



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 5, 2023 – 11:08 PM EDT

PDB ID : 6UU1
Title : E. coli sigma-S transcription initiation complex with a 4-nt RNA and a CTP
("Fresh" crystal soaked with CTP, GTP, and ddTTP for 30 minutes)
Authors : Zuo, Y.; De, S.; Steitz, T.A.
Deposited on : 2019-10-30
Resolution : 4.10 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 ⓘ 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 : 2.35.1
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) : 2.35.1

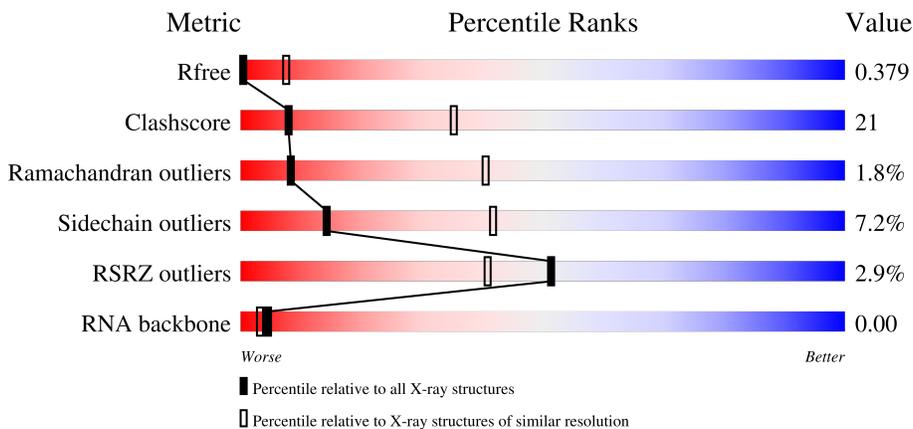
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 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	1193 (4.50-3.70)
Clashscore	141614	1003 (4.44-3.76)
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)
RSRZ outliers	127900	1034 (4.50-3.70)
RNA backbone	3102	1049 (5.04-3.00)

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 ≥ 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	242	
1	BBB	242	
2	CCC	1342	
3	DDD	1407	

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Mol	Chain	Length	Quality of chain
4	EEE	90	
5	FFF	336	
6	111	50	
7	222	50	
8	333	4	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CTP	333	201	-	-	X	-
9	ZN	DDD	1502	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 29064 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	230	1787	1112	317	352	6	0	0	0
1	BBB	228	1767	1100	312	349	6	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-6	ALA	-	expression tag	UNP A0A377D9Q8
AAA	-5	HIS	-	expression tag	UNP A0A377D9Q8
AAA	-4	HIS	-	expression tag	UNP A0A377D9Q8
AAA	-3	HIS	-	expression tag	UNP A0A377D9Q8
AAA	-2	HIS	-	expression tag	UNP A0A377D9Q8
AAA	-1	HIS	-	expression tag	UNP A0A377D9Q8
AAA	0	HIS	-	expression tag	UNP A0A377D9Q8
BBB	-6	ALA	-	expression tag	UNP A0A377D9Q8
BBB	-5	HIS	-	expression tag	UNP A0A377D9Q8
BBB	-4	HIS	-	expression tag	UNP A0A377D9Q8
BBB	-3	HIS	-	expression tag	UNP A0A377D9Q8
BBB	-2	HIS	-	expression tag	UNP A0A377D9Q8
BBB	-1	HIS	-	expression tag	UNP A0A377D9Q8
BBB	0	HIS	-	expression tag	UNP A0A377D9Q8

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	CCC	1341	10576	6636	1842	2055	43	0	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	DDD	1362	10568	6633	1887	1998	50	0	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	EEE	79	627	382	118	126	1	0	0	0

- Molecule 5 is a protein called RNA polymerase sigma factor RpoS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	FFF	277	2253	1411	415	423	4	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
FFF	2	GLY	SER	conflict	UNP P13445
FFF	33	GLU	GLN	conflict	UNP P13445
FFF	329	LEU	-	expression tag	UNP P13445
FFF	330	GLU	-	expression tag	UNP P13445
FFF	331	HIS	-	expression tag	UNP P13445
FFF	332	HIS	-	expression tag	UNP P13445
FFF	333	HIS	-	expression tag	UNP P13445
FFF	334	HIS	-	expression tag	UNP P13445
FFF	335	HIS	-	expression tag	UNP P13445
FFF	336	HIS	-	expression tag	UNP P13445

- Molecule 6 is a DNA chain called Synthetic DNA 50-MER (promoter non-template strand).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
6	111	30	619	294	114	181	30	0	0	0

- Molecule 7 is a DNA chain called Synthetic DNA 50-MER (promoter template strand).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
7	222	36	738	352	137	214	35	0	0	0

- Molecule 8 is a RNA chain called RNA 4-mer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
8	333	4	96	40	17	33	6	0	0	0

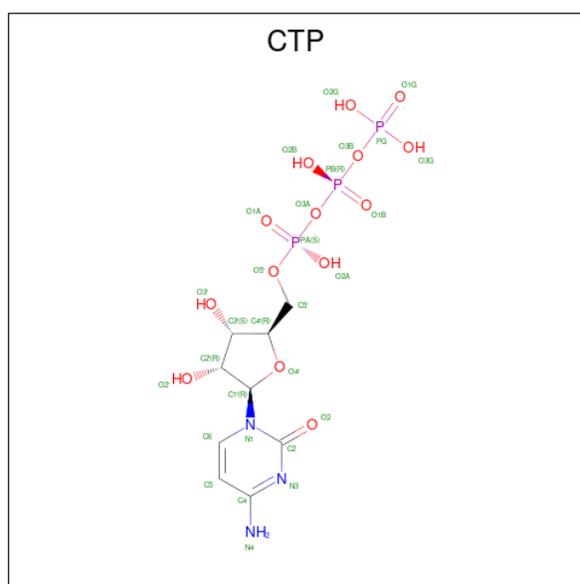
- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
9	DDD	2	2	2	0	0

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
10	DDD	2	2	2	0	0

- Molecule 11 is CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CTP) (formula: C₉H₁₆N₃O₁₄P₃).

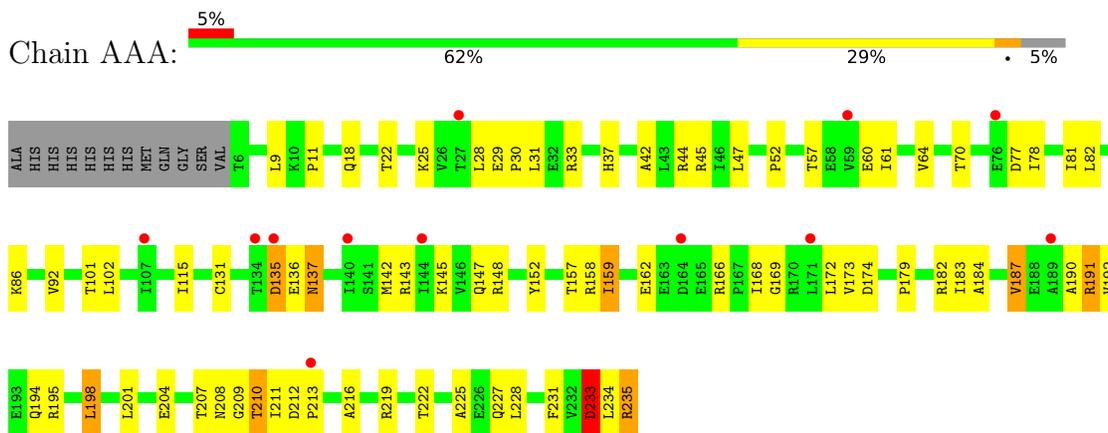


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
11	333	1	29	9	3	14	3	0	0

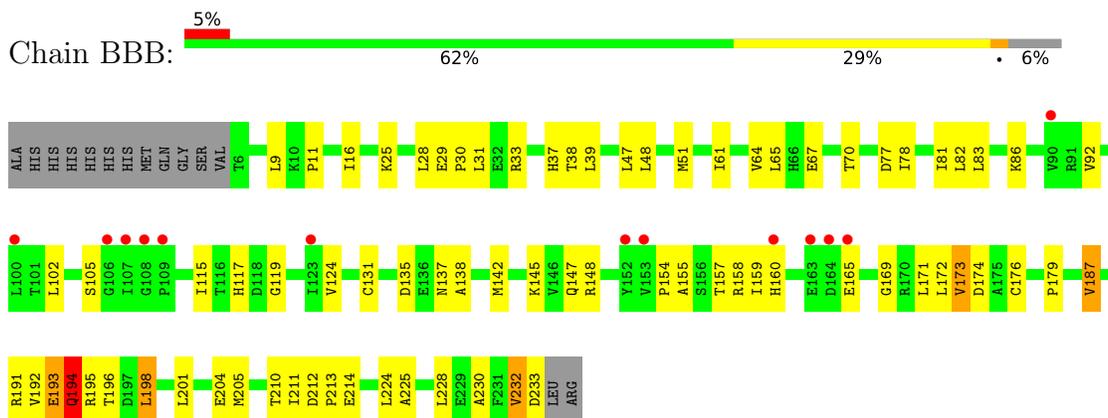
3 Residue-property plots

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.

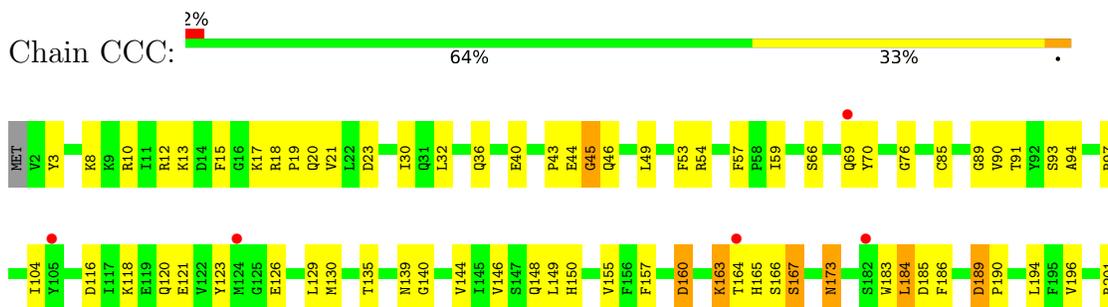
- Molecule 1: DNA-directed RNA polymerase subunit alpha

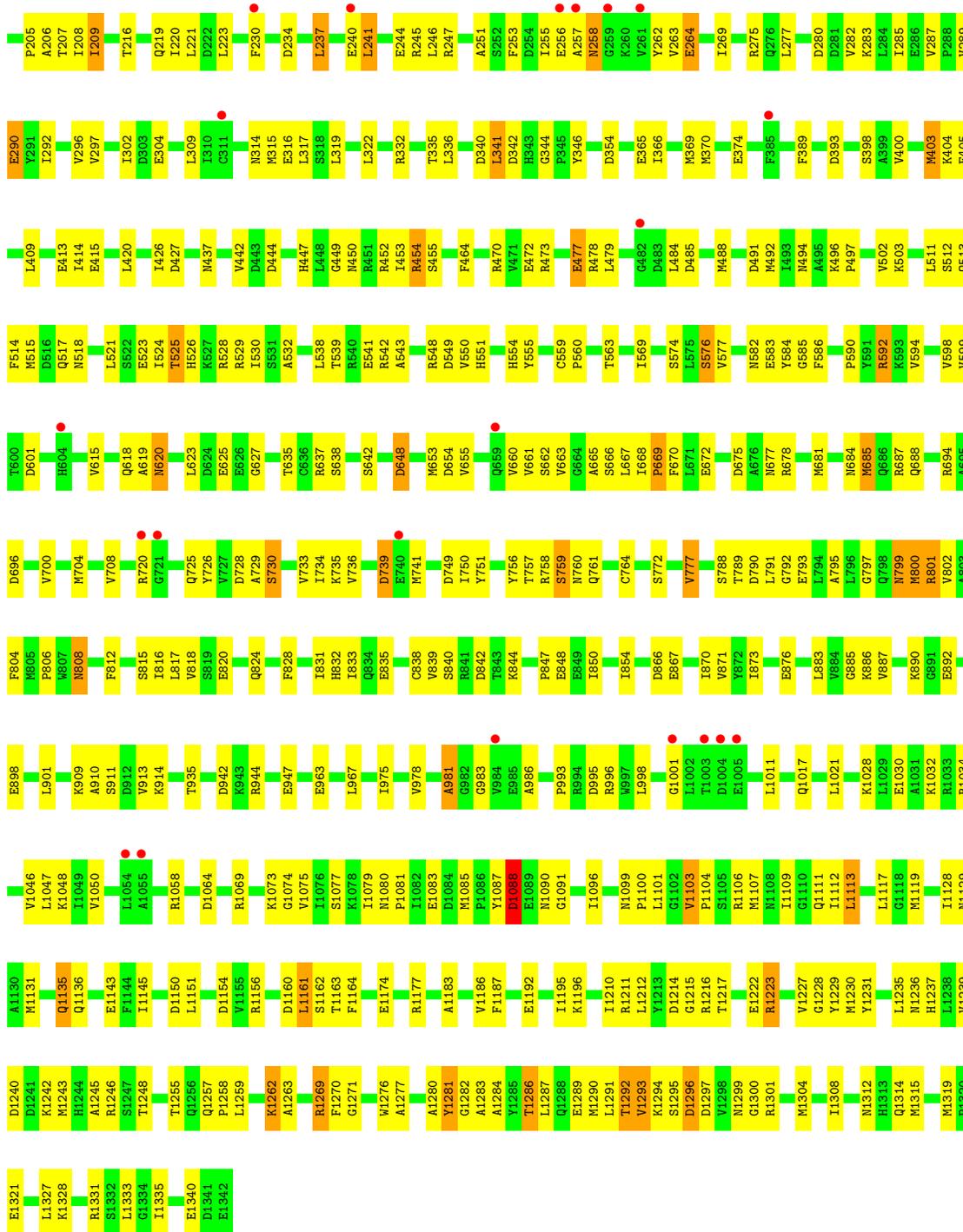


- Molecule 1: DNA-directed RNA polymerase subunit alpha

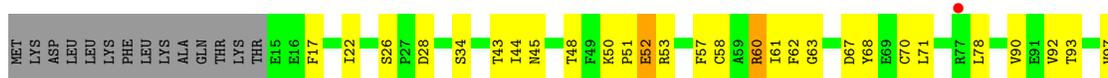


- Molecule 2: DNA-directed RNA polymerase subunit beta





• Molecule 3: DNA-directed RNA polymerase subunit beta'



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.85Å 154.25Å 230.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.18 – 4.10 49.18 – 4.10	Depositor EDS
% Data completeness (in resolution range)	98.0 (49.18-4.10) 98.2 (49.18-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 4.14Å)	Xtrriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.332 , 0.396 0.319 , 0.379	Depositor DCC
R_{free} test set	1774 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	187.4	Xtrriage
Anisotropy	0.501	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 211.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	29064	wwPDB-VP
Average B, all atoms (Å ²)	288.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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: 2DT, MG, CTP, GTP, ZN

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	0.63	0/1809	0.74	0/2450
1	BBB	0.64	0/1789	0.73	0/2425
2	CCC	0.62	0/10745	0.81	3/14499 (0.0%)
3	DDD	0.63	0/10729	0.80	5/14487 (0.0%)
4	EEE	0.62	0/629	0.80	0/847
5	FFF	0.65	0/2282	0.66	0/3076
6	111	0.29	0/693	0.61	0/1066
7	222	0.27	0/828	0.70	0/1277
8	333	0.19	0/50	0.56	0/76
All	All	0.62	0/29554	0.78	8/40203 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	CCC	0	1
3	DDD	0	2
All	All	0	3

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	DDD	636	GLY	C-N-CA	-7.74	102.34	121.70
3	DDD	636	GLY	N-CA-C	-7.16	95.20	113.10
3	DDD	636	GLY	CA-C-N	-6.29	103.37	117.20
2	CCC	1048	LYS	CB-CA-C	-5.97	98.46	110.40
3	DDD	637	ALA	CB-CA-C	5.75	118.72	110.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	CCC	1282	GLY	Peptide
3	DDD	636	GLY	Peptide,Mainchain

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	1787	0	1813	61	0
1	BBB	1767	0	1789	67	0
2	CCC	10576	0	10591	454	0
3	DDD	10568	0	10782	638	0
4	EEE	627	0	634	17	0
5	FFF	2253	0	2298	109	1
6	111	619	0	340	22	0
7	222	738	0	407	74	0
8	333	96	0	46	13	0
9	DDD	2	0	0	3	0
10	DDD	2	0	0	0	0
11	333	29	0	12	11	0
All	All	29064	0	28712	1238	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 21.

The worst 5 of 1238 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)
3:DDD:504:GLN:NE2	3:DDD:731:ARG:HH21	1.12	1.39
3:DDD:750:PRO:HA	3:DDD:781:LYS:CG	1.57	1.35
7:222:21:DG:H4'	7:222:22:DA:C5'	1.54	1.34
3:DDD:750:PRO:CA	3:DDD:781:LYS:HG2	1.61	1.28
7:222:21:DG:C4'	7:222:22:DA:H5'	1.68	1.24

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FFF:67:TYR:O	5:FFF:299:ARG:NH2[3_644]	1.95	0.25

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	228/242 (94%)	210 (92%)	12 (5%)	6 (3%)	5	34
1	BBB	226/242 (93%)	207 (92%)	14 (6%)	5 (2%)	6	37
2	CCC	1339/1342 (100%)	1241 (93%)	72 (5%)	26 (2%)	8	39
3	DDD	1360/1407 (97%)	1246 (92%)	92 (7%)	22 (2%)	9	43
4	EEE	77/90 (86%)	73 (95%)	4 (5%)	0	100	100
5	FFF	275/336 (82%)	254 (92%)	16 (6%)	5 (2%)	8	40
All	All	3505/3659 (96%)	3231 (92%)	210 (6%)	64 (2%)	8	40

5 of 64 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	117	HIS
1	BBB	119	GLY
1	BBB	193	GLU
1	BBB	194	GLN
2	CCC	46	GLN

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	198/208 (95%)	180 (91%)	18 (9%)	9	33
1	BBB	196/208 (94%)	182 (93%)	14 (7%)	14	42
2	CCC	1156/1157 (100%)	1065 (92%)	91 (8%)	12	39
3	DDD	1135/1168 (97%)	1059 (93%)	76 (7%)	16	44
4	EEE	67/74 (90%)	64 (96%)	3 (4%)	27	54
5	FFF	240/292 (82%)	226 (94%)	14 (6%)	20	48
All	All	2992/3107 (96%)	2776 (93%)	216 (7%)	14	42

5 of 216 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	CCC	1262	LYS
3	DDD	515	ARG
4	EEE	8	ASP
2	CCC	1293	VAL
3	DDD	176	PHE

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

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	333	1/4 (25%)	1 (100%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	333	16	G

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

1 non-standard protein/DNA/RNA residue is 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
8	2DT	333	101	7	17,20,21	1.51	4 (23%)	22,28,31	2.70	8 (36%)

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
8	2DT	333	101	7	-	1/7/18/19	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	333	101	2DT	C2-N1	2.76	1.42	1.38
8	333	101	2DT	C6-C5	2.70	1.39	1.34
8	333	101	2DT	C4-C5	2.28	1.48	1.44
8	333	101	2DT	C4-N3	-2.14	1.34	1.38

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	333	101	2DT	C4-N3-C2	-5.22	120.59	127.35
8	333	101	2DT	C5-C4-N3	4.80	119.41	115.31
8	333	101	2DT	O4-C4-C5	-4.80	119.34	124.90
8	333	101	2DT	C3'-C2'-C1'	4.73	108.24	102.78
8	333	101	2DT	N3-C2-N1	4.50	120.86	114.89

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	333	101	2DT	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	333	101	2DT	6	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	$\# Z > 2$
11	CTP	333	201	10	26,30,30	0.54	0	39,47,47	0.52	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CTP	333	201	10	-	5/22/38/38	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	333	201	CTP	PB-O3A-PA-O1A
11	333	201	CTP	PB-O3B-PG-O1G
11	333	201	CTP	PB-O3B-PG-O2G

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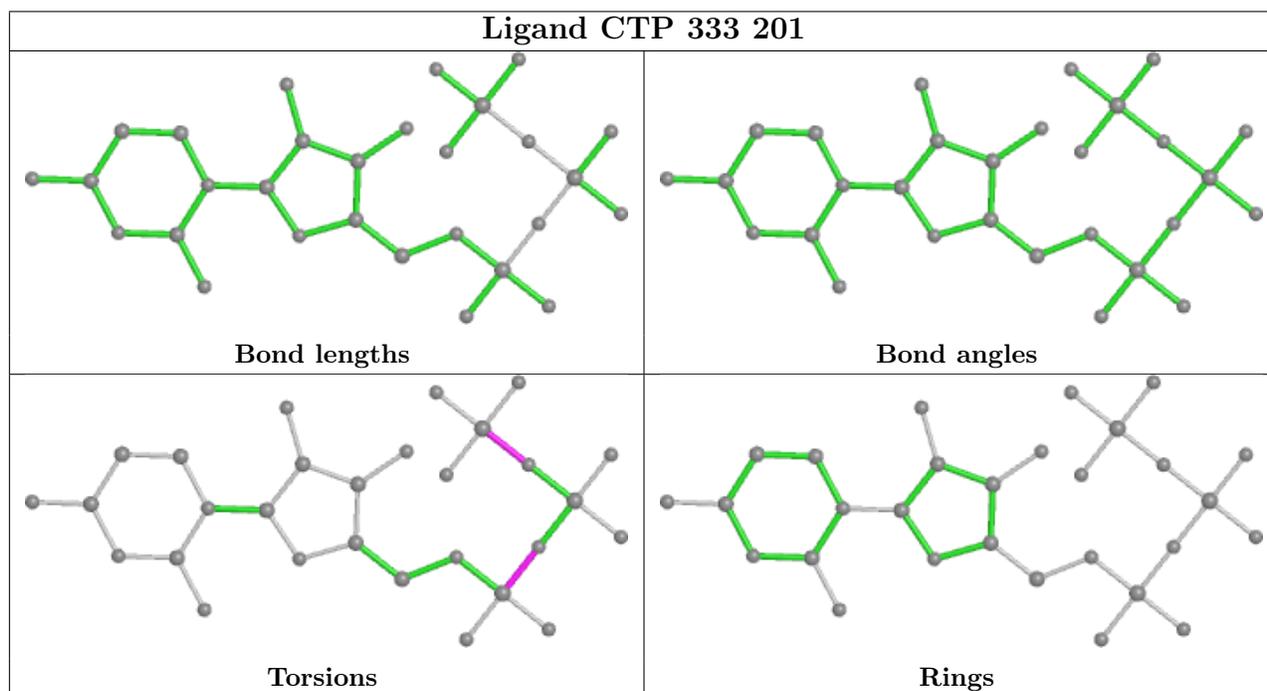
Mol	Chain	Res	Type	Atoms
11	333	201	CTP	PB-O3B-PG-O3G
11	333	201	CTP	PB-O3A-PA-O2A

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	333	201	CTP	11	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	333	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	333	16:G	O3'	101:2DT	P	1.78

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	AAA	230/242 (95%)	0.12	12 (5%) 27 23	232, 309, 389, 488	0
1	BBB	228/242 (94%)	0.02	13 (5%) 23 20	215, 331, 426, 456	0
2	CCC	1341/1342 (99%)	-0.11	26 (1%) 66 58	149, 259, 404, 485	0
3	DDD	1362/1407 (96%)	-0.17	27 (1%) 65 56	142, 269, 383, 504	0
4	EEE	79/90 (87%)	-0.29	1 (1%) 77 68	249, 322, 473, 567	0
5	FFF	277/336 (82%)	0.15	19 (6%) 16 13	215, 334, 439, 467	0
6	111	30/50 (60%)	-0.16	3 (10%) 7 7	272, 329, 405, 531	0
7	222	36/50 (72%)	0.40	4 (11%) 5 6	230, 334, 489, 507	0
8	333	2/4 (50%)	0.92	0 100 100	231, 231, 231, 302	0
All	All	3585/3763 (95%)	-0.09	105 (2%) 51 41	142, 281, 411, 567	0

The worst 5 of 105 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	DDD	853	THR	5.5
7	222	36	DG	5.3
3	DDD	1272	SER	4.9
1	AAA	144	ILE	4.7
1	BBB	108	GLY	4.5

6.2 Non-standard residues in protein, DNA, RNA chains [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(\AA^2)	Q<0.9
8	2DT	333	101	19/20	0.89	0.27	223,258,283,290	0

6.3 Carbohydrates [i](#)

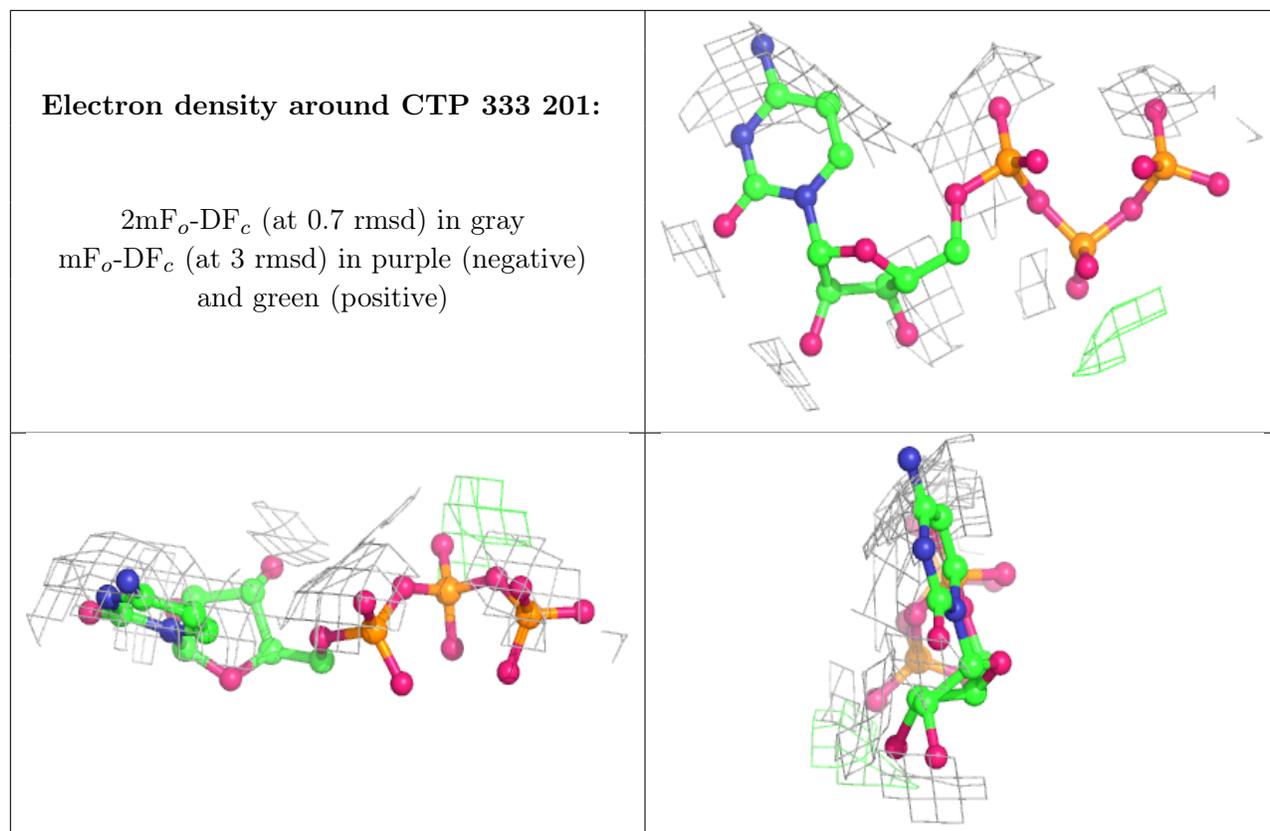
There are no monosaccharides in this entry.

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(\AA^2)	Q<0.9
9	ZN	DDD	1502	1/1	0.94	0.17	293,293,293,293	0
11	CTP	333	201	29/29	0.94	0.29	172,203,288,301	0
9	ZN	DDD	1501	1/1	0.96	0.19	421,421,421,421	0
10	MG	DDD	1504	1/1	0.97	0.20	205,205,205,205	0
10	MG	DDD	1503	1/1	0.99	0.30	133,133,133,133	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.