



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2023 – 04:12 PM EDT

PDB ID : 8FV6
Title : E coli. CTP synthase in complex with dF-dCTP
Authors : Holyoak, T.; McLeod, M.J.; Tran, N.
Deposited on : 2023-01-18
Resolution : 2.25 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.32.2
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) : 2.32.2

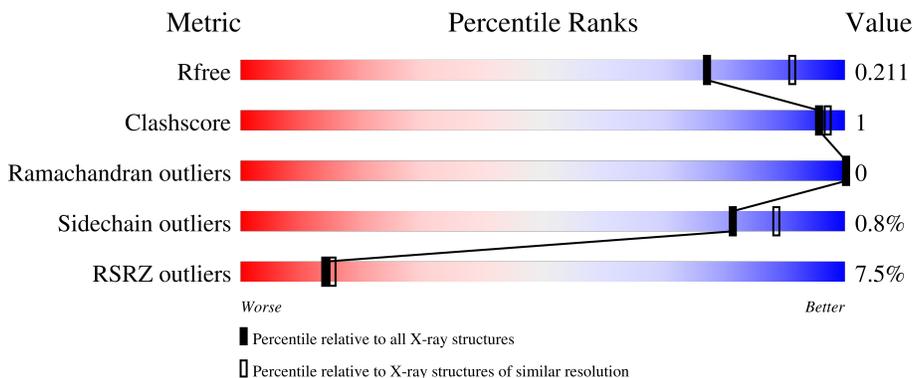
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	
1	BBB	545	

2 Entry composition [i](#)

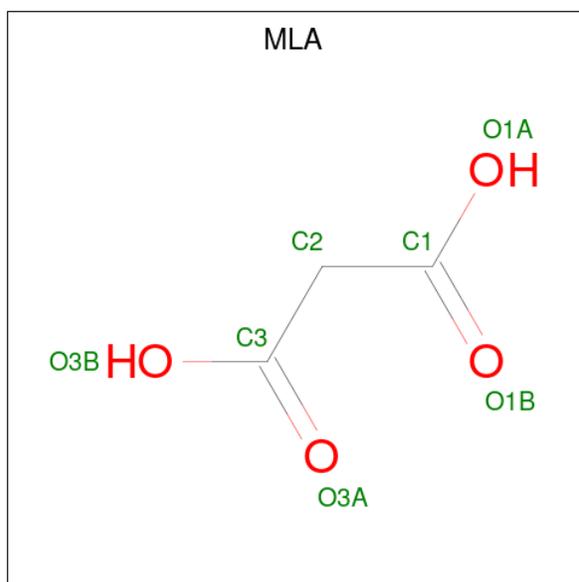
There are 5 unique types of molecules in this entry. The entry contains 8994 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

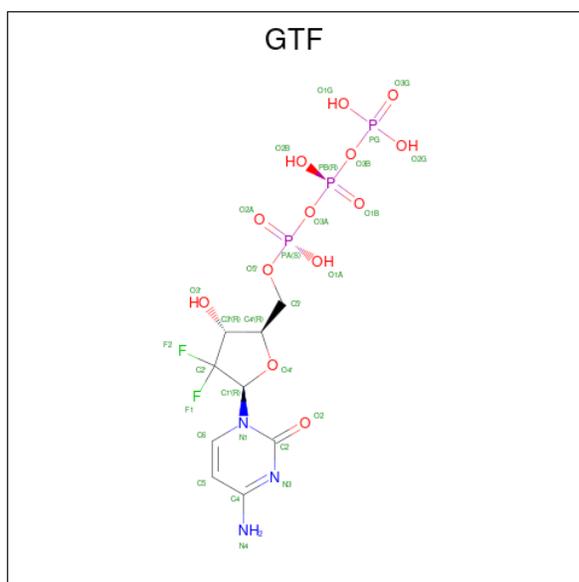
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	535	Total 4212	C 2665	N 732	O 792	S 23	0	8	0
1	BBB	535	Total 4208	C 2663	N 730	O 793	S 22	0	8	0

- Molecule 2 is MALONIC ACID (three-letter code: MLA) (formula: C₃H₄O₄).



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

- Molecule 3 is 2'-deoxy-2',2'-difluorocytidine 5'-(tetrahydrogen triphosphate) (three-letter code: GTF) (formula: C₉H₁₄F₂N₃O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
4	AAA	1	1	1	0	0
4	BBB	1	1	1	0	0

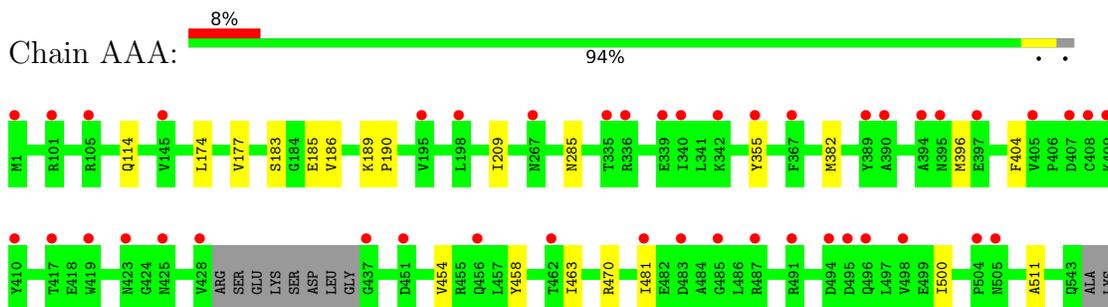
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	AAA	241	241	241	0	0
5	BBB	257	257	257	0	0

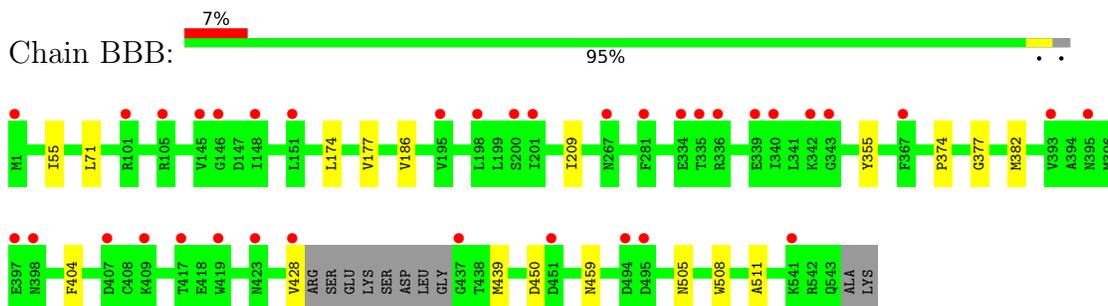
3 Residue-property plots [i](#)

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	158.40Å 108.95Å 129.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.90 – 2.25 48.87 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.90-2.25) 99.9 (48.87-2.25)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.24Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.190 , 0.210 0.193 , 0.211	Depositor DCC
R_{free} test set	5316 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtrriage
Anisotropy	0.071	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8994	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% 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

5.1 Standard geometry

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

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	0.65	0/4313	0.71	0/5841
1	BBB	0.65	0/4309	0.71	0/5836
All	All	0.65	0/8622	0.71	0/11677

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	4212	0	4242	11	0
1	BBB	4208	0	4238	7	0
2	AAA	7	0	2	0	0
2	BBB	7	0	2	0	0
3	AAA	30	0	10	0	0
3	BBB	30	0	10	0	0
4	AAA	1	0	0	0	0
4	BBB	1	0	0	0	0
5	AAA	241	0	0	2	0
5	BBB	257	0	0	0	0
All	All	8994	0	8504	18	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 (18) 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:AAA:396:MET:HE3	1:AAA:481:ILE:HG13	1.86	0.56
1:AAA:382:MET:HA	1:AAA:511:ALA:HB1	1.89	0.54
1:BBB:355:TYR:CD1	1:BBB:404:PHE:HB3	2.43	0.53
1:AAA:355:TYR:CD1	1:AAA:404:PHE:HB3	2.45	0.52
1:BBB:382:MET:HA	1:BBB:511:ALA:HB1	1.94	0.50
1:AAA:183:SER:OG	1:AAA:185[A]:GLU:HG2	2.14	0.48
1:AAA:177:VAL:HG12	1:AAA:186:VAL:HB	1.96	0.47
1:AAA:285:ASN:ND2	5:AAA:709:HOH:O	2.48	0.46
1:BBB:174:LEU:HG	1:BBB:209:ILE:HB	1.98	0.45
1:BBB:71:LEU:HD12	1:BBB:71:LEU:C	2.37	0.44
1:BBB:374:PRO:HA	1:BBB:508:TRP:O	2.19	0.42
1:AAA:458:TYR:CD1	1:AAA:463:ILE:HG21	2.55	0.41
1:AAA:114:GLN:NE2	5:AAA:718:HOH:O	2.53	0.41
1:BBB:177:VAL:HG12	1:BBB:186:VAL:HB	2.02	0.41
1:AAA:189:LYS:HB3	1:AAA:190:PRO:HD3	2.02	0.41
1:AAA:174:LEU:HG	1:AAA:209:ILE:HB	2.01	0.41
1:AAA:454:VAL:HG11	1:AAA:500:ILE:HG21	2.02	0.40
1:BBB:377:GLY:O	1:BBB:511:ALA:HA	2.21	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	539/545 (99%)	531 (98%)	8 (2%)	0	100	100
1	BBB	539/545 (99%)	526 (98%)	13 (2%)	0	100	100
All	All	1078/1090 (99%)	1057 (98%)	21 (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	461/461 (100%)	460 (100%)	1 (0%)	93	96
1	BBB	461/461 (100%)	455 (99%)	6 (1%)	69	79
All	All	922/922 (100%)	915 (99%)	7 (1%)	81	88

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

Mol	Chain	Res	Type
1	AAA	470	ARG
1	BBB	55	ILE
1	BBB	428	VAL
1	BBB	439	MET
1	BBB	450	ASP
1	BBB	459	ASN
1	BBB	505	ASN

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 monosaccharides 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	GTF	AAA	602	4	25,31,31	0.53	0	35,50,50	0.86	2 (5%)
2	MLA	BBB	703	-	6,6,6	1.09	0	7,7,7	0.91	0
2	MLA	AAA	601	-	6,6,6	1.02	0	7,7,7	1.08	0
3	GTF	BBB	701	4	25,31,31	0.54	0	35,50,50	0.85	2 (5%)

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	GTF	AAA	602	4	-	5/22/42/42	0/2/2/2
2	MLA	BBB	703	-	-	2/4/4/4	-
2	MLA	AAA	601	-	-	4/4/4/4	-
3	GTF	BBB	701	4	-	6/22/42/42	0/2/2/2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AAA	602	GTF	F2-C2'-F1	2.59	108.17	105.20
3	BBB	701	GTF	F2-C2'-F1	2.37	107.91	105.20
3	AAA	602	GTF	C4'-O4'-C1'	-2.09	105.70	109.45
3	BBB	701	GTF	C4'-O4'-C1'	-2.07	105.73	109.45

There are no chirality outliers.

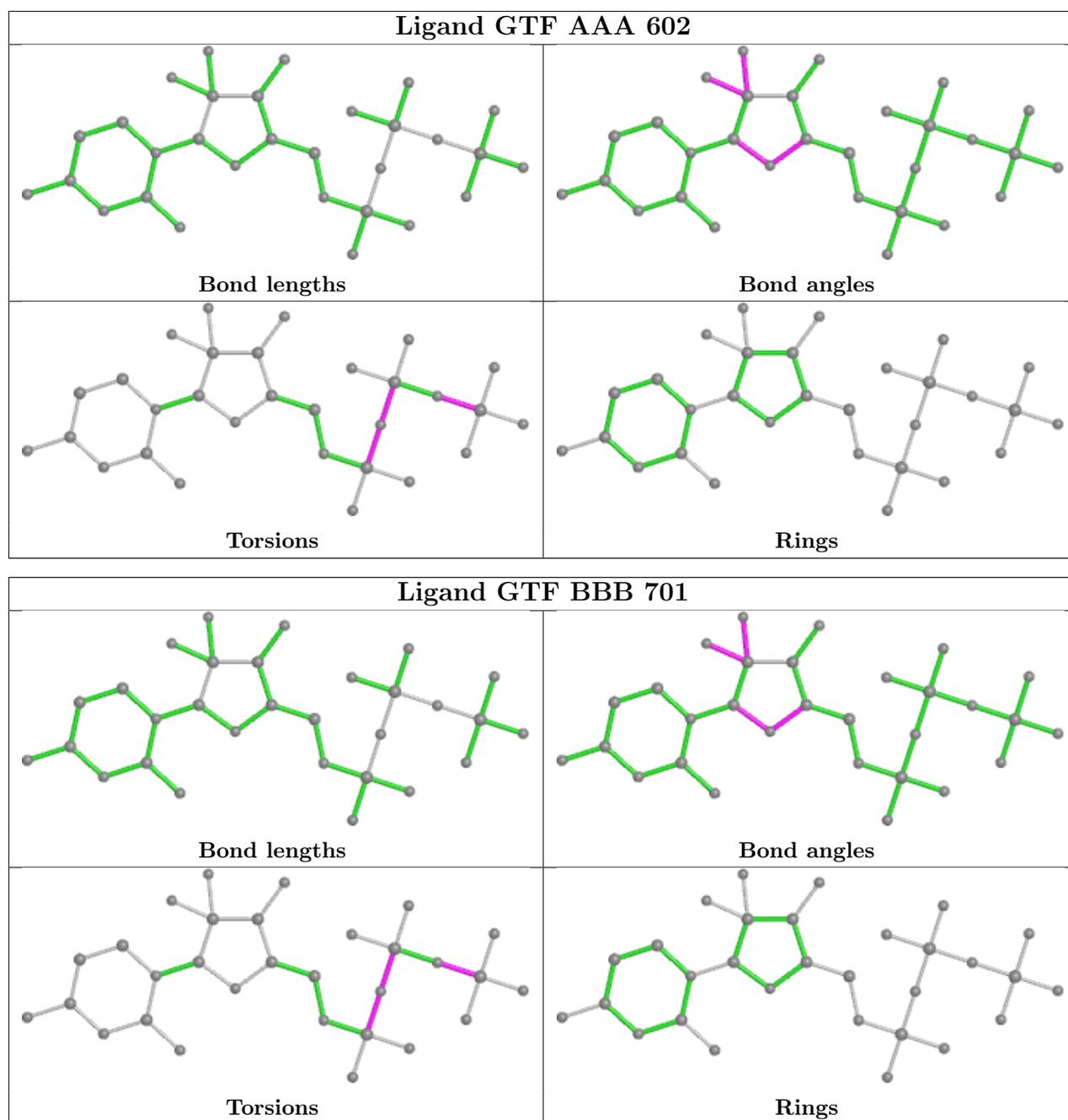
All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	BBB	701	GTF	PB-O3B-PG-O2G
2	BBB	703	MLA	O1A-C1-C2-C3
3	BBB	701	GTF	PA-O3A-PB-O1B
2	AAA	601	MLA	O1B-C1-C2-C3
3	AAA	602	GTF	PB-O3B-PG-O2G
3	AAA	602	GTF	PA-O3A-PB-O1B
3	BBB	701	GTF	PB-O3A-PA-O1A
2	AAA	601	MLA	O1A-C1-C2-C3
3	BBB	701	GTF	PB-O3B-PG-O3G
2	BBB	703	MLA	O1B-C1-C2-C3
3	BBB	701	GTF	PA-O3A-PB-O2B
3	AAA	602	GTF	PB-O3A-PA-O2A
2	AAA	601	MLA	C1-C2-C3-O3B
3	AAA	602	GTF	PB-O3A-PA-O1A
3	AAA	602	GTF	PA-O3A-PB-O2B
3	BBB	701	GTF	PB-O3A-PA-O2A
2	AAA	601	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, 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	535/545 (98%)	0.39	44 (8%) 11 12	23, 49, 83, 99	0
1	BBB	535/545 (98%)	0.26	36 (6%) 17 19	23, 47, 82, 96	0
All	All	1070/1090 (98%)	0.33	80 (7%) 14 15	23, 48, 82, 99	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	342	LYS	4.8
1	AAA	339	GLU	4.8
1	BBB	494	ASP	4.8
1	AAA	340	ILE	4.7
1	AAA	342	LYS	4.5
1	AAA	494	ASP	4.4
1	BBB	495	ASP	4.3
1	AAA	1	MET	4.3
1	BBB	335	THR	4.1
1	BBB	1	MET	4.1
1	BBB	267[A]	ASN	3.9
1	AAA	487	ARG	3.9
1	AAA	335	THR	3.9
1	AAA	405	VAL	3.9
1	BBB	437	GLY	3.8
1	BBB	339	GLU	3.8
1	AAA	336	ARG	3.7
1	AAA	395	ASN	3.6
1	BBB	340	ILE	3.5
1	BBB	101	ARG	3.4
1	BBB	407	ASP	3.3
1	AAA	481	ILE	3.3
1	AAA	407	ASP	3.3
1	AAA	495	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	BBB	336	ARG	3.2
1	BBB	397	GLU	3.2
1	BBB	145	VAL	3.1
1	AAA	437	GLY	3.0
1	BBB	428	VAL	2.9
1	AAA	485	GLY	2.9
1	BBB	395	ASN	2.9
1	BBB	451	ASP	2.8
1	AAA	195	VAL	2.7
1	AAA	505	ASN	2.7
1	AAA	428	VAL	2.7
1	AAA	491	ARG	2.7
1	BBB	423	ASN	2.7
1	BBB	148	ILE	2.7
1	AAA	267	ASN	2.7
1	BBB	409	LYS	2.6
1	BBB	393	VAL	2.6
1	AAA	451	ASP	2.6
1	AAA	367	PHE	2.6
1	BBB	367	PHE	2.6
1	AAA	355	TYR	2.6
1	AAA	425	ASN	2.6
1	AAA	496	GLN	2.5
1	AAA	145	VAL	2.5
1	AAA	419	TRP	2.5
1	AAA	417	THR	2.5
1	AAA	397	GLU	2.4
1	BBB	200	SER	2.4
1	BBB	201	ILE	2.4
1	BBB	151	LEU	2.4
1	AAA	410	TYR	2.4
1	AAA	101	ARG	2.4
1	BBB	198	LEU	2.3
1	AAA	389	TYR	2.3
1	BBB	541	LYS	2.3
1	AAA	390	ALA	2.3
1	AAA	409	LYS	2.2
1	BBB	195	VAL	2.2
1	AAA	504	PRO	2.2
1	BBB	105	ARG	2.2
1	BBB	343	GLY	2.2
1	AAA	198	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	BBB	417	THR	2.2
1	AAA	462	THR	2.1
1	BBB	146	GLY	2.1
1	BBB	419	TRP	2.1
1	AAA	394	ALA	2.1
1	AAA	423	ASN	2.1
1	AAA	456	GLN	2.1
1	BBB	281	PHE	2.1
1	AAA	483	ASP	2.1
1	BBB	334	GLU	2.1
1	AAA	498	VAL	2.0
1	AAA	408	CYS	2.0
1	BBB	398	ASN	2.0
1	AAA	105	ARG	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 monosaccharides in this entry.

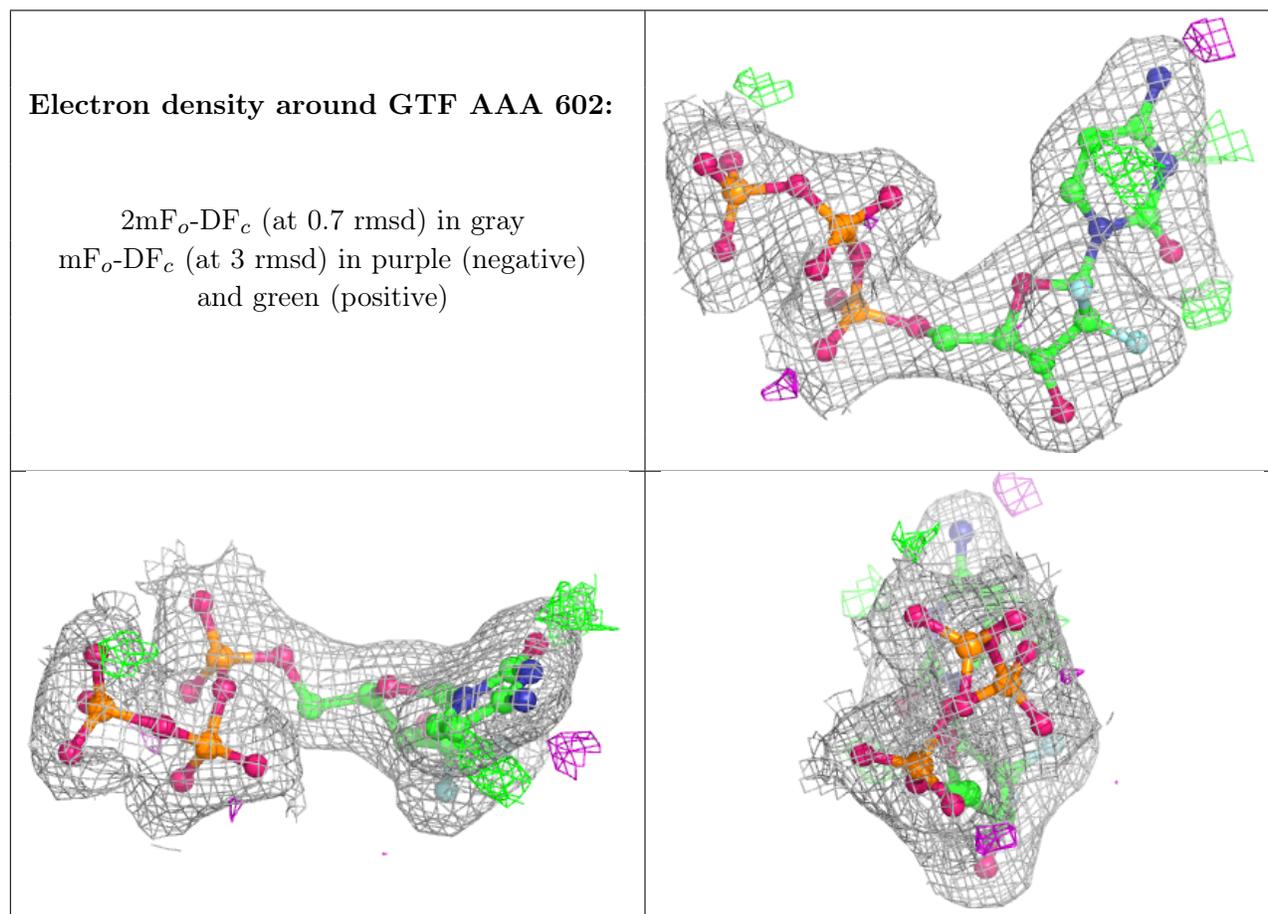
6.4 Ligands [i](#)

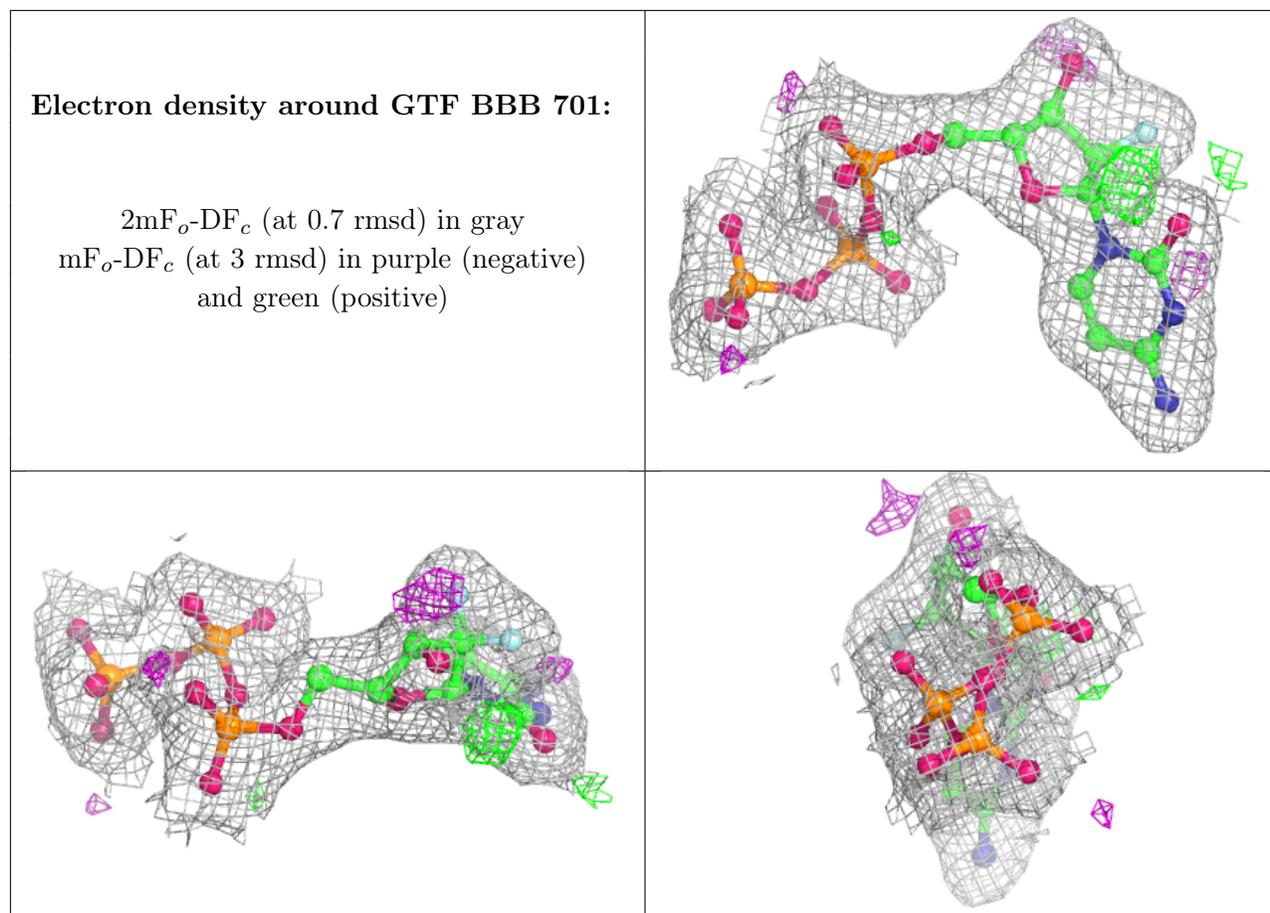
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MLA	AAA	601	7/7	0.87	0.23	51,55,59,64	0
2	MLA	BBB	703	7/7	0.93	0.16	51,53,57,61	0
4	NA	AAA	603	1/1	0.98	0.06	46,46,46,46	0
4	NA	BBB	702	1/1	0.98	0.05	41,41,41,41	0
3	GTF	AAA	602	30/30	0.99	0.15	24,25,30,30	0
3	GTF	BBB	701	30/30	0.99	0.14	22,25,29,31	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.