DIHYDROFURAN-2-YL]METHYL DIHYDROGEN PHOSPHATE (three-letter code: D4M) (formula: C<sub>10</sub>H<sub>13</sub>N<sub>2</sub>O<sub>7</sub>P) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	P	1	Total	C	N	O	P	0	0
			19	10	2	6	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

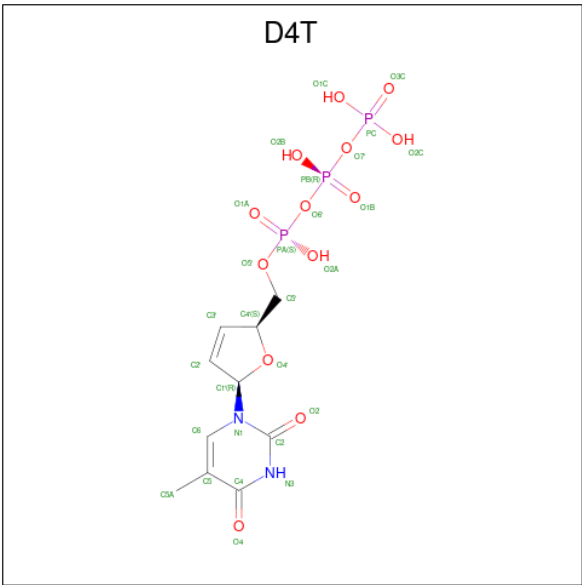


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	P	1	Total	O	S	0	0
			5	4	1		
6	T	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

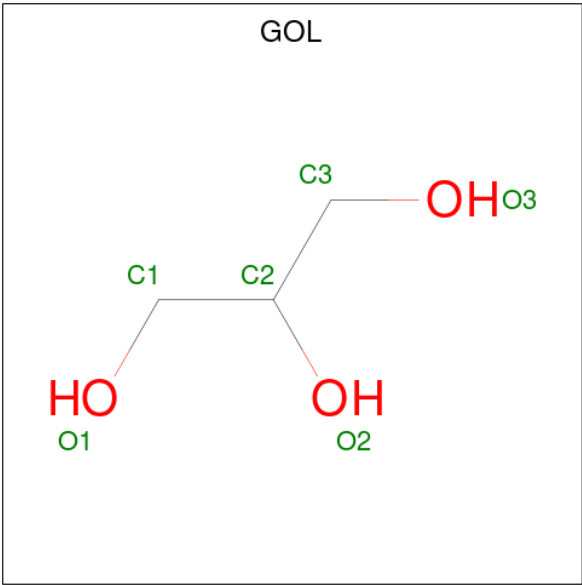
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	P	1	Total	Mg	0	0
			1	1		
7	A	2	Total	Mg	0	0
			2	2		

- Molecule 8 is 2',3'-DEHYDRO-2',3'-DEOXY-THYMIDINE 5'-TRIPHOSPHATE (three-letter code: D4T) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>2</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	0	0
			28	10	2	13	3		

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 10 is water.

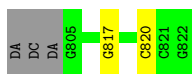
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	P	7	Total 7	O 7	0	0
10	T	6	Total 6	O 6	0	0
10	A	86	Total 86	O 86	0	0
10	B	40	Total 40	O 40	0	0

### 3 Residue-property plots


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

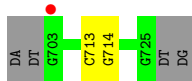
- Molecule 1: DNA Primer 21-mer

Chain P: 




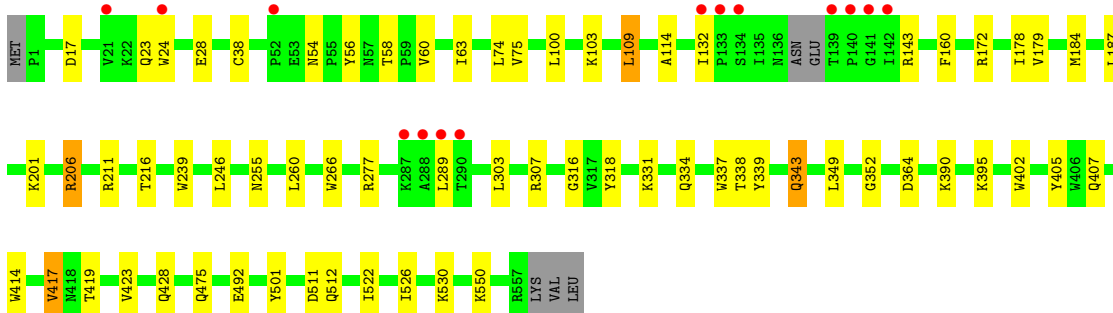
- Molecule 2: DNA template 27-mer

Chain T: 




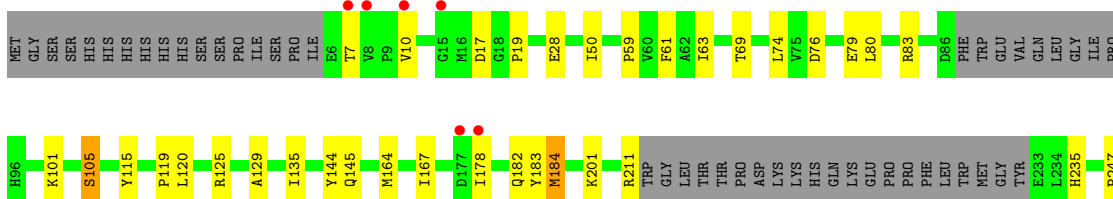
- Molecule 3: Reverse transcriptase/ribonuclease H

Chain A: 

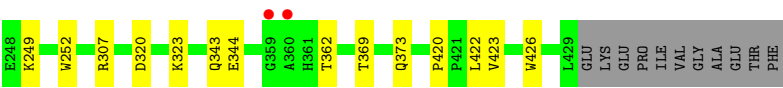


- Molecule 4: p51 RT

Chain B: 







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	165.57Å 170.47Å 103.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.68 – 2.53 47.68 – 2.53	Depositor EDS
% Data completeness (in resolution range)	97.9 (47.68-2.53) 97.9 (47.68-2.53)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, $R_{free}$	0.182 , 0.231 0.182 , 0.231	Depositor DCC
$R_{free}$ test set	2399 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.1	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 45.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8601	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, D4M, SO4, G47, D4T

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	P	0.79	0/380	1.01	0/582
2	T	0.82	0/538	0.84	0/829
3	A	0.38	0/4543	0.55	1/6185 (0.0%)
4	B	0.35	0/3200	0.52	0/4371
All	All	0.44	0/8661	0.59	1/11967 (0.0%)

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
4	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	A	343	GLN	C-N-CA	5.47	135.38	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	B	183	TYR	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	P	367	0	206	1	0
2	T	478	0	255	1	0
3	A	4427	0	4389	35	0
4	B	3114	0	3016	27	0
5	P	19	0	11	0	0
6	A	10	0	0	0	0
6	P	5	0	0	0	0
6	T	5	0	0	0	0
7	A	2	0	0	0	0
7	P	1	0	0	0	0
8	A	28	0	11	0	0
9	B	6	0	8	0	0
10	A	86	0	0	2	0
10	B	40	0	0	0	0
10	P	7	0	0	0	0
10	T	6	0	0	0	0
All	All	8601	0	7896	63	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 (63) 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)
4:B:320:ASP:H	4:B:343:GLN:HE22	1.09	0.97
3:A:364:ASP:HB3	3:A:423:VAL:HG13	1.75	0.69
3:A:260:LEU:HD21	3:A:303:LEU:HD13	1.76	0.67
4:B:79:GLU:HG3	4:B:83:ARG:HE	1.60	0.65
4:B:323:LYS:NZ	4:B:344:GLU:OE2	2.27	0.64
4:B:167:ILE:HG23	4:B:211:ARG:HH11	1.67	0.60
3:A:114:ALA:HB1	3:A:160:PHE:CZ	2.37	0.59
3:A:492:GLU:HG2	3:A:530:LYS:HB2	1.83	0.59
3:A:339:TYR:CZ	3:A:352:GLY:HA3	2.39	0.58
4:B:59:PRO:HG2	4:B:76:ASP:HB3	1.85	0.58
3:A:405:TYR:CE2	3:A:407:GLN:HB2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:60:VAL:HG22	3:A:75:VAL:HG22	1.87	0.55
3:A:54:ASN:O	3:A:143:ARG:NH1	2.39	0.55
3:A:38:CYS:SG	3:A:132:ILE:HD11	2.47	0.54
3:A:23:GLN:HE22	3:A:60:VAL:H	1.56	0.54
4:B:7:THR:HG22	4:B:119:PRO:HB2	1.91	0.53
3:A:172:ARG:HA	10:A:731:HOH:O	2.10	0.52
4:B:178:ILE:HD11	4:B:201:LYS:HG2	1.92	0.52
2:T:713:DC:H2''	2:T:714:DG:C8	2.46	0.51
3:A:303:LEU:O	3:A:307:ARG:HG3	2.11	0.50
4:B:320:ASP:N	4:B:343:GLN:HE22	1.93	0.49
3:A:17:ASP:OD1	3:A:56:TYR:OH	2.23	0.49
3:A:239:TRP:CE2	3:A:316:GLY:HA3	2.48	0.49
4:B:61:PHE:CZ	4:B:74:LEU:HD23	2.48	0.48
3:A:343:GLN:HG3	3:A:349:LEU:HD11	1.96	0.48
3:A:160:PHE:HE2	3:A:184:MET:O	1.97	0.47
4:B:184:MET:HG2	4:B:184:MET:H	1.38	0.47
3:A:417:VAL:HG13	3:A:419:THR:HG23	1.97	0.47
4:B:105:SER:HB3	4:B:235:HIS:CE1	2.50	0.47
4:B:164:MET:HG2	4:B:182:GLN:NE2	2.30	0.46
4:B:19:PRO:HG3	4:B:80:LEU:HB2	1.96	0.46
3:A:109:LEU:HD12	3:A:187:LEU:HB2	1.98	0.46
3:A:343:GLN:HG3	3:A:349:LEU:CD1	2.45	0.46
4:B:28:GLU:HA	4:B:135:ILE:HD11	1.97	0.46
3:A:511:ASP:OD1	3:A:512:GLN:HG3	2.16	0.46
4:B:249:LYS:HB2	4:B:252:TRP:CE2	2.51	0.46
3:A:475:GLN:HB3	3:A:501:TYR:CE2	2.50	0.46
4:B:120:LEU:HD23	4:B:125:ARG:HG2	1.99	0.45
4:B:369:THR:HG22	4:B:373:GLN:HE21	1.81	0.45
3:A:246:LEU:HD13	3:A:260:LEU:HD11	1.99	0.45
3:A:178:ILE:HD11	3:A:201:LYS:HG2	1.99	0.45
4:B:423:VAL:HA	4:B:426:TRP:CD1	2.52	0.45
1:P:820:DC:H4'	3:A:266:TRP:CE2	2.52	0.44
3:A:395:LYS:HD3	3:A:414:TRP:CZ2	2.53	0.44
4:B:422:LEU:HA	4:B:422:LEU:HD23	1.81	0.43
3:A:100:LEU:O	3:A:318:TYR:HB3	2.17	0.43
4:B:247:PRO:O	4:B:307:ARG:NH2	2.48	0.43
3:A:522:ILE:O	3:A:526:ILE:HG13	2.17	0.43
3:A:103:LYS:HE3	3:A:179:VAL:HG11	2.01	0.43
3:A:390:LYS:HB3	3:A:417:VAL:HG21	2.01	0.42
3:A:331:LYS:HB2	3:A:337:TRP:CZ3	2.54	0.42
3:A:550:LYS:HB2	3:A:550:LYS:HE3	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:255:ASN:HD22	3:A:289:LEU:HD22	1.85	0.42
4:B:129:ALA:HA	4:B:144:TYR:O	2.20	0.41
4:B:115:TYR:OH	4:B:184:MET:O	2.25	0.41
3:A:407:GLN:HG2	10:A:703:HOH:O	2.20	0.41
3:A:206:ARG:NH1	3:A:216:THR:O	2.54	0.41
4:B:17:ASP:O	4:B:83:ARG:HD3	2.20	0.41
4:B:50:ILE:HD13	4:B:145:GLN:HB3	2.03	0.41
4:B:7:THR:CG2	4:B:119:PRO:HB2	2.51	0.40
4:B:420:PRO:O	4:B:423:VAL:HG12	2.21	0.40
4:B:369:THR:HG22	4:B:373:GLN:NE2	2.36	0.40
3:A:63:ILE:HD13	3:A:74:LEU:HD11	2.02	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	
3	A	551/561 (98%)	537 (98%)	14 (2%)	0	100	100
4	B	388/452 (86%)	379 (98%)	9 (2%)	0	100	100
All	All	939/1013 (93%)	916 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	
3	A	468/501 (93%)	456 (97%)	12 (3%)	46	70
4	B	322/411 (78%)	315 (98%)	7 (2%)	52	75
All	All	790/912 (87%)	771 (98%)	19 (2%)	49	73

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	24	TRP
3	A	28	GLU
3	A	58	THR
3	A	109	LEU
3	A	206	ARG
3	A	211	ARG
3	A	277	ARG
3	A	334	GLN
3	A	338	THR
3	A	402	TRP
3	A	417	VAL
3	A	428	GLN
4	B	10	VAL
4	B	63	ILE
4	B	69	THR
4	B	101	LYS
4	B	105	SER
4	B	184	MET
4	B	362	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	255	ASN
3	A	407	GLN
3	A	474	ASN
3	A	507	GLN
3	A	520	GLN
3	A	524	GLN
3	A	547	GLN
4	B	182	GLN
4	B	343	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	G47	P	817	1,3,2	20,27,28	1.30	2 (10%)	21,38,41	2.30	6 (28%)

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
1	G47	P	817	1,3,2	-	4/7/25/26	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	817	G47	C6-C5	4.68	1.49	1.41
1	P	817	G47	C5-C4	2.54	1.47	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	817	G47	C2-N3-C4	6.46	122.62	115.28
1	P	817	G47	C5-C6-N1	-4.04	117.91	123.43
1	P	817	G47	C6-N1-C2	3.82	122.02	115.18
1	P	817	G47	C4-C5-N7	-3.25	106.01	109.40
1	P	817	G47	C6-C5-C4	-3.17	117.77	120.80
1	P	817	G47	N3-C2-N1	-2.44	122.37	126.23



There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	P	817	G47	O4'-C4'-C5'-O5'
1	P	817	G47	C3'-C4'-C5'-O5'
1	P	817	G47	N1-C2-N2-C6A
1	P	817	G47	N3-C2-N2-C6A

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 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
6	SO4	P	902	-	4,4,4	0.14	0	6,6,6	0.09	0
9	GOL	B	501	-	5,5,5	0.99	0	5,5,5	1.20	0
8	D4T	A	603	7	23,29,29	4.73	7 (30%)	31,45,45	2.37	12 (38%)
6	SO4	T	801	-	4,4,4	0.13	0	6,6,6	0.17	0
6	SO4	A	605	-	4,4,4	0.10	0	6,6,6	0.32	0
5	D4M	P	901	1,7	14,20,21	1.33	1 (7%)	14,28,31	2.50	5 (35%)
6	SO4	A	604	-	4,4,4	0.24	0	6,6,6	0.25	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
8	D4T	A	603	7	-	6/22/31/31	0/2/2/2
9	GOL	B	501	-	-	4/4/4/4	-
5	D4M	P	901	1,7	-	3/4/18/19	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	603	D4T	C1'-C2'	-12.89	1.32	1.49
8	A	603	D4T	C4'-C3'	-12.36	1.28	1.50
8	A	603	D4T	C6-N1	-8.48	1.36	1.46
8	A	603	D4T	O4'-C4'	6.51	1.58	1.44
8	A	603	D4T	O4'-C1'	5.88	1.52	1.42
8	A	603	D4T	C3'-C2'	4.68	1.46	1.32
8	A	603	D4T	C6-C5	-4.05	1.39	1.51
5	P	901	D4M	C4-C5	3.88	1.49	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	603	D4T	C4'-O4'-C1'	-7.27	103.03	109.99
5	P	901	D4M	C4-N3-C2	7.16	121.19	115.14
8	A	603	D4T	C4-N3-C2	-4.76	121.04	126.86
8	A	603	D4T	C5-C6-N1	4.65	120.27	111.11
8	A	603	D4T	C5A-C5-C6	4.01	120.90	112.34
5	P	901	D4M	C2'-C1'-N1	3.40	117.08	113.44
8	A	603	D4T	O2-C2-N1	-2.99	119.35	123.11
8	A	603	D4T	O4'-C4'-C5'	-2.79	108.80	110.61
8	A	603	D4T	C6-C5-C4	2.70	119.28	111.53
5	P	901	D4M	O4'-C4'-C5'	-2.65	108.90	110.61
8	A	603	D4T	O2C-PC-O7'	2.64	113.49	104.64
5	P	901	D4M	C4'-O4'-C1'	-2.46	107.64	109.99
8	A	603	D4T	N3-C2-N1	2.42	119.22	116.65
8	A	603	D4T	C1'-C2'-C3'	2.12	112.26	109.68
8	A	603	D4T	O4'-C4'-C3'	2.10	106.02	103.06
8	A	603	D4T	C5'-C4'-C3'	-2.03	111.89	115.61
5	P	901	D4M	C5'-C4'-C3'	-2.02	111.91	115.61

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	501	GOL	C1-C2-C3-O3

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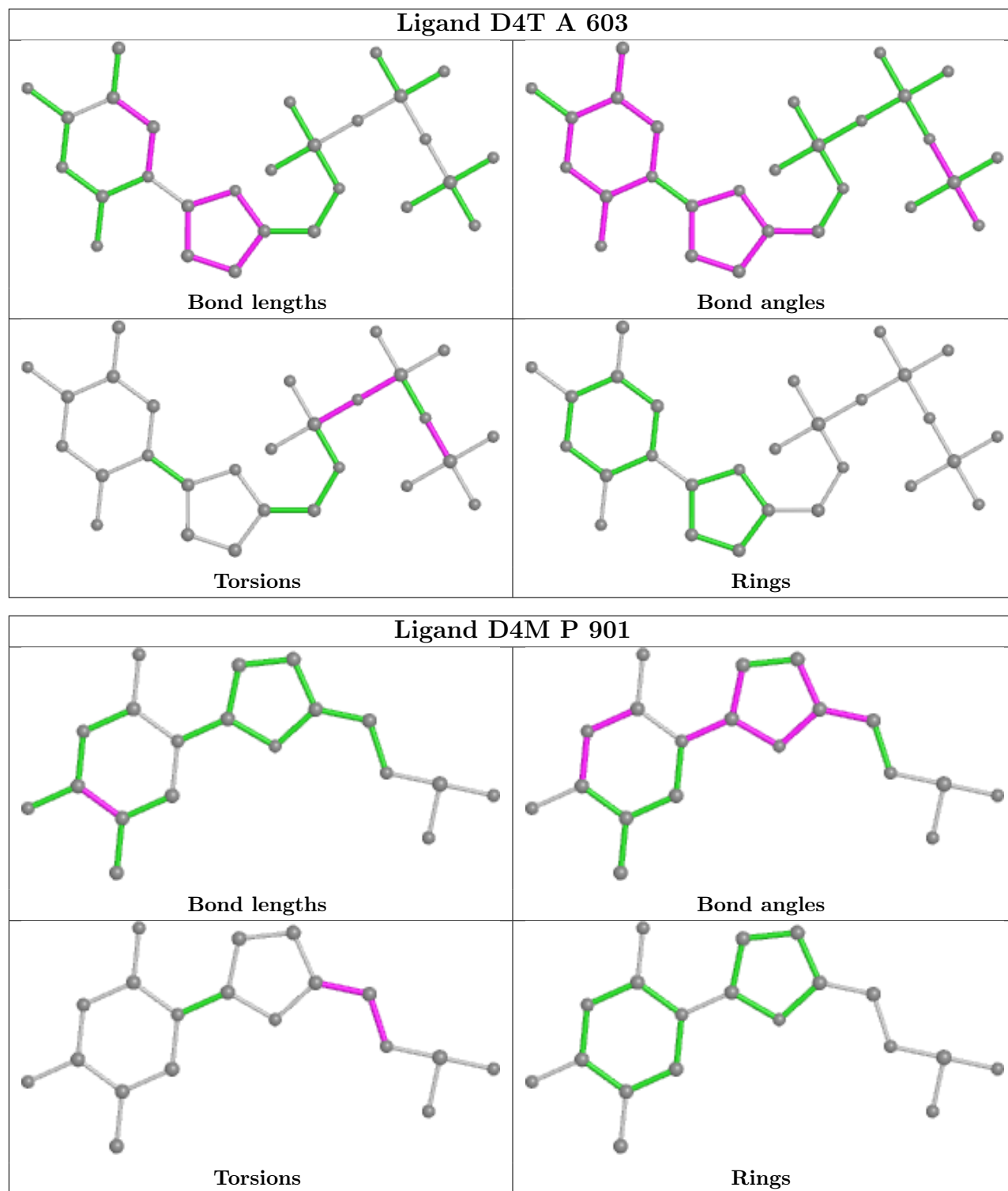
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Mol	Chain	Res	Type	Atoms
8	A	603	D4T	PB-O7'-PC-O1C
8	A	603	D4T	PB-O7'-PC-O2C
5	P	901	D4M	O4'-C4'-C5'-O5'
5	P	901	D4M	C3'-C4'-C5'-O5'
9	B	501	GOL	O1-C1-C2-C3
9	B	501	GOL	O1-C1-C2-O2
9	B	501	GOL	O2-C2-C3-O3
8	A	603	D4T	PA-O6'-PB-O1B
8	A	603	D4T	PB-O6'-PA-O1A
5	P	901	D4M	C4'-C5'-O5'-P
8	A	603	D4T	PB-O6'-PA-O2A
8	A	603	D4T	PB-O7'-PC-O3C

There are no ring outliers.

No monomer is involved in short contacts.

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.



## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	P	17/21 (80%)	-0.56	0 100 100	40, 60, 86, 96	0
2	T	23/27 (85%)	-0.15	1 (4%) 35 39	39, 73, 101, 119	0
3	A	555/561 (98%)	-0.05	14 (2%) 57 61	26, 45, 90, 121	0
4	B	394/452 (87%)	-0.01	8 (2%) 65 68	28, 55, 90, 126	0
All	All	989/1061 (93%)	-0.05	23 (2%) 60 64	26, 50, 92, 126	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	133	PRO	4.1
3	A	288	ALA	3.9
3	A	290	THR	3.4
3	A	141	GLY	3.0
3	A	134	SER	3.0
4	B	360	ALA	2.8
3	A	142	ILE	2.7
3	A	139	THR	2.6
4	B	8	VAL	2.5
3	A	287	LYS	2.5
3	A	140	PRO	2.4
3	A	132	ILE	2.4
3	A	52	PRO	2.3
4	B	177	ASP	2.3
4	B	359	GLY	2.3
3	A	289	LEU	2.3
4	B	10	VAL	2.3
4	B	15	GLY	2.2
4	B	178	ILE	2.2
2	T	703	DG	2.1
3	A	21	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
3	A	24	TRP	2.1
4	B	7	THR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	G47	P	817	25/26	0.94	0.12	44,57,68,74	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

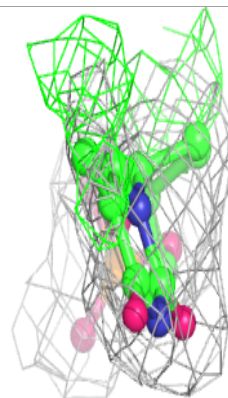
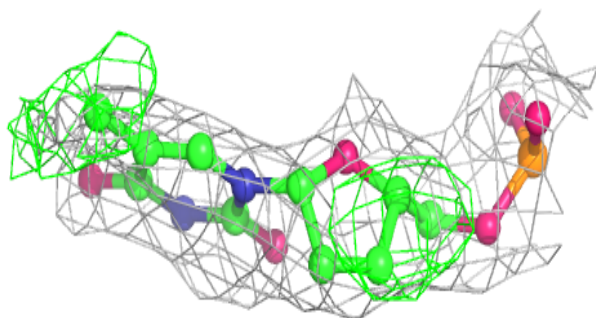
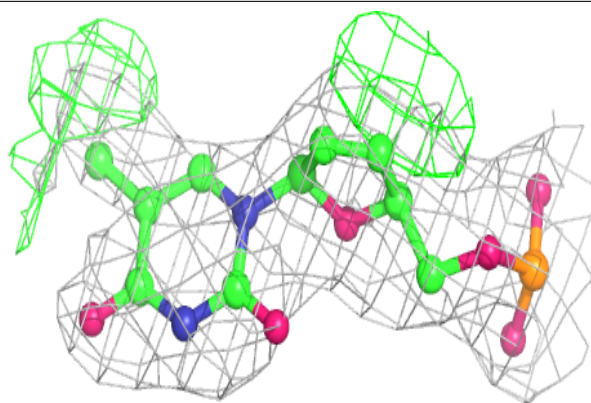
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
6	SO4	P	902	5/5	0.82	0.23	122,122,124,126	0
6	SO4	A	605	5/5	0.86	0.20	113,114,115,116	0
9	GOL	B	501	6/6	0.87	0.29	46,48,57,61	0
6	SO4	T	801	5/5	0.88	0.14	105,108,109,109	0
5	D4M	P	901	19/20	0.89	0.20	40,71,82,84	0
7	MG	A	601	1/1	0.95	0.18	24,24,24,24	0
7	MG	P	903	1/1	0.97	0.05	43,43,43,43	0
7	MG	A	602	1/1	0.97	0.05	32,32,32,32	0
8	D4T	A	603	28/28	0.97	0.12	32,46,51,54	0
6	SO4	A	604	5/5	0.99	0.15	52,58,61,61	0

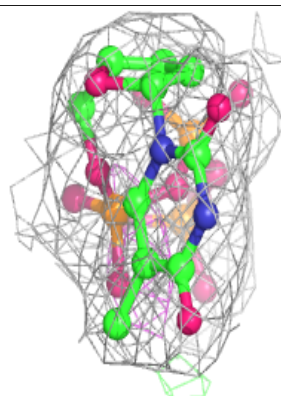
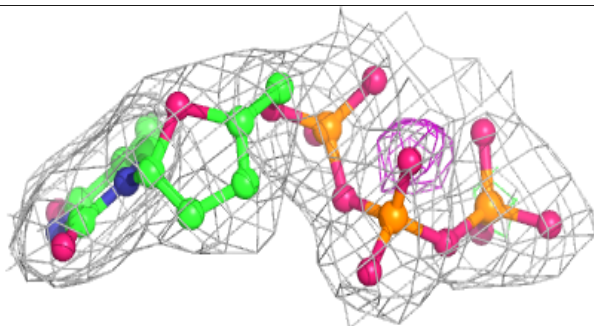
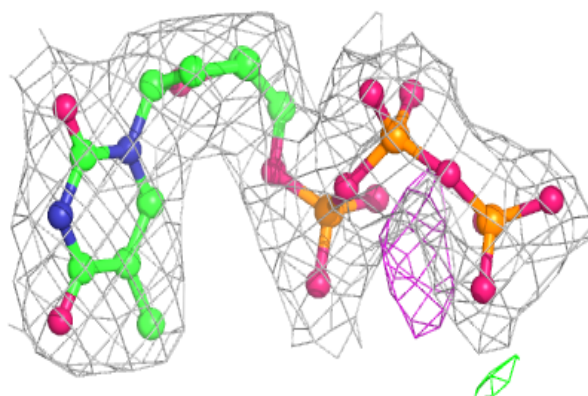
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around D4M P 901:**

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

**Electron density around D4T 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.