



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 10:24 AM UTC

PDB ID : 2AD5 / pdb_00002ad5
Title : Mechanisms of feedback regulation and drug resistance of CTP synthetases: structure of the E. coli CTPS/CTP complex at 2.8-Angstrom resolution.
Authors : Endrizzi, J.A.; Kim, H.; Anderson, P.M.; Baldwin, E.P.
Deposited on : 2005-07-19
Resolution : 2.80 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)
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	:	9.0.010 (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

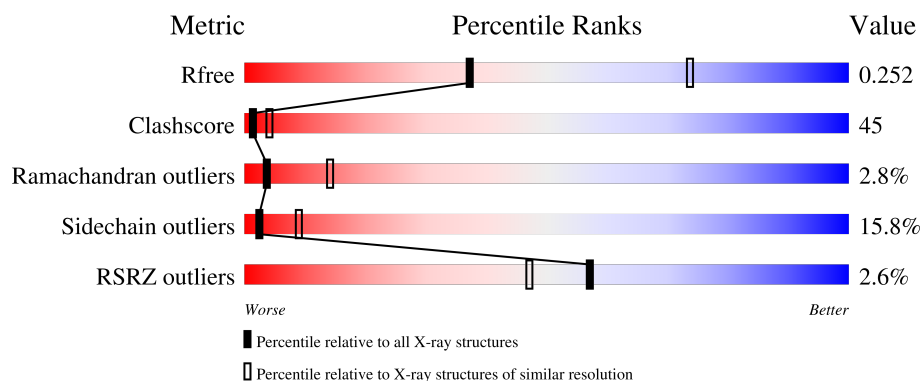
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	545	3% 34% 49% 13% ..
1	B	545	2% 34% 52% 12% ..

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8694 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.

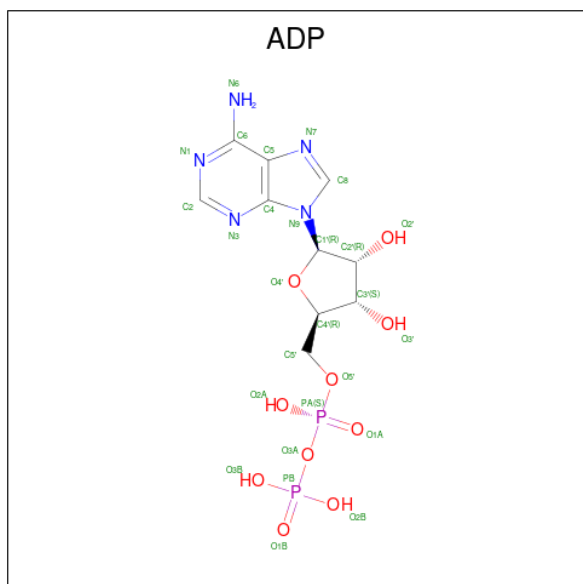
- Molecule 1 is a protein called CTP synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	534	Total	C	N	O	S	16	0	0
			4156	2625	726	784	21			
1	B	536	Total	C	N	O	S	11	0	0
			4172	2636	729	786	21			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

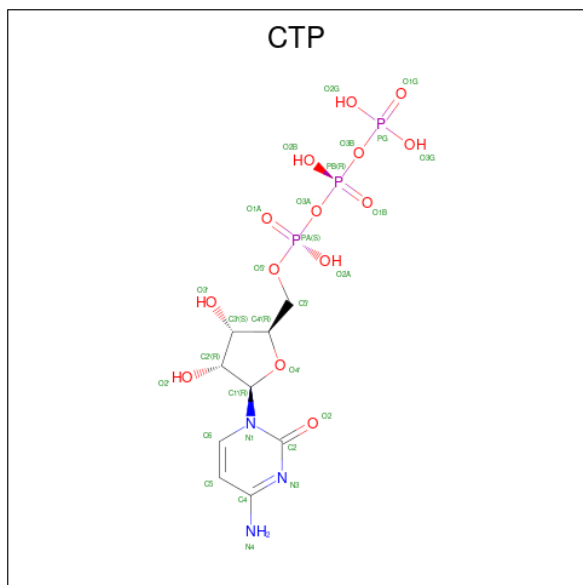
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is CYTIDINE-5'-TRIPHOSPHATE (CCD ID: CTP) (formula: $C_9H_{16}N_3O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			29	9	3	14	3		
4	B	1	Total	C	N	O	P	0	0
			29	9	3	14	3		

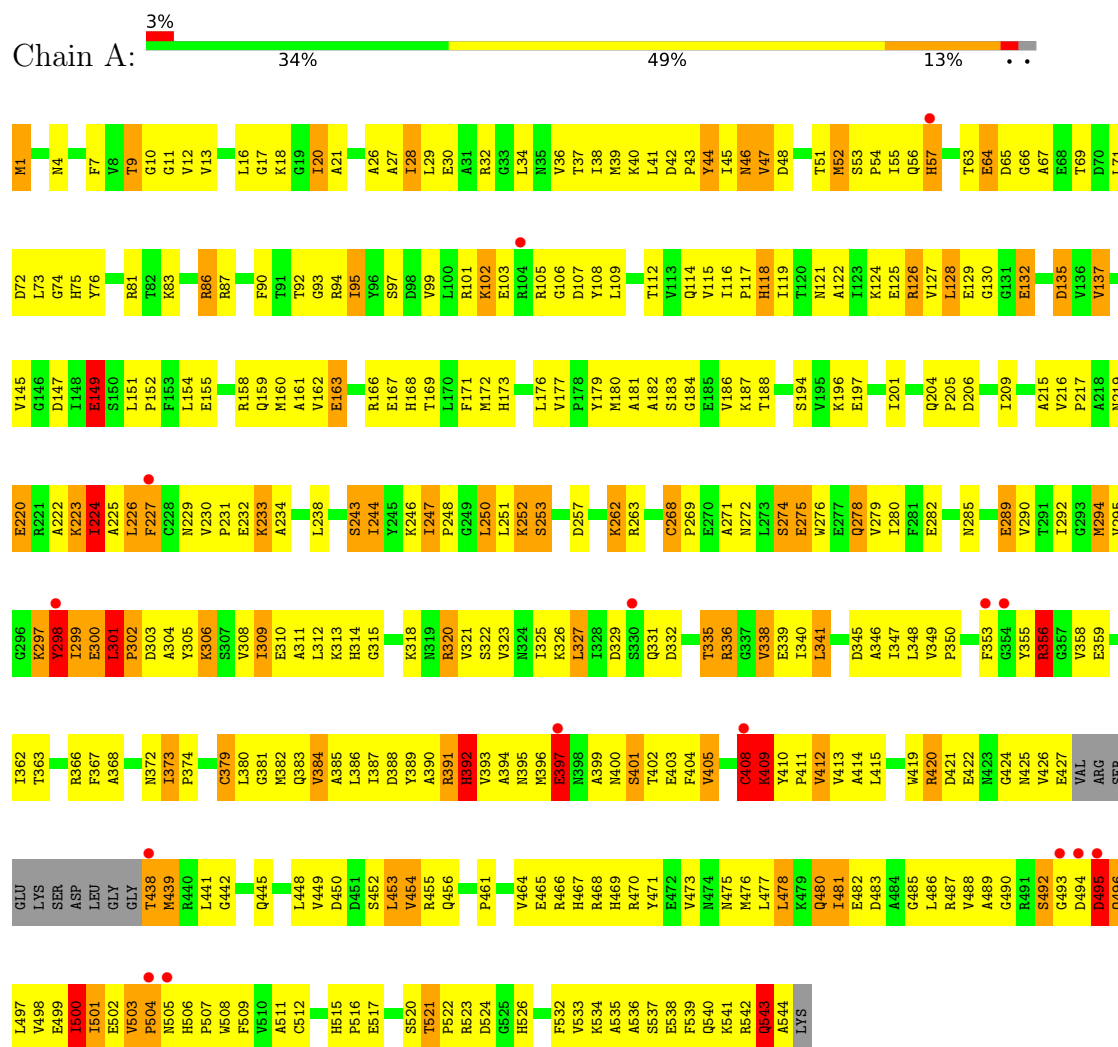
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	130	Total	O	0	0
			130	130		
5	B	122	Total	O	0	0
			122	122		

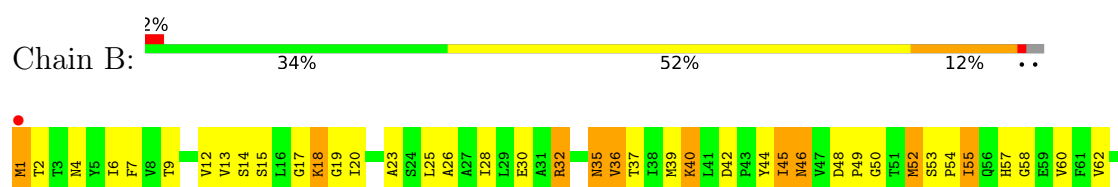
3 Residue-property plots

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: CTP synthase



• Molecule 1: CTP synthase



G66	E132	P217	V279	L348	E418	G485
A67	G133	A218	I280	V349	W419	L486
E68	H134	E219	F281	P350	R420	R487
T69	D135	E220	E282	F353	D421	
D70	V136	R221	A283	G354	E422	G490
L71	D72	A222	E284	N285	N423	R491
D73	E140	Y223	N285	Y355	G424	S492
G74	D147	I224	P286	R356	N425	S493
H75	D148	A225	V287	G357	V426	D494
Y76	I148	L226	S288	V358	E427	D495
E77	Y76	F227	E289	E359	V428	Q496
R78	E149	C228	V290	G360	ARG	L497
F79	S150	W298	T291	M361	SER	Y498
R80	L151	V230	I292	I362	GLU	E499
R81	P152	P231	G293	T363	LYS	I500
T82	M150	E232	M294	T364	SER	I501
S85	I164	A233	V295	A365	ASP	E502
R86	G165	A234	G296	R366	LEU	F503
N88	E167	V235	K297	F367	GLY	P504
H89	H168	I236	Y298	N372	T438	H505
F90	T169	S237	I299	I373	M439	H506
T91	L170	L238	E300	P374	R440	P507
T92	F171	K239	L301	Y375	L441	W508
G93	L174	D242	P302	C379	G442	F509
R94	L175	S243	Y305	L380	A443	V510
I95	T176	K246	R306	G381	Q444	A511
Y96	L176	I247	I309	M382	L448	C512
S97	V177	P248	E310	Q383	V449	Q513
D98	P178	G248	K313	V384	D450	H515
V99	Y179	L280	K319	A385	D451	P516
L100	M180	L251	N320	L386	S452	E517
R101	A181	K252	R320	I387	L453	F518
K102	K187	S253	V321	Y389	R454	T519
E103	T188	Q254	S322	H392	R455	S520
R104	K189	G255	K326	V393	Y458	T521
R105	P190	L256	L327	A394	N459	P522
D107	T191	D257	I328	M396	A460	R523
Y108	Q192	Y259	D329	E397	P461	H526
L109	H193	I260	M396	E400	E465	P527
Q114	S194	C261	S330	S401	R466	L528
V115	E197	K262	Q331	T402	H467	F529
I116	L198	R263	D332	E403	R468	A530
P117	E197	F264	V333	V405	H469	G531
H118	I201	S265	E334	C408	Y470	F532
I119	I207	L266	T335	Y410	R471	V533
T120	L208	N267	R336	F404	E472	K534
N121	L209	C268	G337	V405	V473	A535
E125	I209	P269	V338	C408	N474	A536
R126	C210	A271	I340	K409	N475	F539
V127	R211	N272	L341	Y410	M476	Q540
L128	S212	L273	K342	P411	L477	K541
E129	D213	S274	G343	V412	L478	R542
G130	R214	E275	L344	V413	K479	Q543
G131	A215	W276	D345	L414	Q480	A544
	V216	E277	A346	L415	I481	K545
		Q278	I347		E482	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	163.27Å 106.38Å 130.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.80) 98.3 (20.00-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.81Å)	Xtriage
Refinement program	TNT 5F	Depositor
R, R_{free}	0.202 , 0.277 0.195 , 0.252	Depositor DCC
R_{free} test set	1865 reflections (3.34%)	wwPDB-VP
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 107.8	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	0.94	EDS
Total number of atoms	8694	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.16% 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: ADP, CTP, MG

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	0.92	0/4232	1.46	32/5734 (0.6%)
1	B	0.92	0/4248	1.48	32/5755 (0.6%)
All	All	0.92	0/8480	1.47	64/11489 (0.6%)

There are no bond length outliers.

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	118	HIS	CA-CB-CG	-9.12	104.68	113.80
1	A	118	HIS	CA-CB-CG	-8.79	105.01	113.80
1	A	216	VAL	CA-C-O	7.70	123.69	119.15
1	B	495	ASP	N-CA-C	-7.58	102.89	113.20
1	B	503	VAL	O-C-N	7.36	127.97	121.57

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	4156	0	4162	395	0
1	B	4172	0	4184	358	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	27	0	12	5	0
3	B	27	0	12	4	0
4	A	29	0	12	5	0
4	B	29	0	12	5	0
5	A	130	0	0	10	0
5	B	122	0	0	12	1
All	All	8694	0	8394	753	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 45.

The worst 5 of 753 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:127:VAL:HB	1:A:160:MET:HE1	1.23	1.15
1:A:301:LEU:HD12	1:A:302:PRO:HD2	1.36	1.06
1:A:39:MET:HE1	1:A:130:GLY:HA3	1.40	1.01
1:A:521:THR:HG22	1:A:524:ASP:H	1.27	0.99
1:A:521:THR:HG23	1:A:522:PRO:HD2	1.41	0.99

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)
5:B:1724:HOH:O	5:B:1724:HOH:O[2_555]	0.81	1.39

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	530/545 (97%)	445 (84%)	66 (12%)	19 (4%)	2 10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	532/545 (98%)	461 (87%)	60 (11%)	11 (2%)	5	20
All	All	1062/1090 (97%)	906 (85%)	126 (12%)	30 (3%)	4	14

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	298	TYR
1	A	335	THR
1	A	356	ARG
1	A	391	ARG
1	A	392	HIS

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	451/461 (98%)	373 (83%)	78 (17%)	2	7
1	B	453/461 (98%)	388 (86%)	65 (14%)	3	11
All	All	904/922 (98%)	761 (84%)	143 (16%)	2	9

5 of 143 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	306	LYS
1	B	330	SER
1	B	400	ASN
1	A	300	GLU
1	A	298	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	46	ASN
1	B	204	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	425	ASN
1	B	193	HIS
1	B	229	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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	CTP	A	602	-	29,30,30	1.90	4 (13%)	43,47,47	1.14	5 (11%)
3	ADP	B	1601	2	28,29,29	1.13	2 (7%)	43,45,45	0.74	0
4	CTP	B	1602	-	29,30,30	1.98	5 (17%)	43,47,47	1.56	5 (11%)
3	ADP	A	601	2	28,29,29	0.98	2 (7%)	43,45,45	1.10	3 (6%)

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
4	CTP	A	602	-	-	7/22/38/38	0/2/2/2
3	ADP	B	1601	2	-	8/16/32/32	0/3/3/3
4	CTP	B	1602	-	-	7/22/38/38	0/2/2/2
3	ADP	A	601	2	-	5/16/32/32	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	CTP	PB-O3A	7.35	1.67	1.59
4	B	1602	CTP	PB-O3B	7.18	1.67	1.59
3	B	1601	ADP	PA-O3A	4.82	1.64	1.59
3	A	601	ADP	PA-O3A	3.66	1.63	1.59
4	A	602	CTP	PA-O3A	3.51	1.63	1.59

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1602	CTP	O4'-C1'-N1	-6.31	94.05	108.36
3	A	601	ADP	C1'-N9-C8	4.57	137.24	127.09
3	A	601	ADP	C4-N9-C1'	-4.09	117.08	126.63
4	B	1602	CTP	C2'-C1'-N1	3.81	123.85	113.25
4	A	602	CTP	C4'-O4'-C1'	-2.50	103.95	109.47

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

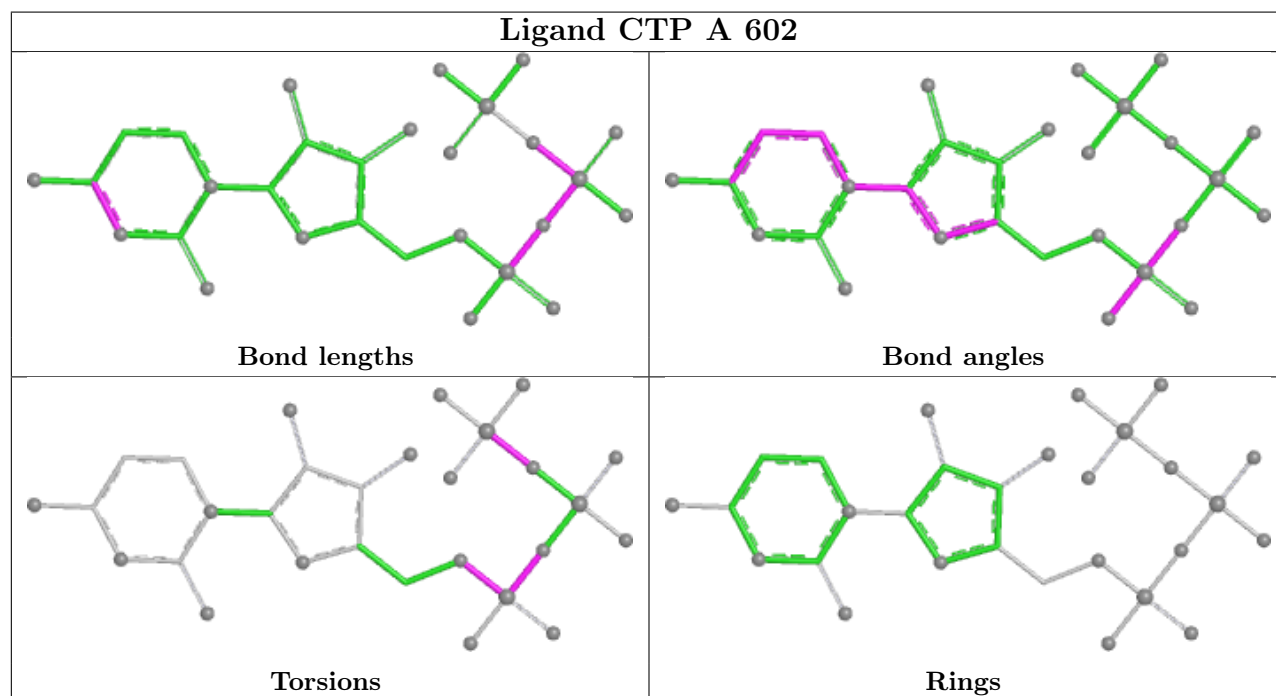
Mol	Chain	Res	Type	Atoms
3	A	601	ADP	PA-O3A-PB-O2B
3	A	601	ADP	C5'-O5'-PA-O1A
3	A	601	ADP	C5'-O5'-PA-O3A
3	A	601	ADP	O4'-C4'-C5'-O5'
3	B	1601	ADP	C5'-O5'-PA-O1A

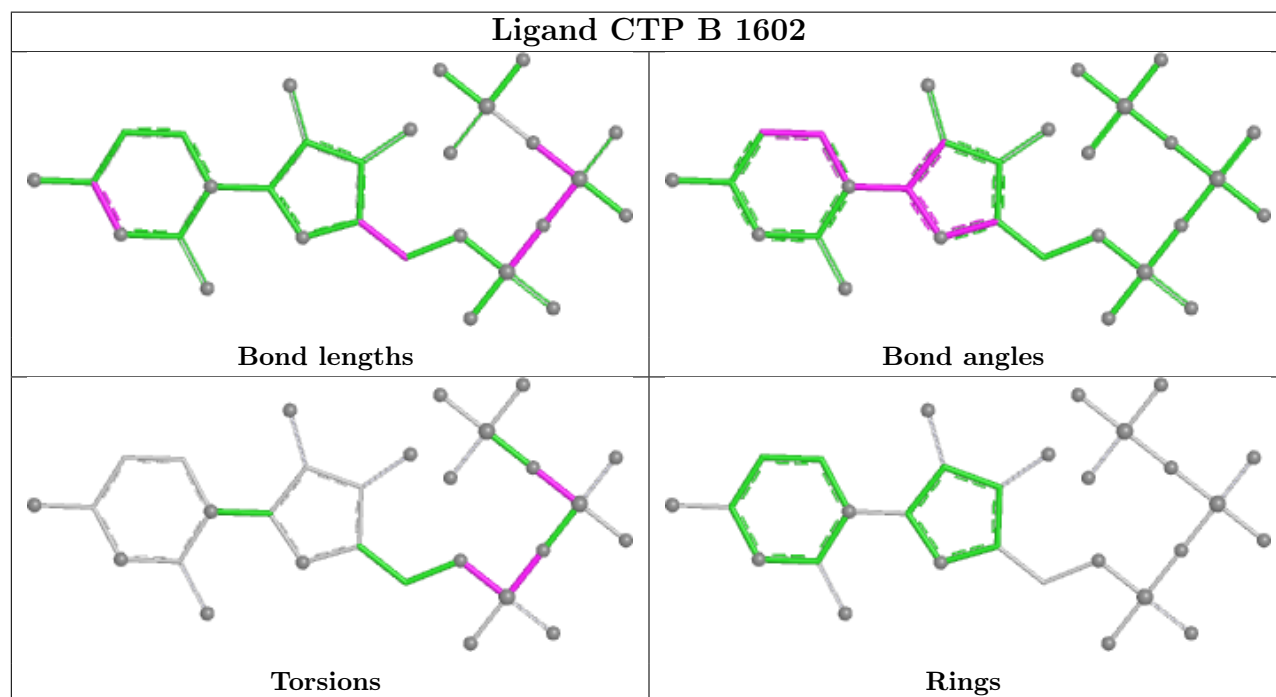
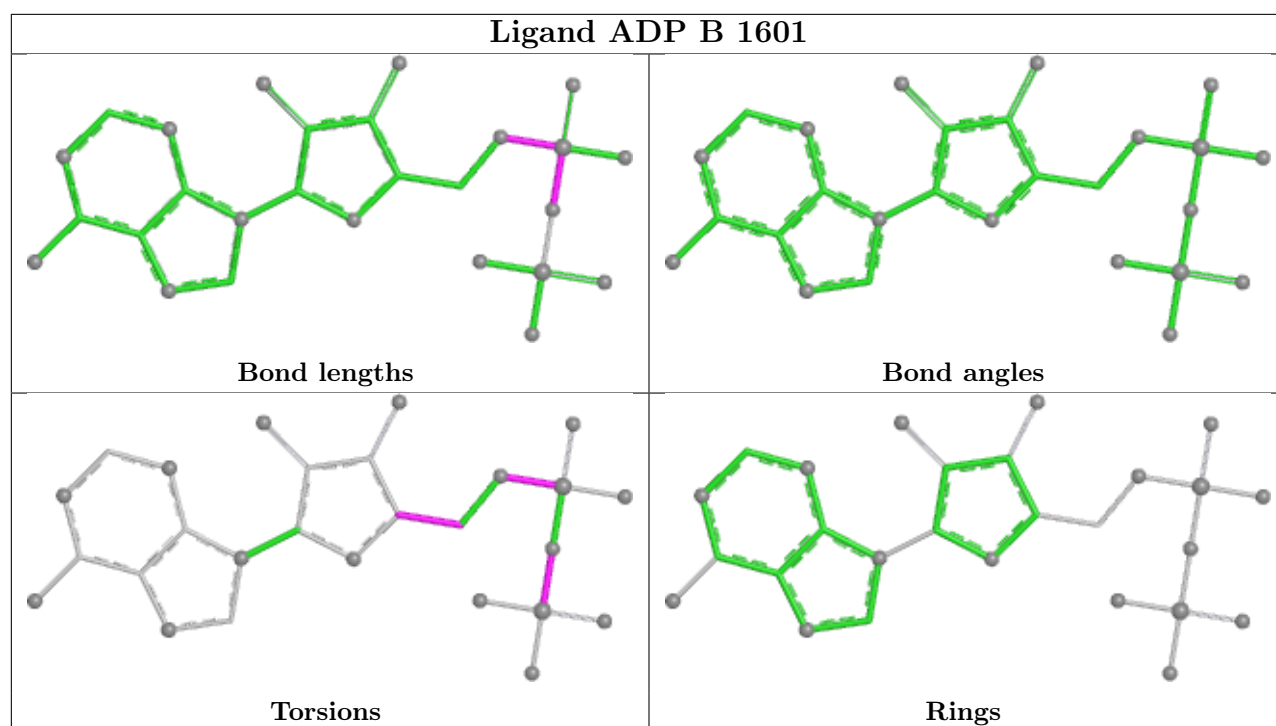
There are no ring outliers.

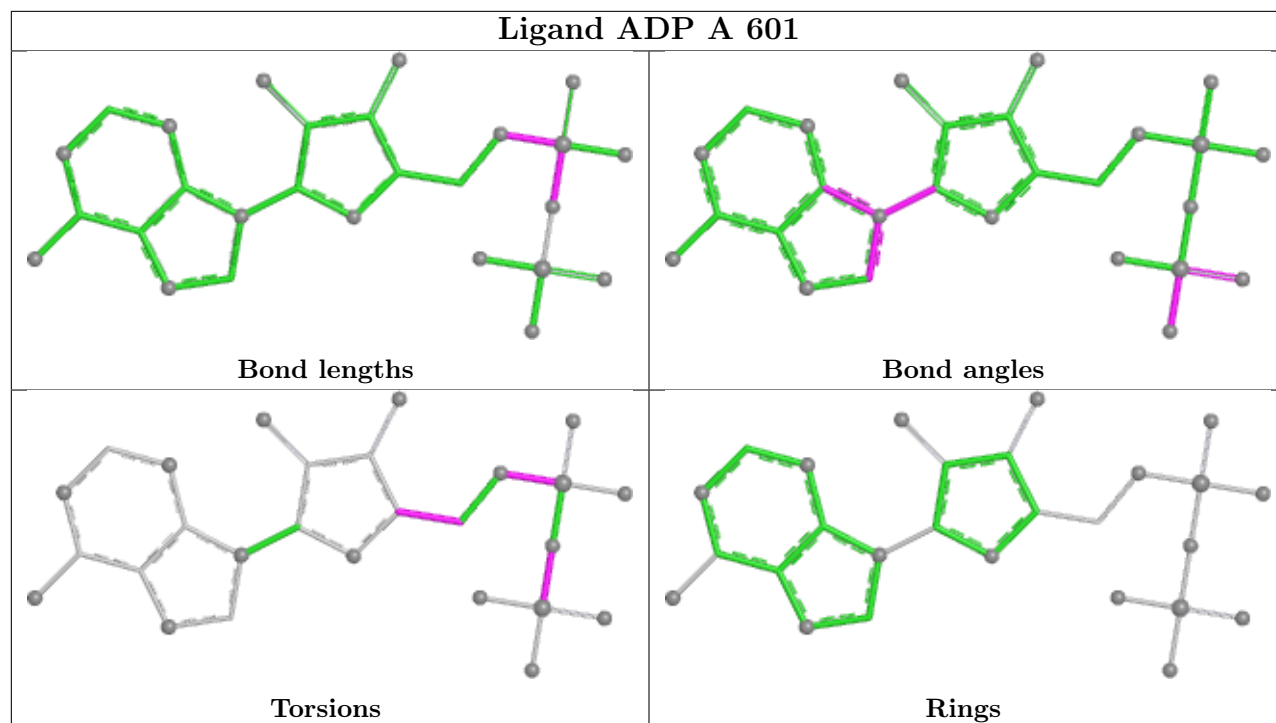
4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	CTP	5	0
3	B	1601	ADP	4	0
4	B	1602	CTP	5	0
3	A	601	ADP	5	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	534/545 (97%)	-0.11	15 (2%)	55 45	30, 57, 92, 99	5 (0%)
1	B	536/545 (98%)	-0.14	13 (2%)	59 49	25, 56, 92, 100	3 (0%)
All	All	1070/1090 (98%)	-0.12	28 (2%)	57 47	25, 57, 92, 100	8 (0%)

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	227	PHE	4.4
1	A	438	THR	3.4
1	B	272	ASN	3.3
1	B	494	ASP	3.2
1	B	544	ALA	3.0

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](#)

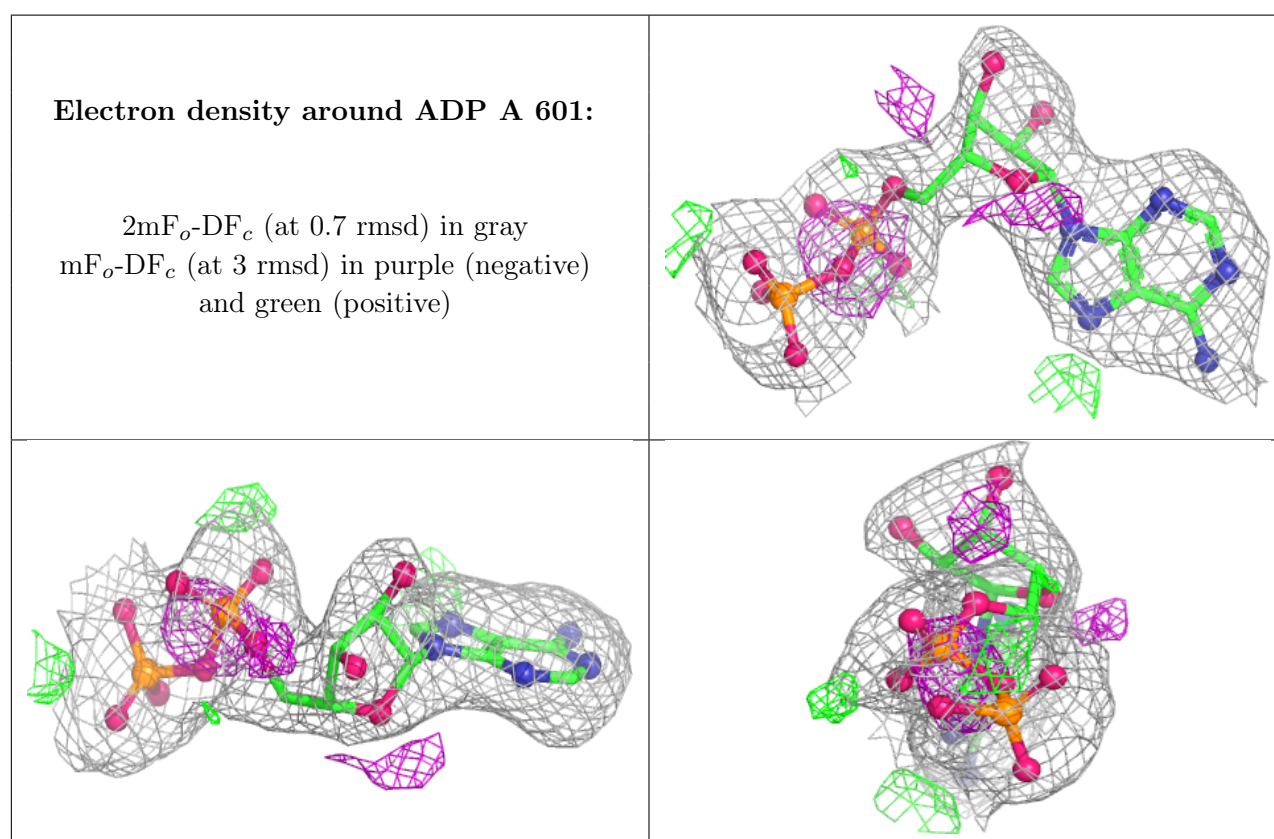
There are no oligosaccharides in this entry.

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.

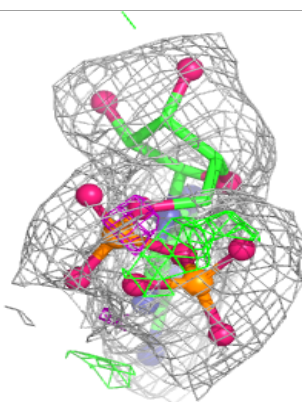
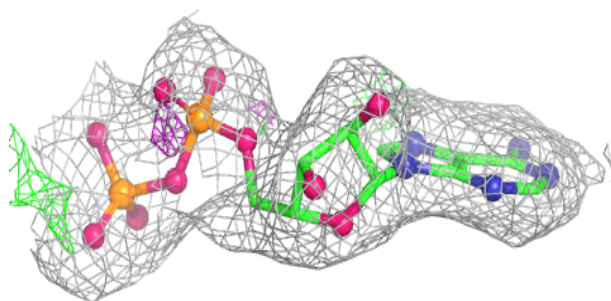
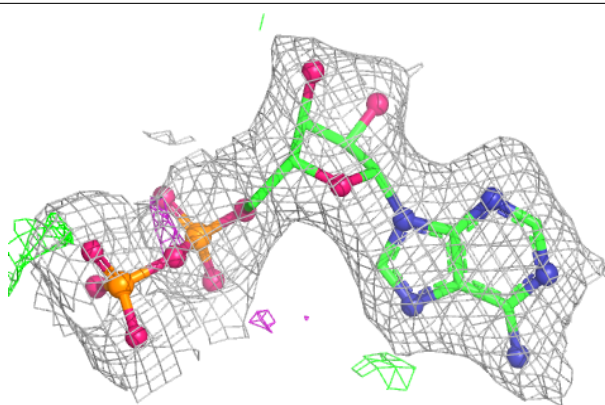
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ADP	A	601	27/27	0.94	0.11	38,72,98,100	0
3	ADP	B	1601	27/27	0.95	0.09	45,78,94,100	0
4	CTP	A	602	29/29	0.97	0.07	29,41,48,52	0
4	CTP	B	1602	29/29	0.98	0.06	39,44,48,50	0
2	MG	B	1701	1/1	0.99	0.04	45,45,45,45	0
2	MG	A	701	1/1	1.00	0.01	32,32,32,32	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.

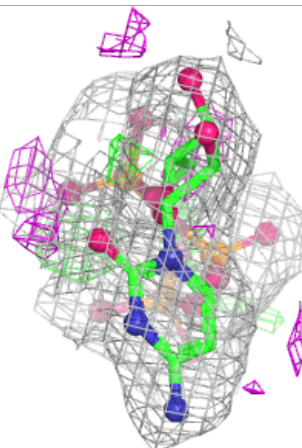
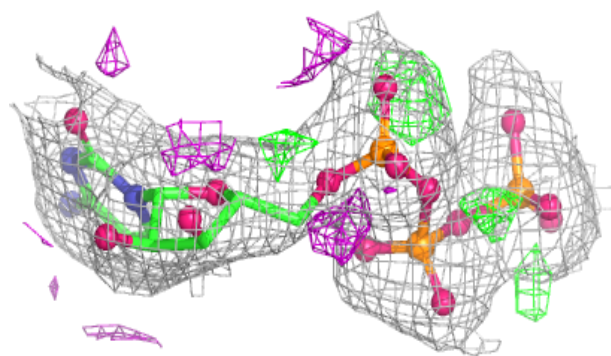
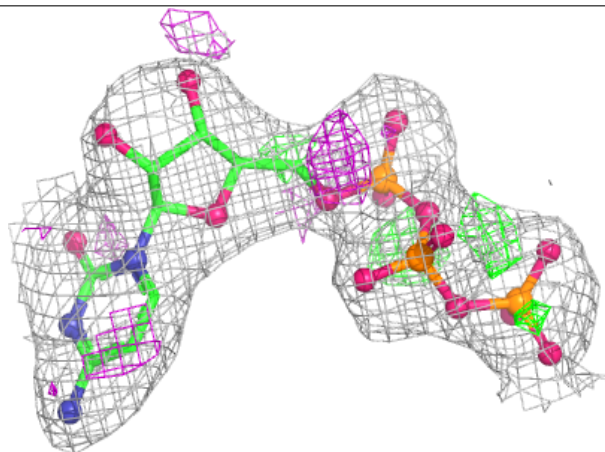


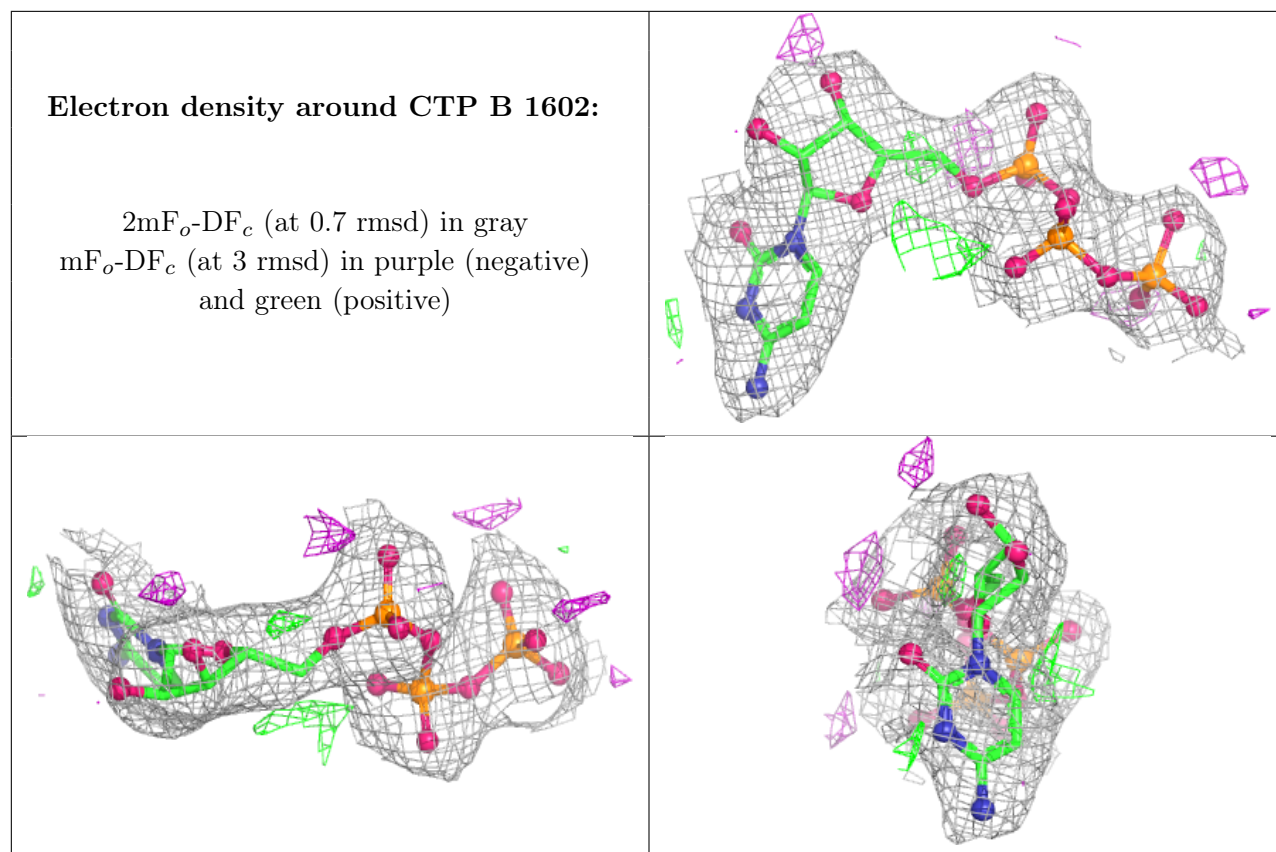
Electron density around ADP B 1601:

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

**Electron density around CTP A 602:**

$2mF_o-DF_c$ (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.