



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2023 – 10:28 PM EDT

PDB ID : 6WOX
Title : Thermus thermophilus RNA polymerase initially transcribing complex with 2'dCTP
Authors : Shin, Y.; Murakami, K.S.
Deposited on : 2020-04-26
Resolution : 3.14 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

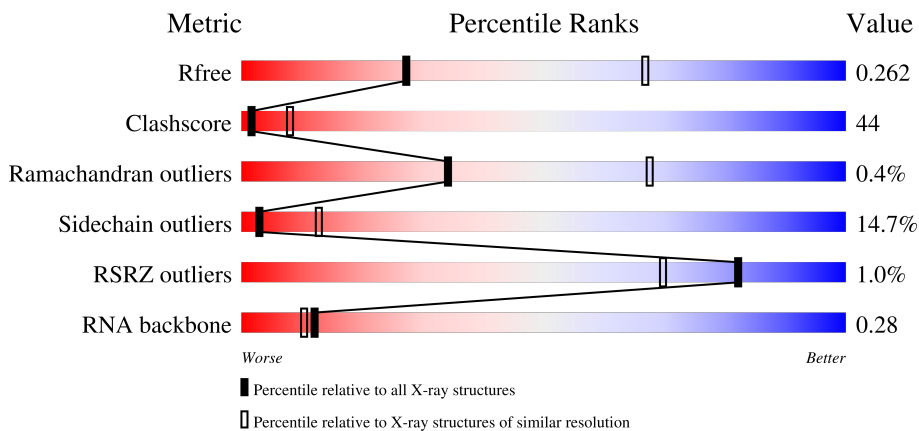
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.14 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	1626 (3.18-3.10)
Clashscore	141614	1735 (3.18-3.10)
Ramachandran outliers	138981	1677 (3.18-3.10)
Sidechain outliers	138945	1677 (3.18-3.10)
RSRZ outliers	127900	1588 (3.18-3.10)
RNA backbone	3102	1000 (3.46-2.82)

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	
1	B	315	
2	C	1119	
3	D	1505	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	E	99	<p>%</p> <p>33% 56% 6% 5%</p>
5	F	423	<p>4%</p> <p>24% 46% 11% 18%</p>
6	G	22	<p>14% 59% 5% 23%</p>
7	H	27	<p>4%</p> <p>15% 74% 7%</p>
8	I	3	<p>100%</p>

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 28581 atoms, of which 12 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	A	226	Total	C	N	O	S	0	0	0
			1782	1138	310	332	2			
1	B	224	Total	C	N	O	S	0	0	0
			1767	1129	307	329	2			

- 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	C	1111	Total	C	N	O	S	0	0	0
			8770	5548	1564	1634	24			

- 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	D	1485	Total	C	N	O	S	0	0	0
			11721	7431	2063	2192	35			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	86	LYS	ARG	conflict	UNP Q8RQE8

- 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	E	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	346	2807	1770	509	524	4	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	46	THR	ALA	conflict	UNP Q72L95

- Molecule 6 is a DNA chain called DNA (5'-D(P*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*GP*CP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
6	G	17	351	166	65	103	17	0	0	0

- Molecule 7 is a DNA chain called DNA (25-MER).

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

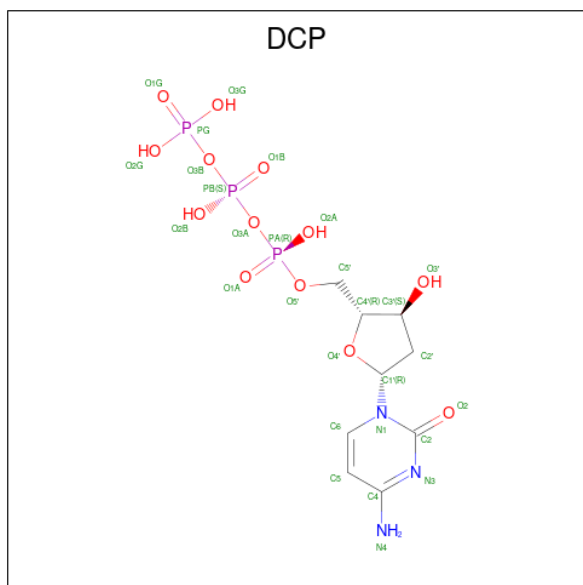
- Molecule 8 is a RNA chain called RNA (5'-R(*GP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
8	I	3	62	29	13	18	2	0	0	0

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	1	Total	Na	0	0
			1	1		

- Molecule 10 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (three-letter code: DCP) (formula: C₉H₁₆N₃O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
10	D	1	Total	C	H	N	O	P	0	0
			40	9	12	3	13	3		

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	1	Total	Mg	0	0
			1	1		

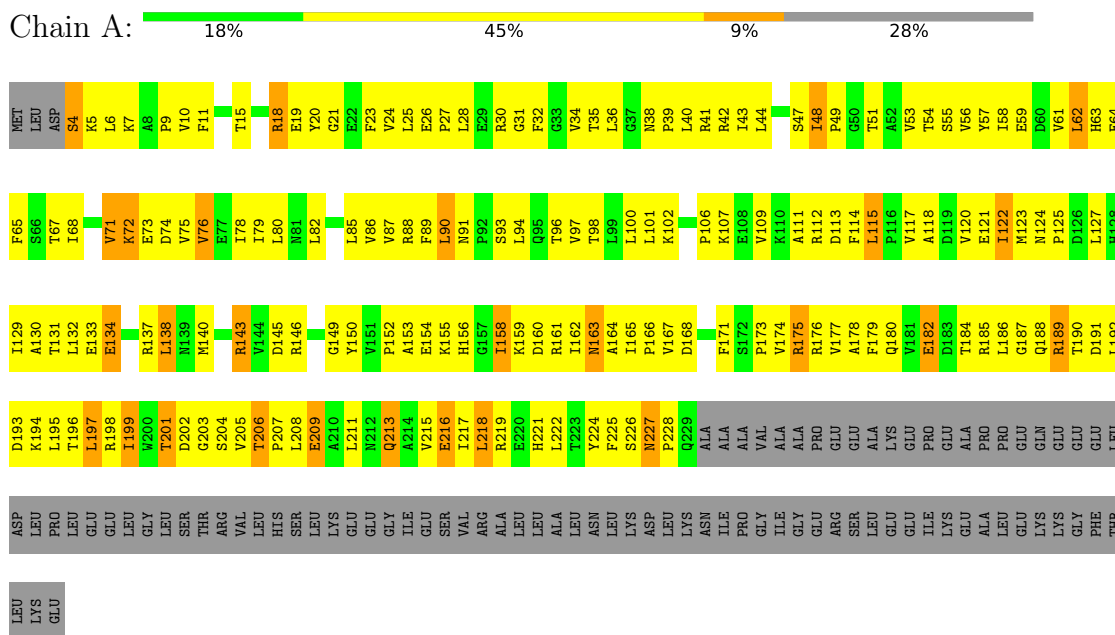
- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

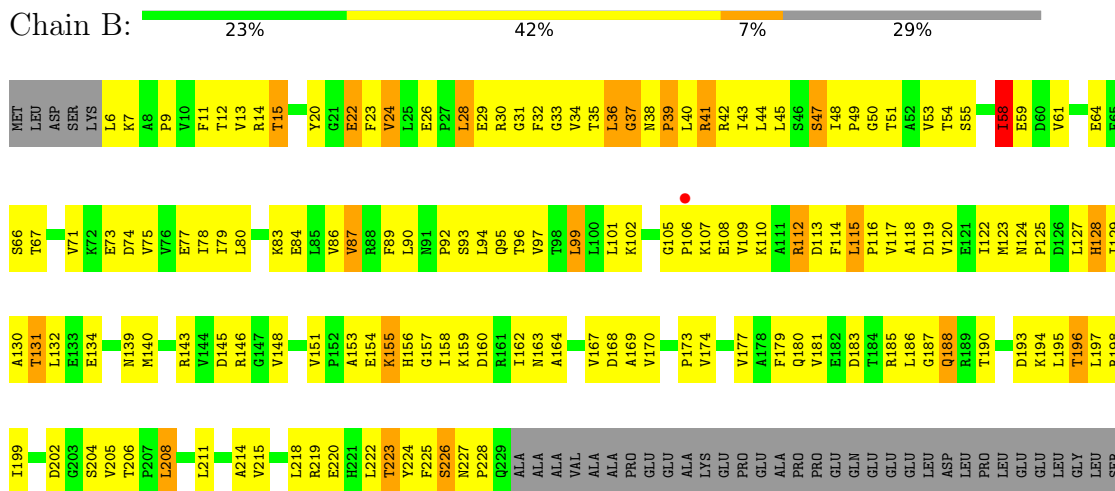
3 Residue-property plots

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

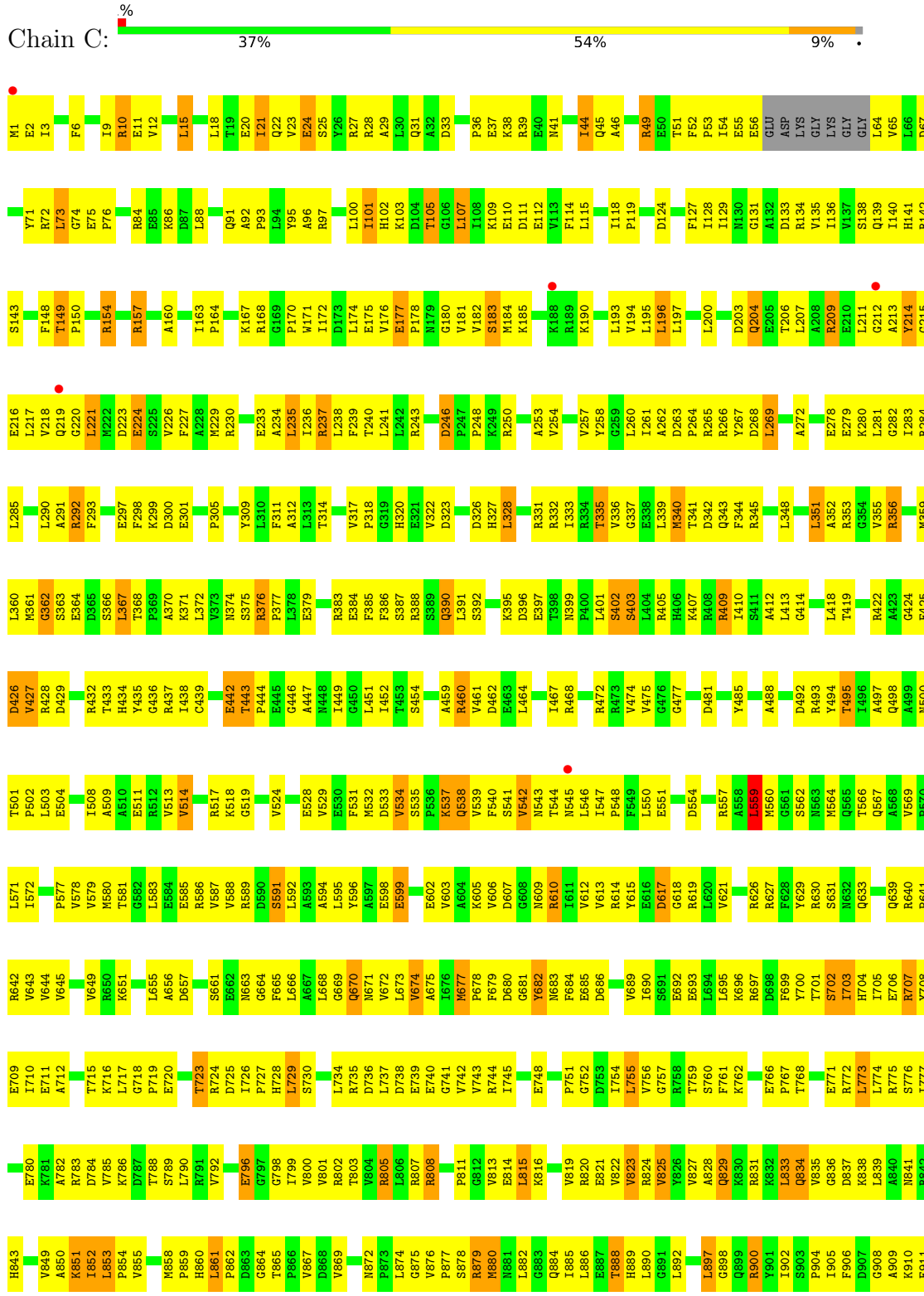


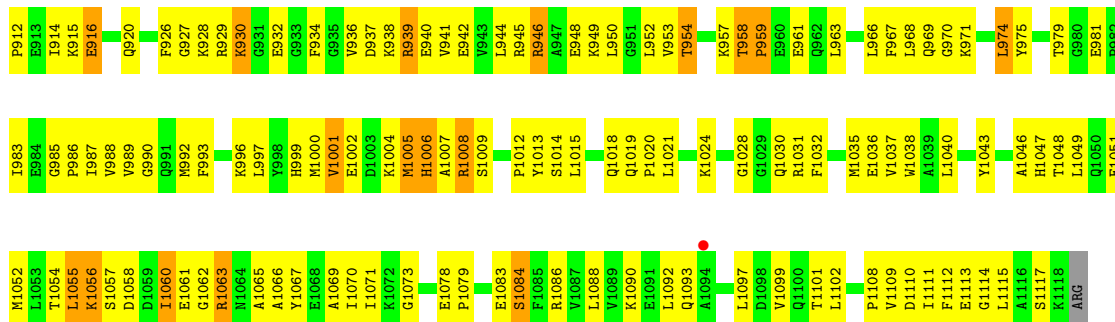
- Molecule 1: DNA-directed RNA polymerase subunit alpha



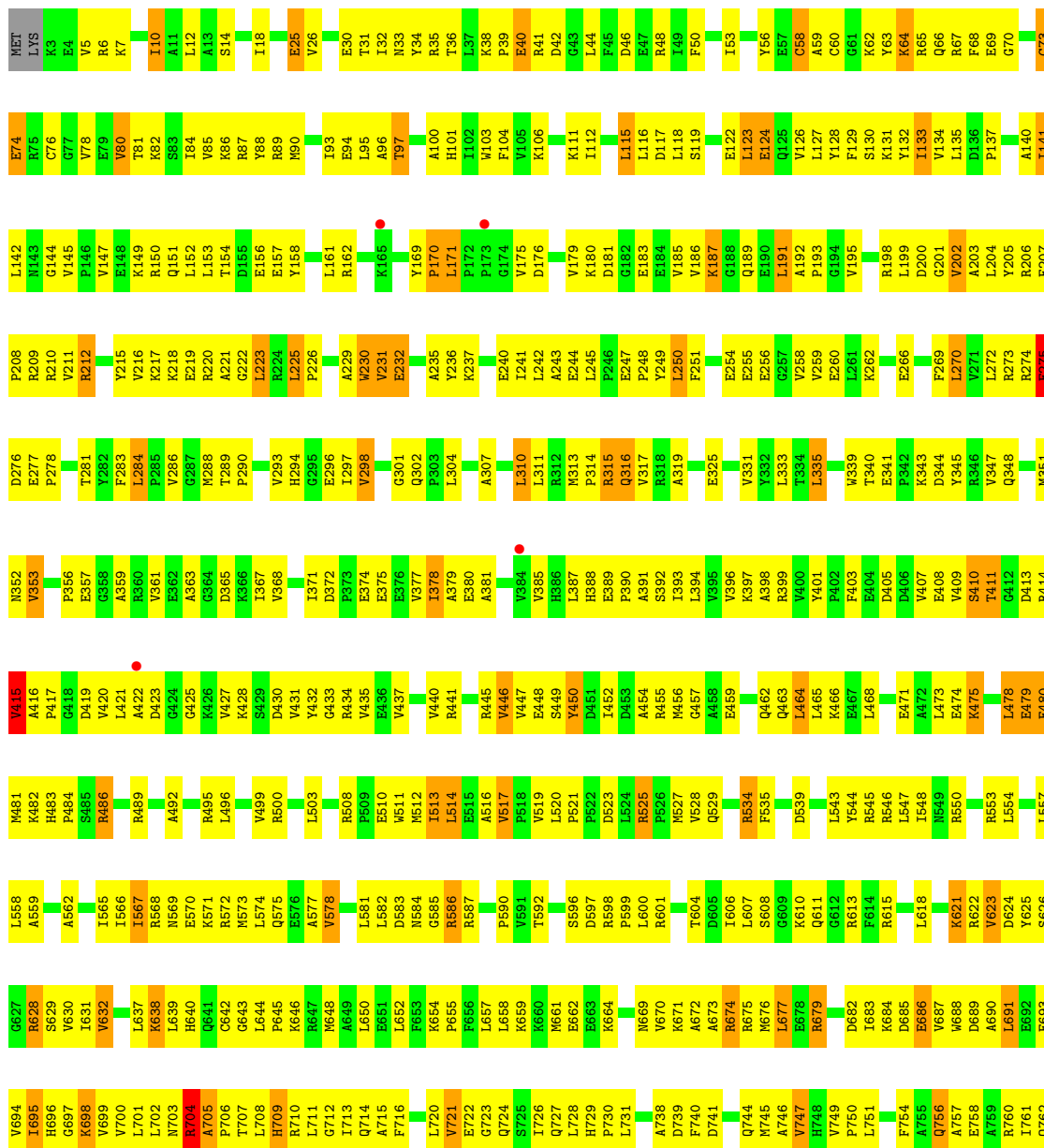
THR	ARG	VAL	LEU	HIS	SER	SER	LEU	LEU	GLU	GLY	GLY	ILE	GLU	SER	VAL	ARG	ALA	ALA	LEU	LEU	ALA	LEU	LEU	ASN	ASN	ASN	ILE	PRO	PRO	GLY	ILE	GLY	GLY	ARG	SER	LEU	LEU	GLU	GLU	ILE	GLY	GLY	ALA	ALA	LEU	LEU	LYS	LYS	LYS	GLY	PHE	THR	LEU	LYS	GLU
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

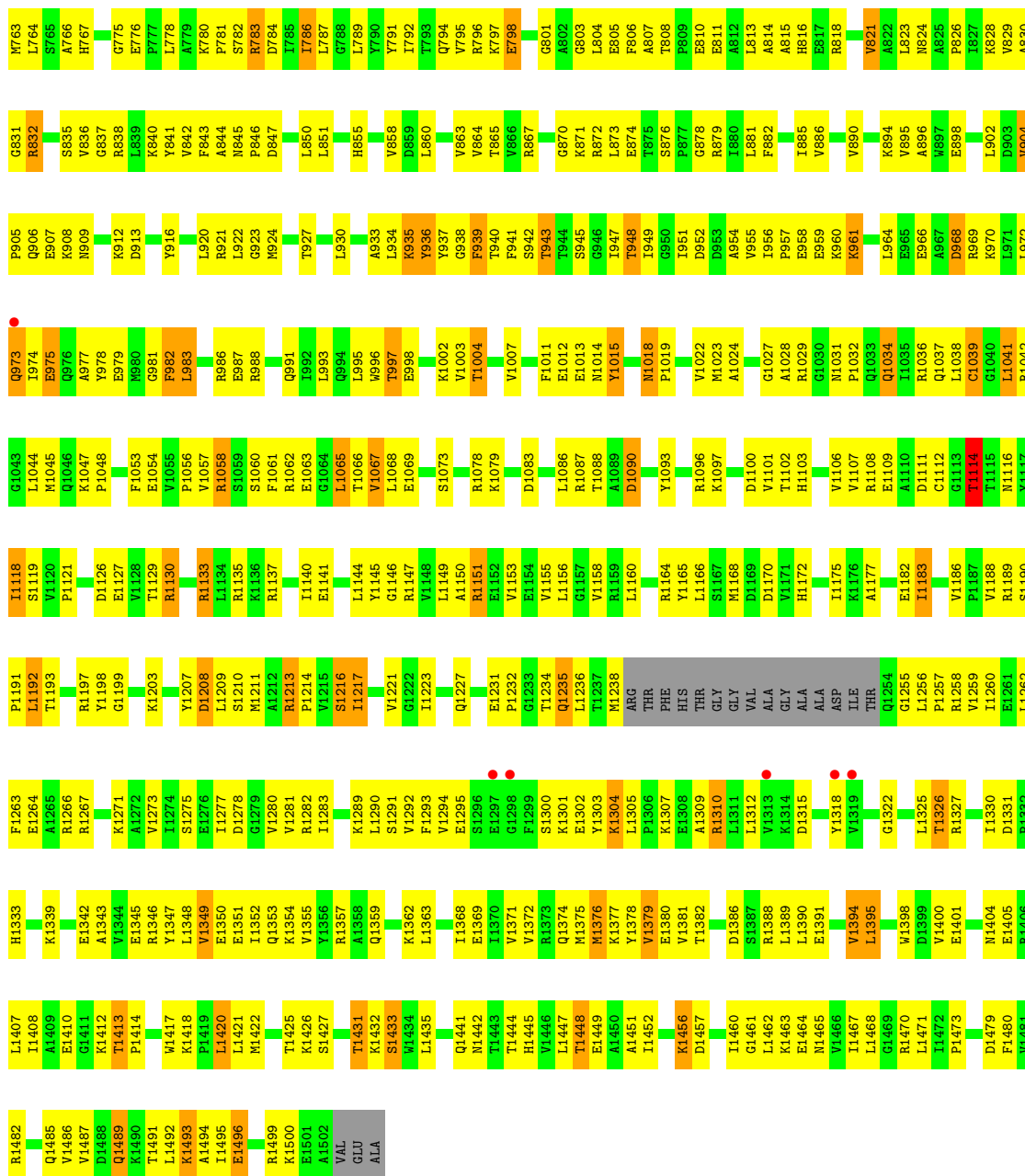
• Molecule 2: DNA-directed RNA polymerase subunit beta



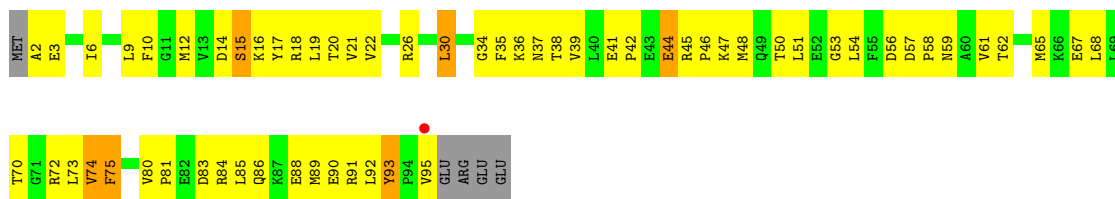


• Molecule 3: DNA-directed RNA polymerase subunit beta'





• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 5: RNA polymerase sigma factor SigA

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	185.44Å 102.65Å 295.38Å 90.00° 98.91° 90.00°	Depositor
Resolution (Å)	29.93 – 3.14 29.93 – 3.14	Depositor EDS
% Data completeness (in resolution range)	93.7 (29.93-3.14) 93.7 (29.93-3.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 3.11Å)	Xtrriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.196 , 0.261 0.197 , 0.262	Depositor DCC
R_{free} test set	2001 reflections (2.23%)	wwPDB-VP
Wilson B-factor (Å ²)	87.4	Xtrriage
Anisotropy	0.743	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 52.2	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	0.95	EDS
Total number of atoms	28581	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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: NA, MG, ZN, DCP

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	0.53	0/1814	0.67	0/2466
1	B	0.51	0/1799	0.70	1/2447 (0.0%)
2	C	0.51	0/8937	0.69	5/12087 (0.0%)
3	D	0.54	2/11927 (0.0%)	0.70	4/16127 (0.0%)
4	E	0.49	0/775	0.64	0/1045
5	F	0.49	0/2852	0.63	0/3837
6	G	1.24	1/393 (0.3%)	1.17	3/605 (0.5%)
7	H	1.15	1/580 (0.2%)	1.11	0/895
8	I	0.89	0/69	1.57	0/106
All	All	0.56	4/29146 (0.0%)	0.71	13/39615 (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
1	B	0	1
2	C	0	1
3	D	0	5
5	F	0	1
All	All	0	8

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	301	GLY	C-N	7.80	1.51	1.34
3	D	1114	THR	CB-CG2	5.39	1.70	1.52
6	G	13	DA	C3'-O3'	-5.39	1.36	1.44
7	H	1	DT	C1'-N1	5.34	1.56	1.49

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
6	G	13	DA	O4'-C4'-C3'	-7.78	101.33	106.00
3	D	170	PRO	C-N-CA	-6.65	105.08	121.70
3	D	225	LEU	CA-CB-CG	6.03	129.18	115.30
2	C	107	LEU	CA-CB-CG	5.92	128.92	115.30
6	G	14	DG	O5'-P-OP1	-5.87	100.42	105.70

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	58	ILE	Peptide
2	C	362	GLY	Peptide
3	D	275	GLU	Peptide
3	D	64	LYS	Peptide
3	D	704	ARG	Peptide

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	A	1782	0	1834	219	0
1	B	1767	0	1816	214	0
2	C	8770	0	8874	815	0
3	D	11721	0	11941	1119	0
4	E	761	0	778	81	0
5	F	2807	0	2882	288	0
6	G	351	0	192	17	0
7	H	516	0	283	41	0
8	I	62	0	34	0	0
9	C	1	0	0	0	0
10	D	28	12	12	3	0
11	D	1	0	0	0	0
12	D	2	0	0	0	0
All	All	28569	12	28646	2541	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 44.

The worst 5 of 2541 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:D:203:ALA:HB1	3:D:393:ILE:HD11	1.17	1.15
5:F:338:LEU:HD23	5:F:339:PRO:HD2	1.21	1.14
3:D:1234:THR:HB	3:D:1235:GLN:HB2	1.31	1.13
3:D:1065:LEU:HD23	3:D:1069:GLU:HB3	1.21	1.12
1:A:88:ARG:HB3	1:A:123:MET:HE3	1.29	1.11

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	224/315 (71%)	192 (86%)	32 (14%)	0	100	100
1	B	222/315 (70%)	192 (86%)	28 (13%)	2 (1%)	17	50
2	C	1107/1119 (99%)	960 (87%)	146 (13%)	1 (0%)	51	82
3	D	1481/1505 (98%)	1255 (85%)	218 (15%)	8 (0%)	29	63
4	E	92/99 (93%)	83 (90%)	9 (10%)	0	100	100
5	F	344/423 (81%)	291 (85%)	51 (15%)	2 (1%)	25	59
All	All	3470/3776 (92%)	2973 (86%)	484 (14%)	13 (0%)	34	67

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	37	GLY
3	D	276	ASP
1	B	154	GLU
5	F	168	LYS
2	C	212	GLY

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	A	199/273 (73%)	164 (82%)	35 (18%)	2	8
1	B	197/273 (72%)	171 (87%)	26 (13%)	4	16
2	C	936/941 (100%)	799 (85%)	137 (15%)	3	13
3	D	1249/1265 (99%)	1082 (87%)	167 (13%)	4	16
4	E	83/88 (94%)	73 (88%)	10 (12%)	5	19
5	F	301/371 (81%)	241 (80%)	60 (20%)	1	5
All	All	2965/3211 (92%)	2530 (85%)	435 (15%)	3	13

5 of 435 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	284	LEU
3	D	754	PHE
5	F	211	ASP
3	D	378	ILE
3	D	525	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	1075	HIS
3	D	1441	GLN
3	D	1195	GLN
3	D	1333	HIS
3	D	1489	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	2/3 (66%)	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 [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 [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
10	DCP	D	1601	9	25,29,29	3.92	11 (44%)	37,45,45	1.94	12 (32%)

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	DCP	D	1601	9	-	9/22/34/34	0/2/2/2

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	1601	DCP	C2'-C1'	-10.24	1.23	1.52
10	D	1601	DCP	O4'-C4'	-8.59	1.25	1.45
10	D	1601	DCP	O4'-C1'	8.36	1.61	1.42
10	D	1601	DCP	C6-C5	5.51	1.47	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	1601	DCP	C2-N3	4.47	1.45	1.36

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	1601	DCP	PB-O3B-PG	-4.36	117.88	132.83
10	D	1601	DCP	C1'-N1-C2	4.29	125.27	117.74
10	D	1601	DCP	O3G-PG-O3B	3.93	117.81	104.64
10	D	1601	DCP	C4-N3-C2	3.49	125.89	120.25
10	D	1601	DCP	C2'-C1'-N1	-3.13	106.56	113.77

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

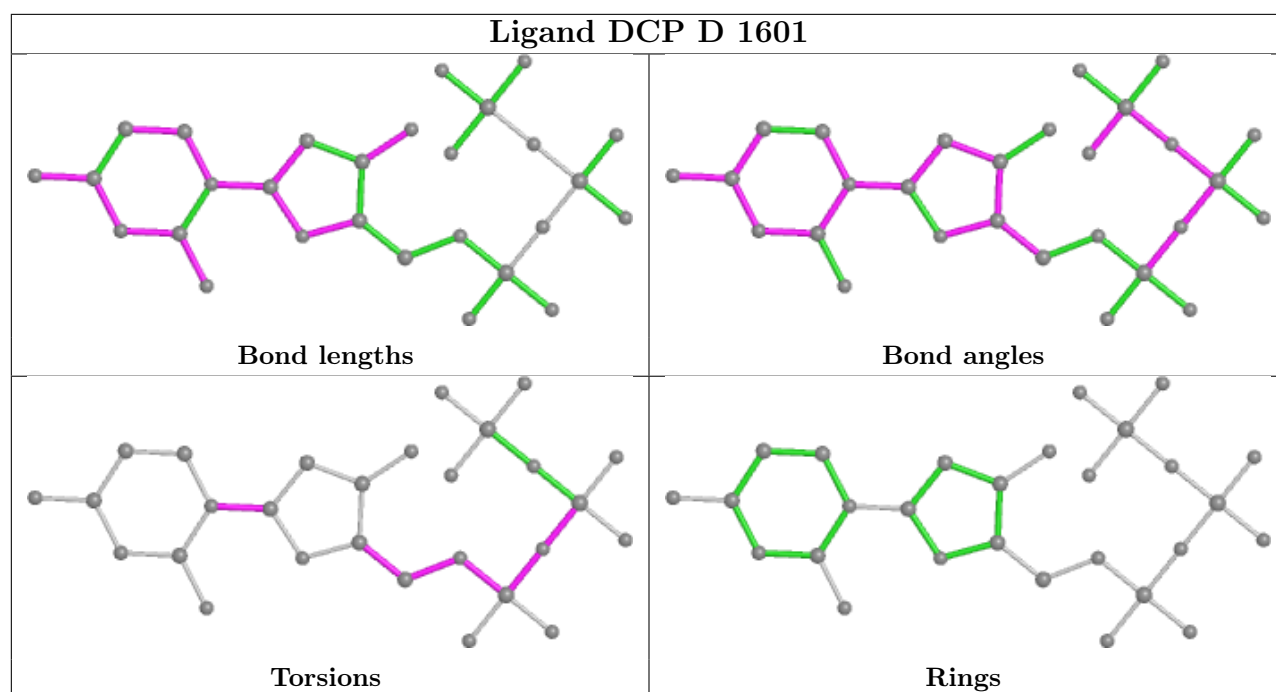
Mol	Chain	Res	Type	Atoms
10	D	1601	DCP	C5'-O5'-PA-O1A
10	D	1601	DCP	C5'-O5'-PA-O3A
10	D	1601	DCP	C2'-C1'-N1-C6
10	D	1601	DCP	PB-O3A-PA-O5'
10	D	1601	DCP	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	1601	DCP	3	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	226/315 (71%)	-0.39	0 100 100	73, 91, 110, 124	0
1	B	224/315 (71%)	-0.39	1 (0%) 92 86	66, 96, 121, 133	0
2	C	1111/1119 (99%)	-0.30	6 (0%) 91 83	56, 91, 138, 160	0
3	D	1485/1505 (98%)	-0.28	10 (0%) 87 77	50, 85, 138, 160	0
4	E	94/99 (94%)	-0.30	1 (1%) 80 66	64, 101, 132, 139	0
5	F	346/423 (81%)	-0.08	17 (4%) 29 14	64, 101, 153, 163	0
6	G	17/22 (77%)	0.11	0 100 100	69, 95, 169, 171	0
7	H	25/27 (92%)	-0.15	1 (4%) 38 20	90, 121, 169, 179	0
8	I	3/3 (100%)	-0.50	0 100 100	73, 73, 76, 87	0
All	All	3531/3828 (92%)	-0.28	36 (1%) 82 70	50, 91, 142, 179	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	391	GLY	4.6
3	D	1313	VAL	4.3
5	F	375	LEU	4.2
3	D	1297	GLU	4.0
5	F	389	PHE	4.0

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](#)

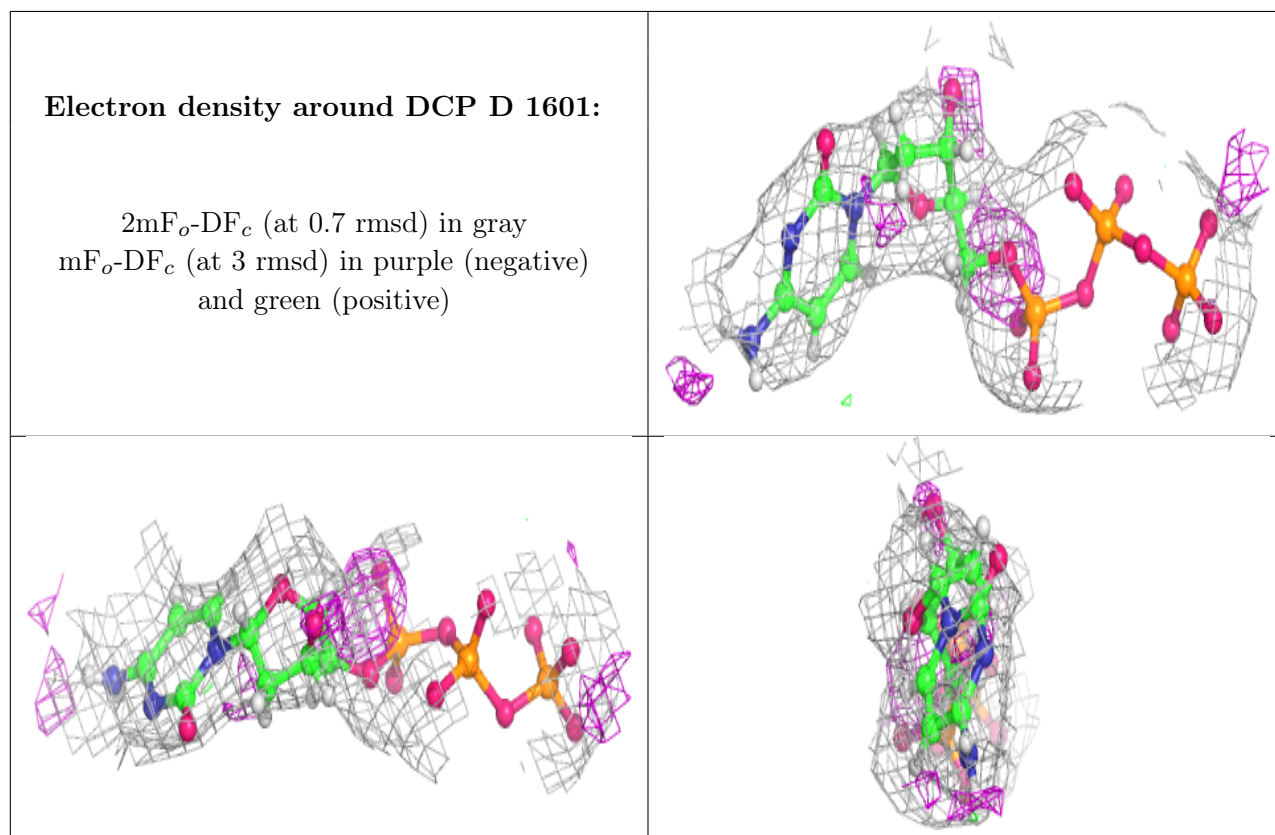
There are no monosaccharides in this entry.

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
9	NA	C	1201	1/1	0.81	0.20	70,70,70,70	0
10	DCP	D	1601	28/28	0.91	0.18	80,93,112,115	0
12	ZN	D	1604	1/1	0.96	0.12	120,120,120,120	0
12	ZN	D	1603	1/1	0.97	0.12	125,125,125,125	0
11	MG	D	1602	1/1	0.98	0.17	67,67,67,67	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.