



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:06 PM GMT

PDB ID : 1WCM
Title : COMPLETE 12-SUBUNIT RNA POLYMERASE II AT 3.8 ANG
Authors : Armache, K.-J.; Mitterweger, S.; Meinhart, A.; Cramer, P.
Deposited on : 2004-11-17
Resolution : 3.80 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

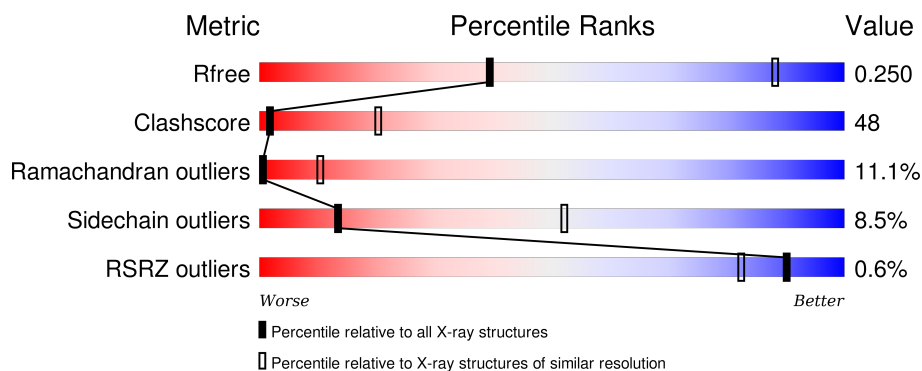
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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. 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>27%</div> <div>43%</div> <div>10%</div> <div>18%</div> </div>
2	B	1224	<div> <div>29%</div> <div>48%</div> <div>12%</div> <div>10%</div> </div>
3	C	318	<div> <div>23%</div> <div>48%</div> <div>12%</div> <div>16%</div> </div>
4	D	177	<div> <div>42%</div> <div>46%</div> <div>11%</div> </div>
5	E	215	<div> <div>40%</div> <div>54%</div> <div>6%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	F	155	<div><div></div><div>18%30%6%46%</div></div>
7	G	171	<div><div></div><div>39%51%9%</div></div>
8	H	146	<div><div>%</div><div></div><div>32%49%10%9%</div></div>
9	I	122	<div><div>2%</div><div></div><div>40%43%12%.</div></div>
10	J	70	<div><div></div><div>17%53%23%7%</div></div>
11	K	120	<div><div></div><div>41%47%8%.</div></div>
12	L	70	<div><div>%</div><div></div><div>16%31%19%34%</div></div>

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 30945 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 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1416	Total	C	N	O	S	0	0	0
			11140	7021	1946	2111	62			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SECOND LARGEST SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1097	Total	C	N	O	S	0	0	0
			8720	5526	1523	1617	54			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II 45 KDA 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 32 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	177	Total	C	N	O	S	0	0	0
			1356	840	241	273	2			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 27 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 23

KDA POLYPEPTIDE.

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

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II 19 KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 14.5 KDA POLYPEPTIDE.

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

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II 14.2 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II AND III 8.3 KDA POLYPEPTIDE.

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

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II 13.6 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	115	Total	C	N	O	S	0	0	1
			920	590	157	171	2			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 7.7 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

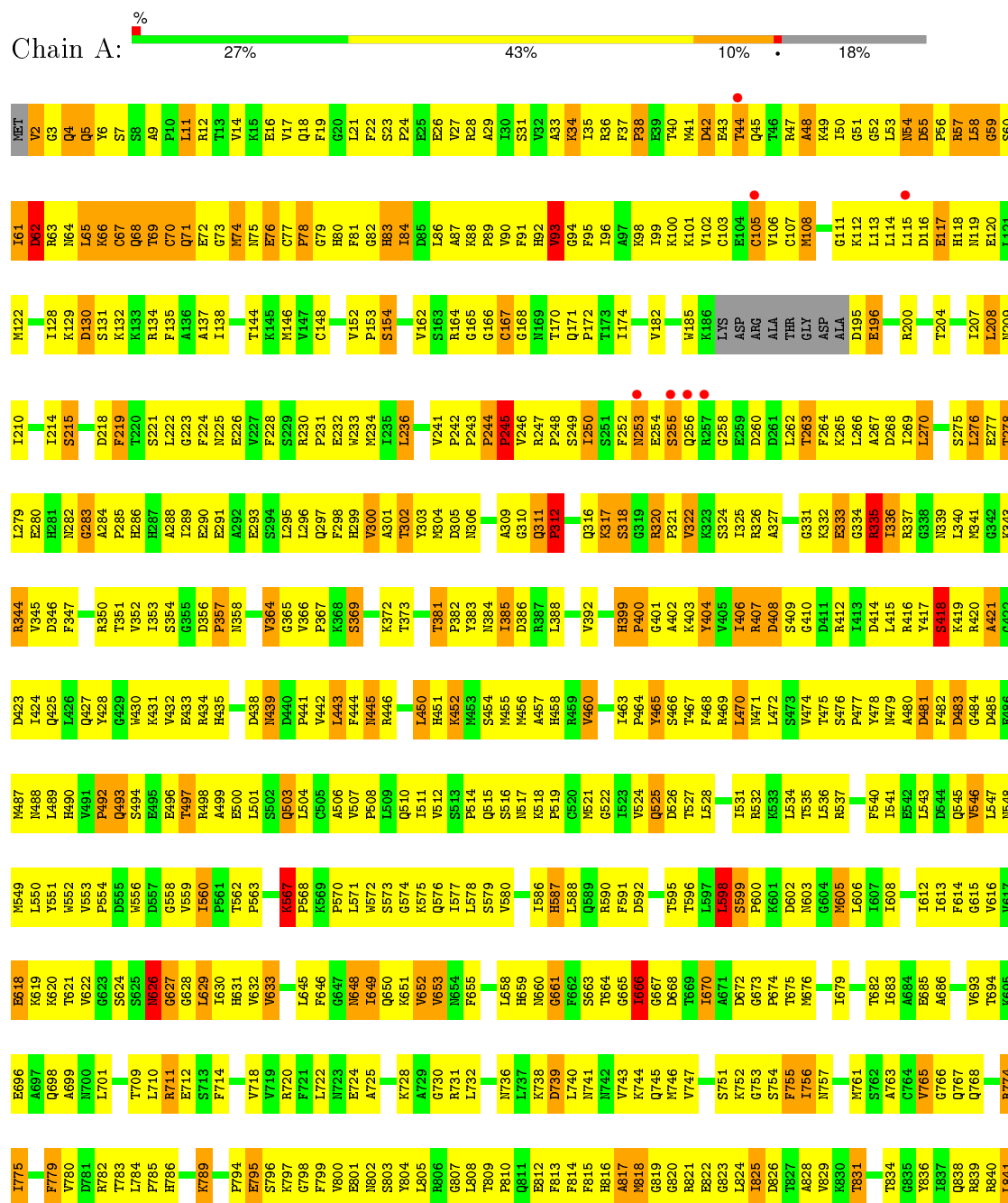
- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

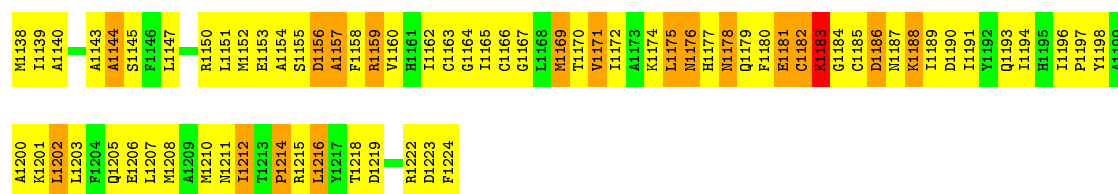
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 II LARGEST SUBUNIT

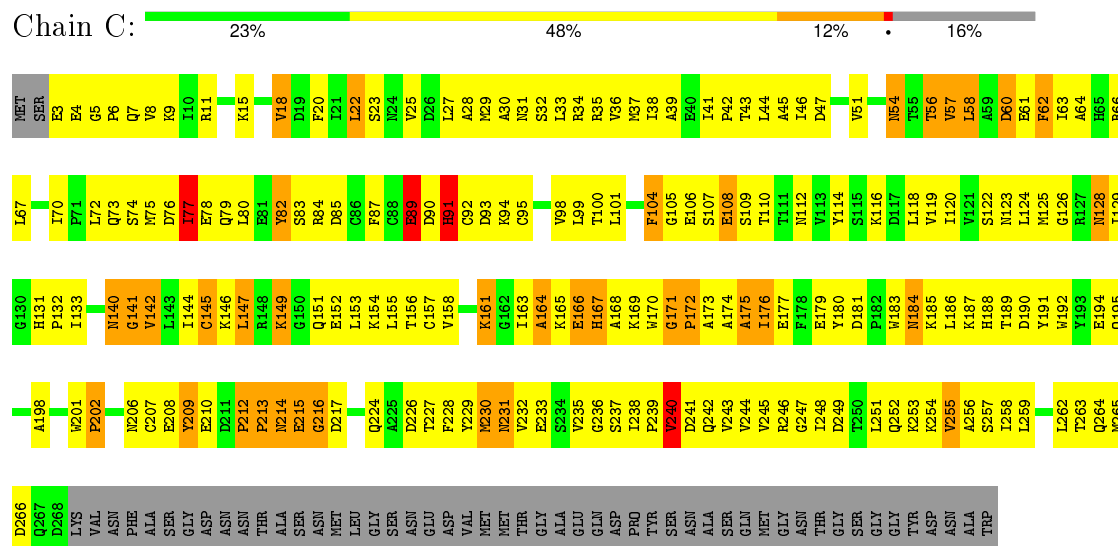




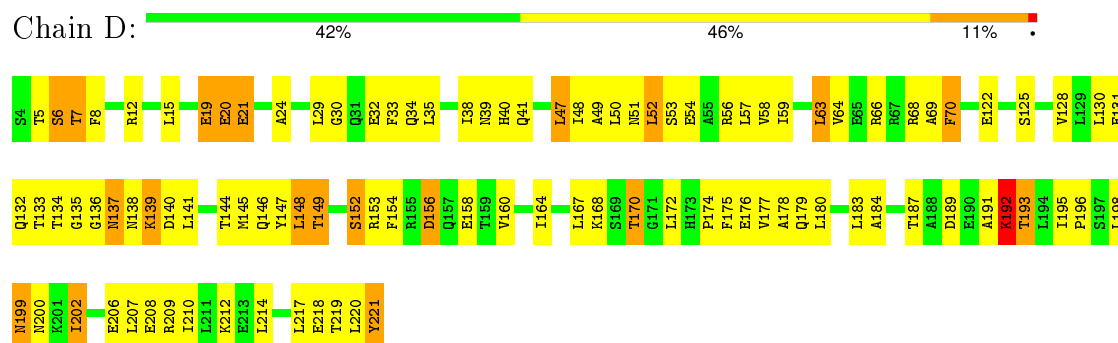
G1068	E997	H1S	G867	L803	C741	E678	V613	G548	C478	A409	LEU	K270	K193	F129	E85
F1069	D998	S933	R668	T806	E742	T679	S614	T649	V479	G410	GLY	K273	E194	V130	D66
M1072	P1000	R935	S869	T807	E743	T680	M615	D550	S480	P411	ILE	L273	E195	D131	S67
N1073	F1001	D936	T871	A808	T745	G682	I616	P551	N483	L412	LVS		P196	V132	T68
N1074	T1002	A937	E872	M909	P745	S633	R617	N552	N484	L413	K345	I276	F197	K133	L69
T1077	A1003	S938	T873	E810	S746	L684	R620	T554	R485	A414	K347	K277	D198	K134	I70
		T939		Y811	T747	L685	E621	T555	T486	Q415		Q278	M199	ARG	LEU
		P940	P877		I748	R686	K622	T556	T487	R418	Y351	I280	G201	THR	GLU
K1080	V1007	R878	Q878	R815	L749	G687	E623	F587	Y488	T419		I281	G202	TYR	GLN
L1081	P1008	R879	G688	R816	G750	G688	E624	L588	Y489	L420		I282	F203	GLU	LEU
M1082	D1009	S943	T880	L817	T751	L689	K625	S559	S490	F421	I355	I283	I204	ALA	ALA
A1083	L1010	R881	T881	P813	K752	V690	K626	E560	T491		L356	V283	I205	GLN	GLN
Q1084	I1011	T882	E891	A819	A753	E691	F627	N561	L492	L424	Q357	I284	I206	ASP	HIS
I1085	T1012	L883	T692	G820		T692	T628	G562	S493		K358	I285	N206	VAL	THR
F1086	N1013	R884	D694	Q821	I756	T693	D629	N563	H494	D427	F360	R286	G207	PRO	THR
F1087	P940		D694	N822	F757	D694	A630		L495	F428	L361	R287		GLY	GLU
A1016	G1088		G888	A823	F758	E695	G631	L566	R496	F429	P362	A288	K210	GLU	ASP
I1017	P1089		T889	T824	P759	E696	R632		R497		H363	I289	V211	ASN	ASN
P1018	P1089		T890	V625	D760	E697	V633	T569	T498	T435	I364	I292	I212	ILE	ILE
S1019	S1019		D891	A826	H761	E698	V634	V570	N498	V436	T365	I293	I213	LYS	LYS
Y1091	R1020	V954	K892	R127	N762	E699	R635	P571	T500	E437	K366	I294	A214	TYR	SER
R1094	M1021	T955	L893		Q763	S700	P636	H572	P501	GLU	L367	D295		LEU	ARG
L1095	T1022	T956	D894	Y830	L637	D573	L637	D573	I502	ALA	E368	E296	R217	LVS	LVS
R1096	R1095	N957		S831	P764	E708	F638	S574	GLY	HIS	G369	I297	V223	TYR	TYR
H1097	H1097	Q958		G832	R766	I703	I639	P575	ARG	ASP	F370	L298	Q224	GLU	GLU
M1098	L1026	D959	L898	G833	N767	A704	V640	D676	ASP	PHE	S371	E299	Q225	GLU	S91
P1099	P1089	V952	T899	N834	T768	N705	E641	A577	GLY	ASN	S372	H300	F226	SER	F92
Y1091	E1028	F963	A900	Q835	Q769	Q706	D642	T578	LVS	NET	R373		K227	GLU	GLU
D1100	C1029	V964	P901	E836	Q770	E707	D643	H579	LEU	LVS	K374	V305	K228	ASP	I95
K1102	L1030	K965	G902	D837	S771	E708	E644	V580	A509	L446	A375	N306	A229	ASP	Y96
I1103	L1031	V966	V903	S838	A772	D709	E644	F581	K510	A447	F376	D307	A230	SER	Y97
H1104	S1032		R904	M839	K773	L710	H648	V582	P511	A450	F377	W308	P231	GLU	T98
R1105	R1033	R969	V905	T840	G774	E711	K649	V585	R512		L378	Q309	P232	SER	K99
R1106	T970	S906	M841	N841	K775	P712	E650	H586	Q513	L453	G379	N310	P233	GLY	P100
A1107	A1035	T971	G907	N842	A776		L651	H587	H514	T454	M381	L311	I234	V165	M101
R1108	A1036	K972	E908	Q843	A777	A715	K652	H588	H515	T454	I382	E312	S235	V102	V102
G1109	G1039	I973	D909	S844	M778	ASN	V653	G589	N516	S455	N383	N313	H236	H103	H103
P1110	N1040	P974	V910	S845	G779	GLU	R654	V589	T517	G456	N384	L314	V237	F166	E104
T1115	E1041	Q976	I911	R846	V780	GLU	K655	H590	H518	L457	N384	K315	A238	I167	
R1116		G977	G913	R848	L782	ASP	G656	N591	W519	K458	L386	F316	E239	G168	
Q1117	A1044	D978	K914	G949	T783	LEU	I658	P993	G520	V459	L387	C317	I240	V108	
P1118	S1045	K979	T915	L850	N784			H594	L521	A460	C388	I241		T109	
V1119	P1046	P980	T916	F851	Y785			R595	C523	L461	A389	L344		L112	
	F1047	A981	P917	R852	T786	D722	L661	L596	P524	A462		Q325		Y113	
R1122	R1122	Q982	I918	S853	V787	P725	M662		A525	T463		R326	I251	P114	
S1123	I1050	R983	S919	L854	R788	P726	T664		E526	G464		R327	L254	Q115	
R1124	T1051	H984	PRD	F855		K727	E665		T527	N465		T329		E116	
D1125		G985	ASP	F856	M792	R728			P528	V466		A330	K357	A117	
G1126	G1054	Q986	GLU	R857	A793	I729	D668	L603	E529	G467		L331	L258	R118	
G1127	I1055		GLU	S958	N794	R730	ILE	R604	G530	GLN		D332	Y259	L119	
	S1056	T989	GLU	Y859	T795	V731	GLU	R605	R630	LVS		P333	R261	N121	
G1131		I990	LEU	M860	L796	S732	GLY	K606	N638	LVS	H400	I334	R261	E186	
M1132	L1059	G991	GLN	D661	Y797	H733	GLY	G607	L539	ALA	F401			S187	
E1134	R1060	I992	GLN	Q862	Y798	H734	PHE	D608						D188	
R1135	Q1065	T993	ARG	E863	F799	A735	GLU	T609	M642	SER	K404		A266	L189	
C1137	S1066	R994	THR	K864	Q800	T736	ASP	T609	S546	SER	R405		R267	L190	
		D1136	ALA	K865	T737	V737	VAL	P611		ARG			T268	K191	
		R996	TYR	Y866	F802	F738	GLU	E612		A477	L408		I269	L192	



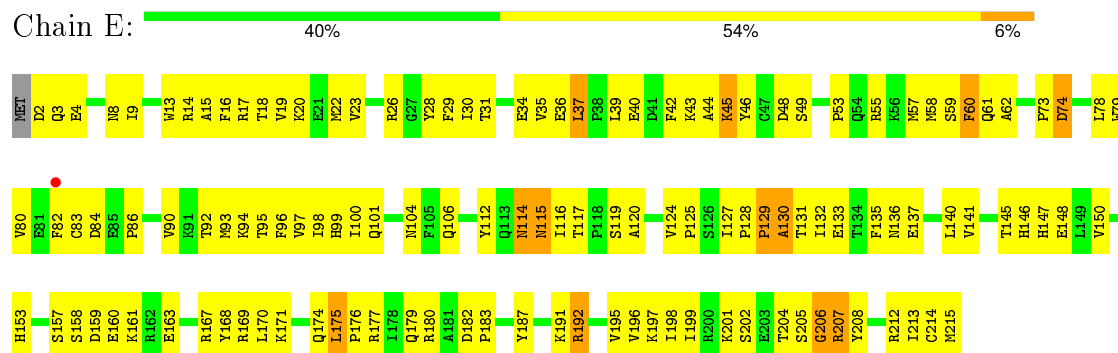
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II 45 KDA POLYPEPTIDE



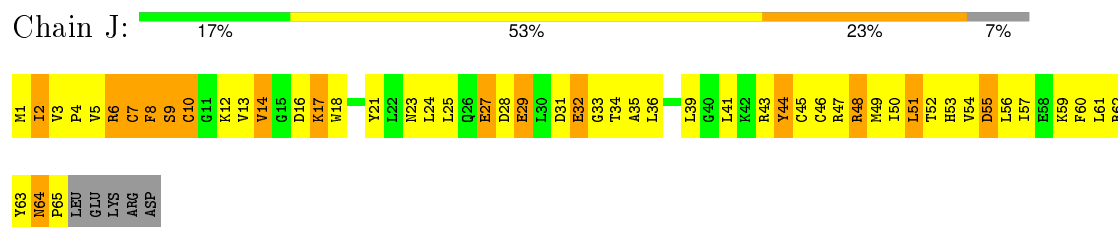
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II 32 KDA POLYPEPTIDE



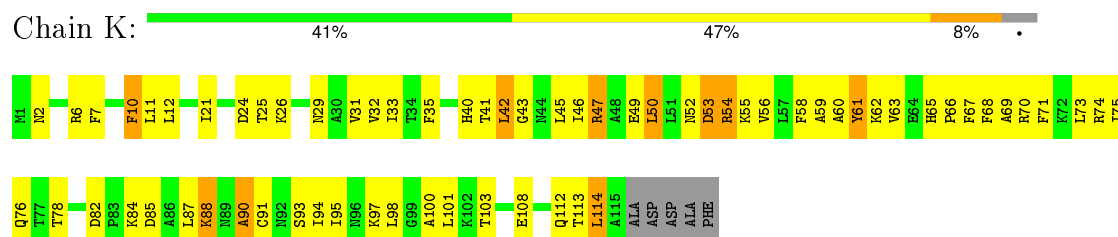
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III 27 KDA POLYPEPTIDE



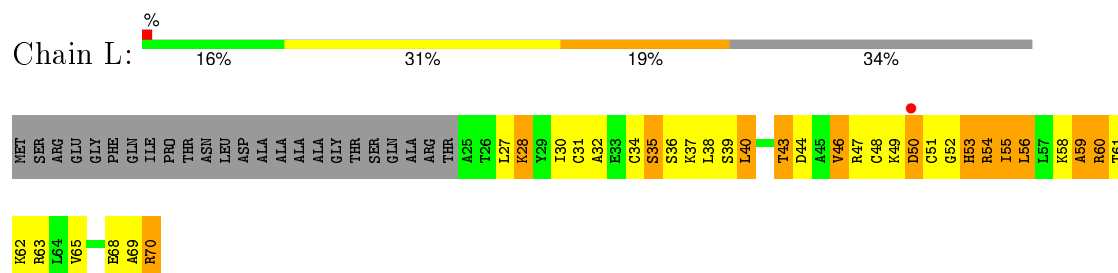
- Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II AND III 8.3 KDA POLYPEPTIDE



- Molecule 11: DNA-DIRECTED RNA POLYMERASE II 13.6 KDA POLYPEPTIDE



- Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III 7.7 KDA POLYPEPTIDE



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	222.72Å 395.13Å 284.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 47.39 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-3.80) 99.2 (47.39-3.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 3.77Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.257 , 0.285 0.222 , 0.250	Depositor DCC
R_{free} test set	2439 reflections (2.04%)	DCC
Wilson B-factor (Å ²)	116.1	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 70.8	EDS
Estimated twinning fraction	0.015 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.021 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 121835 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	30945	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% 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

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	0.48	0/11339	0.73	4/15334 (0.0%)
2	B	0.47	0/8890	0.70	1/11990 (0.0%)
3	C	0.52	0/2133	0.76	0/2891
4	D	0.45	0/1365	0.71	1/1837 (0.1%)
5	E	0.43	0/1788	0.64	0/2406
6	F	0.53	0/691	0.78	0/933
7	G	0.53	0/1368	0.74	0/1844
8	H	0.40	0/1086	0.66	0/1470
9	I	0.48	0/989	0.77	0/1331
10	J	0.54	0/541	0.89	1/727 (0.1%)
11	K	0.50	0/938	0.68	0/1267
12	L	0.55	0/365	0.79	0/485
All	All	0.48	0/31493	0.72	7/42515 (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
1	A	0	1
3	C	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	10	CYS	CA-CB-SG	8.66	129.59	114.00
1	A	1403	GLU	N-CA-C	5.38	125.53	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	567	LYS	C-N-CD	5.34	139.62	128.40
2	B	1185	CYS	N-CA-C	-5.30	96.69	111.00
1	A	452	LYS	N-CA-C	-5.21	96.94	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	303	TYR	Sidechain
3	C	82	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	11140	0	11217	1180	0
2	B	8720	0	8745	919	0
3	C	2095	0	2051	244	0
4	D	1356	0	1319	114	0
5	E	1752	0	1776	154	0
6	F	679	0	701	84	0
7	G	1340	0	1357	150	0
8	H	1068	0	1040	104	0
9	I	971	0	927	94	0
10	J	532	0	542	93	0
11	K	920	0	929	83	0
12	L	363	0	386	45	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
14	A	1	0	0	0	0
All	All	30945	0	30990	2984	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 48.

The worst 5 of 2984 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:77:CYS:O	1:A:78:PRO:O	1.65	1.14
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.30	1.11
7:G:138:THR:HG22	7:G:139:ILE:H	1.12	1.09
1:A:53:LEU:HD23	1:A:54:ASN:N	1.69	1.06
4:D:40:HIS:HB3	7:G:73:LYS:NZ	1.69	1.06

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	1406/1733 (81%)	949 (68%)	293 (21%)	164 (12%)	0	9
2	B	1077/1224 (88%)	735 (68%)	221 (20%)	121 (11%)	0	10
3	C	264/318 (83%)	159 (60%)	66 (25%)	39 (15%)	0	5
4	D	173/177 (98%)	122 (70%)	34 (20%)	17 (10%)	1	14
5	E	212/215 (99%)	148 (70%)	49 (23%)	15 (7%)	1	23
6	F	82/155 (53%)	64 (78%)	14 (17%)	4 (5%)	3	32
7	G	169/171 (99%)	131 (78%)	26 (15%)	12 (7%)	1	23
8	H	129/146 (88%)	84 (65%)	29 (22%)	16 (12%)	0	8
9	I	117/122 (96%)	80 (68%)	29 (25%)	8 (7%)	1	24
10	J	63/70 (90%)	37 (59%)	10 (16%)	16 (25%)	0	1
11	K	113/120 (94%)	89 (79%)	18 (16%)	6 (5%)	2	30
12	L	44/70 (63%)	19 (43%)	14 (32%)	11 (25%)	0	1
All	All	3849/4521 (85%)	2617 (68%)	803 (21%)	429 (11%)	0	10

5 of 429 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	48	ALA
1	A	54	ASN
1	A	55	ASP
1	A	57	ARG

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	1239/1520 (82%)	1135 (92%)	104 (8%)	14	52
2	B	952/1061 (90%)	866 (91%)	86 (9%)	12	49
3	C	234/274 (85%)	212 (91%)	22 (9%)	11	47
4	D	140/159 (88%)	124 (89%)	16 (11%)	7	37
5	E	196/197 (100%)	187 (95%)	9 (5%)	33	72
6	F	74/137 (54%)	65 (88%)	9 (12%)	6	34
7	G	152/152 (100%)	142 (93%)	10 (7%)	21	62
8	H	117/128 (91%)	111 (95%)	6 (5%)	29	69
9	I	113/116 (97%)	99 (88%)	14 (12%)	6	33
10	J	60/65 (92%)	54 (90%)	6 (10%)	9	43
11	K	99/102 (97%)	92 (93%)	7 (7%)	18	59
12	L	40/57 (70%)	37 (92%)	3 (8%)	17	57
All	All	3416/3968 (86%)	3124 (92%)	292 (8%)	13	52

5 of 292 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	485	ARG
2	B	956	THR
9	I	85	PHE
2	B	516	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	701	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	236	HIS
2	B	734	HIS
9	I	12	ASN
2	B	363	HIS
2	B	484	ASN

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 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	1416/1733 (81%)	-0.34	10 (0%) 89 80	19, 87, 162, 200	0
2	B	1097/1224 (89%)	-0.30	8 (0%) 89 80	23, 97, 166, 194	0
3	C	266/318 (83%)	-0.39	0 100 100	37, 81, 139, 160	0
4	D	177/177 (100%)	-0.34	0 100 100	52, 108, 147, 165	0
5	E	214/215 (99%)	-0.31	1 (0%) 91 85	57, 142, 187, 193	0
6	F	84/155 (54%)	-0.63	0 100 100	25, 59, 105, 124	0
7	G	171/171 (100%)	-0.29	0 100 100	57, 84, 114, 138	0
8	H	133/146 (91%)	0.06	2 (1%) 76 62	101, 139, 175, 184	0
9	I	119/122 (97%)	-0.09	2 (1%) 73 58	74, 130, 159, 200	0
10	J	65/70 (92%)	-0.57	0 100 100	42, 79, 120, 127	0
11	K	115/120 (95%)	-0.32	0 100 100	42, 83, 114, 123	0
12	L	46/70 (65%)	-0.22	1 (2%) 65 50	76, 137, 168, 177	0
All	All	3903/4521 (86%)	-0.32	24 (0%) 90 82	19, 94, 166, 200	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1176	LEU	7.5
2	B	882	THR	4.3
9	I	119	THR	3.5
2	B	919	SER	3.3
2	B	92	PHE	3.3

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. 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
13	ZN	I	1121	1/1	0.99	0.14	-0.09	90,90,90,90	0
13	ZN	B	2225	1/1	0.99	0.16	-0.78	44,44,44,44	0
13	ZN	C	1269	1/1	1.00	0.08	-0.88	39,39,39,39	0
13	ZN	A	2457	1/1	1.00	0.10	-1.38	44,44,44,44	0
13	ZN	A	2456	1/1	0.97	0.07	-2.37	86,86,86,86	0
13	ZN	J	1066	1/1	0.99	0.16	-2.55	65,65,65,65	0
13	ZN	I	1122	1/1	0.91	0.06	-2.88	156,156,156,156	0
14	MG	A	2458	1/1	0.98	0.20	-	56,56,56,56	0
13	ZN	L	1071	1/1	0.99	0.12	-	115,115,115,115	0

6.5 Other polymers [i](#)

There are no such residues in this entry.