wwPDB X-ray Structure Validation Summary Report (i)

Aug 16, 2023 – 12:02 PM EDT

PDB ID	:	2AD5
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 (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 (i)) were used in the production of this report:

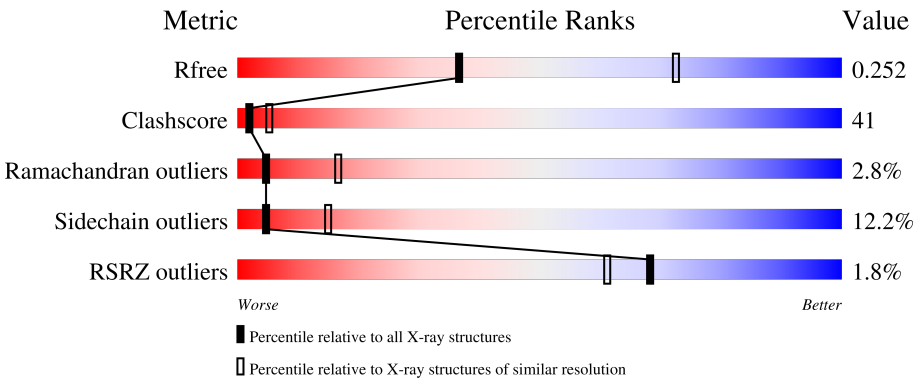
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=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	2% 35% 48% 13% • •
1	B	545	2% 33% 50% 13% • •

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.

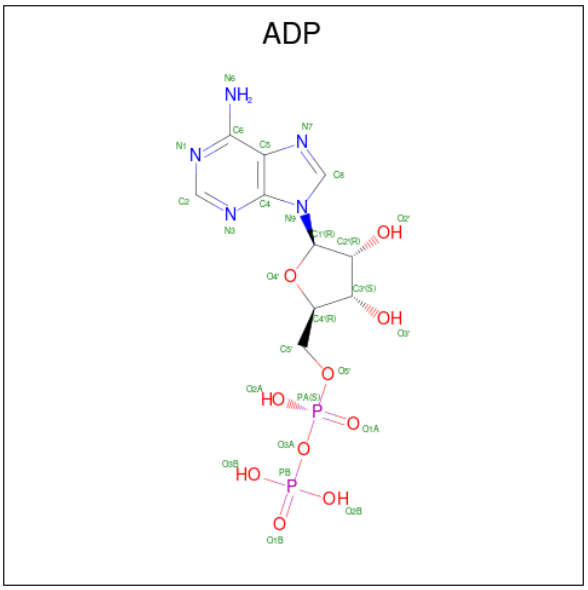
- Molecule 1 is a protein called CTP synthase.

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

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

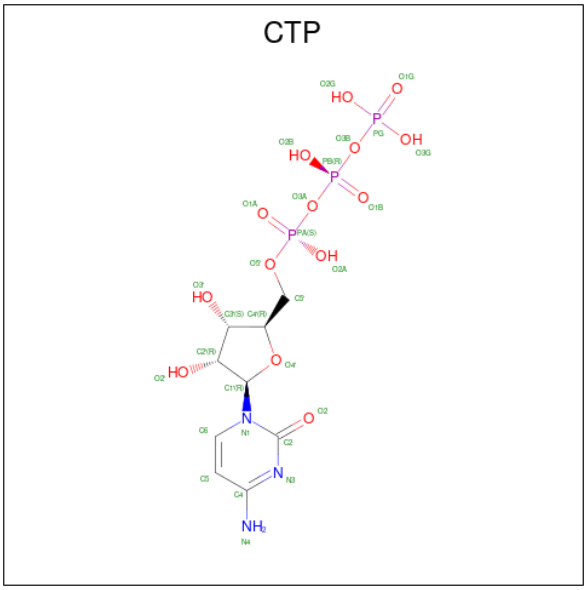
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0
2	B	1	1	1	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

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



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

- Molecule 5 is water.

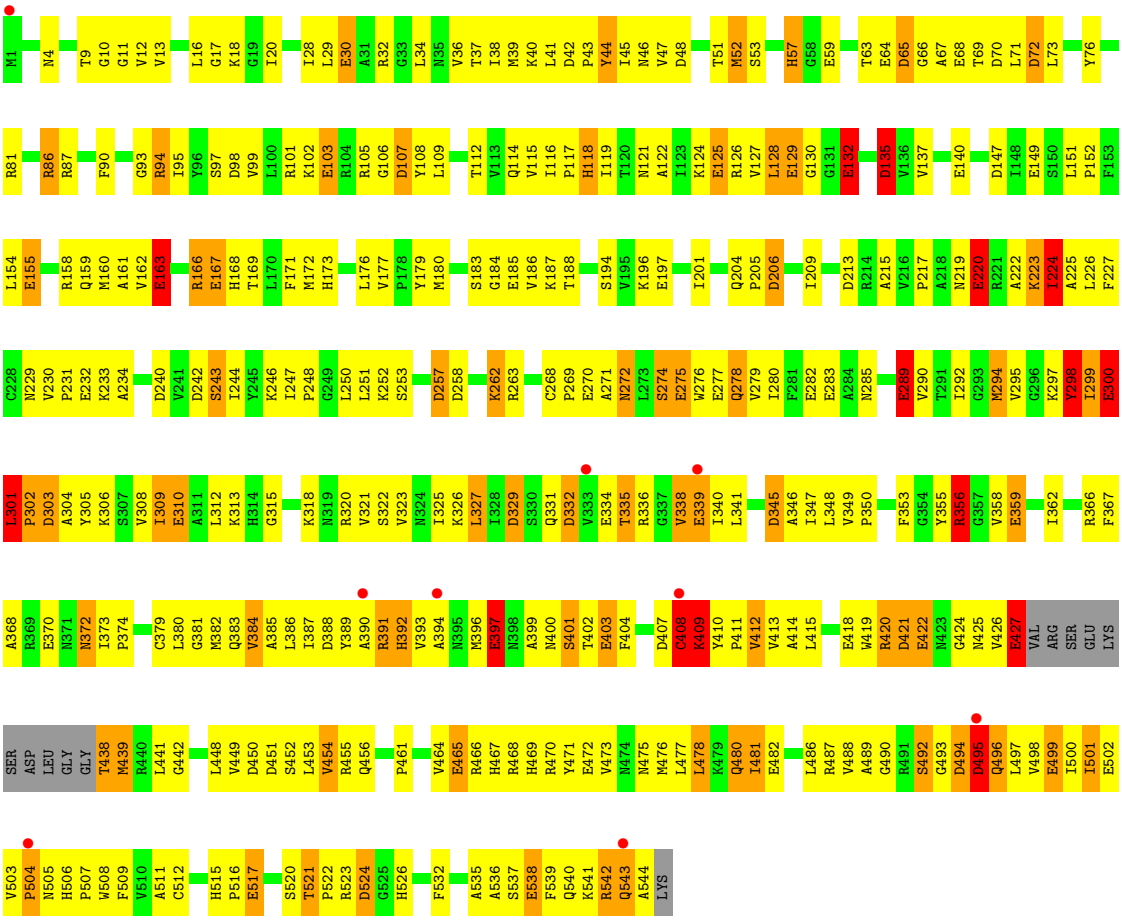
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	130	130	130	0	0
			Total	O		
5	B	122	122	122	0	0

3 Residue-property plots (i)

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.

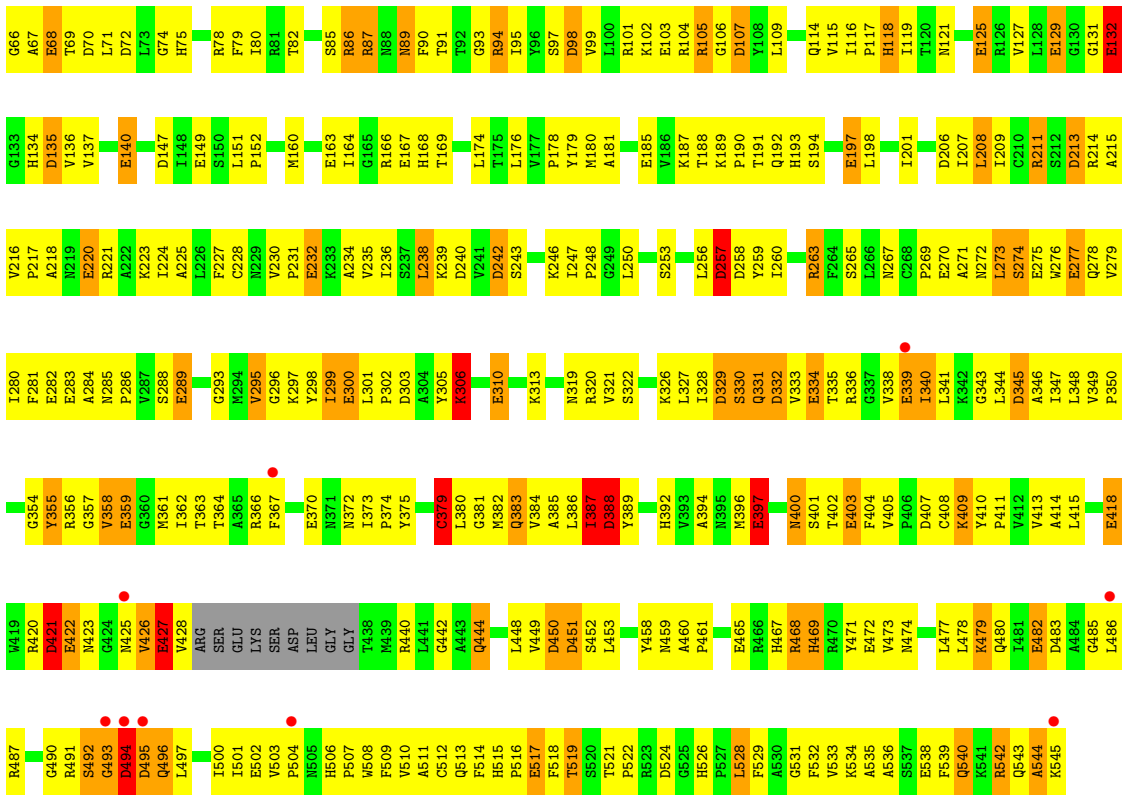
- Molecule 1: CTP synthase

Chain A:



- Molecule 1: CTP synthase

Chain B:


R487 G490 R491 S492 G493 D494 D495 Q496 L497 I500 I501 E502 V503 P504 N505 H506 P507 W508 F509 V510 A511 C512 Q513 F514 H515 P516 E517 F518 T519 S520 T521 P522 R523 D524 G525 H526 P527 L528 F529 A530 G531 F532 V533 K534 A535 A536 S537 E538 F539 Q540 K541 R542 Q543 A544 K545
W419 R420 D421 E422 N423 G424 N425 V426 E427 V428 ARG SER GLU LYS SER ASP LEU GLY GLY T438 M439 R440 L441 G442 A443 Q444 L448 V449 D450 D451 S452 L453 Y458 N459 A460 P461 E465 R466 H467 R468 H469 R470 Y471 E472 V473 N474 L477 L478 K479 Q480 I481 E482 D483 A484 G485 L486
G354 Y355 R356 G357 V358 E359 G360 M361 I362 T363 T364 A365 R366 F367 E370 N371 N372 I373 P374 Y375 G379 L380 G381 M382 Q383 V384 A385 L386 I387 D388 Y389 H392 V393 A394 N395 M396 E397 N400 S401 T402 E403 F404 V405 P406 D407 C408 K409 Y410 P411 V412 V413 A414 L415 E418
I280 F281 E282 E283 A284 N285 P286 V287 S288 E289 G293 M294 V295 G296 K297 Y298 I299 E300 L301 P302 D303 A304 Y305 K306 E310 K313 N319 R320 V321 S322 K326 L327 I328 D329 S330 Q331 D332 V333 E334 T335 R336 G337 V338 E339 I340 L341 K342 G343 L344 D345 A346 I347 L348 V349 P350
V216 P217 A218 N219 E220 R221 A222 K223 I224 A225 L226 F227 C228 N229 V230 P231 E232 K233 A234 V235 I236 S237 L238 K239 D240 V241 D242 S243 K246 I247 P248 G249 L250 S253 L256 D257 D258 Y259 I260 R263 F264 S265 L266 N267 C268 P269 E270 A271 N272 L273 S274 E275 W276 E277 Q278 V279
G133 H134 D135 V136 V137 E140 D147 I148 E149 S150 L151 P152 M160 E163 I164 G165 R166 E167 H168 T169 L174 T175 L176 V177 P178 Y179 M180 A181 E185 V186 K187 T188 K189 P190 T191 Q192 H193 S194 E197 L198 I201 D206 I207 L208 I209 C210 R211 S212 D213 R214 A215
G66 A67 E68 T69 D70 L71 D72 L73 G74 H75 R78 F79 I80 R81 T82 S85 R86 R87 N88 N89 F90 T91 T92 G93 R94 I95 Y96 S97 D98 V99 L100 R101 K102 E103 R104 R105 G106 D107 Y108 L109 Q114 V115 I116 P117 H118 I119 T120 N121 E125 R126 V127 L128 E129 G130 G131 E132

4 Data and refinement statistics (i)

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 45.42 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.80) 98.7 (45.42-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [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)	0.28 , 90.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[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 (i)

5.1 Standard geometry (i)

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	0.89	37/4232 (0.9%)	1.24	47/5734 (0.8%)
1	B	0.87	35/4248 (0.8%)	1.24	46/5755 (0.8%)
All	All	0.88	72/8480 (0.8%)	1.24	93/11489 (0.8%)

The worst 5 of 72 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	129	GLU	CD-OE2	6.69	1.33	1.25
1	A	499	GLU	CD-OE2	6.64	1.32	1.25
1	A	397	GLU	CD-OE2	6.59	1.32	1.25
1	A	300	GLU	CD-OE2	6.42	1.32	1.25
1	B	185	GLU	CD-OE2	6.14	1.32	1.25

The worst 5 of 93 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	301	LEU	C-N-CD	-11.39	95.53	120.60
1	B	107	ASP	CB-CG-OD1	-7.74	111.33	118.30
1	A	450	ASP	CB-CG-OD2	-7.69	111.38	118.30
1	B	303	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	B	494	ASP	CB-CG-OD2	-7.21	111.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4156	0	4162	362	0
1	B	4172	0	4184	327	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
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	6	0
5	A	130	0	0	11	0
5	B	122	0	0	12	1
All	All	8694	0	8394	690	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 41.

The worst 5 of 690 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:39:MET:HE1	1:A:130:GLY:HA3	1.35	1.09
1:A:301:LEU:HD12	1:A:302:PRO:HD2	1.36	1.06
1:A:396:MET:HE1	1:A:480:GLN:HB3	1.39	1.05
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 (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	530/545 (97%)	445 (84%)	66 (12%)	19 (4%)	3	11
1	B	532/545 (98%)	461 (87%)	60 (11%)	11 (2%)	7	23
All	All	1062/1090 (97%)	906 (85%)	126 (12%)	30 (3%)	5	17

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 (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	451/461 (98%)	396 (88%)	55 (12%)	5	15
1	B	453/461 (98%)	398 (88%)	55 (12%)	5	15
All	All	904/922 (98%)	794 (88%)	110 (12%)	5	15

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	20	ILE
1	B	180	MET
1	B	542	ARG
1	B	421	ASP
1	B	40	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	331	GLN
1	B	467	HIS
1	B	480	GLN
1	B	469	HIS
1	A	425	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
3	ADP	A	601	2	24,29,29	0.85	1 (4%)	29,45,45	1.37	4 (13%)
4	CTP	B	1602	-	26,30,30	1.21	1 (3%)	39,47,47	1.63	6 (15%)
3	ADP	B	1601	2	24,29,29	0.84	1 (4%)	29,45,45	0.89	2 (6%)
4	CTP	A	602	-	26,30,30	1.05	1 (3%)	39,47,47	1.08	4 (10%)

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	ADP	A	601	2	-	6/12/32/32	0/3/3/3
4	CTP	B	1602	-	-	6/22/38/38	0/2/2/2
3	ADP	B	1601	2	-	8/12/32/32	0/3/3/3
4	CTP	A	602	-	-	5/22/38/38	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	ADP	PA-O5'	-2.47	1.49	1.59
4	A	602	CTP	C4-N3	2.39	1.39	1.34
3	B	1601	ADP	PA-O5'	-2.34	1.49	1.59
4	B	1602	CTP	C5'-C4'	2.10	1.58	1.51

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1602	CTP	O4'-C1'-N1	-6.26	94.05	108.36
3	A	601	ADP	C1'-N9-C4	-5.44	117.08	126.64
4	B	1602	CTP	C2'-C1'-N1	3.75	123.85	113.22
3	A	601	ADP	PA-O3A-PB	-2.54	124.09	132.83
4	A	602	CTP	C4'-O4'-C1'	-2.50	103.95	109.47

There are no chirality outliers.

5 of 25 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

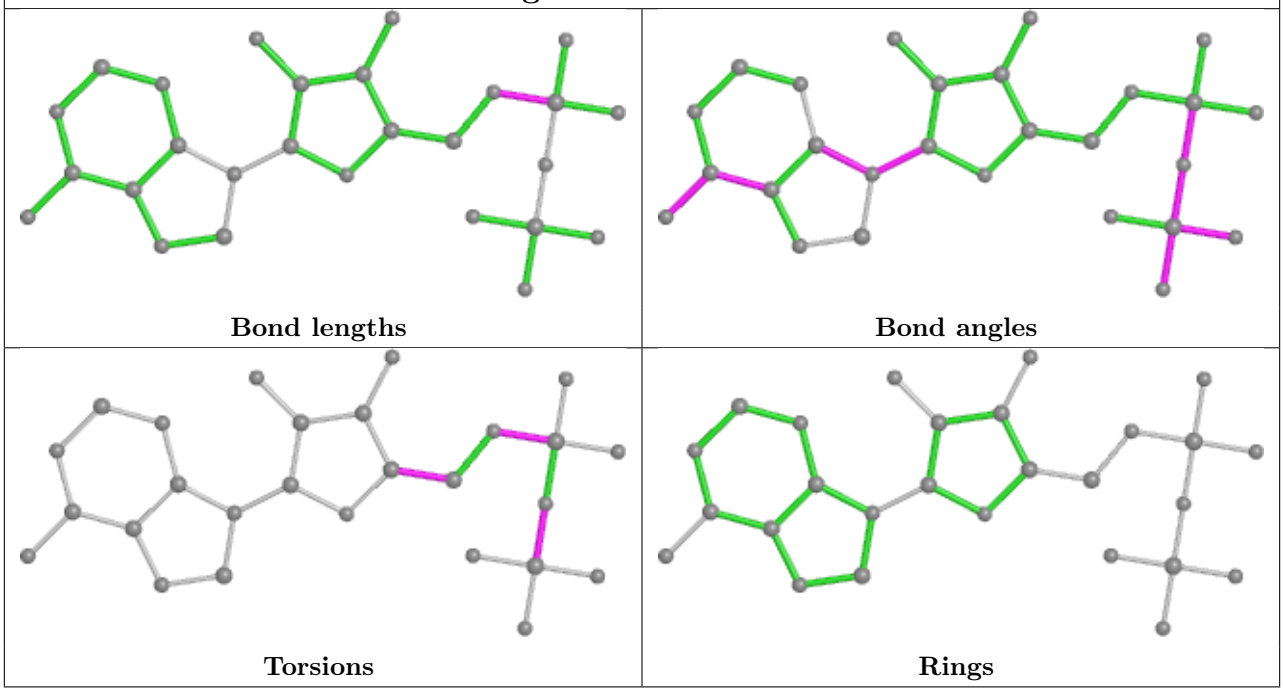
There are no ring outliers.

4 monomers are involved in 20 short contacts:

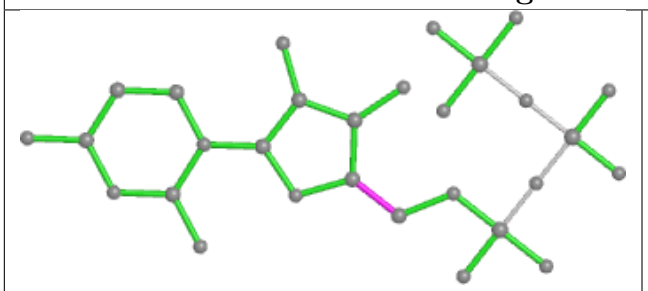
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	ADP	5	0
4	B	1602	CTP	6	0
3	B	1601	ADP	4	0
4	A	602	CTP	5	0

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 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.

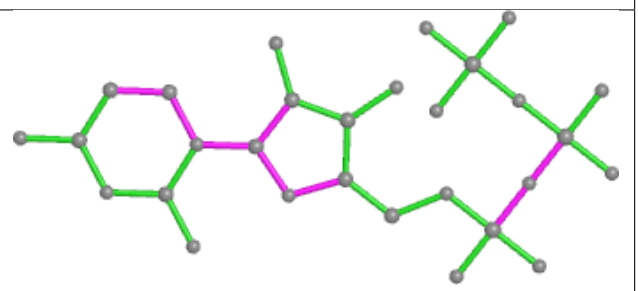
Ligand ADP A 601



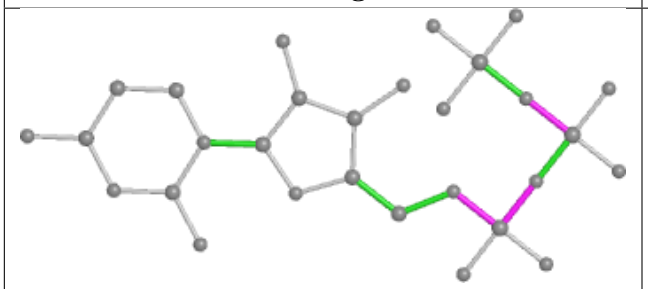
Ligand CTP B 1602



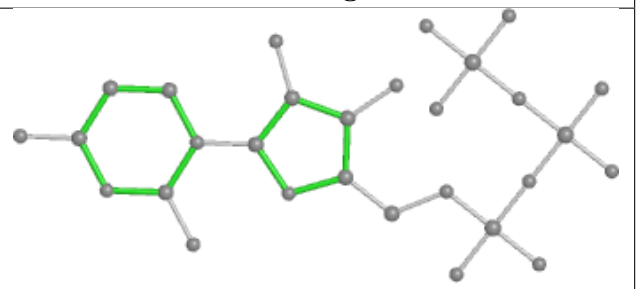
Bond lengths



Bond angles

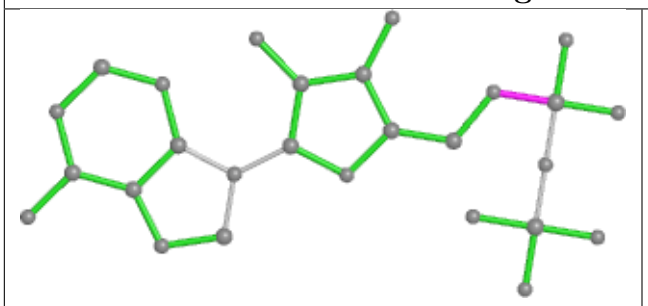


Torsions

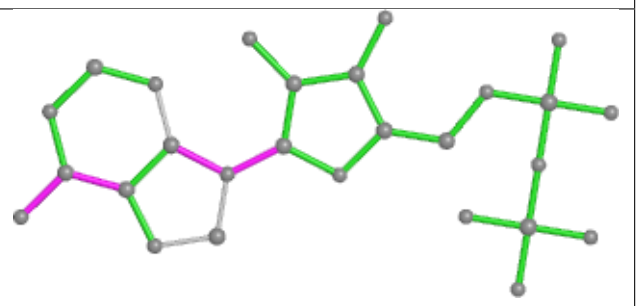


Rings

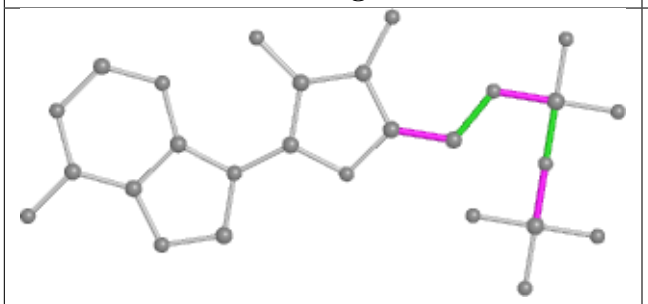
Ligand ADP B 1601



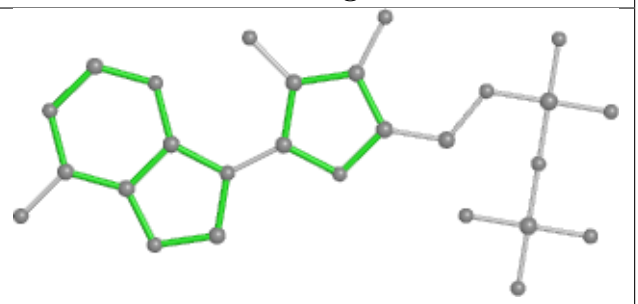
Bond lengths



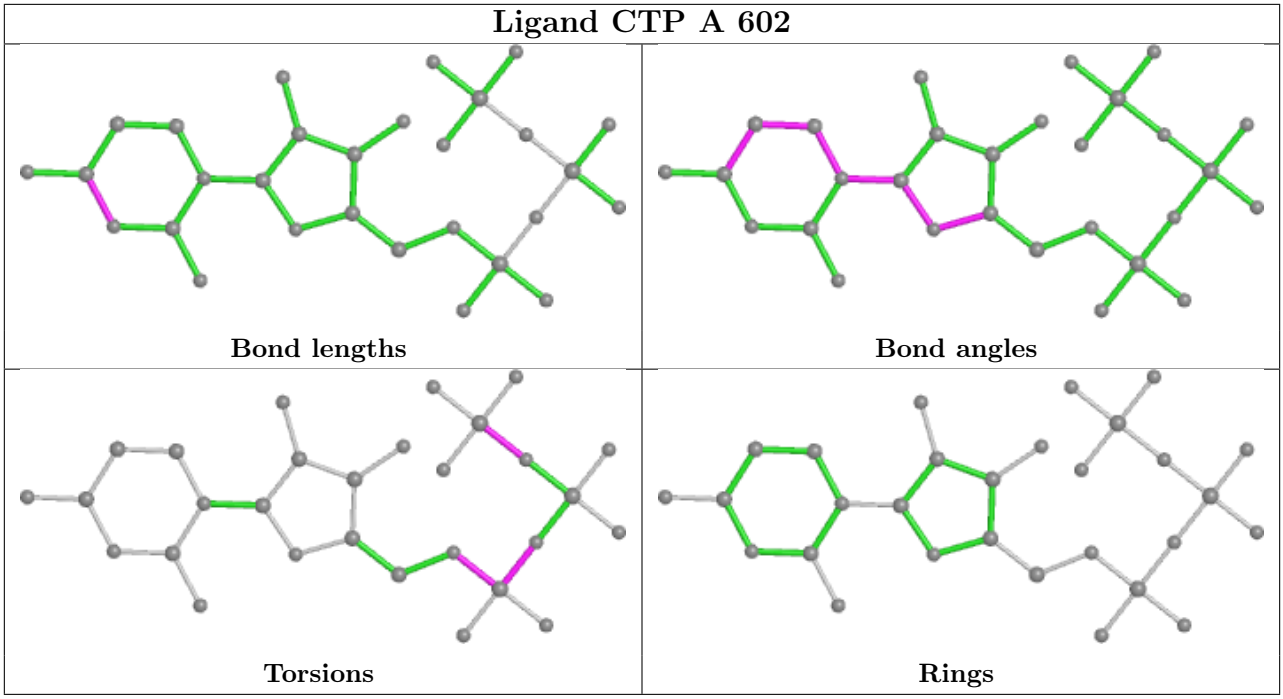
Bond angles



Torsions



Rings



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%)	-0.14	9 (1%)	70	63	30, 58, 92, 99	5 (0%)
1	B	536/545 (98%)	-0.15	10 (1%)	66	59	25, 56, 92, 100	3 (0%)
All	All	1070/1090 (98%)	-0.14	19 (1%)	68	61	25, 57, 92, 100	8 (0%)

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	545	LYS	4.6
1	B	1	MET	4.0
1	A	339	GLU	3.3
1	A	390	ALA	3.0
1	A	394	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 monosaccharides in this entry.

6.4 Ligands (i)

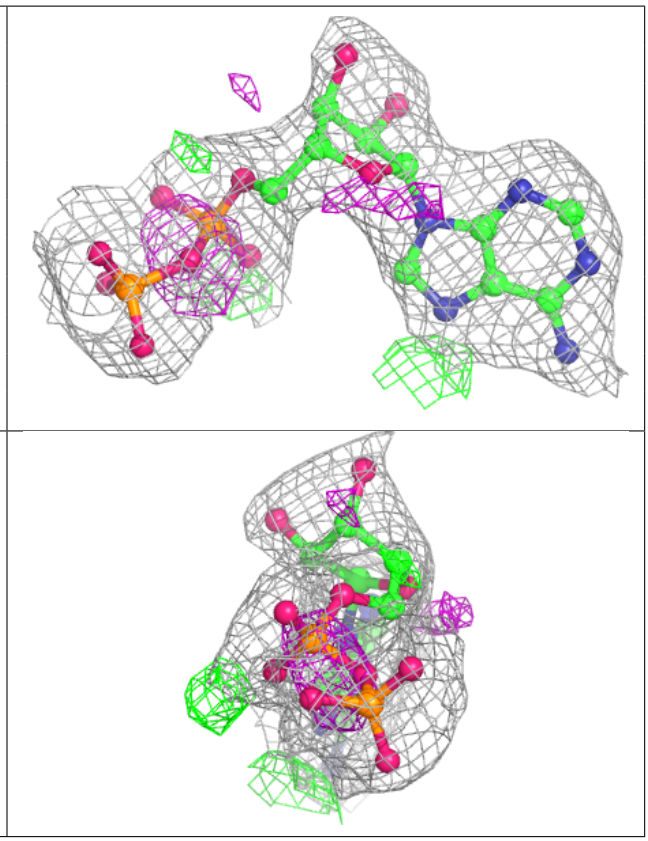
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ADP	A	601	27/27	0.94	0.16	38,72,98,100	0
3	ADP	B	1601	27/27	0.94	0.18	45,78,94,100	0
2	MG	B	1701	1/1	0.96	0.19	45,45,45,45	0
4	CTP	A	602	29/29	0.97	0.15	29,41,48,52	0
4	CTP	B	1602	29/29	0.97	0.15	39,44,48,50	0
2	MG	A	701	1/1	0.99	0.10	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.

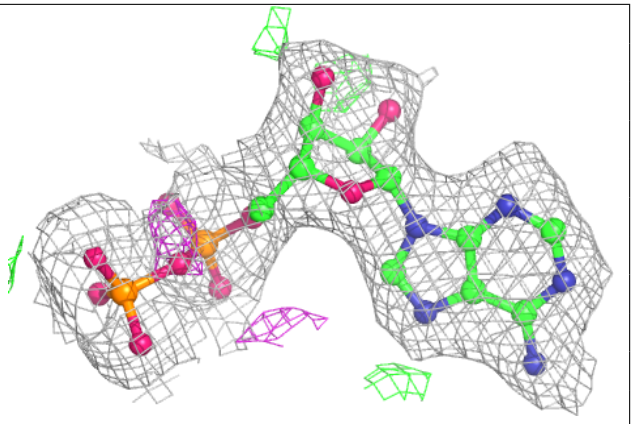
Electron density around ADP A 601:

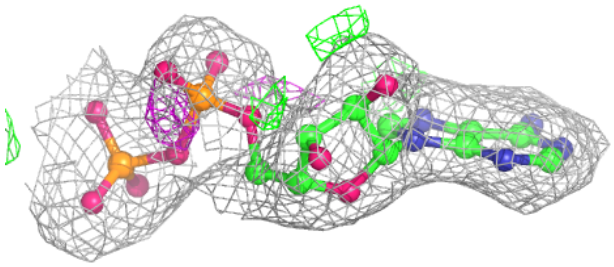
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

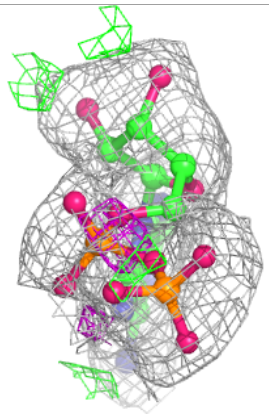


Electron density around ADP B 1601:

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

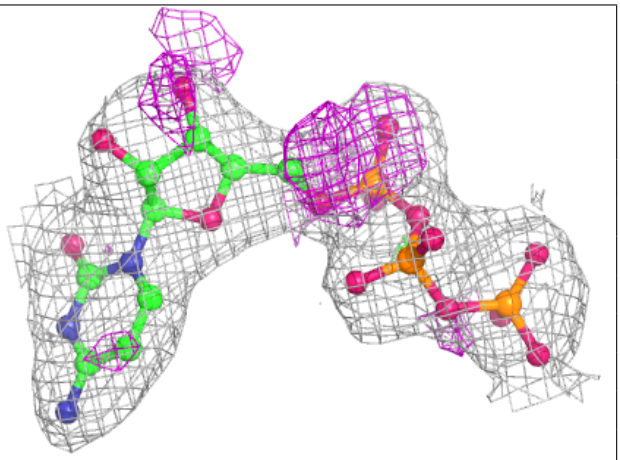


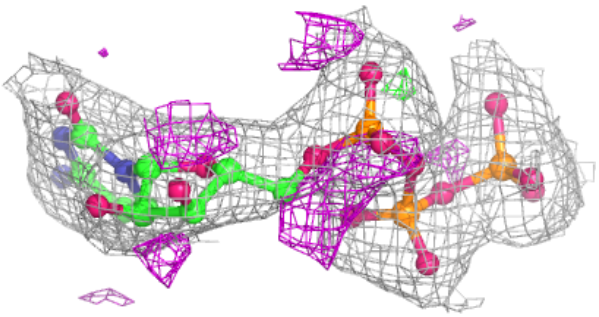


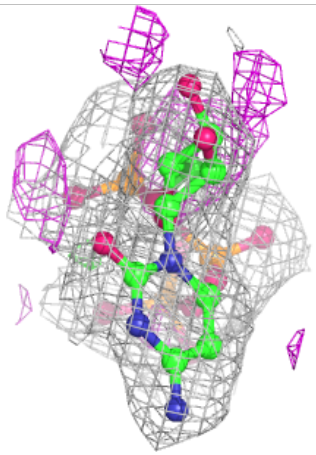


Electron density around CTP A 602:

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

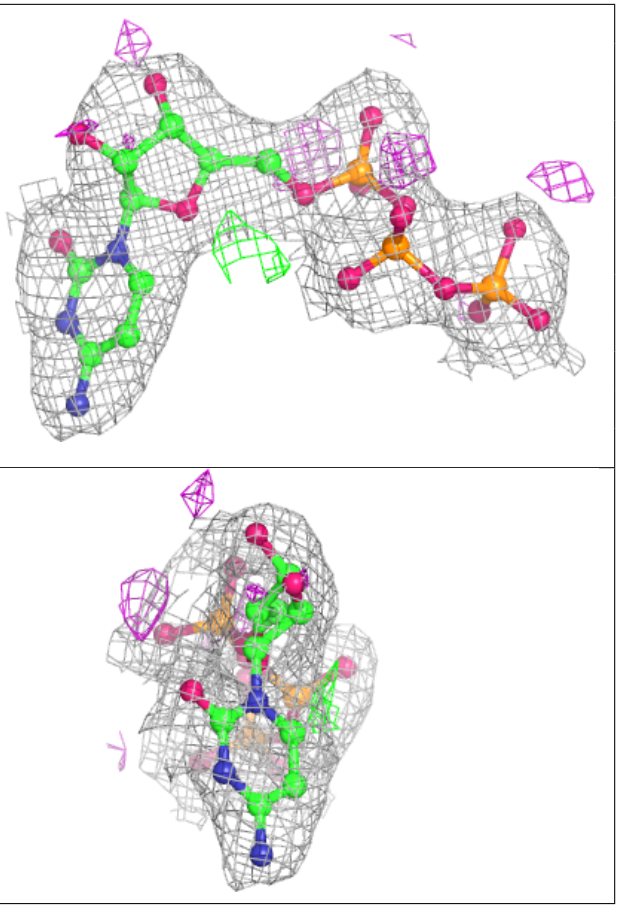






Electron density around CTP B 1602:

$2mF_o$-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.