wwPDB X-ray Structure Validation Summary Report (i)

Oct 24, 2023 – 10:39 PM EDT

PDB ID	:	3H3A
Title	:	The complex structure of CCA-adding enzyme with CTP
Authors	:	Toh, Y.; Tomita, K.
Deposited on	:	2009-04-16
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:

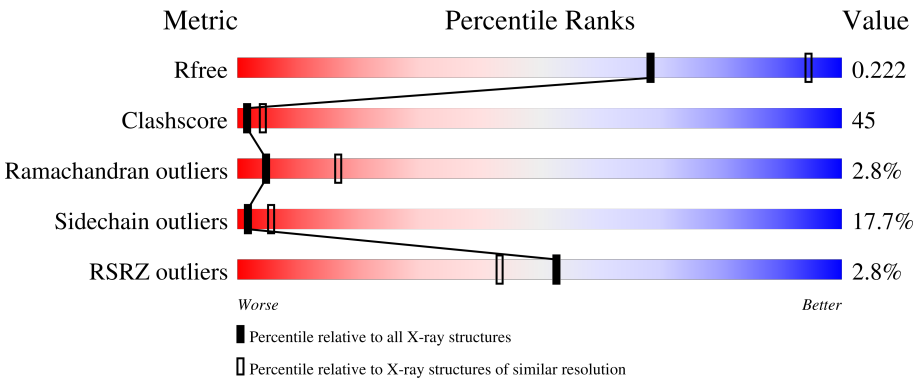
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

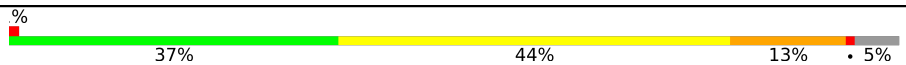
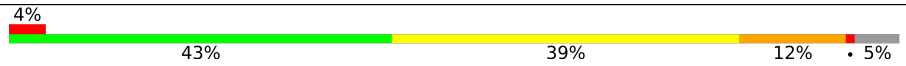
The reported resolution of this entry is 2.80 Å.

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	441	
1	B	441	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6942 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 TRNA nucleotidyl transferase-related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	417	3426	2213	580	622	11	0	0	0
1	B	418	3441	2222	583	625	11	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q9WZH4
A	429	LYS	-	expression tag	UNP Q9WZH4
A	430	LEU	-	expression tag	UNP Q9WZH4
A	431	ALA	-	expression tag	UNP Q9WZH4
A	432	ALA	-	expression tag	UNP Q9WZH4
A	433	ALA	-	expression tag	UNP Q9WZH4
A	434	LEU	-	expression tag	UNP Q9WZH4
A	435	GLU	-	expression tag	UNP Q9WZH4
A	436	HIS	-	expression tag	UNP Q9WZH4
A	437	HIS	-	expression tag	UNP Q9WZH4
A	438	HIS	-	expression tag	UNP Q9WZH4
A	439	HIS	-	expression tag	UNP Q9WZH4
A	440	HIS	-	expression tag	UNP Q9WZH4
A	441	HIS	-	expression tag	UNP Q9WZH4
B	1	MET	-	expression tag	UNP Q9WZH4
B	429	LYS	-	expression tag	UNP Q9WZH4
B	430	LEU	-	expression tag	UNP Q9WZH4
B	431	ALA	-	expression tag	UNP Q9WZH4
B	432	ALA	-	expression tag	UNP Q9WZH4
B	433	ALA	-	expression tag	UNP Q9WZH4
B	434	LEU	-	expression tag	UNP Q9WZH4
B	435	GLU	-	expression tag	UNP Q9WZH4
B	436	HIS	-	expression tag	UNP Q9WZH4
B	437	HIS	-	expression tag	UNP Q9WZH4
B	438	HIS	-	expression tag	UNP Q9WZH4

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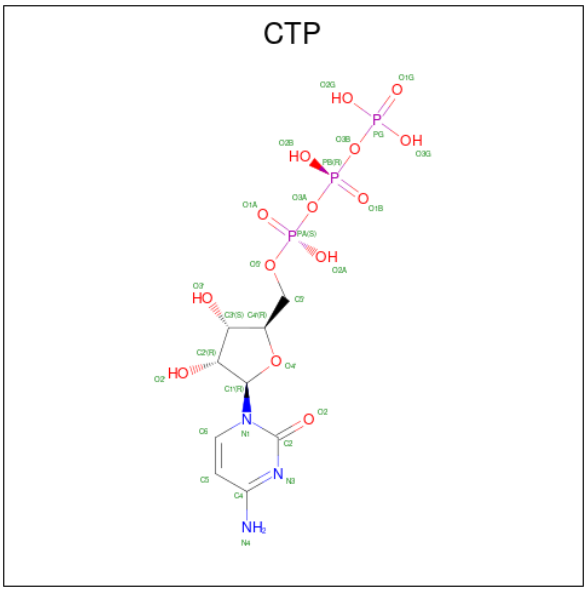
Chain	Residue	Modelled	Actual	Comment	Reference
B	439	HIS	-	expression tag	UNP Q9WZH4
B	440	HIS	-	expression tag	UNP Q9WZH4
B	441	HIS	-	expression tag	UNP Q9WZH4

- Molecule 2 is CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CTP) (formula: $C_9H_{16}N_3O_{14}P_3$).



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

- Molecule 3 is water.

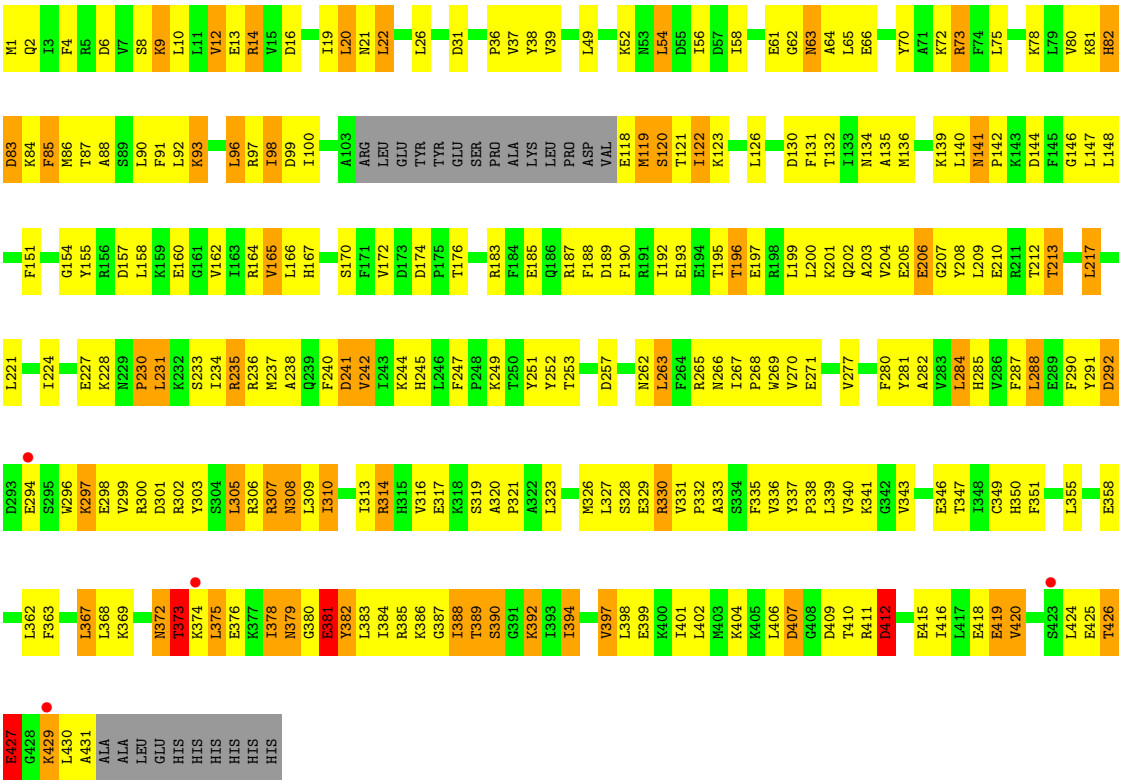
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O	0	0
			6	6		
3	B	11	Total	O	0	0
			11	11		

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.

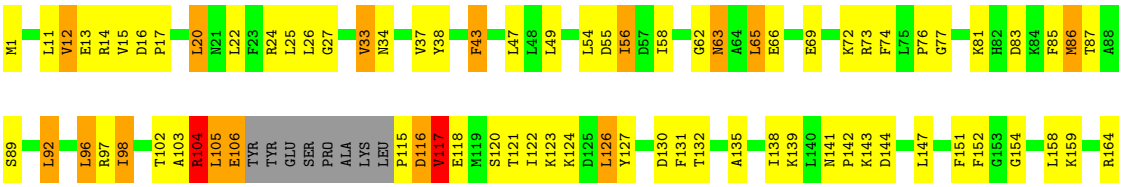
- Molecule 1: TRNA nucleotidyl transferase-related protein

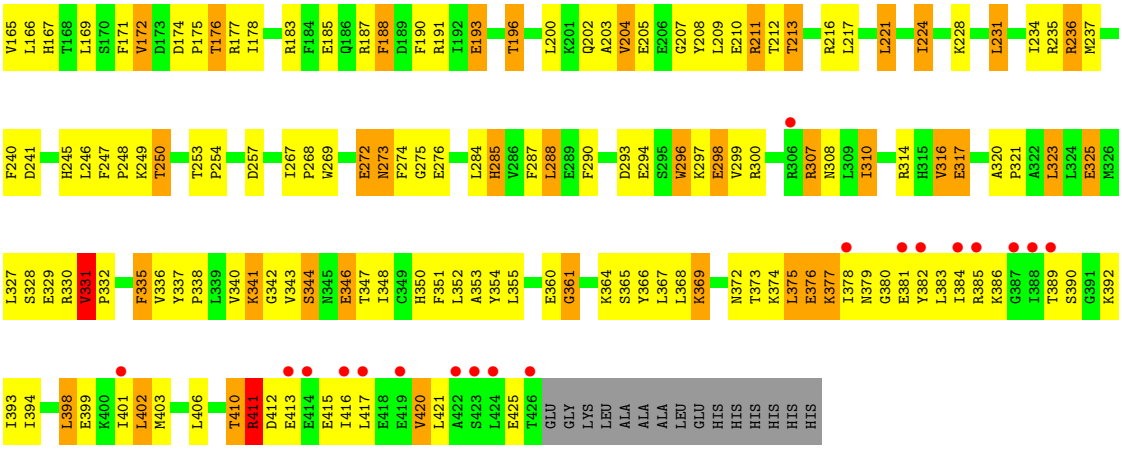
Chain A:



- Molecule 1: TRNA nucleotidyl transferase-related protein

Chain B:




V165 L166 H167 T168 L169 S170 F171 V172 D173 D174 P175 T176 R177 I178 R183 F184 E185 Q186 R187 F188 D189 F190 R191 I192 E193 T196 L200 K201 Q202 A203 V204 E205 E206 G207 Y208 L209 E210 R211 T212 T213 R216 L217 L221 I224 K228 L231 I234 R235 R236 M237
F240 D241 H245 L246 F247 P248 K249 T250 T253 P254 D257 I267 P268 W269 E272 N273 F274 G275 E276 L284 H285 V286 F287 L288 E289 F290 D293 E294 S295 W296 K297 E298 V299 R300 R306 R307 N308 L309 I310 R314 H315 V316 E317 A320 P321 A322 L323 L324 E325 M326
L327 S328 E329 R330 V331 P332 F335 V336 Y337 P338 L339 V340 K341 G342 V343 S344 M345 E346 T347 I348 C349 H350 F351 L352 A353 Y354 L355 E360 G361 K364 S365 Y366 L367 L368 K369 N372 T373 K374 L375 E376 K377 I378 N379 G380 E381 Y382 L383 I384 R385 K386 G387 I388 T389 S390 G391 K392
I393 I394 L398 E399 K400 I401 L402 M403 L406 T410 R411 D412 E413 E414 E415 I416 L417 E418 E419 V420 L421 A422 S423 L424 E425 T426 GLU GLY LYS LEU ALA ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	190.45Å 63.59Å 152.58Å 90.00° 103.31° 90.00°	Depositor
Resolution (Å)	31.79 – 2.80 31.79 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.4 (31.79-2.80) 95.4 (31.79-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.234 , 0.269 0.229 , 0.222	Depositor DCC
R_{free} test set	2099 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	86.3	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 83.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6942	wwPDB-VP
Average B, all atoms (Å^2)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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: CTP

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	0.47	0/3487	0.74	6/4684 (0.1%)
1	B	0.47	0/3503	0.70	4/4707 (0.1%)
All	All	0.47	0/6990	0.72	10/9391 (0.1%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	412	ASP	CB-CA-C	-9.88	90.64	110.40
1	A	373	THR	CB-CA-C	-9.25	86.62	111.60
1	B	331	VAL	CB-CA-C	-8.81	94.65	111.40
1	A	381	GLU	N-CA-C	8.54	134.05	111.00
1	A	381	GLU	CB-CA-C	-6.98	96.45	110.40

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	3426	0	3525	345	1
1	B	3441	0	3538	286	0
2	A	29	0	12	1	0
2	B	29	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	6	0	0	0	0
3	B	11	0	0	0	0
All	All	6942	0	7087	630	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 630 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:272:GLU:C	1:B:273:ASN:HD22	1.33	1.28
1:B:401:ILE:CD1	1:B:416:ILE:HG12	1.72	1.20
1:A:90:LEU:HB3	1:A:98:ILE:HD11	1.23	1.18
1:B:375:LEU:N	1:B:375:LEU:HD23	1.59	1.18
1:A:90:LEU:CB	1:A:98:ILE:HD11	1.73	1.17

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)
1:A:281:TYR:OH	1:A:382:TYR:OH[4_546]	2.08	0.12

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	413/441 (94%)	356 (86%)	43 (10%)	14 (3%)	3 13
1	B	414/441 (94%)	371 (90%)	34 (8%)	9 (2%)	6 22
All	All	827/882 (94%)	727 (88%)	77 (9%)	23 (3%)	5 17

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	SER
1	A	373	THR
1	A	381	GLU
1	A	388	ILE
1	B	341	LYS

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	374/395 (95%)	308 (82%)	66 (18%)	2 5
1	B	377/395 (95%)	310 (82%)	67 (18%)	2 5
All	All	751/790 (95%)	618 (82%)	133 (18%)	2 5

5 of 133 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	323	LEU
1	B	344	SER
1	B	411	ARG
1	A	367	LEU
1	A	358	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	266	ASN
1	B	350	HIS
1	B	345	ASN
1	B	63	ASN
1	B	245	HIS

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)

2 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	$\#\|Z\| > 2$
2	CTP	B	502	-	26,30,30	0.88	1 (3%)	39,47,47	1.35	3 (7%)
2	CTP	A	501	-	26,30,30	0.88	2 (7%)	39,47,47	1.35	3 (7%)

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
2	CTP	B	502	-	-	0/22/38/38	0/2/2/2
2	CTP	A	501	-	-	0/22/38/38	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	CTP	C6-C5	2.28	1.40	1.35
2	A	501	CTP	C6-C5	2.27	1.40	1.35
2	A	501	CTP	C4-N3	2.01	1.38	1.34

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	CTP	PB-O3B-PG	-4.94	115.86	132.83
2	B	502	CTP	PB-O3B-PG	-4.94	115.89	132.83
2	B	502	CTP	PB-O3A-PA	-3.27	121.61	132.83
2	A	501	CTP	PB-O3A-PA	-3.26	121.64	132.83
2	B	502	CTP	O2A-PA-O5'	2.14	117.70	107.75

There are no chirality outliers.

There are no torsion outliers.

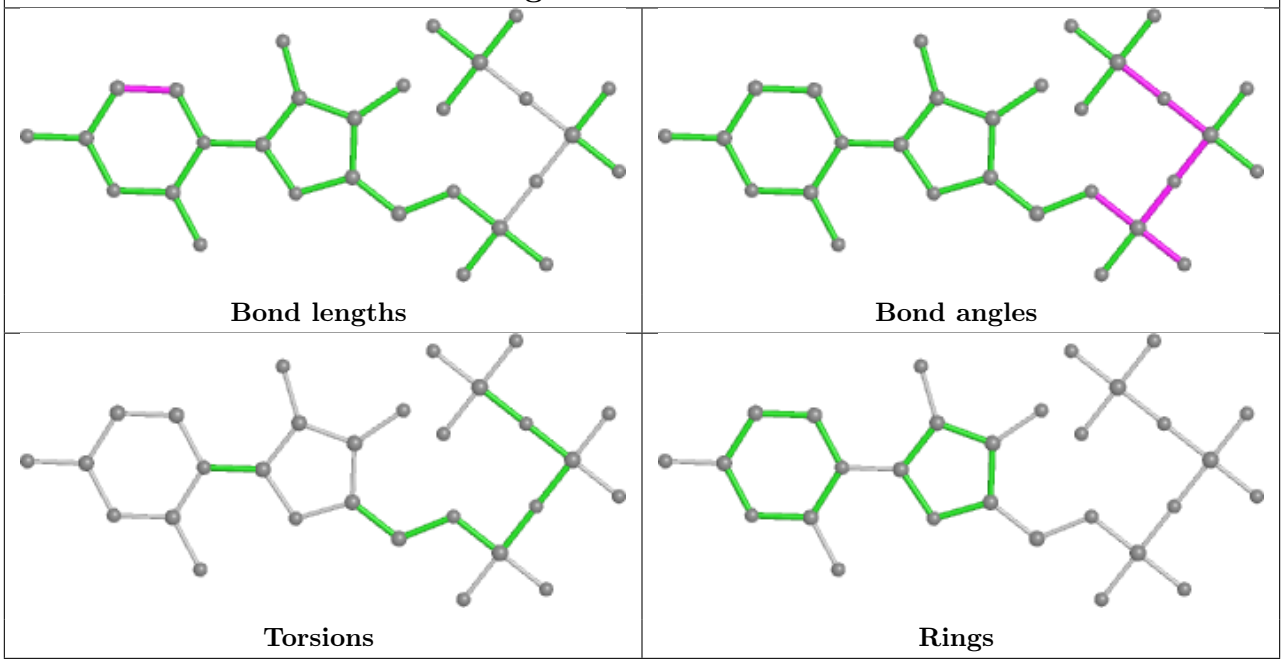
There are no ring outliers.

2 monomers are involved in 3 short contacts:

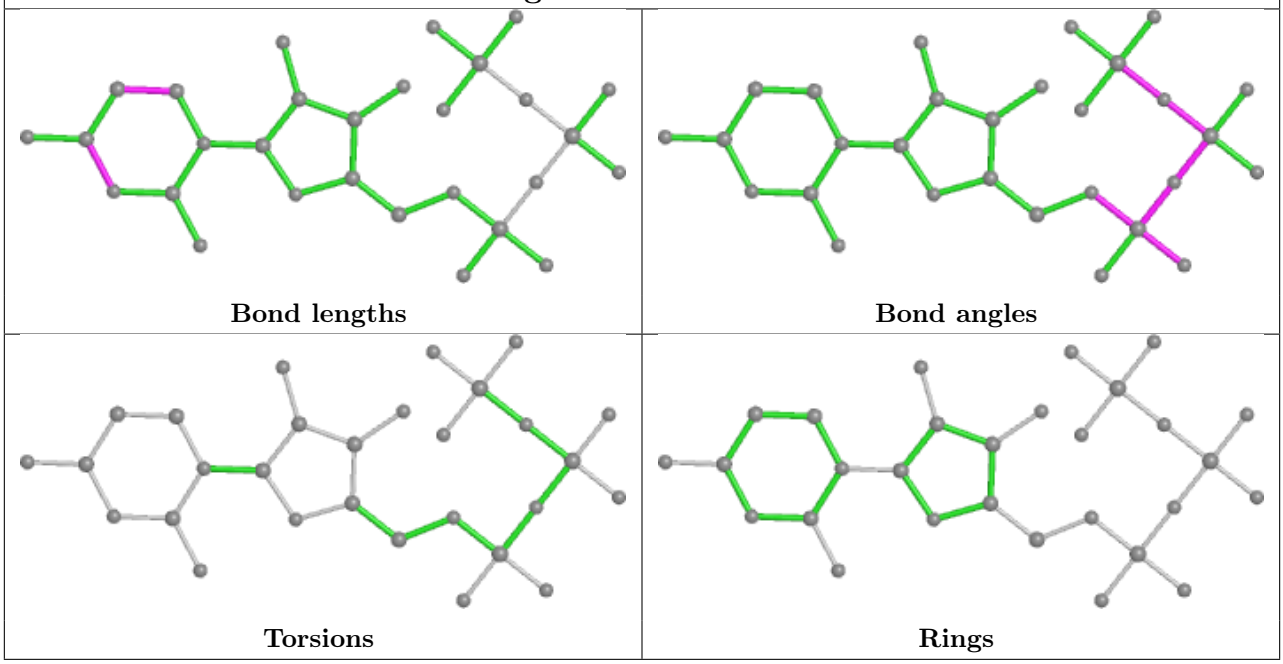
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	CTP	2	0
2	A	501	CTP	1	0

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 CTP B 502



Ligand CTP A 501



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	417/441 (94%)	-0.32	4 (0%)	82	77	50, 121, 169, 215	0
1	B	418/441 (94%)	-0.18	19 (4%)	33	23	55, 94, 213, 319	0
All	All	835/882 (94%)	-0.25	23 (2%)	53	43	50, 109, 187, 319	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	417	LEU	6.2
1	B	414	GLU	4.5
1	B	426	THR	4.2
1	B	387	GLY	4.2
1	B	388	ILE	4.2

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)

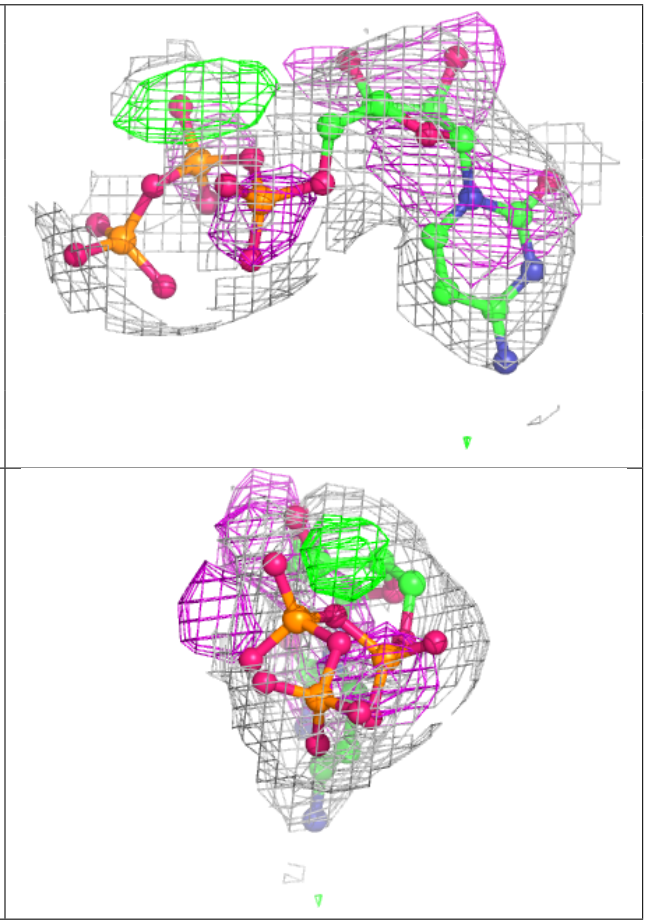
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CTP	A	501	29/29	0.86	0.19	90,111,159,387	0
2	CTP	B	502	29/29	0.93	0.18	90,111,159,387	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.

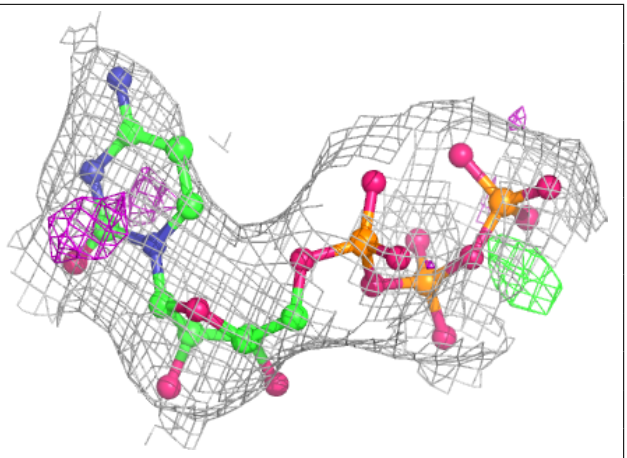
Electron density around CTP A 501:

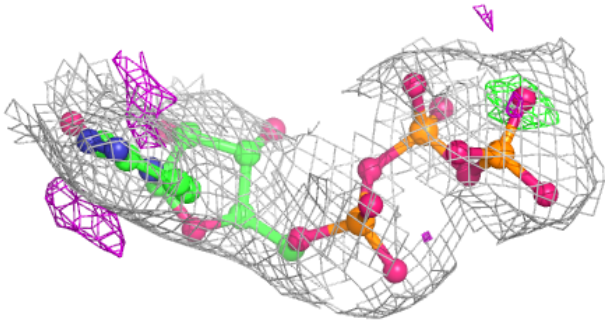
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

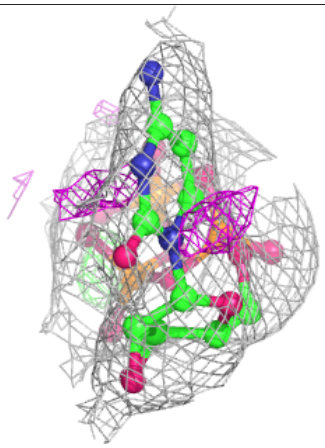


Electron density around CTP B 502:

$2mF_o$-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.