



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 03:07 PM GMT

PDB ID : 3S1M
Title : RNA Polymerase II Initiation Complex with a 5-nt RNA (variant 1)
Authors : Liu, X.; Bushnell, D.A.; Silva, D.A.; Huang, X.; Kornberg, R.D.
Deposited on : 2011-05-15
Resolution : 3.13 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

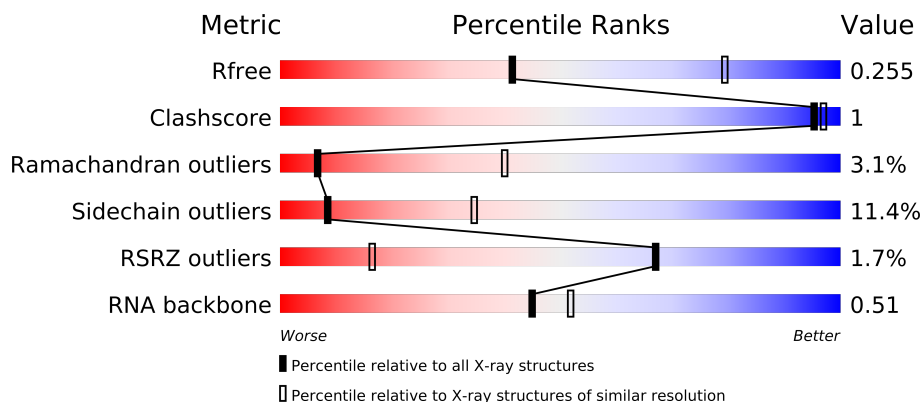
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.13 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}	66092	1337 (3.20-3.08)
Clashscore	79885	1656 (3.20-3.08)
Ramachandran outliers	78287	1614 (3.20-3.08)
Sidechain outliers	78261	1613 (3.20-3.08)
RSRZ outliers	66119	1338 (3.20-3.08)
RNA backbone	1838	1002 (3.66-2.62)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1733	
2	B	1224	
3	C	318	
4	E	215	
5	F	155	
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	R	5	
12	T	29	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 28570 atoms, of which 0 are hydrogen and 0 are deuterium.

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(*AP*GP*AP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	5	Total	C	N	O	P	0	0	0
			107	49	23	31	4			

- 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*GP*TP*CP*TP*CP*GP*AP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	8	Total	C	N	O	P	0	0	0
			162	77	28	49	8			

- 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		

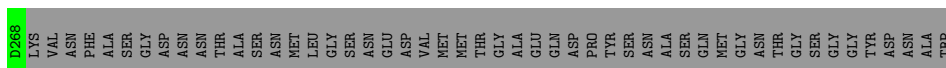
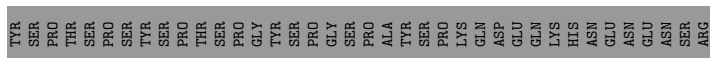
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	1	Total 1	Zn 1	0	0
13	I	2	Total 2	Zn 2	0	0
13	C	1	Total 1	Zn 1	0	0
13	A	2	Total 2	Zn 2	0	0
13	L	1	Total 1	Zn 1	0	0

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

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



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

HIS GLU GLN ILE ARG LYS THR LEU LYS E71 K72 A73 T82 D110 L118 K128 R136 Y137 L138 S142 D154 L155

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

Chain H:

MET S2 P17 N21 K22 D34 Q35 V44 E45 L46 L55 L63 ASN LEU ASP THR PRO ALA ASN ASP SER SER ALA T76 G85 D86 R87 A90 Y95 E106 V107 S108 K109 D110 L111 N128 Y129 R130 N131 L132 K136 M139 A140 R146

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

Chain I:

MET T2 R24 E37 N51 T55 Q60 D61 L62 G63 S64 R70 C75 F76 K77 C78 V84 Q87 R91 R97 F101 F110 T111 Q120 PHE SER

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

Chain J:

M1 I2 V3 R6 C7 F8 L22 Q26 D31 S37 R43 R48 T52 I57 E58 K59 R62 P65 LEU GLU LYS ARG ASP

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

Chain K:

M1 R6 L12 G13 E14 K20 D22 V31 R47 L51 V63 L101 L114 ALA ALA ASP ASP ALA PHE

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

Chain L:

MET SER ARG GLY PHE GLN ILE THR ASN LEU ASP ALA ALA ALA GLY THR SER GLN ALA ARG THR A25 T26 L27 I30 E33 C34 S35 S39 R42 T43 D44 A45 V46 R47 C51 T55 L56 L57 K58 A59 R60 L64 V65 R70

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

Chain R:

A6 G7 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*GP*TP*CP*TP*CP*GP*AP*TP*G)-3')

Chain T:

DC DA DC DC DC DG DA DA DA DA DA DA DA DA DA DA DA DA DA DA DA C16 T19 C20 G21 T22 C23 DT DC DG DA DT DG

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	156.92Å 220.71Å 191.77Å 90.00° 97.48° 90.00°	Depositor
Resolution (Å)	47.72 – 3.13 47.72 – 3.12	Depositor EDS
% Data completeness (in resolution range)	(Not available) (47.72-3.13) 98.7 (47.72-3.12)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.183 , 0.233 0.206 , 0.255	Depositor DCC
R_{free} test set	5662 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	79.3	Xtriage
Anisotropy	0.725	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 83.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 113128 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28570	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage'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.

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	0.47	0/11241	0.75	2/15199 (0.0%)
2	B	0.48	0/9033	0.76	1/12181 (0.0%)
3	C	0.44	0/2133	0.77	0/2891
4	E	0.43	0/1788	0.67	0/2406
5	F	0.44	0/700	0.68	0/945
6	H	0.44	0/1086	0.78	1/1470 (0.1%)
7	I	0.47	0/989	0.81	0/1331
8	J	0.49	0/541	0.83	0/727
9	K	0.43	0/937	0.68	0/1265
10	L	0.51	0/365	0.90	0/485
11	R	0.95	0/120	1.47	0/186
12	T	1.24	0/180	1.92	7/275 (2.5%)
All	All	0.48	0/29113	0.77	11/39361 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	22	DT	O4'-C1'-N1	7.68	113.38	108.00
1	A	218	ASP	C-N-CA	6.95	139.08	121.70
12	T	23	DC	O4'-C1'-N1	6.54	112.58	108.00
12	T	20	DC	O4'-C1'-N1	6.33	112.43	108.00
12	T	19	DT	O4'-C1'-N1	5.92	112.14	108.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11043	0	23	16	0
2	B	8861	0	0	14	0
3	C	2095	0	0	3	0
4	E	1752	0	0	0	0
5	F	688	0	5	2	0
6	H	1068	0	0	0	0
7	I	971	0	0	4	0
8	J	532	0	0	4	0
9	K	919	0	0	2	0
10	L	363	0	0	1	0
11	R	107	0	0	0	0
12	T	162	0	0	0	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
All	All	28570	0	28	37	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 1.

The worst 5 of 37 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:756:ILE:CD1	1:A:756:ILE:CG1	1.74	1.57
1:A:567:LYS:O	1:A:569:LYS:N	2.24	0.69
1:A:596:THR:O	1:A:598:LEU:N	2.27	0.68
1:A:399:HIS:O	1:A:401:GLY:N	2.30	0.65
3:C:66:ARG:NH2	8:J:3:VAL:O	2.35	0.59

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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%)	1242 (89%)	110 (8%)	43 (3%)	7	40
2	B	1096/1224 (90%)	949 (87%)	112 (10%)	35 (3%)	6	39
3	C	264/318 (83%)	239 (90%)	18 (7%)	7 (3%)	8	44
4	E	212/215 (99%)	202 (95%)	8 (4%)	2 (1%)	25	75
5	F	83/155 (54%)	74 (89%)	6 (7%)	3 (4%)	5	35
6	H	129/146 (88%)	107 (83%)	14 (11%)	8 (6%)	2	18
7	I	117/122 (96%)	101 (86%)	15 (13%)	1 (1%)	25	75
8	J	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	6	39
9	K	112/120 (93%)	105 (94%)	6 (5%)	1 (1%)	25	75
10	L	44/70 (63%)	26 (59%)	10 (23%)	8 (18%)	0	0
All	All	3515/4173 (84%)	3102 (88%)	303 (9%)	110 (3%)	7	40

5 of 110 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	55	ASP
1	A	325	ILE
1	A	399	HIS
1	A	543	LEU

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%)	1067 (87%)	158 (13%)	6	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	967/1061 (91%)	863 (89%)	104 (11%)	9	37
3	C	234/274 (85%)	213 (91%)	21 (9%)	14	49
4	E	196/197 (100%)	181 (92%)	15 (8%)	18	60
5	F	75/137 (55%)	73 (97%)	2 (3%)	57	91
6	H	117/128 (91%)	101 (86%)	16 (14%)	5	24
7	I	113/116 (97%)	103 (91%)	10 (9%)	14	51
8	J	60/65 (92%)	48 (80%)	12 (20%)	2	9
9	K	99/102 (97%)	90 (91%)	9 (9%)	14	48
10	L	40/57 (70%)	31 (78%)	9 (22%)	1	6
All	All	3126/3657 (86%)	2770 (89%)	356 (11%)	8	34

5 of 356 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	58	THR
2	B	604	ARG
8	J	22	LEU
2	B	102	VAL
2	B	416	LEU

Some 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
11	R	4/5 (80%)	1 (25%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	7	G

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 9 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.

5.7 Other polymers ⓘ

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1405/1733 (81%)	0.08	46 (3%) 44 7	62, 106, 212, 241	0
2	B	1114/1224 (91%)	-0.06	10 (0%) 81 29	60, 101, 178, 207	0
3	C	266/318 (83%)	-0.22	0 100 100	72, 98, 138, 170	0
4	E	214/215 (99%)	-0.09	0 100 100	79, 137, 185, 197	0
5	F	85/155 (54%)	-0.27	0 100 100	87, 119, 155, 169	0
6	H	133/146 (91%)	0.11	3 (2%) 57 11	100, 141, 173, 184	0
7	I	119/122 (97%)	-0.23	0 100 100	77, 107, 146, 158	0
8	J	65/70 (92%)	-0.13	0 100 100	64, 94, 131, 144	0
9	K	114/120 (95%)	-0.18	0 100 100	64, 101, 127, 143	0
10	L	46/70 (65%)	-0.09	1 (2%) 59 12	79, 135, 168, 176	0
11	R	5/5 (100%)	0.65	0 100 100	211, 213, 220, 220	0
12	T	8/29 (27%)	0.23	0 100 100	193, 198, 203, 205	0
All	All	3574/4207 (84%)	-0.03	60 (1%) 67 16	60, 107, 200, 241	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1087	ALA	6.5
1	A	1088	GLY	5.6
1	A	317	LYS	4.9
1	A	1176	LEU	4.2
1	A	141	LEU	4.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
13	ZN	I	204	1/1	0.15	-0.15	83,83,83,83	0
13	ZN	I	203	1/1	0.12	-0.26	108,108,108,108	0
13	ZN	L	105	1/1	0.12	-0.41	129,129,129,129	0
13	ZN	C	319	1/1	0.12	-0.44	92,92,92,92	0
13	ZN	A	1734	1/1	0.25	-0.49	300,300,300,300	0
13	ZN	B	1307	1/1	0.06	-1.45	202,202,202,202	0
14	MG	A	2001	1/1	0.15	-1.59	60,60,60,60	0
13	ZN	J	101	1/1	0.22	-1.78	85,85,85,85	0
13	ZN	A	1735	1/1	0.06	-2.10	190,190,190,190	0

6.5 Other polymers ⓘ

There are no such residues in this entry.