



wwPDB X-ray Structure Validation Summary Report

Nov 7, 2014 – 07:33 AM EST

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 validation summary report for a publicly released PDB entry.

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

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

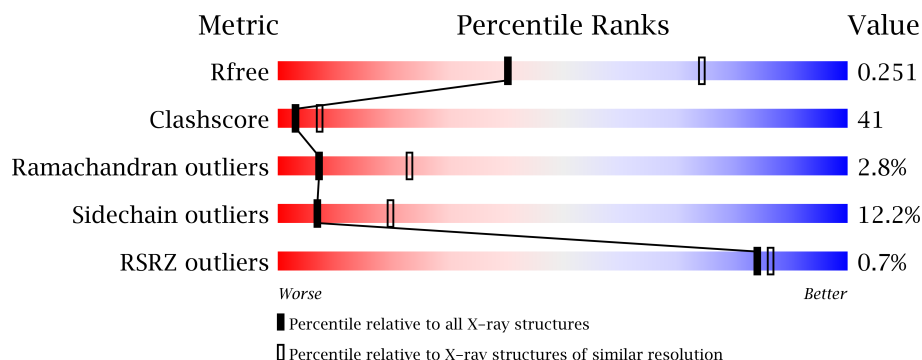
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : trunk24103
Percentile statistics : 23426
Refmac : 5.8.0049
CCP4 : 6.1.3
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk24103

1 Overall quality at a glance

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}	77520	2045 (2.80-2.80)
Clashscore	88313	2463 (2.80-2.80)
Ramachandran outliers	86584	2419 (2.80-2.80)
C α geometry	86677	2429 (2.80-2.80)
Sidechain outliers	86556	2421 (2.80-2.80)
RSRZ outliers	77580	2048 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	545	
1	B	545	

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 8694 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

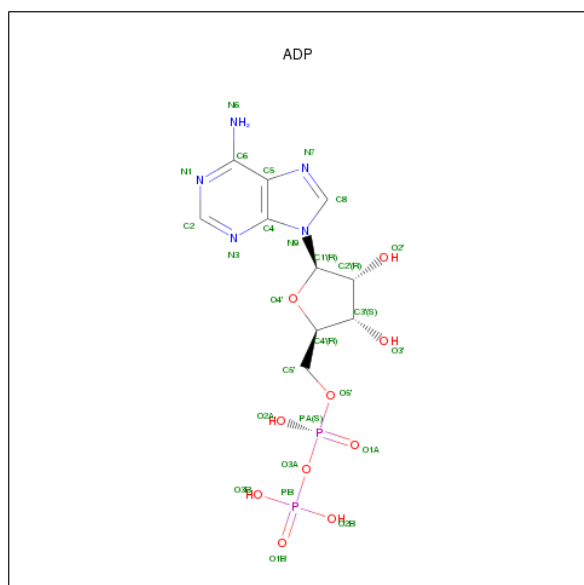
- Molecule 1 is a protein called CTP synthase.

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 (three-letter code: MG) (formula: Mg).

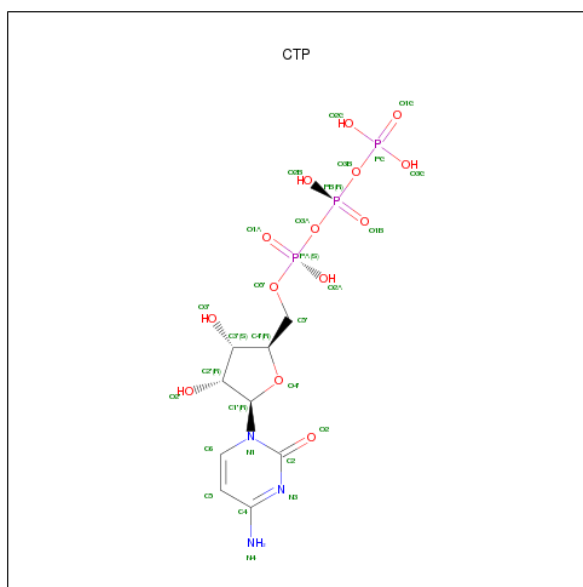
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- 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
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 (three-letter code: 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		

R487	G480	R491	S492	G493	D494	D495	Q496	L497	I500	E501	L502	V503	P504	N505	H506	P507	V508	F509	V510	A511	C512	O513	F514	H515	E516	E517	F518	T519	S520	T521	P522	R523	D524	G525	H526	F527	L528	F529	A530	G531	F532	V533	K534	A535	A536	S537	E538	F539	Q540	R541	R542	Q543	A544	K545
V419	R420	D421	E422	N423	G424	N425	V426	E427	V428	ARG	SER	GLU	LYS	SER	ASP	LEU	GLY	GLY	T438	P439	R440	L441	G442	A443	Q444	L448	V449	D450	D451	S452	L453	Y458	N459	A460	P461	E465	R466	H467	B468	H469	R470	Y471	E472	V473	N474	L477	L478	K479	Q480	L481	E482	D483	A484	L486
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	L209	C210	R211	S212	D213	R214	A215				
P216	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
I280	F281	E282	E283	A284	N285	P286	V287	S288	E289	G293	N294	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	G342	L343	D344	A345	T346	L347	V348	P349	
G354	Y355	R356	G357	V358	E359	G360	M361	I362	T363	T364	A365	R366	F367	E370	N371	N372	I373	P374	Y375	C379	L380	G381	M382	Q383	V384	A385	L386	I387	D388	Y389	H392	V393	A394	N395	K396	E397	N400	S401	T402	E403	F404	V405	P406	D407	C408	R409	Y410	P411	V412	V413	A414	L415	E418	

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 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
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.81Å)	Xtriage
Refinement program	TNT V. 5-F	Depositor
R, R_{free}	0.202 , 0.277 0.194 , 0.251	Depositor DCC
R_{free} test set	1865 reflections (3.45%)	DCC
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 91.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 55879 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, CTP, ADP

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(°)	Ideal(°)
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 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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 41.

The worst 5 of 690 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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%)	5	16
1	B	532/545 (98%)	461 (87%)	60 (11%)	11 (2%)	10	32
All	All	1062/1090 (97%)	906 (85%)	126 (12%)	30 (3%)	7	23

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%)	396 (88%)	55 (12%)	7	20
1	B	453/461 (98%)	398 (88%)	55 (12%)	7	20
All	All	904/922 (98%)	794 (88%)	110 (12%)	7	20

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

Mol	Chain	Res	Type
1	A	480	GLN
1	B	86	ARG
1	B	428	VAL
1	A	495	ASP
1	B	1	MET

Some 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	46	ASN

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Mol	Chain	Res	Type
1	B	134	HIS
1	B	425	ASN
1	A	469	HIS
1	A	506	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	29,29,29	0.91	2 (6%)	45,45,45	1.49	4 (8%)
4	CTP	A	602	-	30,30,30	1.93	6 (20%)	44,47,47	1.70	5 (11%)
3	ADP	B	1601	2	29,29,29	0.99	3 (10%)	45,45,45	0.91	1 (2%)
4	CTP	B	1602	-	30,30,30	1.63	4 (13%)	44,47,47	1.86	7 (15%)

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	-	0/16/32/32	0/3/3/3
4	CTP	A	602	-	-	0/20/38/38	0/2/2/2
3	ADP	B	1601	2	-	0/16/32/32	0/3/3/3
4	CTP	B	1602	-	-	0/20/38/38	0/2/2/2

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	CTP	C2-N1	4.94	1.43	1.38
4	A	602	CTP	PG-O3B	4.68	1.68	1.60
4	A	602	CTP	PB-O3A	4.26	1.67	1.59
4	B	1602	CTP	PB-O3B	4.15	1.67	1.59
4	B	1602	CTP	PG-O3B	3.55	1.66	1.60

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	CTP	C6-C5-C4	7.30	120.99	117.51
4	B	1602	CTP	O4'-C1'-N1	-6.40	94.05	108.08
3	A	601	ADP	C8-N9-C1'	5.89	137.24	126.15
3	A	601	ADP	C1'-N9-C4	-5.53	117.08	126.64
4	A	602	CTP	C4'-O4'-C1'	-5.25	103.95	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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%)	-0.57	4 (0%)	84 86	30, 58, 93, 99	5 (0%)
1	B	536/545 (98%)	-0.56	4 (0%)	84 86	25, 56, 92, 100	3 (0%)
All	All	1070/1090 (98%)	-0.57	8 (0%)	84 86	25, 57, 92, 100	8 (0%)

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	3.2
1	B	494	ASP	3.1
1	B	545	LYS	2.7
1	A	339	GLU	2.4
1	B	495	ASP	2.4

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MG	B	1701	1/1	0.14	0.59	45,45,45,45	0
3	ADP	B	1601	27/27	0.14	0.05	45,78,94,100	0
3	ADP	A	601	27/27	0.12	-0.13	38,72,98,100	0
4	CTP	A	602	29/29	0.13	-0.28	29,41,48,52	0
4	CTP	B	1602	29/29	0.13	-0.70	39,44,48,50	0
2	MG	A	701	1/1	0.09	-0.83	32,32,32,32	0

6.5 Other polymers ⓘ

There are no such residues in this entry.