



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2018 – 08:28 pm GMT

PDB ID : 1WCM
Title : Complete 12-Subunit RNA Polymerase II at 3.8 Angstrom
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

<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	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

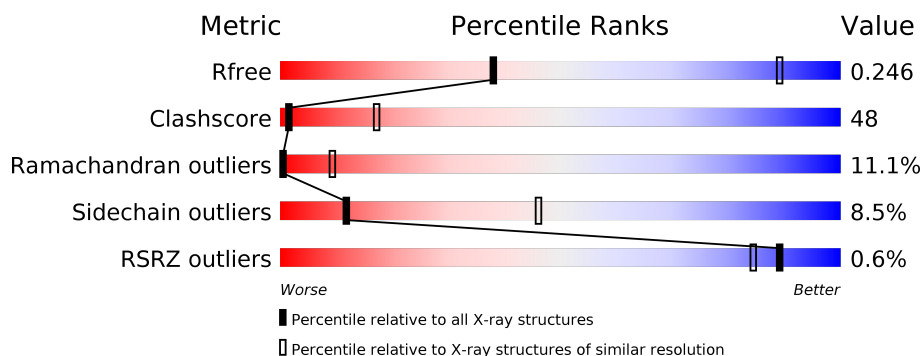
1 Overall quality at a glance

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}	111664	1028 (4.02-3.58)
Clashscore	122126	1061 (4.00-3.60)
Ramachandran outliers	120053	1025 (4.00-3.60)
Sidechain outliers	120020	1019 (4.00-3.60)
RSRZ outliers	108989	1021 (4.06-3.54)

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></div> <div> <div></div> <div>27%</div> <div>43%</div> <div>10%</div> <div>•</div> <div>18%</div> </div> </div>
2	B	1224	<div> <div></div> <div> <div></div> <div>29%</div> <div>48%</div> <div>12%</div> <div>10%</div> </div> </div>
3	C	318	<div> <div></div> <div> <div></div> <div>23%</div> <div>48%</div> <div>12%</div> <div>•</div> <div>16%</div> </div> </div>
4	D	177	<div> <div></div> <div> <div></div> <div>42%</div> <div>46%</div> <div>11%</div> <div>•</div> </div> </div>
5	E	215	<div> <div></div> <div> <div></div> <div>40%</div> <div>54%</div> <div>6%</div> </div> </div>
6	F	155	<div> <div></div> <div> <div></div> <div>18%</div> <div>30%</div> <div>6%</div> <div>•</div> <div>46%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
7	G	171	<div><div></div><div>39%51%9%</div></div>
8	H	146	<div>%<div><div></div><div>32%49%10%9%</div></div></div>
9	I	122	<div>2%<div><div></div><div>40%43%12%••</div></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>16%31%19%34%</div></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		

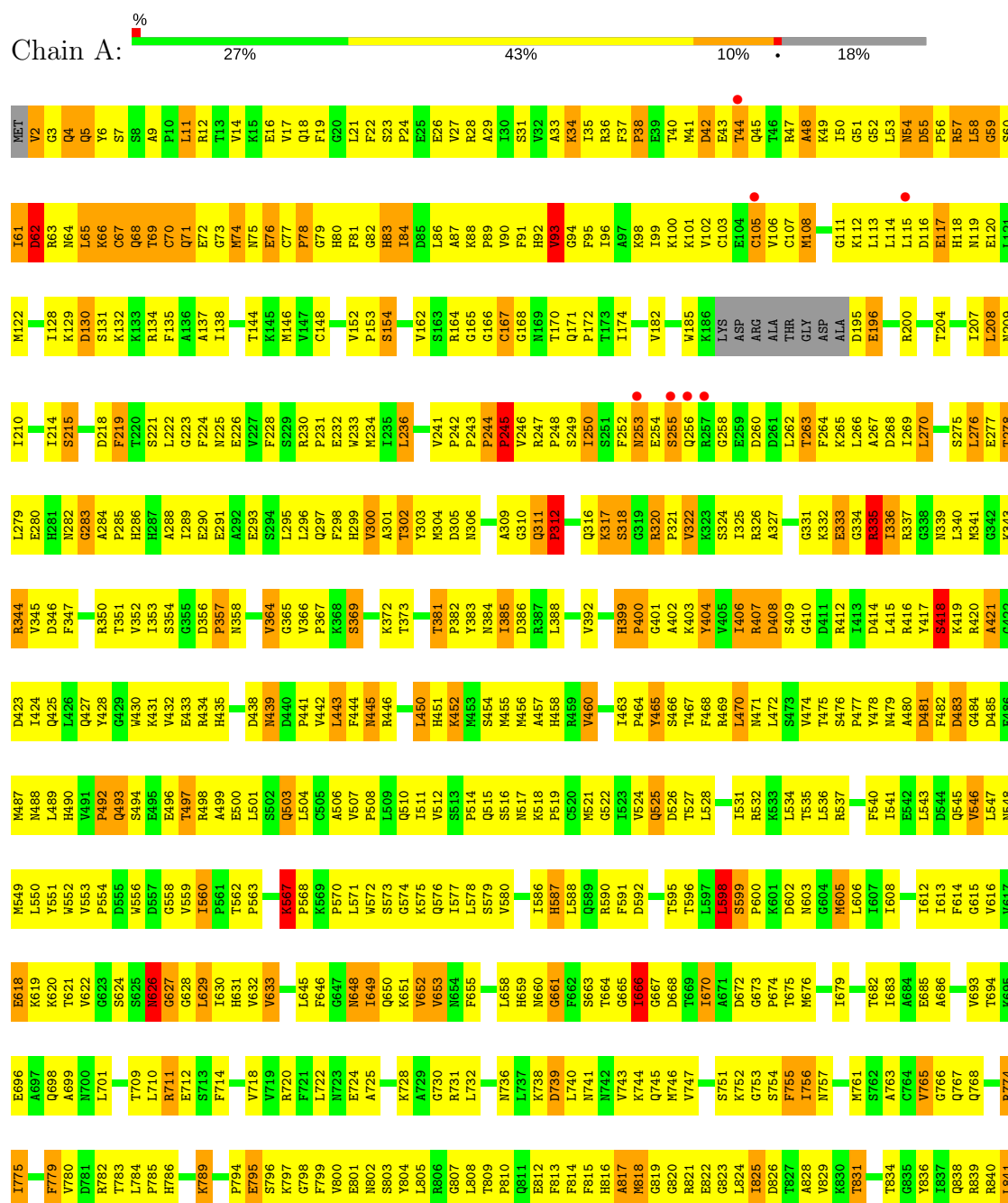
- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

3 Residue-property plots

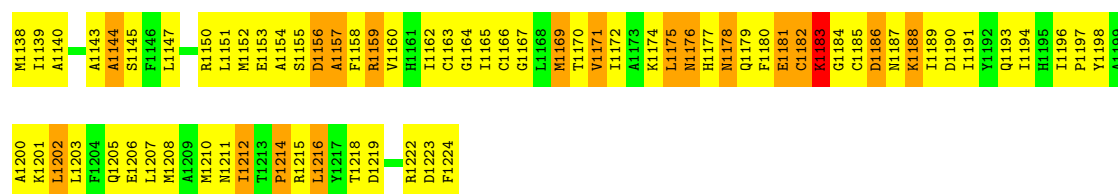
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



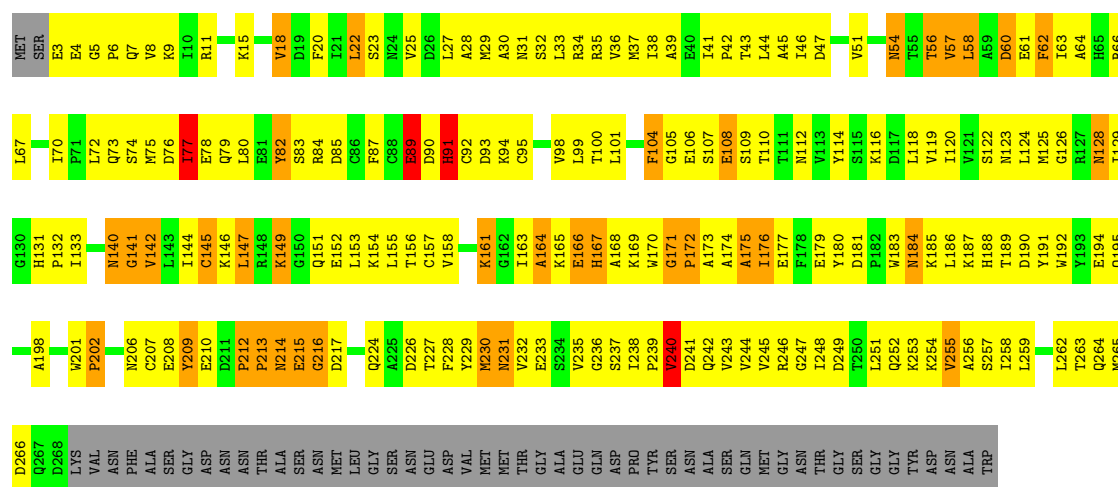


G1068	E997	HIS	G867	L803	C741	E678	V613	G548	G478	A409	LEU	K270	K193	F129	E85
F1069	D998	S933	R668	T806	E742	T679	S614	T549	V479	G410	GLY	L273	E194	V130	D66
M1072	M999	R935	S869	T807	E743	T680	M615	D550	S480	P411	ILE	L273	E196	D131	T68
Y1073	F1000	R936	T871	A808	H745	S882	R617	P552	N483	L413	LVS	K276	F197	V132	L69
N1074	T1002	D937	T872	M809	P745	S883	R620	P553	N484	A414	ARG	K277	D198	K133	I70
T1077	A1003	S938	T873	E810	S746	L684	R621	T554	R485	Q415	K347	Q278	M199	K134	LEU
		P940	P877	Y811	M747	L685	E622	T555	Y466	K418	Y351	T280	G200	ARG	LEU
K1080	V1007	R815	Q878	R815	L748	R686	K622	T556	T487	T419		T281	G201	THR	GLU
L1081	P1008	R942	R879	R816	G750	G888	E623	F557	Y488	L420		T282	F203	GLU	GLN
M1082	D1009	S943	T880	L817	W751	L689	K625	S549	S490	F421		T283	F204	ALA	ALA
A1083	L1010	R944	R881	P813	K752	V690	E626	E560	T491	L424		T284	I204	ILE	GLN
Q1084	I1011	E945	T882	A819	A753	V691	F627	E561	L492			T285	I205	ASP	HIS
F1086	L1012		L883	G820		T692	T628	G562	S493			T286	N206	VAL	THR
T1087	N1013	I948	R884	Q821	I756	T693	D629	S563	H494	D427		T287	G207	PRO	THR
F1088		V949		N822	F757	D694	A630	N563	R496	F428		T288	K210	GLY	GLU
A1016	A1016	G888	G888	A823	F758	E695	G631	L566	R497	F429		T289	K211	ARG	ASP
I1017	G1088	Q951	T889	I824	P759	E696	R632		R498			T290	V211	GLU	ASP
P1018	P1089	V952	T890	V825	D760	E697	V633		T498			T291	L212	LEU	ASN
T1089		D891		A826	H761	E698	Y634		N499	T436		T292	I213	LYS	ILE
Y1091	S1019	L953	K892	R1020	N762	E699	R635		P501	V436		T293	A214	TYR	SER
R1094	M1021	T955	L893		Q763	S700	P636		P502	E437		T294	GLU	ARG	GLU
L1095	T1022	T956	D894	S830	S764	T707	L637		I502	ALA		T295	R217	LEU	LVS
R1096		N957		S831	P765	E708	F638		GLY	HIS		T297	V223	ILE	TYR
H1097	H1025	Q958		G832	R766	I703	L639		ARG	ASP		T298	Q224	GLU	GLU
M1098	L1026	D959	G897	G833	N767	A704	V640		ASP	PHE		T299	V225	GLU	S91
T1099	I1027	T899	L898	N834	E641	M705	E641		GLY	ASN		T300	F226	SER	F92
D1100	E1028	A900		Q835	Y769	Q706	D642		LVS	MET		T301	K227	GLU	
D1101	C1029	V964	P901	E836	Q770	D643	D643		LEU	LVS		T302	K228	ASP	I95
K1102	L1030	K965	G902	D837	S771	E709	E644		A509	L446		T303	A229	ASP	Y96
I1103	L1031	V966	V903	S838	A772	D708			K510	A447		T304	A230	SER	Y97
H1104	S1032		R904	M839	K773	T709	H648		P511			T305	P231	GLU	T98
A1105	K1033	R969	V905	R841	G774	E711	K649		Q513	A450		T306	P232	SER	K99
R1106	A1035	T971	S906	N842	K775	P712	E650		L514	L453		T307	P233	GLY	P100
A1107	A1036	T972	G907	Q843	A776		L652		H515	T454		T308	S235	K164	M101
G1108		I973	E908	S844	M778		V653		N516	S455		T309	H236	V165	V102
P1110	G1039	P974	D909	S845	G779		R654		T517	G456		T310	V237	F166	M103
T1115	N1040	Q975	V910	L845	V780		K655		H518	L457		T311	A238	I167	E104
Q1117	S1045	I976	I911	R846	L782		G656		W519			T312	E239	G168	
P1118	P1046	G977	G913	R848	L783		H657		G520	V459		T313	C317		V108
V1119	F1047	A981	T916	F851	Y785		I658		L521	A460		T314	I240	P171	T109
R1122	S1123	S982	P917	R852	N787		L651		C523	A462		T315	L244	M172	L112
L1124	T1051	H984	S919	L854	P725		A663		A525	T463		T316	I251	M173	Y113
D1125	G1054	Q985	F855	F855	T726		T664		E526	G464		T317	L254	R175	P114
G1126		Q986	R857	R857	K727		E665		T527	N465		T318	L254	M178	E116
G1127	S1056	T989	S858	S858	R728				P528	K393		T319	K257	C179	A117
G1131	L1059	I990	Y859	Y859	I729		D668		G530	V466		T320	L258	Y180	R118
E1132	Q1065	I992	M860	L796	R730		L603		G530	GLU		T321	Y259	L181	L119
M1133	R1060	I993	G861	L796	V731		R604		N538	LVS		T322	G260	T185	N121
E1134	Q1065	T993	Q862	Y798	H733		G607		L539	ALA		T323	R261	E186	L122
R1136	R1066	Y994	Q863	F799	H734		PHE		M642	MET		T324	S265	S187	T123
C1137	D1136	S1066	K864	Q800	A735		GLU		N610	SER		T325	A266	L189	S125
			ALA	T736	T736		ASP		S646	SER		T326	R267	Y190	S126
			VAL	F738	F738		VAL		S646	ARG		T327	T268	K191	G127
			GLU				GLU		E512	A477		T328	I269	L192	L128



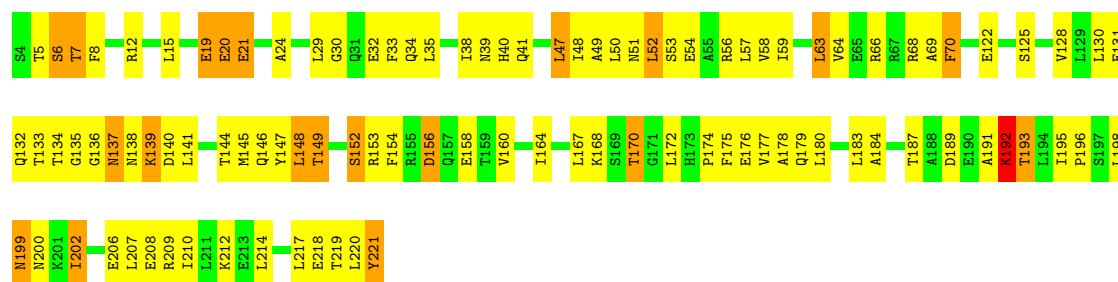
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II 45 KDA POLYPEPTIDE

Chain C:



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

Chain D:

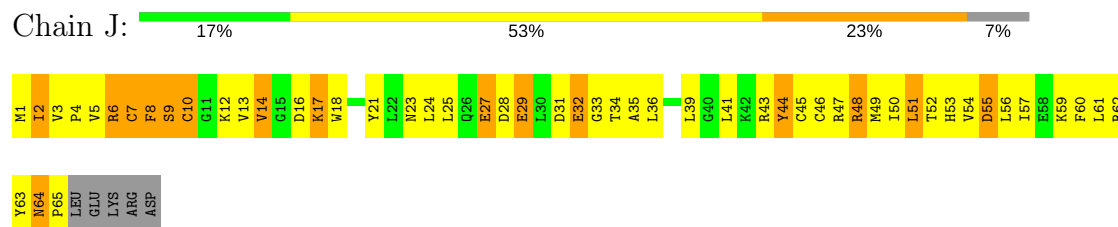


• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III 27 KDA POLYPEPTIDE

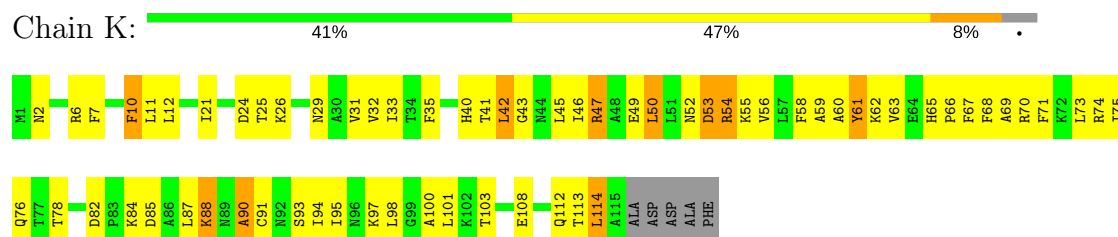
Chain E:



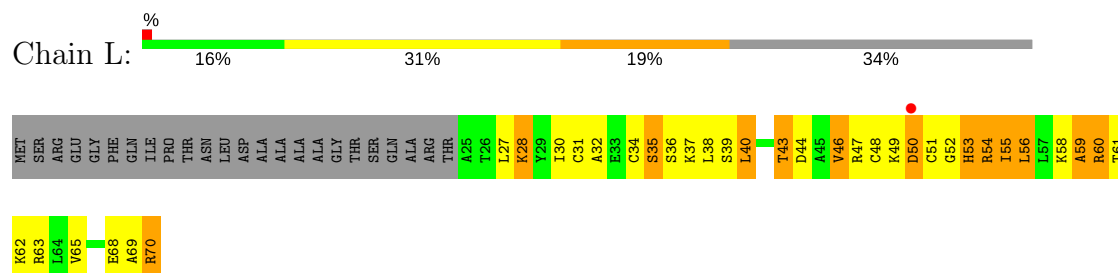
- Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II AND III 8.3 KDA POLYPEPTIDE



- 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 0.208 , 0.246	Depositor DCC
R_{free} test set	2439 reflections (2.00%)	wwPDB-VP
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 , 70.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
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
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, 0.333 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	0.48	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

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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	8
2	B	1077/1224 (88%)	735 (68%)	221 (20%)	121 (11%)	0	9
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	12
5	E	212/215 (99%)	148 (70%)	49 (23%)	15 (7%)	1	20
6	F	82/155 (53%)	64 (78%)	14 (17%)	4 (5%)	2	28
7	G	169/171 (99%)	131 (78%)	26 (15%)	12 (7%)	1	20
8	H	129/146 (88%)	84 (65%)	29 (22%)	16 (12%)	0	7
9	I	117/122 (96%)	80 (68%)	29 (25%)	8 (7%)	1	21
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	27
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	9

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%)	12	46
2	B	952/1061 (90%)	866 (91%)	86 (9%)	10	42
3	C	234/274 (85%)	212 (91%)	22 (9%)	9	40
4	D	140/159 (88%)	124 (89%)	16 (11%)	6	32
5	E	196/197 (100%)	187 (95%)	9 (5%)	29	64
6	F	74/137 (54%)	65 (88%)	9 (12%)	5	29
7	G	152/152 (100%)	142 (93%)	10 (7%)	18	55
8	H	117/128 (91%)	111 (95%)	6 (5%)	26	62
9	I	113/116 (97%)	99 (88%)	14 (12%)	5	28
10	J	60/65 (92%)	54 (90%)	6 (10%)	8	37
11	K	99/102 (97%)	92 (93%)	7 (7%)	16	52
12	L	40/57 (70%)	37 (92%)	3 (8%)	15	50
All	All	3416/3968 (86%)	3124 (92%)	292 (8%)	12	46

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

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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 [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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	76:LYS	C	118:THR	N	35.50

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%)	-0.37	10 (0%) 87 82	19, 87, 162, 200	0
2	B	1097/1224 (89%)	-0.33	8 (0%) 87 82	23, 97, 166, 194	0
3	C	266/318 (83%)	-0.42	0 100 100	37, 81, 139, 160	0
4	D	177/177 (100%)	-0.36	0 100 100	52, 108, 147, 165	0
5	E	214/215 (99%)	-0.34	1 (0%) 90 86	57, 142, 187, 193	0
6	F	84/155 (54%)	-0.65	0 100 100	25, 59, 105, 124	0
7	G	171/171 (100%)	-0.31	0 100 100	57, 84, 114, 138	0
8	H	133/146 (91%)	0.04	1 (0%) 86 80	101, 139, 175, 184	0
9	I	119/122 (97%)	-0.11	2 (1%) 70 60	74, 130, 159, 200	0
10	J	65/70 (92%)	-0.60	0 100 100	42, 79, 120, 127	0
11	K	115/120 (95%)	-0.34	0 100 100	42, 83, 114, 123	0
12	L	46/70 (65%)	-0.24	1 (2%) 62 51	76, 137, 168, 177	0
All	All	3903/4521 (86%)	-0.34	23 (0%) 89 84	19, 94, 166, 200	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1176	LEU	7.7
2	B	882	THR	4.2
9	I	119	THR	3.3
2	B	92	PHE	3.2
2	B	919	SER	3.1

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
13	ZN	I	1122	1/1	0.91	0.06	156,156,156,156	0
13	ZN	A	2456	1/1	0.97	0.07	86,86,86,86	0
14	MG	A	2458	1/1	0.98	0.21	56,56,56,56	0
13	ZN	I	1121	1/1	0.99	0.14	90,90,90,90	0
13	ZN	L	1071	1/1	0.99	0.12	115,115,115,115	0
13	ZN	B	2225	1/1	0.99	0.16	44,44,44,44	0
13	ZN	J	1066	1/1	0.99	0.16	65,65,65,65	0
13	ZN	C	1269	1/1	1.00	0.08	39,39,39,39	0
13	ZN	A	2457	1/1	1.00	0.10	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.