



wwPDB EM Map/Model Validation Report

Apr 10, 2016 – 01:56 PM BST

PDB ID : 3LU0
EMDB ID: : EMD-5169
Title : Molecular model of Escherichia coli core RNA polymerase
Authors : Darst, S.A.
Deposited on : 2010-02-16
Resolution : 11.20 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

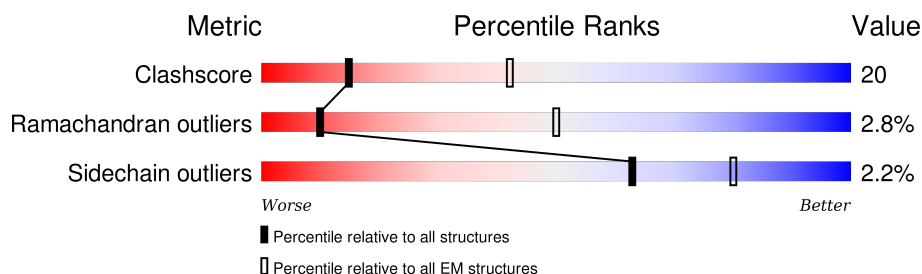
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 11.20 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	329	
1	B	329	
2	C	1342	
3	D	1407	
4	E	91	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 25410 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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					AltConf	Trace
1	A	235	Total	C	N	O	S	0	0
			1820	1132	323	358	7		
1	B	235	Total	C	N	O	S	0	0
			1820	1132	323	358	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1335	Total	C	N	O	S	0	0
			10523	6602	1836	2042	43		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	516	VAL	ASP	CONFLICT	UNP P0A8V2

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1364	Total	C	N	O	S	0	0
			10547	6624	1879	1994	50		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	89	Total	C	N	O	S	0	0
			697	424	132	140	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
5	D	1	Total	Mg	0
			1	1	

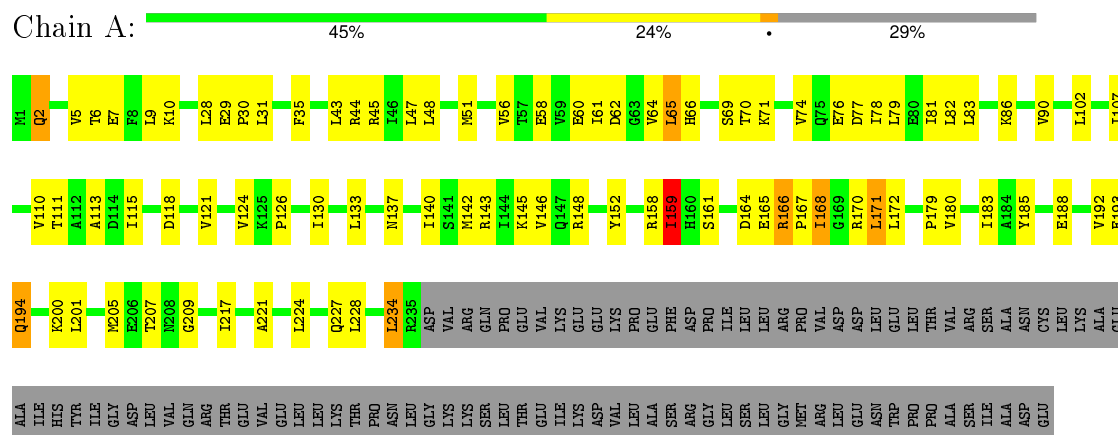
- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
6	D	2	Total	Zn	0
			2	2	

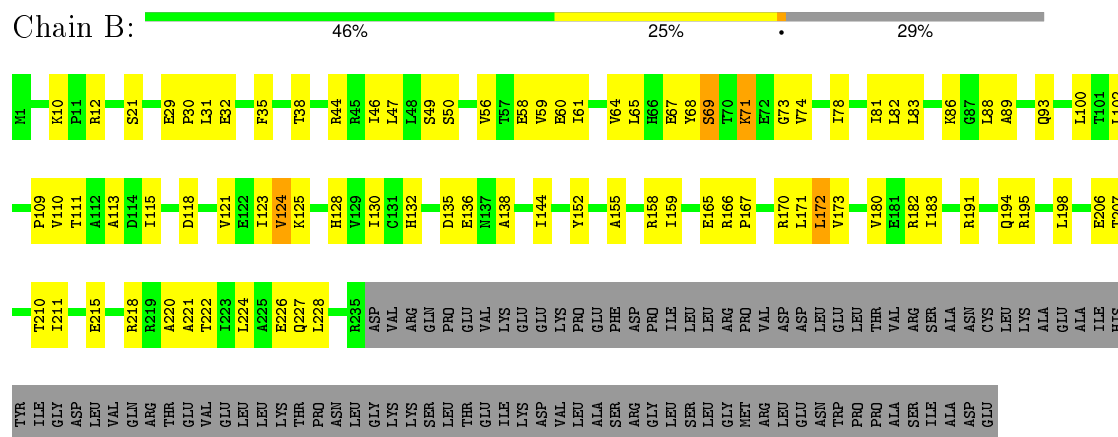
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

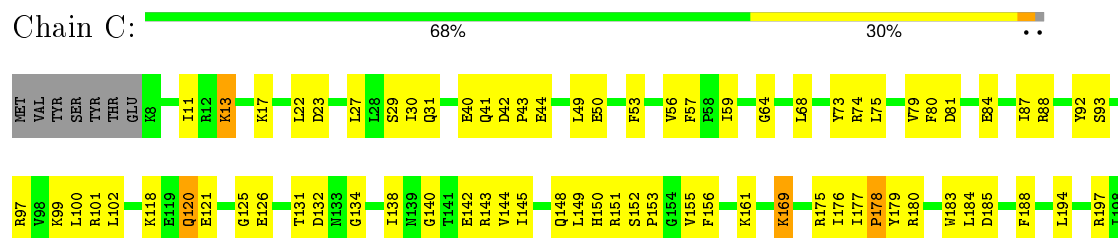
• Molecule 1: DNA-directed RNA polymerase subunit alpha

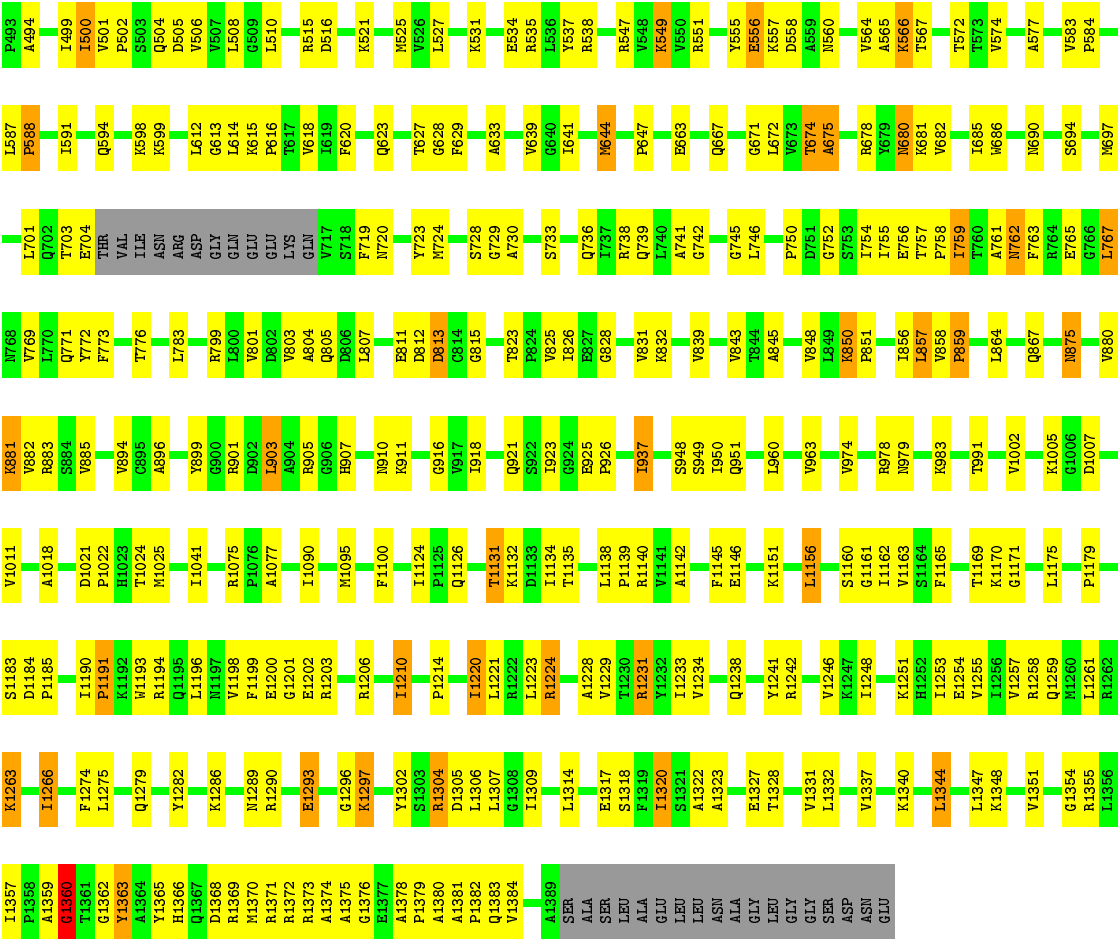


• Molecule 1: DNA-directed RNA polymerase subunit alpha

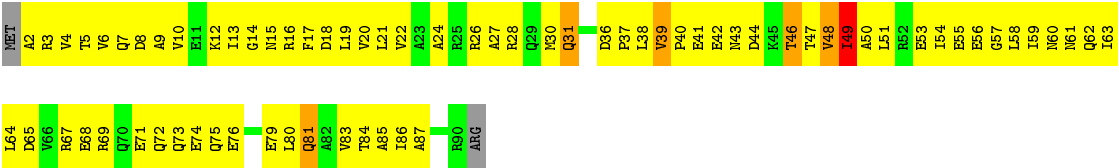
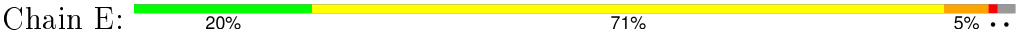


• Molecule 2: DNA-directed RNA polymerase subunit beta





● Molecule 4: DNA-directed RNA polymerase subunit omega



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	10	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	50000	Depositor
Image detector	Kodak SO163 film	Depositor

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: 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 >2	RMSZ	# Z >2
1	A	0.19	0/1842	0.37	0/2495
1	B	0.19	0/1842	0.36	0/2495
2	C	0.21	1/10690 (0.0%)	0.34	0/14422
3	D	0.26	0/10710	0.63	3/14470 (0.0%)
4	E	1.09	2/699 (0.3%)	1.79	4/942 (0.4%)
All	All	0.29	3/25783 (0.0%)	0.56	7/34824 (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	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	49	ILE	C-N	5.62	1.47	1.34
2	C	951	MET	CG-SD	5.51	1.95	1.81
4	E	49	ILE	CA-C	5.30	1.66	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1360	GLY	CA-C-N	-50.05	7.09	117.20
4	E	81	GLN	CG-CD-OE1	-38.65	44.30	121.60
3	D	1360	GLY	C-N-CA	-31.89	41.97	121.70
4	E	81	GLN	CG-CD-NE2	-9.65	93.55	116.70
4	E	49	ILE	C-N-CA	8.22	142.25	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	1360	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	1820	0	1850	78	0
1	B	1820	0	1850	59	0
2	C	10523	0	10551	327	0
3	D	10547	0	10751	495	0
4	E	697	0	706	209	0
5	D	1	0	0	0	0
6	D	2	0	0	0	0
All	All	25410	0	25708	1011	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 20.

The worst 5 of 1011 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:615:LYS:CD	4:E:5:THR:CA	1.80	1.59
3:D:615:LYS:CE	4:E:5:THR:HA	1.37	1.53
3:D:615:LYS:CD	4:E:5:THR:HA	1.34	1.46
3:D:615:LYS:HD3	4:E:5:THR:C	1.31	1.46
3:D:615:LYS:HD3	4:E:5:THR:CA	1.34	1.45

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 PDB entries followed by that with respect to all EM entries.

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	233/329 (71%)	196 (84%)	31 (13%)	6 (3%)	7	45
1	B	233/329 (71%)	197 (84%)	28 (12%)	8 (3%)	5	40
2	C	1333/1342 (99%)	1109 (83%)	190 (14%)	34 (3%)	7	45
3	D	1362/1407 (97%)	1124 (82%)	198 (14%)	40 (3%)	6	43
4	E	87/91 (96%)	74 (85%)	10 (12%)	3 (3%)	5	40
All	All	3248/3498 (93%)	2700 (83%)	457 (14%)	91 (3%)	10	44

5 of 91 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	ILE
1	A	166	ARG
1	B	124	VAL
2	C	489	PRO
2	C	582	ASN

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 PDB entries followed by that with respect to all EM entries.

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	202/286 (71%)	195 (96%)	7 (4%)	43	74
1	B	202/286 (71%)	199 (98%)	3 (2%)	72	88
2	C	1150/1157 (99%)	1139 (99%)	11 (1%)	82	92
3	D	1129/1168 (97%)	1091 (97%)	38 (3%)	44	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	E	73/75 (97%)	71 (97%)	2 (3%)	52 79
All	All	2756/2972 (93%)	2695 (98%)	61 (2%)	63 83

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	201	LEU
3	D	500	ILE
3	D	1297	LYS
3	D	222	LYS
3	D	255	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	1090	ASN
3	D	158	GLN
3	D	1295	ASN
2	C	1108	ASN
2	C	1236	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 3 ligands modelled in this entry, 3 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.