



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 28, 2026 – 08:39 PM UTC

PDB ID : 1IW7 / pdb_00001iw7
Title : Crystal structure of the RNA polymerase holoenzyme from *Thermus thermophilus* at 2.6Å resolution
Authors : RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2002-04-22
Resolution : 2.60 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

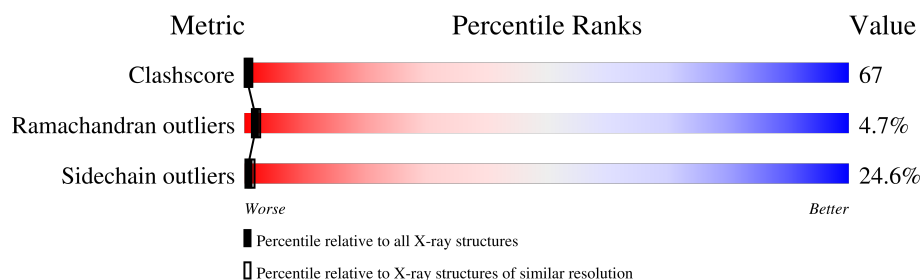
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

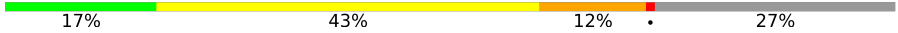
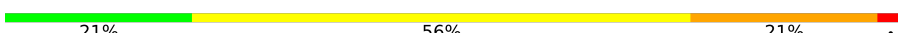
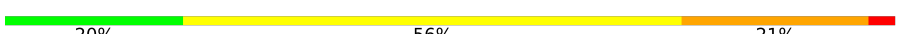
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

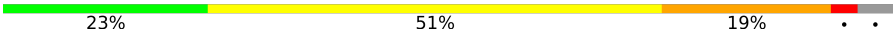
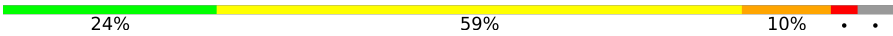
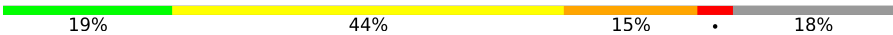
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	315	
1	B	315	
1	K	315	
1	L	315	
2	C	1119	
2	M	1119	
3	D	1524	
3	N	1524	

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Mol	Chain	Length	Quality of chain
4	E	99	 23% 51% 19% . .
4	O	99	 24% 59% 10% . .
5	F	423	 19% 44% 13% 5% 18%
5	P	423	 19% 44% 15% . 18%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 59529 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 RNA polymerase alpha subunit.

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 RNA polymerase beta subunit.

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 RNA polymerase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1392	Total	C	N	O	S	0	0	0
			10801	6823	1925	2020	33			
3	N	1392	Total	C	N	O	S	0	0	0
			10801	6823	1925	2020	33			

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

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-70 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	345	Total	C	N	O	S	0	0	0
			2771	1744	504	519	4			
5	P	345	Total	C	N	O	S	0	0	0
			2771	1744	504	519	4			

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	18	Total	Mg	0	0
			18	18		
6	B	24	Total	Mg	0	0
			24	24		
6	C	63	Total	Mg	0	0
			63	63		
6	D	118	Total	Mg	0	0
			118	118		
6	E	6	Total	Mg	0	0
			6	6		
6	F	31	Total	Mg	0	0
			31	31		
6	K	20	Total	Mg	0	0
			20	20		
6	L	19	Total	Mg	0	0
			19	19		
6	M	64	Total	Mg	0	0
			64	64		
6	N	92	Total	Mg	0	0
			92	92		
6	O	8	Total	Mg	0	0
			8	8		
6	P	22	Total	Mg	0	0
			22	22		

- Molecule 7 is LEAD (II) ION (CCD ID: PB) (formula: Pb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	2	Total	Pb	0	0
			2	2		
7	N	2	Total	Pb	0	0
			2	2		

- Molecule 8 is water.

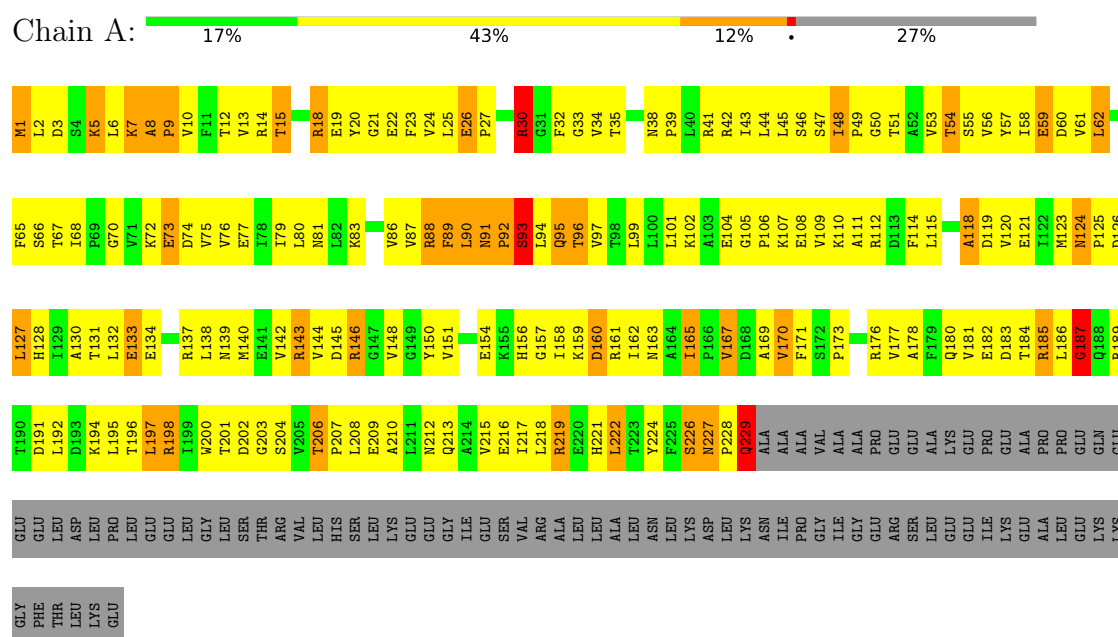
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	194	Total 194	O 194	0	0
8	B	193	Total 193	O 193	0	0
8	C	869	Total 869	O 869	0	0
8	D	1163	Total 1163	O 1163	0	0
8	E	114	Total 114	O 114	0	0
8	F	381	Total 381	O 381	0	0
8	K	161	Total 161	O 161	0	0
8	L	157	Total 157	O 157	0	0
8	M	822	Total 822	O 822	0	0
8	N	983	Total 983	O 983	0	0
8	O	114	Total 114	O 114	0	0
8	P	325	Total 325	O 325	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

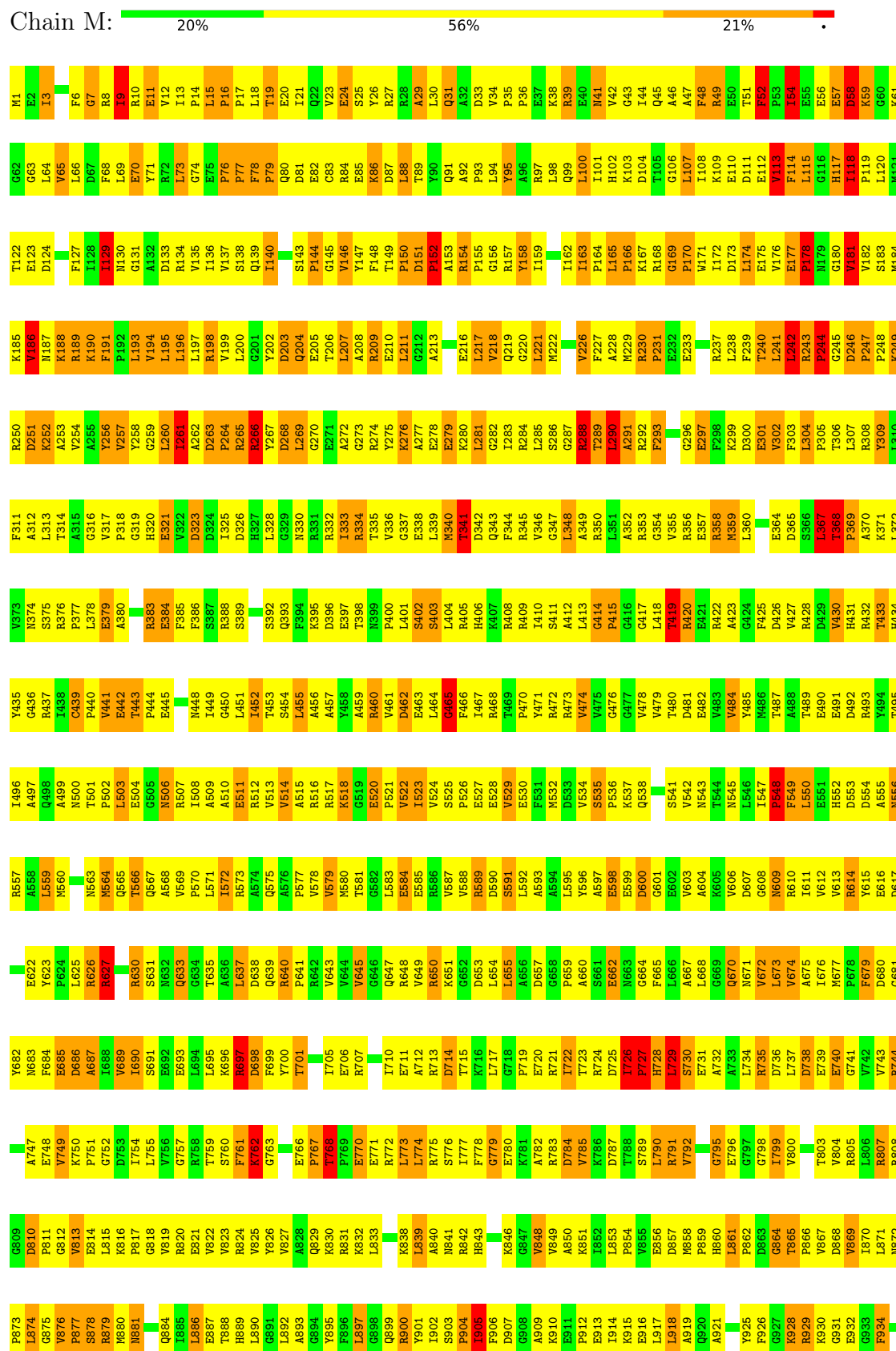
Note EDS was not executed.

• Molecule 1: RNA polymerase alpha subunit



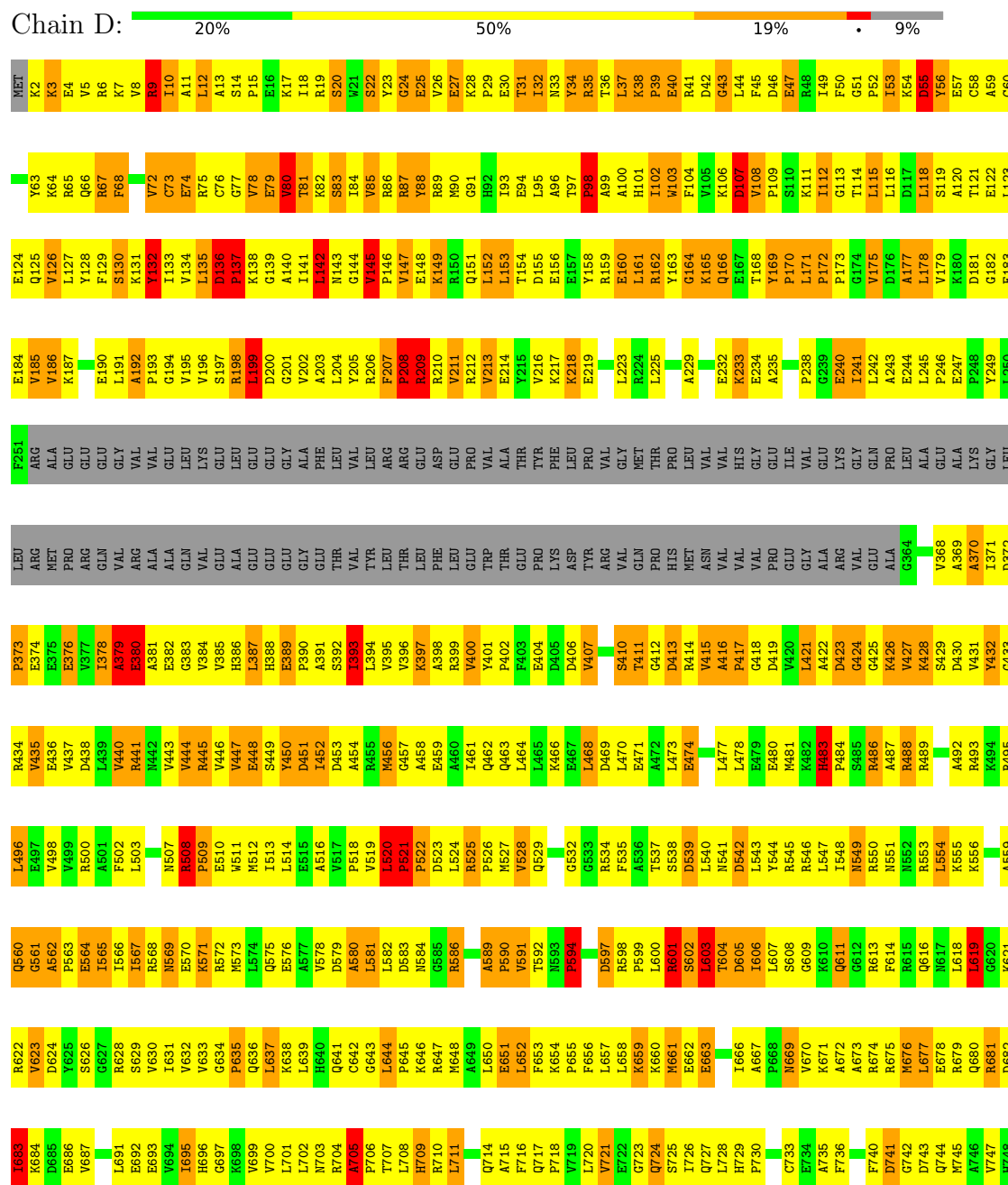


● Molecule 2: RNA polymerase beta subunit

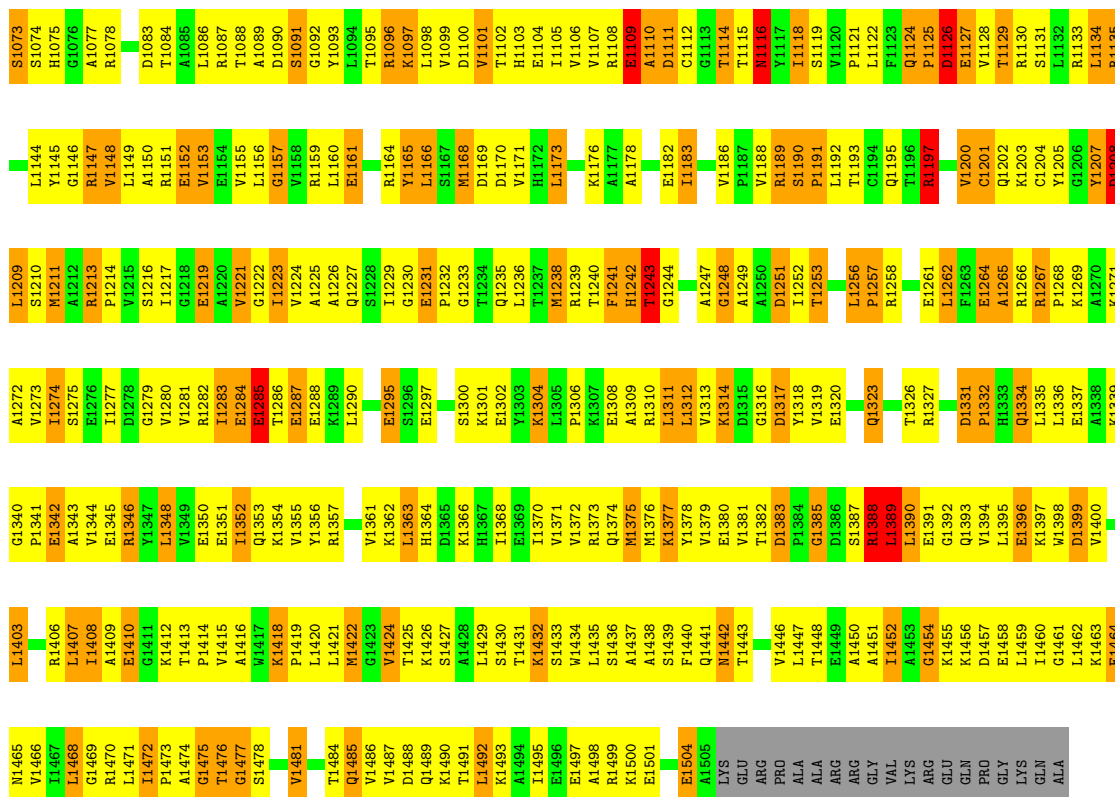




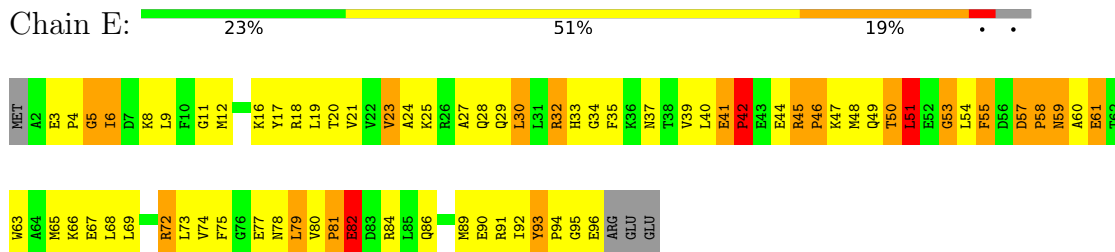
• Molecule 3: RNA polymerase beta subunit



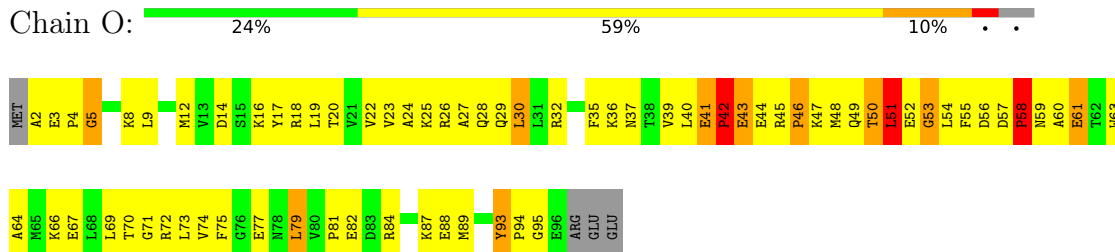
F1008	G938	T875	E811	H748	K621	A559	V499	L439	A379	GLN	GLY	E190	Q125	K62
F939	F939	S876	A812	V749	R622	Q560	R500	V440	E380	VAL	GLY	L191	V126	K65
T940	T940	G877	L813	P750	G623	G561	A501	R441	E381	ALA	VAL	L192	L127	R66
F941	F941	G878	A814	P751	D624	A562	F502	R442	E382	ALA	VAL	F193	Y128	Q66
S942	S942	R879	A815	S752	Y625	E563	L503	V443	G383	ALA	GLU	G194	F129	R67
T943	T943	I880	E817	S753	S626	E564	D504	V444	V384	GLN	LEU	V195	S130	F68
T944	T944	L881	R818	F754	G627	I565	S505	R445	V385	VAL	LYS	V196	K131	E69
L1021	L1021	F883	G819	A755	R628	I566	G506	V446	H386	GLU	LYS	S197	Y132	
Y1022	Y1022	E884	E820	Q756	S629	I567	M507	V447	L387	LEU	GLU	L198	I133	V72
M1023	M1023	R884	R821	A757	F630	R568	R508	S448	H388	GLU	GLU	L199	V134	C73
A1024	A1024	I885	H696	A758	G631	R569	P509	S449	H389	GLU	GLU	D200	L135	E74
Q1025	Q1025	V886	G697	A759	V632	E570	E510	Y450	P390	GLY	GLY	G201	D136	R75
T951	T951	R887	R823	R760	V633	K571	M511	D451	A391	ALA	ALA	V202	P137	C76
D952	D952	E888	A825	I761	G634	R572	M512	I452	S392	GLU	PHE	A203	K138	G77
A1027	A1027	A889	R826	Q762	P635	M573	I513	D453	I393	THR	LEU	L204	G139	V78
G1028	G1028	R890	I827	M763	Q636	L574	L514	A454	L394	VAL	VAL	Y205	A140	E79
R1029	R1029	E891	K828	L764	L637	E575	E515	R455	V395	THR	LEU	R206	L141	V80
G1030	G1030	V892	N703	S765	K638	E576	A516	M456	V396	LEU	ARG	F207	I142	T81
N1031	N1031	E893	R704	A766	L639	A577	V517	G457	K397	THR	ARG	P208	N143	K82
P1032	P1032	K894	A705	H767	H640	V578	P518	A458	A398	GLU	GLU	R209	G144	S83
Q1033	Q1033	V895	P706	N768	Q641	V579	V519	E458	A399	ASP	ASP	R210	V145	I84
Q1034	Q1034	A896	L707	L769	C642	A580	L520	A460	Y401	GLU	GLU	V211	P146	V85
I1035	I1035	R897	L708	L770		L581	P521	I461	Y401	GLU	PRO	R212	P147	R86
R1036	R1036	E898	H709	S771	P645	L582	P522	Q462	P402	THR	VAL	Y213	E148	R87
Q1037	Q1037	L899	R710		K646	D583	D523	Q463	F403	THR	ALA	E214	K149	Y88
L1038	L1038	I900	L711	S774	R647	N584	L524	L464	E404	GLU	THR	Y215	R150	R89
G1039	G1039	Q901	G712	G775	M648	R587	R525	L465	D405	PRO	THR	V216	Q151	M90
C1040	C1040	L839	I713	E776	M649	P526	K466	K466	D406	LYS	PHE	K217	L152	G91
R1041	R1041	D903	K840	P777	L650	G588	M527	E467	A407	ASP	LEU	K218	L153	H92
L1042	L1042	K841	Y841	L778	E651	A589	V528	L468	E408	THR	PRO	E219	T154	I93
G1043	G1043	P905	R716	A779	L652	P590	Q529	D469	V409	ARG	VAL	R220	D155	E94
L1044	L1044	Q906	Q717	K780	F653	V591	V530	L470	S410	VAL	GLY	A221	E156	L95
M1045	M1045	R907	P718	R781	K654	I592	D531	E471	T411	GLN	MET	L225	E157	A96
Q1046	Q1046	K908	L719	S782	P655	N593	G532	A472	G412	THR	THR	L226	Y158	T97
P1048	P1048		L720	R783	F656	P594	G533	L473	D413	PRO	PRO	L227	L161	A99
S1049	S1049	L911	V721	D784	L657		R534	E474	R414	ASN	VAL	A228	R162	A100
G1050	G1050	K912	E722	I785	L658	D597	F535	K475	V415	VAL	VAL	A229	Y163	H101
E1051	E1051	D913	G723	L786	K659	R598	A536	E476	A416	VAL	VAL		G164	I102
T1052	T1052	L914	Q724	L787	K660	P599	T537	L477	P417	VAL	HIS	E232	K165	W103
F1053	F1053	V915		G788	M661	L600	S538	L478	G418	VAL	GLY	R233	Q166	F104
E1054	E1054	Y916	Q727	L789	E662	R601	D539	E479	D419	PRO	GLU	E234	E167	
V1055	V1055	Q917	L728	E663	K664	S602	L540	E480	V420	GLU	ILE		T168	D107
P1056	P1056	A918	H729	K800		L603	N541	M481	L421	GLY	VAL	P238	Y169	V108
V1057	V1057	F919	P730		N669	T604	D542	K482	A422	ALA	GLU	G239	P170	P109
S1058	S1058	L920	L731	Q794	V670	D605	L543	R483	D423	ARG	LYS	E240	P171	
R1059	R1059	R921	V732	V795	K671	L606	Y544	P484	G424	VAL	GLY	I241	L171	S110
S1060	S1060	L922	C733	R796	K671	L607	R545	S485	G425	GLU	GLN	L242	P172	K111
F1061	F1061	D862	E734	K797	A672	S508	R546	R486	K426	ALA	PRO	A243	P173	I112
R1062	R1062	V925	A735	E798	A673	G609	L547	A487	V427	LEU	LEU	E244	G113	G113
E1063	E1063	K926	F736	K799	R674	K610	I548	R488	K428	ALA	ALA	L245	A177	T114
G1064	G1064	T927	N737	K800	R675	Q611	N549	R489	S429	GLU	GLU	P246	L178	L115
L1065	L1065	V866	A738	Q794	M676	G612	R550	A490	D430	ALA	ALA	E247	V179	L116
T1066	T1066	R867	D739	L804	L677	R613	N551	K491	V431	LYS	LYS	P248	K180	D117
V1067	V1067	Y868	F740	E678	E678	F614	N552	A492	Y432	GLY	GLY	Y249	L181	L118
L1068	L1068	M869	D741	R679	R679	R615	R553	K493	R434	LEU	LEU	L250	G182	S119
V1069	V1069	G870	G742	Q680	Q680	Q616	L554	K494	R434	LEU	LEU	F251	V185	A120
E1069	E1069	A807		R681	R681	N617	K555	R495	V435	ARG	ARG		V186	T121
Q1005	Q1005	T808	M745	D682	D682	L618	K556	L496	E436	MET	MET	ALA	V187	E122
F1071	F1071	L873	A746	I683	I683	L619	L557	E497	V377	PRO	PRO	GLU	K187	L123
I1072	I1072	E810	V747		K684	G620	L558	V498	D438	ARG	ARG	GLU		E124



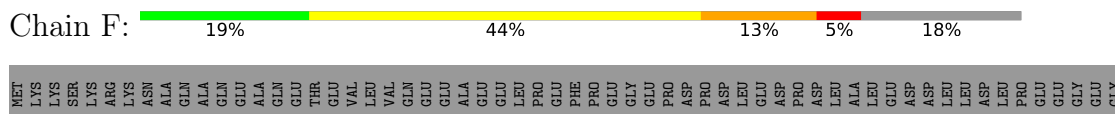
- Molecule 4: RNA polymerase omega subunit

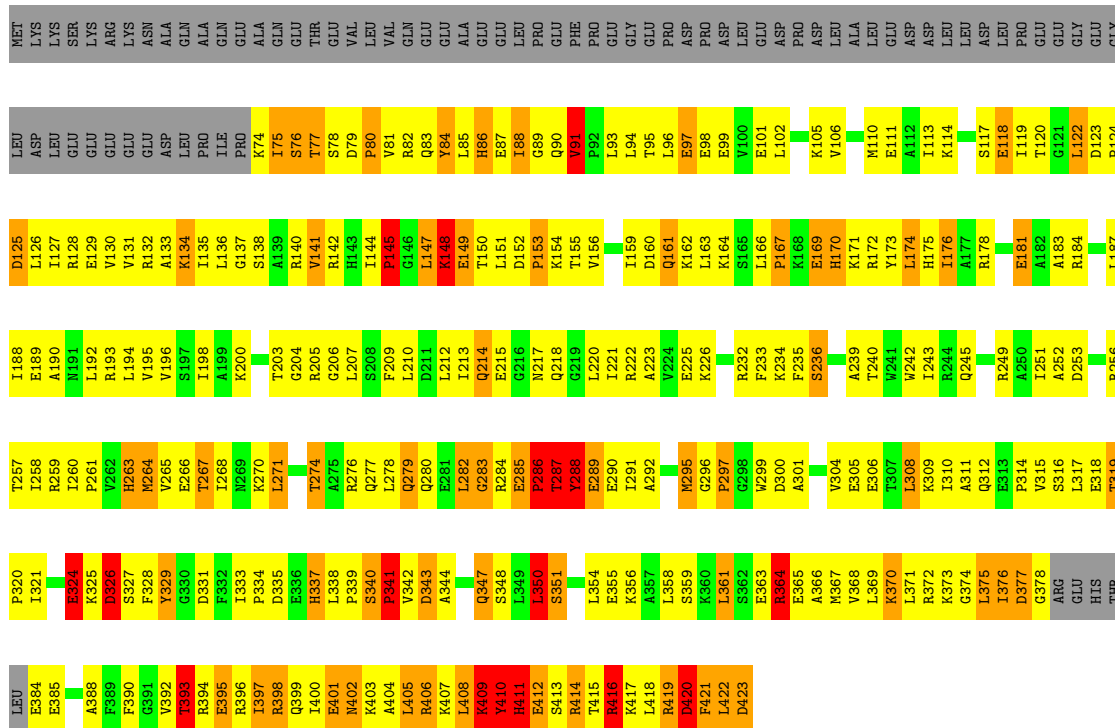


- Molecule 4: RNA polymerase omega subunit



- Molecule 5: RNA polymerase sigma-70 subunit





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	236.35Å 236.35Å 249.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.60)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.228 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	59529	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PB, 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	0.76	2/1838 (0.1%)	1.29	19/2498 (0.8%)
1	B	0.74	0/1838	1.19	20/2498 (0.8%)
1	K	0.71	1/1838 (0.1%)	1.21	17/2498 (0.7%)
1	L	0.73	0/1838	1.24	15/2498 (0.6%)
2	C	0.82	8/8997 (0.1%)	1.45	129/12164 (1.1%)
2	M	0.82	9/8997 (0.1%)	1.44	119/12164 (1.0%)
3	D	0.84	18/10979 (0.2%)	1.47	168/14844 (1.1%)
3	N	0.84	20/10979 (0.2%)	1.48	167/14844 (1.1%)
4	E	0.84	0/783	1.47	11/1054 (1.0%)
4	O	0.81	0/783	1.50	9/1054 (0.9%)
5	F	1.00	13/2812 (0.5%)	1.44	47/3781 (1.2%)
5	P	0.92	9/2812 (0.3%)	1.44	38/3781 (1.0%)
All	All	0.83	80/54494 (0.1%)	1.43	759/73678 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	3
3	N	0	3
5	F	0	1
All	All	0	7

The worst 5 of 80 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	380	GLU	C-N	-11.84	1.17	1.33
2	C	58	ASP	CA-C	-11.64	1.39	1.52
3	N	380	GLU	C-N	-11.54	1.17	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	423	ASP	C-OXT	10.80	1.45	1.23
5	F	420	ASP	CA-C	-9.97	1.40	1.52

The worst 5 of 759 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	380	GLU	CA-C-O	-21.63	96.85	120.43
1	L	229	GLN	CA-C-O	21.37	157.12	120.80
3	N	380	GLU	CA-C-O	-20.66	97.86	120.80
2	C	243	ARG	CA-C-N	19.93	144.75	119.84
2	C	243	ARG	C-N-CA	19.93	144.75	119.84

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	132	TYR	Sidechain
3	D	379	ALA	Peptide
3	D	380	GLU	Mainchain
5	F	421	PHE	Sidechain
3	N	132	TYR	Sidechain

5.2 Too-close contacts [i](#)

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	255	0
1	B	1806	0	1861	218	0
1	K	1806	0	1861	215	0
1	L	1806	0	1861	213	0
2	C	8829	0	8933	1337	0
2	M	8829	0	8933	1310	0
3	D	10801	0	10888	1589	0
3	N	10801	0	10885	1588	0
4	E	769	0	775	102	0
4	O	769	0	775	111	0
5	F	2771	0	2843	408	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	2771	0	2844	435	0
6	A	18	0	0	0	0
6	B	24	0	0	0	0
6	C	63	0	0	0	0
6	D	118	0	0	1	0
6	E	6	0	0	0	0
6	F	31	0	0	0	0
6	K	20	0	0	0	0
6	L	19	0	0	0	0
6	M	64	0	0	0	0
6	N	92	0	0	0	0
6	O	8	0	0	0	0
6	P	22	0	0	0	0
7	D	2	0	0	0	0
7	N	2	0	0	0	0
8	A	194	0	0	46	0
8	B	193	0	0	51	0
8	C	869	0	0	256	0
8	D	1163	0	0	330	0
8	E	114	0	0	30	0
8	F	381	0	0	67	0
8	K	161	0	0	49	0
8	L	157	0	0	53	0
8	M	822	0	0	269	0
8	N	983	0	0	293	0
8	O	114	0	0	32	0
8	P	325	0	0	75	0
All	All	59529	0	54320	7258	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 67.

The worst 5 of 7258 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)
5:F:419:ARG:CB	5:F:419:ARG:CG	1.76	1.60
5:P:401:GLU:CG	5:P:401:GLU:CB	1.76	1.56
5:F:401:GLU:CB	5:F:401:GLU:CG	1.77	1.55
3:N:218:LYS:CB	8:N:9902:HOH:O	1.85	1.18
1:A:94:LEU:HD21	1:A:119:ASP:HB2	1.26	1.16

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 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%)	201 (88%)	21 (9%)	5 (2%)	5	10
1	B	227/315 (72%)	200 (88%)	24 (11%)	3 (1%)	9	21
1	K	227/315 (72%)	199 (88%)	24 (11%)	4 (2%)	6	14
1	L	227/315 (72%)	199 (88%)	25 (11%)	3 (1%)	9	21
2	C	1117/1119 (100%)	923 (83%)	139 (12%)	55 (5%)	1	2
2	M	1117/1119 (100%)	928 (83%)	135 (12%)	54 (5%)	2	2
3	D	1388/1524 (91%)	1119 (81%)	196 (14%)	73 (5%)	1	1
3	N	1388/1524 (91%)	1113 (80%)	200 (14%)	75 (5%)	1	1
4	E	93/99 (94%)	72 (77%)	13 (14%)	8 (9%)	0	0
4	O	93/99 (94%)	71 (76%)	15 (16%)	7 (8%)	1	1
5	F	341/423 (81%)	295 (86%)	31 (9%)	15 (4%)	2	2
5	P	341/423 (81%)	288 (84%)	34 (10%)	19 (6%)	1	1
All	All	6786/7590 (89%)	5608 (83%)	857 (13%)	321 (5%)	2	2

5 of 321 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	GLY
2	C	111	ASP
2	C	152	PRO
2	C	231	PRO
2	C	244	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	202/273 (74%)	162 (80%)	40 (20%)	1	2
1	B	202/273 (74%)	164 (81%)	38 (19%)	1	2
1	K	202/273 (74%)	160 (79%)	42 (21%)	1	2
1	L	202/273 (74%)	163 (81%)	39 (19%)	1	2
2	C	941/941 (100%)	712 (76%)	229 (24%)	1	1
2	M	941/941 (100%)	694 (74%)	247 (26%)	0	1
3	D	1123/1279 (88%)	840 (75%)	283 (25%)	0	1
3	N	1123/1279 (88%)	810 (72%)	313 (28%)	0	1
4	E	83/87 (95%)	65 (78%)	18 (22%)	1	2
4	O	83/87 (95%)	68 (82%)	15 (18%)	2	3
5	F	295/370 (80%)	220 (75%)	75 (25%)	0	1
5	P	295/370 (80%)	232 (79%)	63 (21%)	1	2
All	All	5692/6446 (88%)	4290 (75%)	1402 (25%)	1	1

5 of 1402 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	673	LEU
3	N	752	SER
2	M	791	ARG
2	M	672	VAL
3	N	121	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 180 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	431	HIS
3	N	714	GLN
2	M	834	GLN
2	M	1064	ASN

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Mol	Chain	Res	Type
3	N	962	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 489 ligands modelled in this entry, 489 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	D	1
3	N	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	380:GLU	C	381:ALA	N	1.17
1	N	380:GLU	C	381:ALA	N	1.17

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.