



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 2, 2021 – 12:05 PM EDT

PDB ID : 1J3K  
Title : Quadruple mutant (N51I+C59R+S108N+I164L) Plasmodium falciparum dihydrofolate reductase-thymidylate synthase (PfDHFR-TS) complexed with WR99210, NADPH, and dUMP  
Authors : Yuvaniyama, J.; Chitnumsub, P.; Kamchonwongpaisan, S.; Vanichtanankul, J.; Sirawaraporn, W.; Taylor, P.; Walkinshaw, M.; Yuthavong, Y.  
Deposited on : 2003-02-03  
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
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) : 2.23.2

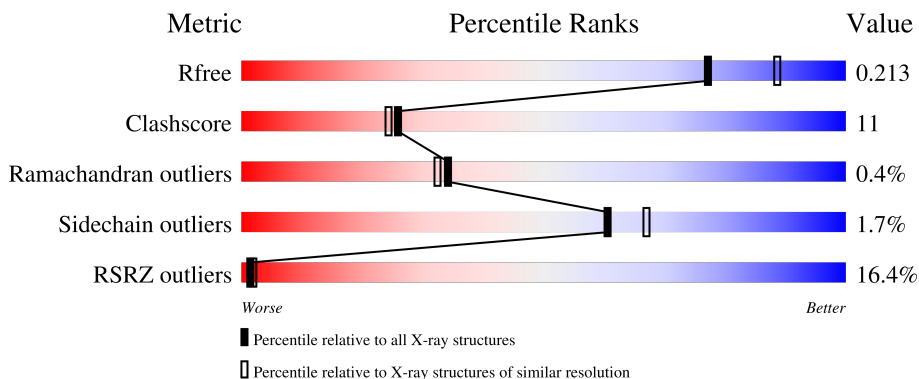
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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  $\geq 3$ , 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	280	 15% 62% 15% 21%
1	B	280	 34% 48% 29% 21%
2	C	328	 7% 91% 8% ..
2	D	328	 6% 87% 12% ..

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10528 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 Bifunctional dihydrofolate reductase-thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	221	1837	1190	297	338	12	0	0	0
1	B	221	1834	1189	297	336	12	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	ILE	ASN	engineered mutation	UNP P13922
A	59	ARG	CYS	engineered mutation	UNP P13922
A	108	ASN	SER	engineered mutation	UNP P13922
A	164	LEU	ILE	engineered mutation	UNP P13922
B	51	ILE	ASN	engineered mutation	UNP P13922
B	59	ARG	CYS	engineered mutation	UNP P13922
B	108	ASN	SER	engineered mutation	UNP P13922
B	164	LEU	ILE	engineered mutation	UNP P13922

- Molecule 2 is a protein called Bifunctional dihydrofolate reductase-thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	326	2713	1747	456	495	15	0	0	0
2	D	326	2713	1747	456	495	15	0	0	0

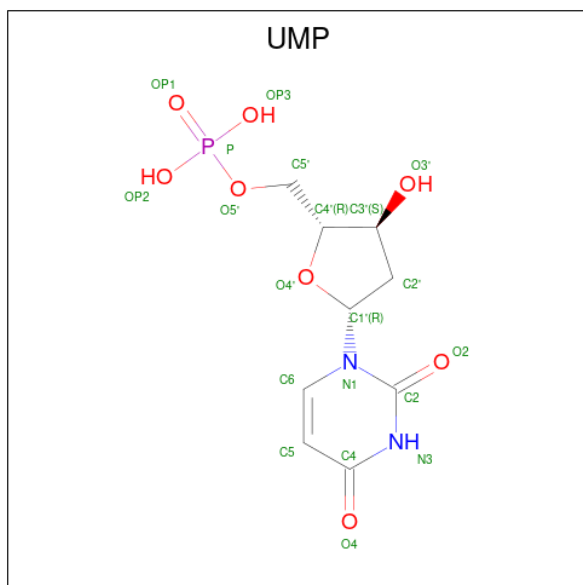
- Molecule 3 is 6,6-DIMETHYL-1-[3-(2,4,5-TRICHLOROPHENOXY)PROPOXY]-1,6-DIHYDRO-1,3,5-TRIAZINE-2,4-DIAMINE (three-letter code: WRA) (formula: C<sub>14</sub>H<sub>18</sub>Cl<sub>3</sub>N<sub>5</sub>O<sub>2</sub>).



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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
4	B	1	48	21	7	17	3	0	0

- Molecule 5 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: C<sub>9</sub>H<sub>13</sub>N<sub>2</sub>O<sub>8</sub>P).




Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
5	C	1	20	9	2	8	1	0	0
5	D	1	20	9	2	8	1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	238	Total	O	0	0
			238	238		
6	B	102	Total	O	0	0
			102	102		
6	C	428	Total	O	0	0
			428	428		
6	D	479	Total	O	0	0
			479	479		



## ● Molecule 2: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain D:  6% 87% 12% ..

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.68Å 158.09Å 165.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.98 – 2.10 28.98 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.8 (28.98-2.10) 96.9 (28.98-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.43 (at 2.10Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.182 , 0.222 0.176 , 0.213	Depositor DCC
$R_{free}$ test set	4523 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.0	Xtrriage
Anisotropy	0.446	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 65.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.006 for -h,l,k	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10528	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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: UMP, WRA, NDP

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	0.64	0/1871	0.88	5/2515 (0.2%)
1	B	0.46	0/1869	0.76	1/2512 (0.0%)
2	C	0.74	1/2784 (0.0%)	0.85	2/3766 (0.1%)
2	D	0.73	1/2784 (0.0%)	0.84	1/3766 (0.0%)
All	All	0.67	2/9308 (0.0%)	0.83	9/12559 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	494	CYS	CB-SG	-9.88	1.65	1.82
2	D	494	CYS	CB-SG	-7.79	1.69	1.82

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	SER	N-CA-C	-8.83	87.17	111.00
2	C	304	LYS	N-CA-C	6.75	129.22	111.00
2	C	351	LEU	N-CA-C	-6.23	94.19	111.00
2	D	351	LEU	N-CA-C	-6.21	94.23	111.00
1	B	30	GLU	N-CA-C	5.85	126.79	111.00

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	1837	0	1873	42	0
1	B	1834	0	1873	86	0
2	C	2713	0	2638	22	0
2	D	2713	0	2638	44	0
3	A	24	0	18	1	0
3	B	24	0	18	0	0
4	A	48	0	26	4	0
4	B	48	0	26	6	0
5	C	20	0	11	1	0
5	D	20	0	11	0	0
6	A	238	0	0	12	1
6	B	102	0	0	11	0
6	C	428	0	0	4	1
6	D	479	0	0	13	0
All	All	10528	0	9132	194	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 194 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:A:1:MET:HG3	1:A:2:MET:H	0.97	1.11
1:A:1:MET:HG3	1:A:2:MET:N	1.78	0.98
2:D:300:GLU:HG3	2:D:304:LYS:NZ	1.78	0.98
2:D:605:ASP:HB3	2:D:608:ALA:HB2	1.46	0.98
1:B:210:VAL:HB	6:B:2028:HOH:O	1.64	0.95

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1592:HOH:O	6:C:1593:HOH:O[3_645]	2.18	0.02

## 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	217/280 (78%)	208 (96%)	8 (4%)	1 (0%)	29	26
1	B	217/280 (78%)	198 (91%)	18 (8%)	1 (0%)	29	26
2	C	324/328 (99%)	312 (96%)	11 (3%)	1 (0%)	41	41
2	D	324/328 (99%)	307 (95%)	16 (5%)	1 (0%)	41	41
All	All	1082/1216 (89%)	1025 (95%)	53 (5%)	4 (0%)	34	32

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	430	TYR
1	A	26	GLY
1	B	28	LYS
2	D	430	TYR

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	210/268 (78%)	203 (97%)	7 (3%)	38	40
1	B	210/268 (78%)	203 (97%)	7 (3%)	38	40
2	C	300/302 (99%)	298 (99%)	2 (1%)	84	88
2	D	300/302 (99%)	299 (100%)	1 (0%)	92	95
All	All	1020/1140 (90%)	1003 (98%)	17 (2%)	60	67

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	286	GLU
2	D	304	LYS
1	B	4	GLN
1	B	23	LYS
1	B	49	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	171	GLN
2	D	424	ASN
1	B	231	ASN
2	D	450	ASN
2	C	424	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	WRA	A	609	-	22,25,25	2.97	14 (63%)	25,36,36	1.29	3 (12%)
3	WRA	B	709	-	22,25,25	3.25	12 (54%)	25,36,36	1.16	2 (8%)
4	NDP	B	710	-	45,52,52	2.68	22 (48%)	53,80,80	1.90	15 (28%)
5	UMP	D	711	-	18,21,21	1.91	4 (22%)	21,31,31	1.69	7 (33%)
5	UMP	C	611	-	18,21,21	1.86	4 (22%)	21,31,31	1.60	7 (33%)
4	NDP	A	610	-	45,52,52	2.68	19 (42%)	53,80,80	1.83	14 (26%)

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	WRA	A	609	-	-	2/8/27/27	0/2/2/2
3	WRA	B	709	-	-	2/8/27/27	0/2/2/2
4	NDP	B	710	-	-	11/30/77/77	0/5/5/5
5	UMP	D	711	-	-	1/7/22/22	0/2/2/2
5	UMP	C	611	-	-	2/7/22/22	0/2/2/2
4	NDP	A	610	-	-	5/30/77/77	0/5/5/5

The worst 5 of 75 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	610	NDP	O4B-C1B	8.99	1.53	1.41
3	B	709	WRA	C17-C12	6.11	1.49	1.38
4	A	610	NDP	C4A-N3A	5.89	1.43	1.35
4	B	710	NDP	C5D-C4D	5.83	1.69	1.51
3	B	709	WRA	C17-C16	5.37	1.47	1.38

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	610	NDP	C1D-N1N-C2N	-5.19	112.47	121.11
4	B	710	NDP	O2X-P2B-O1X	4.62	128.76	110.68
4	B	710	NDP	O3X-P2B-O1X	-4.15	94.44	110.68
4	B	710	NDP	C3N-C2N-N1N	-4.12	117.22	123.10
4	B	710	NDP	C1D-N1N-C2N	-4.12	114.25	121.11

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

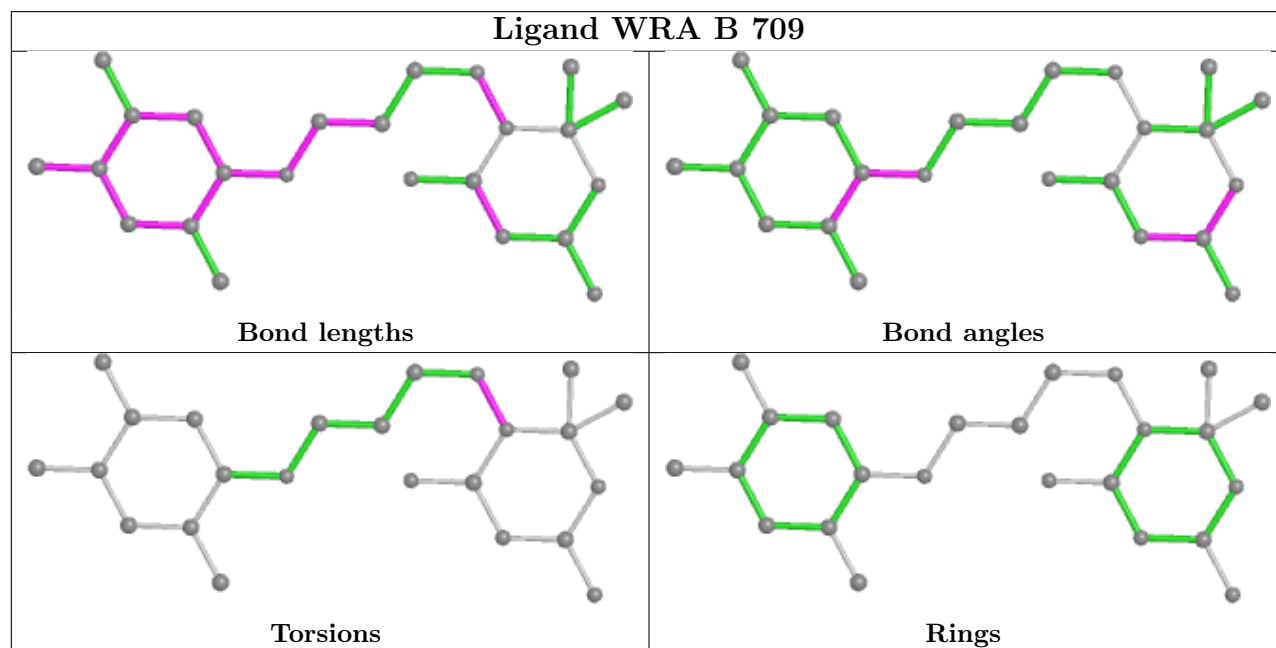
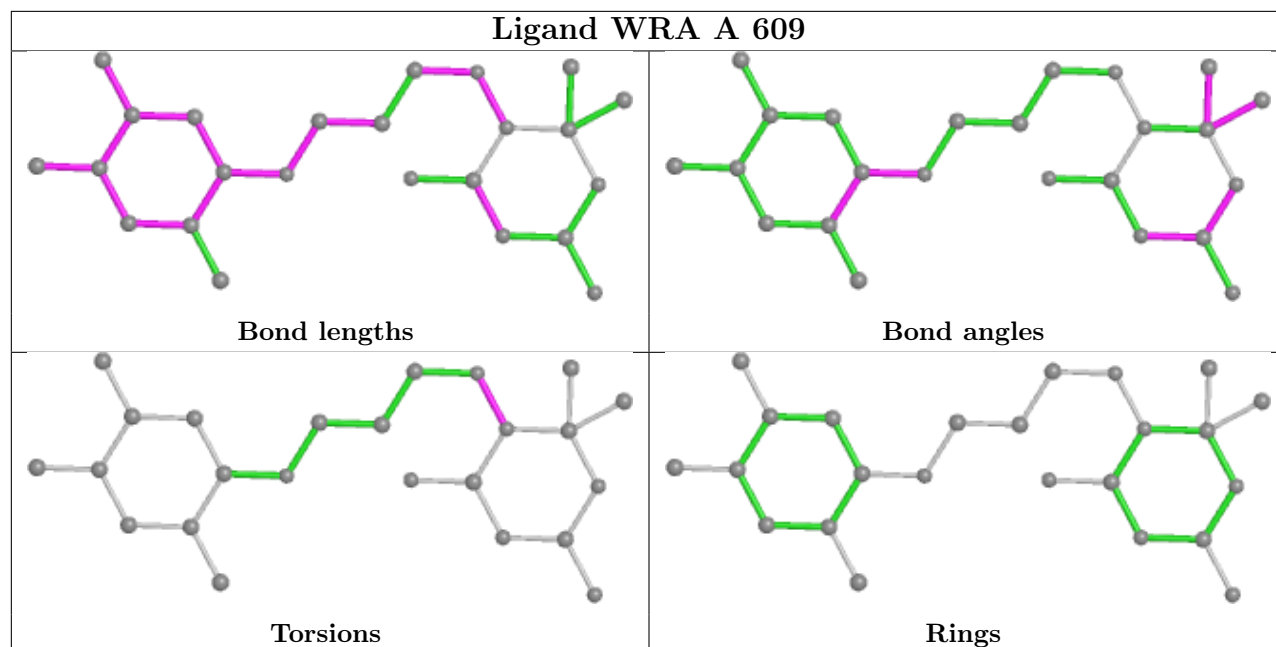
Mol	Chain	Res	Type	Atoms
3	A	609	WRA	C5-N6-O7-C8
3	B	709	WRA	C1-N6-O7-C8
3	B	709	WRA	C5-N6-O7-C8
4	A	610	NDP	PA-O3-PN-O5D
4	A	610	NDP	C5D-O5D-PN-O1N

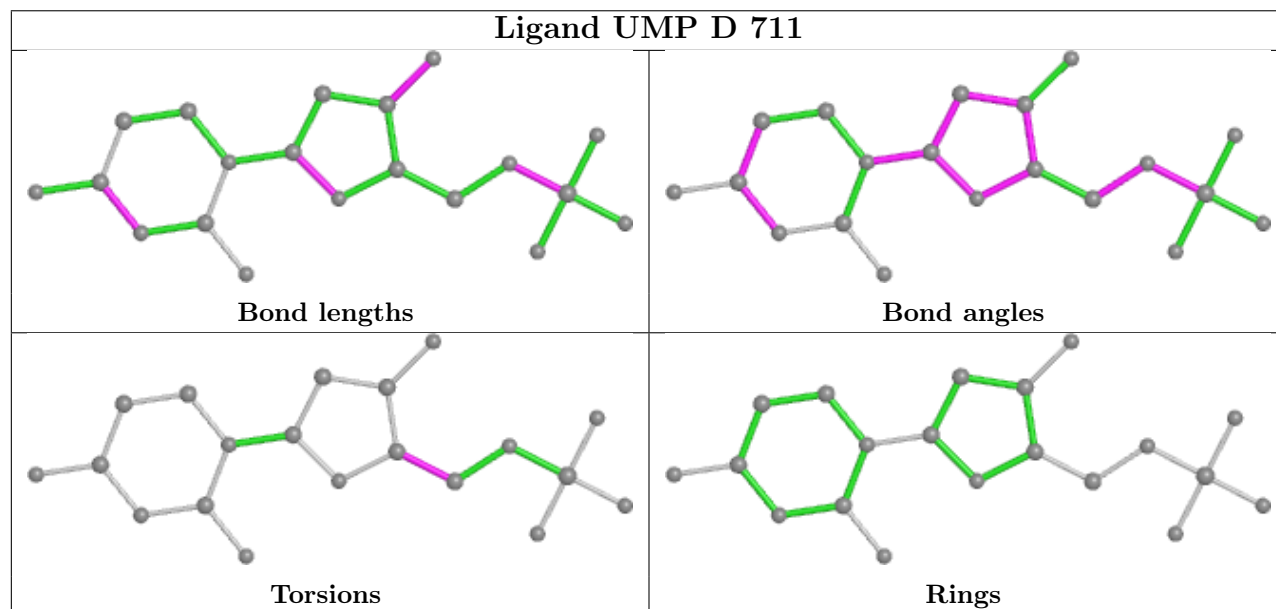
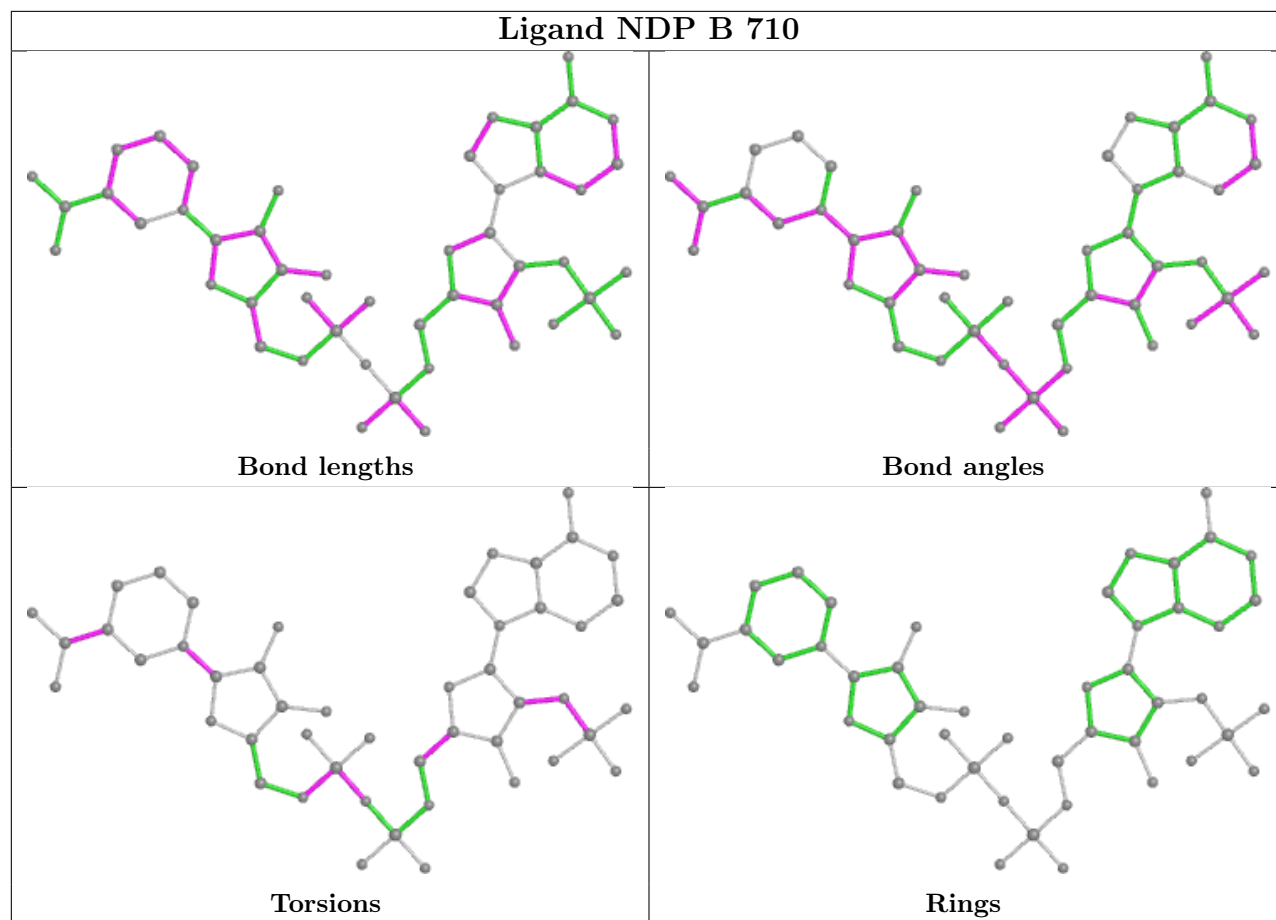
There are no ring outliers.

4 monomers are involved in 12 short contacts:

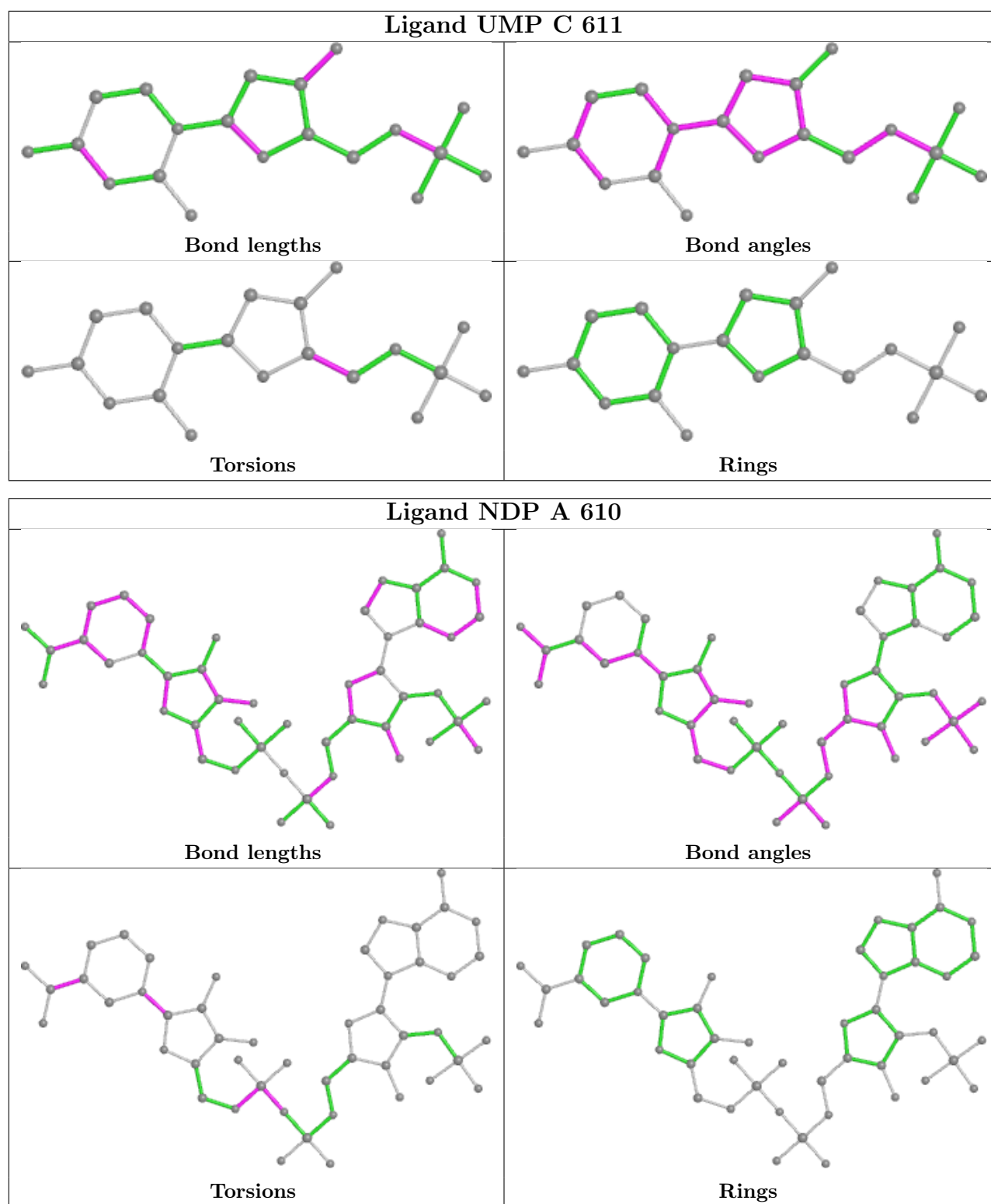
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	609	WRA	1	0
4	B	710	NDP	6	0
5	C	611	UMP	1	0
4	A	610	NDP	4	0

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.









## 5.7 Other polymers [\(i\)](#)

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 [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, 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	221/280 (78%)	0.92	41 (18%) <b>1</b> <b>1</b>	23, 41, 87, 95	0
1	B	221/280 (78%)	2.23	95 (42%) <b>0</b> <b>0</b>	29, 73, 95, 95	0
2	C	326/328 (99%)	0.17	23 (7%) <b>16</b> <b>20</b>	21, 31, 90, 95	0
2	D	326/328 (99%)	0.09	20 (6%) <b>21</b> <b>26</b>	19, 32, 86, 95	0
All	All	1094/1216 (89%)	0.71	179 (16%) <b>1</b> <b>2</b>	19, 37, 94, 95	0

The worst 5 of 179 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	11.8
1	A	2	MET	10.7
1	B	75	TYR	9.8
1	A	23	LYS	9.5
1	A	26	GLY	9.5

### 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](#)

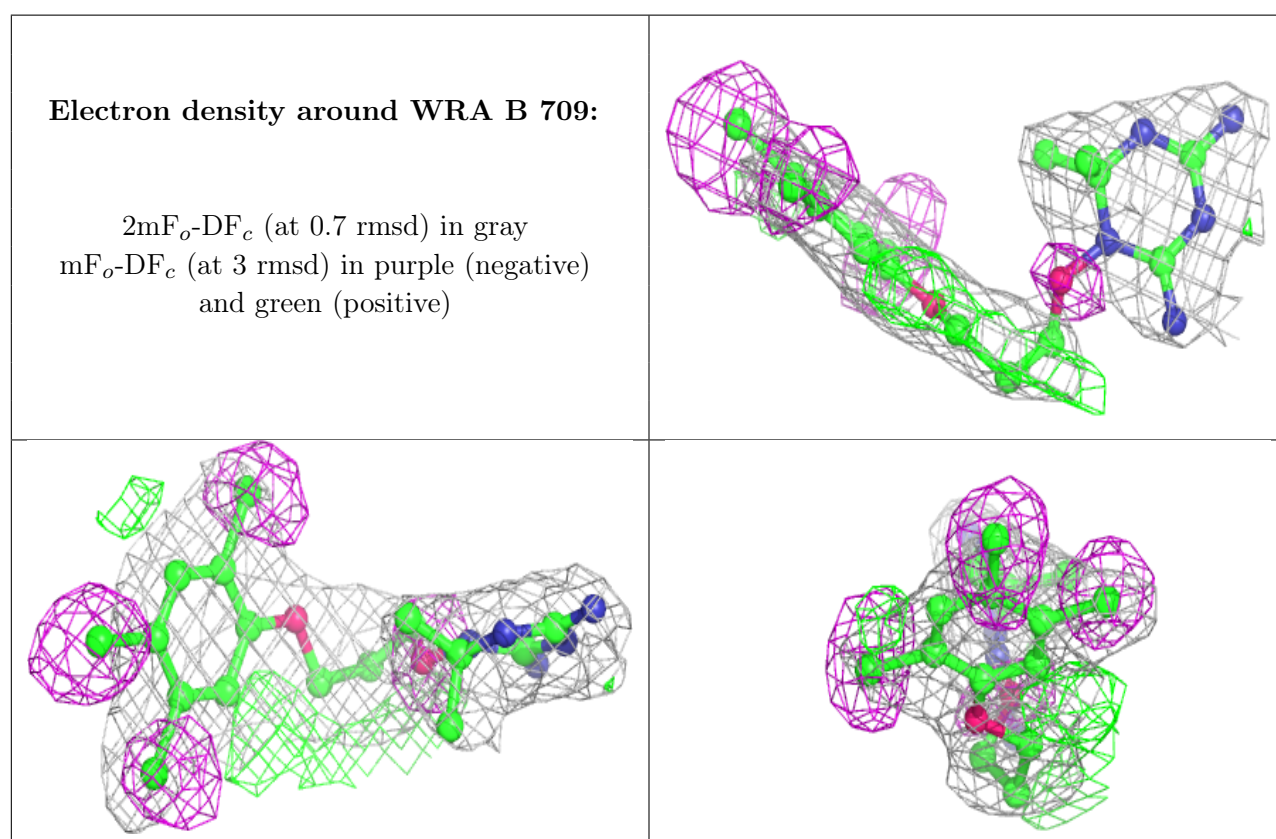
There are no monosaccharides in this entry.

### 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.

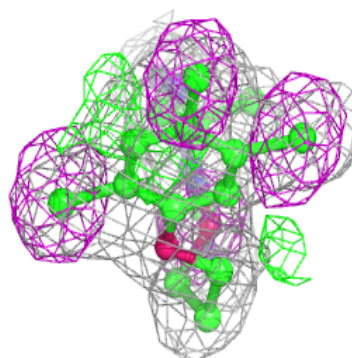
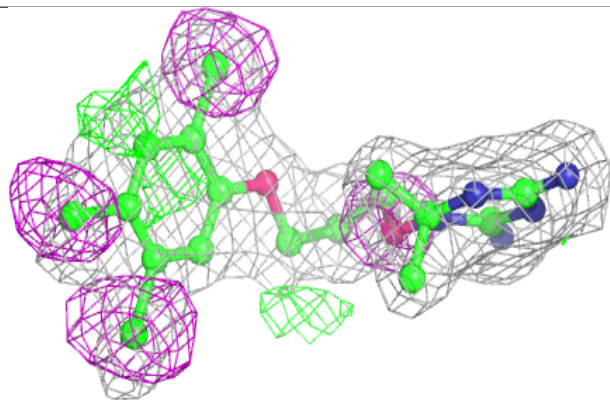
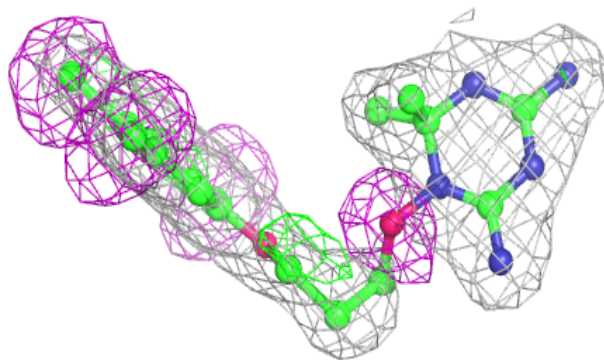
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	WRA	B	709	24/24	0.40	0.32	57,64,65,67	0
3	WRA	A	609	24/24	0.55	0.27	29,41,47,49	0
4	NDP	B	710	48/48	0.75	0.27	76,85,95,95	0
4	NDP	A	610	48/48	0.95	0.10	32,40,49,50	0
5	UMP	D	711	20/20	0.98	0.08	27,31,36,37	0
5	UMP	C	611	20/20	0.99	0.08	23,27,32,32	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.

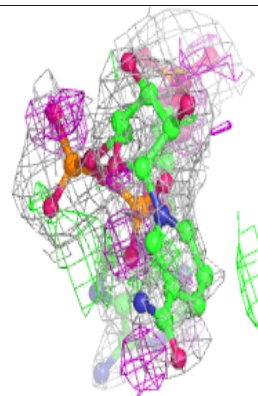
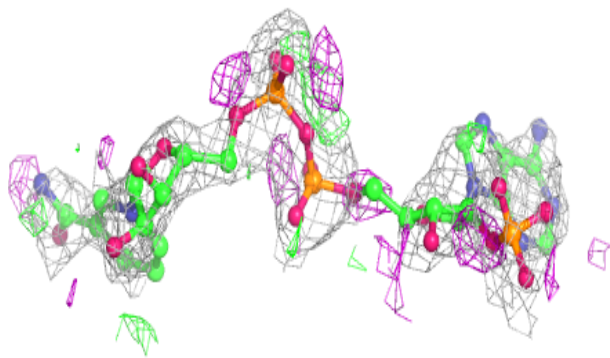
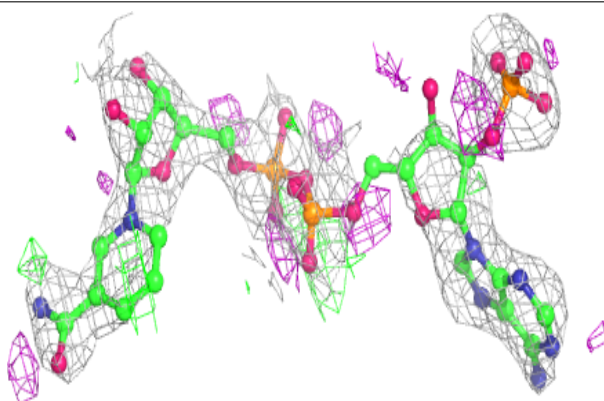


**Electron density around WRA A 609:**

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

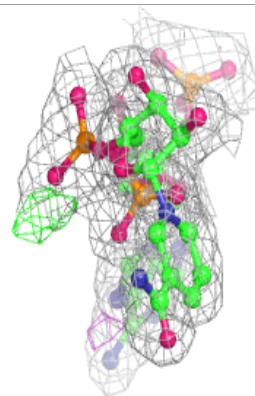
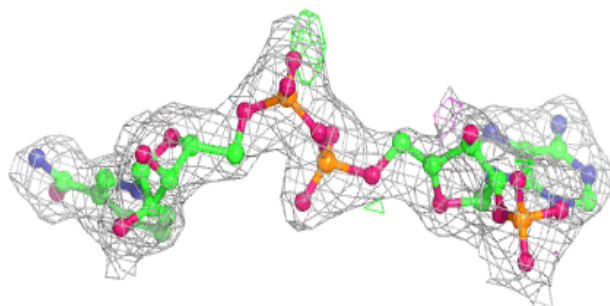
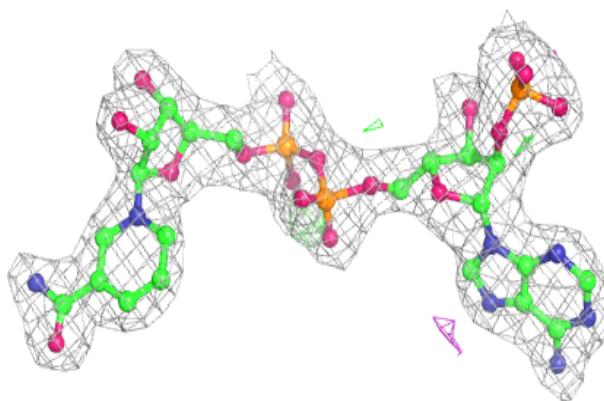
**Electron density around NDP B 710:**

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

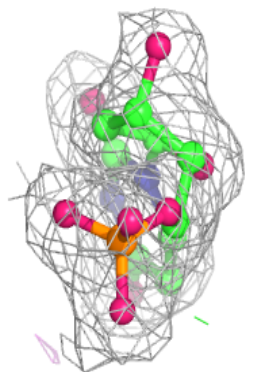
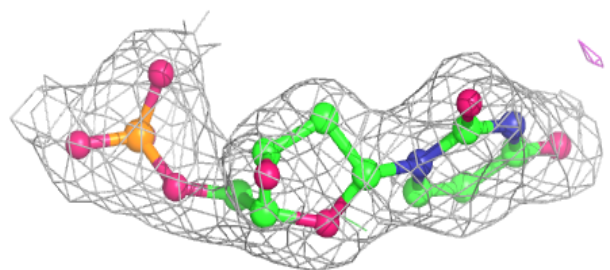
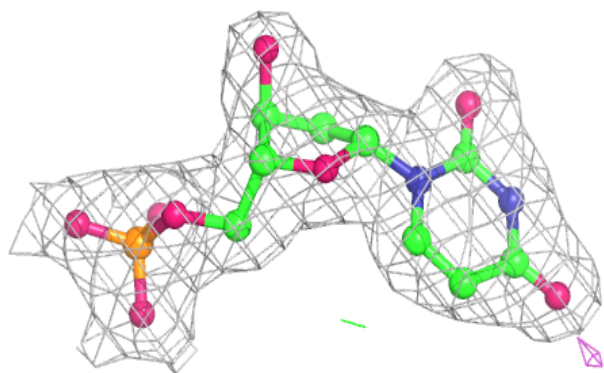


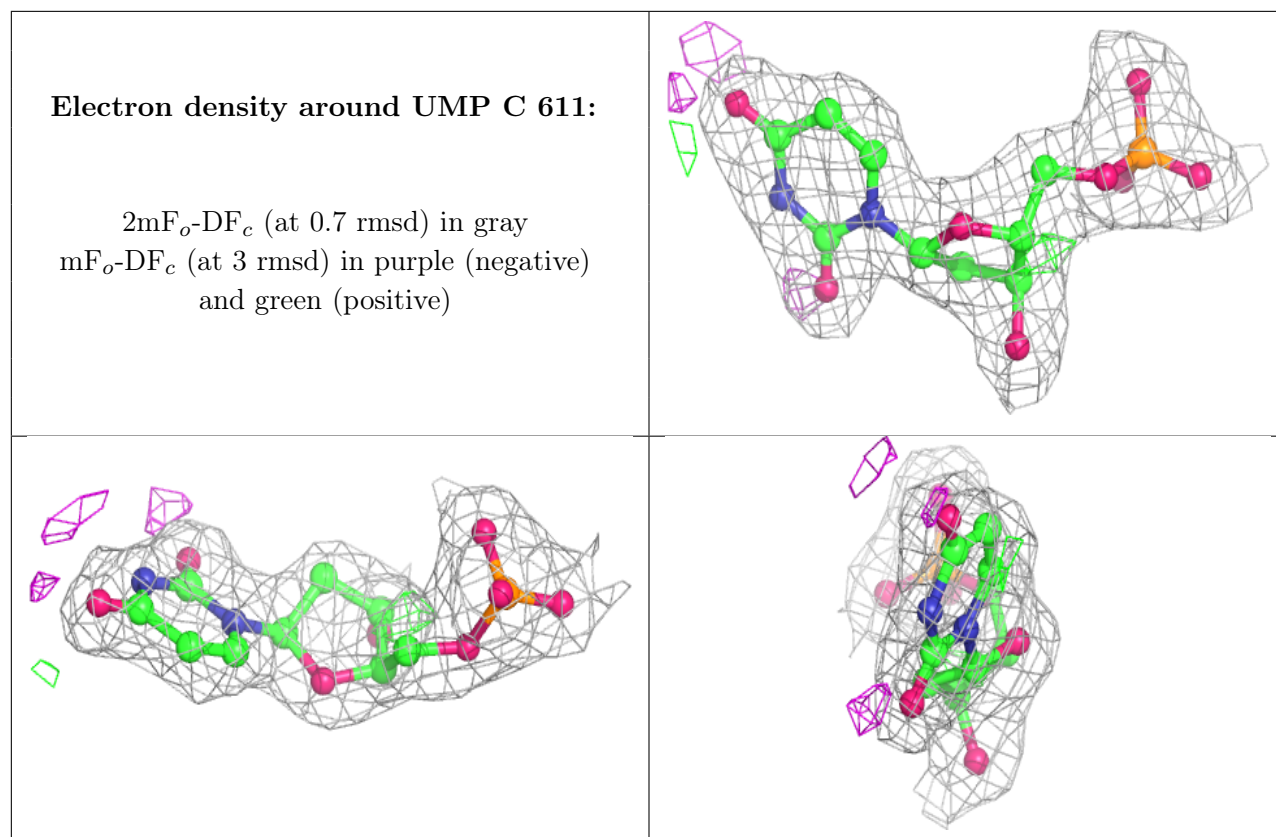
**Electron density around NDP A 610:**

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

**Electron density around UMP D 711:**

$2mF_o-DF_c$  (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.