



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 06:33 am BST

PDB ID : 4YG2
Title : X-ray crystal structur of Escherichia coli RNA polymerase sigma70 holoenzyme
Authors : Murakami, K.S.
Deposited on : 2015-02-25
Resolution : 3.70 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	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

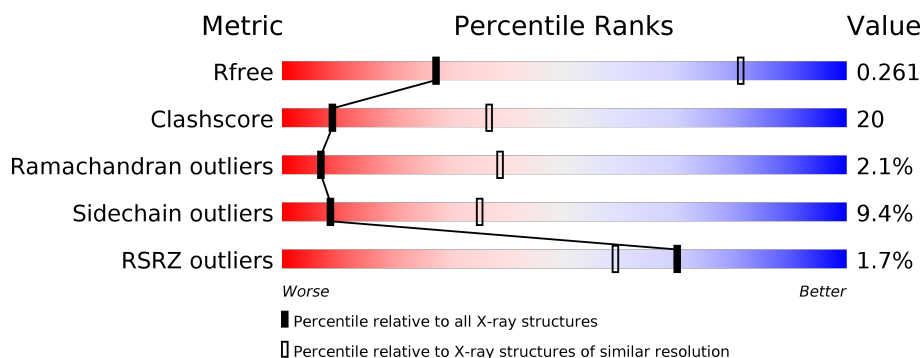
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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}	130704	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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 respectively. 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	329	<div> <div>46%</div> <div>41%</div> <div>9%</div> <div>••</div> </div>
1	B	329	<div>2%</div> <div>37%</div> <div>27%</div> <div>•</div> <div>34%</div>
1	G	329	<div>34%</div> <div>28%</div> <div>5%</div> <div>•</div> <div>31%</div>
1	H	329	<div>%</div> <div>34%</div> <div>29%</div> <div>•</div> <div>34%</div>
2	C	1342	<div>%</div> <div>54%</div> <div>40%</div> <div>5%</div>
2	I	1342	<div>3%</div> <div>59%</div> <div>37%</div> <div>•</div>

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Mol	Chain	Length	Quality of chain
3	D	1407	<div><div></div><div>44%33%5%17%</div></div>
3	J	1407	<div><div>%</div><div>45%32%5%18%</div></div>
4	E	91	<div><div></div><div>62%27%9%•</div></div>
4	K	91	<div><div>%</div><div>47%33%7%13%</div></div>
5	F	613	<div><div>3%</div><div>41%33%•24%</div></div>
5	L	613	<div><div>2%</div><div>40%33%•23%</div></div>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 55741 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 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2490	1557	439	486	8			
1	B	217	Total	C	N	O	S	0	0	0
			1677	1047	295	329	6			
1	G	227	Total	C	N	O	S	0	0	0
			1755	1093	311	345	6			
1	H	216	Total	C	N	O	S	0	0	0
			1662	1038	292	326	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0	0
			10570	6631	1841	2055	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10566	6629	1840	2054	43			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1166	Total	C	N	O	S	0	0	0
			9060	5697	1621	1696	46			
3	J	1155	Total	C	N	O	S	0	0	0
			9001	5659	1612	1684	46			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	S	0	0	0
			691	421	129	140	1			
4	K	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	468	Total	C	N	O	S	0	0	0
			3813	2389	678	723	23			
5	L	469	Total	C	N	O	S	0	0	0
			3821	2393	679	726	23			

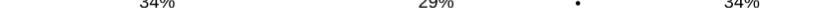
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	1	Total	Mg	0	0
			1	1		
6	I	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	2	Total	Zn	0	0
			2	2		
7	D	2	Total	Zn	0	0
			2	2		

[illegible]

Chain H: 

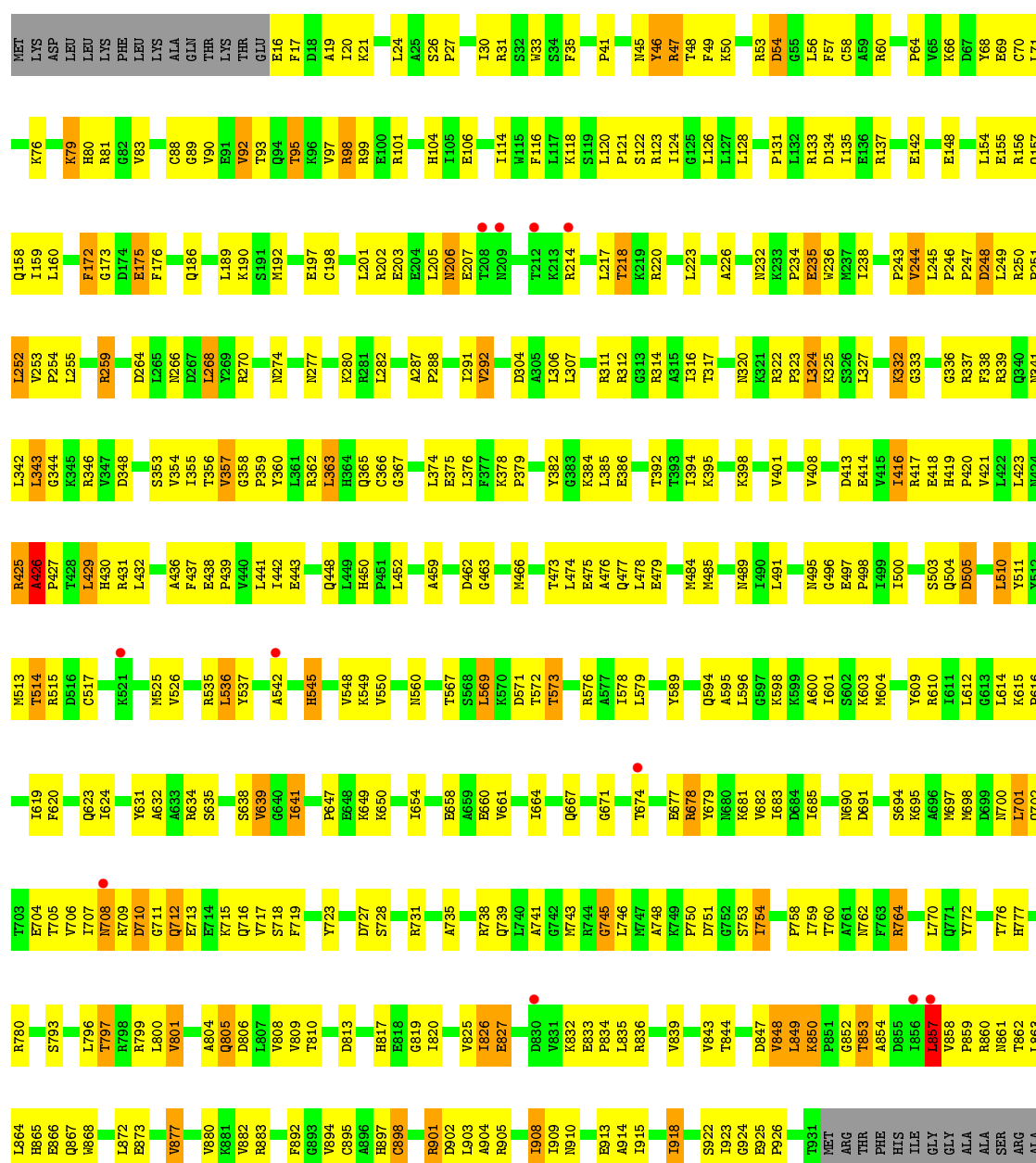
Residue	Category	Residue	Category	Residue	Category	Residue	Category	Residue	Category
LYS	Grey	VAL	Grey	Y153	Yellow	GLN	Grey	GLN	Grey
LEU	Grey	ARG	Grey	R158	Yellow	GLY	Grey	GLY	Grey
SER	Grey	PRO	Grey	ILE	Yellow	ASP	Grey	SER	Grey
THR	Grey	GLU	Grey	HIS	Yellow	LEU	Grey	VAL	Grey
GLU	Grey	VAL	Grey	SER	Yellow	GLU	Grey	T6	Yellow
ILE	Grey	LYS	Grey	GLU	Yellow	GLU	Grey	E7	Yellow
GLY	Grey	GLU	Grey	ASP	Yellow	GLU	Grey	F8	Yellow
ASP	Grey	GLY	Grey	GLU	Yellow	GLY	Grey	L9	Yellow
VAL	Grey	LYS	Grey	GLU	Yellow	GLY	Grey	K10	Yellow
LEU	Grey	PRO	Grey	ARG	Yellow	GLY	Grey	P11	Yellow
ALA	Grey	GLU	Grey	PRO	Yellow	GLY	Grey	R12	Yellow
SER	Grey	PHE	Grey	ILE	Yellow	GLY	Grey	L13	Yellow
ARG	Grey	ASP	Grey	GLY	Yellow	GLY	Grey	Q18	Orange
GLY	Grey	PRO	Grey	ARG	Yellow	GLY	Grey	V19	Orange
GLY	Grey	ILE	Grey	L171	Yellow	GLY	Grey	S20	Orange
LEU	Grey	LEU	Grey	L172	Yellow	GLY	Grey	S21	Orange
SER	Grey	LEU	Grey	V173	Yellow	GLY	Grey	T22	Orange
LEU	Grey	LEU	Grey	ARG	Yellow	GLY	Grey	H23	Orange
GLY	Grey	ARG	Grey	Y177	Yellow	GLY	Grey	A24	Orange
MET	Grey	VAL	Grey	S178	Yellow	GLY	Grey	T27	Orange
LEU	Grey	ARG	Grey	P179	Yellow	GLY	Grey	L28	Orange
GLU	Grey	ASP	Grey	V180	Yellow	GLY	Grey	E29	Orange
ASN	Grey	ASP	Grey	LEU	Yellow	GLY	Grey	P30	Orange
TRP	Grey	LEU	Grey	I183	Orange	GLY	Grey	F35	Orange
PRO	Grey	GLU	Grey	A184	Orange	GLY	Grey	G36	Orange
PRO	Grey	THR	Grey	Y185	Orange	GLY	Grey	H37	Orange
ALA	Grey	VAL	Grey	ALA	Orange	GLY	Grey	T38	Orange
SER	Grey	ARG	Grey	A190	Orange	GLY	Grey	R44	Orange
ILE	Grey	SER	Grey	ILE	Orange	GLY	Grey	R45	Orange
ALA	Grey	ALA	Grey	E193	Orange	GLY	Grey	I46	Orange
ASP	Grey	ALA	Grey	Q194	Orange	GLY	Grey	L47	Orange
GLU	Grey	ASN	Grey	R195	Orange	GLY	Grey	S49	Orange
LEU	Grey	CYS	Grey	R196	Orange	GLY	Grey	M51	Orange
GLY	Grey	LEU	Grey	D197	Orange	GLY	Grey	T57	Orange
ALA	Grey	LYS	Grey	I198	Orange	GLY	Grey	E58	Orange
GLU	Grey	ALA	Grey	D199	Orange	GLY	Grey	V59	Orange
GLU	Grey	ALA	Grey	K200	Orange	GLY	Grey	E60	Orange
ILE	Grey	ILE	Grey	L201	Orange	GLY	Grey	I61	Orange
HIS	Grey	HIS	Grey	V202	Orange	GLY	Grey	D62	Orange
TVR	Grey	TVR	Grey	M205	Orange	GLY	Grey	G63	Orange
ILE	Grey	ILE	Grey	E206	Orange	GLY	Grey	V64	Orange
GLY	Grey	GLY	Grey	T207	Orange	GLY	Grey	L65	Orange
ASP	Grey	ASP	Grey	LEU	Orange	GLY	Grey	H66	Orange
LEU	Grey	LEU	Grey	T210	Orange	GLY	Grey	E67	Orange
VAL	Grey	VAL	Grey	K221	Orange	GLY	Grey	V68	Orange
GLN	Grey	ARG	Grey	L224	Orange	GLY	Grey	S69	Orange
ARG	Grey	THR	Grey	Q227	Orange	GLY	Grey	I70	Orange
THR	Grey	GLU	Grey	L228	Orange	GLY	Grey	K71	Orange
VAL	Grey	VAL	Grey	F231	Orange	GLY	Grey	E73	Orange
GLU	Grey	GLU	Grey	V232	Orange	GLY	Grey	V74	Orange
LEU	Grey	LEU	Grey	D233	Orange	GLY	Grey	C75	Orange
LEU	Grey	LEU	Grey	ASN	Orange	GLY	Grey		
LYS	Grey	LYS	Grey	LEU	Orange	GLY	Grey		
THR	Grey	THR	Grey	ASP	Orange	GLY	Grey		
ASP	Grey	ASP	Grey	GLY	Orange	GLY	Grey		
GLU	Grey	GLU	Grey	ASP	Orange	GLY	Grey		

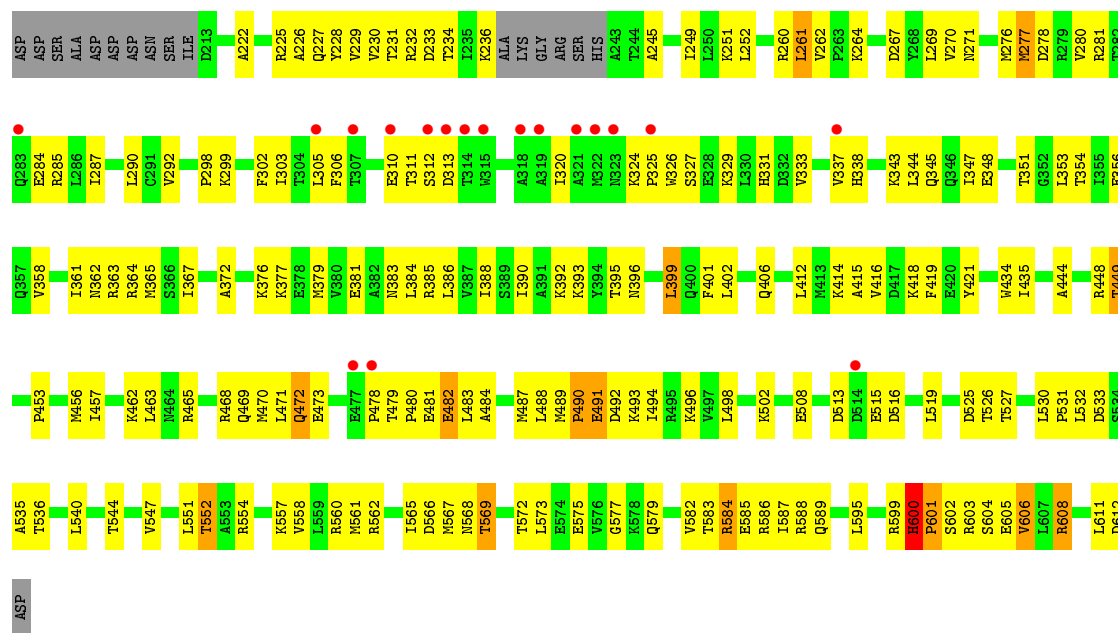
Chain C: 

A1283	L1204	Q1134	L1054	L979	V884	R687	V594	F506	L420	A298	L171	S93
A1284	P1205	Q1135	R1058	V980	G885	Q688	T595	S512	S421	A299	Y172	A94
T1285	T1206	Q1136	R1059	A981	X886	A689	D596	Q513	K422	L310	R175	P95
T1286	E1137	R1059	R1059	G982	T887	E775	G597	F514	D423	I314	I176	L96
L1287	R1210	Q1061	Q1061	G983	T888	E778	T600	M515	D423	N314	I177	R97
G1288	K1140	P1062	P1062	V984	R889	R694	D601	D516	V428	D320	V183	V98
E1289	L1141	G1063	G1063	E985	K890	R694	E601	Q517	D320	L321	L184	K99
M1290	R1142	E986	E986	A986	C891	D696	H604	N518	K431	L321	L184	L100
D1296	Q1146	K988	K988	K988	R892	V782	Y606	N519	K431	L322	L185	R101
D1297	R1147	L989	L989	K989	R892	L783	L606	P520	I433	A323	F186	L102
V1298	A1148	D990	D990	K990	T896	L699	S607	L521	K324	K324	E187	V103
M1299	Y1149	K991	K991	R991	R897	L699	A608	S522	E441	L325	F188	R107
G1300	D1150	L992	L992	E992	E896	E705	I609	E523	S526	S526	D189	E108
R1301	G1151	P993	P993	R993	R903	S712	E610	I324	Q327	Q327	P190	A109
K1303	G1152	R994	R994	D995	R903	S712	V615	T325	I445	F337	L194	E111
M1304	A1153	D996	D996	R996	E908	V714	I616	H526	L448	F337	L194	K115
Y1305	R1156	Q1077	Q1077	W997	Q909	T715	A617	R528	R452	F338	V196	D116
I1308	Q1157	K1078	K1078	L998	A910	T716	Q618	R529	R452	D342	R197	I117
H1313	Q1158	I1079	I1079	L999	E910	T717	A619	I530	R454	D342	I198	I118
Q1314	V1159	M1080	M1080	K1000	K914	R720	N620	G534	S455	P345	K201	K118
P1317	L1160	P1081	P1081	L1001	K914	R720	N620	G534	S455	P345	K201	E119
L1327	L1161	I1082	I1082	L1002	D915	G721	F629	P535	V456	I347	R202	Q120
R1331	S1162	E1083	E1083	T1003	S916	G722	F629	P535	V456	I347	R202	Q120
S1332	T1163	D1084	D1084	D1004	S917	G723	L633	L538	R465	I360	A206	V122
L1333	F1164	M1085	M1085	E1005	R918	V724	V634	T539	R465	L363	T207	Y123
E1340	D1241	P1086	P1086	E1006	R919	G725	T635	R540	V466	L363	T208	M124
E1342	D1242	Y1087	Y1087	K1007	R920	V726	C636	E541	G467	V364	I208	G125
R1343	L1171	G1091	G1091	Q1008	N922	V727	R637	R542	G467	E365	I209	E126
S1344	R1172	T1092	T1092	Q1009	G923	D728	S642	V550	R470	R368	L213	M130
S1345	L1176	P1093	P1093	Q1010	V924	A729	S642	H551	V471	R369	L221	T131
S1346	R1177	V1094	V1094	L1011	D930	R731	F645	P552	E472	R370	K227	D132
S1347	R1178	L1098	L1098	Q1012	V931	V732	S646	T553	R473	K227	V228	F136
S1348	M1180	M1099	M1099	L1014	K941	V733	Q649	H554	A474	P375	I229	I137
S1349	P1181	P1100	P1100	Q1017	D942	V735	V650	G556	K476	P376	F230	I138
S1350	L1182	S1105	S1105	Y1018	R943	V736	D654	R557	L481	K381	D234	M139
S1351	Q1256	P1106	P1106	D1019	R944	N737	V655	V558	E382	E382	D234	R143
S1352	Q1257	M1107	M1107	E1020	E949	E738	S656	C559	S383	N235	K236	S147
S1353	V1186	M1108	M1108	L1021	E949	D739	T657	P560	L384	K236	L237	Q148
S1354	F1187	Q1111	Q1111	E1024	R951	V741	Q658	I561	F385	K236	Q238	L149
S1355	D1188	Q1112	Q1112	F1025	R951	V742	Q658	S576	L487	K387	R239	H150
S1356	G1189	L1113	L1113	K1028	E963	P743	V660	V577	M488	L388	E240	R151
S1357	K1190	H1116	H1116	K1032	R966	E745	S662	Q490	P489	F389	L241	F156
S1358	E1192	L1117	L1117	K1033	R967	A746	S662	D491	M492	F390	V242	F157
S1359	A1193	G1118	G1118	K1035	R968	G747	V670	N582	M492	V395	R245	D158
S1360	E1194	M1119	M1119	I1036	A969	V748	E672	E583	N494	G396	L246	S159
S1361	K1196	I1124	I1124	T1037	R971	L753	E672	Y584	I493	L397	T250	D160
S1362	E1197	I1124	I1124	A1043	R972	V754	R678	G585	G401	G401	R268	H164
S1363	L1198	I1128	I1128	P1044	R973	K755	R678	F586	I498	R402	R268	H165
S1364	L1199	I1129	I1129	R974	R974	Y756	M681	L587	S499	S499	E413	G168
S1365	K1200	M1129	M1129	R975	R975	T757	M681	P590	K503	K503	L284	K169
S1366	L1201	A1130	A1130	K1048	R976	C764	M685	R591	K503	K503	L285	K169
S1367	G1202	M1131	M1131	I1049	R977	I765	Q686	R592	K503	K503	L292	V170

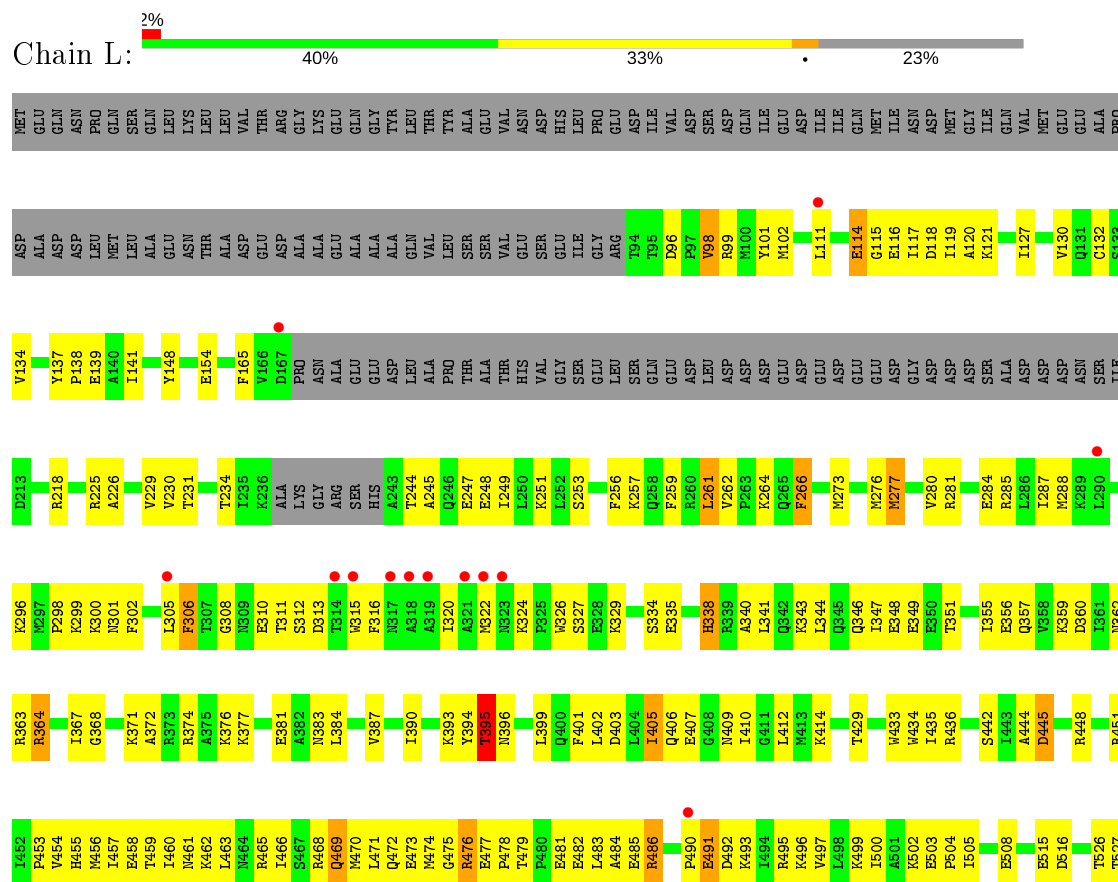
- Molecule 3: DNA-directed RNA polymerase subunit beta'







• Molecule 5: RNA polymerase sigma factor RpoD



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	187.31Å 205.90Å 309.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 3.70 29.98 – 3.70	Depositor EDS
% Data completeness (in resolution range)	96.8 (29.98-3.70) 92.5 (29.98-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 3.75Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.191 , 0.260 0.194 , 0.261	Depositor DCC
R_{free} test set	6183 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	116.2	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 61.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	55741	wwPDB-VP
Average B, all atoms (Å ²)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% 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	0.62	0/2524	0.81	2/3421 (0.1%)
1	B	0.58	0/1697	0.84	0/2300
1	G	0.57	0/1777	0.78	0/2408
1	H	0.51	0/1681	0.83	3/2278 (0.1%)
2	C	0.69	2/10739 (0.0%)	0.86	7/14489 (0.0%)
2	I	0.57	0/10735	0.77	3/14484 (0.0%)
3	D	0.70	0/9200	0.90	12/12423 (0.1%)
3	J	0.64	0/9140	0.83	5/12341 (0.0%)
4	E	0.66	0/693	0.82	0/935
4	K	0.61	0/629	0.77	0/847
5	F	0.56	0/3864	0.81	3/5194 (0.1%)
5	L	0.52	0/3872	0.71	1/5205 (0.0%)
All	All	0.63	2/56551 (0.0%)	0.82	36/76325 (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
2	C	0	2
2	I	0	2
3	D	0	2
3	J	0	3
5	F	0	2
All	All	0	11

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	949	GLU	CB-CG	6.52	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	838	CYS	CB-SG	-6.02	1.72	1.82

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	484	LEU	CA-CB-CG	9.03	136.06	115.30
2	C	796	LEU	CB-CG-CD2	-8.02	97.36	111.00
2	C	1161	LEU	CA-CB-CG	-7.43	98.22	115.30
3	D	268	LEU	CA-CB-CG	-7.05	99.09	115.30
2	C	544	GLY	N-CA-C	-6.83	96.01	113.10

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	109	ALA	Peptide
2	C	236	LYS	Peptide
3	D	1184	ASP	Peptide
3	D	901	ARG	Peptide
5	F	600	HIS	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	2490	0	2542	129	0
1	B	1677	0	1703	75	0
1	G	1755	0	1773	96	0
1	H	1662	0	1687	79	0
2	C	10570	0	10582	460	0
2	I	10566	0	10576	403	1
3	D	9060	0	9209	451	1
3	J	9001	0	9168	412	0
4	E	691	0	695	24	0
4	K	627	0	634	27	0
5	F	3813	0	3880	150	0
5	L	3821	0	3884	163	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
7	D	2	0	0	0	0
7	J	2	0	0	0	0
All	All	55741	0	56333	2271	1

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 2271 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:G:190:ALA:HB2	1:G:200:LYS:HB2	1.42	1.01
1:A:296:GLY:H	1:A:299:SER:HB2	1.26	1.00
5:L:484:ALA:HB1	5:L:491:GLU:HB2	1.41	0.99
3:D:210:SER:HB2	3:D:213:LYS:HB2	1.47	0.97
3:D:1183:SER:HA	3:J:206:ASN:HD21	1.29	0.96

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:712:GLN:NE2	2:I:862:LEU:O[4_545]	2.14	0.06

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	317/329 (96%)	246 (78%)	53 (17%)	18 (6%)	1 19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	213/329 (65%)	193 (91%)	16 (8%)	4 (2%)	8	40
1	G	225/329 (68%)	198 (88%)	18 (8%)	9 (4%)	3	26
1	H	212/329 (64%)	196 (92%)	12 (6%)	4 (2%)	8	40
2	C	1338/1342 (100%)	1205 (90%)	112 (8%)	21 (2%)	9	43
2	I	1338/1342 (100%)	1197 (90%)	120 (9%)	21 (2%)	9	43
3	D	1162/1407 (83%)	1030 (89%)	105 (9%)	27 (2%)	6	36
3	J	1151/1407 (82%)	1027 (89%)	98 (8%)	26 (2%)	6	36
4	E	87/91 (96%)	81 (93%)	5 (6%)	1 (1%)	14	50
4	K	77/91 (85%)	71 (92%)	3 (4%)	3 (4%)	3	27
5	F	462/613 (75%)	423 (92%)	32 (7%)	7 (2%)	10	44
5	L	463/613 (76%)	425 (92%)	30 (6%)	8 (2%)	9	42
All	All	7045/8222 (86%)	6292 (89%)	604 (9%)	149 (2%)	7	38

5 of 149 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	107	ILE
1	A	136	GLU
1	A	162	GLU
1	A	167	PRO

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	278/286 (97%)	227 (82%)	51 (18%)	1	10
1	B	186/286 (65%)	171 (92%)	15 (8%)	11	41
1	G	193/286 (68%)	164 (85%)	29 (15%)	3	18
1	H	183/286 (64%)	170 (93%)	13 (7%)	14	45
2	C	1155/1157 (100%)	1053 (91%)	102 (9%)	10	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	1154/1157 (100%)	1053 (91%)	101 (9%)	10	38
3	D	962/1168 (82%)	876 (91%)	86 (9%)	9	37
3	J	960/1168 (82%)	873 (91%)	87 (9%)	9	36
4	E	72/75 (96%)	63 (88%)	9 (12%)	4	23
4	K	67/75 (89%)	60 (90%)	7 (10%)	7	30
5	F	417/540 (77%)	385 (92%)	32 (8%)	13	43
5	L	418/540 (77%)	379 (91%)	39 (9%)	9	35
All	All	6045/7024 (86%)	5474 (91%)	571 (9%)	8	35

5 of 571 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	21	LEU
1	G	200	LYS
4	K	18	ASP
5	F	154	GLU
5	F	572	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	469	GLN
2	I	620	ASN
5	L	258	GLN
5	F	545	HIS
1	G	66	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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 [i](#)

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	319/329 (96%)	-0.36	1 (0%) 94 90	84, 129, 182, 196	0
1	B	217/329 (65%)	-0.18	5 (2%) 60 48	91, 164, 203, 214	0
1	G	227/329 (68%)	-0.28	1 (0%) 92 88	126, 154, 181, 218	0
1	H	216/329 (65%)	-0.10	3 (1%) 75 64	118, 174, 198, 207	0
2	C	1340/1342 (99%)	-0.38	18 (1%) 77 67	58, 114, 218, 253	0
2	I	1340/1342 (99%)	-0.19	44 (3%) 46 35	93, 148, 222, 378	0
3	D	1166/1407 (82%)	-0.39	2 (0%) 95 93	63, 107, 168, 218	0
3	J	1155/1407 (82%)	-0.27	14 (1%) 79 69	85, 128, 189, 228	0
4	E	89/91 (97%)	-0.59	0 100 100	67, 116, 140, 152	0
4	K	79/91 (86%)	-0.27	1 (1%) 77 67	99, 139, 205, 222	0
5	F	468/613 (76%)	-0.17	19 (4%) 37 27	93, 160, 273, 305	0
5	L	469/613 (76%)	-0.15	13 (2%) 53 40	114, 172, 279, 307	0
All	All	7085/8222 (86%)	-0.28	121 (1%) 70 59	58, 135, 209, 378	0

The worst 5 of 121 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	982	GLY	11.1
5	F	319	ALA	6.7
2	I	983	GLY	5.3
5	L	318	ALA	5.0
2	I	981	ALA	4.9

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 [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(\AA^2)	Q<0.9
6	MG	C	1401	1/1	0.95	0.51	94,94,94,94	0
6	MG	J	2001	1/1	0.96	0.25	94,94,94,94	0
6	MG	I	1401	1/1	0.96	0.44	94,94,94,94	0
6	MG	D	2001	1/1	0.96	0.35	94,94,94,94	0
7	ZN	J	2002	1/1	0.97	0.04	105,105,105,105	0
7	ZN	J	2003	1/1	0.98	0.11	94,94,94,94	0
7	ZN	D	2002	1/1	0.99	0.09	113,113,113,113	0
7	ZN	D	2003	1/1	0.99	0.17	94,94,94,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.