



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:17 AM UTC

PDB ID : 8FVC / pdb_00008fvc
Title : E coli. CTP synthase in complex with dF-dCTP (potassium malonate + 5 mM MgCl₂)
Authors : Holyoak, T.; McLeod, M.J.; Tran, N.
Deposited on : 2023-01-18
Resolution : 2.28 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

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

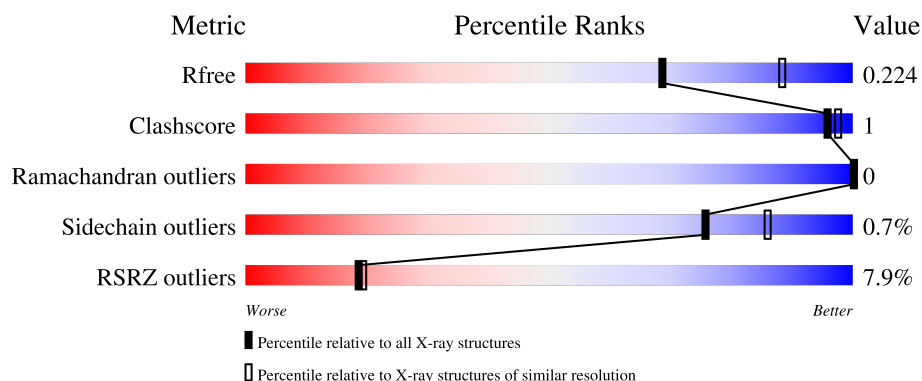
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	AAA	545	8% 94% ..
1	BBB	545	7% 94% ..

2 Entry composition [i](#)

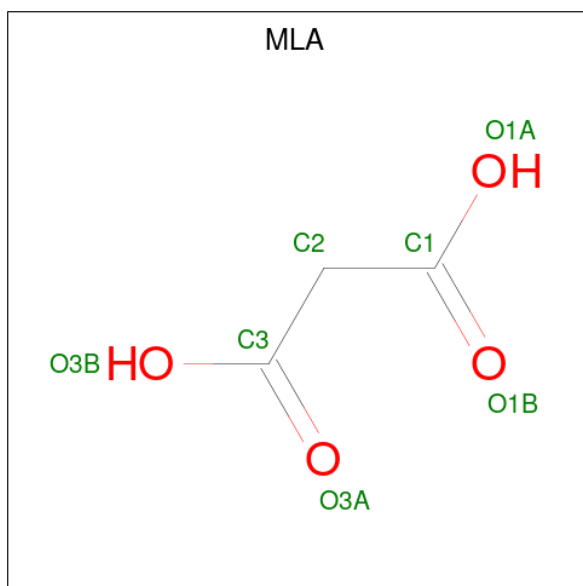
There are 4 unique types of molecules in this entry. The entry contains 9019 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

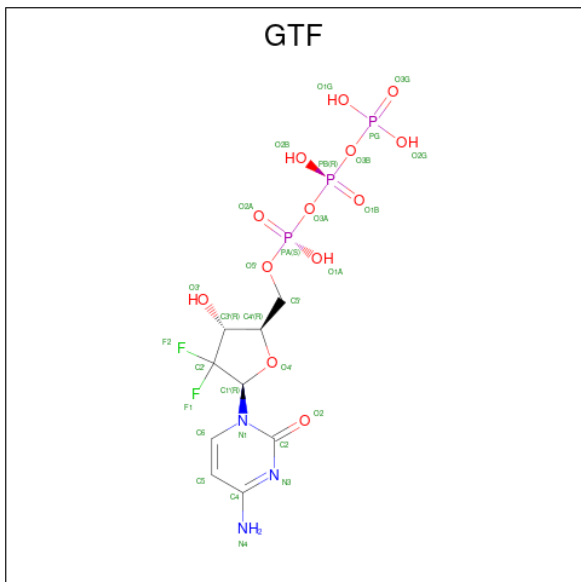
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	534	Total	C	N	O	S	0	10	0
			4243	2685	738	797	23			
1	BBB	534	Total	C	N	O	S	0	6	0
			4212	2661	737	791	23			

- Molecule 2 is MALONIC ACID (CCD ID: MLA) (formula: $C_3H_4O_4$).



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

- Molecule 3 is 2'-deoxy-2',2'-difluorocytidine 5'-(tetrahydrogen triphosphate) (CCD ID: GTF) (formula: $\text{C}_9\text{H}_{14}\text{F}_2\text{N}_3\text{O}_{13}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	AAA	1	Total 30	C 9	F 2	N 3	O 13	P 3	0	0
3	BBB	1	Total 30	C 9	F 2	N 3	O 13	P 3	0	0

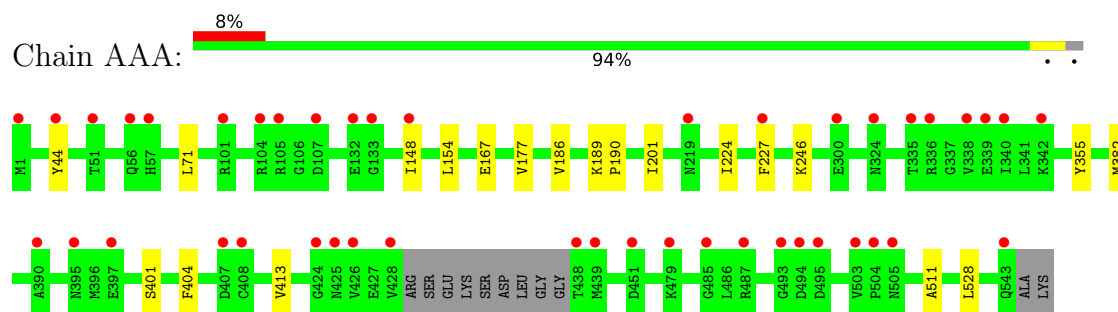
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	253	Total O 253 253	0	0
4	BBB	223	Total O 223 223	0	0

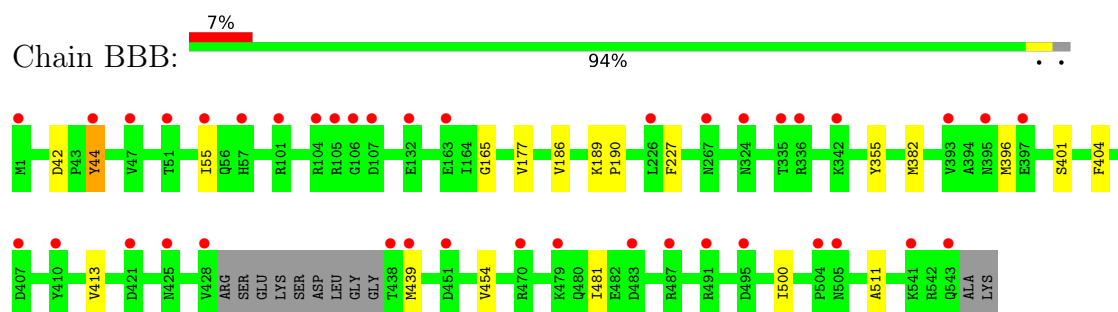
3 Residue-property plots [i](#)

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



- Molecule 1: CTP synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	165.80Å 103.97Å 131.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.70 – 2.28 81.70 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.7 (81.70-2.28) 99.7 (81.70-2.28)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.193 , 0.218 0.199 , 0.224	Depositor DCC
R_{free} test set	5239 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 27.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9019	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.25% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GTF, MLA

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	0/4320	1.41	2/5853 (0.0%)
1	BBB	1.02	0/4288	1.40	1/5808 (0.0%)
All	All	1.01	0/8608	1.41	3/11661 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	165	GLY	CA-C-O	-5.53	118.41	122.23
1	AAA	246	LYS	CA-C-N	5.29	123.57	120.24
1	AAA	246	LYS	C-N-CA	5.29	123.57	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	4243	0	4257	11	0
1	BBB	4212	0	4229	8	0
2	AAA	14	0	4	0	0
2	BBB	14	0	4	0	0
3	AAA	30	0	10	0	0
3	BBB	30	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	AAA	253	0	0	0	0
4	BBB	223	0	0	0	0
All	All	9019	0	8514	19	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 (19) 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	2.40	0.56
1:BBB:382:MET:HA	1:BBB:511:ALA:HB1	1.88	0.55
1:AAA:154:LEU:HD13	1:AAA:201:ILE:CD1	2.37	0.55
1:AAA:382:MET:HA	1:AAA:511:ALA:HB1	1.94	0.48
1:BBB:396:MET:HE1	1:BBB:481:ILE:HG13	1.99	0.45
1:AAA:189:LYS:HB3	1:AAA:190:PRO:HD3	1.99	0.45
1:AAA:224:ILE:HA	1:AAA:227[B]:PHE:CE2	2.53	0.44
1:BBB:42:ASP:HB3	1:BBB:44:TYR:CE2	2.53	0.44
1:AAA:71:LEU:C	1:AAA:71:LEU:HD12	2.42	0.44
1:AAA:355:TYR:CD1	1:AAA:404:PHE:HB3	2.54	0.43
1:AAA:401:SER:HA	1:AAA:413:VAL:O	2.19	0.43
1:BBB:177:VAL:HG12	1:BBB:186:VAL:HB	2.01	0.43
1:AAA:167[A]:GLU:H	1:AAA:167[A]:GLU:CD	2.26	0.42
1:AAA:227[B]:PHE:CD1	1:AAA:227[B]:PHE:C	2.96	0.42
1:BBB:189:LYS:HB3	1:BBB:190:PRO:HD3	2.02	0.42
1:BBB:401:SER:HA	1:BBB:413:VAL:O	2.20	0.42
1:AAA:177:VAL:HG12	1:AAA:186:VAL:HB	2.02	0.41
1:AAA:148[B]:ILE:HD13	3:BBB:603:GTF:N3	2.36	0.41
1:BBB:454:VAL:HG11	1:BBB:500:ILE:HG21	2.03	0.40

There are no symmetry-related clashes.

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	AAA	540/545 (99%)	532 (98%)	8 (2%)	0	100	100
1	BBB	536/545 (98%)	528 (98%)	8 (2%)	0	100	100
All	All	1076/1090 (99%)	1060 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	463/461 (100%)	460 (99%)	3 (1%)	78	87
1	BBB	459/461 (100%)	455 (99%)	4 (1%)	70	82
All	All	922/922 (100%)	915 (99%)	7 (1%)	76	84

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	44	TYR
1	AAA	528[A]	LEU
1	AAA	528[B]	LEU
1	BBB	44	TYR
1	BBB	55	ILE
1	BBB	227	PHE
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 ⓘ

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	AAA	601	-	6,6,6	1.36	0	7,7,7	0.98	0
3	GTF	BBB	603	-	28,31,31	0.64	0	39,50,50	0.71	1 (2%)
2	MLA	BBB	601	-	6,6,6	1.33	0	7,7,7	1.02	0
2	MLA	BBB	602	-	6,6,6	1.35	0	7,7,7	1.00	0
3	GTF	AAA	603	-	28,31,31	0.61	0	39,50,50	0.66	1 (2%)
2	MLA	AAA	602	-	6,6,6	1.36	0	7,7,7	0.98	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	AAA	601	-	-	2/4/4/4	-
3	GTF	BBB	603	-	-	1/22/42/42	0/2/2/2
2	MLA	BBB	601	-	-	0/4/4/4	-
2	MLA	BBB	602	-	-	2/4/4/4	-
3	GTF	AAA	603	-	-	1/22/42/42	0/2/2/2
2	MLA	AAA	602	-	-	4/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BBB	603	GTF	F2-C2'-F1	2.13	108.11	105.55
3	AAA	603	GTF	F2-C2'-F1	2.05	108.01	105.55

There are no chirality outliers.

All (10) torsion outliers are listed below:

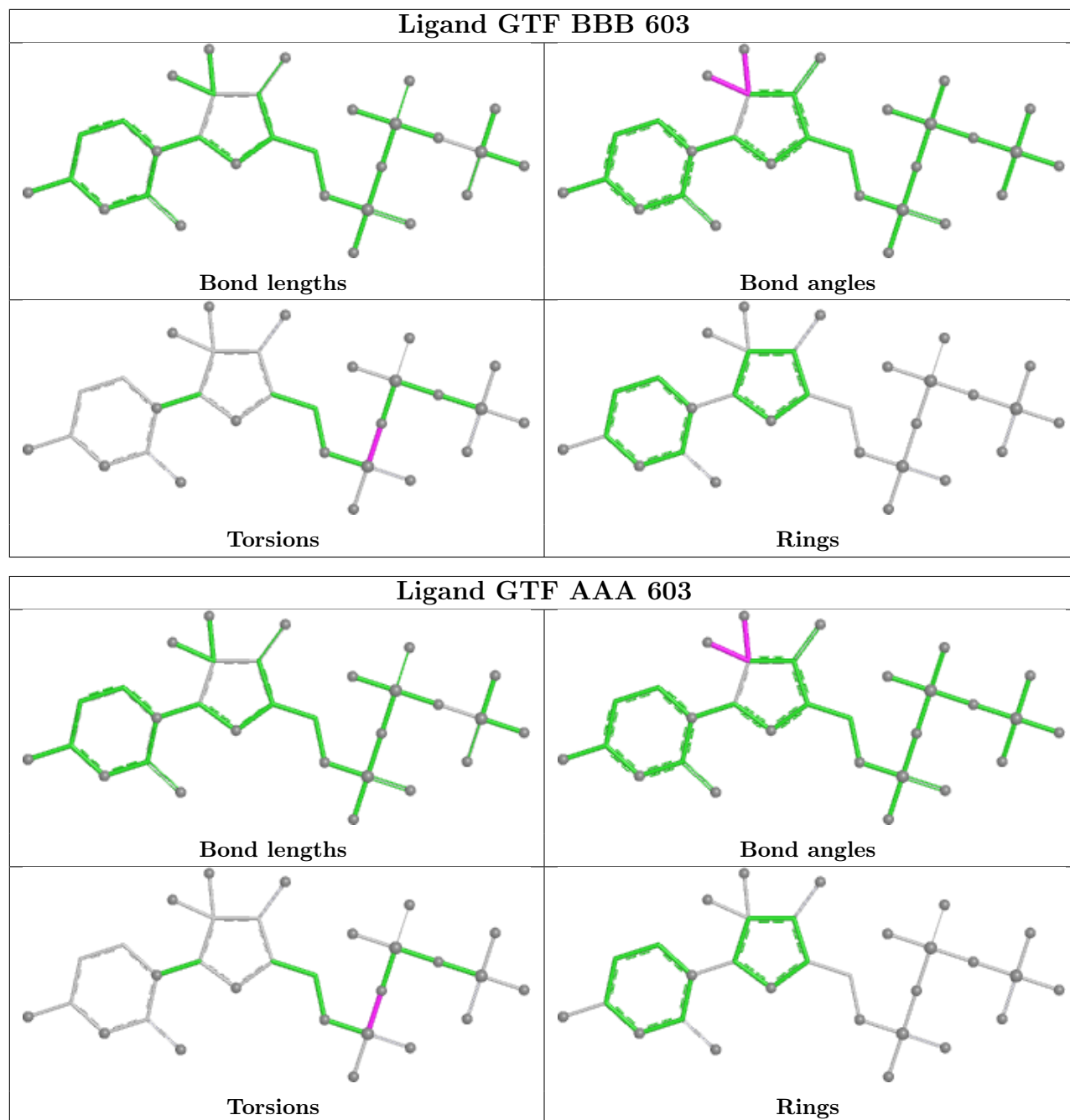
Mol	Chain	Res	Type	Atoms
2	AAA	602	MLA	O1A-C1-C2-C3
2	AAA	602	MLA	O1B-C1-C2-C3
3	AAA	603	GTF	PB-O3A-PA-O5'
3	BBB	603	GTF	PB-O3A-PA-O5'
2	AAA	601	MLA	C1-C2-C3-O3B
2	AAA	601	MLA	C1-C2-C3-O3A
2	AAA	602	MLA	C1-C2-C3-O3A
2	AAA	602	MLA	C1-C2-C3-O3B
2	BBB	602	MLA	C1-C2-C3-O3A
2	BBB	602	MLA	C1-C2-C3-O3B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	BBB	603	GTF	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 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, 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	AAA	534/545 (97%)	0.38	44 (8%)	17 18	17, 45, 74, 98	10 (1%)
1	BBB	534/545 (97%)	0.43	40 (7%)	20 21	17, 46, 74, 104	6 (1%)
All	All	1068/1090 (97%)	0.40	84 (7%)	18 19	17, 45, 74, 104	16 (1%)

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	428	VAL	11.8
1	BBB	438	THR	8.6
1	AAA	428	VAL	7.3
1	AAA	1	MET	6.8
1	AAA	438	THR	6.7
1	BBB	1	MET	6.2
1	BBB	104	ARG	5.8
1	BBB	44	TYR	5.2
1	AAA	104	ARG	5.2
1	AAA	44	TYR	4.7
1	BBB	342	LYS	4.5
1	BBB	51	THR	4.1
1	AAA	339	GLU	4.0
1	AAA	57	HIS	4.0
1	AAA	105	ARG	3.9
1	AAA	451	ASP	3.8
1	AAA	505	ASN	3.7
1	BBB	105	ARG	3.7
1	AAA	342	LYS	3.7
1	AAA	227[A]	PHE	3.7
1	BBB	504	PRO	3.6
1	AAA	504	PRO	3.5
1	BBB	101	ARG	3.5
1	BBB	57	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
1	BBB	543	GLN	3.3
1	AAA	51	THR	3.2
1	BBB	505	ASN	3.2
1	BBB	479	LYS	3.1
1	BBB	407	ASP	3.1
1	BBB	487	ARG	2.9
1	AAA	300	GLU	2.8
1	BBB	495	ASP	2.8
1	AAA	397	GLU	2.8
1	BBB	397	GLU	2.8
1	BBB	106	GLY	2.7
1	AAA	487	ARG	2.7
1	AAA	543	GLN	2.7
1	AAA	424	GLY	2.7
1	AAA	493	GLY	2.7
1	AAA	335	THR	2.7
1	AAA	495	ASP	2.6
1	BBB	491[A]	ARG	2.6
1	AAA	407	ASP	2.6
1	AAA	395	ASN	2.5
1	AAA	340	ILE	2.5
1	BBB	439	MET	2.5
1	AAA	494	ASP	2.4
1	BBB	163	GLU	2.4
1	BBB	451	ASP	2.4
1	BBB	226[A]	LEU	2.4
1	AAA	133	GLY	2.3
1	BBB	470	ARG	2.3
1	BBB	395	ASN	2.2
1	BBB	47	VAL	2.2
1	AAA	148[A]	ILE	2.2
1	BBB	336	ARG	2.2
1	AAA	408	CYS	2.2
1	BBB	335	THR	2.2
1	BBB	410	TYR	2.1
1	BBB	55	ILE	2.1
1	AAA	439	MET	2.1
1	BBB	421	ASP	2.1
1	BBB	425	ASN	2.1
1	BBB	483	ASP	2.1
1	BBB	541	LYS	2.1
1	AAA	101	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	AAA	479	LYS	2.1
1	AAA	56	GLN	2.1
1	AAA	503	VAL	2.1
1	BBB	393	VAL	2.1
1	AAA	336	ARG	2.1
1	AAA	107	ASP	2.1
1	AAA	219	ASN	2.1
1	AAA	425	ASN	2.1
1	BBB	107	ASP	2.1
1	BBB	324[A]	ASN	2.1
1	AAA	132	GLU	2.0
1	AAA	390	ALA	2.0
1	AAA	338	VAL	2.0
1	AAA	426	VAL	2.0
1	AAA	485	GLY	2.0
1	BBB	132	GLU	2.0
1	AAA	324[A]	ASN	2.0
1	BBB	267	ASN	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, 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	MLA	AAA	602	7/7	0.82	0.15	89,91,91,92	0
2	MLA	BBB	602	7/7	0.85	0.15	86,91,96,98	0
2	MLA	AAA	601	7/7	0.93	0.11	42,48,62,63	0
2	MLA	BBB	601	7/7	0.94	0.10	48,53,67,69	0
3	GTF	AAA	603	30/30	0.99	0.04	29,32,34,35	0

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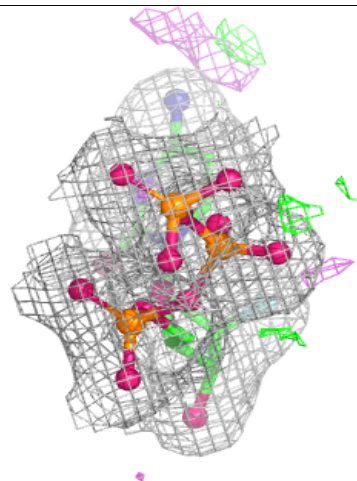
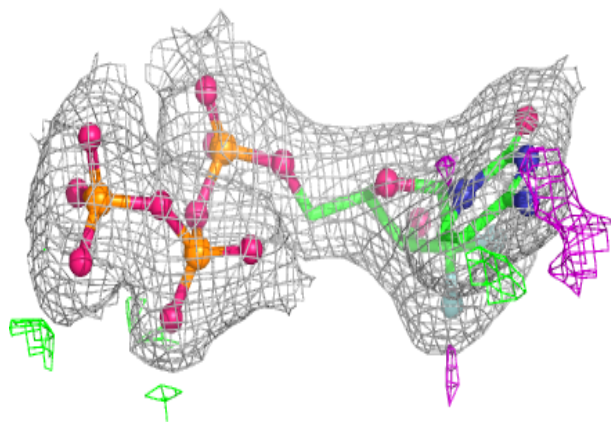
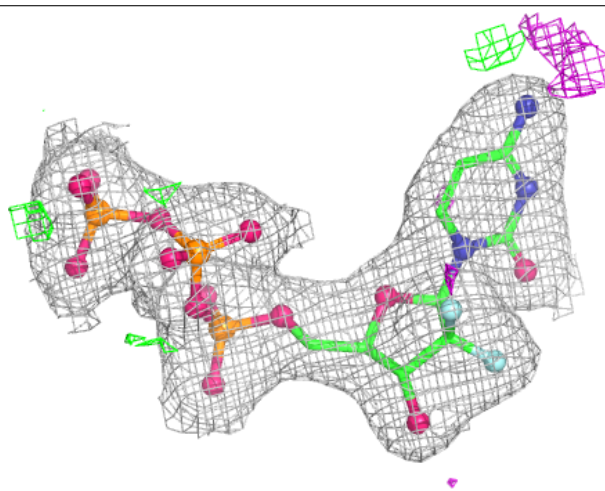
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GTF	BBB	603	30/30	0.99	0.04	30,32,35,36	0

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.

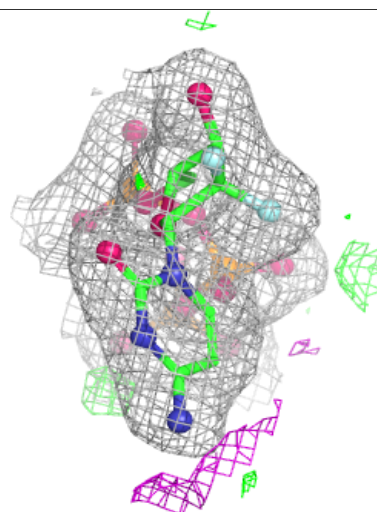
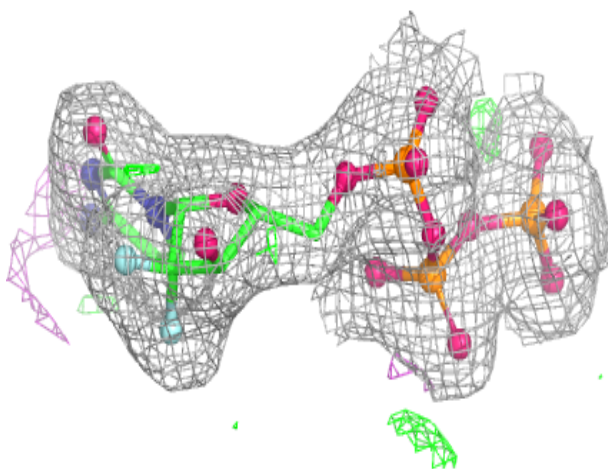
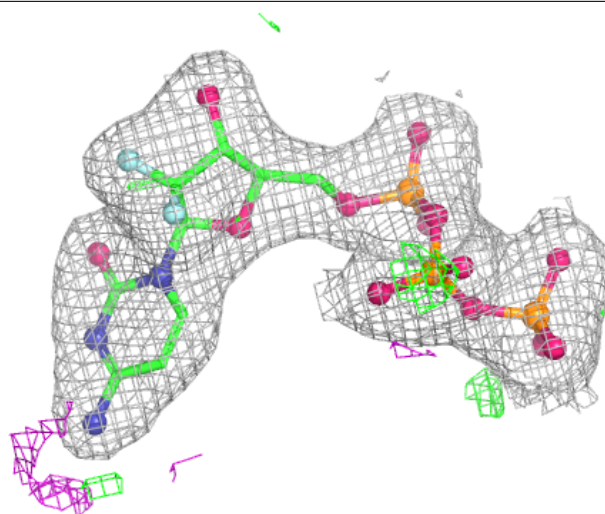
Electron density around GTF AAA 603:

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



Electron density around GTF BBB 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.