



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 01:51 PM UTC

PDB ID : 6A2P / pdb_00006a2p
Title : Crystal structure of quadruple mutant (N51I+C59R+S108N+I164L) Plasmodium falciparum DHFR-TS complexed with BT3, NADPH, and dUMP
Authors : Chitnumsub, P.; Jaruwat, A.; Tarnchampoo, B.; Yuthavong, Y.
Deposited on : 2018-06-12
Resolution : 2.60 Å (reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

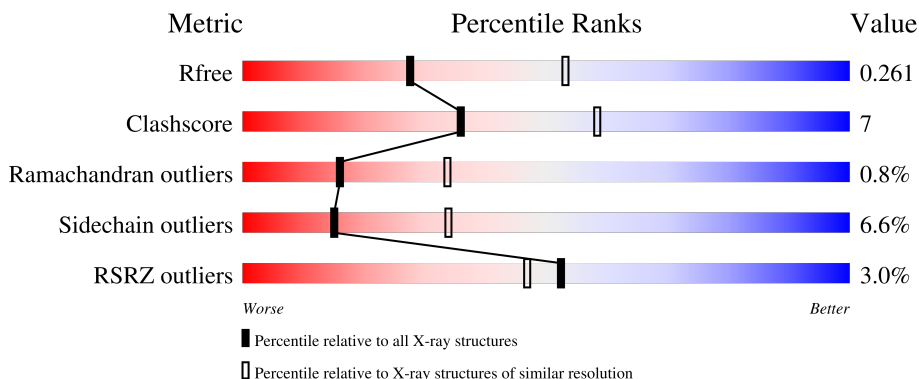
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	608	 4% 70% 17% • 9% 10%
1	B	608	 4% 65% 22% • 9% 9%

2 Entry composition [i](#)

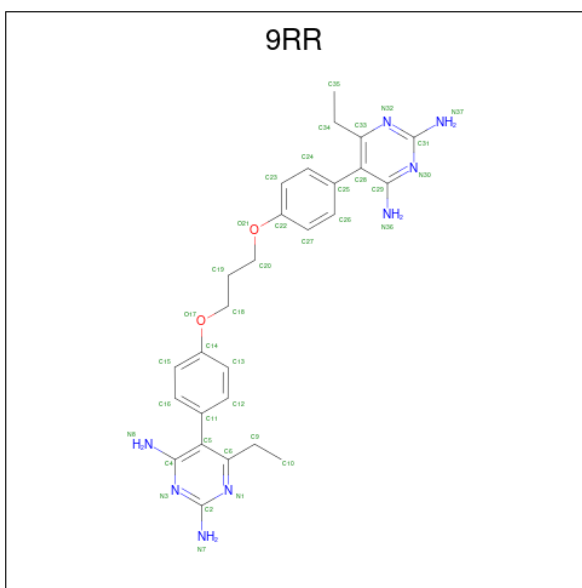
There are 5 unique types of molecules in this entry. The entry contains 9490 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	547	Total	C	N	O	S	0	0	0
			4550	2937	753	833	27			
1	B	551	Total	C	N	O	S	0	0	0
			4580	2955	759	839	27			

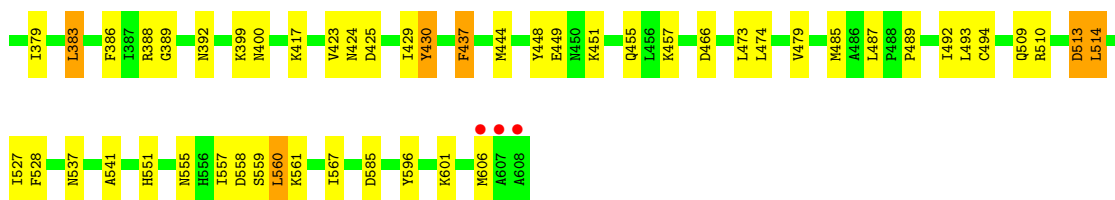
- Molecule 2 is 5,5'-[propane-1,3-diylbis(oxy-4,1-phenylene)]bis(6-ethylpyrimidine-2,4-diamine) (CCD ID: 9RR) (formula: C₂₇H₃₂N₈O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total	C	N	O	0	0
			37	27	8	2		
2	B	1	Total	C	N	O	0	0
			37	27	8	2		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	100	Total 100	O 100	0	0
5	B	98	Total 98	O 98	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.24Å 158.90Å 167.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.28 – 2.60 25.28 – 2.60	Depositor EDS
% Data completeness (in resolution range)	92.8 (25.28-2.60) 92.8 (25.28-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 2.60Å)	Xtrriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.206 , 0.267 0.204 , 0.261	Depositor DCC
R_{free} test set	2309 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	54.6	Xtrriage
Anisotropy	0.515	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9490	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, UMP, 9RR

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	1.21	18/4655 (0.4%)	1.30	11/6281 (0.2%)
1	B	1.20	30/4686 (0.6%)	1.28	18/6322 (0.3%)
All	All	1.20	48/9341 (0.5%)	1.29	29/12603 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	4
All	All	0	9

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	596	TYR	N-CA	-7.41	1.37	1.46
1	B	541	ALA	CA-C	7.33	1.55	1.52
1	A	299	LYS	N-CA	6.68	1.53	1.46
1	A	455	GLN	C-O	-6.58	1.16	1.24
1	B	567	ILE	N-CA	-6.53	1.40	1.46

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284	ASP	CA-CB-CG	8.98	121.58	112.60
1	A	481	ASP	CA-CB-CG	6.71	119.31	112.60
1	B	386	PHE	CA-CB-CG	6.49	120.29	113.80
1	B	194	ASP	CA-CB-CG	6.36	118.96	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	38	ARG	CB-CA-C	-6.19	101.04	109.28

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	ARG	Sidechain
1	A	165	GLY	Peptide
1	A	350	VAL	Peptide
1	A	352	SER	Peptide
1	A	402	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4550	0	4511	55	0
1	B	4580	0	4543	77	0
2	A	37	0	0	2	0
2	B	37	0	0	3	0
3	A	48	0	25	12	0
4	A	20	0	11	0	0
4	B	20	0	11	0	0
5	A	100	0	0	5	0
5	B	98	0	0	1	0
All	All	9490	0	9101	134	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 7.

The worst 5 of 134 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:ASN:HA	1:B:444:MET:CE	1.74	1.15
1:B:392:ASN:HA	1:B:444:MET:HE2	1.19	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:ASN:CA	1:B:444:MET:HE2	1.86	1.05
1:A:166:GLY:H	3:A:702:NAP:H5N	1.35	0.89
1:B:392:ASN:CB	1:B:444:MET:HE2	2.05	0.87

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	541/608 (89%)	503 (93%)	34 (6%)	4 (1%)	18	38
1	B	545/608 (90%)	493 (90%)	47 (9%)	5 (1%)	14	30
All	All	1086/1216 (89%)	996 (92%)	81 (8%)	9 (1%)	16	34

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	24	ASN
1	B	173	PHE
1	A	300	GLU
1	A	305	ASN
1	B	95	SER

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	510/570 (90%)	481 (94%)	29 (6%)	18	40
1	B	514/570 (90%)	475 (92%)	39 (8%)	12	27
All	All	1024/1140 (90%)	956 (93%)	68 (7%)	15	34

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	314	ILE
1	B	357	ILE
1	B	514	LEU
1	A	417	LYS
1	A	379	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	424	ASN
1	B	537	ASN
1	A	424	ASN
1	B	121	ASN
1	B	144	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	NAP	A	702	-	50,52,52	3.13	21 (42%)	71,80,80	2.16	26 (36%)
2	9RR	A	701	-	40,40,40	1.65	9 (22%)	55,55,55	2.97	22 (40%)
2	9RR	B	701	-	40,40,40	1.01	3 (7%)	55,55,55	2.58	18 (32%)
4	UMP	A	703	-	21,21,21	1.37	3 (14%)	30,31,31	2.66	12 (40%)
4	UMP	B	702	-	21,21,21	1.57	5 (23%)	30,31,31	2.17	12 (40%)

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	NAP	A	702	-	-	9/35/67/67	0/5/5/5
2	9RR	A	701	-	-	4/20/20/20	0/4/4/4
2	9RR	B	701	-	-	8/20/20/20	0/4/4/4
4	UMP	A	703	-	-	3/10/22/22	0/2/2/2
4	UMP	B	702	-	-	1/10/22/22	0/2/2/2

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	NAP	PA-O3	9.68	1.69	1.59
3	A	702	NAP	PN-O3	8.35	1.68	1.59
3	A	702	NAP	C3N-C7N	7.12	1.61	1.50
3	A	702	NAP	O4D-C1D	7.00	1.50	1.40
3	A	702	NAP	C5A-C4A	5.89	1.49	1.39

The worst 5 of 90 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	9RR	C9-C6-C5	-9.98	115.82	122.47
2	B	701	9RR	C31-N32-C33	8.06	122.14	116.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	9RR	C34-C33-C28	-7.93	117.19	122.47
2	B	701	9RR	C2-N1-C6	7.65	121.84	116.26
2	A	701	9RR	C5-C4-N3	-7.44	118.23	122.55

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

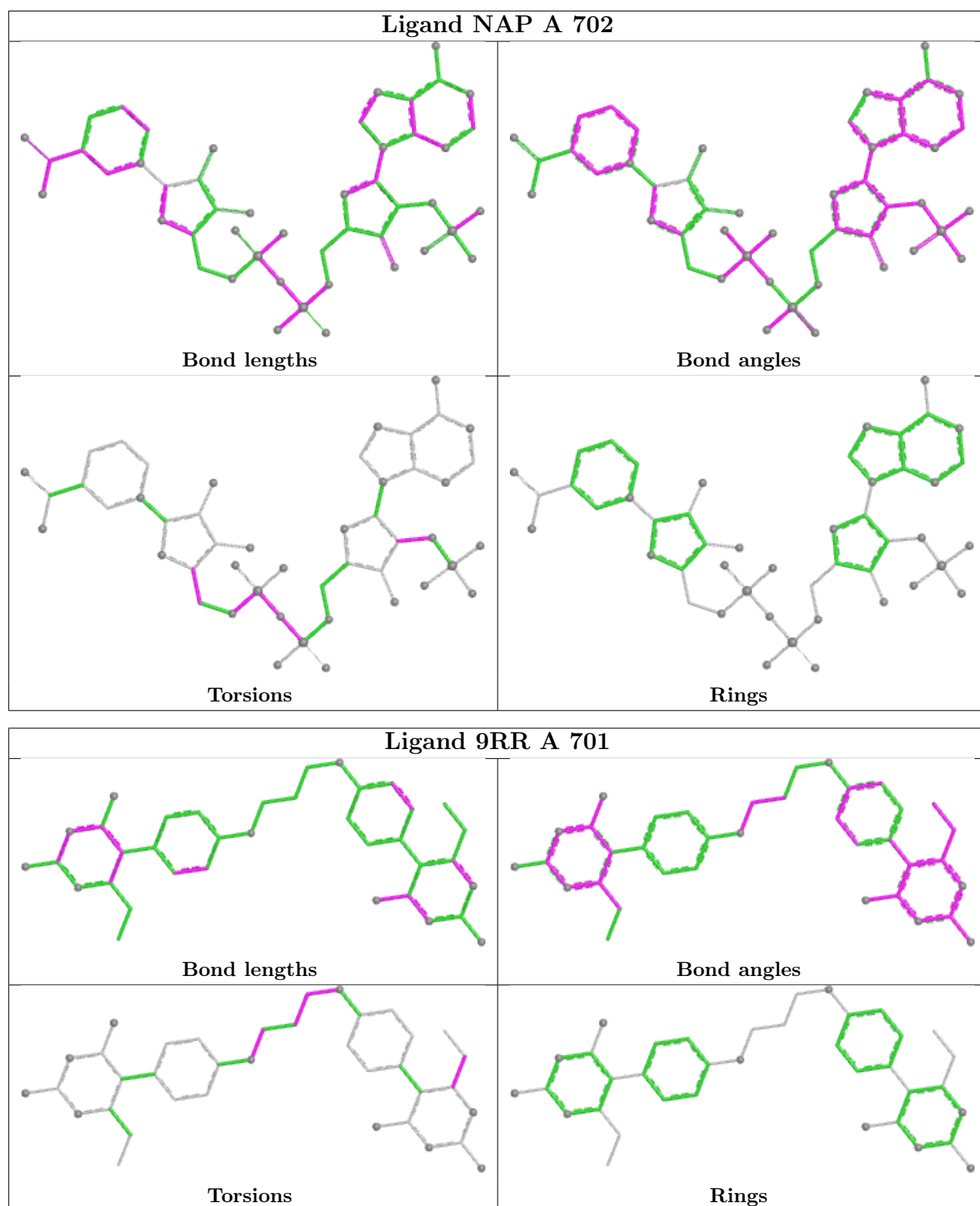
Mol	Chain	Res	Type	Atoms
3	A	702	NAP	C5D-O5D-PN-O1N
3	A	702	NAP	C3B-C2B-O2B-P2B
2	A	701	9RR	C18-C19-C20-O21
2	B	701	9RR	C23-C22-O21-C20
2	B	701	9RR	C27-C22-O21-C20

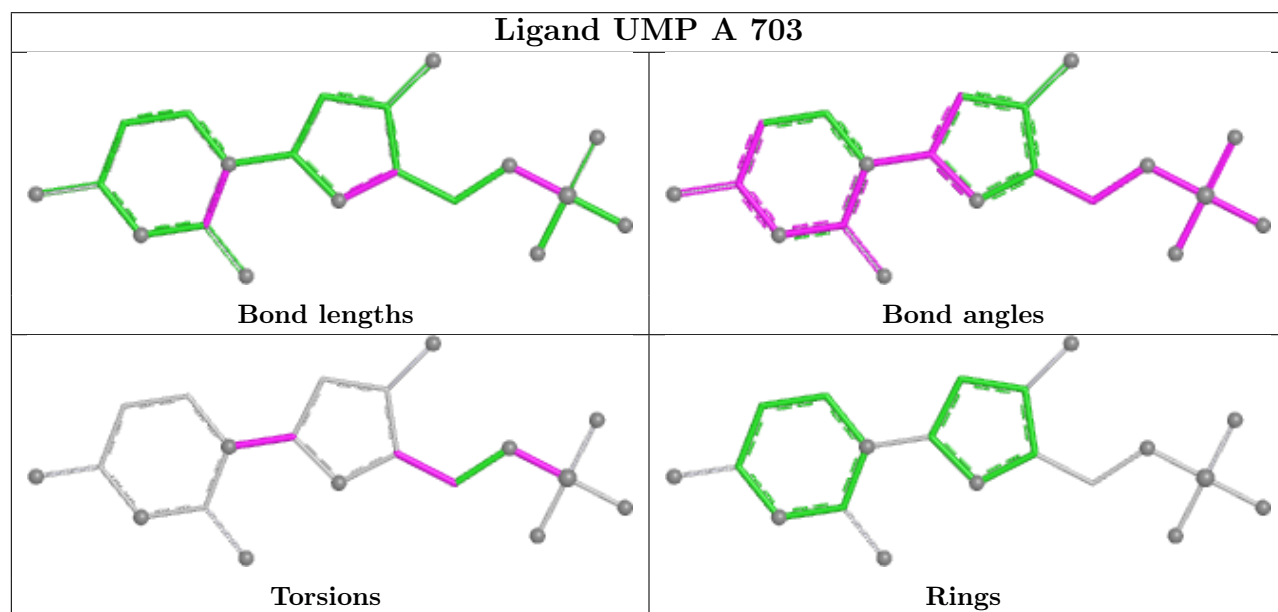
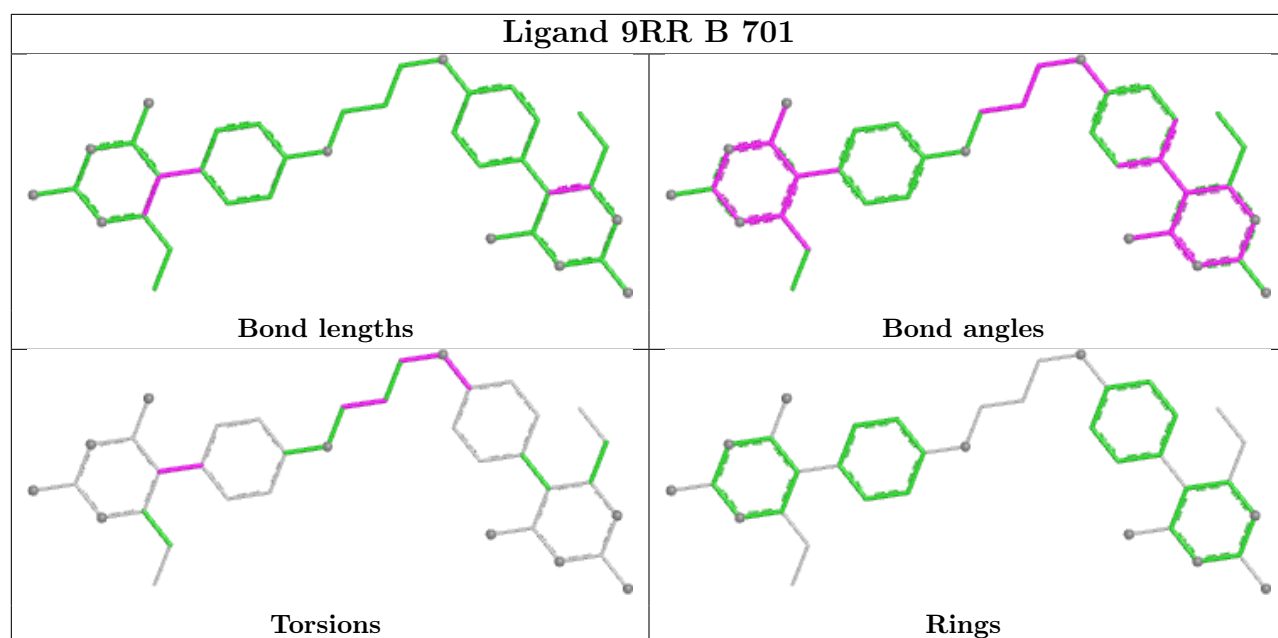
There are no ring outliers.

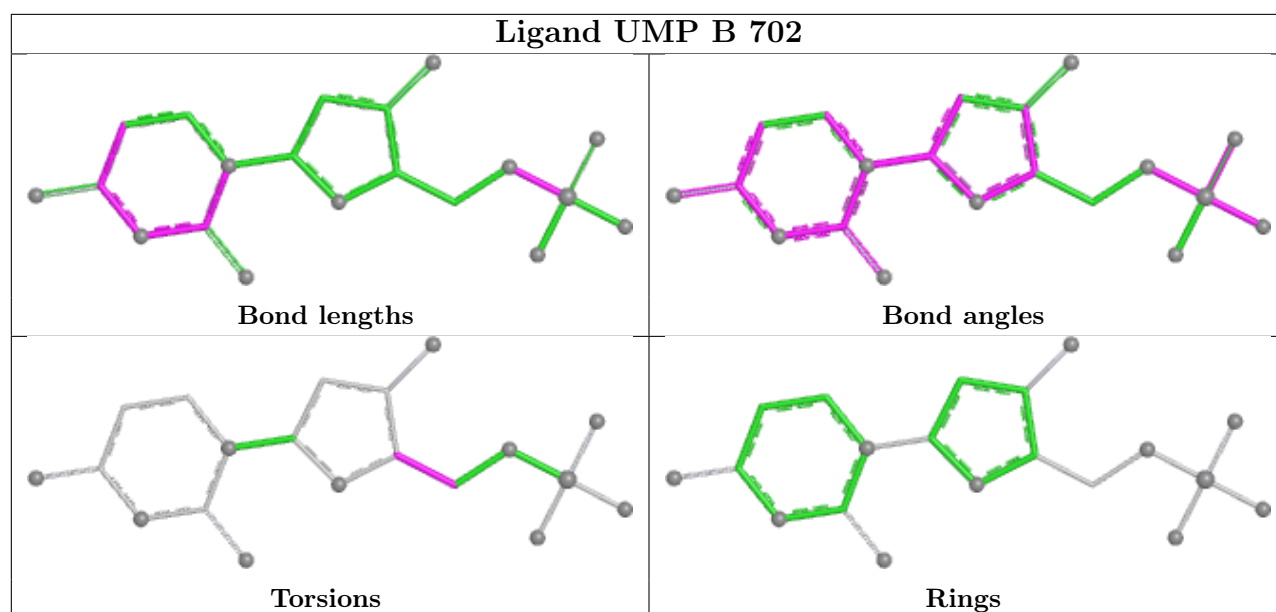
3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	NAP	12	0
2	A	701	9RR	2	0
2	B	701	9RR	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.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	547/608 (89%)	-0.31	8 (1%) 72 68	30, 52, 115, 120	0
1	B	551/608 (90%)	-0.00	25 (4%) 38 32	31, 59, 119, 120	0
All	All	1098/1216 (90%)	-0.16	33 (3%) 52 47	30, 54, 118, 120	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	607	ALA	4.8
1	A	607	ALA	3.4
1	B	85	THR	3.2
1	B	83	LYS	3.0
1	B	104	MET	2.9

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

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

6.3 Carbohydrates [i](#)

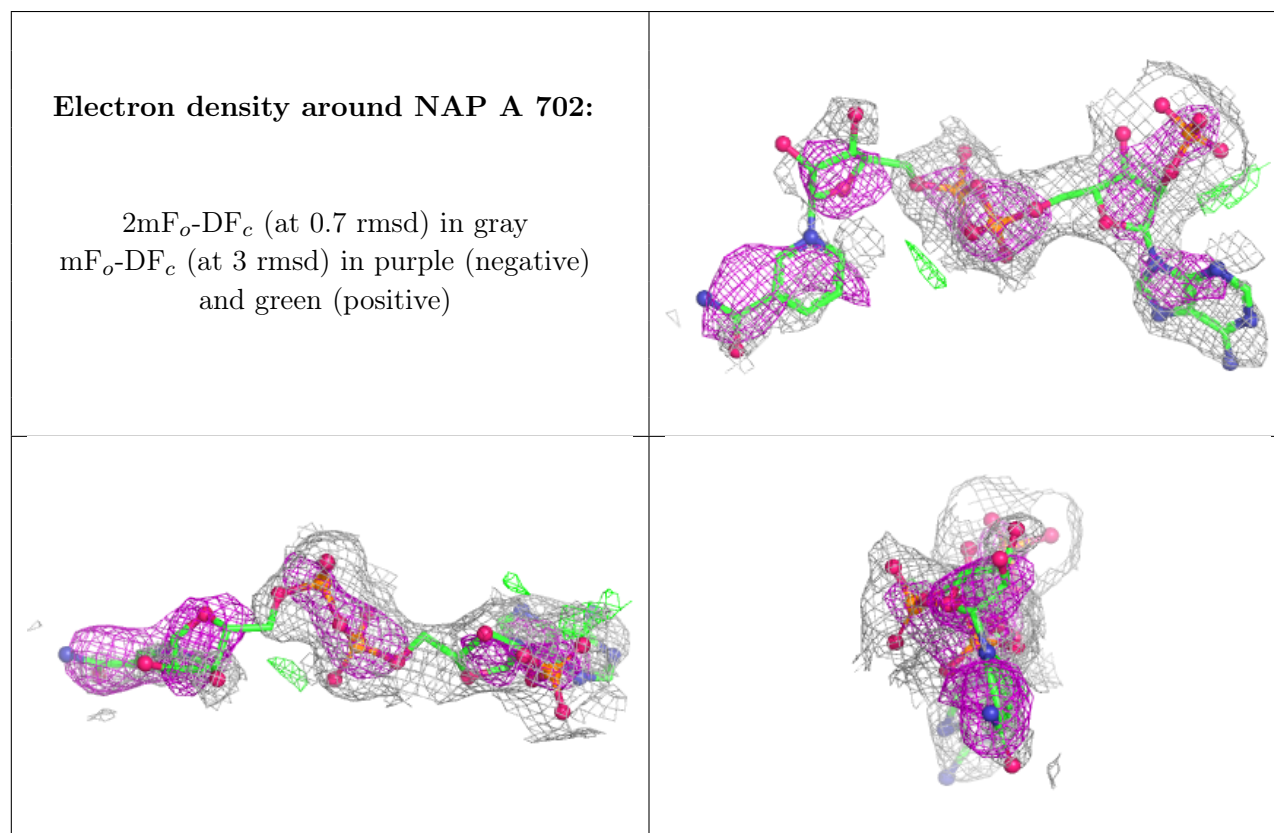
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

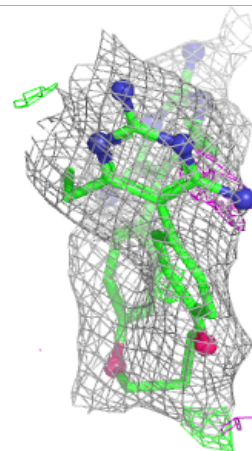
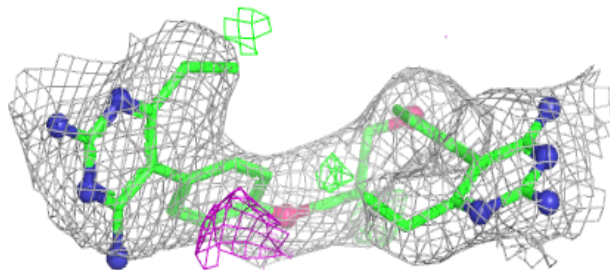
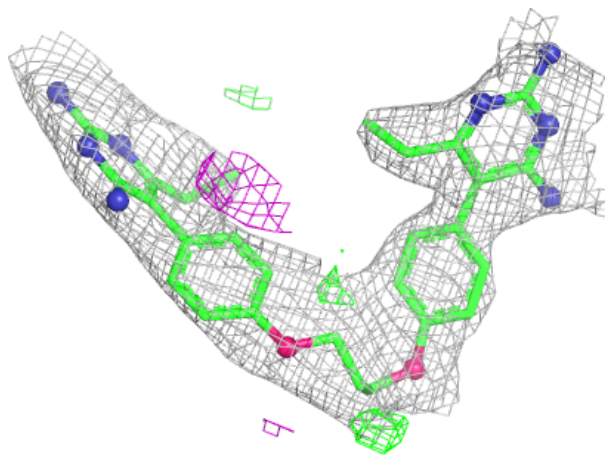
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAP	A	702	48/48	0.84	0.13	44,68,92,107	0
2	9RR	B	701	37/37	0.85	0.12	61,82,100,104	0
2	9RR	A	701	37/37	0.92	0.09	29,48,64,74	0
4	UMP	A	703	20/20	0.97	0.06	40,47,70,72	0
4	UMP	B	702	20/20	0.97	0.06	42,53,69,78	0

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.



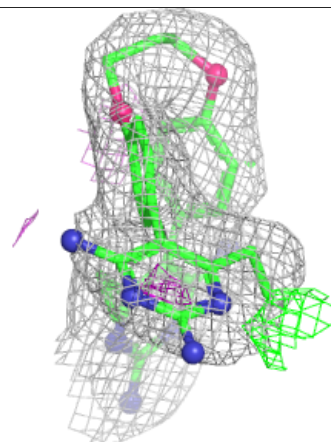
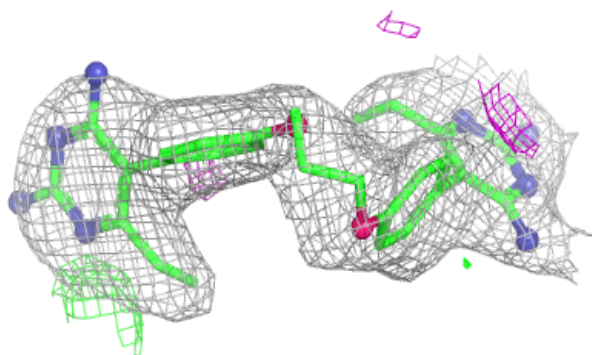
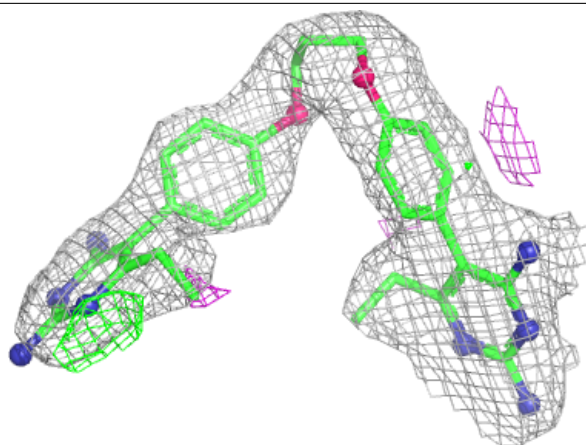
Electron density around 9RR B 701:

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

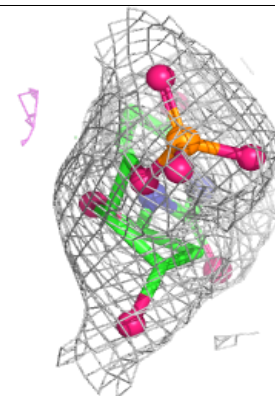
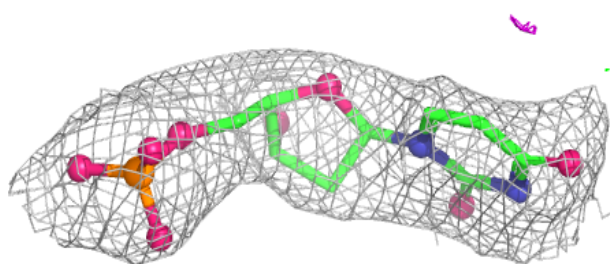


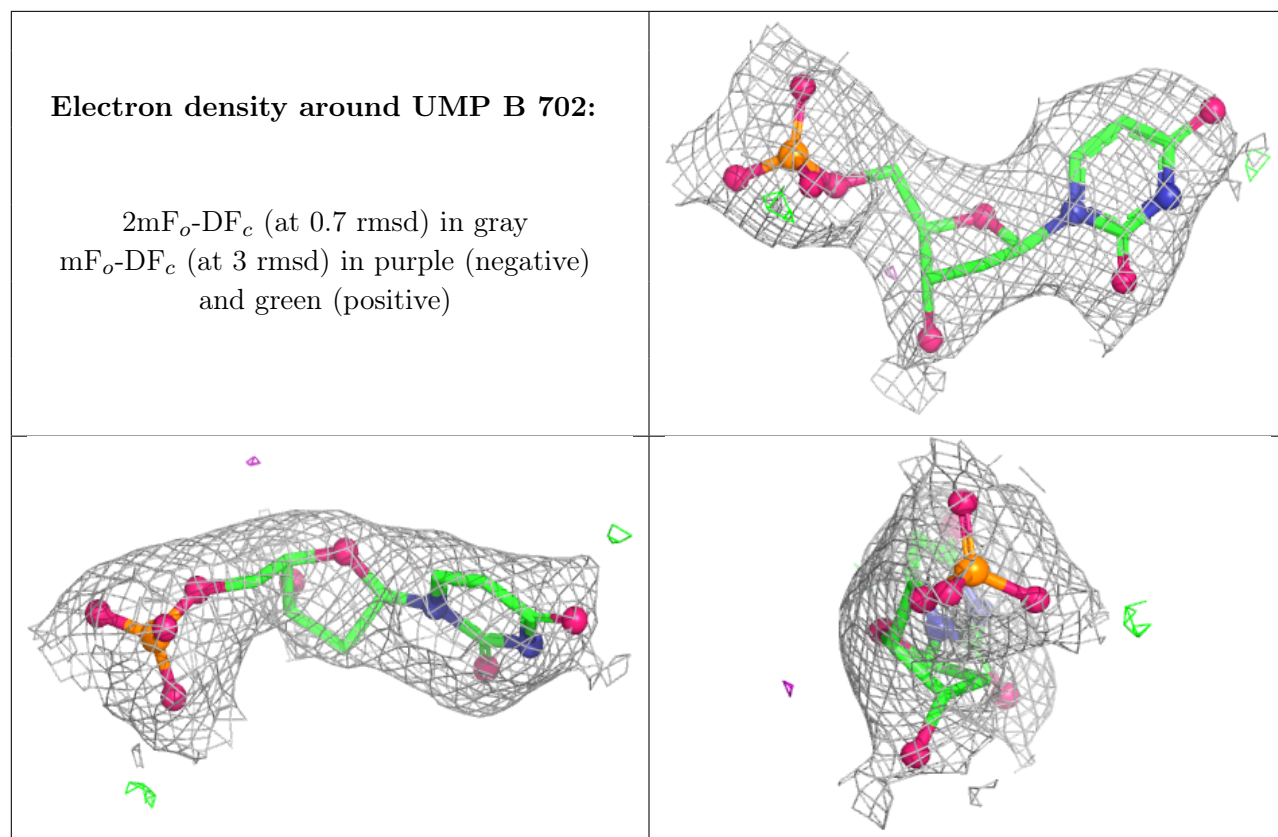
Electron density around 9RR A 701:

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

**Electron density around UMP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.