



wwPDB X-ray Structure Validation Summary Report ⓘ

May 28, 2020 – 10:03 pm BST

PDB ID : 2CW0
Title : Crystal structure of Thermus thermophilus RNA polymerase holoenzyme at 3.3 angstroms resolution
Authors : Tuske, S.; Sarafianos, S.G.; Wang, X.; Hudson, B.; Sineva, E.; Mukhopadhyay, J.; Birktoft, J.J.; Leroy, O.; Ismail, S.; Clark Jr., A.D.; Dharia, C.; Napoli, A.; Laptenko, O.; Lee, J.; Borukhov, S.; Ebright, R.H.; Arnold, E.
Deposited on : 2005-06-15
Resolution : 3.30 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

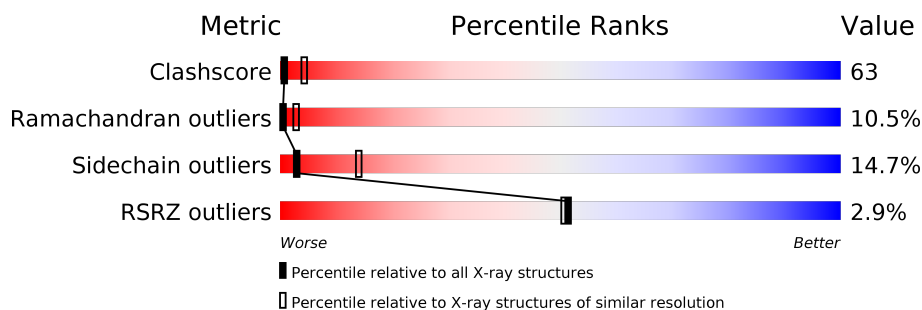
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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))
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	315	<div> <div>18%</div> <div>44%</div> <div>10%</div> <div>27%</div> </div>
1	B	315	<div>5%</div> <div>19%</div> <div>43%</div> <div>11%</div> <div>27%</div>
1	K	315	<div>%</div> <div>23%</div> <div>38%</div> <div>10%</div> <div>27%</div>
1	L	315	<div>2%</div> <div>17%</div> <div>48%</div> <div>8%</div> <div>27%</div>
2	C	1119	<div>2%</div> <div>25%</div> <div>59%</div> <div>14%</div> <div>•</div>
2	M	1119	<div>3%</div> <div>24%</div> <div>59%</div> <div>15%</div> <div>•</div>
3	D	1524	<div>2%</div> <div>20%</div> <div>52%</div> <div>18%</div> <div>•</div> <div>9%</div>

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Mol	Chain	Length	Quality of chain
3	N	1524	<div><div></div><div>3%</div><div>21%</div><div>52%</div><div>17%</div><div>•</div><div>9%</div></div>
4	E	99	<div><div></div><div>2%</div><div>29%</div><div>52%</div><div>11%</div><div>•</div><div>•</div></div>
4	O	99	<div><div></div><div>4%</div><div>34%</div><div>47%</div><div>9%</div><div>5%</div><div>•</div></div>
5	F	423	<div><div></div><div>2%</div><div>22%</div><div>48%</div><div>10%</div><div>•</div><div>18%</div></div>
5	P	423	<div><div></div><div>2%</div><div>26%</div><div>44%</div><div>10%</div><div>•</div><div>18%</div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 53962 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 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	B	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	K	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	L	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	24			
2	M	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1392	Total	C	N	O	S	0	0	0
			10975	6953	1941	2048	33			
3	N	1392	Total	C	N	O	S	0	0	0
			10975	6953	1941	2048	33			

- Molecule 4 is a protein called RNA polymerase omega chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	95	Total	C	N	O	S	0	0	0
			769	488	133	144	4			
4	O	95	Total	C	N	O	S	0	0	0
			769	488	133	144	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	345	Total	C	N	O	S	0	0	0
			2793	1762	504	523	4			
5	P	345	Total	C	N	O	S	0	0	0
			2793	1762	504	523	4			

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

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

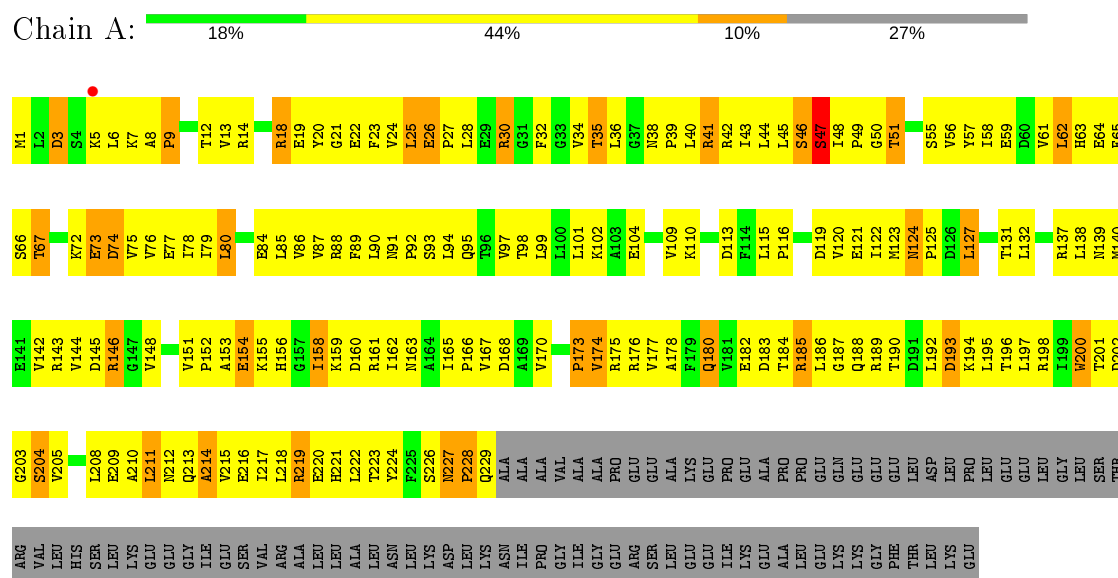
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	Mg	0	0
			1	1		
7	N	1	Total	Mg	0	0
			1	1		

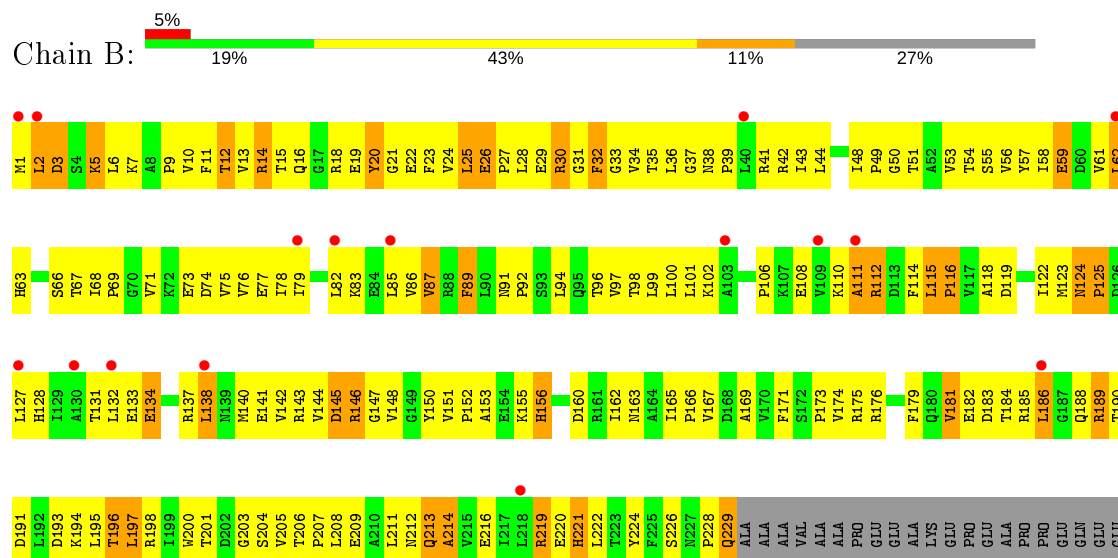
3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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 alpha chain

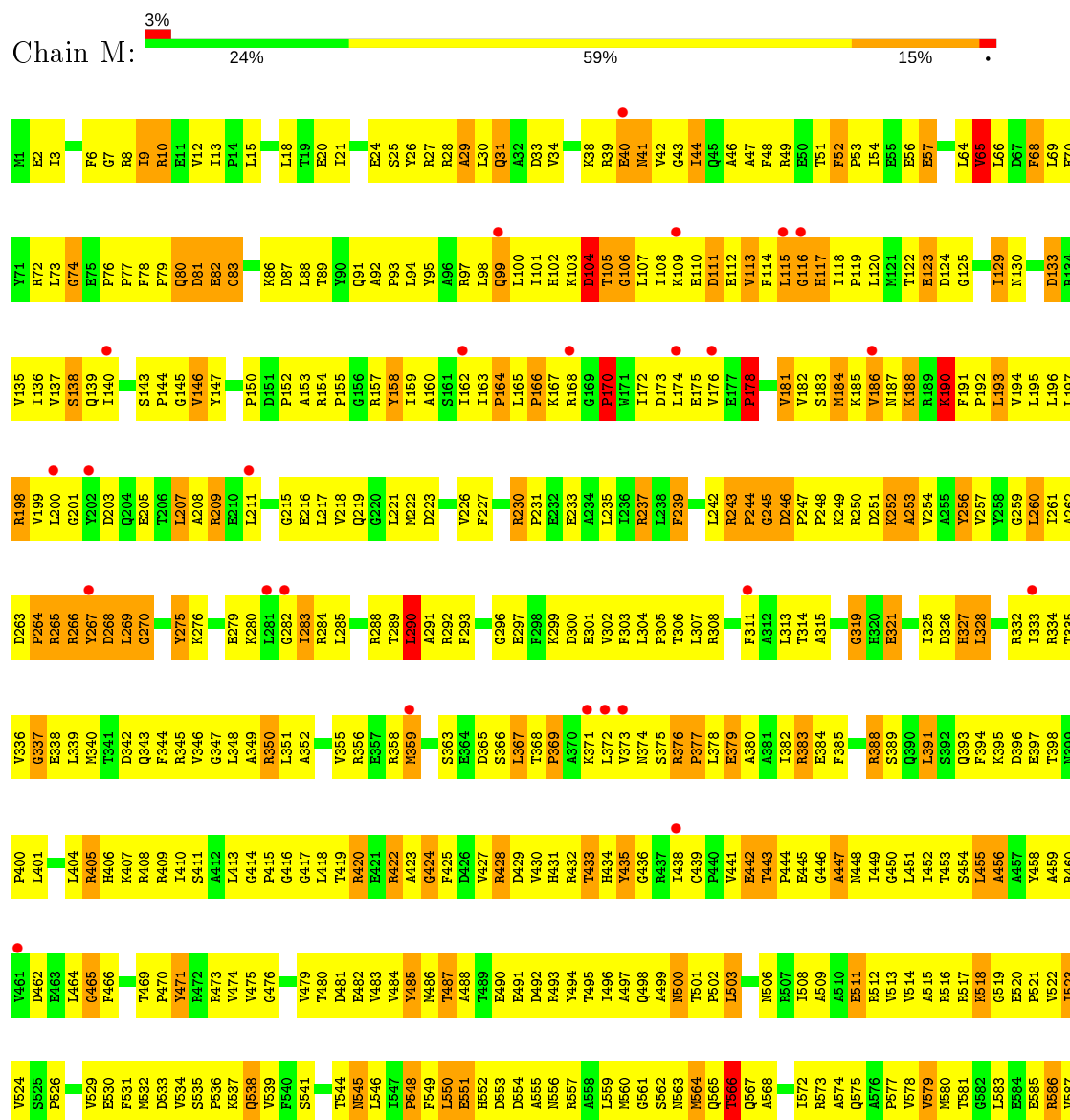


• Molecule 1: DNA-directed RNA polymerase alpha chain



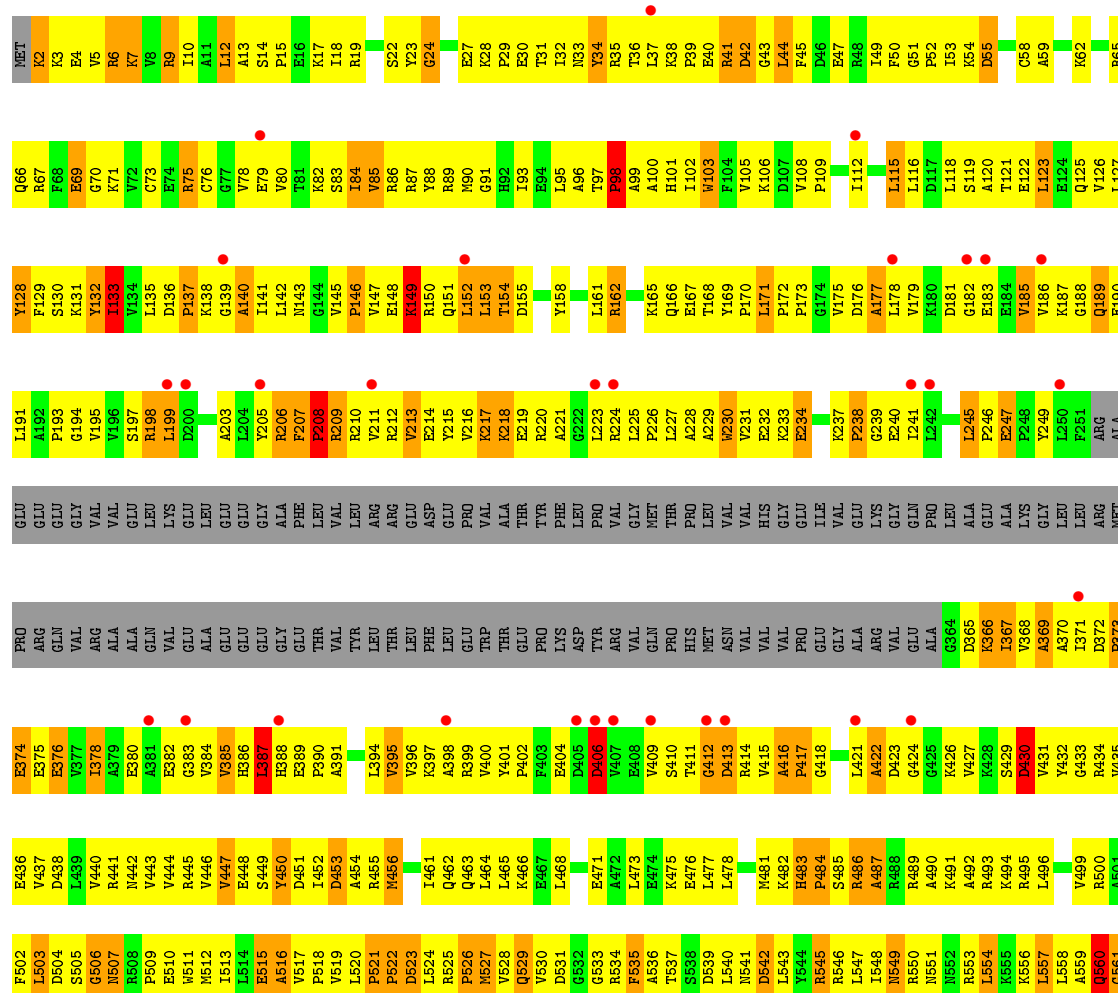
- Molecule 2: DNA-directed RNA polymerase beta chain







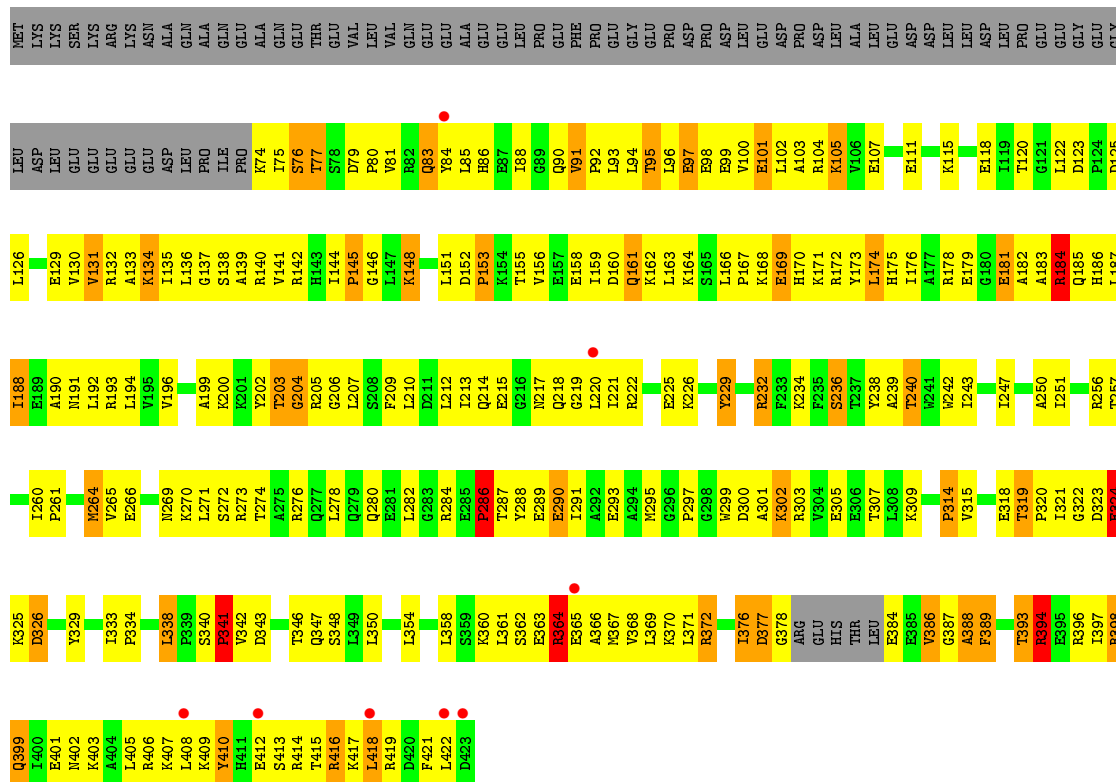
C1194	S1131	Y1070	H1010	T940	I880	E811	L751	V687	D624	E564	F502	V495	I371	LEU
Q1195	L1132	F1071	F1011	F941	L881	A812	S752	W688	I625	E565	F503	E496	D372	ARG
R1196	T1133	I1072	E1012		F882	L813	F754		S626	I566	D504	V437	P373	PRO
R1197	L1134	S1073	E1013	T944	A883	A814	F754	L691	G627	I567	D504	D438	E374	MET
V1198	K1135	H1074	N1014	S945	R884	A815	A755	E692	R628	R568	S505	I439	E375	ARG
G1199	K1136	H1075	Y1015	G946	I885	B816	A756	E693	S629	N569		V440	E376	GLN
V1200	R1137	G1076	P1016	T947	V886	E817	A757	V694	V630	E570	B508	R441	V377	VAL
C1201	A1138	A1077	F1017	T948	A887	R818	E758	I695	I631	K571	P509	K442	I378	ARG
K1202	D1139	R1078	N1018	T949	E888	G819	A759	H696	V632	R572	B510	V443	A379	ALA
K1203	T1140	K1079	P1019	G950	A889	E820	R760	G697	V633	R573	W511	V444	E380	ALA
K1204	E1141	G1080	L1020	T951	A890	V821	I761	X698	G634	L574	W512	R445	A381	GLN
Y1205	A1142	G1081	Y1021	D952	E891	V822	Q762	V699	P635	D575	J513	V446	E382	VAL
G1206	G1143	A1082	V1022	D953	D892	N824	W763	V700	P636	E576		V447	E383	GLU
Y1207	L1144	D1083	M1023	A954	E893	A825	L764	L701	L637	A577	A516	E448	V384	ALA
D1208	Y1145	T1084	A1024	V955	R894	P826	A766	L702	R638	W578	W517	S449	V385	GLU
L1209	V1146	A1085	Q1025	T956	V895	I827	S765	W703	L639	D579	P518		V386	GLU
S1210	R1147	L1086	S1026	P957	A896	R828	H767	R709	H640	A580	W519	I452	L387	GLY
S1211	V1148	R1087	G1027	E958	W897	V829	W768	A705	Q641	L581	L520	I453	H388	GLY
A1212	L1149	T1088	A1028	E959	E898	A830	L769	P706	G642	L582	P521	A454	E389	GLU
R1213	A1150	A1089	R1029	V960	L899	G831	L770	T707	G643	D583	P522	R455	P390	THR
P1214	L1151		G1030		I900	R832	S771	L708	L644	N584	D523	R456		VAL
V1215	E1152	Y1093	N1031	L964	Q901	E833	L778	R709	L650	P590	Q529	I393	T393	TYR
S1216	V1153	Y1099	P1032	T958	R908	T834	A772	A710	L652	W591	W530	I457	L394	LEU
I1217	E1154	L1094	Q1033	R969	D903	W835	Q717	R716	L652	T592	D531	A458	V395	THR
G1218	V1155	T1095	Q1034	K970	W904	V836	W774	G712	R647	R587	W527	I460	V396	LEU
E1219	L1156	R1096	L1035	L971	P905	G837	E776	I713	L649	A588	W528	I461	K397	PHE
A1220		K1097	R1036	L972	Q906	R838	P777	Q714	L650	P590	Q529	Q462	A398	LEU
V1221	R1159	L1098	Q1037	T972	R907	E873	A779	A715	L652	W591	W530	Q463	V400	THR
G1222	L1160	Y1099	L1038	R974	K908	T834	W778	F716	L652	T592	D531		Y401	THR
I1223	E1161	D1100	G1039	E975	N909	W842	K780	Q717	P655	N593	G532	D469	P402	GLU
V1224	L1162	Y1101	L1040	Q976	S910	F843	P781	P718	K654	P594	G533	L470	F403	PRO
A1225	G1163	T1102	G1041	A977	L911		S782	W720	P655	G595	R534	L473	E404	LYS
I1226	R1164	H1103	R1042	T978	K912	P846	L783	L720	F656	S596	P535	E474	E408	ASP
Q1227	Y1165	E1104	G1043	T984	D913	A849	D784	V721	L657	D597	A536	K475		TYR
S1228	L1166	T1105	L1044		R914	L850	I785	E722	L658	R598	T537	K476	E409	ARG
I1229	S1167	V1106	M1045	D985	W915	L850	I786	G723	X659	P599	S538	E477	S410	VAL
G1230	M1168	V1107	Q1046	R986	Y916		L787	Q724	K660	L600	D539	L477	T411	GLN
E1231	D1169	R1108	K1047	E987	Q917	W853	G788	S725	H661	R601	L540	L478		PRO
P1232	D1170	E1109	P1048	R988	A918		L789	L728	E662	S602	W541	E479		GLN
G1233	V1171	A1110	S1049	F989	F919	W858	Y790		E663	L603	D542	E480	D413	HIS
T1234	H1172	D1111	G1050	D990	L920	D859	I792	H729		T604	L543	M481	R414	MET
L1235	L1173	C1112	E1051	Q991	R921	L860	Y793	P730	P668	D605	W544	K482	V415	ASN
T1237	L1174	G1113	T1052	I992	L922	Q861	T793	L731	N669	T606	R545	H483	A422	VAL
M1238	T1114	T1114	F1053	L993	G923	D862	Q794	W732	V670	L607	R546	P484	A416	VAL
F1241	T1115	M1116	E1054	Q994	W924	W863	Y795	C733	K671	S606	L547	S485	P417	VAL
T1242	K1176	M1117	V1055	N995	E925	V864	K796	E734	A672	G609	W548	R486	V420	PRO
T1243	A1177	Y1117	V1057	N996	K926	T865	K797	A735	A673	W610	W549	A487	L421	GLU
G1244	E1179		V1058	T997	T927	V866	E798	F736	R674	Q611	R550	R488	A422	GLY
G1245		S1119	R1058	E998	A928	E867	K799	W737	R675	G612	W551	R489	D423	ALA
L1246		V1120	S1059	T999	R929	W868	K800	A738	W676	R613	W552	K490	G424	ARG
A1247	L1182	P1121	S1060	T1000	L930	W869	G801	D739	L677	R614	W553	K491	G425	VAL
G1248	V1186	F1122	F1061	E1001	L931	R872	A802	F740	E678	W615	L554	A492	K426	GLU
A1249	P1187	F1123	R1062	K1002	D932	G803	G803	D741	R679	Q616	W555	R493	V427	ALA
	V1188	Q1124	E1063	V1003	A933	L873	L804	G742	G680	W617		K494	K428	
	R1189	P1125	G1064	T1004	L934	E874	E805	D743	R681	L618	R495	S429	D365	G364
	D1126	Q1105	L1065	Q1005	K935	T875	F806	W745	D682	L619	A569	D430	K366	
	E1127	T1066	T1066	A1006	Y936	S876	A807	M745	L683	G620	W560	E497	I367	
	V1128	V1067	V1067	V1007	Y937	P877	T808	M745	R684	W621	G561	V498	V368	
T1253	L1191	F1068	L1068	Q938	G938	G878	P809	W749	H682	A562	W499	G433	A369	
G1255	T1193	R1130	E1069	K1009	F939	R879	E810	P750	E886	W623	P563	R500	A370	







• Molecule 5: RNA polymerase sigma factor rpoD



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	236.15Å 236.15Å 249.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.30 29.87 – 3.30	Depositor EDS
% Data completeness (in resolution range)	84.1 (30.00-3.30) 47.2 (29.87-3.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 3.31Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.282 , 0.320 0.286 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	97.4	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , -23.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.499 for -h,-k,l 0.499 for h,-h-k,-l 0.064 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	53962	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.25% 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	0.46	0/1838	0.75	0/2498
1	B	0.36	0/1838	0.64	0/2498
1	K	0.46	0/1838	0.75	0/2498
1	L	0.39	0/1838	0.68	0/2498
2	C	0.45	0/8997	0.79	8/12164 (0.1%)
2	M	0.46	0/8997	0.79	8/12164 (0.1%)
3	D	0.48	0/11165	0.83	16/15088 (0.1%)
3	N	0.46	0/11165	0.81	15/15088 (0.1%)
4	E	0.42	0/783	0.80	3/1054 (0.3%)
4	O	0.42	0/783	0.80	1/1054 (0.1%)
5	F	0.40	0/2836	0.73	0/3812
5	P	0.41	0/2836	0.72	0/3812
All	All	0.45	0/54914	0.78	51/74228 (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
3	D	0	1
3	N	0	3
5	F	0	1
All	All	0	5

There are no bond length outliers.

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1209	LEU	N-CA-C	-10.12	83.67	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	728	HIS	N-CA-C	7.66	131.69	111.00
2	C	728	HIS	N-CA-C	7.62	131.58	111.00
3	N	1209	LEU	N-CA-C	-7.26	91.39	111.00
2	M	319	GLY	N-CA-C	-7.22	95.05	113.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	132	TYR	Sidechain
5	F	84	TYR	Sidechain
3	N	1015	TYR	Sidechain
3	N	1318	TYR	Sidechain
3	N	132	TYR	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	1806	0	1861	249	0
1	B	1806	0	1861	193	0
1	K	1806	0	1861	190	0
1	L	1806	0	1861	208	0
2	C	8829	0	8933	1143	0
2	M	8829	0	8933	1183	0
3	D	10975	0	11211	1725	0
3	N	10975	0	11210	1681	0
4	E	769	0	775	94	0
4	O	769	0	775	83	0
5	F	2793	0	2873	301	0
5	P	2793	0	2873	364	0
6	D	2	0	0	0	0
6	N	2	0	0	0	0
7	D	1	0	0	0	0
7	N	1	0	0	0	0
All	All	53962	0	55027	6832	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 63.

The worst 5 of 6832 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:1101:VAL:HG21	3:D:1424:VAL:HG22	1.21	1.20
2:C:1016:ILE:H	2:C:1016:ILE:HD13	1.06	1.16
3:D:907:GLU:HG2	3:D:1027:GLY:H	1.02	1.16
3:D:136:ASP:HB3	3:D:137:PRO:HD3	1.22	1.15
3:D:145:VAL:HG22	3:D:146:PRO:HD2	1.27	1.15

There are no symmetry-related clashes.

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	227/315 (72%)	167 (74%)	39 (17%)	21 (9%)	0	4
1	B	227/315 (72%)	177 (78%)	37 (16%)	13 (6%)	1	11
1	K	227/315 (72%)	161 (71%)	39 (17%)	27 (12%)	0	2
1	L	227/315 (72%)	166 (73%)	44 (19%)	17 (8%)	1	7
2	C	1117/1119 (100%)	781 (70%)	226 (20%)	110 (10%)	0	3
2	M	1117/1119 (100%)	769 (69%)	215 (19%)	133 (12%)	0	2
3	D	1388/1524 (91%)	941 (68%)	293 (21%)	154 (11%)	0	2
3	N	1388/1524 (91%)	907 (65%)	332 (24%)	149 (11%)	0	3
4	E	93/99 (94%)	67 (72%)	17 (18%)	9 (10%)	0	3
4	O	93/99 (94%)	59 (63%)	20 (22%)	14 (15%)	0	1
5	F	341/423 (81%)	241 (71%)	67 (20%)	33 (10%)	0	3
5	P	341/423 (81%)	249 (73%)	57 (17%)	35 (10%)	0	3
All	All	6786/7590 (89%)	4685 (69%)	1386 (20%)	715 (10%)	0	3

5 of 715 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	SER
1	B	3	ASP
1	B	118	ALA
1	B	160	ASP
2	C	7	GLY

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	202/273 (74%)	177 (88%)	25 (12%)	4	19
1	B	202/273 (74%)	172 (85%)	30 (15%)	3	13
1	K	202/273 (74%)	173 (86%)	29 (14%)	3	15
1	L	202/273 (74%)	182 (90%)	20 (10%)	8	28
2	C	941/941 (100%)	808 (86%)	133 (14%)	3	16
2	M	941/941 (100%)	805 (86%)	136 (14%)	3	14
3	D	1170/1279 (92%)	970 (83%)	200 (17%)	2	9
3	N	1170/1279 (92%)	980 (84%)	190 (16%)	2	10
4	E	83/87 (95%)	72 (87%)	11 (13%)	4	17
4	O	83/87 (95%)	70 (84%)	13 (16%)	2	12
5	F	300/370 (81%)	264 (88%)	36 (12%)	5	20
5	P	300/370 (81%)	269 (90%)	31 (10%)	7	26
All	All	5796/6446 (90%)	4942 (85%)	854 (15%)	3	14

5 of 854 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	1462	LEU
1	L	156	HIS
3	N	1326	THR
4	E	66	LYS

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Mol	Chain	Res	Type
5	F	416	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 168 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	1442	ASN
1	L	38	ASN
3	N	1441	GLN
3	D	1489	GLN
1	K	95	GLN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	229/315 (72%)	-0.13	1 (0%) 92 93	41, 64, 87, 113	0
1	B	229/315 (72%)	0.09	16 (6%) 16 16	47, 121, 143, 143	0
1	K	229/315 (72%)	-0.06	3 (1%) 77 77	28, 63, 88, 111	0
1	L	229/315 (72%)	-0.03	7 (3%) 49 48	41, 79, 99, 117	0
2	C	1119/1119 (100%)	-0.07	25 (2%) 62 60	12, 67, 133, 143	0
2	M	1119/1119 (100%)	-0.06	31 (2%) 53 51	6, 71, 122, 133	0
3	D	1392/1524 (91%)	-0.00	37 (2%) 54 52	7, 60, 125, 143	0
3	N	1392/1524 (91%)	0.05	53 (3%) 40 37	5, 65, 134, 143	0
4	E	95/99 (95%)	-0.03	2 (2%) 63 62	54, 84, 100, 106	0
4	O	95/99 (95%)	0.04	4 (4%) 36 34	46, 86, 117, 121	0
5	F	345/423 (81%)	-0.06	9 (2%) 56 53	48, 81, 113, 121	0
5	P	345/423 (81%)	-0.08	8 (2%) 60 59	47, 73, 110, 123	0
All	All	6818/7590 (89%)	-0.02	196 (2%) 51 50	5, 70, 129, 143	0

The worst 5 of 196 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	1247	ALA	14.8
3	D	1246	VAL	9.4
2	C	211	LEU	8.7
3	N	1246	VAL	8.3
1	B	1	MET	7.4

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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	ZN	D	1525	1/1	0.85	0.29	107,107,107,107	0
6	ZN	N	1526	1/1	0.89	0.28	72,72,72,72	0
6	ZN	N	1525	1/1	0.92	0.32	108,108,108,108	0
7	MG	D	1527	1/1	0.94	0.09	19,19,19,19	0
7	MG	N	1527	1/1	0.96	0.17	29,29,29,29	0
6	ZN	D	1526	1/1	0.99	0.26	78,78,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.