Full wwPDB X-ray Structure Validation Report (i)

Aug 17, 2023 – 02:09 PM JST

PDB ID	:	8JFC
Title	:	V1/S quadruple mutant Plasmodium falciparum dihydrofolate reductase-thymidylate synthase (PfDHFR-TS) complexed with compound 6 (B21591), NADPH and dUMP
Authors	:	Vanichtanankul, J.; Saeyang, T.; Vitsupakorn, D.; Saepua, S.; Thongpanchang, C.; Yuthavong, Y.; Kamchonwongpaisan, S.; Hoarau, M.
Deposited on	:	2023-05-17
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

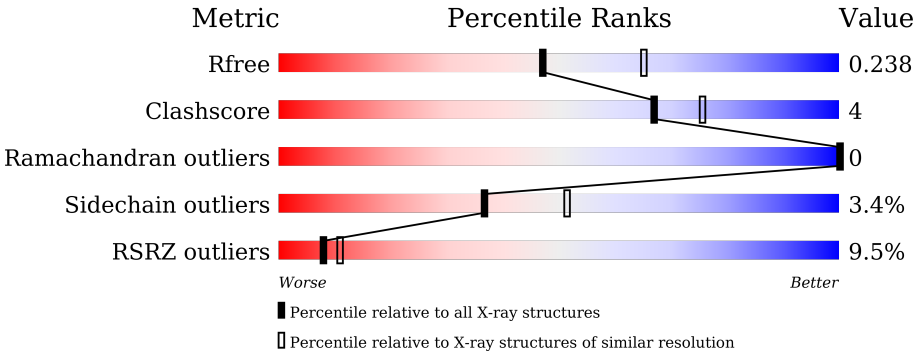
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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 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 <=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	5% 79% 7% 13%
1	B	608	12% 74% 12% • 13%

2 Entry composition

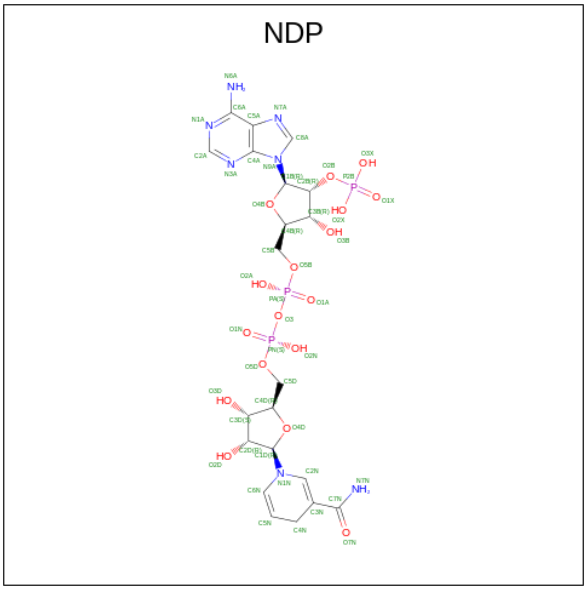
There are 6 unique types of molecules in this entry. The entry contains 9649 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

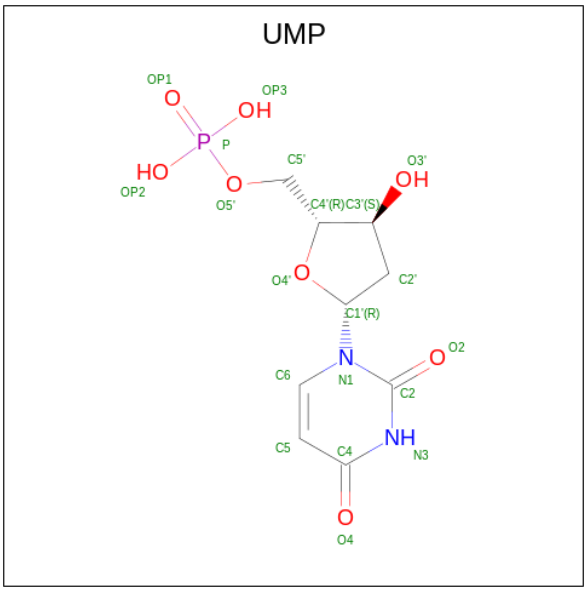
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	528	Total	C	N	O	S	0	0	0
			4395	2846	724	800	25			
1	B	531	Total	C	N	O	S	0	0	0
			4412	2855	727	805	25			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



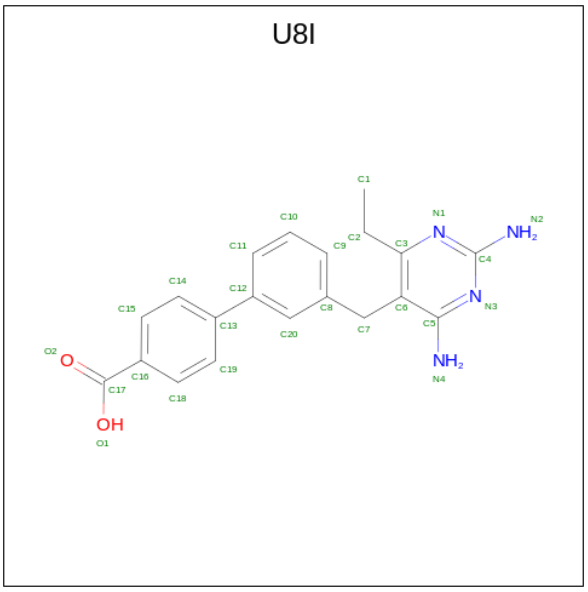
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: $C_9H_{13}N_2O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
3	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 4 is 4-[3-[[2,4-bis(azanyl)-6-ethyl-pyrimidin-5-yl]methyl]phenyl]benzoic acid (three-letter code: U8I) (formula: $C_{20}H_{20}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			26	20	4	2		

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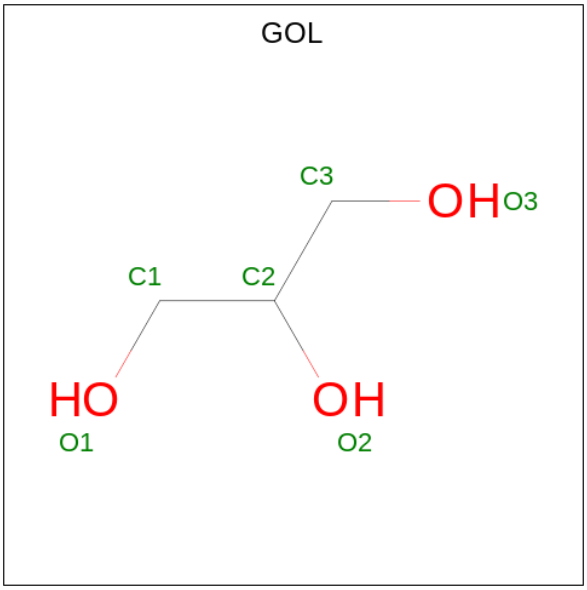
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 26 20 4 2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

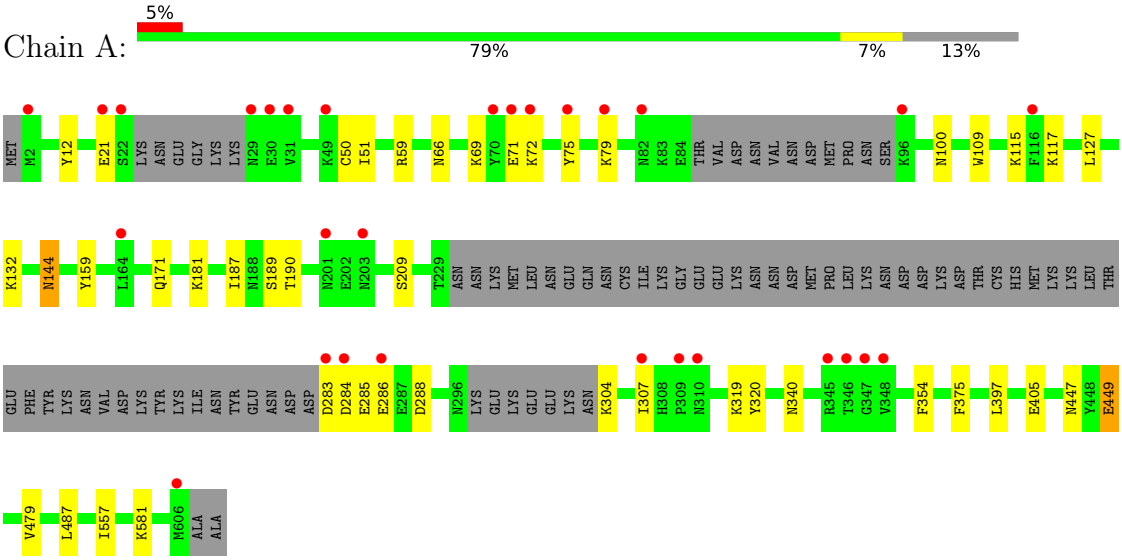
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	358	Total O 358 358	0	0
6	B	284	Total O 284 284	0	0

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.

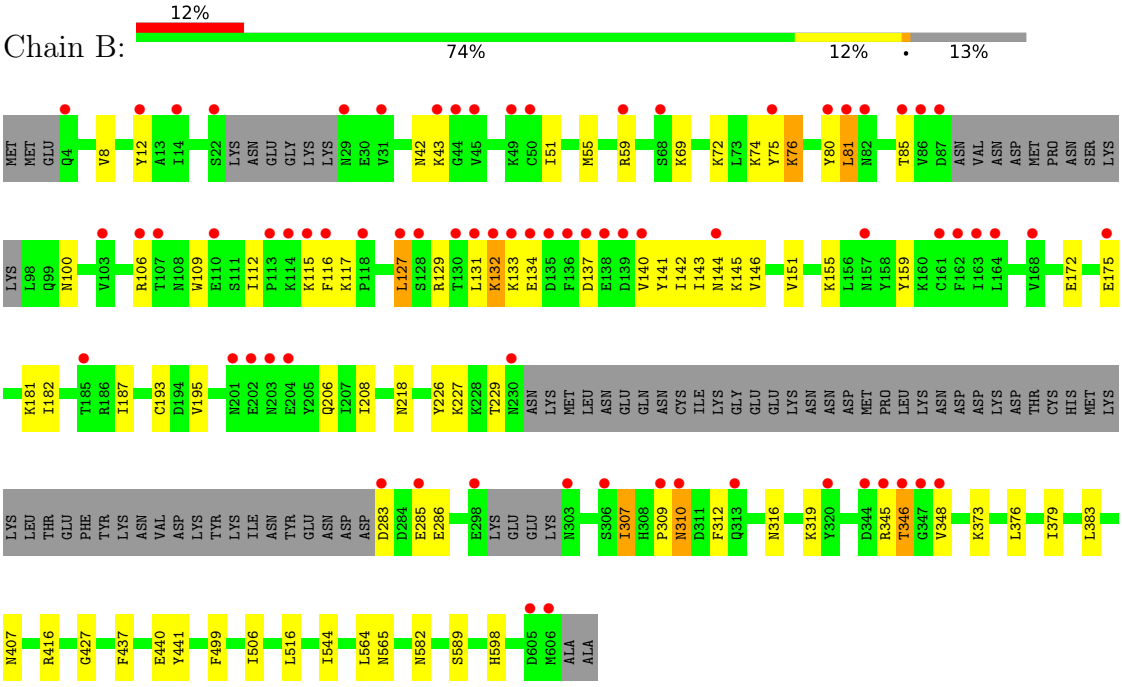
• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain A:



• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	56.98Å 155.76Å 165.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.31 – 2.30 24.31 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (24.31-2.30) 99.2 (24.31-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.188 , 0.238 0.188 , 0.238	Depositor DCC
R_{free} test set	3445 reflections (5.25%)	wwPDB-VP
Wilson B-factor (Å^2)	25.0	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 55.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9649	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NDP, U8I, GOL, UMP

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	0.44	0/4498	0.61	0/6075
1	B	0.41	0/4515	0.59	0/6101
All	All	0.42	0/9013	0.60	0/12176

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

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	4395	0	4344	25	0
1	B	4412	0	4353	53	0
2	A	48	0	26	1	0
2	B	48	0	26	2	0
3	A	20	0	11	0	0
3	B	20	0	11	1	0
4	A	26	0	0	0	0
4	B	26	0	0	1	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
6	A	358	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	284	0	0	4	0
All	All	9649	0	8787	69	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 (69) 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:182:ILE:HB	1:B:226:TYR:HB2	1.68	0.76
1:B:133:LYS:HE3	1:B:141:TYR:HA	1.69	0.73
1:B:346:THR:HB	1:B:348:VAL:HG23	1.76	0.67
1:A:51:ILE:HD13	1:A:187:ILE:HD12	1.82	0.61
1:B:8:VAL:HA	1:B:76:LYS:HD3	1.84	0.60
1:A:284:ASP:OD2	1:B:72:LYS:NZ	2.34	0.60
1:B:51:ILE:HD13	1:B:187:ILE:HD12	1.84	0.59
1:B:132:LYS:HG3	1:B:134:GLU:HG2	1.83	0.58
1:B:407:ASN:ND2	6:B:806:HOH:O	2.37	0.57
1:B:312:PHE:HA	1:B:565:ASN:HD21	1.71	0.55
1:B:506:ILE:HG12	1:B:544:ILE:HB	1.88	0.55
1:B:80:TYR:CD2	1:B:81:LEU:HD13	2.42	0.54
1:A:581:LYS:NZ	6:A:809:HOH:O	2.38	0.54
1:B:172:GLU:HA	1:B:175:GLU:HG2	1.90	0.53
1:A:397:LEU:HD21	1:A:405:GLU:HB2	1.89	0.53
1:A:75:TYR:CZ	1:A:79:LYS:HD2	2.43	0.53
1:B:373:LYS:HG3	1:B:598:HIS:CE1	2.44	0.53
1:B:582:ASN:HB3	6:B:980:HOH:O	2.08	0.53
1:B:112:ILE:O	1:B:117:LYS:NZ	2.37	0.52
1:B:42:ASN:ND2	1:B:43:LYS:HD3	2.25	0.52
1:B:208:ILE:HG21	1:B:227:LYS:HD2	1.93	0.50
1:B:312:PHE:HB2	1:B:316:ASN:ND2	2.25	0.50
1:A:209:SER:HB3	1:A:320:TYR:HB2	1.94	0.50
1:A:354:PHE:CE2	1:B:506:ILE:HG13	2.49	0.48
1:B:145:LYS:HD3	1:B:146:VAL:N	2.28	0.48
1:B:12:TYR:HD2	1:B:181:LYS:HB2	1.78	0.47
1:A:319:LYS:HG2	1:B:286:GLU:HG2	1.95	0.47
1:B:80:TYR:HD2	1:B:81:LEU:HD13	1.77	0.47
1:B:312:PHE:HB2	1:B:316:ASN:HD21	1.79	0.47
1:B:589:SER:HB3	6:B:1047:HOH:O	2.14	0.47
1:A:21:GLU:HG2	1:A:190:THR:HG22	1.97	0.47
1:A:307:ILE:HD11	1:A:557:ILE:HD13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:VAL:HG12	1:B:155:LYS:HE2	1.96	0.46
1:A:127:LEU:O	2:A:701:NDP:H1B	2.16	0.46
1:B:106:ARG:NH1	2:B:704:NDP:O3X	2.49	0.46
1:A:340:ASN:HB3	1:B:499:PHE:CE1	2.51	0.45
1:B:307:ILE:H	1:B:307:ILE:HG12	1.56	0.45
1:B:309:PRO:HG2	6:B:892:HOH:O	2.16	0.45
1:B:127:LEU:HD12	1:B:143:ILE:HG13	1.99	0.45
1:B:376:LEU:HD22	1:B:379:ILE:HD11	1.99	0.45
1:A:66:ASN:HD22	1:A:69:LYS:HE3	1.81	0.44
1:B:109:TRP:CE2	1:B:117:LYS:HD2	2.52	0.44
1:A:109:TRP:CE2	1:A:117:LYS:HD2	2.53	0.44
1:A:144:ASN:H	1:A:144:ASN:HD22	1.65	0.44
1:A:479:VAL:HB	1:B:437:PHE:CD1	2.52	0.43
1:B:100:ASN:OD1	1:B:159:TYR:HB3	2.18	0.43
1:B:206:GLN:NE2	1:B:229:THR:HG22	2.33	0.43
1:B:137:ASP:HB2	1:B:140:VAL:HG23	2.00	0.43
1:A:12:TYR:HD2	1:A:181:LYS:HB2	1.84	0.42
1:A:72:LYS:HE3	1:A:72:LYS:HB3	1.81	0.42
1:B:72:LYS:HE2	1:B:72:LYS:HB3	1.79	0.42
1:B:131:LEU:HB3	1:B:142:ILE:HD13	2.01	0.42
1:B:383:LEU:HA	1:B:383:LEU:HD12	1.83	0.42
1:A:340:ASN:HB3	1:B:499:PHE:CD1	2.54	0.42
1:B:345:ARG:NH2	3:B:701:UMP:OP3	2.42	0.42
1:B:427:GLY:HA2	1:B:441:TYR:CE2	2.55	0.42
1:B:42:ASN:HB2	1:B:193:CYS:HA	2.01	0.42
1:B:115:LYS:HE2	1:B:115:LYS:HB2	1.91	0.42
1:A:288:ASP:OD1	1:B:69:LYS:NZ	2.46	0.42
1:B:310:ASN:ND2	1:B:310:ASN:H	2.18	0.42
1:A:285:GLU:OE2	1:B:12:TYR:OH	2.38	0.41
1:A:447:ASN:HD21	1:A:449:GLU:HB2	1.85	0.41
1:A:286:GLU:HG3	1:B:319:LYS:HG2	2.02	0.41
1:A:581:LYS:HA	1:A:581:LYS:HD3	1.81	0.41
1:B:76:LYS:HE3	1:B:76:LYS:HB3	1.97	0.41
1:B:129:ARG:HG3	2:B:704:NDP:C2A	2.51	0.41
1:B:42:ASN:HD21	1:B:43:LYS:HD3	1.85	0.40
1:B:116:PHE:CE1	4:B:702:U8I:O2	2.74	0.40
1:A:100:ASN:OD1	1:A:159:TYR:HB3	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	518/608 (85%)	499 (96%)	19 (4%)	0	100	100
1	B	521/608 (86%)	505 (97%)	16 (3%)	0	100	100
All	All	1039/1216 (85%)	1004 (97%)	35 (3%)	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	
1	A	493/570 (86%)	480 (97%)	13 (3%)	46	63
1	B	495/570 (87%)	474 (96%)	21 (4%)	30	42
All	All	988/1140 (87%)	954 (97%)	34 (3%)	37	51

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	CYS
1	A	59	ARG
1	A	71	GLU
1	A	115	LYS
1	A	132	LYS
1	A	144	ASN
1	A	171	GLN
1	A	189	SER

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Mol	Chain	Res	Type
1	A	283	ASP
1	A	304	LYS
1	A	375	PHE
1	A	449	GLU
1	A	487	LEU
1	B	55	MET
1	B	59	ARG
1	B	74	LYS
1	B	75	TYR
1	B	76	LYS
1	B	81	LEU
1	B	85	THR
1	B	127	LEU
1	B	132	LYS
1	B	144	ASN
1	B	195	VAL
1	B	218	ASN
1	B	283	ASP
1	B	285	GLU
1	B	307	ILE
1	B	310	ASN
1	B	346	THR
1	B	416	ARG
1	B	440	GLU
1	B	516	LEU
1	B	564	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	144	ASN
1	A	171	GLN
1	A	218	ASN
1	A	316	ASN
1	A	394	ASN
1	A	424	ASN
1	B	42	ASN
1	B	99	GLN
1	B	108	ASN
1	B	206	GLN
1	B	310	ASN

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Mol	Chain	Res	Type
1	B	316	ASN
1	B	394	ASN
1	B	407	ASN
1	B	415	ASN
1	B	424	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

8 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	UMP	A	702	-	21,21,21	0.90	0	31,31,31	1.55	6 (19%)
2	NDP	A	701	-	45,52,52	2.08	7 (15%)	53,80,80	1.53	7 (13%)
3	UMP	B	701	-	21,21,21	0.91	1 (4%)	31,31,31	1.53	5 (16%)
5	GOL	B	703	-	5,5,5	0.80	0	5,5,5	0.97	0
2	NDP	B	704	-	45,52,52	2.24	6 (13%)	53,80,80	1.52	9 (16%)
4	U8I	B	702	-	27,28,28	0.46	0	34,39,39	0.86	2 (5%)
5	GOL	A	704	-	5,5,5	1.19	0	5,5,5	0.96	0
4	U8I	A	703	-	27,28,28	0.47	0	34,39,39	0.82	2 (5%)

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	UMP	A	702	-	-	1/10/22/22	0/2/2/2
2	NDP	A	701	-	-	5/30/77/77	0/5/5/5
3	UMP	B	701	-	-	2/10/22/22	0/2/2/2
5	GOL	B	703	-	-	2/4/4/4	-
2	NDP	B	704	-	-	3/30/77/77	0/5/5/5
4	U8I	B	702	-	-	2/14/14/14	0/3/3/3
5	GOL	A	704	-	-	2/4/4/4	-
4	U8I	A	703	-	-	0/14/14/14	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	704	NDP	P2B-O2B	11.47	1.81	1.59
2	A	701	NDP	P2B-O2B	9.37	1.77	1.59
2	A	701	NDP	PN-O5D	5.21	1.80	1.59
2	B	704	NDP	PN-O5D	5.16	1.80	1.59
2	A	701	NDP	C7N-N7N	3.63	1.43	1.33
2	B	704	NDP	C7N-N7N	3.31	1.42	1.33
2	B	704	NDP	O2B-C2B	-3.12	1.32	1.44
2	A	701	NDP	O2B-C2B	-3.06	1.33	1.44
2	A	701	NDP	O4B-C1B	3.04	1.45	1.41
2	A	701	NDP	C2A-N1A	2.82	1.39	1.33
2	B	704	NDP	C4A-N3A	2.62	1.39	1.35
2	B	704	NDP	C2A-N1A	2.55	1.38	1.33
3	B	701	UMP	C5-C4	-2.16	1.38	1.43
2	A	701	NDP	C3B-C2B	2.02	1.57	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	704	NDP	PN-O3-PA	-5.43	114.18	132.83
2	A	701	NDP	PN-O3-PA	-5.04	115.54	132.83
3	A	702	UMP	C4-N3-C2	-3.84	121.52	126.58
3	B	701	UMP	C4-N3-C2	-3.77	121.61	126.58
3	B	701	UMP	C5-C4-N3	3.64	120.29	114.84
3	A	702	UMP	C5-C4-N3	3.48	120.05	114.84
2	A	701	NDP	O2B-P2B-O1X	-3.34	96.49	109.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	701	UMP	O4-C4-C5	-3.31	119.34	125.16
2	B	704	NDP	O2B-P2B-O1X	-3.23	96.91	109.39
3	B	701	UMP	C1'-N1-C6	-2.95	115.72	121.55
4	B	702	U8I	C7-C6-C5	-2.91	118.05	122.14
3	A	702	UMP	O4-C4-C5	-2.76	120.31	125.16
2	B	704	NDP	PA-O5B-C5B	-2.75	105.55	121.68
3	A	702	UMP	C1'-N1-C2	2.68	122.92	117.64
2	A	701	NDP	O3X-P2B-O2X	2.66	117.79	107.64
3	B	701	UMP	C1'-N1-C2	2.65	122.85	117.64
3	A	702	UMP	N3-C2-N1	2.60	118.34	114.89
4	B	702	U8I	C6-C3-N1	-2.58	121.31	123.49
2	B	704	NDP	O3X-P2B-O2X	2.56	117.41	107.64
3	A	702	UMP	C1'-N1-C6	-2.54	116.54	121.55
4	A	703	U8I	C7-C6-C5	-2.46	118.67	122.14
2	A	701	NDP	C3N-C2N-N1N	-2.41	119.65	123.10
2	B	704	NDP	O5D-PN-O1N	-2.39	99.72	109.07
2	B	704	NDP	PN-O5D-C5D	-2.31	108.14	121.68
2	B	704	NDP	O4B-C4B-C3B	2.31	109.68	105.11
2	A	701	NDP	C2A-N1A-C6A	-2.30	114.81	118.75
2	B	704	NDP	C2A-N1A-C6A	-2.25	114.91	118.75
2	A	701	NDP	PA-O5B-C5B	-2.24	108.53	121.68
2	B	704	NDP	O2A-PA-O1A	2.15	122.85	112.24
4	A	703	U8I	C6-C3-N1	-2.12	121.70	123.49
2	A	701	NDP	N3A-C2A-N1A	2.04	131.86	128.68

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	NDP	PA-O3-PN-O5D
5	A	704	GOL	O1-C1-C2-C3
5	B	703	GOL	C1-C2-C3-O3
5	A	704	GOL	O1-C1-C2-O2
5	B	703	GOL	O2-C2-C3-O3
3	B	701	UMP	C3'-C4'-C5'-O5'
2	B	704	NDP	O4D-C1D-N1N-C2N
3	B	701	UMP	O4'-C4'-C5'-O5'
2	A	701	NDP	C5B-O5B-PA-O3
2	B	704	NDP	C2B-O2B-P2B-O3X
2	A	701	NDP	O4D-C1D-N1N-C2N
4	B	702	U8I	C1-C2-C3-C6
2	B	704	NDP	C2B-O2B-P2B-O2X

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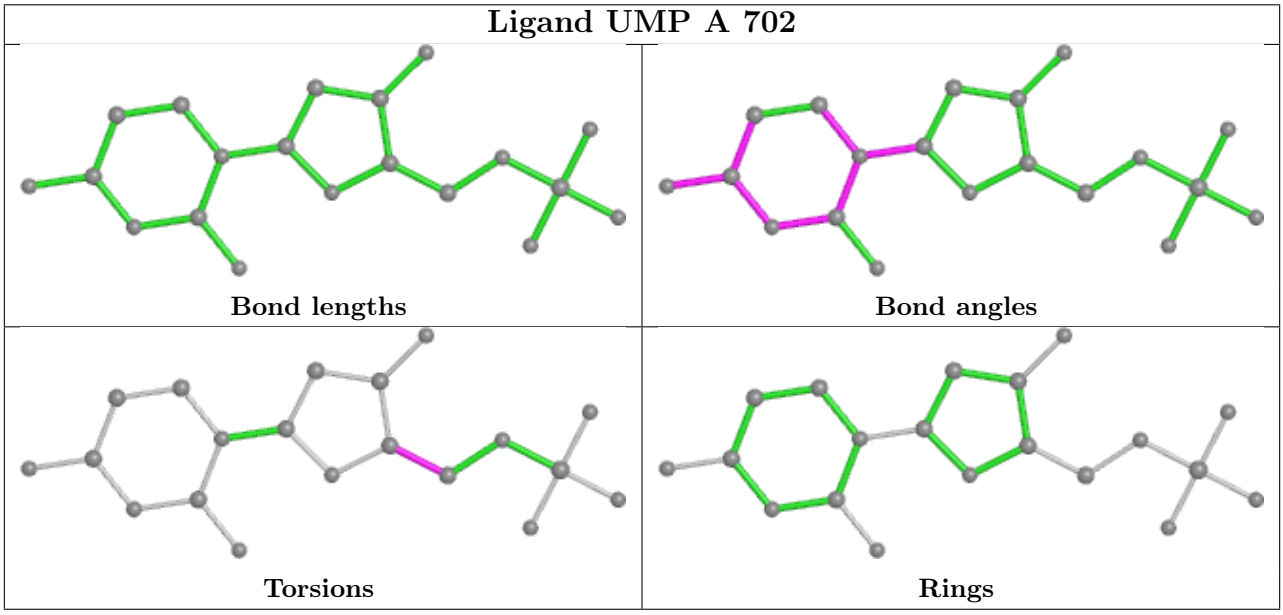
Mol	Chain	Res	Type	Atoms
3	A	702	UMP	O4'-C4'-C5'-O5'
2	A	701	NDP	C5B-O5B-PA-O1A
2	A	701	NDP	C2N-C3N-C7N-N7N
4	B	702	U8I	C1-C2-C3-N1

There are no ring outliers.

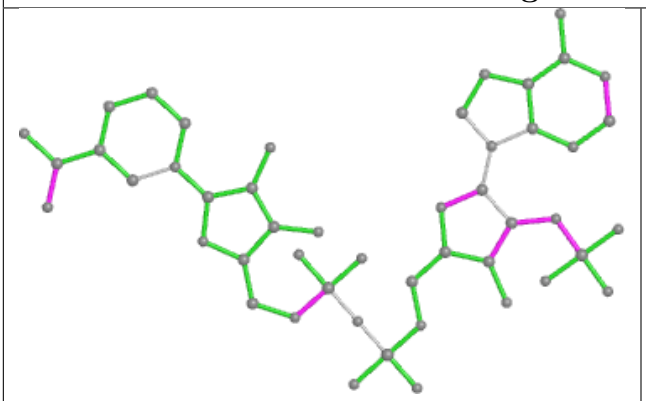
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	NDP	1	0
3	B	701	UMP	1	0
2	B	704	NDP	2	0
4	B	702	U8I	1	0

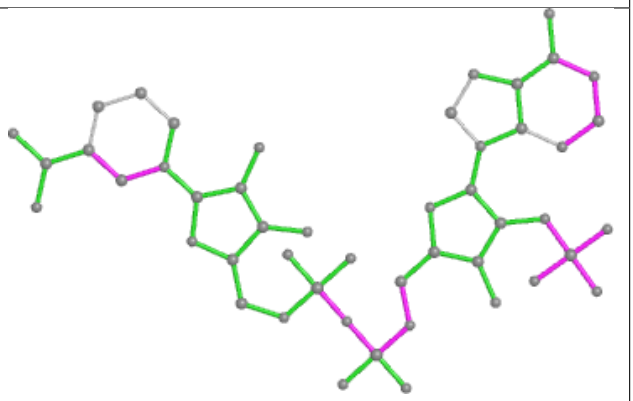
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



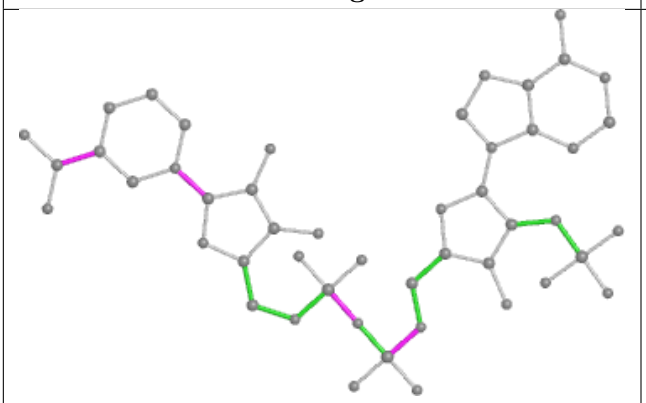
Ligand NDP A 701



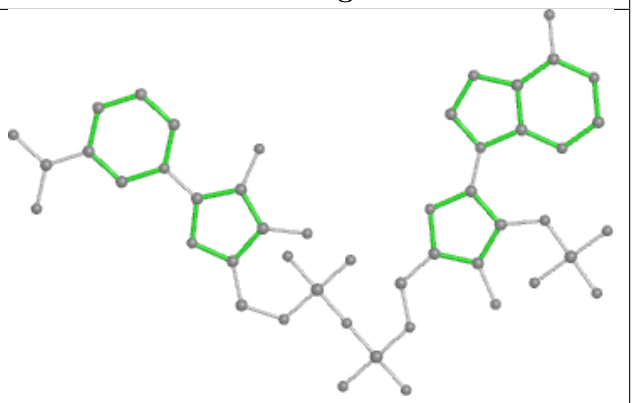
Bond lengths



Bond angles

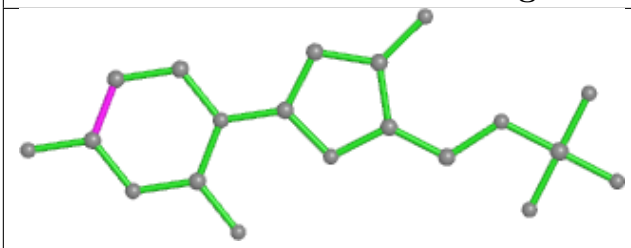


Torsions

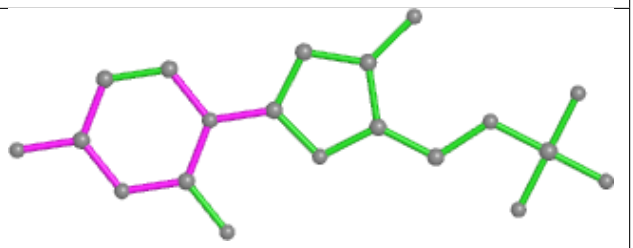


Rings

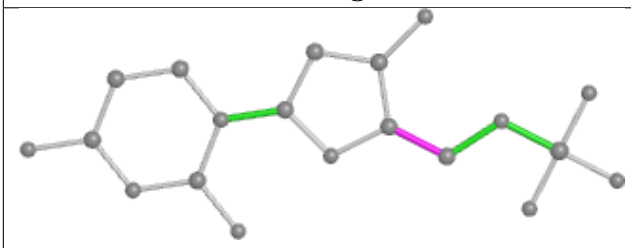
Ligand UMP B 701



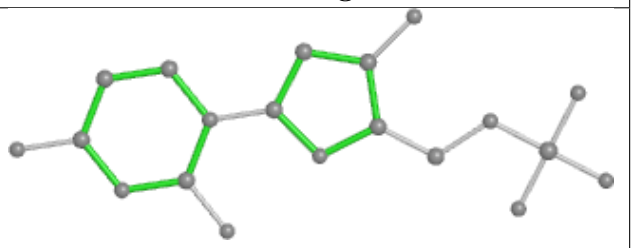
Bond lengths



Bond angles

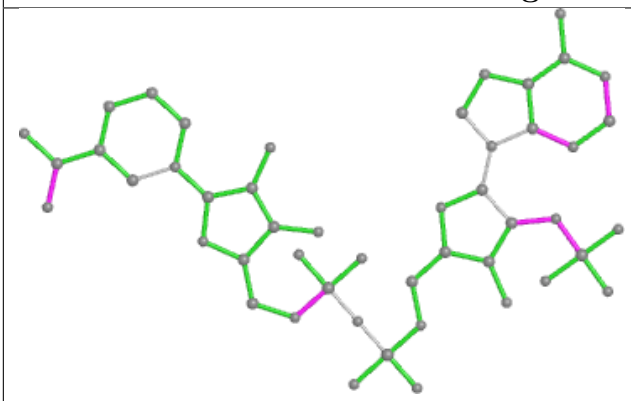


Torsions

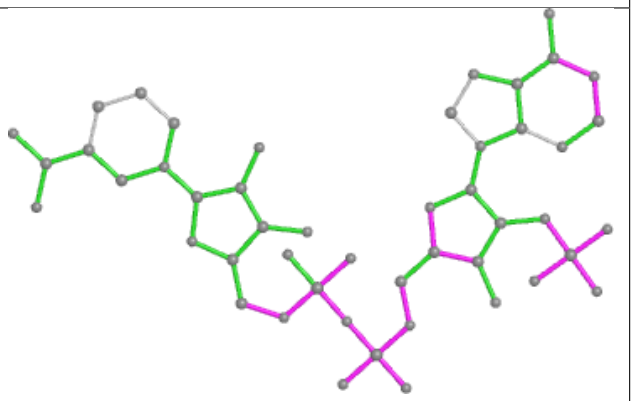


Rings

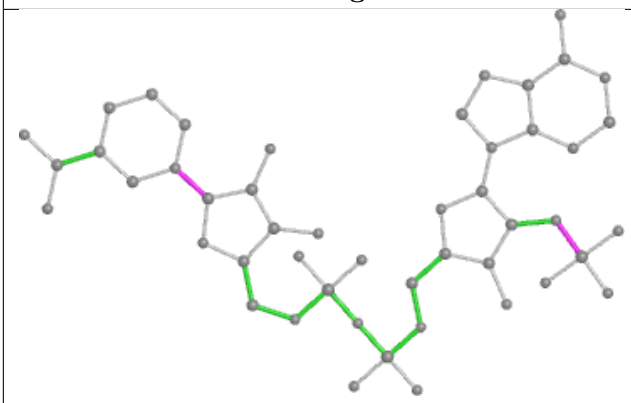
Ligand NDP B 704



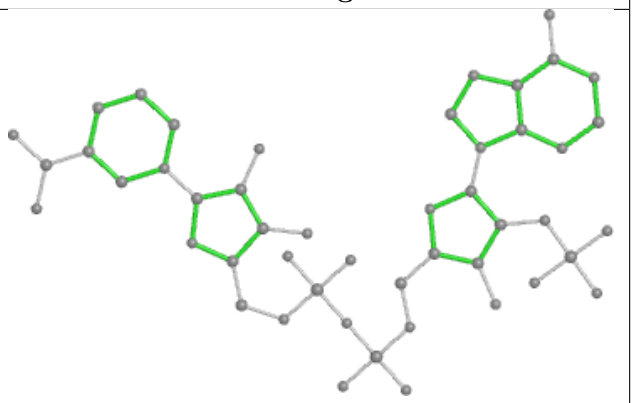
Bond lengths



Bond angles

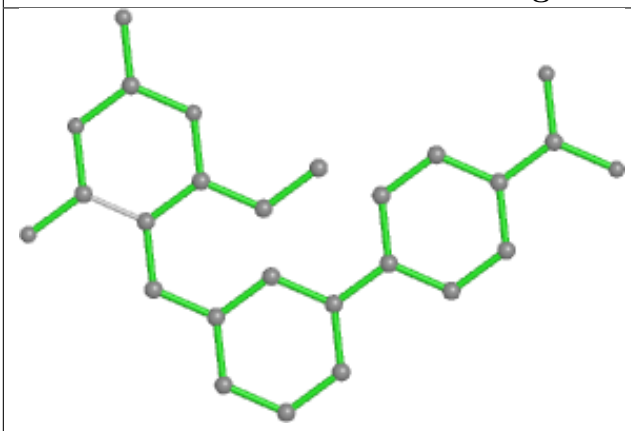


Torsions

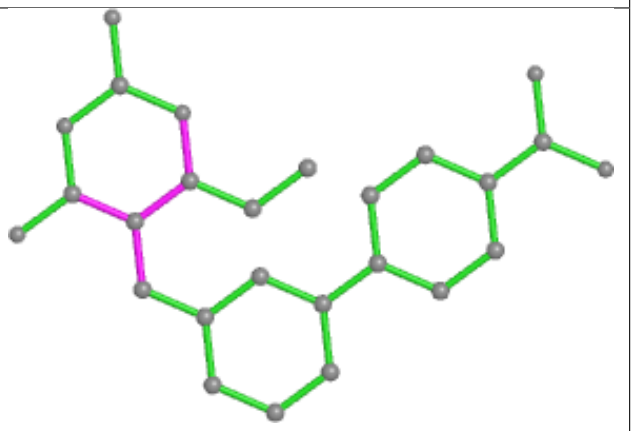


Rings

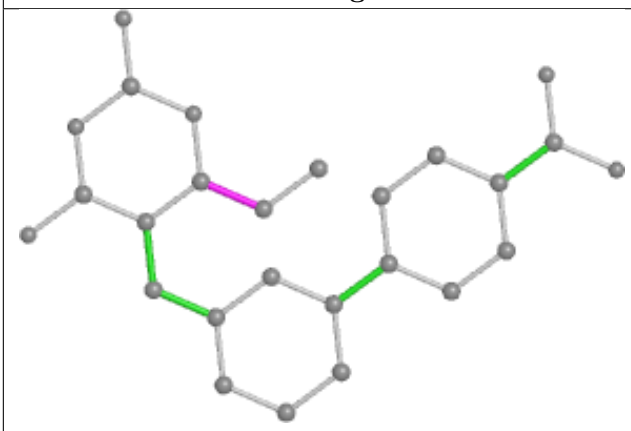
Ligand U8I B 702



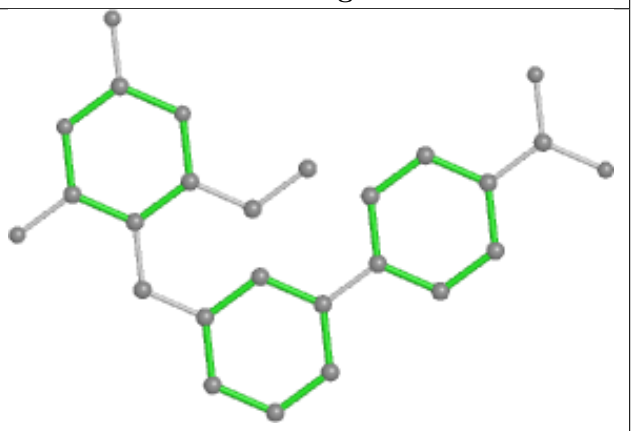
Bond lengths



Bond angles

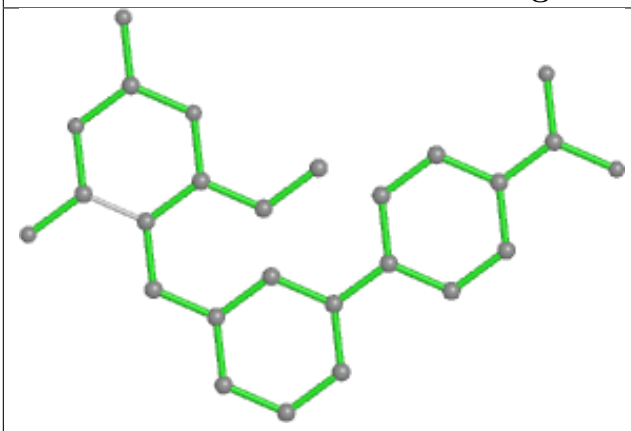


Torsions

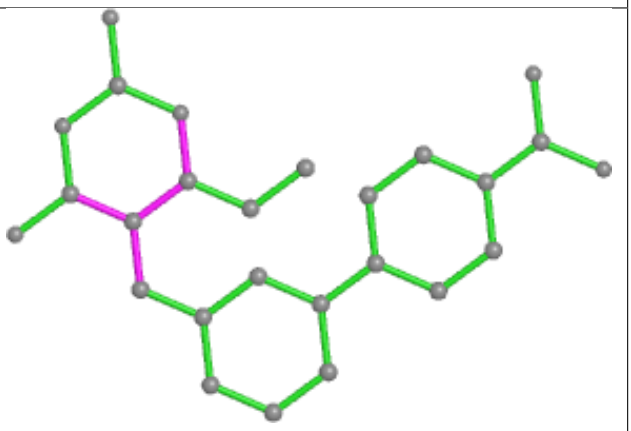


Rings

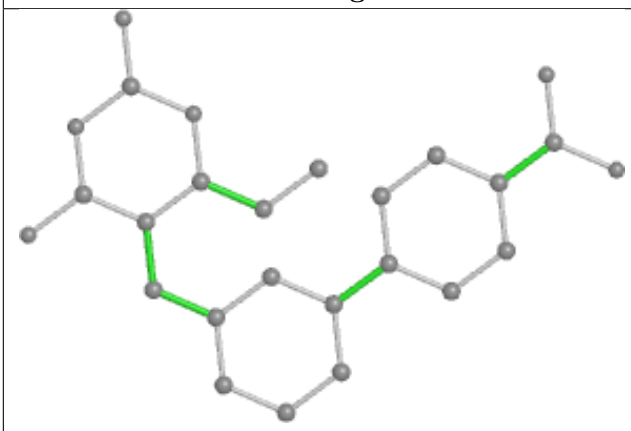
Ligand U8I A 703



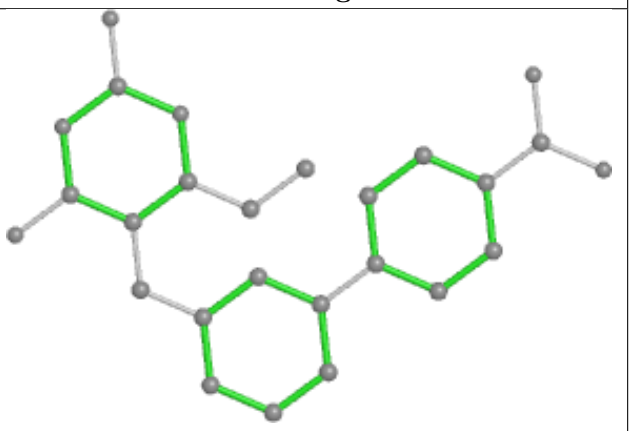
Bond lengths



Bond angles



Torsions



Rings

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^{th} 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	528/608 (86%)	0.08	29 (5%) 25 31	12, 25, 56, 87	0
1	B	531/608 (87%)	0.51	72 (13%) 3 4	13, 30, 75, 102	0
All	All	1059/1216 (87%)	0.29	101 (9%) 8 11	12, 26, 68, 102	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	136	PHE	7.8
1	A	2	MET	7.2
1	B	116	PHE	7.1
1	B	309	PRO	6.3
1	B	75	TYR	6.0
1	A	346	THR	5.9
1	B	138	GLU	5.9
1	B	346	THR	5.7
1	A	22	SER	5.3
1	A	284	ASP	5.2
1	B	49	LYS	5.1
1	B	85	THR	5.1
1	B	134	GLU	4.9
1	A	96	LYS	4.9
1	A	283	ASP	4.9
1	B	130	THR	4.8
1	B	230	ASN	4.6
1	B	29	ASN	4.5
1	A	29	ASN	4.3
1	B	345	ARG	4.3
1	B	135	ASP	4.1
1	B	348	VAL	4.1
1	B	140	VAL	4.0
1	B	303	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	81	LEU	4.0
1	B	283	ASP	4.0
1	B	131	LEU	3.9
1	B	162	PHE	3.9
1	B	132	LYS	3.9
1	B	44	GLY	3.9
1	B	161	CYS	3.8
1	B	204	GLU	3.7
1	B	86	VAL	3.7
1	B	175	GLU	3.7
1	B	113	PRO	3.7
1	A	347	GLY	3.7
1	B	115	LYS	3.6
1	A	75	TYR	3.6
1	A	307	ILE	3.5
1	B	106	ARG	3.5
1	B	4	GLN	3.4
1	B	107	THR	3.4
1	A	310	ASN	3.4
1	B	50	CYS	3.4
1	B	133	LYS	3.3
1	A	71	GLU	3.3
1	B	201	ASN	3.3
1	B	139	ASP	3.2
1	A	82	ASN	3.2
1	B	137	ASP	3.2
1	B	163	ILE	3.1
1	A	116	PHE	3.1
1	A	309	PRO	3.1
1	B	14	ILE	3.1
1	B	110	GLU	3.1
1	B	31	VAL	2.9
1	B	203	ASN	2.9
1	B	306	SER	2.9
1	A	21	GLU	2.9
1	B	298	GLU	2.9
1	A	49	LYS	2.9
1	B	144	ASN	2.8
1	B	285	GLU	2.8
1	B	87	ASP	2.8
1	B	202	GLU	2.8
1	B	605	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	30	GLU	2.8
1	A	203	ASN	2.8
1	B	82	ASN	2.8
1	B	128	SER	2.7
1	B	45	VAL	2.7
1	B	310	ASN	2.7
1	A	286	GLU	2.6
1	B	164	LEU	2.6
1	B	168	VAL	2.6
1	B	22	SER	2.5
1	B	157	ASN	2.5
1	A	31	VAL	2.5
1	B	80	TYR	2.4
1	B	606	MET	2.4
1	A	348	VAL	2.4
1	B	103	VAL	2.4
1	A	72	LYS	2.4
1	B	68	SER	2.4
1	B	43	LYS	2.3
1	B	114	LYS	2.3
1	A	345	ARG	2.3
1	B	59	ARG	2.3
1	A	201	ASN	2.3
1	B	320	TYR	2.3
1	A	79	LYS	2.3
1	B	313	GLN	2.3
1	B	118	PRO	2.2
1	A	606	MET	2.2
1	B	12	TYR	2.2
1	A	164	LEU	2.2
1	B	344	ASP	2.2
1	B	347	GLY	2.2
1	B	185	THR	2.1
1	B	127	LEU	2.1
1	A	70	TYR	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

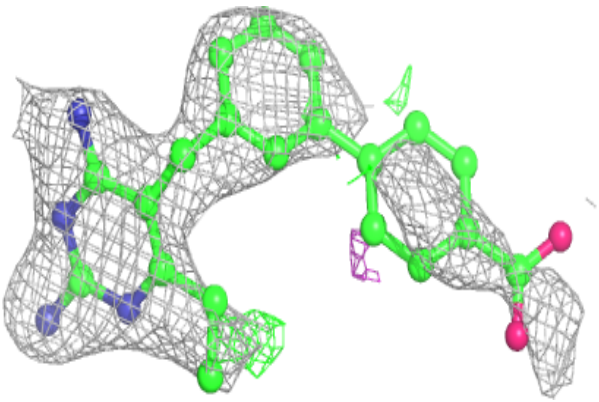
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

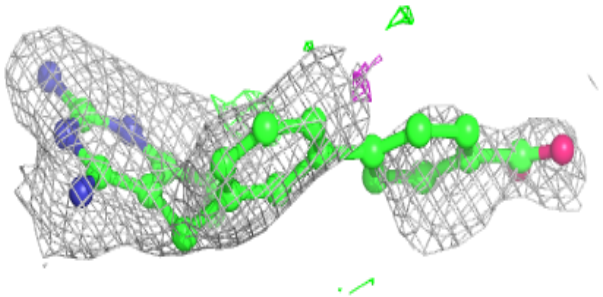
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	U8I	B	702	26/26	0.73	0.29	34,55,86,92	0
2	NDP	B	704	48/48	0.80	0.29	44,77,90,91	0
4	U8I	A	703	26/26	0.81	0.25	17,35,53,58	0
5	GOL	B	703	6/6	0.91	0.13	21,24,31,33	0
5	GOL	A	704	6/6	0.94	0.14	18,21,24,27	0
3	UMP	A	702	20/20	0.96	0.13	20,30,36,36	0
3	UMP	B	701	20/20	0.96	0.16	22,31,40,41	0
2	NDP	A	701	48/48	0.96	0.13	18,32,38,41	0

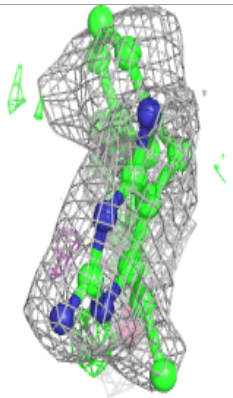
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around U8I 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)

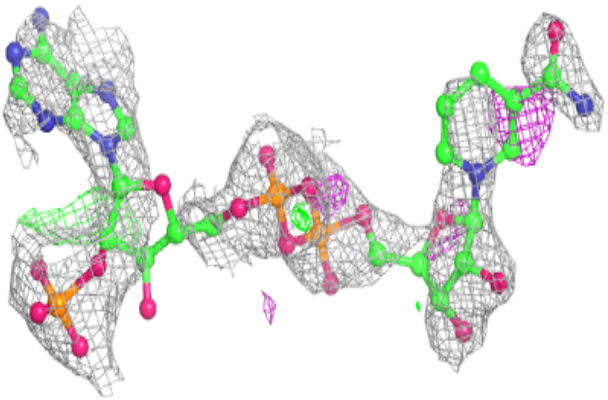


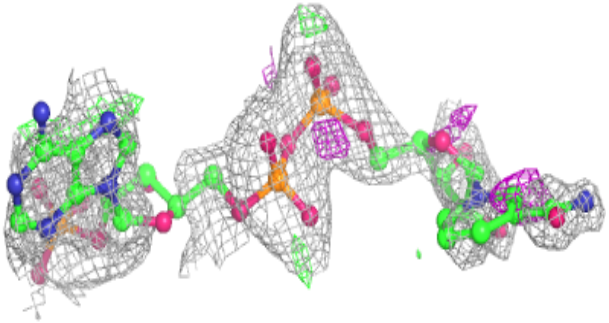


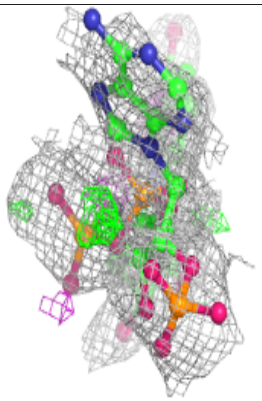


Electron density around NDP B 704:

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

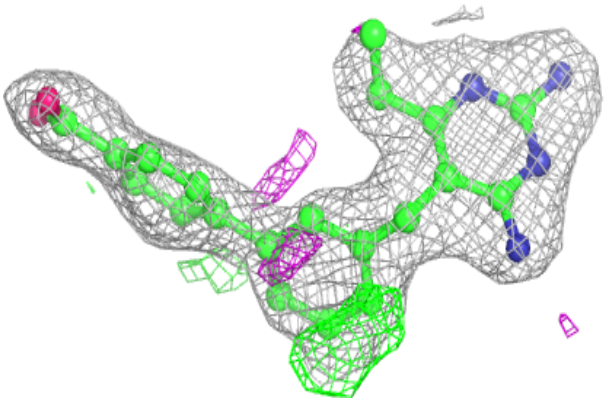


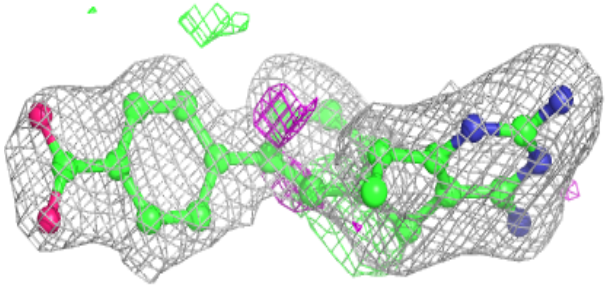


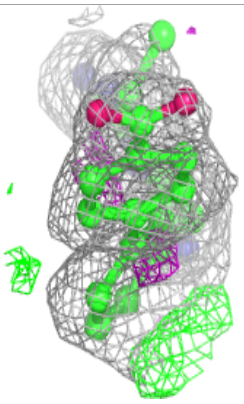


Electron density around U8I A 703:

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

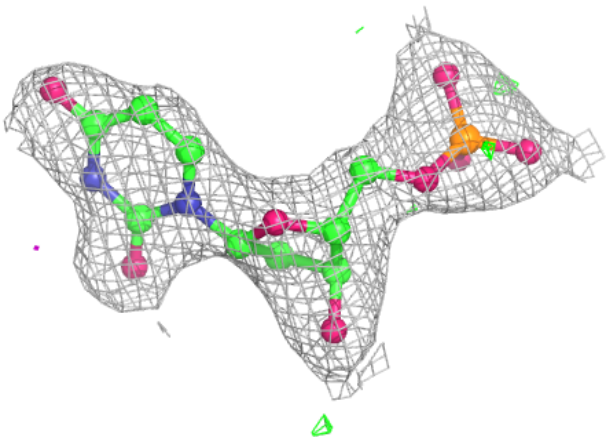


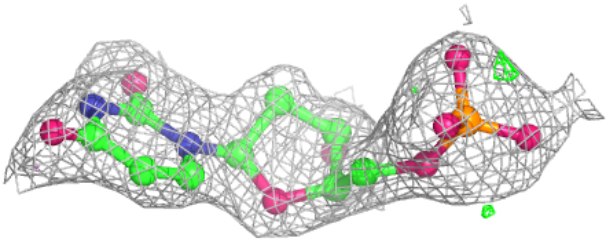


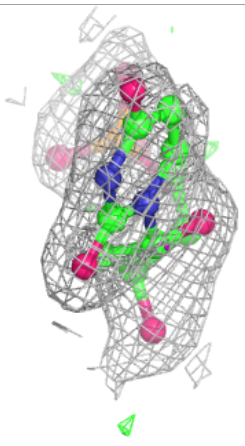


Electron density around UMP A 702:

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

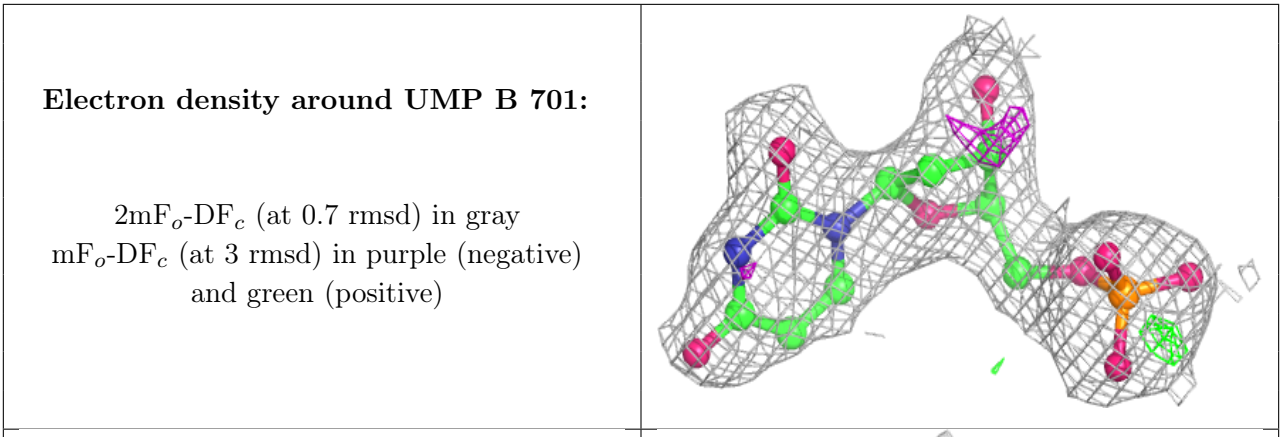






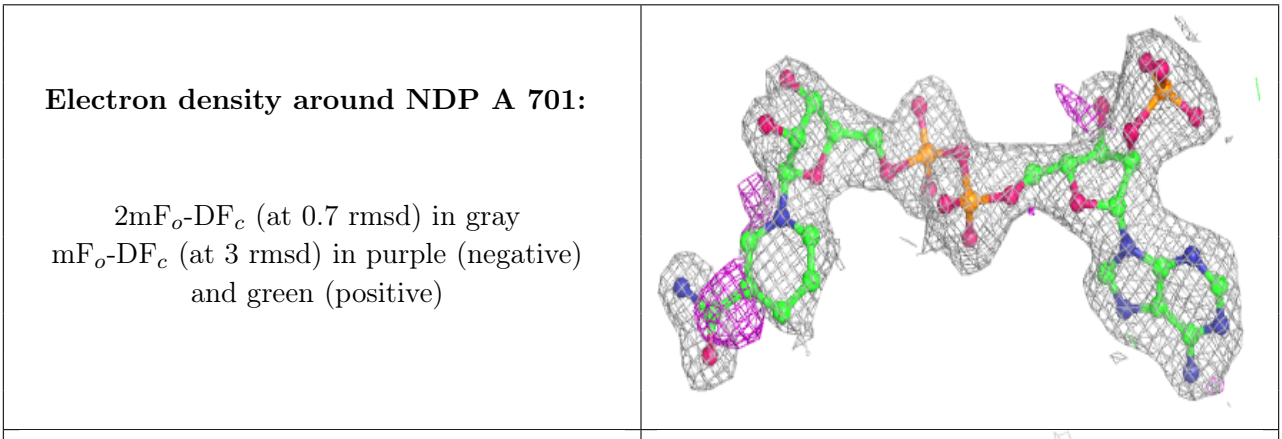
Electron density around UMP B 701:

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



Electron density around NDP 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.