



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:48 PM UTC

PDB ID : 8FVB / pdb\_00008fvb  
Title : E coli. CTP synthase in complex with CTP  
Authors : Holyoak, T.; McLeod, M.J.; Tran, N.  
Deposited on : 2023-01-18  
Resolution : 2.03 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](mailto: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>.

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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

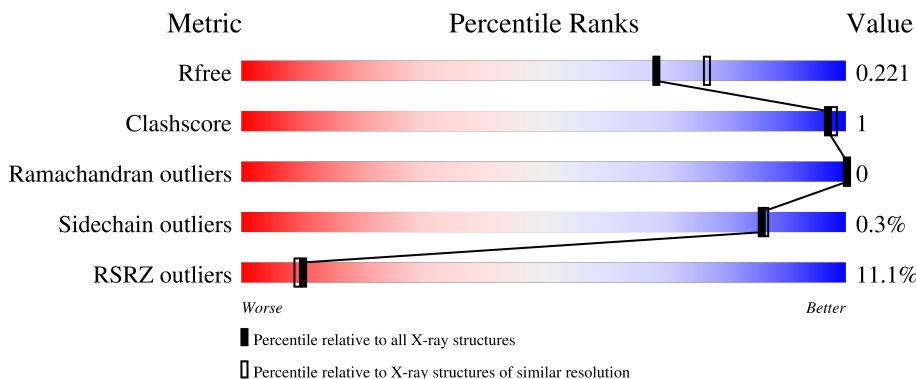
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

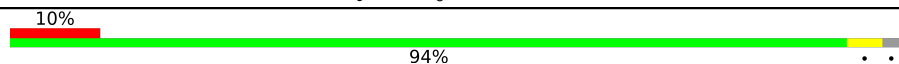
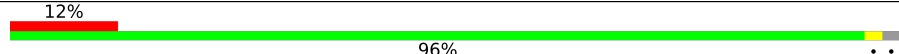
The reported resolution of this entry is 2.03 Å.

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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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  $\geq 3$ , 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	AAA	545	
1	BBB	545	

## 2 Entry composition [i](#)

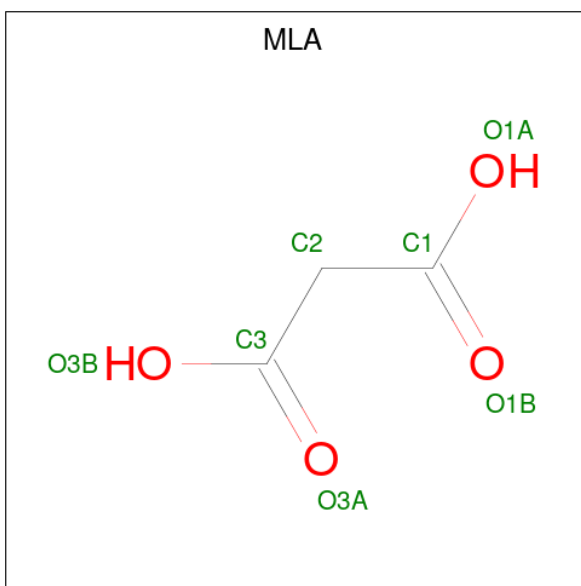
There are 4 unique types of molecules in this entry. The entry contains 9436 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

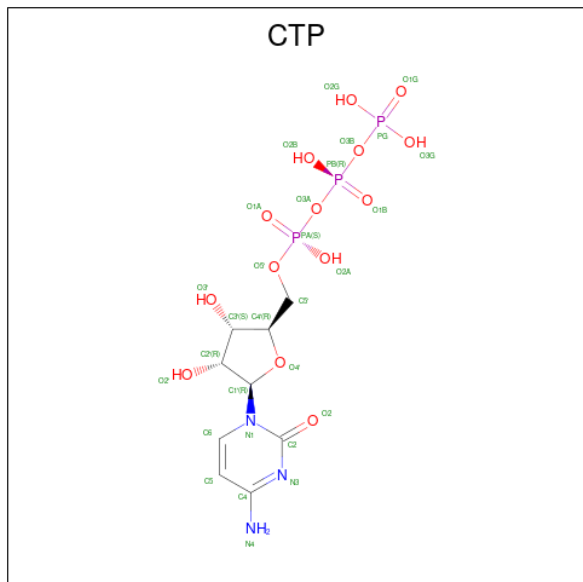
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	534	Total 4265	C 2703	N 736	O 804	S 22	0	17	0
1	BBB	534	Total 4238	C 2685	N 734	O 796	S 23	0	14	0

- Molecule 2 is MALONIC ACID (CCD ID: MLA) (formula: C<sub>3</sub>H<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	AAA	1	Total 7	C 3	O 4	0	0
2	AAA	1	Total 7	C 3	O 4	0	0
2	BBB	1	Total 7	C 3	O 4	0	0
2	BBB	1	Total 7	C 3	O 4	0	0

- Molecule 3 is CYTIDINE-5'-TRIPHOSPHATE (CCD ID: CTP) (formula:  $C_9H_{16}N_3O_{14}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	AAA	1	29	9	3	14	3	0	0
3	BBB	1	29	9	3	14	3	0	0

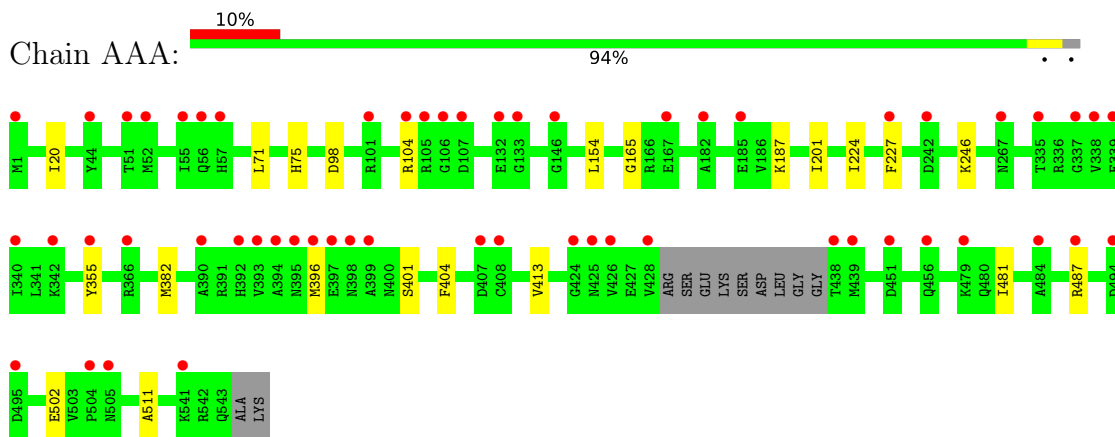
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	433	Total	O	0	0
			433	433		
4	BBB	414	Total	O	0	0
			414	414		

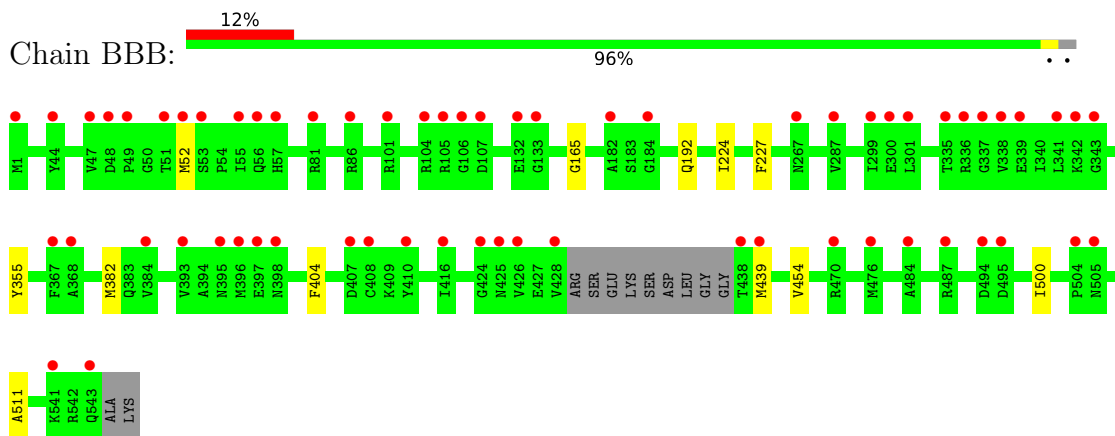
### 3 Residue-property plots [i](#)

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



- Molecule 1: CTP synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	164.71Å 103.91Å 131.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.00 – 2.03 44.00 – 2.03	Depositor EDS
% Data completeness (in resolution range)	97.4 (44.00-2.03) 97.4 (44.00-2.03)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 2.03Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.192 , 0.214 0.199 , 0.221	Depositor DCC
$R_{free}$ test set	7162 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.4	Xtrriage
Anisotropy	0.018	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 39.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9436	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.43% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MLA, 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	AAA	1.01	0/4382	1.40	3/5936 (0.1%)
1	BBB	1.02	0/4354	1.41	1/5898 (0.0%)
All	All	1.01	0/8736	1.41	4/11834 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	165	GLY	CA-C-O	-5.58	118.38	122.23
1	BBB	165	GLY	CA-C-O	-5.49	118.44	122.23
1	AAA	246	LYS	CA-C-N	5.14	123.48	120.24
1	AAA	246	LYS	C-N-CA	5.14	123.48	120.24

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	AAA	4265	0	4298	11	0
1	BBB	4238	0	4281	5	0
2	AAA	14	0	4	0	0
2	BBB	14	0	4	0	0
3	AAA	29	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	BBB	29	0	12	0	0
4	AAA	433	0	0	2	0
4	BBB	414	0	0	0	0
All	All	9436	0	8611	16	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 1.

All (16) 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:BBB:355:TYR:CD1	1:BBB:404:PHE:HB3	2.44	0.52
1:AAA:355:TYR:CD1	1:AAA:404:PHE:HB3	2.45	0.51
1:BBB:382:MET:HA	1:BBB:511:ALA:HB1	1.92	0.51
1:AAA:382:MET:HA	1:AAA:511:ALA:HB1	1.92	0.50
1:BBB:224:ILE:HA	1:BBB:227[A]:PHE:CE2	2.48	0.49
1:AAA:98:ASP:OD1	4:AAA:701:HOH:O	2.20	0.48
1:AAA:224:ILE:HA	1:AAA:227[A]:PHE:CE2	2.49	0.47
1:AAA:20:ILE:HD11	1:AAA:75:HIS:CE1	2.49	0.47
1:AAA:487:ARG:NH1	1:AAA:502:GLU:OE1	2.51	0.44
1:BBB:192:GLN:HA	1:BBB:227[B]:PHE:CE1	2.53	0.44
1:AAA:71:LEU:C	1:AAA:71:LEU:HD12	2.43	0.43
1:AAA:396:MET:HE1	1:AAA:481:ILE:HG13	1.99	0.43
1:AAA:154:LEU:HD13	1:AAA:201:ILE:CD1	2.50	0.42
1:AAA:401:SER:HA	1:AAA:413:VAL:O	2.19	0.42
1:AAA:187:LYS:NZ	4:AAA:716:HOH:O	2.54	0.41
1:BBB:454:VAL:HG11	1:BBB:500:ILE:HG21	2.02	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	AAA	547/545 (100%)	536 (98%)	11 (2%)	0	100	100
1	BBB	544/545 (100%)	536 (98%)	8 (2%)	0	100	100
All	All	1091/1090 (100%)	1072 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	AAA	470/461 (102%)	469 (100%)	1 (0%)	87	88
1	BBB	467/461 (101%)	465 (100%)	2 (0%)	84	84
All	All	937/922 (102%)	934 (100%)	3 (0%)	86	86

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	104	ARG
1	BBB	52	MET
1	BBB	439	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

6 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	MLA	BBB	803	-	6,6,6	1.11	0	7,7,7	1.03	0
2	MLA	AAA	602	-	6,6,6	1.13	0	7,7,7	1.02	0
2	MLA	AAA	601	-	6,6,6	1.14	0	7,7,7	0.84	0
3	CTP	AAA	603	-	29,30,30	0.64	0	43,47,47	0.63	0
3	CTP	BBB	801	-	29,30,30	0.61	0	43,47,47	0.65	0
2	MLA	BBB	802	-	6,6,6	1.11	0	7,7,7	1.18	0

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	MLA	BBB	803	-	-	2/4/4/4	-
2	MLA	AAA	602	-	-	4/4/4/4	-
2	MLA	AAA	601	-	-	0/4/4/4	-
3	CTP	AAA	603	-	-	1/22/38/38	0/2/2/2
3	CTP	BBB	801	-	-	1/22/38/38	0/2/2/2
2	MLA	BBB	802	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

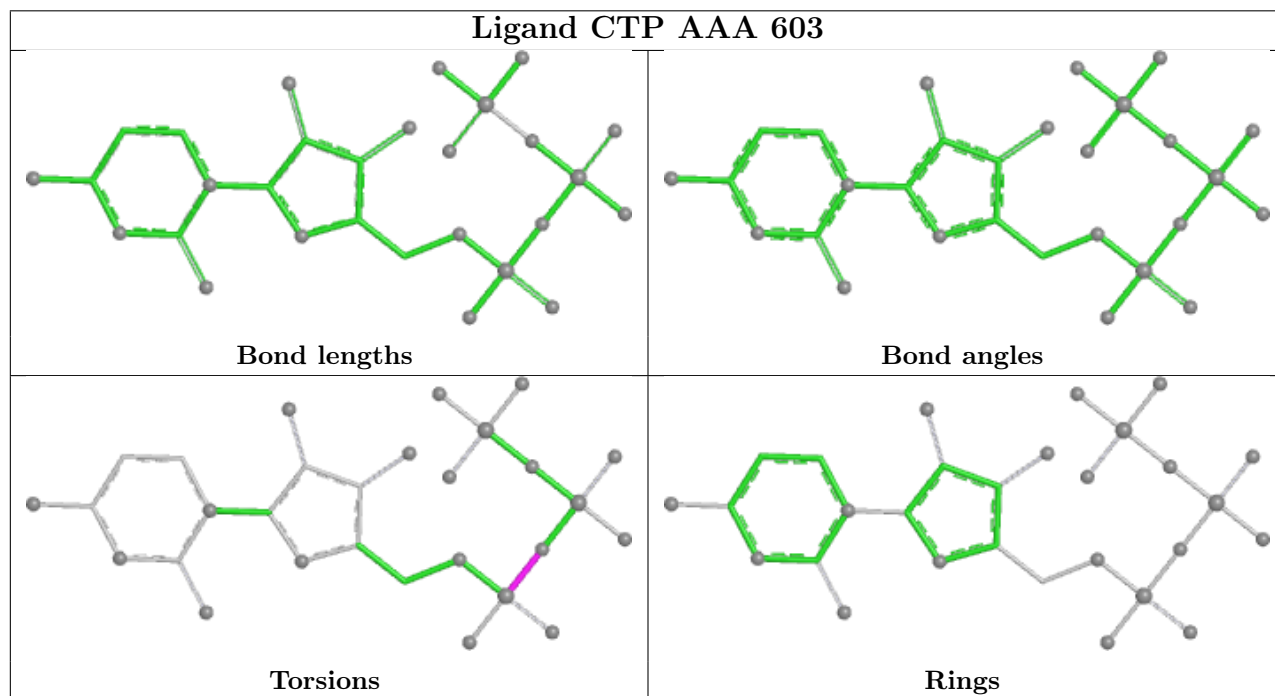
All (8) torsion outliers are listed below:

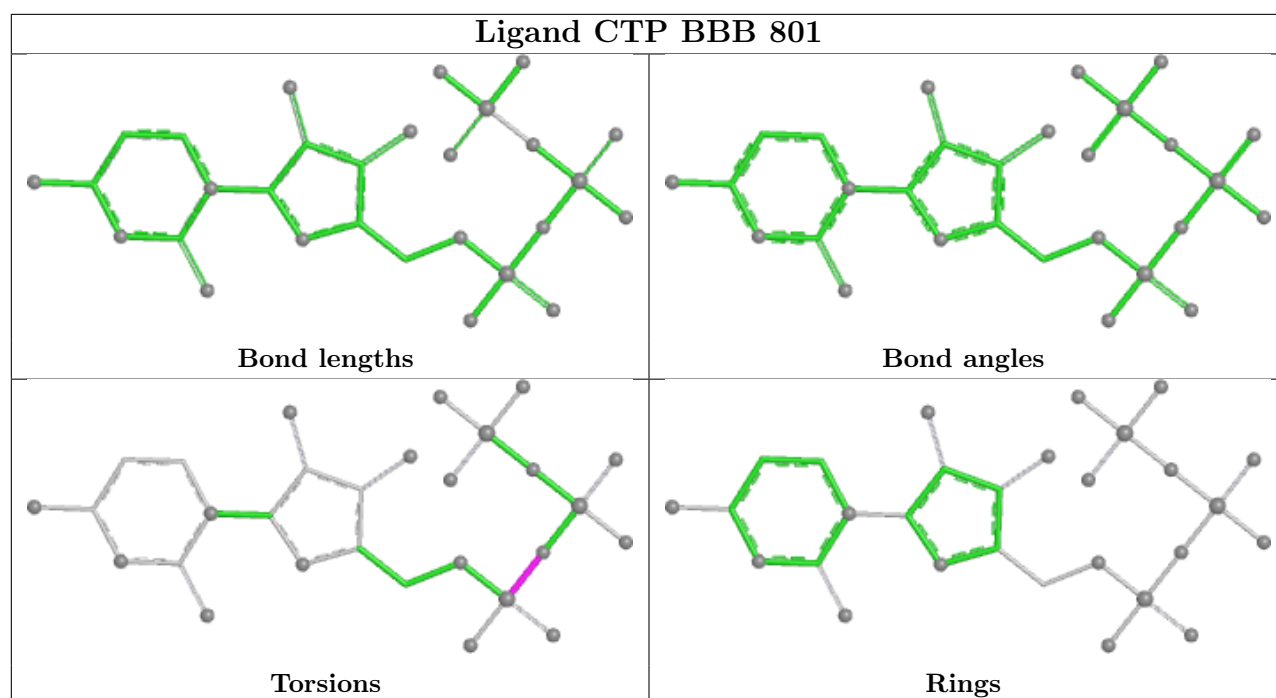
Mol	Chain	Res	Type	Atoms
2	AAA	602	MLA	O1A-C1-C2-C3
2	AAA	602	MLA	O1B-C1-C2-C3
3	AAA	603	CTP	PB-O3A-PA-O5'
3	BBB	801	CTP	PB-O3A-PA-O5'
2	AAA	602	MLA	C1-C2-C3-O3A
2	AAA	602	MLA	C1-C2-C3-O3B
2	BBB	803	MLA	C1-C2-C3-O3B
2	BBB	803	MLA	C1-C2-C3-O3A

There are no ring outliers.

No monomer is involved in short contacts.

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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AAA	534/545 (97%)	0.63	56 (10%) <b>11</b>   <b>10</b>	12, 35, 58, 74	17 (3%)
1	BBB	534/545 (97%)	0.73	63 (11%) <b>9</b>   <b>8</b>	15, 36, 60, 76	14 (2%)
All	All	1068/1090 (97%)	0.68	119 (11%) <b>10</b>   <b>9</b>	12, 36, 59, 76	31 (2%)

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	428	VAL	8.4
1	BBB	51	THR	6.0
1	AAA	1	MET	5.9
1	BBB	438	THR	5.9
1	AAA	227[A]	PHE	5.4
1	AAA	438	THR	5.2
1	AAA	57	HIS	5.1
1	BBB	1	MET	5.0
1	BBB	397	GLU	4.6
1	AAA	504	PRO	4.6
1	AAA	104	ARG	4.5
1	AAA	51	THR	4.4
1	AAA	505	ASN	4.2
1	BBB	342	LYS	4.0
1	AAA	451	ASP	3.9
1	AAA	339	GLU	3.9
1	BBB	44	TYR	3.8
1	BBB	55	ILE	3.8
1	BBB	106	GLY	3.8
1	AAA	397	GLU	3.7
1	BBB	47	VAL	3.7
1	AAA	342	LYS	3.6
1	BBB	504	PRO	3.6
1	AAA	55	ILE	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	AAA	182	ALA	3.5
1	AAA	56	GLN	3.5
1	AAA	428	VAL	3.5
1	AAA	494	ASP	3.4
1	BBB	393	VAL	3.4
1	BBB	395	ASN	3.4
1	BBB	52	MET	3.4
1	BBB	439	MET	3.4
1	AAA	132	GLU	3.4
1	BBB	396	MET	3.3
1	AAA	133	GLY	3.3
1	BBB	105	ARG	3.3
1	AAA	105	ARG	3.2
1	AAA	487	ARG	3.2
1	BBB	132	GLU	3.2
1	BBB	505	ASN	3.2
1	BBB	487	ARG	3.2
1	AAA	44[A]	TYR	3.1
1	AAA	393	VAL	3.1
1	AAA	426	VAL	3.1
1	BBB	339	GLU	3.1
1	BBB	182	ALA	3.0
1	AAA	106	GLY	3.0
1	BBB	133	GLY	3.0
1	BBB	335	THR	3.0
1	BBB	495	ASP	3.0
1	BBB	426	VAL	3.0
1	AAA	335	THR	2.9
1	AAA	495	ASP	2.9
1	AAA	267	ASN	2.9
1	BBB	56	GLN	2.8
1	BBB	104	ARG	2.7
1	BBB	425	ASN	2.7
1	BBB	86	ARG	2.7
1	BBB	300	GLU	2.7
1	BBB	408	CYS	2.7
1	AAA	395	ASN	2.7
1	BBB	267[A]	ASN	2.7
1	AAA	101	ARG	2.6
1	BBB	107	ASP	2.6
1	BBB	407	ASP	2.6
1	BBB	101	ARG	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	AAA	185	GLU	2.6
1	BBB	494	ASP	2.5
1	AAA	407[A]	ASP	2.5
1	BBB	49	PRO	2.5
1	AAA	52	MET	2.5
1	AAA	337	GLY	2.5
1	AAA	424	GLY	2.5
1	BBB	416	ILE	2.5
1	AAA	408	CYS	2.5
1	AAA	107	ASP	2.5
1	AAA	456	GLN	2.5
1	BBB	543	GLN	2.5
1	BBB	81	ARG	2.5
1	AAA	146	GLY	2.5
1	BBB	337	GLY	2.5
1	BBB	424	GLY	2.5
1	BBB	384	VAL	2.4
1	AAA	439	MET	2.4
1	BBB	57	HIS	2.4
1	AAA	392	HIS	2.4
1	BBB	301	LEU	2.4
1	AAA	340	ILE	2.4
1	BBB	336	ARG	2.3
1	BBB	287	VAL	2.3
1	AAA	167	GLU	2.3
1	AAA	394	ALA	2.3
1	BBB	484	ALA	2.3
1	BBB	470	ARG	2.3
1	BBB	53	SER	2.3
1	BBB	367	PHE	2.2
1	BBB	48	ASP	2.2
1	BBB	368	ALA	2.2
1	BBB	341	LEU	2.2
1	BBB	410	TYR	2.2
1	AAA	338	VAL	2.2
1	BBB	476	MET	2.2
1	BBB	343	GLY	2.1
1	AAA	242	ASP	2.1
1	AAA	399	ALA	2.1
1	AAA	484	ALA	2.1
1	BBB	184	GLY	2.1
1	BBB	299	ILE	2.1

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	BBB	338	VAL	2.1
1	AAA	479	LYS	2.1
1	BBB	541	LYS	2.1
1	AAA	396	MET	2.1
1	AAA	366	ARG	2.1
1	AAA	541	LYS	2.1
1	AAA	390	ALA	2.0
1	AAA	398	ASN	2.0
1	AAA	425	ASN	2.0
1	BBB	398	ASN	2.0
1	AAA	355	TYR	2.0

## 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](#)

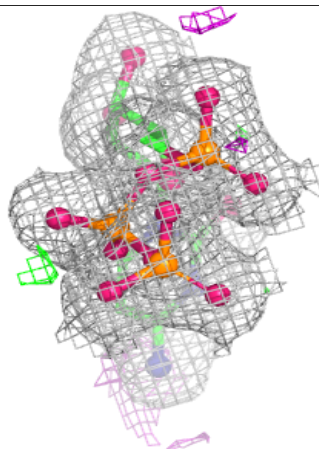
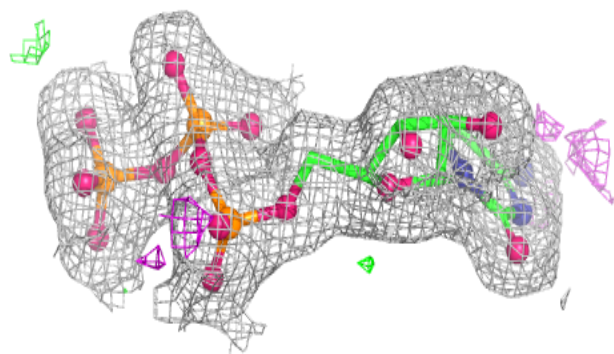
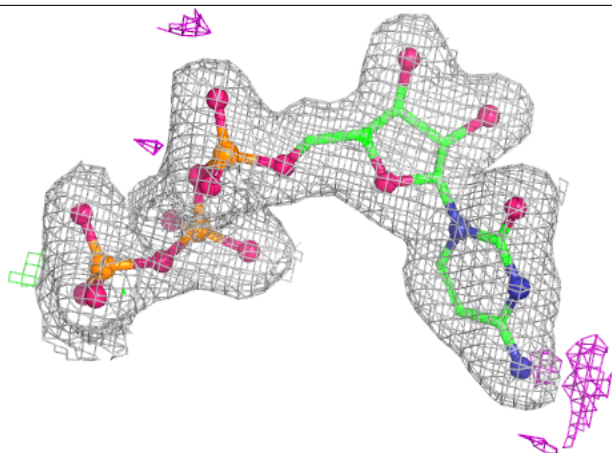
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

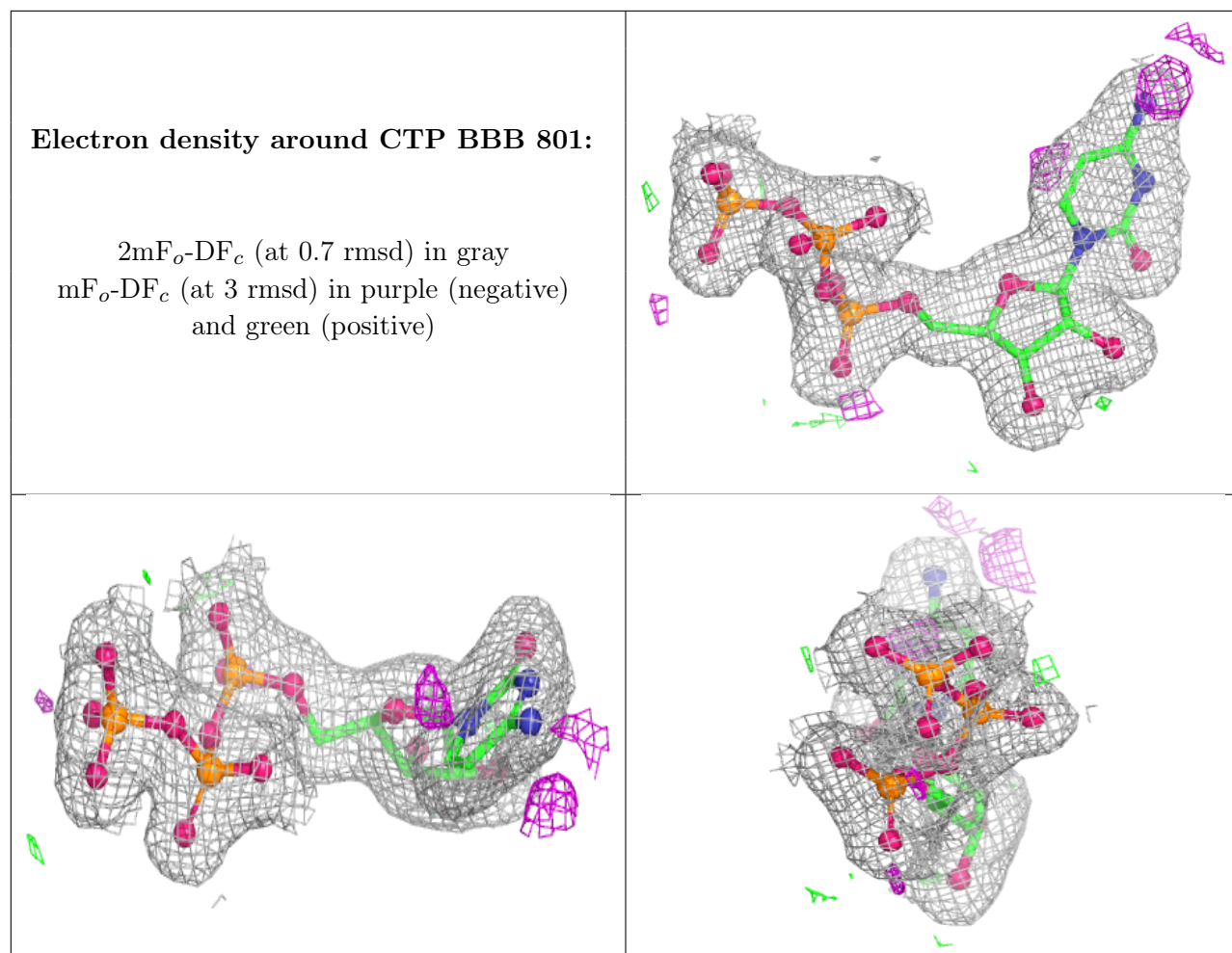
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MLA	AAA	602	7/7	0.77	0.18	72,75,75,76	0
2	MLA	BBB	803	7/7	0.78	0.17	77,78,79,80	0
2	MLA	AAA	601	7/7	0.89	0.14	31,33,39,40	0
2	MLA	BBB	802	7/7	0.91	0.11	35,37,43,45	0
3	CTP	AAA	603	29/29	0.99	0.04	21,22,23,23	0
3	CTP	BBB	801	29/29	0.99	0.04	22,23,25,25	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 AAA 603:**

$2mF_o-DF_c$  (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.