



## wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Jul 24, 2017 – 01:15 PM EDT

PDB ID : 5NSS  
EMDB ID: : EMD-3696  
Title : Cryo-EM structure of RNA polymerase-sigma54 holoenzyme with promoter  
DNA and transcription activator PspF intermediate complex  
Authors : Glyde, R.; Ye, F.Z.; Darbari, V.C.; Zhang, N.; Buck, M.; Zhang, X.D.  
Deposited on : unknown  
Resolution : 5.80 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](mailto: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.

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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

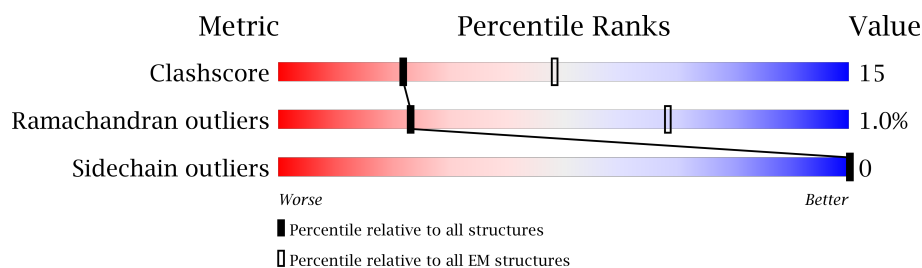
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*










The reported resolution of this entry is 5.80 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.





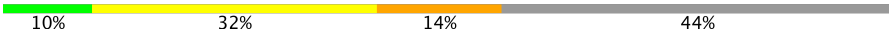


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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  $\geq 3$ , 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	 48% 24% . 28%
1	B	329	 50% 20% . 29%
2	C	1342	 72% 27% .
3	D	1449	 73% 20% 7%
4	E	91	 60% 21% 19%
5	F	295	 74% 11% 16%
5	G	295	 75% 9% 15%
5	J	295	 75% 10% 15%
5	K	295	 76% 8% 16%

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Mol	Chain	Length	Quality of chain
5	L	295	 75% 9% 15%
5	N	295	 76% 9% 15%
6	H	63	 10% 32% 14% 44%
7	M	581	 61% 5% 33%
8	I	63	 37% 10% 51%

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 32252 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	238	Total	C	N	O	S	0	0
			1691	1057	301	327	6		
1	B	235	Total	C	N	O	S	0	0
			1665	1040	295	325	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0
			9347	5862	1629	1823	33		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1352	Total	C	N	O	S	0	0
			8312	5137	1533	1616	26		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	74	Total	C	N	O	S	0	0
			520	320	98	101	1		

- Molecule 5 is a protein called Psp operon transcriptional activator.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	248	Total	C	N	O		0	0
			1222	726	248	248			
5	G	251	Total	C	N	O		0	0
			1237	735	251	251			
5	J	251	Total	C	N	O		0	0
			1237	735	251	251			

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Mol	Chain	Residues	Atoms				AltConf	Trace
5	K	248	Total	C	N	O	0	0
			1222	726	248	248		
5	L	250	Total	C	N	O	0	0
			1232	732	250	250		
5	N	251	Total	C	N	O	0	0
			1237	735	251	251		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	initiating methionine	UNP P37344
F	-18	GLY	-	expression tag	UNP P37344
F	-17	SER	-	expression tag	UNP P37344
F	-16	SER	-	expression tag	UNP P37344
F	-15	HIS	-	expression tag	UNP P37344
F	-14	HIS	-	expression tag	UNP P37344
F	-13	HIS	-	expression tag	UNP P37344
F	-12	HIS	-	expression tag	UNP P37344
F	-11	HIS	-	expression tag	UNP P37344
F	-10	HIS	-	expression tag	UNP P37344
F	-9	SER	-	expression tag	UNP P37344
F	-8	SER	-	expression tag	UNP P37344
F	-7	GLY	-	expression tag	UNP P37344
F	-6	LEU	-	expression tag	UNP P37344
F	-5	VAL	-	expression tag	UNP P37344
F	-4	PRO	-	expression tag	UNP P37344
F	-3	ARG	-	expression tag	UNP P37344
F	-2	GLY	-	expression tag	UNP P37344
F	-1	SER	-	expression tag	UNP P37344
F	0	HIS	-	expression tag	UNP P37344
G	-19	MET	-	initiating methionine	UNP P37344
G	-18	GLY	-	expression tag	UNP P37344
G	-17	SER	-	expression tag	UNP P37344
G	-16	SER	-	expression tag	UNP P37344
G	-15	HIS	-	expression tag	UNP P37344
G	-14	HIS	-	expression tag	UNP P37344
G	-13	HIS	-	expression tag	UNP P37344
G	-12	HIS	-	expression tag	UNP P37344
G	-11	HIS	-	expression tag	UNP P37344
G	-10	HIS	-	expression tag	UNP P37344
G	-9	SER	-	expression tag	UNP P37344
G	-8	SER	-	expression tag	UNP P37344

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	GLY	-	expression tag	UNP P37344
G	-6	LEU	-	expression tag	UNP P37344
G	-5	VAL	-	expression tag	UNP P37344
G	-4	PRO	-	expression tag	UNP P37344
G	-3	ARG	-	expression tag	UNP P37344
G	-2	GLY	-	expression tag	UNP P37344
G	-1	SER	-	expression tag	UNP P37344
G	0	HIS	-	expression tag	UNP P37344
J	-19	MET	-	initiating methionine	UNP P37344
J	-18	GLY	-	expression tag	UNP P37344
J	-17	SER	-	expression tag	UNP P37344
J	-16	SER	-	expression tag	UNP P37344
J	-15	HIS	-	expression tag	UNP P37344
J	-14	HIS	-	expression tag	UNP P37344
J	-13	HIS	-	expression tag	UNP P37344
J	-12	HIS	-	expression tag	UNP P37344
J	-11	HIS	-	expression tag	UNP P37344
J	-10	HIS	-	expression tag	UNP P37344
J	-9	SER	-	expression tag	UNP P37344
J	-8	SER	-	expression tag	UNP P37344
J	-7	GLY	-	expression tag	UNP P37344
J	-6	LEU	-	expression tag	UNP P37344
J	-5	VAL	-	expression tag	UNP P37344
J	-4	PRO	-	expression tag	UNP P37344
J	-3	ARG	-	expression tag	UNP P37344
J	-2	GLY	-	expression tag	UNP P37344
J	-1	SER	-	expression tag	UNP P37344
J	0	HIS	-	expression tag	UNP P37344
K	-19	MET	-	initiating methionine	UNP P37344
K	-18	GLY	-	expression tag	UNP P37344
K	-17	SER	-	expression tag	UNP P37344
K	-16	SER	-	expression tag	UNP P37344
K	-15	HIS	-	expression tag	UNP P37344
K	-14	HIS	-	expression tag	UNP P37344
K	-13	HIS	-	expression tag	UNP P37344
K	-12	HIS	-	expression tag	UNP P37344
K	-11	HIS	-	expression tag	UNP P37344
K	-10	HIS	-	expression tag	UNP P37344
K	-9	SER	-	expression tag	UNP P37344
K	-8	SER	-	expression tag	UNP P37344
K	-7	GLY	-	expression tag	UNP P37344
K	-6	LEU	-	expression tag	UNP P37344

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-5	VAL	-	expression tag	UNP P37344
K	-4	PRO	-	expression tag	UNP P37344
K	-3	ARG	-	expression tag	UNP P37344
K	-2	GLY	-	expression tag	UNP P37344
K	-1	SER	-	expression tag	UNP P37344
K	0	HIS	-	expression tag	UNP P37344
L	-19	MET	-	initiating methionine	UNP P37344
L	-18	GLY	-	expression tag	UNP P37344
L	-17	SER	-	expression tag	UNP P37344
L	-16	SER	-	expression tag	UNP P37344
L	-15	HIS	-	expression tag	UNP P37344
L	-14	HIS	-	expression tag	UNP P37344
L	-13	HIS	-	expression tag	UNP P37344
L	-12	HIS	-	expression tag	UNP P37344
L	-11	HIS	-	expression tag	UNP P37344
L	-10	HIS	-	expression tag	UNP P37344
L	-9	SER	-	expression tag	UNP P37344
L	-8	SER	-	expression tag	UNP P37344
L	-7	GLY	-	expression tag	UNP P37344
L	-6	LEU	-	expression tag	UNP P37344
L	-5	VAL	-	expression tag	UNP P37344
L	-4	PRO	-	expression tag	UNP P37344
L	-3	ARG	-	expression tag	UNP P37344
L	-2	GLY	-	expression tag	UNP P37344
L	-1	SER	-	expression tag	UNP P37344
L	0	HIS	-	expression tag	UNP P37344
N	-19	MET	-	initiating methionine	UNP P37344
N	-18	GLY	-	expression tag	UNP P37344
N	-17	SER	-	expression tag	UNP P37344
N	-16	SER	-	expression tag	UNP P37344
N	-15	HIS	-	expression tag	UNP P37344
N	-14	HIS	-	expression tag	UNP P37344
N	-13	HIS	-	expression tag	UNP P37344
N	-12	HIS	-	expression tag	UNP P37344
N	-11	HIS	-	expression tag	UNP P37344
N	-10	HIS	-	expression tag	UNP P37344
N	-9	SER	-	expression tag	UNP P37344
N	-8	SER	-	expression tag	UNP P37344
N	-7	GLY	-	expression tag	UNP P37344
N	-6	LEU	-	expression tag	UNP P37344
N	-5	VAL	-	expression tag	UNP P37344
N	-4	PRO	-	expression tag	UNP P37344

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-3	ARG	-	expression tag	UNP P37344
N	-2	GLY	-	expression tag	UNP P37344
N	-1	SER	-	expression tag	UNP P37344
N	0	HIS	-	expression tag	UNP P37344

- | Mol | Chain | Residues | Atoms        |          |          |          |         | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|---------|---------|-------|
| 6   | H     | 35       | Total<br>719 | C<br>340 | N<br>134 | O<br>210 | P<br>35 | 0       | 0     |

- | Mol | Chain | Residues | Atoms |      |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 7   | M     | 388      | Total | C    | N   | O   | 0       | 0     |
|     |       |          | 1977  | 1191 | 388 | 398 |         |       |

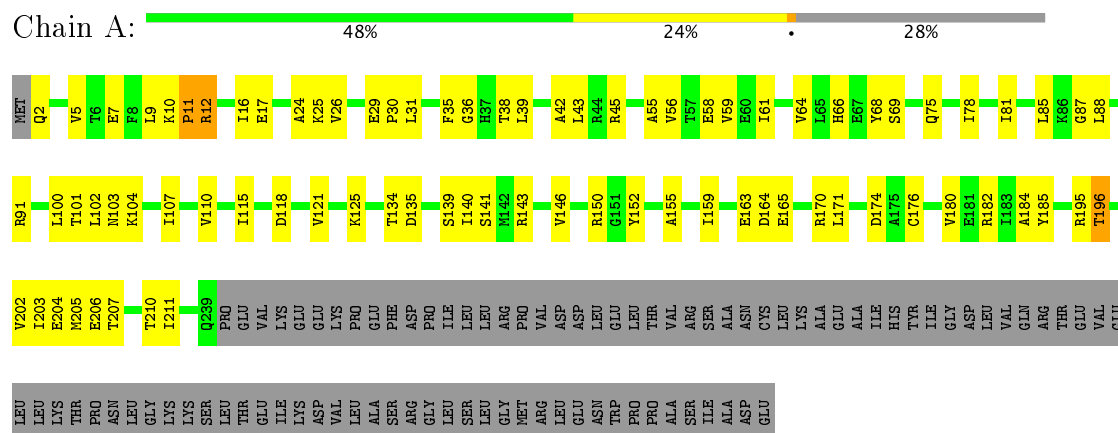
- | Mol | Chain | Residues | Atoms        |          |          |          |         | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|---------|---------|-------|
| 8   | I     | 31       | Total<br>634 | C<br>300 | N<br>117 | O<br>186 | P<br>31 | 0       | 0     |



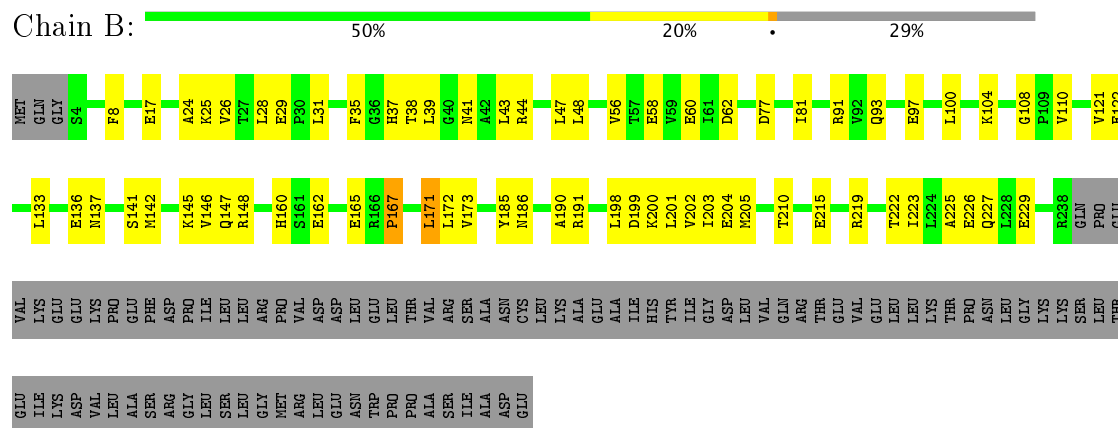
### 3 Residue-property plots

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. 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.

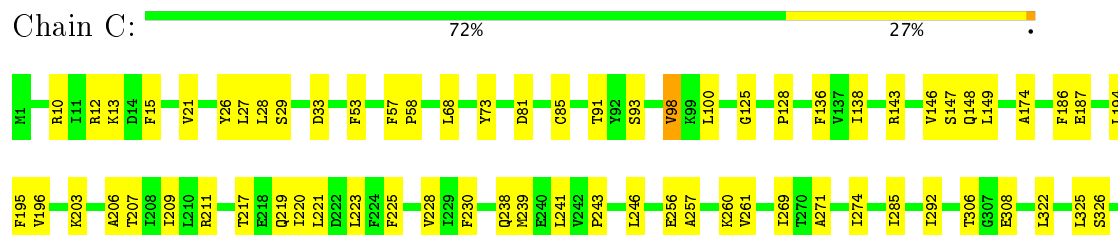
- Molecule 1: DNA-directed RNA polymerase subunit alpha

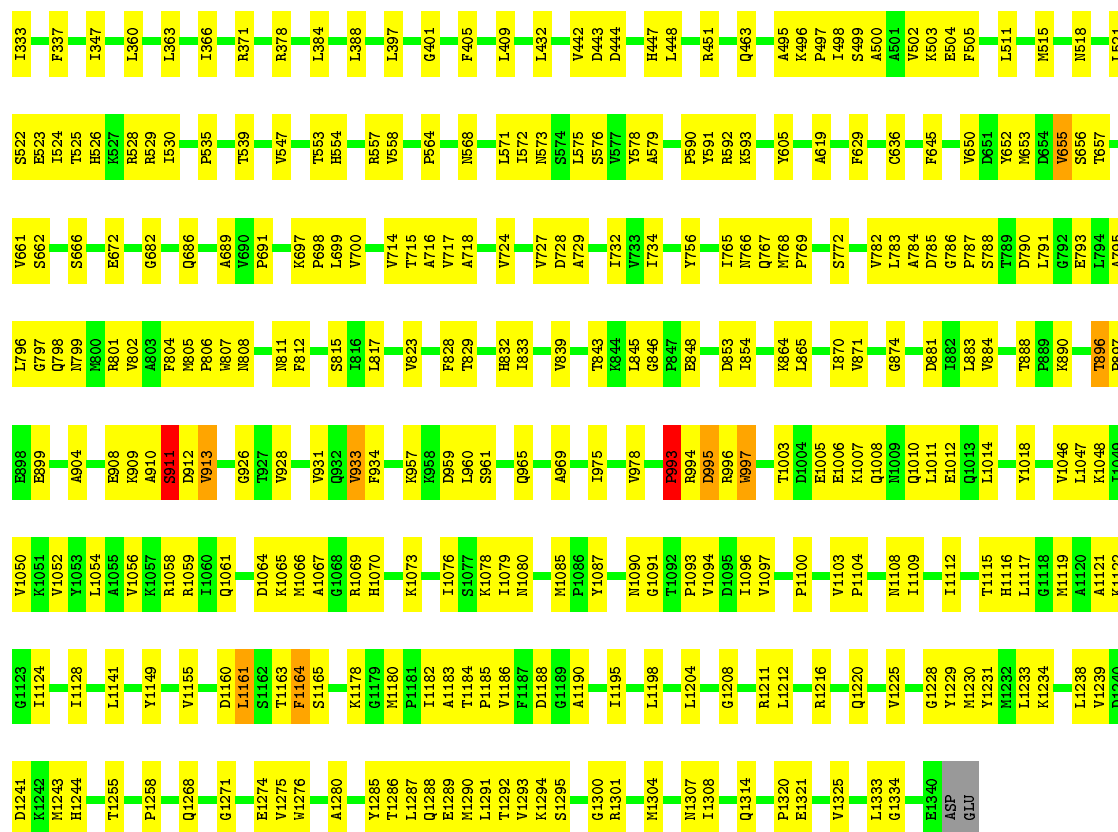


- Molecule 1: DNA-directed RNA polymerase subunit alpha



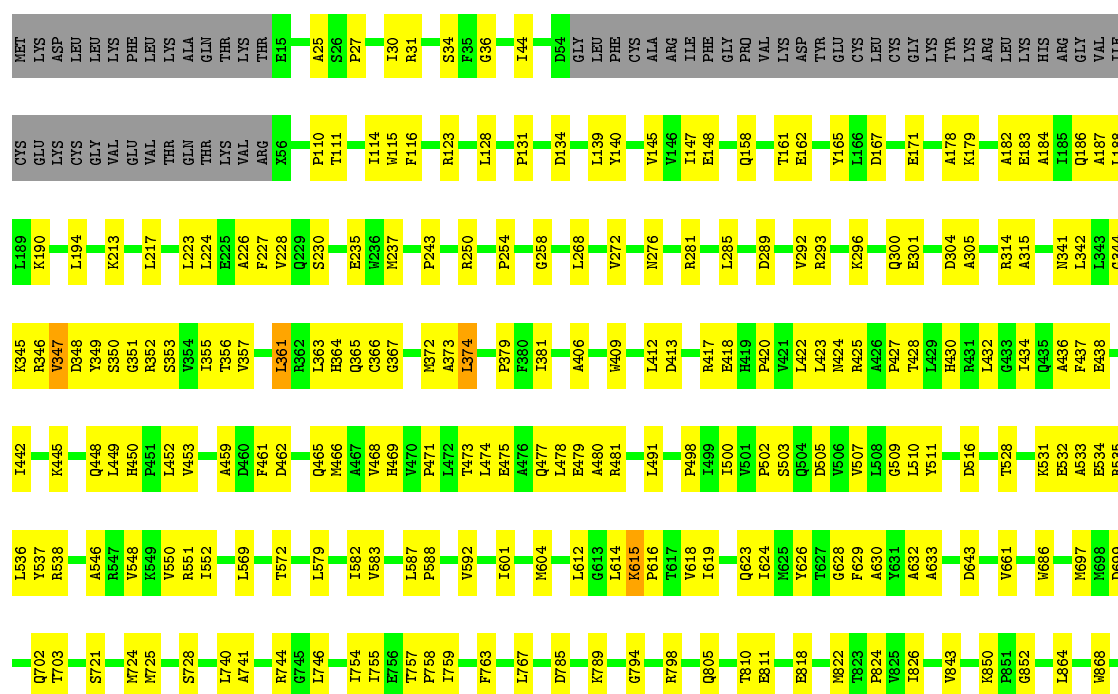
- Molecule 2: DNA-directed RNA polymerase subunit beta

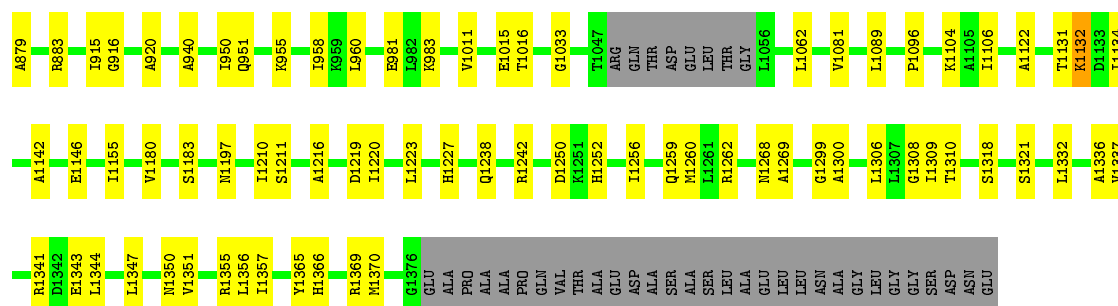




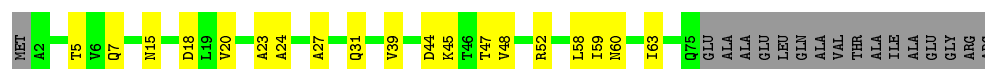
- Molecule 3: DNA-directed RNA polymerase subunit beta',DNA-directed RNA polymerase subunit beta',DNA-directed RNA polymerase subunit beta'

Chain D: 73% 20% 7%

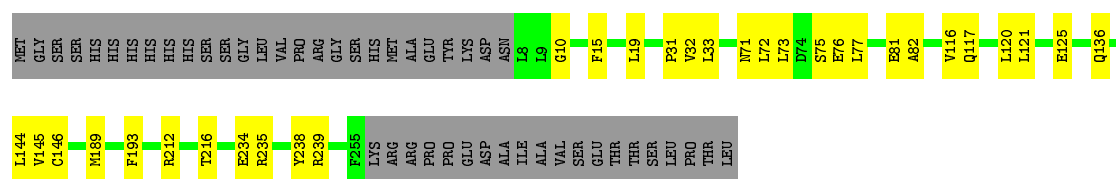




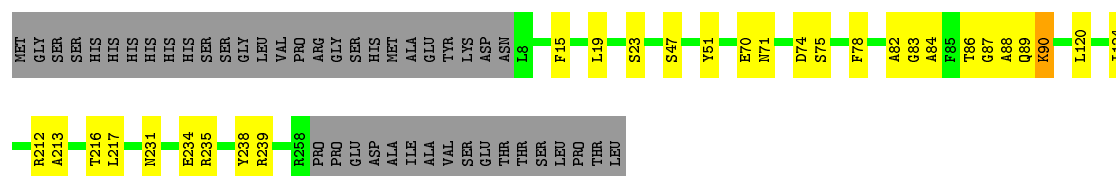
- Molecule 4: DNA-directed RNA polymerase subunit omega



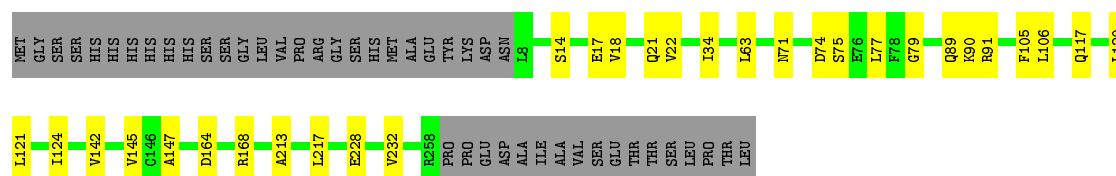
- Molecule 5: Psp operon transcriptional activator



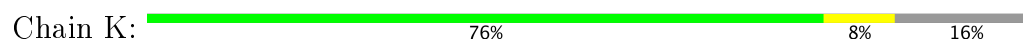
- Molecule 5: Psp operon transcriptional activator



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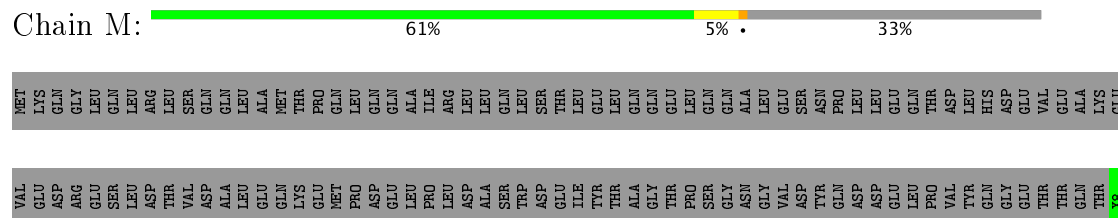


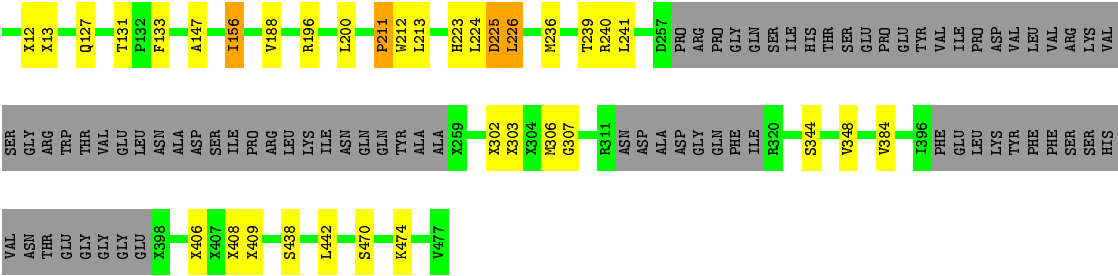
- Molecule 5: Psp operon transcriptional activator

- Molecule 5: Psp operon transcriptional activator

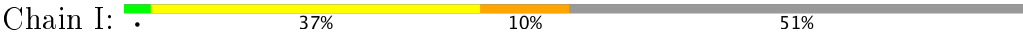
- Molecule 6: Non-template promoter DNA

- [illegible]





● Molecule 8: Template promoter DNA



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	79355	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.25	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

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	0.24	0/1708	0.48	0/2328
1	B	0.24	0/1680	0.48	1/2291 (0.0%)
2	C	0.25	1/9475 (0.0%)	0.47	3/12931 (0.0%)
3	D	0.25	0/8180	0.49	3/11220 (0.0%)
4	E	0.23	0/521	0.45	0/711
5	F	0.23	0/1221	0.41	0/1697
5	G	0.25	0/1236	0.45	0/1718
5	J	0.24	0/1236	0.42	0/1718
5	K	0.24	0/1221	0.42	0/1697
5	L	0.24	0/1231	0.44	0/1711
5	N	0.24	0/1236	0.40	0/1718
6	H	2.14	8/806 (1.0%)	1.74	11/1242 (0.9%)
7	M	0.24	0/1459	0.50	0/2034
8	I	1.14	9/709 (1.3%)	1.15	5/1089 (0.5%)
All	All	0.45	18/31919 (0.1%)	0.57	23/44105 (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	C	0	1
3	D	0	3
7	M	0	1
All	All	0	5

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	68	DT	O3'-P	-40.57	1.12	1.61
6	H	83	DC	O3'-P	-33.28	1.21	1.61
8	I	-22	DC	O3'-P	-10.42	1.48	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	-21	DG	O3'-P	8.36	1.71	1.61
6	H	75	DG	C1'-N9	-7.03	1.37	1.47

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	83	DC	P-O3'-C3'	37.54	164.75	119.70
6	H	69	DG	P-O3'-C3'	-23.90	91.02	119.70
8	I	-13	DC	P-O3'-C3'	12.84	135.11	119.70
6	H	83	DC	OP1-P-O3'	11.25	129.95	105.20
6	H	83	DC	C5'-C4'-O4'	11.09	130.37	109.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	896	THR	Peptide
3	D	1183	SER	Peptide
3	D	250	ARG	Peptide
3	D	614	LEU	Peptide
7	M	133	PHE	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	1691	0	1625	55	0
1	B	1665	0	1603	53	0
2	C	9347	0	8545	275	0
3	D	8312	0	6467	228	0
4	E	520	0	493	15	0
5	F	1222	0	556	16	0
5	G	1237	0	562	18	0
5	J	1237	0	562	18	0
5	K	1222	0	556	12	0
5	L	1232	0	560	18	0
5	N	1237	0	562	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	719	0	395	64	0
7	M	1977	0	888	34	0
8	I	634	0	349	44	0
All	All	32252	0	23723	813	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 15.

The worst 5 of 813 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)
6:H:68:DT:O3'	6:H:69:DG:P	1.12	1.51
6:H:72:DC:H41	7:M:13:UNK:CB	1.33	1.42
6:H:74:DT:H2''	6:H:75:DG:C5'	1.52	1.40
6:H:68:DT:HO3'	6:H:69:DG:P	0.90	1.38
3:D:366:CYS:SG	3:D:437:PHE:HB2	1.70	1.32

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	234/329 (71%)	211 (90%)	18 (8%)	5 (2%)	8	45
1	B	233/329 (71%)	212 (91%)	17 (7%)	4 (2%)	11	51
2	C	1338/1342 (100%)	1221 (91%)	103 (8%)	14 (1%)	18	61
3	D	1304/1449 (90%)	1161 (89%)	135 (10%)	8 (1%)	28	70
4	E	72/91 (79%)	68 (94%)	4 (6%)	0	100	100
5	F	246/295 (83%)	231 (94%)	14 (6%)	1 (0%)	38	77
5	G	249/295 (84%)	236 (95%)	11 (4%)	2 (1%)	22	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	J	249/295 (84%)	232 (93%)	15 (6%)	2 (1%)	22	66
5	K	246/295 (83%)	229 (93%)	15 (6%)	2 (1%)	22	66
5	L	248/295 (84%)	236 (95%)	10 (4%)	2 (1%)	22	66
5	N	249/295 (84%)	235 (94%)	13 (5%)	1 (0%)	38	77
7	M	276/581 (48%)	233 (84%)	37 (13%)	6 (2%)	8	44
All	All	4944/5891 (84%)	4505 (91%)	392 (8%)	47 (1%)	23	61

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	10	LYS
1	A	11	PRO
1	A	12	ARG
1	A	196	THR

### 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	166/286 (58%)	166 (100%)	0	100	100
1	B	162/286 (57%)	162 (100%)	0	100	100
2	C	857/1157 (74%)	857 (100%)	0	100	100
3	D	509/1168 (44%)	509 (100%)	0	100	100
4	E	48/75 (64%)	48 (100%)	0	100	100
7	M	23/423 (5%)	23 (100%)	0	100	100
All	All	1765/3395 (52%)	1765 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	1061	GLN
2	C	1080	ASN
3	D	805	GLN
2	C	832	HIS
3	D	1244	GLN

### 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](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	M	3
6	H	2
1	A	1
3	D	1

The worst 5 of 7 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	49:UNK	C	120:LEU	N	59.90
1	M	413:UNK	C	415:ALA	N	4.42
1	A	237:VAL	C	238:ARG	N	3.50
1	M	304:UNK	C	306:MET	N	3.31
1	D	97:UNK	C	99:ARG	N	3.04