



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 13, 2018 – 01:37 pm GMT

PDB ID : 3S15
Title : RNA Polymerase II Initiation Complex with a 7-nt RNA
Authors : Liu, X.; Bushnell, D.A.; Silva, D.A.; Huang, X.; Kornberg, R.D.
Deposited on : 2011-05-14
Resolution : 3.30 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
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

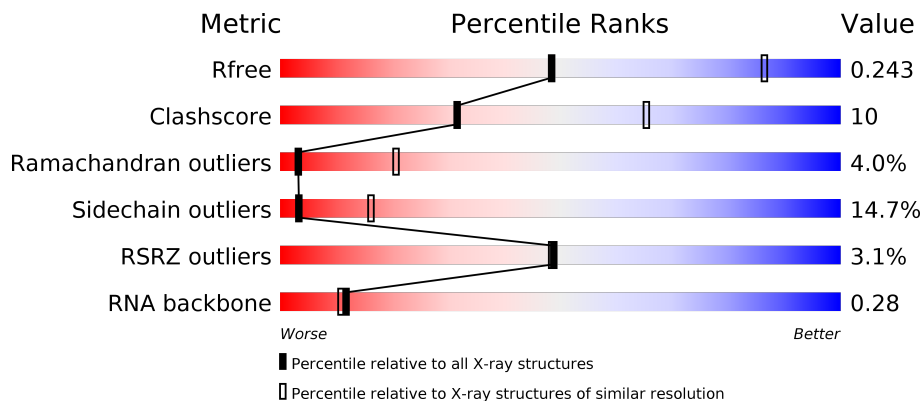
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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.



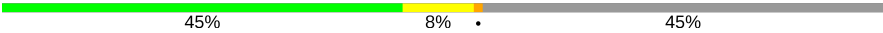


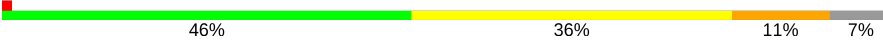




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	1168 (3.36-3.24)
Clashscore	122126	1022 (3.34-3.26)
Ramachandran outliers	120053	1004 (3.34-3.26)
Sidechain outliers	120020	1003 (3.34-3.26)
RSRZ outliers	108989	1133 (3.36-3.24)
RNA backbone	2636	1009 (3.74-2.86)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	1733	<div> <div>3%</div> <div> <div></div> <div>54%</div> <div>23%</div> <div>• •</div> <div>19%</div> </div> </div>
2	B	1224	<div> <div>2%</div> <div> <div></div> <div>59%</div> <div>26%</div> <div>5%</div> <div>•</div> <div>9%</div> </div> </div>
3	C	318	<div> <div></div> <div> <div></div> <div>56%</div> <div>25%</div> <div>•</div> <div>16%</div> </div> </div>
4	E	215	<div> <div>7%</div> <div> <div></div> <div>70%</div> <div>26%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	F	155	
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	R	7	
12	T	29	

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
14	MG	B	2002[A]	-	-	-	X
14	MG	B	2002[B]	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 28717 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1405	Total	C	N	O	S	0	0	0
			11043	6965	1936	2081	61			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1114	Total	C	N	O	S	0	0	0
			8861	5610	1549	1647	55			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	85	Total	C	N	O	S	0	0	0
			688	439	116	130	3			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 11 is a RNA chain called RNA (5'-R(*CP*GP*AP*GP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	7	Total	C	N	O	P	0	0	0
			153	69	33	45	6			

- Molecule 12 is a DNA chain called DNA (5'-D(*CP*TP*AP*CP*CP*GP*AP*TP*AP*AP*GP*CP*AP*GP*AP*CP*GP*AP*TP*CP*CP*TP*CP*TP*CP*GP*AP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	13	Total	C	N	O	P	0	0	0
			261	125	43	80	13			

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	J	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	1	Total 1	Zn 1	0	0
13	I	2	Total 2	Zn 2	0	0
13	C	1	Total 1	Zn 1	0	0
13	A	2	Total 2	Zn 2	0	0
13	L	1	Total 1	Zn 1	0	0

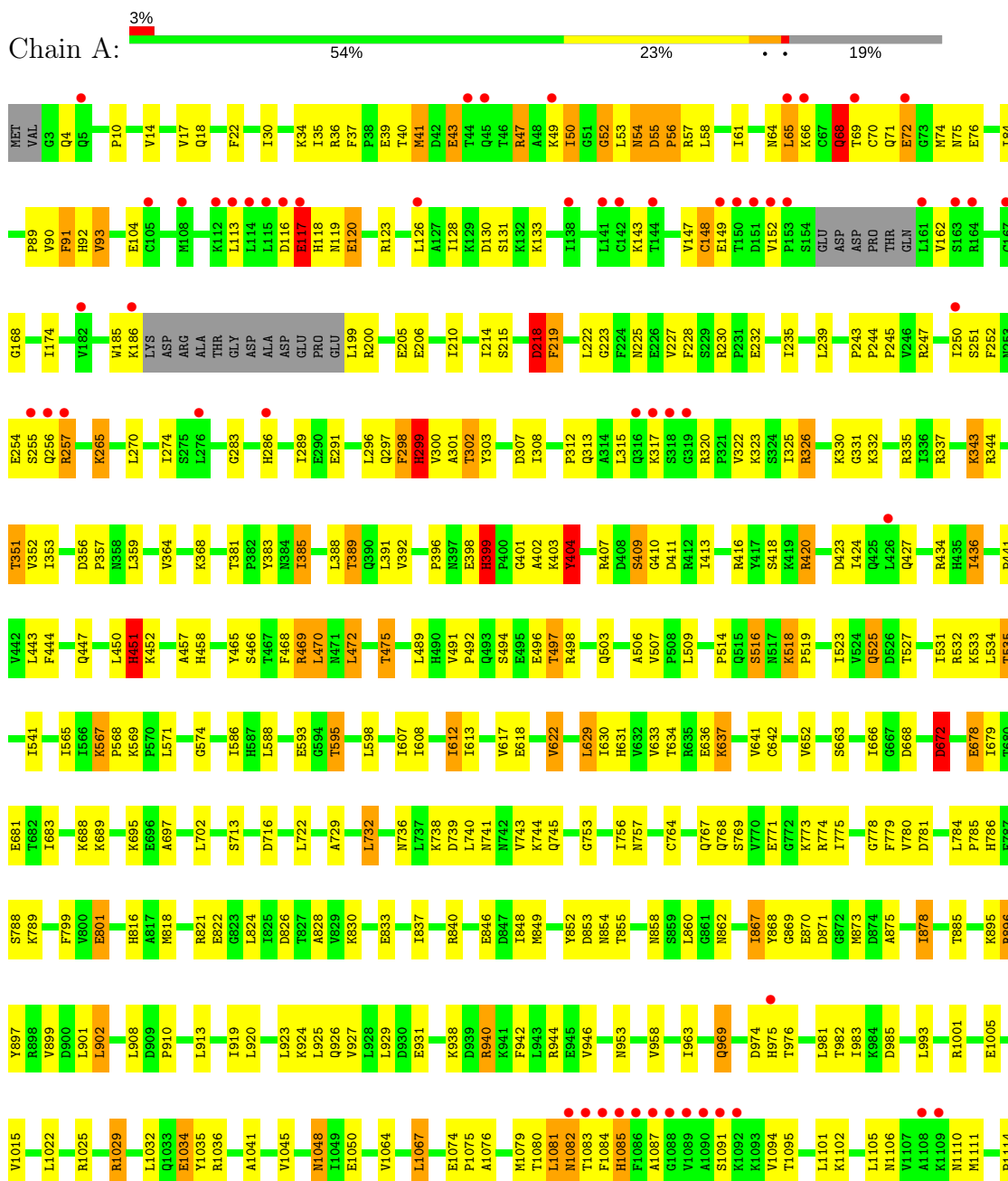
- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

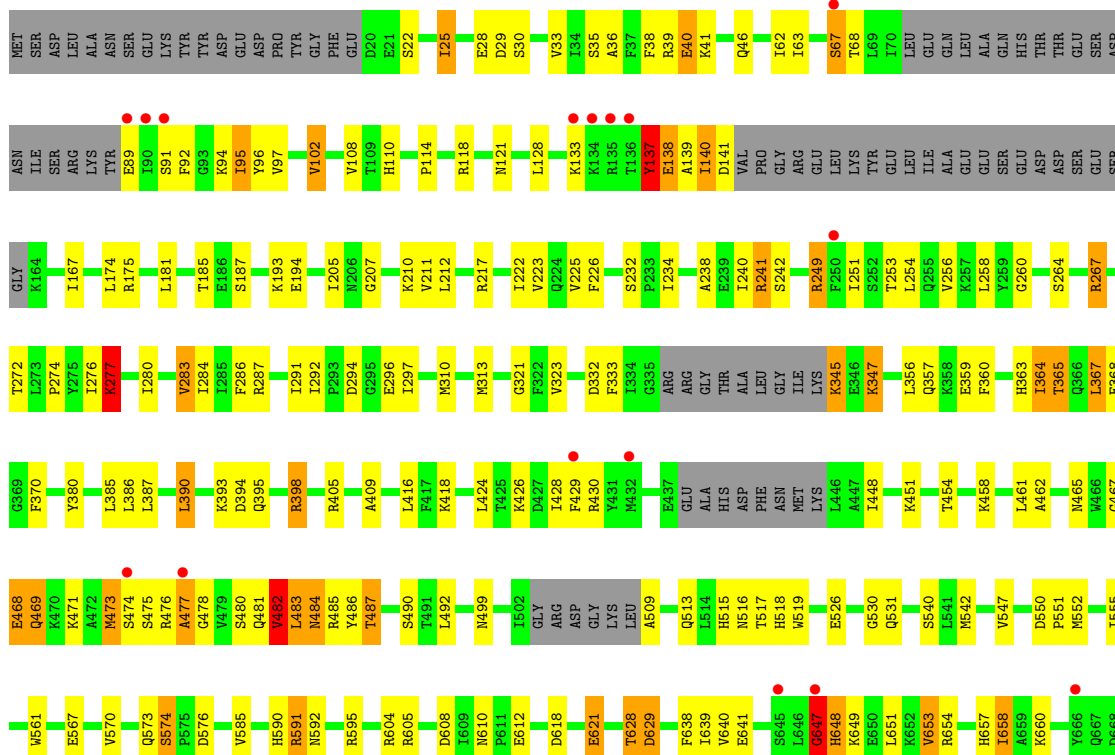
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	B	1	Total 2	Mg 2	0	1
14	A	1	Total 1	Mg 1	0	0

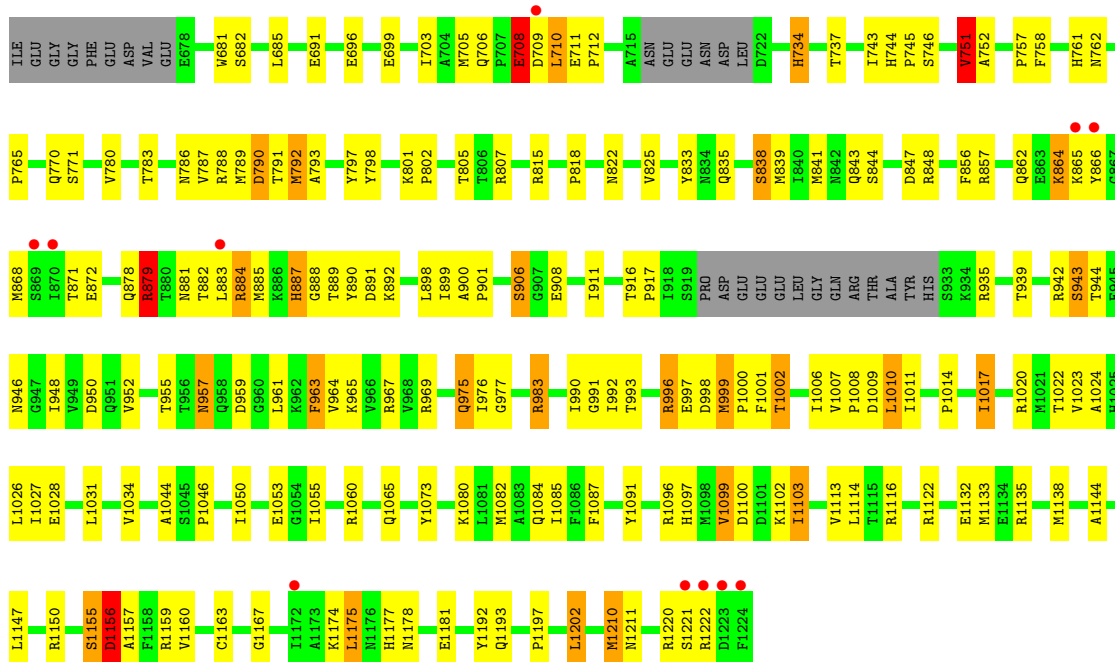
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 II subunit RPB1

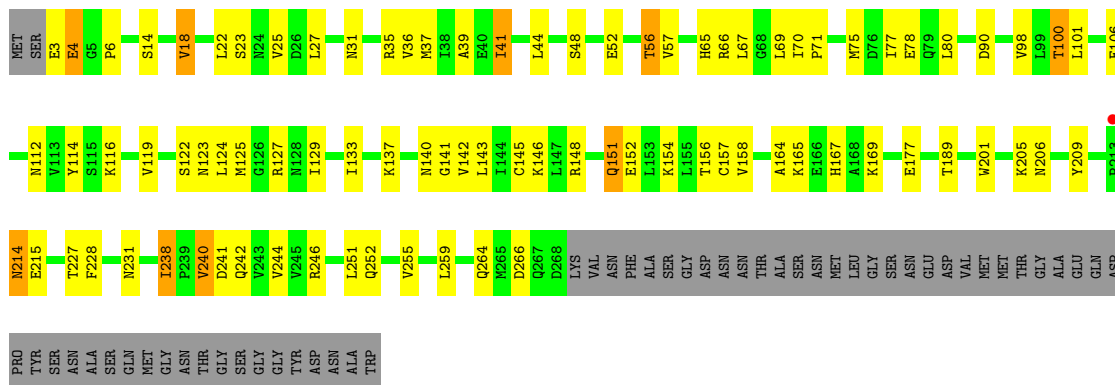






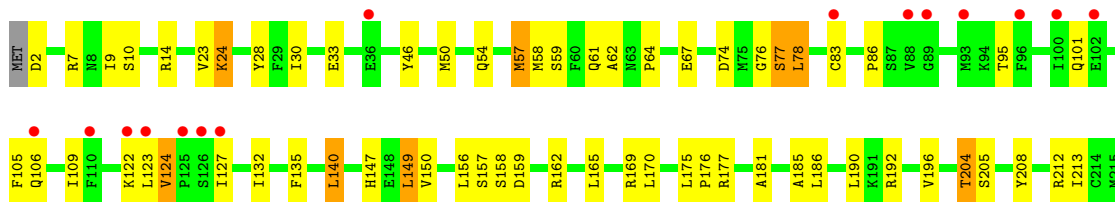
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 56% 25% 16%



• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 7% 70% 26%



• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 45% 8% 45%

MET SER ASP TYR GLU ALA PHE ASN ASP GLY ASN GLU ASN PHE GLU ASP PHE ASP VAL GLU HIS PHE SER ASP GLU THR THR TYR GLU GLU LYS PRO GLN PHE LYS ASP GLY THR THR ASP ALA ASN GLY LYS THR THR ILE VAL THR GLY GLY ASN GLY PRO GLU ASP PHE GLN

HIS GLU GLN ILE ARG LYS THR LEU LYS E71 R79 T62 M85 E89 R90 A91 R92 R93 D110 L111 L118 K123 T134 E144 D145 D154 L155

- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 3% 59% 26% 5% 9%

MET S2 N3 D8 I9 F10 Q11 G18 R19 R22 V23 C24 R25 I26 E27 A28 Q35 L38 T39 L40 V44 E45 L46 F47 P48 D83 I59 A60 S61 S62 L63 ASN LEU GLU THR ASP THR PRO ALA ASN ASP SER SER ALA T76 Q83 A84 G85 D86 R87

A90 Y95 M97 T100 S108 K109 D110 M123 R124 L125 M128 Y129 R130 M131 L132 K136 Q137 E138 W138 A140 R145 R146

- Molecule 7: DNA-directed RNA polymerase II subunit RPB9

Chain I: 72% 22%

MET T2 T3 M12 R17 E28 S9 V35 Y44 I52 T55 V58 V59 Q60 D61 I62 G63 S64 D65 L68 P69 R70 C75 P76 K77 C78 V84 Q90 R91 D94 M97 V102 C103 C106 S107 H108 M116 G120 PHE SER

- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: % 46% 36% 11% 7%

H1 I2 V3 P4 V5 R6 C7 F8 S9 C10 G11 K12 V13 V14 W18 E19 L22 E27 D31 E32 L36 Y44 R47 R48 R49 I50 T52 H53 H54 P55 L56 I57 F58 K59 R62 Y63 R64 P65 LEU GLU LYS ARG ASP

- Molecule 9: DNA-directed RNA polymerase II subunit RPB11

Chain K: 70% 22% 5%

M1 R6 E16 S17 K18 L19 K20 T25 K26 V31 K37 E38 D39 H40 T41 L42 E49 R54 K55 F58 V63 R64 R65 P66 P67 R70 R74 R76 F78 E79 C91 T94 I95 L101 W109 L114 ALA ALA ASP ASP ALA PHE

- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L: % 34% 21% 6% 34%

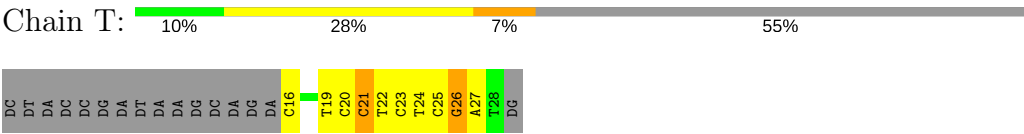
MET SER ARG GLU GLY PHE GLN ILE THR PRO ASN ASP ALA ALA ALA ALA GLY THR SER GLN ARG THR A25 T26 L27 C31 A32 K37 R42 T43 D44 A45 A46 D50 C51 R54 R55 L56 L57 Y58 X58 A59 R60 T61 R62 R63 L64 V65 Q66 P67 E68 A69 R70

- Molecule 11: RNA (5'-R(*CP*GP*AP*GP*AP*GP*G)-3')

Chain R: 57% 43%

C4 G9 G10

● Molecule 12: DNA (5'-D(*CP*TP*AP*CP*CP*GP*AP*TP*AP*AP*GP*CP*AP*GP*AP*CP*GP*AP*TP*CP*CP*TP*CP*TP*CP*GP*AP*TP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	167.93Å 220.89Å 194.62Å 90.00° 100.16° 90.00°	Depositor
Resolution (Å)	44.11 – 3.30 44.11 – 3.29	Depositor EDS
% Data completeness (in resolution range)	(Not available) (44.11-3.30) 99.8 (44.11-3.29)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 3.32Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.8.0, BUSTER 2.8.0	Depositor
R, R_{free}	0.174 , 0.228 0.191 , 0.243	Depositor DCC
R_{free} test set	5242 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	75.8	Xtriage
Anisotropy	0.604	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 104.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28717	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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: ZN, 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	0.51	0/11241	0.82	6/15199 (0.0%)
2	B	0.54	0/9033	0.84	7/12181 (0.1%)
3	C	0.48	0/2133	0.81	0/2891
4	E	0.45	0/1788	0.71	0/2406
5	F	0.50	0/700	0.70	0/945
6	H	0.47	0/1086	0.83	2/1470 (0.1%)
7	I	0.50	0/989	0.84	0/1331
8	J	0.56	0/541	0.90	1/727 (0.1%)
9	K	0.45	0/937	0.71	0/1265
10	L	0.56	0/365	1.03	1/485 (0.2%)
11	R	0.88	0/172	1.62	3/268 (1.1%)
12	T	1.20	0/290	2.48	30/444 (6.8%)
All	All	0.53	0/29275	0.86	50/39612 (0.1%)

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	B	0	1

There are no bond length outliers.

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	16	DC	P-O3'-C3'	11.73	133.77	119.70
12	T	21	DC	O4'-C4'-C3'	-9.95	100.03	106.00
12	T	26	DG	P-O3'-C3'	9.52	131.12	119.70
12	T	20	DC	O4'-C4'-C3'	-8.84	100.69	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	19	DT	O4'-C4'-C3'	-8.80	100.72	106.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	647	GLY	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	11043	0	11133	237	0
2	B	8861	0	8884	214	0
3	C	2095	0	2051	48	0
4	E	1752	0	1776	27	0
5	F	688	0	707	8	0
6	H	1068	0	1040	27	0
7	I	971	0	927	10	0
8	J	532	0	542	26	0
9	K	919	0	929	17	0
10	L	363	0	386	13	0
11	R	153	0	78	0	0
12	T	261	0	148	5	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
14	A	1	0	0	0	0
14	B	2	0	0	0	0
All	All	28717	0	28601	554	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 10.

The worst 5 of 554 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:A:867:ILE:CD1	1:A:867:ILE:CG1	1.77	1.60
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.42	1.01
1:A:494:SER:HB3	1:A:497:THR:HB	1.45	0.98
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	1.97	0.97
1:A:567:LYS:HD2	1:A:568:PRO:HD2	1.46	0.94

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	1395/1733 (80%)	1210 (87%)	126 (9%)	59 (4%)	3	19
2	B	1096/1224 (90%)	948 (86%)	102 (9%)	46 (4%)	3	19
3	C	264/318 (83%)	237 (90%)	21 (8%)	6 (2%)	7	33
4	E	212/215 (99%)	197 (93%)	11 (5%)	4 (2%)	9	38
5	F	83/155 (54%)	76 (92%)	6 (7%)	1 (1%)	14	47
6	H	129/146 (88%)	109 (84%)	9 (7%)	11 (8%)	1	6
7	I	117/122 (96%)	95 (81%)	18 (15%)	4 (3%)	4	25
8	J	63/70 (90%)	56 (89%)	5 (8%)	2 (3%)	4	26
9	K	112/120 (93%)	104 (93%)	6 (5%)	2 (2%)	9	39
10	L	44/70 (63%)	29 (66%)	9 (20%)	6 (14%)	0	2
All	All	3515/4173 (84%)	3061 (87%)	313 (9%)	141 (4%)	3	21

5 of 141 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	THR

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Mol	Chain	Res	Type
1	A	55	ASP
1	A	56	PRO
1	A	69	THR
1	A	72	GLU

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	1225/1520 (81%)	1033 (84%)	192 (16%)	3	14
2	B	967/1061 (91%)	838 (87%)	129 (13%)	4	19
3	C	234/274 (85%)	205 (88%)	29 (12%)	5	22
4	E	196/197 (100%)	169 (86%)	27 (14%)	4	18
5	F	75/137 (55%)	69 (92%)	6 (8%)	13	41
6	H	117/128 (91%)	97 (83%)	20 (17%)	2	11
7	I	113/116 (97%)	99 (88%)	14 (12%)	5	22
8	J	60/65 (92%)	45 (75%)	15 (25%)	0	2
9	K	99/102 (97%)	84 (85%)	15 (15%)	3	15
10	L	40/57 (70%)	28 (70%)	12 (30%)	0	1
All	All	3126/3657 (86%)	2667 (85%)	459 (15%)	3	16

5 of 459 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	194	GLU
2	B	649	LYS
8	J	22	LEU
2	B	241	ARG
2	B	394	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1432	GLN
2	B	499	ASN
7	I	12	ASN
2	B	121	ASN
2	B	357	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	6/7 (85%)	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	1405/1733 (81%)	0.03	60 (4%) 35 35	48, 92, 168, 202	0
2	B	1114/1224 (91%)	-0.11	27 (2%) 59 56	43, 79, 139, 202	0
3	C	266/318 (83%)	-0.29	1 (0%) 92 92	52, 80, 117, 169	0
4	E	214/215 (99%)	0.25	15 (7%) 16 17	69, 130, 190, 204	0
5	F	85/155 (54%)	-0.13	0 100 100	66, 97, 133, 162	0
6	H	133/146 (91%)	0.22	5 (3%) 40 38	86, 127, 158, 170	0
7	I	119/122 (97%)	-0.31	0 100 100	59, 97, 131, 150	0
8	J	65/70 (92%)	-0.30	1 (1%) 73 71	47, 70, 100, 127	0
9	K	114/120 (95%)	-0.28	0 100 100	60, 87, 112, 127	0
10	L	46/70 (65%)	-0.10	1 (2%) 62 61	65, 109, 149, 161	0
11	R	7/7 (100%)	-0.59	0 100 100	89, 97, 131, 139	0
12	T	13/29 (44%)	-0.29	0 100 100	110, 124, 160, 169	0
All	All	3581/4209 (85%)	-0.05	110 (3%) 49 48	43, 90, 161, 204	0

The worst 5 of 110 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1082	ASN	10.5
1	A	1176	LEU	9.8
1	A	318	SER	7.9
1	A	1087	ALA	7.9
1	A	1086	PHE	7.2

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 carbohydrates 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
14	MG	B	2002[A]	1/1	0.56	0.68	41,41,41,41	1
14	MG	B	2002[B]	1/1	0.56	0.68	3,3,3,3	1
13	ZN	A	1734	1/1	0.88	0.06	236,236,236,236	0
13	ZN	A	1735	1/1	0.96	0.11	112,112,112,112	0
14	MG	A	2001	1/1	0.98	0.08	68,68,68,68	0
13	ZN	B	1307	1/1	0.98	0.12	147,147,147,147	0
13	ZN	L	105	1/1	0.99	0.08	112,112,112,112	0
13	ZN	I	204	1/1	0.99	0.10	74,74,74,74	0
13	ZN	I	203	1/1	0.99	0.14	98,98,98,98	0
13	ZN	J	101	1/1	0.99	0.19	75,75,75,75	0
13	ZN	C	319	1/1	1.00	0.09	78,78,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.