



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:27 PM GMT

PDB ID : 1K83
Title : Crystal Structure of Yeast RNA Polymerase II Complexed with the Inhibitor Alpha Amanitin
Authors : Bushnell, D.A.; Cramer, P.; Kornberg, R.D.
Deposited on : 2001-10-22
Resolution : 2.80 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

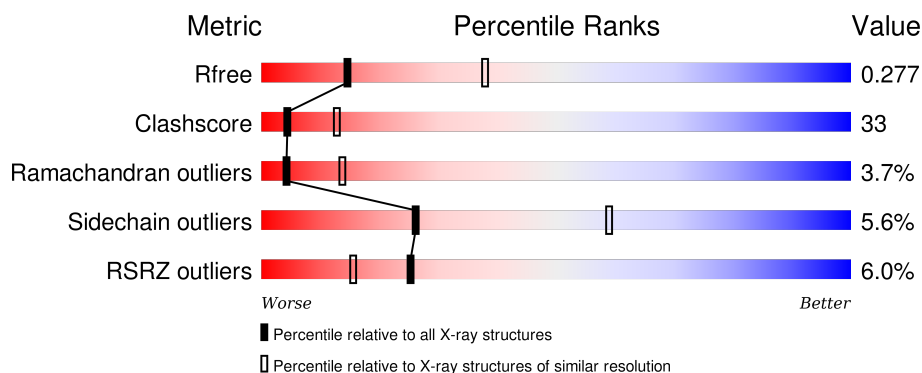
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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. 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	1733	<div> <div>4%</div> <div>40% 33% 5% 21%</div> </div>
2	B	1224	<div> <div>6%</div> <div>47% 38% • 12%</div> </div>
3	C	318	<div> <div>2%</div> <div>36% 43% • 16%</div> </div>
4	E	215	<div> <div>3%</div> <div>56% 39% 5% •</div> </div>
5	F	155	<div> <div>•</div> <div>25% 27% • 46%</div> </div>

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Mol	Chain	Length	Quality of chain
6	H	146	<div><div></div><div>21%31%50%10%9%</div></div>
7	I	122	<div><div></div><div>4%48%45%7%</div></div>
8	J	70	<div><div></div><div>%47%43%7%</div></div>
9	K	120	<div><div></div><div>3%43%43%9%5%</div></div>
10	L	70	<div><div></div><div>14%13%39%13%36%</div></div>
11	M	8	<div><div></div><div>13%50%38%13%</div></div>

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 27902 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 II LARGEST SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1366	Total	C	N	O	S	0	0	0
			10751	6785	1871	2036	59			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II 140KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1082	Total	C	N	O	S	0	0	0
			8616	5467	1503	1594	52			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II 45KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II 27KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	213	Total	C	N	O	S	0	0	0
			1744	1107	308	318	11			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASE II 23KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASE II 14.5KD POLYPEPTIDE.

TIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II 14.2KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	122	Total	C	N	O	S	0	0	0
			997	613	182	191	11			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASE II 8.3KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II 13.6KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASE II 7.7KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	45	Total	C	N	O	S	0	0	0
			359	221	71	63	4			

- Molecule 11 is a protein called ALPHA AMANITIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	M	8	Total	C	N	O	S	0	0	0
			64	39	10	14	1			

- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	J	1	Total 1	Zn 1	0	0
12	B	1	Total 1	Zn 1	0	0
12	I	2	Total 2	Zn 2	0	0
12	C	1	Total 1	Zn 1	0	0
12	A	2	Total 2	Zn 2	0	0
12	L	1	Total 1	Zn 1	0	0

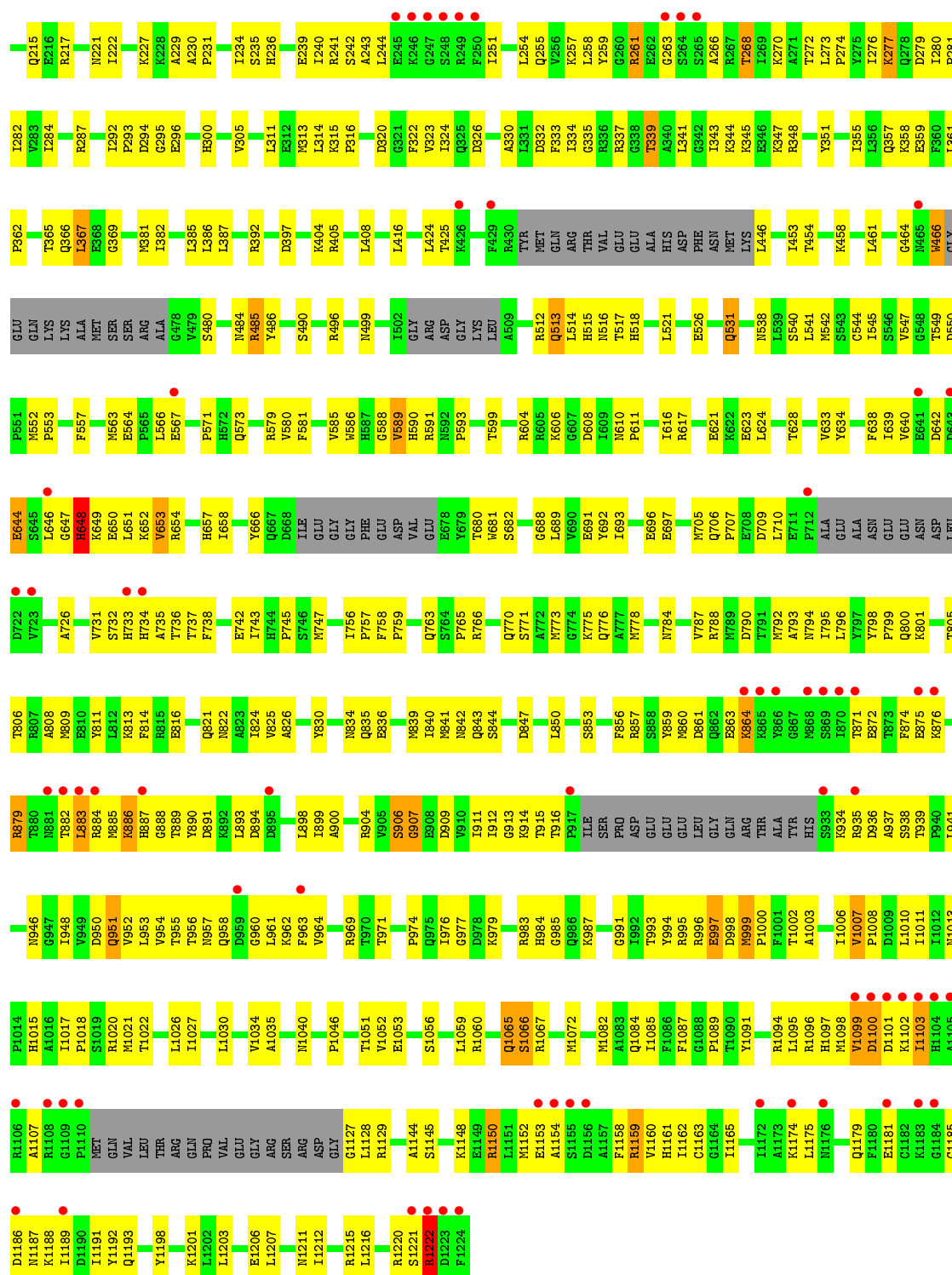
- Molecule 13 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	1	Total 1	Mn 1	0	0

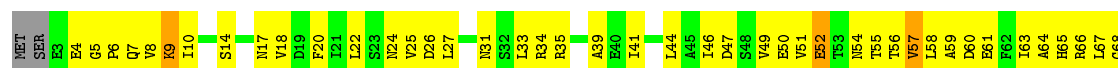
- Molecule 14 is water.

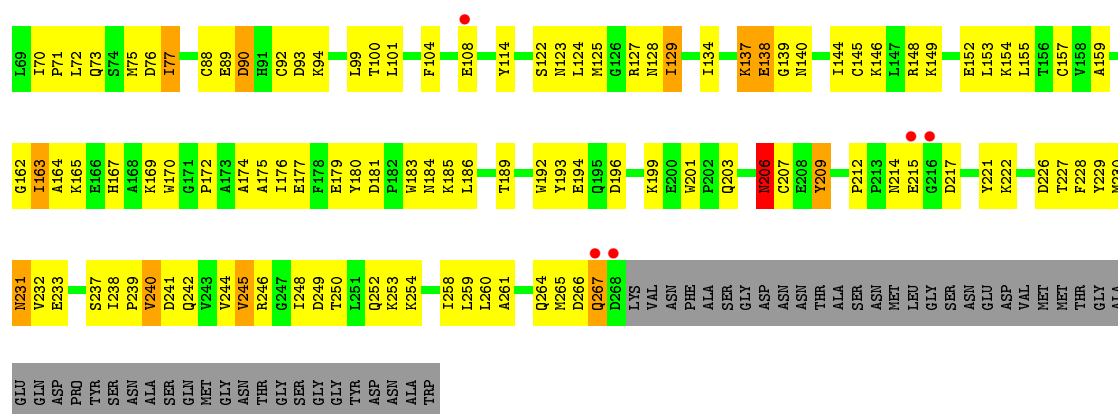
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	31	Total 31	O 31	0	0
14	B	23	Total 23	O 23	0	0
14	C	3	Total 3	O 3	0	0
14	E	6	Total 6	O 6	0	0
14	F	4	Total 4	O 4	0	0
14	J	1	Total 1	O 1	0	0
14	M	1	Total 1	O 1	0	0

PI099	PI100	PI101	PI102	LI105	MI106	VI107	MI111	LI112	FI108	GLI113	PI114	SI115	LI116	LI117	VI118	QI103	EI034	YI035	YI036	QI039	QI040	AI041	VI045	NI048	HI059	PI060	GI061	VI066	NI070	NI071	NI072	NI073	NI074	NI075	NI076	NI077	NI078	NI079	NI080	NI081	NI082	NI083	NI084	NI085	NI086	NI087	NI088	NI089	NI090	NI091	NI092	NI093	NI094	NI095	NI096	NI097	NI098	NI099	NI100	NI101	NI102	NI103	NI104	NI105	NI106	NI107	NI108	NI109	NI110	NI111	NI112	NI113	NI114	NI115	NI116	NI117	NI118	NI119	NI120	NI121	NI122	NI123	NI124	NI125	NI126	NI127	NI128	NI129	NI130	NI131	NI132	NI133	NI134	NI135	NI136	NI137	NI138	NI139	NI140	NI141	NI142	NI143	NI144	NI145	NI146	NI147	NI148	NI149	NI150	NI151	NI152	NI153	NI154	NI155	NI156	NI157	NI158	NI159	NI160	NI161	NI162	NI163	NI164	NI165	NI166	NI167	NI168	NI169	NI170	NI171	NI172	NI173	NI174	NI175	NI176	NI177	NI178	NI179	NI180	NI181	NI182	NI183	NI184	NI185	NI186	NI187	NI188	NI189	NI190	NI191	NI192	NI193	NI194	NI195	NI196	NI197	NI198	NI199	NI200	NI201	NI202	NI203	NI204	NI205	NI206	NI207	NI208	NI209	NI210	NI211	NI212	NI213	NI214	NI215	NI216	NI217	NI218	NI219	NI220	NI221	NI222	NI223	NI224	NI225	NI226	NI227	NI228	NI229	NI230	NI231	NI232	NI233	NI234	NI235	NI236	NI237	NI238	NI239	NI240	NI241	NI242	NI243	NI244	NI245	NI246	NI247	NI248	NI249	NI250	NI251	NI252	NI253	NI254	NI255	NI256	NI257	NI258	NI259	NI260	NI261	NI262	NI263	NI264	NI265	NI266	NI267	NI268	NI269	NI270	NI271	NI272	NI273	NI274	NI275	NI276	NI277	NI278	NI279	NI280	NI281	NI282	NI283	NI284	NI285	NI286	NI287	NI288	NI289	NI290	NI291	NI292	NI293	NI294	NI295	NI296	NI297	NI298	NI299	NI300	NI301	NI302	NI303	NI304	NI305	NI306	NI307	NI308	NI309	NI310	NI311	NI312	NI313	NI314	NI315	NI316	NI317	NI318	NI319	NI320	NI321	NI322	NI323	NI324	NI325	NI326	NI327	NI328	NI329	NI330	NI331	NI332	NI333	NI334	NI335	NI336	NI337	NI338	NI339	NI340	NI341	NI342	NI343	NI344	NI345	NI346	NI347	NI348	NI349	NI350	NI351	NI352	NI353	NI354	NI355	NI356	NI357	NI358	NI359	NI360	NI361	NI362	NI363	NI364	NI365	NI366	NI367	NI368	NI369	NI370	NI371	NI372	NI373	NI374	NI375	NI376	NI377	NI378	NI379	NI380	NI381	NI382	NI383	NI384	NI385	NI386	NI387	NI388	NI389	NI390	NI391	NI392	NI393	NI394	NI395	NI396	NI397	NI398	NI399	NI400	NI401	NI402	NI403	NI404	NI405	NI406	NI407	NI408	NI409	NI410	NI411	NI412	NI413	NI414	NI415	NI416	NI417	NI418	NI419	NI420	NI421	NI422	NI423	NI424	NI425	NI426	NI427	NI428	NI429	NI430	NI431	NI432	NI433	NI434	NI435	NI436	NI437	NI438	NI439	NI440	NI441	NI442	NI443	NI444	NI445	NI446	NI447	NI448	NI449	NI450	NI451	NI452	NI453	NI454	NI455	NI456	NI457	NI458	NI459	NI460	NI461	NI462	NI463	NI464	NI465	NI466	NI467	NI468	NI469	NI470	NI471	NI472	NI473	NI474	NI475	NI476	NI477	NI478	NI479	NI480	NI481	NI482	NI483	NI484	NI485	NI486	NI487	NI488	NI489	NI490	NI491	NI492	NI493	NI494	NI495	NI496	NI497	NI498	NI499	NI500	NI501	NI502	NI503	NI504	NI505	NI506	NI507	NI508	NI509	NI510	NI511	NI512	NI513	NI514	NI515	NI516	NI517	NI518	NI519	NI520	NI521	NI522	NI523	NI524	NI525	NI526	NI527	NI528	NI529	NI530	NI531	NI532	NI533	NI534	NI535	NI536	NI537	NI538	NI539	NI540	NI541	NI542	NI543	NI544	NI545	NI546	NI547	NI548	NI549	NI550	NI551	NI552	NI553	NI554	NI555	NI556	NI557	NI558	NI559	NI560	NI561	NI562	NI563	NI564	NI565	NI566	NI567	NI568	NI569	NI570	NI571	NI572	NI573	NI574	NI575	NI576	NI577	NI578	NI579	NI580	NI581	NI582	NI583	NI584	NI585	NI586	NI587	NI588	NI589	NI590	NI591	NI592	NI593	NI594	NI595	NI596	NI597	NI598	NI599	NI600	NI601	NI602	NI603	NI604	NI605	NI606	NI607	NI608	NI609	NI610	NI611	NI612	NI613	NI614	NI615	NI616	NI617	NI618	NI619	NI620	NI621	NI622	NI623	NI624	NI625	NI626	NI627	NI628	NI629	NI630	NI631	NI632	NI633	NI634	NI635	NI636	NI637	NI638	NI639	NI640	NI641	NI642	NI643	NI644	NI645	NI646	NI647	NI648	NI649	NI650	NI651	NI652	NI653	NI654	NI655	NI656	NI657	NI658	NI659	NI660	NI661	NI662	NI663	NI664	NI665	NI666	NI667	NI668	NI669	NI670	NI671	NI672	NI673	NI674	NI675	NI676	NI677	NI678	NI679	NI680	NI681	NI682	NI683	NI684	NI685	NI686	NI687	NI688	NI689	NI690	NI691	NI692	NI693	NI694	NI695	NI696	NI697	NI698	NI699	NI700	NI701	NI702	NI703	NI704	NI705	NI706	NI707	NI708	NI709	NI710	NI711	NI712	NI713	NI714	NI715	NI716	NI717	NI718	NI719	NI720	NI721	NI722	NI723	NI724	NI725	NI726	NI727	NI728	NI729	NI730	NI731	NI732	NI733	NI734	NI735	NI736	NI737	NI738	NI739	NI740	NI741	NI742	NI743	NI744	NI745	NI746	NI747	NI748	NI749	NI750	NI751	NI752	NI753	NI754	NI755	NI756	NI757	NI758	NI759	NI760	NI761	NI762	NI763	NI764	NI765	NI766	NI767	NI768	NI769	NI770	NI771	NI772	NI773	NI774	NI775	NI776	NI777	NI778	NI779	NI780	NI781	NI782	NI783	NI784	NI785	NI786	NI787	NI788	NI789	NI790	NI791	NI792	NI793	NI794	NI795	NI796	NI797	NI798	NI799	NI800	NI801	NI802	NI803	NI804	NI805	NI806	NI807	NI808	NI809	NI810	NI811	NI812	NI813	NI814	NI815	NI816	NI817	NI818	NI819	NI820	NI821	NI822	NI823	NI824	NI825	NI826	NI827	NI828	NI829	NI830	NI831	NI832	NI833	NI834	NI835	NI836	NI837	NI838	NI839	NI840	NI841	NI842	NI843	NI844	NI845	NI846	NI847	NI848	NI849	NI850	NI851	NI852	NI853	NI854	NI855	NI856	NI857	NI858	NI859	NI860	NI861	NI862	NI863	NI864	NI865	NI866	NI867	NI868	NI869	NI870	NI871	NI872	NI873	N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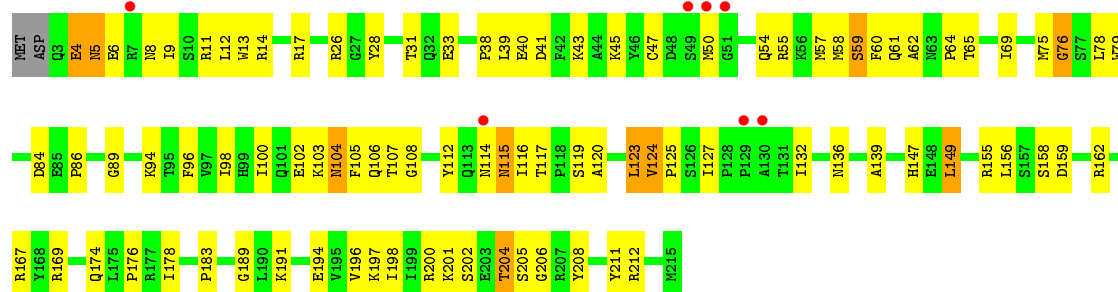


● Molecule 3: DNA-DIRECTED RNA POLYMERASE II 45KD POLYPEPTIDE

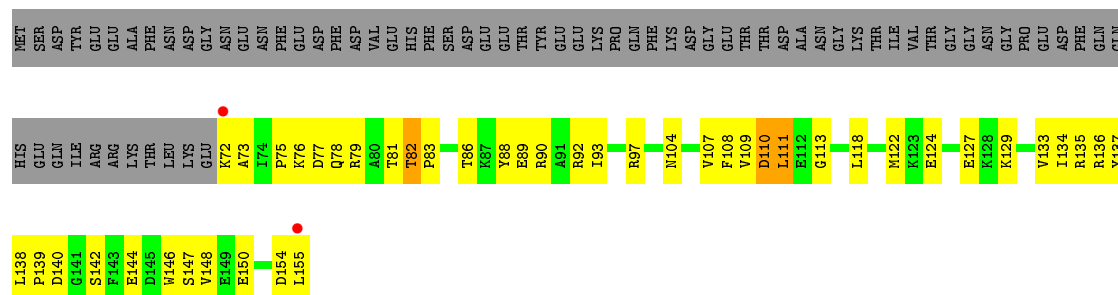
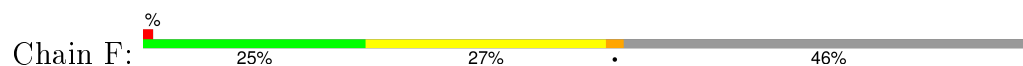




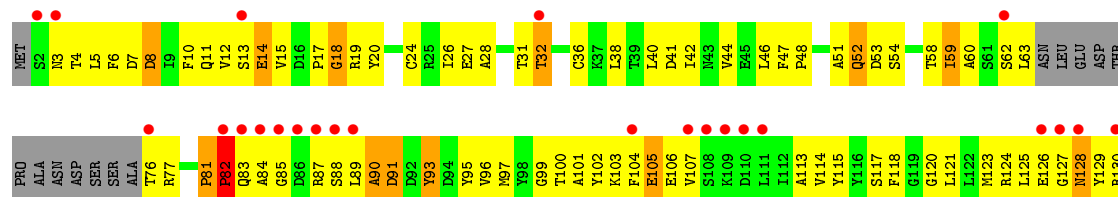
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II 27KD POLYPEPTIDE



• Molecule 5: DNA-DIRECTED RNA POLYMERASE II 23KD POLYPEPTIDE



• Molecule 6: DNA-DIRECTED RNA POLYMERASE II 14.5KD POLYPEPTIDE





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	122.51Å 222.48Å 374.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.80) 93.4 (20.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.79Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.280 0.227 , 0.277	Depositor DCC
R_{free} test set	3507 reflections (3.01%)	DCC
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 125151 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	27902	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MN, HYP, TRX, CSX, ILX

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	0.42	0/10940	0.68	2/14792 (0.0%)
2	B	0.42	0/8786	0.68	1/11847 (0.0%)
3	C	0.40	0/2133	0.66	0/2891
4	E	0.40	0/1780	0.67	0/2395
5	F	0.46	0/691	0.67	0/933
6	H	0.36	0/1086	0.68	0/1470
7	I	0.48	0/1016	0.68	0/1365
8	J	0.44	0/541	0.70	0/727
9	K	0.39	0/937	0.62	0/1265
10	L	0.47	0/361	0.71	0/478
11	M	2.39	1/22 (4.5%)	1.63	0/26
All	All	0.42	1/28293 (0.0%)	0.68	3/38189 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	7	ASN	CA-C	5.26	1.66	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	200	GLY	N-CA-C	5.82	127.64	113.10
1	A	798	GLY	N-CA-C	5.55	126.98	113.10
1	A	472	LEU	CA-CB-CG	-5.01	103.78	115.30

There are no chirality outliers.

There are no planarity outliers.

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	10751	0	10819	759	0
2	B	8616	0	8645	586	0
3	C	2095	0	2051	165	0
4	E	1744	0	1772	87	0
5	F	679	0	701	55	0
6	H	1068	0	1040	115	0
7	I	997	0	953	75	0
8	J	532	0	542	56	0
9	K	919	0	929	71	0
10	L	359	0	382	61	1
11	M	64	0	51	7	0
12	A	2	0	0	0	0
12	B	1	0	0	0	0
12	C	1	0	0	0	0
12	I	2	0	0	0	0
12	J	1	0	0	0	0
12	L	1	0	0	0	0
13	A	1	0	0	0	0
14	A	31	0	0	1	0
14	B	23	0	0	5	0
14	C	3	0	0	0	0
14	E	6	0	0	1	0
14	F	4	0	0	0	0
14	J	1	0	0	0	0
14	M	1	0	0	0	0
All	All	27902	0	27885	1826	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 33.

The worst 5 of 1826 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:A:1161:THR:HG22	1:A:1163:ILE:H	1.09	1.15
2:B:1051:THR:HG22	2:B:1053:GLU:H	1.17	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:871:THR:HG22	2:B:872:GLU:H	1.09	1.09
1:A:855:THR:HG21	1:A:857:ARG:HE	1.10	1.08
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.33	1.07

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)
10:L:28:LYS:NZ	10:L:28:LYS:NZ[3_655]	2.05	0.15

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	1348/1733 (78%)	1160 (86%)	134 (10%)	54 (4%)	4	12
2	B	1062/1224 (87%)	931 (88%)	107 (10%)	24 (2%)	8	26
3	C	264/318 (83%)	223 (84%)	30 (11%)	11 (4%)	3	11
4	E	211/215 (98%)	180 (85%)	23 (11%)	8 (4%)	4	13
5	F	82/155 (53%)	71 (87%)	10 (12%)	1 (1%)	16	47
6	H	129/146 (88%)	88 (68%)	23 (18%)	18 (14%)	0	1
7	I	120/122 (98%)	102 (85%)	16 (13%)	2 (2%)	11	36
8	J	63/70 (90%)	58 (92%)	5 (8%)	0	100	100
9	K	112/120 (93%)	98 (88%)	13 (12%)	1 (1%)	21	55
10	L	43/70 (61%)	23 (54%)	13 (30%)	7 (16%)	0	0
11	M	4/8 (50%)	4 (100%)	0	0	100	100
All	All	3438/4181 (82%)	2938 (86%)	374 (11%)	126 (4%)	4	14

5 of 126 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ASP
1	A	56	PRO
1	A	399	HIS
1	A	464	PRO
1	A	465	TYR

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	1196/1520 (79%)	1116 (93%)	80 (7%)	20	50
2	B	940/1061 (89%)	899 (96%)	41 (4%)	35	69
3	C	234/274 (85%)	221 (94%)	13 (6%)	26	59
4	E	195/197 (99%)	190 (97%)	5 (3%)	54	86
5	F	74/137 (54%)	71 (96%)	3 (4%)	37	72
6	H	117/128 (91%)	114 (97%)	3 (3%)	54	86
7	I	116/116 (100%)	108 (93%)	8 (7%)	19	48
8	J	60/65 (92%)	57 (95%)	3 (5%)	30	64
9	K	99/102 (97%)	88 (89%)	11 (11%)	8	23
10	L	40/57 (70%)	34 (85%)	6 (15%)	3	11
11	M	2/2 (100%)	2 (100%)	0	100	100
All	All	3073/3659 (84%)	2900 (94%)	173 (6%)	26	59

5 of 173 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1426	GLU
2	B	513	GLN
9	K	50	LEU
2	B	18	PHE
2	B	261	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	325	GLN
2	B	648	HIS
6	H	128	ASN
2	B	366	GLN
2	B	515	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	ILX	M	1	11	7,9,10	1.66	2 (28%)	7,11,13	1.84	2 (28%)
11	TRX	M	2	11	14,16,17	2.56	5 (35%)	10,22,24	2.13	5 (50%)
11	CSX	M	6	11	3,6,7	2.65	2 (66%)	3,6,8	1.34	1 (33%)
11	HYP	M	8	11	7,8,9	4.03	1 (14%)	5,10,12	1.45	2 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	ILX	M	1	11	-	0/10/12/14	0/0/0/0
11	TRX	M	2	11	-	0/3/6/8	0/2/2/2
11	CSX	M	6	11	-	0/1/5/7	0/0/0/0
11	HYP	M	8	11	-	0/0/11/13	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	6	CSX	O-C	2.36	1.30	1.19
11	M	2	TRX	CD1-CG	2.48	1.43	1.38
11	M	1	ILX	CA-N	2.58	1.56	1.47
11	M	2	TRX	CZ3-CH2	2.85	1.44	1.38
11	M	1	ILX	OG1-CG1	2.92	1.49	1.43

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	2	TRX	CH2-CZ2-CE2	-4.32	116.37	119.19
11	M	1	ILX	CG2-CB-CG1	-3.50	105.72	111.22
11	M	2	TRX	OH2-CH2-CZ3	-2.91	111.82	120.05
11	M	2	TRX	O-C-CA	-2.68	118.50	125.49
11	M	6	CSX	O-C-CA	-2.30	119.51	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	M	1	ILX	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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	1366/1733 (78%)	-0.04	66 (4%) 34 23	18, 48, 107, 137	0
2	B	1082/1224 (88%)	-0.02	78 (7%) 18 10	20, 46, 105, 128	0
3	C	266/318 (83%)	-0.09	5 (1%) 70 59	30, 53, 83, 124	0
4	E	213/215 (99%)	0.01	7 (3%) 50 38	22, 59, 99, 109	0
5	F	84/155 (54%)	-0.25	2 (2%) 62 50	24, 44, 67, 82	0
6	H	133/146 (91%)	1.15	30 (22%) 1 1	64, 94, 122, 125	0
7	I	122/122 (100%)	0.01	5 (4%) 41 29	30, 51, 89, 106	0
8	J	65/70 (92%)	-0.41	1 (1%) 76 68	26, 47, 76, 85	0
9	K	114/120 (95%)	-0.16	3 (2%) 59 47	31, 60, 79, 97	0
10	L	45/70 (64%)	1.03	10 (22%) 1 1	49, 86, 108, 110	0
11	M	4/8 (50%)	0.88	1 (25%) 1 0	73, 80, 83, 84	0
All	All	3494/4181 (83%)	0.01	208 (5%) 25 15	18, 50, 105, 137	0

The worst 5 of 208 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	69	THR	15.1
1	A	1390	ASN	11.3
2	B	882	THR	9.2
2	B	866	TYR	8.5
1	A	1389	PHE	8.2

6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
11	ILX	M	1	10/11	0.84	0.33	-	72,74,79,80	0
11	CSX	M	6	7/8	0.74	0.24	-	80,82,84,86	0
11	HYP	M	8	8/9	0.91	0.20	-	70,72,72,73	0
11	TRX	M	2	15/16	0.88	0.23	-	75,77,79,80	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
12	ZN	C	3002	1/1	0.99	0.09	-1.29	49,49,49,49	0
12	ZN	B	3007	1/1	0.99	0.07	-1.32	64,64,64,64	0
12	ZN	I	3004	1/1	0.96	0.07	-1.65	62,62,62,62	0
12	ZN	J	3001	1/1	0.99	0.12	-1.68	46,46,46,46	0
12	ZN	L	3005	1/1	0.89	0.06	-1.69	86,86,86,86	0
12	ZN	A	3008	1/1	0.97	0.12	-1.73	81,81,81,81	0
12	ZN	A	3006	1/1	0.98	0.10	-2.19	64,64,64,64	0
12	ZN	I	3003	1/1	0.99	0.08	-2.42	45,45,45,45	0
13	MN	A	3009	1/1	0.72	0.34	-	149,149,149,149	0

6.5 Other polymers [i](#)

There are no such residues in this entry.