



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 4, 2021 – 12:11 PM JST

PDB ID : 7EH1
Title : Thermus thermophilus transcription initiation complex containing a template-strand purine at position TSS-2, GpG RNA primer, and CMPcPP
Authors : Li, L.; Zhang, Y.
Deposited on : 2021-03-27
Resolution : 2.90 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 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	:	2.22
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)	:	2.22

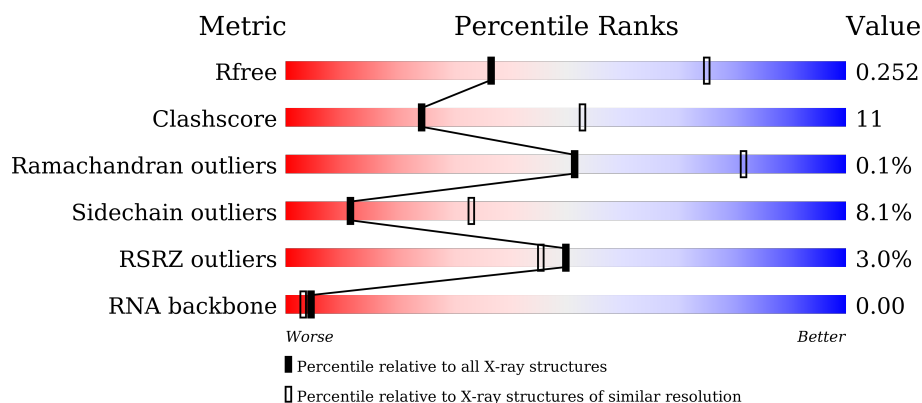
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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	A	315	<div> <div>2%</div> <div>50% 21% • 27%</div> </div>
1	B	315	<div> <div>%</div> <div>48% 23% • 28%</div> </div>
2	C	1119	<div> <div>2%</div> <div>68% 29% ••</div> </div>
3	D	1524	<div> <div>4%</div> <div>68% 27% ••</div> </div>

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Mol	Chain	Length	Quality of chain
4	E	99	<div><div></div><div>68%23%5%</div></div>
5	F	443	<div><div>%</div><div>56%21%22%</div></div>
6	G	27	<div><div></div><div>44%44%7%</div></div>
7	H	19	<div><div>5%</div><div>58%26%5%11%</div></div>
8	I	2	<div><div></div><div>100%</div></div>

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 28630 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
1	A	231	Total	C	N	O	S	0	0	0
			1803	1152	312	337	2			
1	B	227	Total	C	N	O	S	0	0	0
			1758	1124	301	331	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1112	Total	C	N	O	S	0	0	0
			8750	5538	1553	1635	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1486	Total	C	N	O	S	0	1	0
			11714	7428	2061	2190	35			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			759	484	132	139	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total	C	N	O	S	0	0	0
			2803	1767	508	524	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	expression tag	UNP Q5SKW1
F	-18	GLY	-	expression tag	UNP Q5SKW1
F	-17	SER	-	expression tag	UNP Q5SKW1
F	-16	SER	-	expression tag	UNP Q5SKW1
F	-15	HIS	-	expression tag	UNP Q5SKW1
F	-14	HIS	-	expression tag	UNP Q5SKW1
F	-13	HIS	-	expression tag	UNP Q5SKW1
F	-12	HIS	-	expression tag	UNP Q5SKW1
F	-11	HIS	-	expression tag	UNP Q5SKW1
F	-10	HIS	-	expression tag	UNP Q5SKW1
F	-9	SER	-	expression tag	UNP Q5SKW1
F	-8	SER	-	expression tag	UNP Q5SKW1
F	-7	GLY	-	expression tag	UNP Q5SKW1
F	-6	LEU	-	expression tag	UNP Q5SKW1
F	-5	VAL	-	expression tag	UNP Q5SKW1
F	-4	PRO	-	expression tag	UNP Q5SKW1
F	-3	ARG	-	expression tag	UNP Q5SKW1
F	-2	GLY	-	expression tag	UNP Q5SKW1
F	-1	SER	-	expression tag	UNP Q5SKW1
F	0	HIS	-	expression tag	UNP Q5SKW1

- Molecule 6 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	25	Total	C	N	O	P	0	0	0
			516	246	99	147	24			

- Molecule 7 is a DNA chain called DNA (5'-D(*CP*C*TP*GP*CP*AP*TP*CP*CP*GP*T
P*GP*AP*GP*CP*CP*AP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	17	Total	C	N	O	P	0	0	0
			346	165	66	99	16			

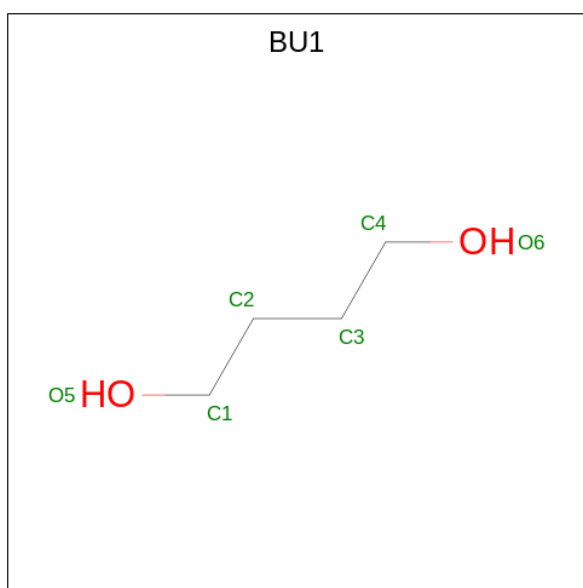
- Molecule 8 is a RNA chain called RNA (5'-R(*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	2	Total	C	N	O	P	0	0	0
			43	20	10	12	1			

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	2	Total	Mg	0	0
			2	2		
9	C	1	Total	Mg	0	0
			1	1		
9	D	1	Total	Mg	0	0
			1	1		
9	F	1	Total	Mg	0	0
			1	1		

- Molecule 10 is 1,4-BUTANEDIOL (three-letter code: BU1) (formula: $C_4H_{10}O_2$).

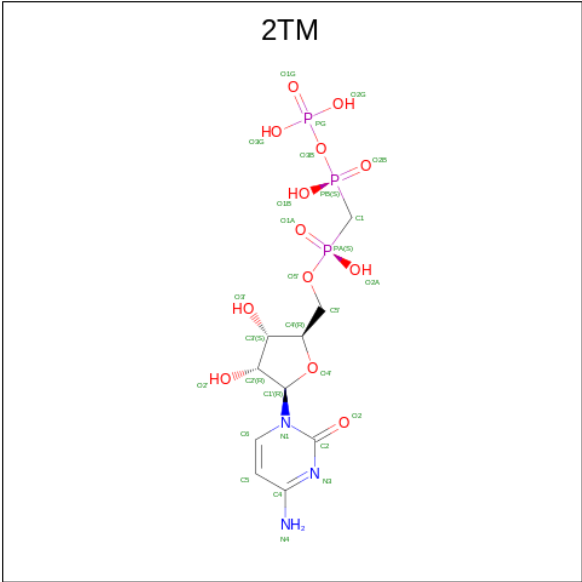


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			6	4	2		
10	D	1	Total	C	O	0	0
			6	4	2		

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	2	Total	Zn	0	0
			2	2		

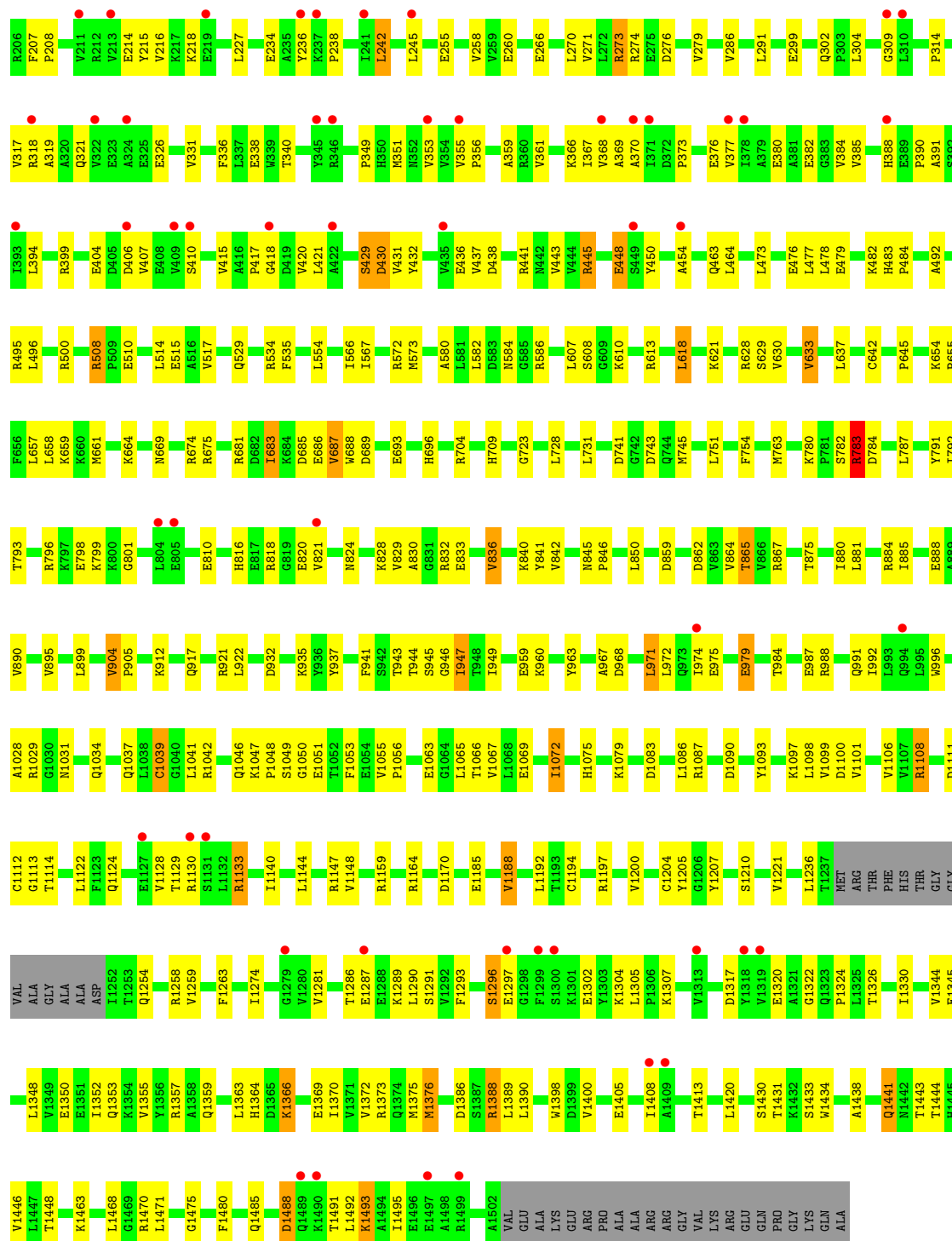
- Molecule 12 is 5'-O-[(S)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]methyl}phosphoryl]cytidine (three-letter code: 2TM) (formula: $C_{10}H_{18}N_3O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	I	1	Total	C	N	O	P	0	0
			29	10	3	13	3		

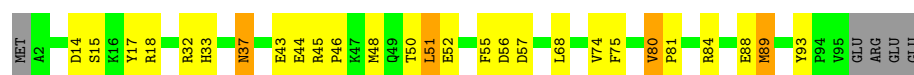
- Molecule 13 is water.

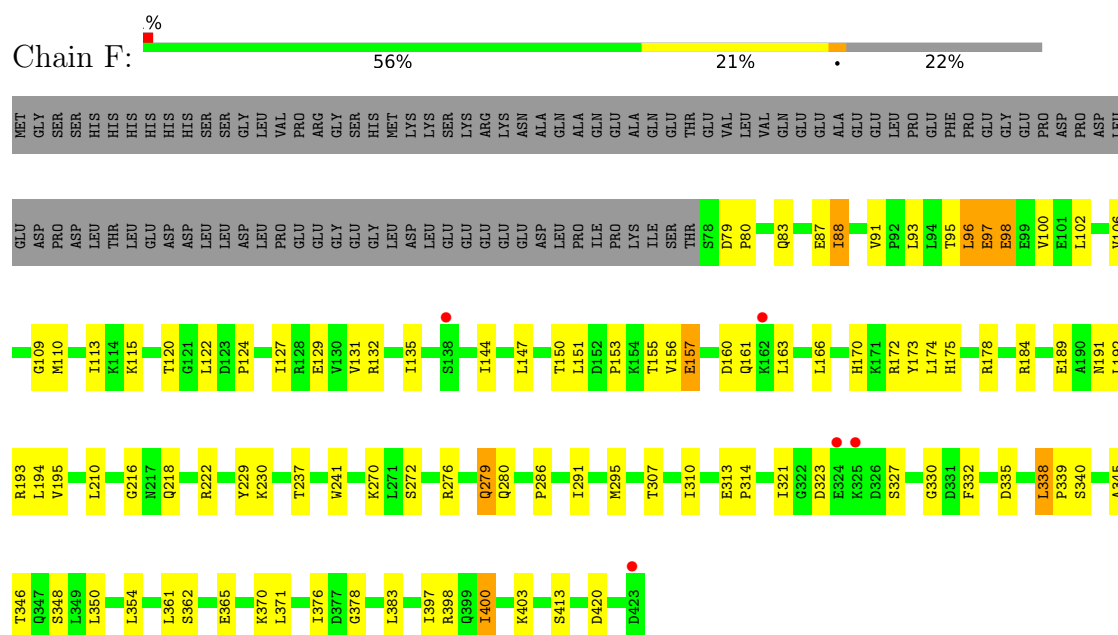
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	4	Total	O	0	0
			4	4		
13	B	4	Total	O	0	0
			4	4		
13	C	28	Total	O	0	0
			28	28		
13	D	42	Total	O	0	0
			42	42		
13	E	3	Total	O	0	0
			3	3		
13	F	5	Total	O	0	0
			5	5		
13	H	1	Total	O	0	0
			1	1		
13	I	3	Total	O	0	0
			3	3		



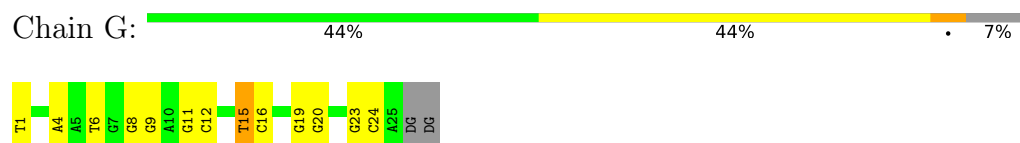
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:

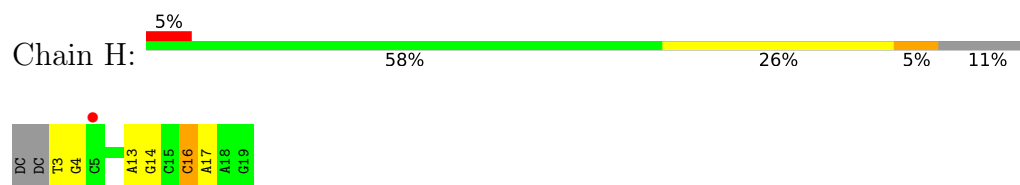




- Molecule 6: DNA (27-MER)



- Molecule 7: DNA (5'-D(*CP*C*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*CP*CP*AP*AP*G)-3')



- Molecule 8: RNA (5'-R(*GP*G)-3')



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	184.12Å 103.32Å 295.65Å 90.00° 98.96° 90.00°	Depositor
Resolution (Å)	25.27 – 2.90 48.88 – 2.90	Depositor EDS
% Data completeness (in resolution range)	82.1 (25.27-2.90) 82.1 (48.88-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.191 , 0.253 0.191 , 0.252	Depositor DCC
R_{free} test set	1971 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	49.9	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.019 for $1/2^*h-3/2^*k,-1/2^*h-1/2^*k,-1/2^*h+1/2^*k-l$ 0.024 for $1/2^*h+3/2^*k,1/2^*h-1/2^*k,-1/2^*h-1/2^*k-l$	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	28630	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 3.16% 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: BU1, ZN, 2TM, MG

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	0.45	0/1835	0.64	0/2497
1	B	0.43	0/1790	0.62	0/2440
2	C	0.48	0/8917	0.63	0/12064
3	D	0.49	1/11923 (0.0%)	0.66	3/16126 (0.0%)
4	E	0.48	0/773	0.65	0/1042
5	F	0.43	0/2848	0.55	0/3833
6	G	1.03	0/580	1.03	1/895 (0.1%)
7	H	0.94	0/388	0.99	2/597 (0.3%)
8	I	0.79	0/48	1.26	0/74
All	All	0.50	1/29102 (0.0%)	0.65	6/39568 (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
3	D	0	3
5	F	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1039	CYS	CB-SG	-5.85	1.72	1.81

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	16	DC	O4'-C4'-C3'	-7.19	101.62	104.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	783	ARG	NE-CZ-NH1	-6.26	117.17	120.30
3	D	1108	ARG	NE-CZ-NH1	6.08	123.34	120.30
3	D	1108	ARG	NE-CZ-NH2	-5.91	117.35	120.30
7	H	13	DA	O4'-C4'-C3'	-5.70	102.22	104.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	1207	TYR	Peptide
3	D	782	SER	Peptide
3	D	829	VAL	Peptide
5	F	330	GLY	Peptide

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	A	1803	0	1852	47	0
1	B	1758	0	1778	50	0
2	C	8750	0	8833	229	0
3	D	11714	0	11926	275	0
4	E	759	0	771	18	0
5	F	2803	0	2871	67	0
6	G	516	0	283	14	0
7	H	346	0	192	3	0
8	I	43	0	23	0	0
9	B	2	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
9	F	1	0	0	0	0
10	B	6	0	10	3	0
10	D	6	0	10	1	0
11	D	2	0	0	0	0
12	I	29	0	14	0	0
13	A	4	0	0	0	0
13	B	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	C	28	0	0	3	0
13	D	42	0	0	2	0
13	E	3	0	0	0	0
13	F	5	0	0	1	0
13	H	1	0	0	0	0
13	I	3	0	0	0	0
All	All	28630	0	28563	628	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 11.

The worst 5 of 628 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)
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.46	0.97
2:C:805:ARG:HH21	2:C:807:ARG:HD3	1.26	0.97
2:C:628:PHE:H	2:C:638:ASP:HB2	1.32	0.93
1:B:176:ARG:NH1	3:D:888:GLU:OE2	2.04	0.88
2:C:715:THR:HG22	2:C:717:LEU:H	1.35	0.88

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	A	229/315 (73%)	211 (92%)	18 (8%)	0	100	100
1	B	225/315 (71%)	212 (94%)	13 (6%)	0	100	100
2	C	1108/1119 (99%)	1034 (93%)	74 (7%)	0	100	100
3	D	1483/1524 (97%)	1389 (94%)	92 (6%)	2 (0%)	51	82
4	E	92/99 (93%)	86 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	F	344/443 (78%)	335 (97%)	9 (3%)	0	100	100
All	All	3481/3815 (91%)	3267 (94%)	212 (6%)	2 (0%)	51	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	830	ALA
3	D	783	ARG

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	A	199/273 (73%)	182 (92%)	17 (8%)	10	31
1	B	193/273 (71%)	177 (92%)	16 (8%)	11	32
2	C	932/941 (99%)	851 (91%)	81 (9%)	10	30
3	D	1247/1279 (98%)	1151 (92%)	96 (8%)	13	35
4	E	82/88 (93%)	73 (89%)	9 (11%)	6	19
5	F	300/388 (77%)	280 (93%)	20 (7%)	16	43
All	All	2953/3242 (91%)	2714 (92%)	239 (8%)	11	33

5 of 239 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	40	GLU
5	F	97	GLU
3	D	443	VAL
5	F	88	ILE
5	F	371	LEU

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

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	1/2 (50%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 7 are monoatomic - leaving 3 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	$\# Z > 2$
10	BU1	B	2002	-	5,5,5	0.43	0	4,4,4	0.30	0
12	2TM	I	2101	-	24,30,30	5.54	14 (58%)	30,47,47	1.66	6 (20%)
10	BU1	D	2004	-	5,5,5	0.38	0	4,4,4	0.17	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
10	BU1	B	2002	-	-	1/3/3/3	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	2TM	I	2101	-	-	6/17/38/38	0/2/2/2
10	BU1	D	2004	-	-	1/3/3/3	-

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	I	2101	2TM	PB-O3B	15.00	1.75	1.58
12	I	2101	2TM	O4'-C1'	11.11	1.56	1.41
12	I	2101	2TM	C2'-C3'	-7.91	1.31	1.53
12	I	2101	2TM	C6-N1	7.49	1.45	1.35
12	I	2101	2TM	O4'-C4'	-7.42	1.28	1.45

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	I	2101	2TM	C2-N3-C4	4.36	120.76	116.34
12	I	2101	2TM	PG-O3B-PB	-3.16	121.50	132.62
12	I	2101	2TM	O4'-C1'-C2'	-2.94	102.63	106.93
12	I	2101	2TM	N4-C4-N3	2.57	120.55	116.49
12	I	2101	2TM	C2'-C3'-C4'	2.11	106.75	102.64

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	I	2101	2TM	C5'-O5'-PA-O2A
12	I	2101	2TM	C2'-C1'-N1-C6
12	I	2101	2TM	PA-C1-PB-O3B
12	I	2101	2TM	PA-C1-PB-O1B
12	I	2101	2TM	PA-C1-PB-O2B

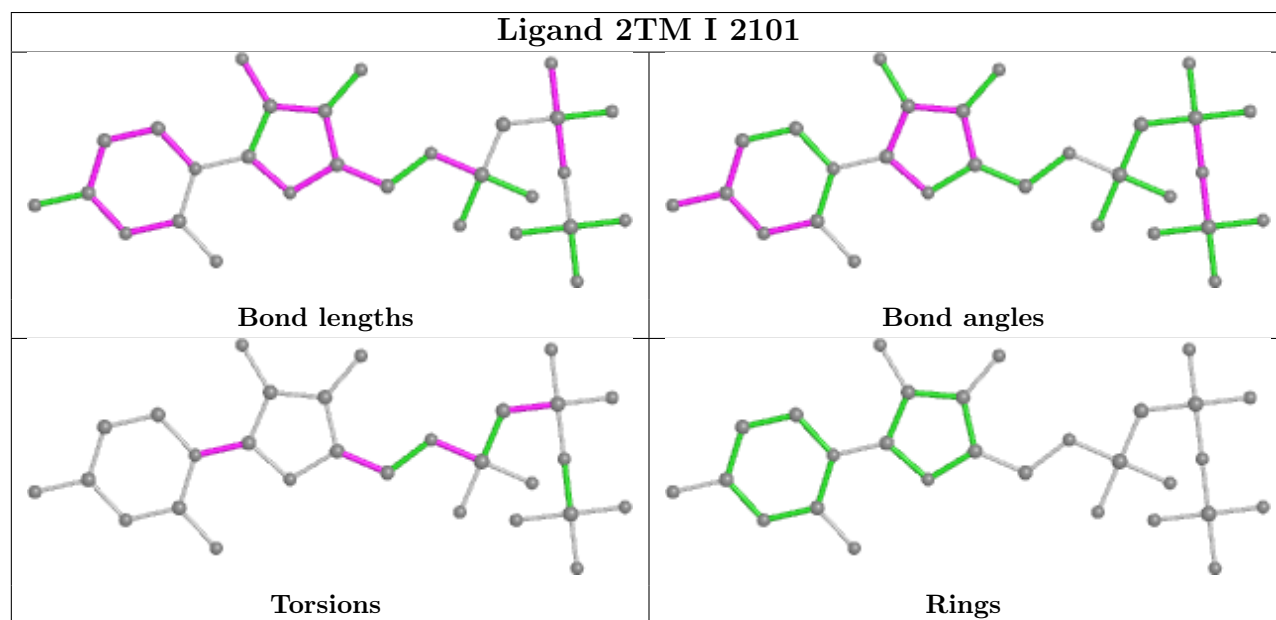
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	2002	BU1	3	0
10	D	2004	BU1	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 [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	231/315 (73%)	-0.25	5 (2%) 62 59	23, 43, 65, 96	0
1	B	227/315 (72%)	-0.17	4 (1%) 68 67	27, 53, 82, 118	0
2	C	1112/1119 (99%)	-0.24	23 (2%) 63 61	12, 37, 87, 121	0
3	D	1486/1524 (97%)	-0.05	67 (4%) 33 29	8, 41, 97, 125	0
4	E	94/99 (94%)	-0.36	0 100 100	20, 40, 71, 82	0
5	F	346/443 (78%)	-0.08	5 (1%) 75 75	24, 56, 94, 114	0
6	G	25/27 (92%)	-0.01	0 100 100	57, 74, 136, 146	0
7	H	17/19 (89%)	0.14	1 (5%) 22 18	31, 60, 140, 144	0
8	I	2/2 (100%)	-0.14	0 100 100	27, 27, 27, 28	2 (100%)
All	All	3540/3863 (91%)	-0.14	105 (2%) 50 45	8, 43, 94, 146	2 (0%)

The worst 5 of 105 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	ASP	5.0
2	C	365	ASP	4.9
1	B	2	LEU	4.5
3	D	422	ALA	4.1
2	C	107	LEU	4.1

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](#)

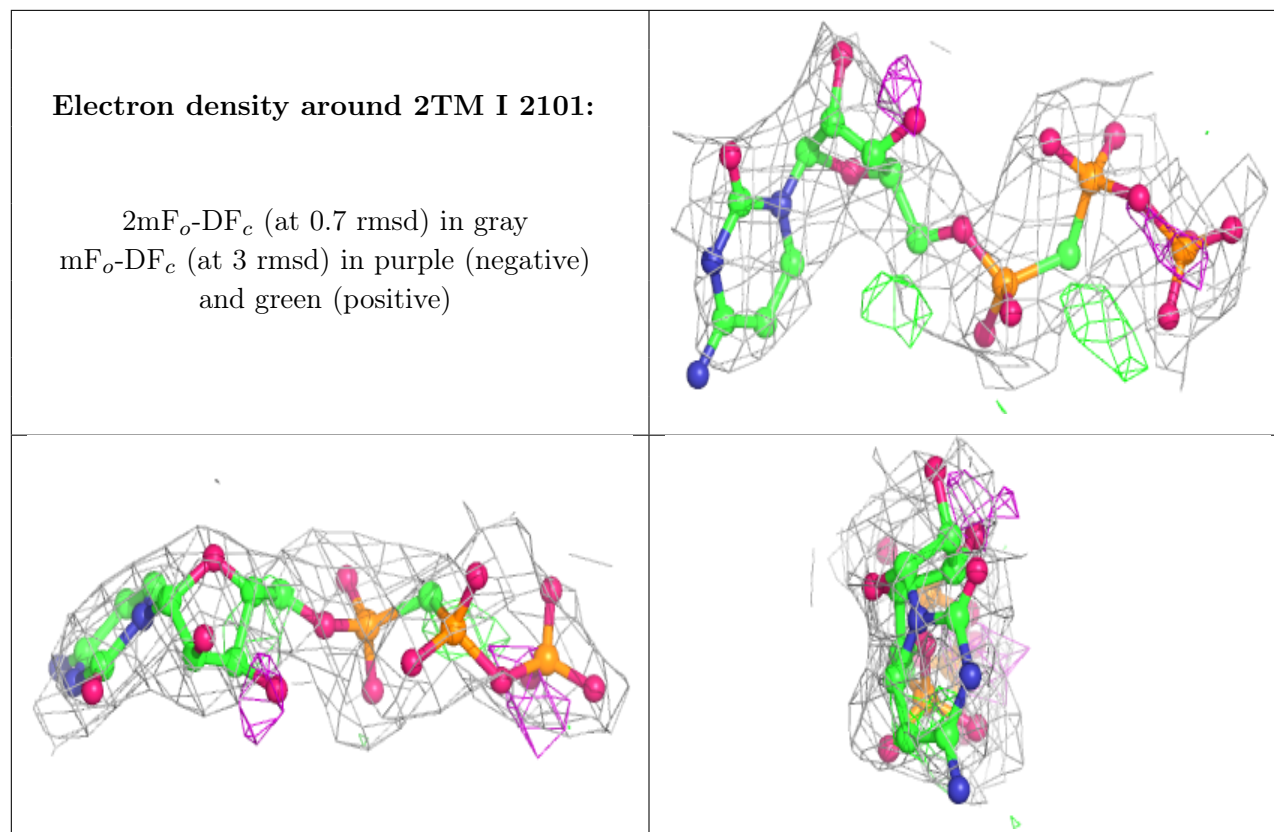
There are no monosaccharides in this entry.

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
9	MG	B	2001	1/1	0.87	0.11	57,57,57,57	0
12	2TM	I	2101	29/29	0.87	0.24	21,38,72,76	29
10	BU1	B	2002	6/6	0.88	0.29	34,40,48,49	0
10	BU1	D	2004	6/6	0.91	0.33	27,30,37,39	0
9	MG	B	2003	1/1	0.92	0.23	41,41,41,41	0
9	MG	C	2001	1/1	0.94	0.27	20,20,20,20	0
9	MG	F	2001	1/1	0.98	0.10	28,28,28,28	0
11	ZN	D	2001	1/1	0.99	0.11	24,24,24,24	0
11	ZN	D	2002	1/1	0.99	0.08	61,61,61,61	0
9	MG	D	2003	1/1	0.99	0.22	8,8,8,8	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.