



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 15, 2026 – 02:06 PM EDT

PDB ID : 9Y7Q / pdb_00009y7q
Title : Crystal structure of Candida auris dihydrofolate reductase in complex with inhibitor 1051 (S-form) and NADPH
Authors : Erlandsen, H.; Wright, D.; Krucinska, J.
Deposited on : 2025-09-11
Resolution : 2.42 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 ⓘ 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)
Xtriage (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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

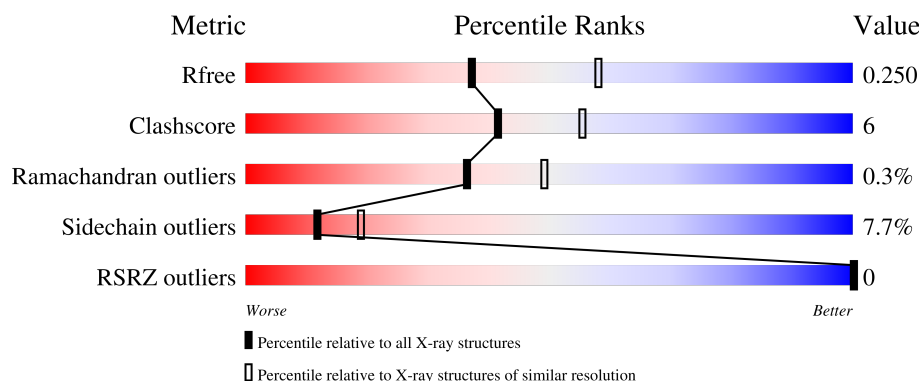
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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	208	
1	B	208	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3508 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 Dihydrofolate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	S	0	3	0
			1654	1061	282	302	9			
1	B	205	Total	C	N	O	S	0	0	0
			1665	1065	287	306	7			

There are 8 discrepancies between the modelled and reference sequences:

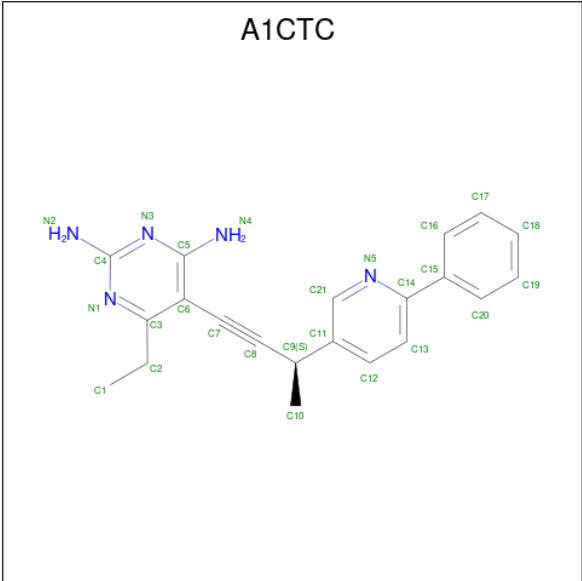
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP A0A0L0P1H8
A	-3	SER	-	expression tag	UNP A0A0L0P1H8
A	-2	HIS	-	expression tag	UNP A0A0L0P1H8
A	-1	MET	-	expression tag	UNP A0A0L0P1H8
B	-3	GLY	-	expression tag	UNP A0A0L0P1H8
B	-2	SER	-	expression tag	UNP A0A0L0P1H8
B	-1	HIS	-	expression tag	UNP A0A0L0P1H8
B	-1A	MET	-	expression tag	UNP A0A0L0P1H8

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



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 6-ethyl-5-[(3S)-3-(6-phenylpyridin-3-yl)but-1-yn-1-yl]pyrimidine-2,4-diamine (CCD ID: A1CTC) (formula: C₂₁H₂₁N₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			26	21	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	N	0	0
			26	21	5		

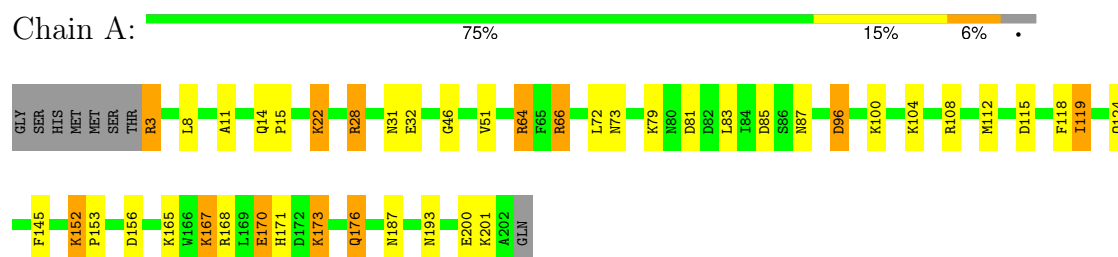
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	31	Total	O	0	0
			31	31		
4	B	10	Total	O	0	0
			10	10		

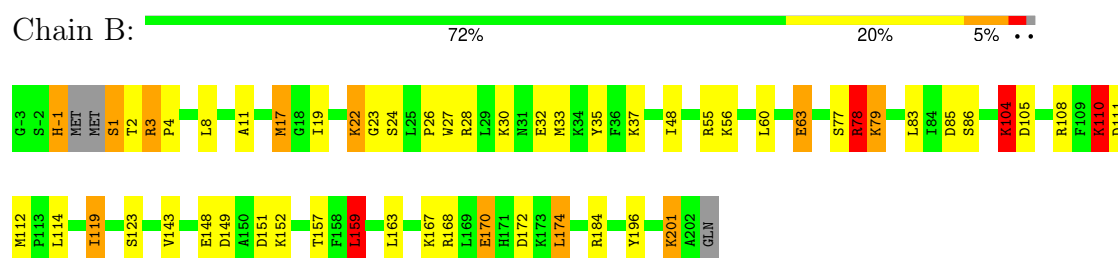
3 Residue-property plots

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: Dihydrofolate reductase



• Molecule 1: Dihydrofolate reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.09Å 69.82Å 112.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.96 – 2.42 32.96 – 2.42	Depositor EDS
% Data completeness (in resolution range)	99.8 (32.96-2.42) 99.8 (32.96-2.42)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.160 , 0.244 0.171 , 0.250	Depositor DCC
R_{free} test set	1022 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	44.7	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3508	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, A1CTC

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	0.94	1/1695 (0.1%)	1.58	19/2283 (0.8%)
1	B	0.92	0/1703	1.61	27/2294 (1.2%)
All	All	0.93	1/3398 (0.0%)	1.60	46/4577 (1.0%)

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
1	A	0	5
1	B	0	5
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	28	ARG	NE-CZ	7.19	1.41	1.33

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	17	MET	CG-SD-CE	-11.26	76.14	100.90
1	B	152	LYS	N-CA-CB	9.43	122.77	110.04
1	A	87	ASN	CB-CA-C	-8.45	96.28	110.56
1	A	66	ARG	CB-CA-C	-7.74	97.93	108.68
1	B	37	LYS	CB-CA-C	7.59	123.76	110.85
1	B	148	GLU	CB-CA-C	-7.45	96.29	109.62
1	A	176	GLN	CB-CA-C	7.05	122.83	110.85
1	A	22	LYS	CB-CA-C	-7.00	101.95	111.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	ARG	CG-CD-NE	-6.95	96.72	112.00
1	A	31	ASN	CA-CB-CG	-6.89	105.71	112.60
1	B	167	LYS	N-CA-CB	-6.78	99.07	110.80
1	B	108	ARG	CB-CA-C	-6.74	95.70	109.38
1	B	159	LEU	N-CA-CB	-6.63	100.22	109.97
1	B	22	LYS	CB-CA-C	-6.62	101.89	112.09
1	B	148	GLU	N-CA-CB	6.57	119.70	110.04
1	A	152	LYS	N-CA-CB	6.53	118.86	110.04
1	A	201	LYS	CG-CD-CE	6.44	126.11	111.30
1	B	151	ASP	CA-CB-CG	6.26	118.86	112.60
1	B	104	LYS	CB-CA-C	6.24	120.79	110.81
1	B	60	LEU	N-CA-CB	-6.19	100.74	110.46
1	B	149	ASP	CA-CB-CG	-6.19	106.41	112.60
1	A	3	ARG	N-CA-CB	-6.17	100.02	110.50
1	B	157	THR	CA-CB-OG1	-6.10	100.45	109.60
1	A	3	ARG	CB-CA-C	6.05	121.60	110.10
1	B	1	SER	CA-C-N	5.85	132.71	121.54
1	B	1	SER	C-N-CA	5.85	132.71	121.54
1	B	85	ASP	CA-CB-CG	5.76	118.36	112.60
1	B	78	ARG	CA-CB-CG	-5.65	102.80	114.10
1	B	108	ARG	CA-CB-CG	-5.62	102.86	114.10
1	A	104	LYS	CB-CG-CD	5.59	124.16	111.30
1	A	167	LYS	CG-CD-CE	5.51	123.97	111.30
1	A	145	PHE	CA-CB-CG	-5.49	108.31	113.80
1	A	173	LYS	CB-CA-C	-5.48	101.53	110.85
1	A	3	ARG	CD-NE-CZ	5.45	132.03	124.40
1	B	56	LYS	N-CA-CB	5.45	118.22	110.16
1	B	2	THR	N-CA-CB	5.41	119.63	110.49
1	B	167	LYS	CB-CA-C	5.40	119.48	109.70
1	B	23	GLY	CA-C-O	-5.37	113.89	119.20
1	A	115	ASP	CB-CA-C	5.27	121.43	112.00
1	A	200	GLU	CB-CG-CD	5.23	121.48	112.60
1	B	112	MET	CG-SD-CE	5.20	112.35	100.90
1	B	3	ARG	CD-NE-CZ	5.20	131.68	124.40
1	A	156	ASP	CA-CB-CG	5.12	117.72	112.60
1	B	63	GLU	CA-CB-CG	-5.09	103.92	114.10
1	B	143	VAL	N-CA-CB	-5.06	104.37	111.25
1	A	171	HIS	CB-CG-CD2	-5.03	124.67	131.20

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	ARG	Sidechain
1	A	168	ARG	Sidechain
1	A	28	ARG	Sidechain
1	A	64	ARG	Sidechain
1	A	66	ARG	Sidechain
1	B	168	ARG	Sidechain
1	B	201	LYS	Peptide
1	B	28	ARG	Sidechain
1	B	55	ARG	Sidechain
1	B	78	ARG	Sidechain

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	1654	0	1653	17	0
1	B	1665	0	1663	25	0
2	A	48	0	26	3	0
2	B	48	0	26	5	0
3	A	26	0	0	1	0
3	B	26	0	0	2	0
4	A	31	0	0	0	0
4	B	10	0	0	0	0
All	All	3508	0	3368	44	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 6.

All (44) 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:17:MET:HE1	1:B:163:LEU:HD11	1.54	0.88
1:B:11:ALA:H	2:B:302:NDP:H72N	1.28	0.80
1:A:11:ALA:H	2:A:300:NDP:H72N	1.40	0.69
1:A:152:LYS:HB2	1:A:153:PRO:HD2	1.75	0.69
1:B:17:MET:HE1	1:B:163:LEU:CD1	2.26	0.66
1:B:170:GLU:OE2	1:B:170:GLU:HA	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:GLU:O	1:B:63:GLU:HG3	2.03	0.59
1:B:26:PRO:HG2	1:B:27:TRP:CZ3	2.39	0.57
1:A:170[A]:GLU:CD	1:A:170[A]:GLU:H	2.09	0.56
1:A:8:LEU:HD23	1:A:119:ILE:HG12	1.87	0.56
1:A:124:GLN:OE1	2:A:300:NDP:H8A	2.05	0.55
1:B:123:SER:HB3	2:B:302:NDP:O2N	2.07	0.54
1:B:78:ARG:HH11	1:B:78:ARG:HG3	1.73	0.53
1:B:-1:HIS:CD2	1:B:-1:HIS:H	2.27	0.53
1:A:170[A]:GLU:HG2	1:A:173:LYS:HG2	1.91	0.52
1:B:110:LYS:O	1:B:111:ASP:HB2	2.10	0.50
1:B:174:LEU:C	1:B:174:LEU:HD12	2.37	0.49
1:A:32:GLU:OE1	3:A:301:A1CTC:N1	2.45	0.49
1:B:19:ILE:O	2:B:302:NDP:H2N	2.12	0.49
1:A:72:LEU:C	1:A:72:LEU:HD23	2.40	0.46
1:B:-1:HIS:CD2	1:B:-1:HIS:N	2.84	0.46
1:B:8:LEU:HD23	1:B:119:ILE:HG12	1.97	0.45
1:B:77:SER:OG	2:B:302:NDP:O1X	2.25	0.45
1:A:85:ASP:OD1	1:A:85:ASP:C	2.60	0.45
1:B:35:TYR:CD2	1:B:196:TYR:CE1	3.05	0.45
1:A:119:ILE:HD13	1:A:119:ILE:N	2.32	0.44
1:B:3:ARG:HB2	1:B:4:PRO:CD	2.48	0.43
1:B:33:MET:HE2	1:B:33:MET:HB2	1.81	0.43
1:B:104:LYS:O	1:B:104:LYS:HE2	2.19	0.43
1:A:51:VAL:HA	1:A:118:PHE:O	2.19	0.43
1:A:96:ASP:OD2	1:A:100:LYS:NZ	2.48	0.42
1:B:32:GLU:OE1	3:B:301:A1CTC:N1	2.53	0.42
1:B:79:LYS:HE2	1:B:79:LYS:N	2.35	0.42
1:B:19:ILE:HD13	1:B:159:LEU:HD13	2.02	0.41
1:B:114:LEU:N	1:B:114:LEU:HD12	2.33	0.41
1:A:187:ASN:O	1:A:193:ASN:HA	2.20	0.41
2:A:300:NDP:H8A	2:A:300:NDP:H3B	2.02	0.41
1:B:1:SER:C	1:B:3:ARG:H	2.28	0.41
1:A:81:ASP:HB2	1:A:83:LEU:HD23	2.03	0.41
3:B:301:A1CTC:C7	2:B:302:NDP:H42N	2.51	0.41
1:A:81:ASP:CB	1:A:83:LEU:HD23	2.51	0.41
1:A:46:GLY:O	1:A:112:MET:HB3	2.22	0.40
1:A:14:GLN:HA	1:A:15:PRO:HA	1.88	0.40
1:B:119:ILE:N	1:B:119:ILE:HD13	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	201/208 (97%)	199 (99%)	2 (1%)	0	100	100
1	B	201/208 (97%)	194 (96%)	6 (3%)	1 (0%)	24	35
All	All	402/416 (97%)	393 (98%)	8 (2%)	1 (0%)	36	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	110	LYS

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	182/186 (98%)	171 (94%)	11 (6%)	17	29
1	B	183/186 (98%)	165 (90%)	18 (10%)	7	11
All	All	365/372 (98%)	336 (92%)	29 (8%)	12	18

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	22	LYS
1	A	73	ASN
1	A	79	LYS
1	A	96	ASP

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Mol	Chain	Res	Type
1	A	119	ILE
1	A	165	LYS
1	A	167	LYS
1	A	170[A]	GLU
1	A	170[B]	GLU
1	A	176	GLN
1	B	-1	HIS
1	B	22	LYS
1	B	24	SER
1	B	30	LYS
1	B	48	ILE
1	B	79	LYS
1	B	83	LEU
1	B	86	SER
1	B	104	LYS
1	B	105	ASP
1	B	110	LYS
1	B	119	ILE
1	B	159	LEU
1	B	170	GLU
1	B	172	ASP
1	B	174	LEU
1	B	184	ARG
1	B	201	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	31	ASN
1	A	176	GLN
1	B	-1	HIS
1	B	14	GLN
1	B	31	ASN
1	B	47	HIS
1	B	142	GLN

5.3.3 RNA ⓘ

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](#)

4 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	A1CTC	A	301	-	27,28,28	0.74	0	34,38,38	1.33	2 (5%)
2	NDP	B	302	-	51,52,52	0.73	1 (1%)	71,80,80	1.09	8 (11%)
3	A1CTC	B	301	-	27,28,28	0.68	0	34,38,38	1.40	3 (8%)
2	NDP	A	300	-	51,52,52	0.75	1 (1%)	71,80,80	1.19	9 (12%)

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	A1CTC	A	301	-	-	2/12/15/15	0/3/3/3
2	NDP	B	302	-	-	3/34/77/77	0/5/5/5
3	A1CTC	B	301	-	-	5/12/15/15	0/3/3/3
2	NDP	A	300	-	-	2/34/77/77	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	302	NDP	P2B-O2X	-2.57	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	NDP	C4N-C3N	-2.51	1.45	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	A1CTC	C10-C9-C8	-5.48	102.24	110.09
3	B	301	A1CTC	C10-C9-C8	-4.73	103.32	110.09
3	B	301	A1CTC	C2-C3-C6	3.54	124.99	122.54
2	A	300	NDP	P2B-O2B-C2B	-3.44	114.25	123.43
2	A	300	NDP	O3-PN-O1N	-3.15	101.24	110.70
2	A	300	NDP	C2B-C1B-N9A	-3.14	108.59	113.75
2	A	300	NDP	O2B-C2B-C1B	-2.93	99.74	110.05
2	B	302	NDP	P2B-O2B-C2B	-2.89	115.71	123.43
2	B	302	NDP	O3-PN-O1N	-2.46	103.30	110.70
3	A	301	A1CTC	C11-C9-C8	2.45	115.83	112.22
3	B	301	A1CTC	C13-C12-C11	-2.41	118.78	121.18
2	B	302	NDP	C1D-N1N-C2N	-2.41	117.17	121.14
2	A	300	NDP	O2X-P2B-O2B	-2.37	96.60	105.85
2	B	302	NDP	C3N-C7N-N7N	-2.37	113.46	117.67
2	A	300	NDP	O2N-PN-O1N	2.35	123.37	112.44
2	B	302	NDP	O2N-PN-O1N	2.32	123.23	112.44
2	B	302	NDP	O2N-PN-O3	2.18	113.17	107.27
2	B	302	NDP	O4D-C4D-C3D	2.18	109.47	105.15
2	A	300	NDP	O2A-PA-O1A	2.17	122.53	112.44
2	B	302	NDP	C2B-C1B-N9A	-2.13	110.24	113.75
2	A	300	NDP	O2D-C2D-C3D	2.13	118.65	111.82
2	A	300	NDP	O3X-P2B-O2X	2.07	115.55	107.80

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	300	NDP	PA-O3-PN-O5D
3	A	301	A1CTC	C6-C7-C8-C9
3	B	301	A1CTC	C1-C2-C3-C6
3	B	301	A1CTC	C6-C7-C8-C9
2	B	302	NDP	C3D-C4D-C5D-O5D
3	B	301	A1CTC	C1-C2-C3-N1
3	B	301	A1CTC	C3-C6-C7-C8
2	A	300	NDP	O4D-C1D-N1N-C2N
2	B	302	NDP	O4D-C1D-N1N-C2N
3	A	301	A1CTC	C3-C6-C7-C8

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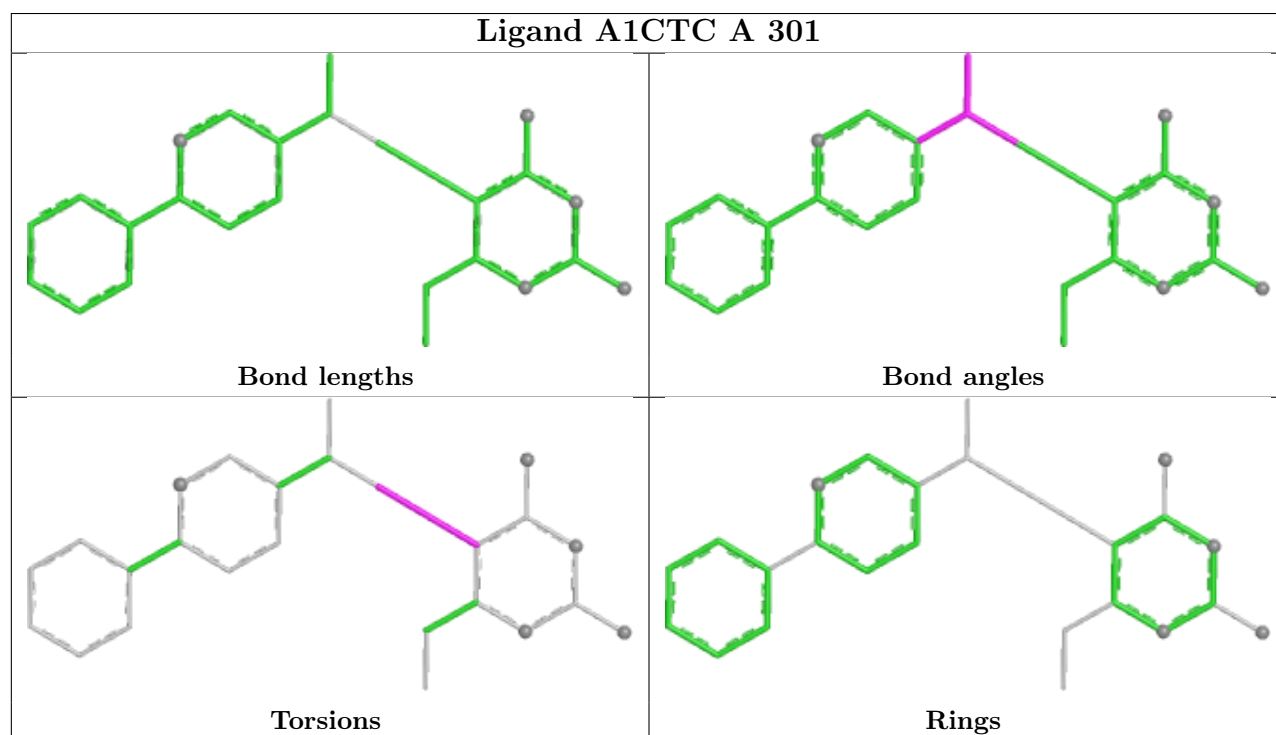
Mol	Chain	Res	Type	Atoms
2	B	302	NDP	PN-O3-PA-O2A
3	B	301	A1CTC	C12-C11-C9-C8

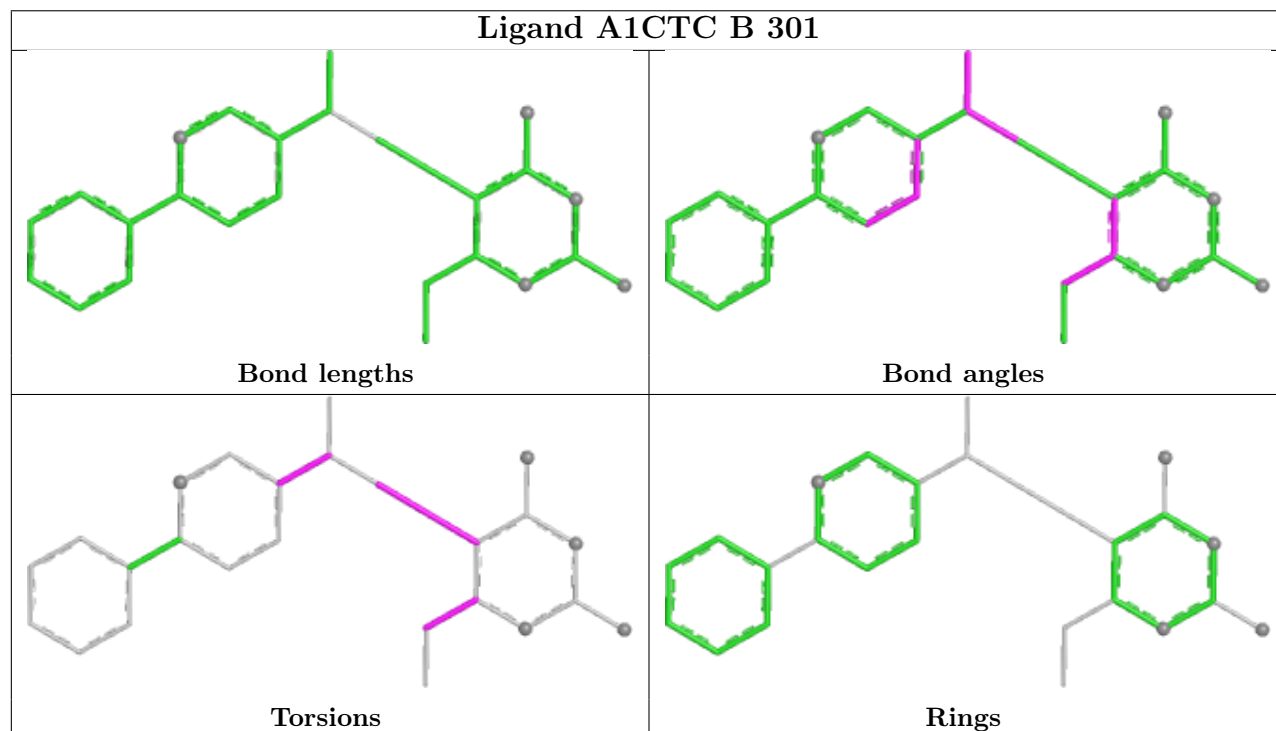
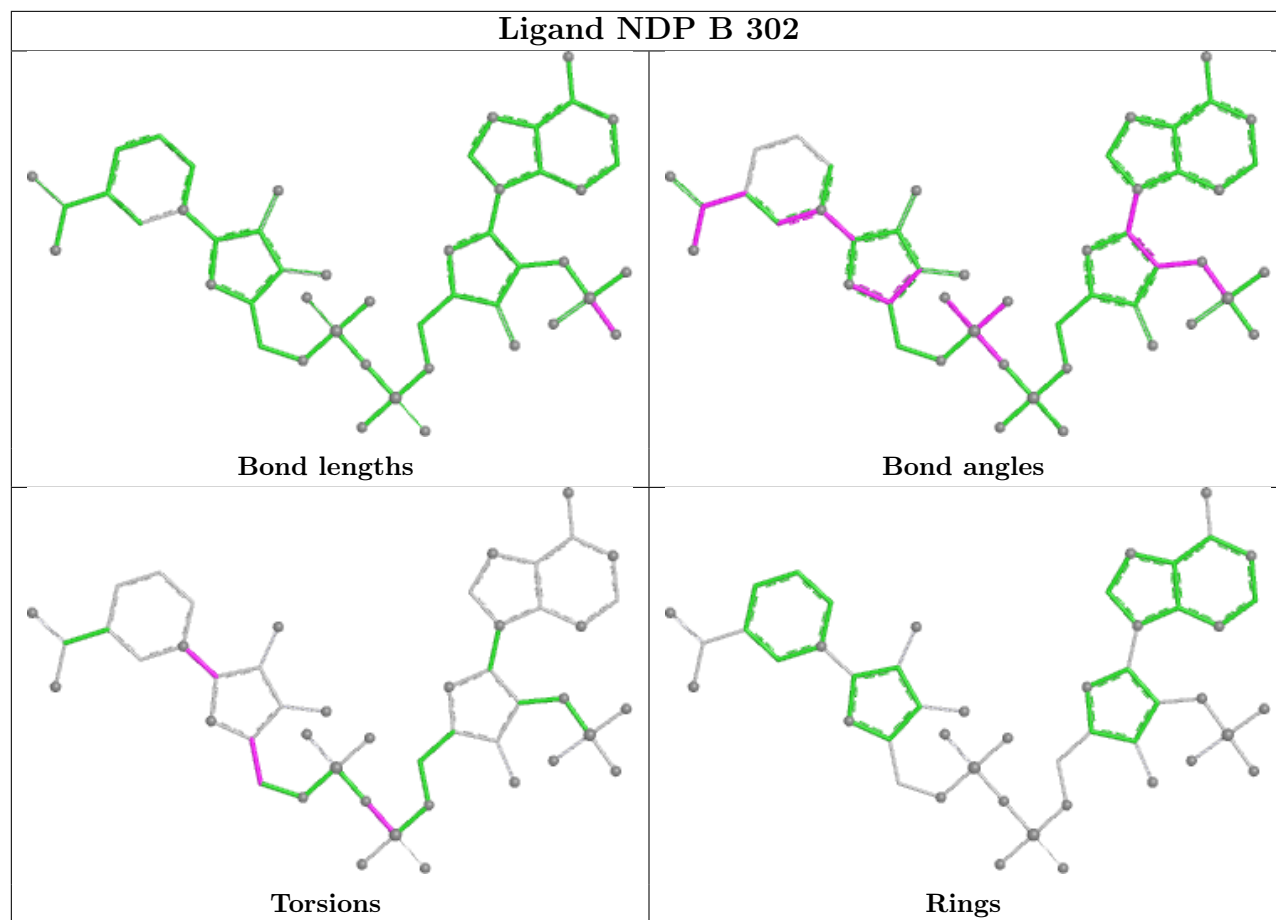
There are no ring outliers.

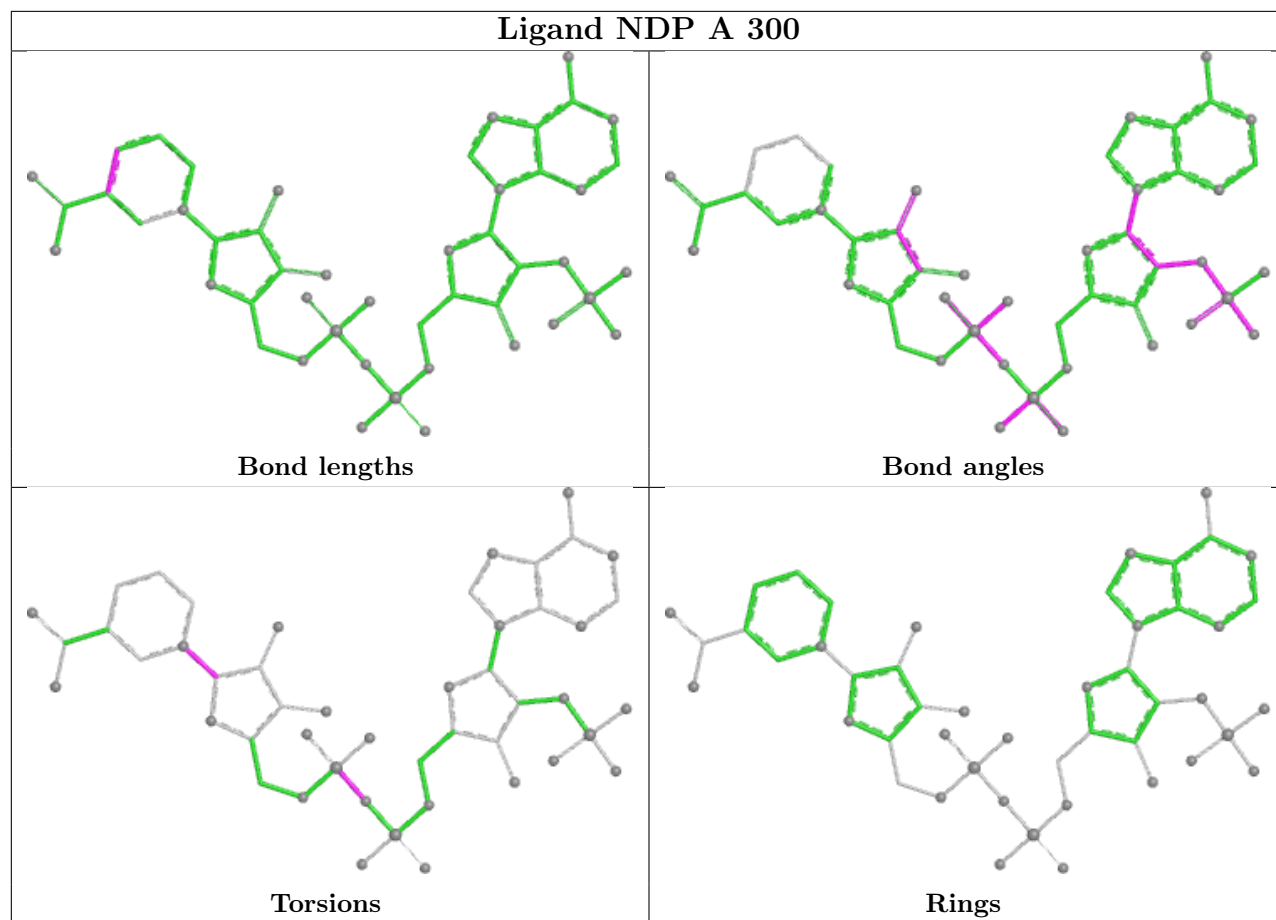
4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	A1CTC	1	0
2	B	302	NDP	5	0
3	B	301	A1CTC	2	0
2	A	300	NDP	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	200/208 (96%)	-0.92	0 100 100	19, 43, 64, 75	3 (1%)
1	B	205/208 (98%)	-0.68	0 100 100	36, 55, 79, 95	0
All	All	405/416 (97%)	-0.80	0 100 100	19, 48, 74, 95	3 (0%)

There are no RSRZ outliers to report.

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.

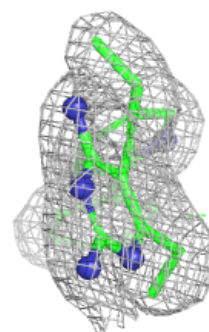
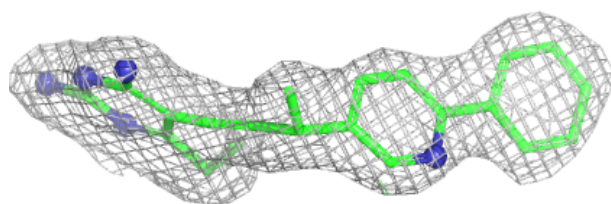
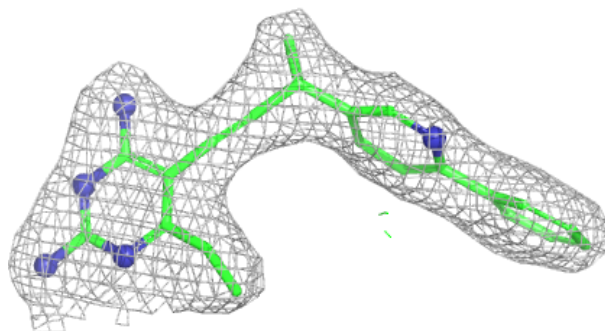
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	A1CTC	A	301	26/26	0.97	0.06	30,35,51,56	0
3	A1CTC	B	301	26/26	0.97	0.06	38,42,60,62	0
2	NDP	A	300	48/48	0.98	0.04	31,44,63,67	0
2	NDP	B	302	48/48	0.99	0.04	34,41,53,54	0

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.

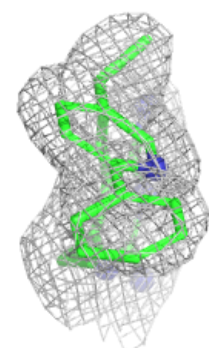
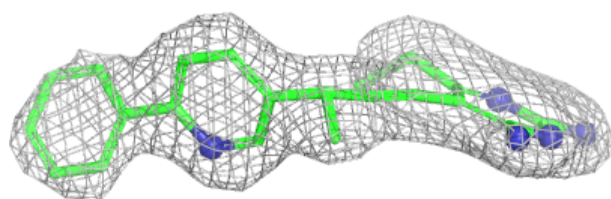
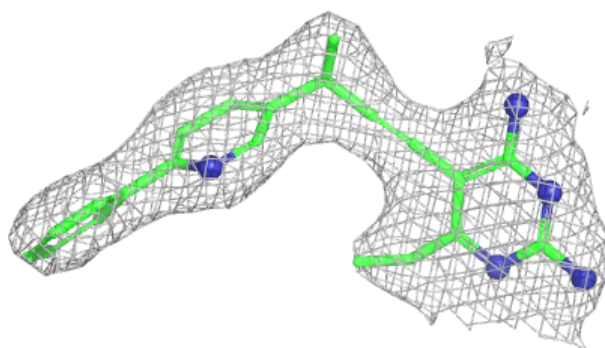
Electron density around A1CTC A 301:

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



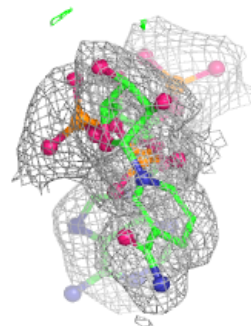
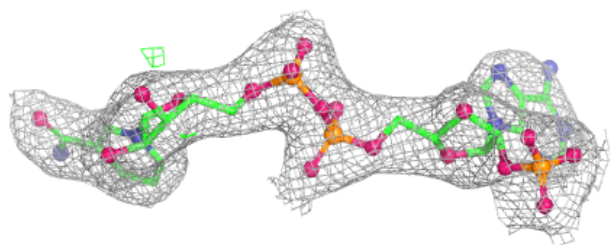
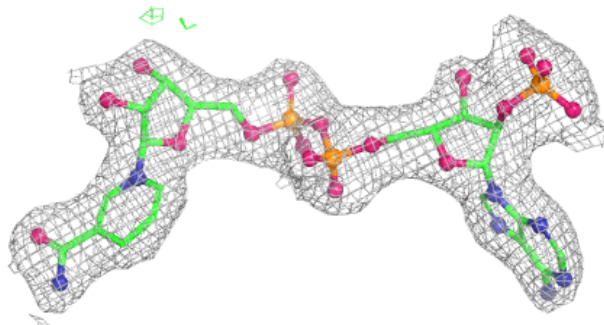
Electron density around A1CTC B 301:

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

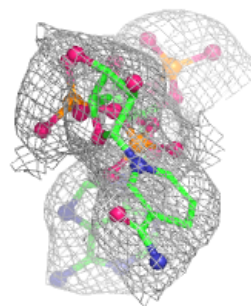
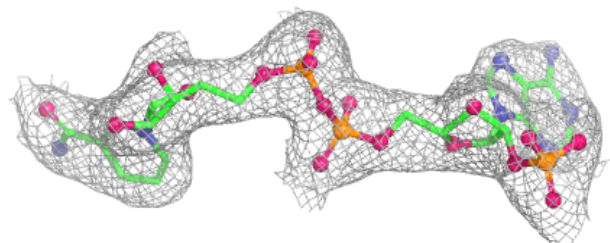
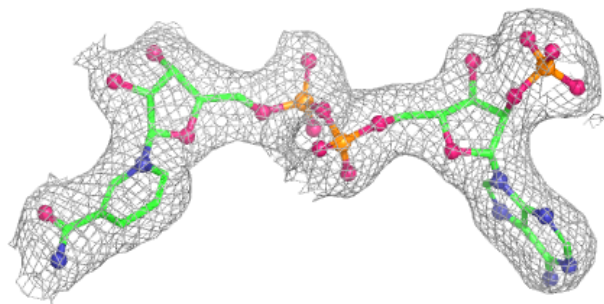


Electron density around NDP A 300:

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

**Electron density around NDP B 302:**

$2mF_o-DF_c$ (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.