



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Aug 20, 2017 – 09:50 PM EDT

PDB ID : 5MY1
EMDB ID: : EMD-3580
Title : E. coli expressome
Authors : Kohler, R.; Mooney, R.A.; Mills, D.J.; Kostrewa, D.; Landick, R.; Cramer, P.
Deposited on : unknown
Resolution : 7.60 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

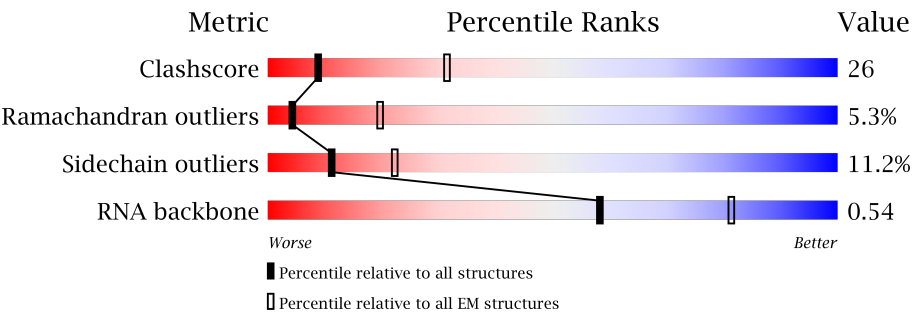
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 7.60 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.



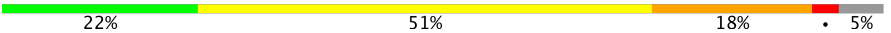
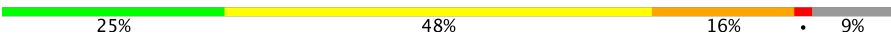
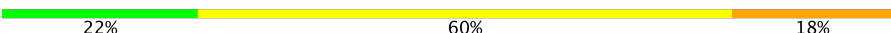
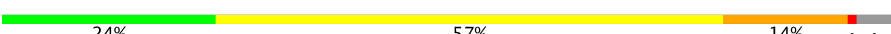
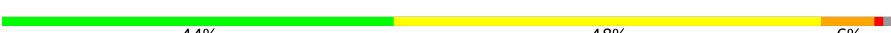
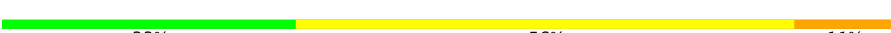







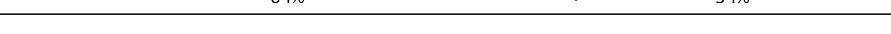
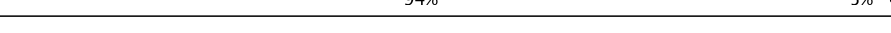
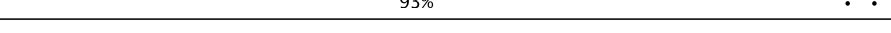
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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	1542	<div><div>26%</div><div>59%</div><div>14%</div><div>.</div></div>
2	C	232	<div><div>25%</div><div>50%</div><div>14%</div><div>11%</div></div>
3	D	205	<div><div>27%</div><div>54%</div><div>19%</div><div>.</div></div>
4	E	166	<div><div>29%</div><div>51%</div><div>10%</div><div>.</div><div>10%</div></div>
5	F	135	<div><div>24%</div><div>37%</div><div>11%</div><div>.</div><div>26%</div></div>
6	G	178	<div><div>25%</div><div>47%</div><div>12%</div><div>.</div><div>16%</div></div>
7	H	129	<div><div>44%</div><div>46%</div><div>10%</div></div>
8	I	129	<div><div>25%</div><div>51%</div><div>22%</div><div>..</div></div>

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Mol	Chain	Length	Quality of chain
9	J	103	
10	K	128	
11	L	123	
12	M	117	
13	N	100	
14	O	89	
15	P	82	
16	Q	83	
17	R	74	
18	S	91	
19	T	86	
20	B	240	
21	U	71	
22	V	329	
22	W	329	
23	X	1342	
24	Y	1407	
25	Z	91	

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 71071 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 RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1530	Total	C	N	O	P	0	0
			32831	14642	6024	10635	1530		

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	150	Total	C	N	O	S	0	0
			1174	730	226	214	4		

- Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 13 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	88	Total	C	N	O	S	0	0
			716	440	146	129	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	79	ARG	GLN	conflict	UNP P0ADZ4

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	R	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 20 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	B	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	51	Total	C	N	O	S	0	0
			425	265	86	73	1		

- Molecule 22 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	225	Total	C	N	O	S	0	0
			1422	884	254	280	4		
22	W	216	Total	C	N	O	S	0	0
			1485	917	271	292	5		

- Molecule 23 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	1319	Total	C	N	O	S	1	0
			8347	5174	1507	1642	24		

- Molecule 24 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	1372	Total	C	N	O	S	0	0
			7824	4771	1488	1552	13		

- Molecule 25 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	79	Total	C	N	O	S	0	0
			623	379	116	127	1		

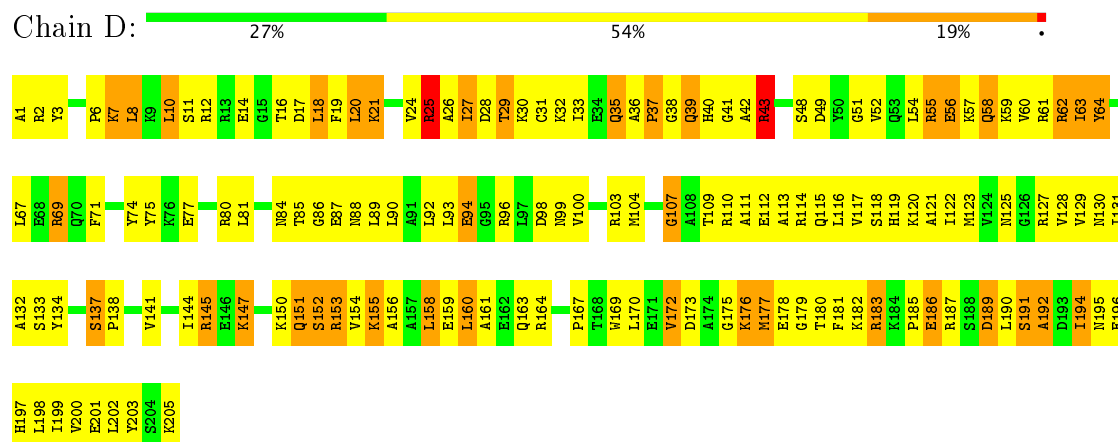
- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
26	Y	1	Total	Zn	0
			1	1	

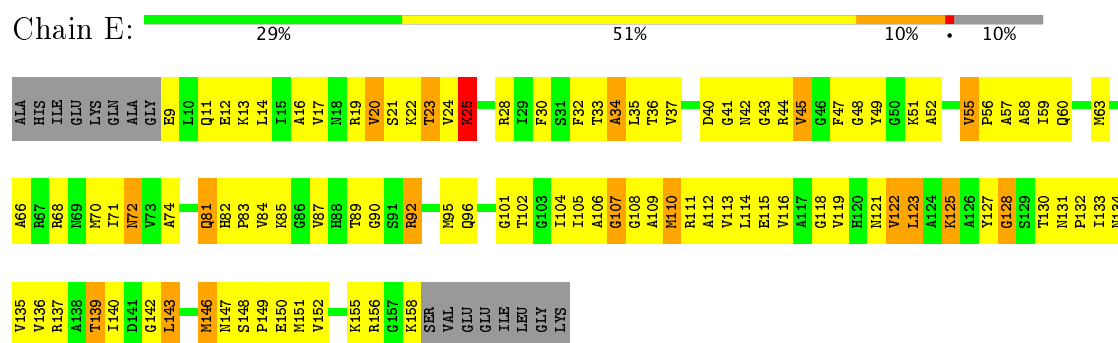
- Molecule 1: 16S ribosomal RNA



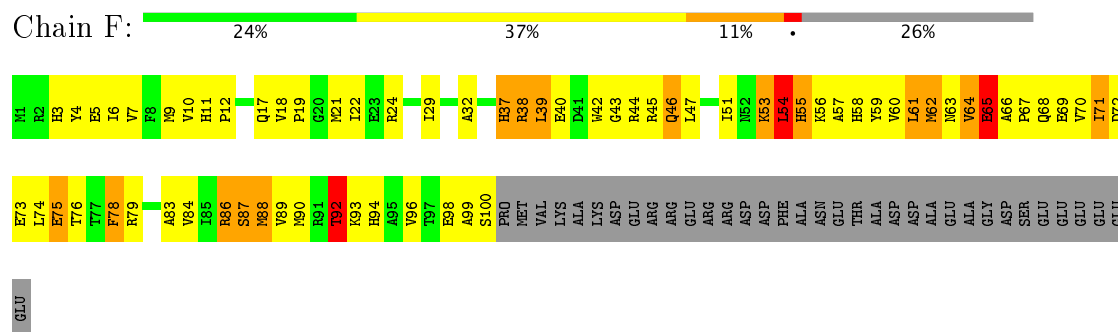
- Molecule 3: 30S ribosomal protein S4



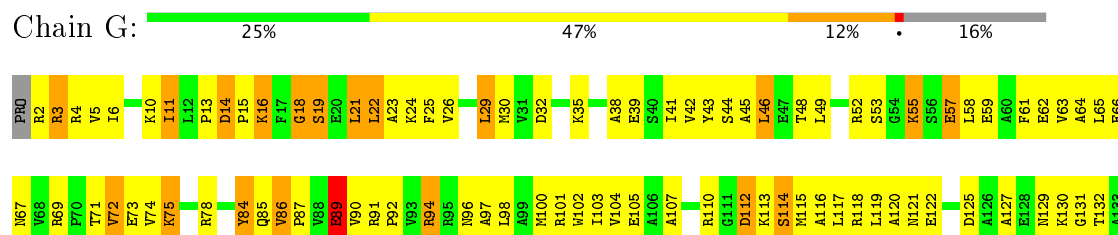
- Molecule 4: 30S ribosomal protein S5

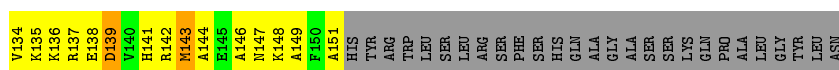


- Molecule 5: 30S ribosomal protein S6

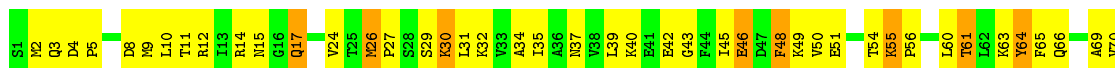


- Molecule 6: 30S ribosomal protein S7

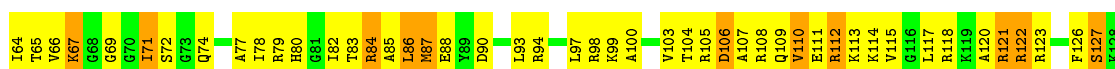
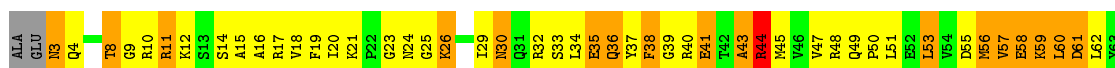




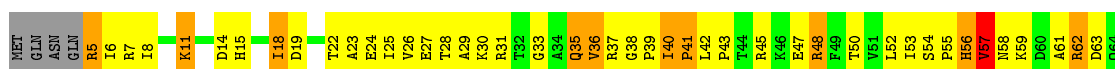
• Molecule 7: 30S ribosomal protein S8



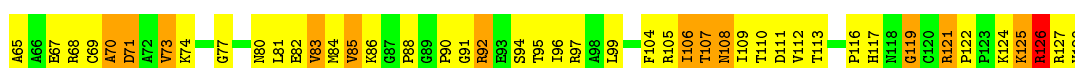
• Molecule 8: 30S ribosomal protein S9



• Molecule 9: 30S ribosomal protein S10

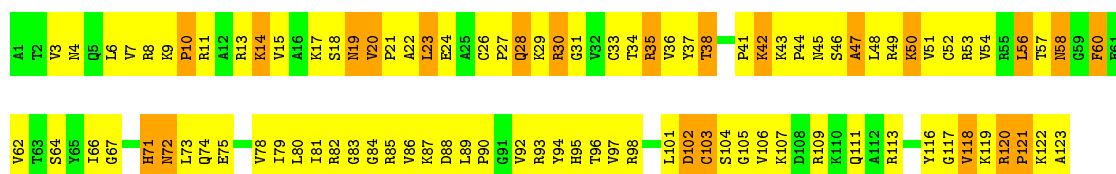


• Molecule 10: 30S ribosomal protein S11

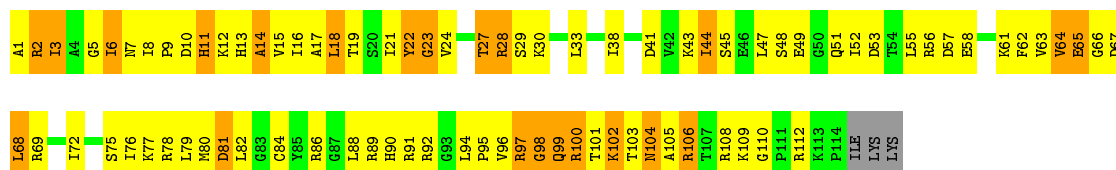


• Molecule 11: 30S ribosomal protein S12

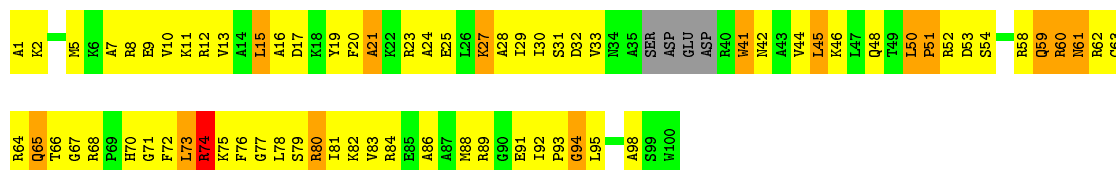
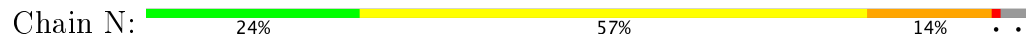




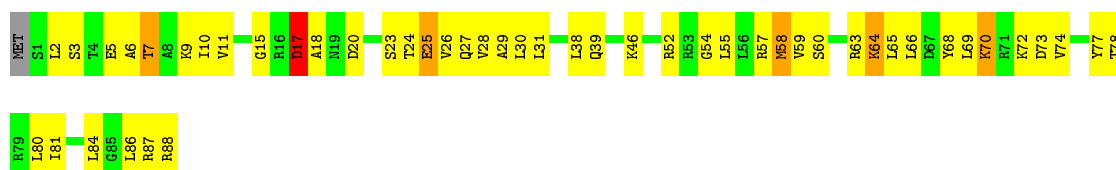
• Molecule 12: 30S ribosomal protein S13



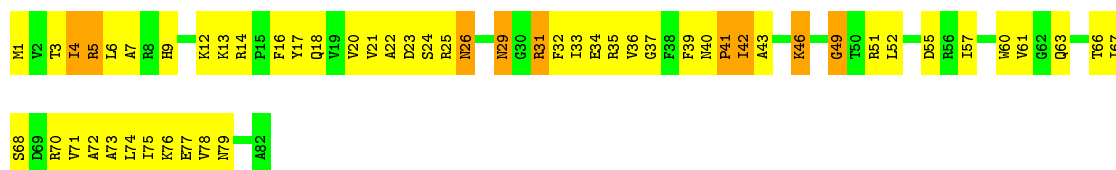
• Molecule 13: 30S ribosomal protein S14



• Molecule 14: 30S ribosomal protein S15

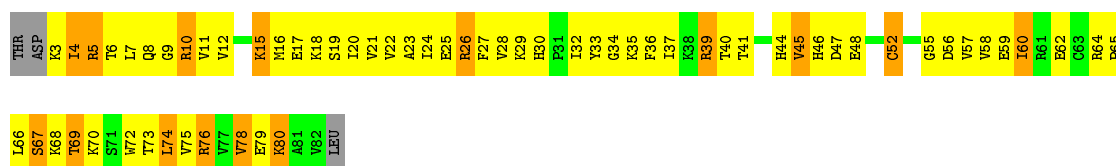


• Molecule 15: 30S ribosomal protein S16



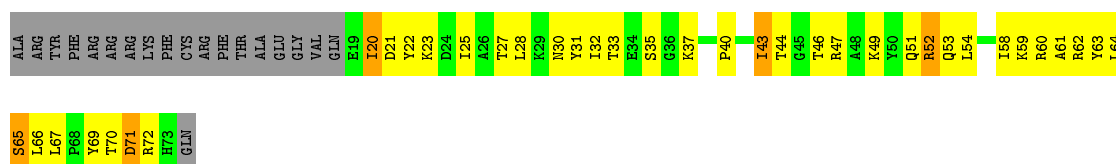
• Molecule 16: 30S ribosomal protein S17





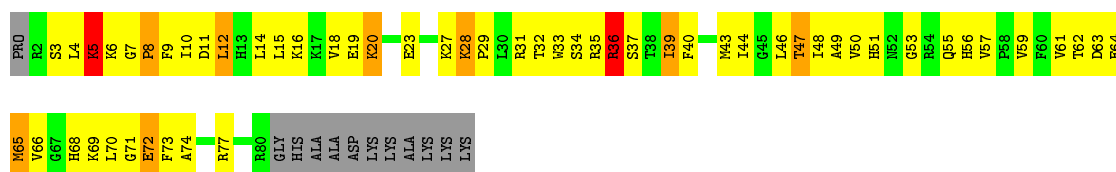
- Molecule 17: 30S ribosomal protein S18

Chain R: 24% 43% 7% 26%



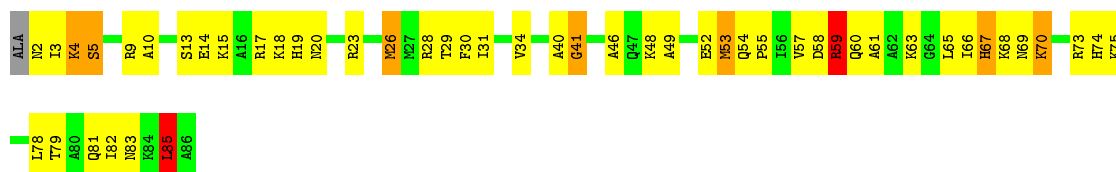
- Molecule 18: 30S ribosomal protein S19

Chain S: 25% 51% 9% 13%



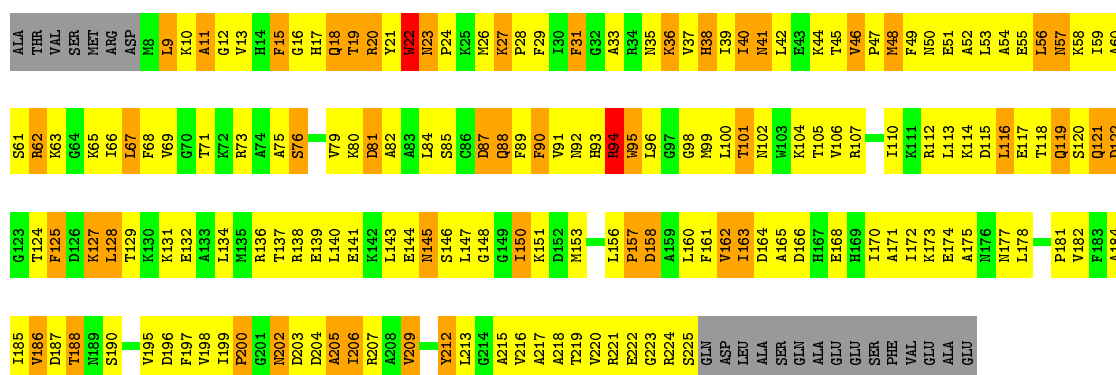
- Molecule 19: 30S ribosomal protein S20

Chain T: 41% 48% 8% ..



- Molecule 20: 30S ribosomal protein S2

Chain B: 20% 51% 20% 9%



- Molecule 21: 30S ribosomal protein S21

Chain U: 

MET PRO VAL I3 K4 V5 R6 E7 N8 E9 P10 F11 D12 V13 A14 L15 R16 R17 F18 K19 R20 S21 C22 E23 K24 A25 G26 V27 L28 A29 E30 V31 R32 R33 R34 E35 F36 Y37 E38 K39 P40 T41 T42 E43 R44 K48 V52 K53 ARG HIS ALA LYS LYS LEU ALA ARG ASN

ALA ARG ARG THR ARG LEU TYR

- Molecule 22: DNA-directed RNA polymerase subunit alpha

Chain V: 

MET GLN GLY SER VAL ASP THR LEU PHE K10 V14 K95 L102 T111 A112 A113 D114 I115 T116 H117 D118 G119 D120 K125 P126 Q127 H128 E163 D164 S178 E193 L234 ARG ASP VAL ARG GLN PRO GLU VAL LYS GLU ASP VAL ARG LYS LYS SER THR LEU ILE LYS ASP VAL VAL SER PHE ASP PRO ILE LEU

LEU ARG PRO VAL ASP LEU GLU THR VAL ARG SER ASN CYS LEU LYS ALA GLU ILE HIS TYR ILE GLY ASP LEU VAL GLN ARG THR VAL GLU LYS THR ASN GLY LYS LYS SER THR LEU ILE LYS ASP VAL VAL SER PHE ASP PRO ILE LEU

LEU GLY MET ARG LEU ASN TRP PRO ALA SER ILE ALA ASP GLU

- Molecule 22: DNA-directed RNA polymerase subunit alpha

Chain W: 

MET GLN GLY S4 L13 L133 A138 H160 SER GLU ASP GLU ARG ARG PRO ILE GLY ARG LEU VAL D174 E193 V232 ASP LEU ARG VAL ARG GLN PRO GLU VAL LYS GLU GLY LYS PRO GLU PHE ASP PRO ILE LEU LEU LEU LEU MET ARG VAL ASP ASP LEU LEU

THR VAL ARG SER ALA ASN CYS LEU LYS ALA ILE HIS TYR ILE ASP GLU LEU VAL GLN ARG THR GLU LEU LEU LYS THR ASN GLY LYS SER LEU THR ILE ASP VAL LEU MET ARG LEU LEU LEU TRP LEU

PRO ALA SER ILE ALA ASP GLU

- Molecule 23: DNA-directed RNA polymerase subunit beta

Chain X: 

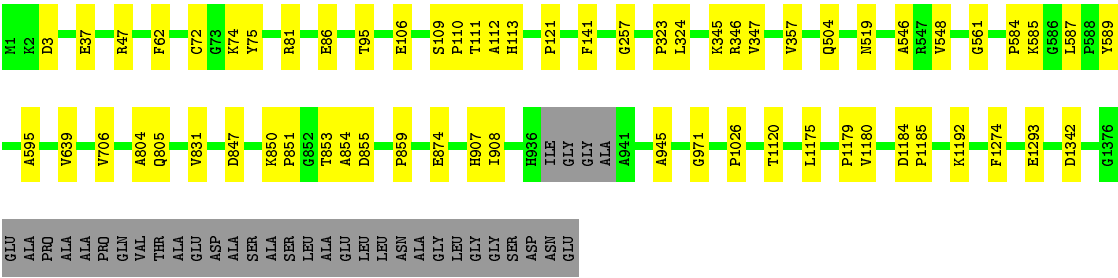
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A860 A861 L862 S863 K864 L865 D866 E867 I873 K886 V887 T893 Q894 L895 T896 P897 E898 E899 K900 L901 L902 R903 A904 I905 K943 R944 E947 G983 VAL GLU ALA GLU LYS LEU ASP LYS LEU ASP LEU PRO ARG ASP ARG TRP LEU LEU LEU GLY LEU THR D1004 L1042 A1043 P1044

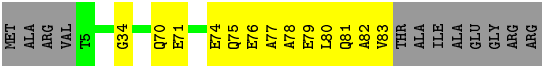
V1138 V1159 T1255 T1292 S1295 P1317 E1321 D1341 GLU

- Molecule 24: DNA-directed RNA polymerase subunit beta'

Chain Y: 



- Molecule 25: DNA-directed RNA polymerase subunit omega



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	15085	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	16	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.27	1/36762 (0.0%)	0.75	7/57350 (0.0%)
10	K	0.24	0/893	0.46	0/1205
11	L	0.22	0/969	0.47	0/1300
12	M	0.21	0/892	0.48	0/1193
13	N	0.25	0/785	0.46	0/1043
14	O	0.23	0/724	0.45	0/966
15	P	0.26	0/659	0.44	0/884
16	Q	0.24	0/657	0.46	0/881
17	R	0.23	0/462	0.46	0/621
18	S	0.26	0/652	0.46	0/877
19	T	0.24	0/671	0.41	0/888
2	C	0.23	0/1651	0.45	0/2225
20	B	0.25	0/1735	0.47	0/2338
21	U	1.01	4/430 (0.9%)	0.74	2/570 (0.4%)
22	V	0.36	0/1438	0.57	0/1982
22	W	0.37	0/1502	0.57	0/2052
23	X	0.35	0/8473	0.54	2/11640 (0.0%)
24	Y	0.34	0/7889	0.52	0/10883
25	Z	0.36	0/625	0.52	0/842
3	D	0.23	0/1665	0.46	0/2227
4	E	0.23	0/1118	0.45	0/1504
5	F	0.25	0/835	0.47	0/1128
6	G	0.23	0/1187	0.45	0/1591
7	H	0.24	0/989	0.45	0/1326
8	I	0.24	0/1034	0.45	0/1375
9	J	0.23	0/796	0.49	0/1077
All	All	0.29	5/75493 (0.0%)	0.64	11/109968 (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	A	0	16
21	U	0	1
23	X	0	1
All	All	0	18

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	U	15	LEU	C-N	-15.10	0.99	1.34
21	U	25	ALA	C-N	-9.37	1.16	1.33
1	A	463	U	O3'-P	-6.66	1.53	1.61
21	U	29	ALA	C-N	6.60	1.49	1.34
21	U	11	PHE	C-N	-5.38	1.21	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	765	G	N9-C1'-C2'	-8.19	102.99	112.00
1	A	438	U	N1-C1'-C2'	-6.31	105.06	112.00
1	A	232	G	C5'-C4'-C3'	-6.22	106.04	116.00
1	A	66	A	N9-C1'-C2'	-5.95	105.45	112.00
21	U	15	LEU	C-N-CA	5.74	136.05	121.70

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	G	Sidechain
1	A	281	G	Sidechain
1	A	437	U	Sidechain
1	A	438	U	Sidechain
1	A	58	C	Sidechain

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	32831	0	16521	1126	0
2	C	1624	0	1697	268	0
3	D	1643	0	1707	213	0
4	E	1105	0	1148	112	0
5	F	817	0	808	75	0
6	G	1174	0	1230	104	0
7	H	979	0	1034	79	0
8	I	1022	0	1070	143	0
9	J	786	0	828	129	0
10	K	877	0	887	109	0
11	L	955	0	1019	101	0
12	M	883	0	944	85	0
13	N	774	0	827	94	0
14	O	716	0	742	49	0
15	P	649	0	666	78	0
16	Q	648	0	691	77	0
17	R	455	0	478	40	0
18	S	637	0	665	76	0
19	T	665	0	714	52	0
20	B	1704	0	1725	314	0
21	U	425	0	447	102	0
22	V	1422	0	1178	38	0
22	W	1485	0	1322	0	0
23	X	8347	0	6484	136	0
24	Y	7824	0	5280	17	0
25	Z	623	0	617	126	0
26	Y	1	0	0	0	0
All	All	71071	0	50729	3201	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 26.

The worst 5 of 3201 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)
9:J:89:ARG:HG3	22:V:116:THR:CB	1.15	1.56
2:C:126:ARG:HB2	23:X:904:ALA:CB	1.15	1.55
20:B:63:LYS:NZ	25:Z:34:GLY:CA	1.70	1.50
2:C:126:ARG:CB	23:X:904:ALA:CB	1.89	1.49
9:J:89:ARG:CG	22:V:116:THR:CB	1.85	1.49

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	
2	C	204/232 (88%)	135 (66%)	50 (24%)	19 (9%)	1	14
3	D	203/205 (99%)	131 (64%)	54 (27%)	18 (9%)	1	15
4	E	148/166 (89%)	107 (72%)	34 (23%)	7 (5%)	3	28
5	F	98/135 (73%)	69 (70%)	23 (24%)	6 (6%)	2	22
6	G	148/178 (83%)	103 (70%)	37 (25%)	8 (5%)	2	25
7	H	127/129 (98%)	105 (83%)	19 (15%)	3 (2%)	7	42
8	I	125/129 (97%)	86 (69%)	28 (22%)	11 (9%)	1	15
9	J	96/103 (93%)	63 (66%)	21 (22%)	12 (12%)	0	7
10	K	115/128 (90%)	75 (65%)	27 (24%)	13 (11%)	0	8
11	L	121/123 (98%)	74 (61%)	30 (25%)	17 (14%)	0	5
12	M	112/117 (96%)	87 (78%)	14 (12%)	11 (10%)	1	12
13	N	92/100 (92%)	59 (64%)	24 (26%)	9 (10%)	1	12
14	O	86/89 (97%)	66 (77%)	18 (21%)	2 (2%)	7	43
15	P	80/82 (98%)	59 (74%)	16 (20%)	5 (6%)	1	22
16	Q	78/83 (94%)	48 (62%)	26 (33%)	4 (5%)	2	26
17	R	53/74 (72%)	27 (51%)	19 (36%)	7 (13%)	0	6
18	S	77/91 (85%)	57 (74%)	14 (18%)	6 (8%)	1	17
19	T	83/86 (96%)	69 (83%)	8 (10%)	6 (7%)	1	19
20	B	216/240 (90%)	145 (67%)	53 (24%)	18 (8%)	1	16
21	U	49/71 (69%)	22 (45%)	12 (24%)	15 (31%)	0	0
22	V	223/329 (68%)	193 (86%)	23 (10%)	7 (3%)	5	36
22	W	212/329 (64%)	186 (88%)	23 (11%)	3 (1%)	13	54
23	X	1312/1342 (98%)	1106 (84%)	173 (13%)	33 (2%)	6	41
24	Y	1368/1407 (97%)	1155 (84%)	159 (12%)	54 (4%)	3	31
25	Z	77/91 (85%)	72 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5503/6059 (91%)	4299 (78%)	910 (16%)	294 (5%)	4	26

5 of 294 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	2	GLN
2	C	91	ALA
2	C	153	SER
3	D	18	LEU
3	D	31	CYS

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	
2	C	170/189 (90%)	142 (84%)	28 (16%)	2	16
3	D	172/172 (100%)	140 (81%)	32 (19%)	2	11
4	E	113/125 (90%)	92 (81%)	21 (19%)	2	11
5	F	87/116 (75%)	68 (78%)	19 (22%)	1	7
6	G	123/146 (84%)	102 (83%)	21 (17%)	2	15
7	H	104/104 (100%)	87 (84%)	17 (16%)	3	17
8	I	105/106 (99%)	83 (79%)	22 (21%)	1	8
9	J	86/90 (96%)	66 (77%)	20 (23%)	1	6
10	K	90/98 (92%)	70 (78%)	20 (22%)	1	7
11	L	103/103 (100%)	88 (85%)	15 (15%)	3	21
12	M	92/95 (97%)	70 (76%)	22 (24%)	1	5
13	N	79/83 (95%)	67 (85%)	12 (15%)	3	19
14	O	76/77 (99%)	69 (91%)	7 (9%)	11	37
15	P	65/65 (100%)	56 (86%)	9 (14%)	4	23
16	Q	74/77 (96%)	60 (81%)	14 (19%)	2	11
17	R	48/64 (75%)	45 (94%)	3 (6%)	21	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	S	70/78 (90%)	60 (86%)	10 (14%)	4	22
19	T	65/65 (100%)	56 (86%)	9 (14%)	4	23
20	B	180/198 (91%)	142 (79%)	38 (21%)	1	8
21	U	44/61 (72%)	36 (82%)	8 (18%)	2	12
22	V	106/286 (37%)	104 (98%)	2 (2%)	62	82
22	W	130/286 (46%)	129 (99%)	1 (1%)	85	92
23	X	567/1157 (49%)	567 (100%)	0	100	100
24	Y	332/1168 (28%)	330 (99%)	2 (1%)	89	94
25	Z	66/75 (88%)	66 (100%)	0	100	100
All	All	3147/5084 (62%)	2795 (89%)	352 (11%)	11	29

5 of 352 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	I	126	PHE
10	K	117	HIS
20	B	122	ASP
9	J	18	ILE
9	J	98	VAL

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

Mol	Chain	Res	Type
8	I	36	GLN
10	K	28	ASN
20	B	121	GLN
8	I	49	GLN
9	J	20	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1529/1542 (99%)	277 (18%)	25 (1%)

5 of 277 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	A
1	A	9	G
1	A	14	U
1	A	31	G
1	A	32	A

5 of 25 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	913	A
1	A	975	A
1	A	1397	C
1	A	960	U
1	A	1025	U

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 1 ligands modelled in this entry, 1 is 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
23	X	2
21	U	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	967:LEU	C	968:GLU	N	4.69
1	X	941:LYS	C	942:ASP	N	3.24
1	U	25:ALA	C	26:GLY	N	1.16
1	U	15:LEU	C	16:ARG	N	0.99