



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:56 AM GMT

PDB ID : 2JA6
Title : CPD LESION CONTAINING RNA POLYMERASE II ELONGATION COM-
PLEX B
Authors : Brueckner, F.; Hennecke, U.; Carell, T.; Cramer, P.
Deposited on : 2006-11-23
Resolution : 4.00 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

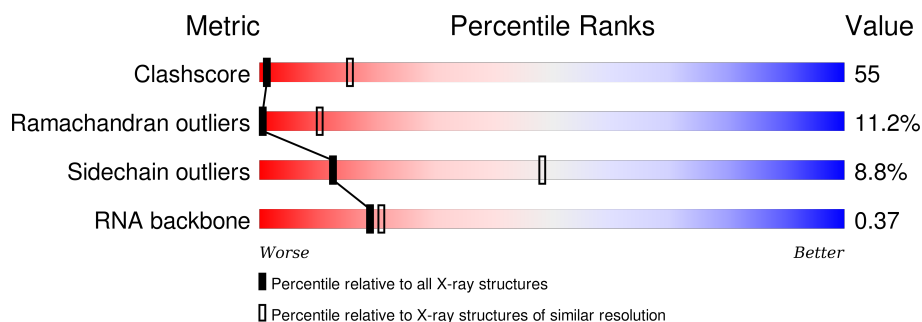
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RNA backbone	2183	1079 (5.04-2.80)


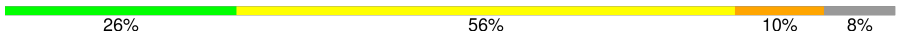







The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1733	
2	B	1224	
3	C	318	
4	D	221	
5	E	215	
6	F	155	

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Mol	Chain	Length	Quality of chain
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	N	14	
14	P	11	
15	T	25	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	TT	T	17	-	-	X	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 32011 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	1421	Total	C	N	O	S	0	0	0
			11186	7048	1958	2118	62			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1115	Total	C	N	O	S	0	0	0
			8866	5614	1553	1644	55			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	267	Total	C	N	O	S	0	0	0
			2101	1320	349	419	13			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II 32KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	177	Total	C	N	O	S	0	0	0
			1427	882	256	287	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	87	Total	C	N	O	S	0	0	0
			705	451	119	132	3			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II 19KDA 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	135	Total	C	N	O	S	0	0	0
			1084	683	183	214	4			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	116	Total	C	N	O	S	0	0	0
			944	581	172	181	10			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I/II/III SUBUNIT 10.

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	114	Total	C	N	O	S	0	0	0
			919	590	156	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
			364	224	72	64	4			

- Molecule 13 is a DNA chain called 5'-D(*TP*AP*AP*GP*TP*AP*CP*TP*TP*GP*AP*GP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	8	Total	C	N	O	P	0	0	0
			165	79	29	49	8			

- Molecule 14 is a RNA chain called 5'-R(*UP*UP*CP*GP*AP*CP*CP*AP*GP*GP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	10	Total	C	N	O	P	0	0	0
			213	95	38	70	10			

- Molecule 15 is a DNA chain called 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*TTP*TP*CP*CP*BRUP*GP*GP*TP*CP*AP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	19	Total	Br	C	N	O	P	0	0
			404	1	196	62	126	19		

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

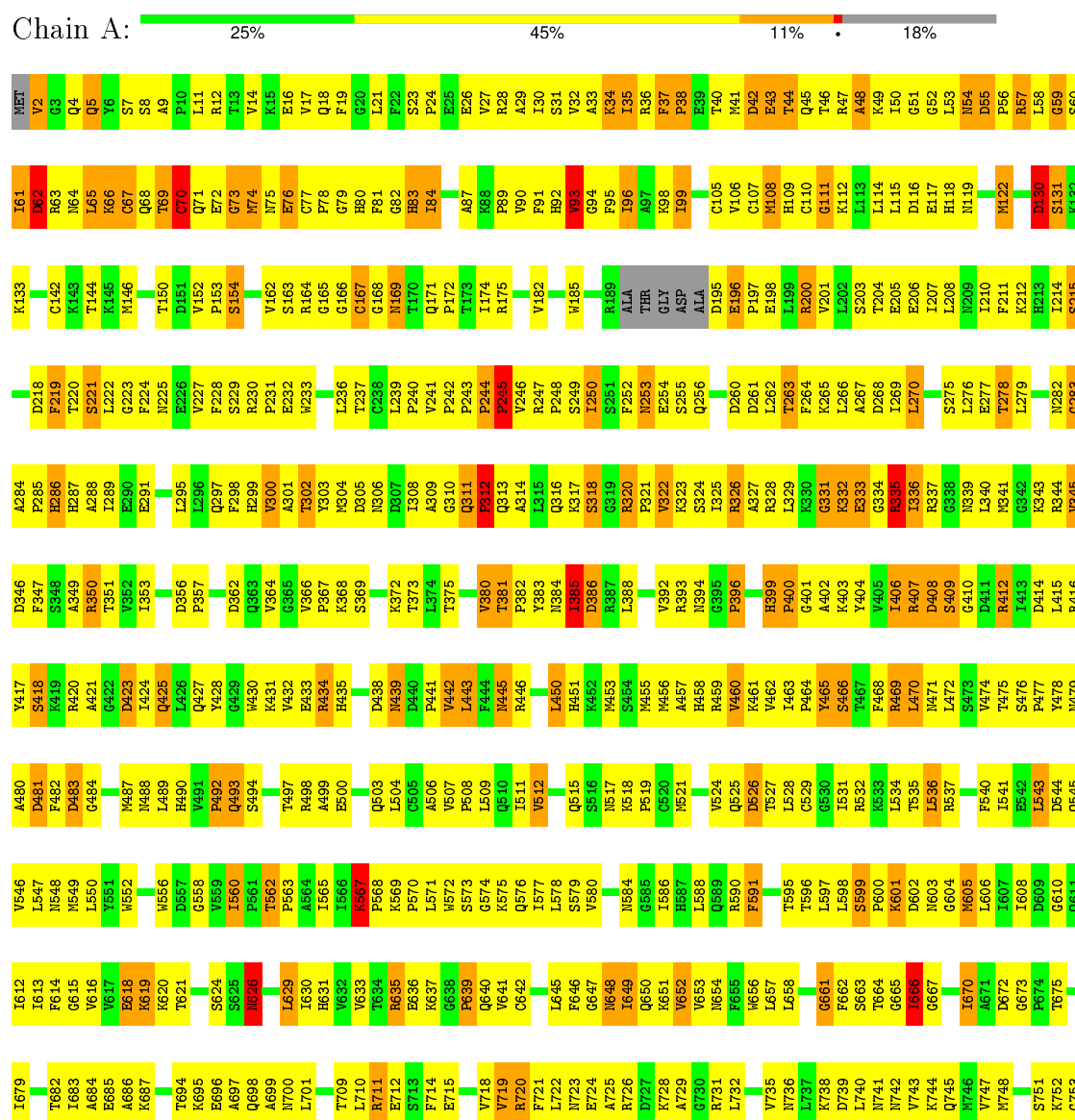
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	8	Total	Zn	0	0
			8	8		

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.

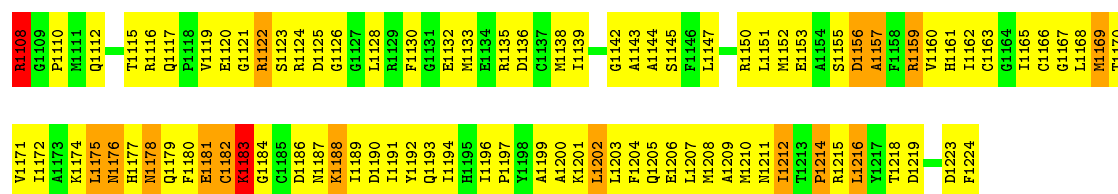
Note EDS was not executed.

• Molecule 1: DNA-DIRECTED RNA POLYMERASE II LARGEST SUBUNIT

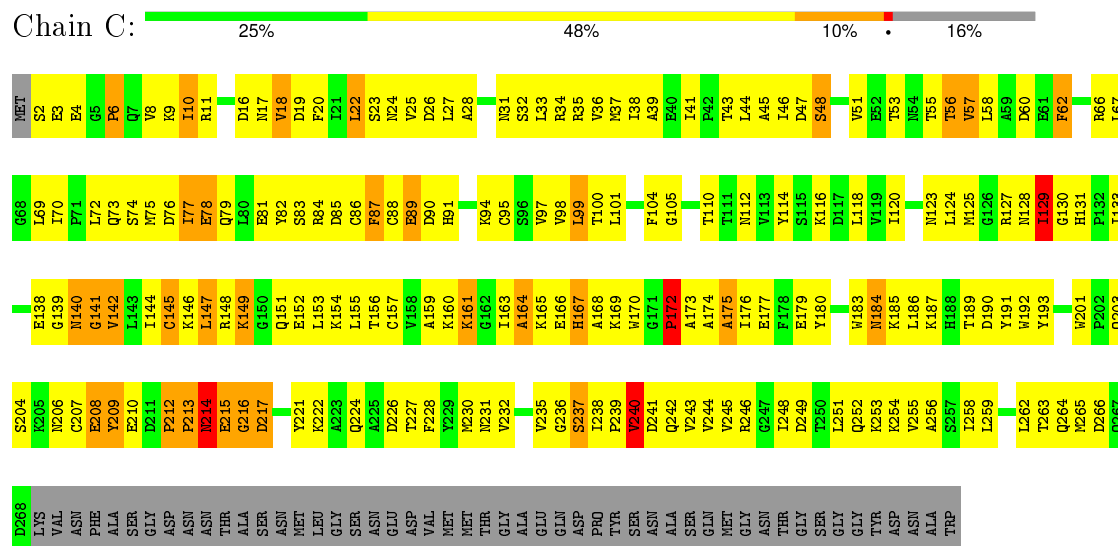




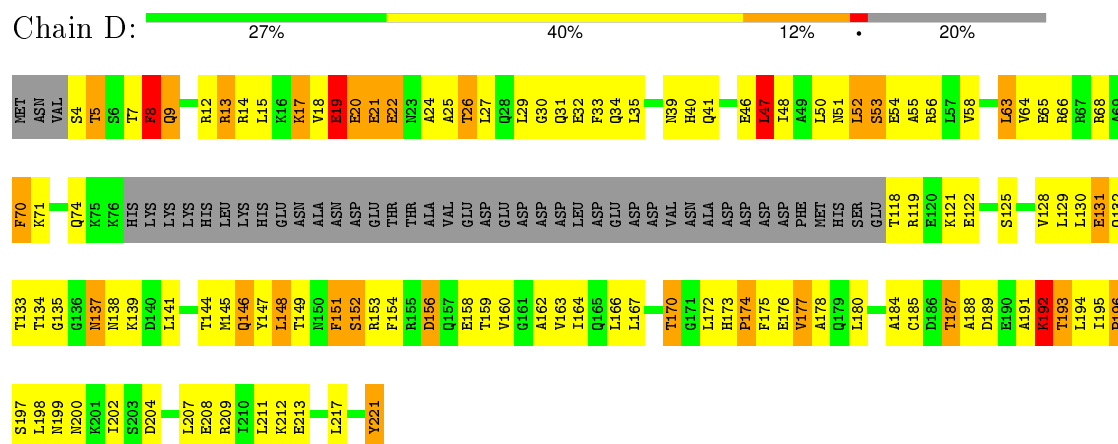
H1040	D978	T915	F851	A726	E526	L457	L385	P916	R249	E186	S126	D61	MET
E1041	K979	T916	R852	K727	T527	K458	L386	C317	F250	S187	G127	I62	SER
E1042	F980	F917	S953	R728	P528	K459	L387	V318	I251	L188	L128	I63	ASP
D1043	A981	T918	L854	I729	E529	A460	C388			L189	F129	D64	LEU
A1044	S932	S919	F855	R730	G530	A461	C389	I324	L254	K191	V130	D65	ALA
S1045	R993	PRD	F856	R731	K537	A462	L390	Q325	K257	L192	D131	D66	ASN
P1046	H984	ASP	R857	S732	N538	T463	D391	D326	L258	L193	V132	S67	SER
F1047	G985	GLU	S858	H733	L539	G464	R392	R327	Y259	K194	K133		GLU
T1050	G986	GLU	Y859		L539	M465	K393	E328	R260	C195	LYS	I70	LYS
T1051	G987	LEU	R860	T737	S540	M466	D394	T329	G260	C196	ARG	LEU	TYR
V1052	G988	LEU	D861	T738	L541	M467	D395	A330	R261	P196	THR	GLU	TYR
R1060	T989	GLY	Q862	F738	M542	D468	D396	L331	E262	F197	TYR	GLN	ASP
E1061	R990	GLN	R863	T739		Q469	D397	D332	G263	D198	GLU	LEU	GLU
H1062	G991	ARG	K864	H740	S546	K470	R398	F333	S264	M199	ALA	ALA	ASP
G1063	T992	THR	R865	C741	F547	K471	D399	T334	S265	Y202	ILE	GLN	PRO
T1064	T993	ALA	Y866	E742	G548	K472	H400	G335	A266	HIS	ASP	GLN	TYR
R1065	G994	THR	G867	I743	T549	M473	F401	R336	R267	F203	VAL	THR	GLY
G1066	R995	HIS	M868	H744	D550	S474	G402	R337	T268	I204	PRO	THR	THR
S1067	E997	TYR	S869	T745	P551	S475	K403	G338	I269	I205	GLY	GLU	E19
R1068	E998	K934	R870	S746	M552		K404	T339	L273	N206	ARG	SER	D20
F1069	T871	R935	E872	M747	P553	V479	K405	A340	P274	G207	GLU	ASP	E21
T1070	R872	L812	T873	I748	T555	S480	L408	I343	Y275	K210	LEU	ASN	A23
E1071	F1001	R813	T874	L749	T556	Q481		K344	I276	V211	LEU	ASN	S22
T1072	A1002	F814	G750	G751	T557	L483	P411	K345	Q277	L212	TYR	SER	P24
H1073	A1003	R815	G752	A752	L558	M484	L412	E346	Q278	I213	GLU	ARG	I25
T1074	T1006	L817	A753	A754	S559	R485	L413	K347	D279	A214	ILE	TYR	T26
G1075	P1007	R818	T755	T756	E560	Y486	A414	R348	I280	Q215	ALA	GLU	A27
H1076	P1008	G820	I756	I757	W561	T487	T419	K349	P281	R217	GLU	GLU	D29
T1077	T1009	R821	G757	G758	G562			Y351	I282	R217	GLU	SER	S30
G1078	L1010	R822	G759	F758	M563	S490	L424	T355	V283	K94	SER	K94	K31
K1079	I1011	A823	E597	F759	L566	T491	L424	L356	I284	I95	GLU	I95	K32
K1080	L1012	R824	E598	D760		T492	D427	Q357	I285	N221	ASP	I96	V33
L1081	M1013	W825	E599	H761	Y569	S493	I428	K358	F286	I222	ASP	T97	I34
M1082	A1016	A826	S700	G762	G571	R496	F429	E359	R287	V223	SER	T98	S35
G1083	I1017	R827	L701	Q763	P571	R497	R430	F360	Q224	Q224	GLU	K99	A36
T1084	P1018	A828	L702	S764	H572	T498	Y431	I361	V225	V225	SER	P100	F37
I1085	S1019	C829	L703	P765	Q573		M432	L362	F226	F226	GLY	M101	F38
F1086	R1020	Y830	M705	R766		T502	Q433	H363	I292	K227	K164	V102	R39
G1087	T1021	S831	Q706	G769	A577	ARG	R434	I364	D294	K228	V165	I103	E40
T1088	P1022	R832	F707	Q770	T579	ASP	E437	T366	G295	A230	I167	E104	K41
P1089	V1023	Y833	E708	S771	R580	GLY	GLU	T367	E296	P231	G168	S105	G42
T1090	A1024	Q835	D709	A772	F581	LYS	ALA	E368	I297	S232	R169	D106	L43
Y1091	L1025	E836	L710		V582	LEU	HIS	E369	E299	S233	P171	G107	V44
R1094	L1026	D837	E711	K775	V585	ALA	ASP	F370	H300	I234	I172	V108	S45
L1095	I1027	S838	F712	A777	W586	P511	PHE	E371	R300	S235	M173	L112	Q46
R1096	E1028	R839	A715	T778	H587		ASN	S372	I304	V237	L174	Y113	L48
H1097	G1029	T840	G715	G779	G588	L514	LYS	R373	V305	E238	S176	O115	D49
K1098	L1030	M841	ASN		G588	H514		F376	W308	I240	R177	E116	S61
V1099	S1032	R842	GLU	F781	V589	H515	L446	F377	I241	R241	M178	A117	R52
D1100	D1030	Q843	GLU	L782	H590	N516	A447	F378	Q309	S242	C179	R118	Q53
L1101	K1033	T971	ASN	L783	K655	T517	L448	L378	R309	S242	C179	L119	F54
K1102	V1034	S845	ASP	T783	G656	H518	M449	G379	M310	A243	Y180	R120	V55
T1103	A1035	R846	LEU	N784	P593	H519	A450	V380	L311	I244	L181	N121	D66
H1104	A1036	D847	ASP	T785	A594	G520	K451	N381	E312	E245	S182	L122	Y57
R1105	L1037	R848	T722	T786	A594	G520	K451	N382	M313	K246	E183	T123	T58
T1106	S1038	G849	T723	T787	M597	L521	T454	N383	L314	K247	E184	T124	L59
A1107	G1039	R850	F725	R788	E598	V522		N384	K315	S248	T185	S125	Q60



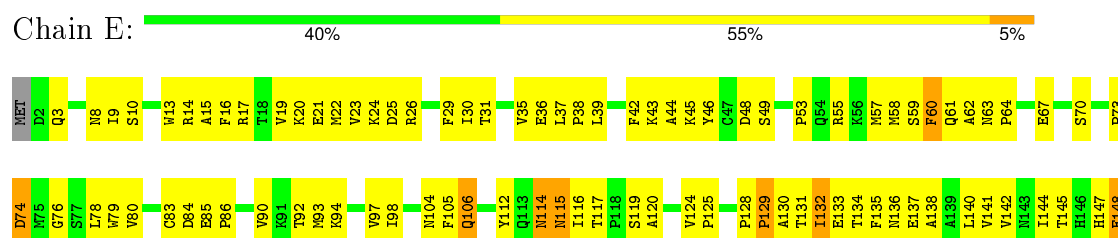
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II 45KDA POLYPEPTIDE



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

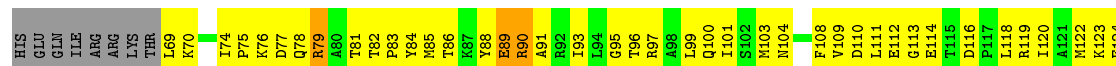
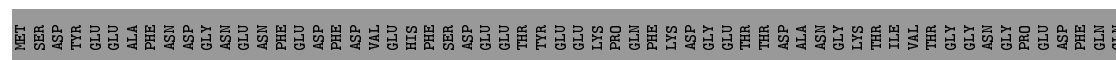


• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III 27 KDA POLYPEPTIDE

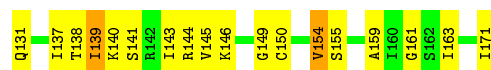
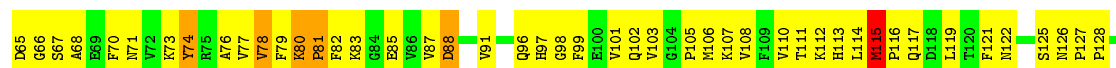




- Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III 23 KDA POLYPEPTIDE



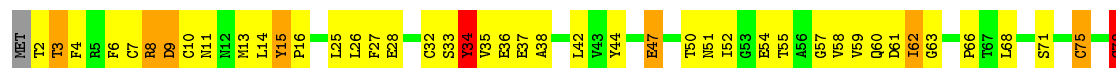
- Molecule 7: DNA-DIRECTED RNA POLYMERASE II 19KDA POLYPEPTIDE



- Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III 14.5 KDA POLYPEPTIDE



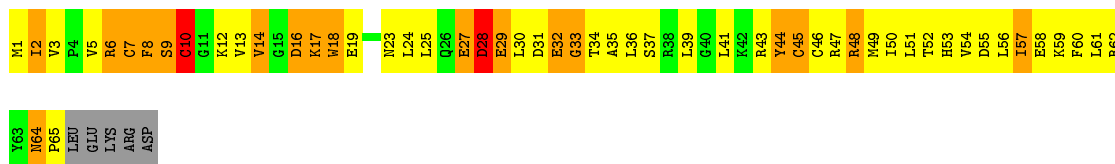
- Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT 9





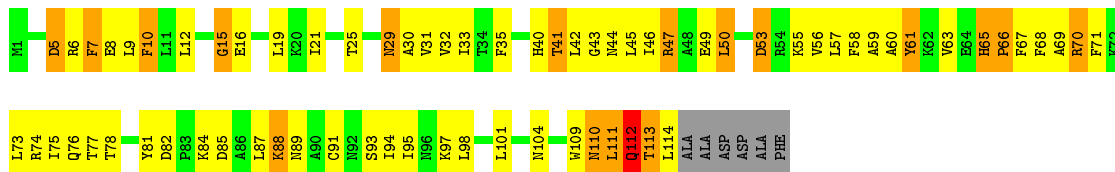
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I/II/III SUBUNIT 10

Chain J: 16% 49% 26% 7%



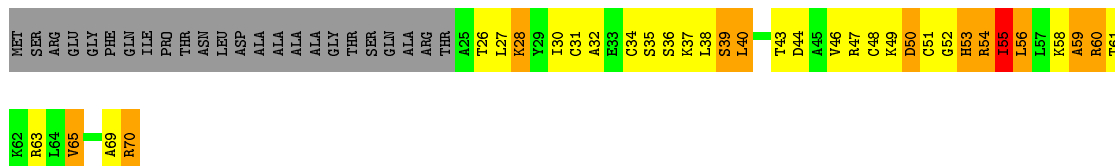
• Molecule 11: DNA-DIRECTED RNA POLYMERASE II 13.6 KDA POLYPEPTIDE

Chain K: 36% 44% 14% 5%



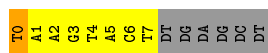
• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III 7.7 KDA POLYPEPTIDE

Chain L: 17% 31% 16% 34%



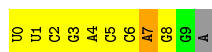
• Molecule 13: 5'-D(*TP*AP*AP*GP*TP*AP*CP*TP*TP*GP *AP*GP*CP*T)-3'

Chain N: 50% 7% 43%



• Molecule 14: 5'-R(*UP*UP*CP*GP*AP*CP*CP*AP*GP*GP*AP)-3'

Chain P: 9% 73% 9% 9%



• Molecule 15: 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP *CP*TP*TP*TTP*TP*CP*CP *BRUP*GP*GP*TP*CP*AP*TP*T)-3'

Chain T: 56% 20% 24%

DA	DG	DC	DT	DC	DA	A10	G11	T12	A13	G14	T15	T16	M17	T19	C20	G21	U22	G23	G24	T25	C26	A27	T28	T29
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4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	223.58 Å 393.49 Å 283.50 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 4.00	Depositor
% Data completeness (in resolution range)	99.3 (50.00-4.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.292 , 0.301	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	32011	wwPDB-VP
Average B, all atoms (Å ²)	116.0	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: MG, ZN, BRU, TT

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	0.47	0/11385	0.73	2/15393 (0.0%)
2	B	0.47	0/9037	0.71	2/12181 (0.0%)
3	C	0.47	0/2138	0.72	0/2896
4	D	0.44	0/1437	0.68	1/1925 (0.1%)
5	E	0.43	0/1788	0.63	0/2406
6	F	0.54	0/716	0.76	0/964
7	G	0.50	0/1368	0.73	0/1844
8	H	0.39	0/1102	0.66	0/1492
9	I	0.39	0/962	0.67	0/1295
10	J	0.50	0/541	0.80	1/727 (0.1%)
11	K	0.54	0/937	0.76	1/1265 (0.1%)
12	L	0.45	0/366	0.71	0/485
13	N	1.16	1/184 (0.5%)	1.01	0/280
14	P	0.63	0/237	1.01	0/367
15	T	1.14	2/383 (0.5%)	1.24	3/582 (0.5%)
All	All	0.49	3/32581 (0.0%)	0.73	10/44102 (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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	N	0	DT	OP3-P	-6.79	1.53	1.61
15	T	10	DA	OP3-P	-6.78	1.53	1.61
15	T	21	DC	C3'-O3'	6.37	1.52	1.44

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1096	ARG	NE-CZ-NH1	-11.17	114.72	120.30
15	T	24	DG	O4'-C1'-N9	7.13	112.99	108.00
10	J	10	CYS	CA-CB-SG	6.47	125.65	114.00
11	K	113	THR	N-CA-C	6.47	128.47	111.00
15	T	28	DT	O4'-C1'-N1	5.56	111.89	108.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	303	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	11186	0	11266	1369	0
2	B	8866	0	8898	1056	0
3	C	2101	0	2055	275	0
4	D	1427	0	1451	150	0
5	E	1752	0	1776	142	0
6	F	705	0	730	77	0
7	G	1340	0	1357	167	0
8	H	1084	0	1057	133	0
9	I	944	0	901	105	0
10	J	532	0	542	101	0
11	K	919	0	929	113	0
12	L	364	0	386	49	0
13	N	165	0	92	14	0
14	P	213	0	109	22	0
15	T	404	0	229	56	0
16	A	1	0	0	0	0
17	A	8	0	0	0	0
All	All	32011	0	31778	3528	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 55.

The worst 5 of 3528 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)
8:H:100:THR:HG23	8:H:138:GLU:HA	1.33	1.11
2:B:343:ILE:HG23	2:B:347:LYS:HB2	1.13	1.11
1:A:34:LYS:HD3	1:A:57:ARG:HH22	1.07	1.10
1:A:53:LEU:HD23	1:A:54:ASN:H	0.94	1.09
7:G:138:THR:HG22	7:G:139:ILE:H	1.19	1.08

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	1410/1733 (81%)	947 (67%)	306 (22%)	157 (11%)	0	10
2	B	1096/1224 (90%)	754 (69%)	222 (20%)	120 (11%)	0	11
3	C	264/318 (83%)	164 (62%)	62 (24%)	38 (14%)	0	5
4	D	173/221 (78%)	118 (68%)	38 (22%)	17 (10%)	1	14
5	E	212/215 (99%)	153 (72%)	42 (20%)	17 (8%)	1	19
6	F	84/155 (54%)	65 (77%)	13 (16%)	6 (7%)	1	23
7	G	169/171 (99%)	128 (76%)	30 (18%)	11 (6%)	1	26
8	H	131/146 (90%)	87 (66%)	26 (20%)	18 (14%)	0	6
9	I	114/122 (93%)	77 (68%)	26 (23%)	11 (10%)	1	14
10	J	63/70 (90%)	34 (54%)	12 (19%)	17 (27%)	0	1
11	K	112/120 (93%)	82 (73%)	20 (18%)	10 (9%)	1	17
12	L	44/70 (63%)	18 (41%)	13 (30%)	13 (30%)	0	0
All	All	3872/4565 (85%)	2627 (68%)	810 (21%)	435 (11%)	0	10

5 of 435 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	THR
1	A	48	ALA
1	A	57	ARG
1	A	62	ASP
1	A	65	LEU

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	1244/1520 (82%)	1123 (90%)	121 (10%)	10	43
2	B	967/1061 (91%)	886 (92%)	81 (8%)	14	51
3	C	235/274 (86%)	218 (93%)	17 (7%)	18	57
4	D	159/200 (80%)	138 (87%)	21 (13%)	5	30
5	E	196/197 (100%)	191 (97%)	5 (3%)	54	81
6	F	77/137 (56%)	71 (92%)	6 (8%)	16	54
7	G	152/152 (100%)	140 (92%)	12 (8%)	15	54
8	H	119/128 (93%)	112 (94%)	7 (6%)	24	64
9	I	110/116 (95%)	98 (89%)	12 (11%)	8	38
10	J	60/65 (92%)	52 (87%)	8 (13%)	5	30
11	K	99/102 (97%)	87 (88%)	12 (12%)	6	33
12	L	40/57 (70%)	36 (90%)	4 (10%)	9	42
All	All	3458/4009 (86%)	3152 (91%)	306 (9%)	12	48

5 of 306 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	396	ASP
2	B	878	GLN
10	J	7	CYS
2	B	429	PHE

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Mol	Chain	Res	Type
2	B	635	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	465	ASN
2	B	821	GLN
9	I	90	GLN
2	B	515	HIS
2	B	538	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	9/11 (81%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	7	A

There are no RNA pucker outliers to report.

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

2 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$
15	TT	T	17	13,15	38,43,44	4.79	7 (18%)	54,69,72	2.54	16 (29%)
15	BRU	T	22	15,14	13,21,22	1.69	3 (23%)	16,30,33	4.18	3 (18%)

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
15	TT	T	17	13,15	-	0/18/105/106	0/3/6/6
15	BRU	T	22	15,14	-	0/3/21/22	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	17	TT	C5T-C6T	-19.98	1.31	1.55
15	T	17	TT	C5-C6	-19.41	1.32	1.55
15	T	17	TT	C6T-N1T	-4.39	1.39	1.46
15	T	17	TT	C6-N1	-3.47	1.40	1.46
15	T	17	TT	C5T-C4T	-3.40	1.45	1.51

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	22	BRU	C5-C4-N3	-7.90	115.56	124.00
15	T	17	TT	C5-C6-C6T	-6.07	79.03	89.27
15	T	17	TT	N3T-C2T-N1T	-4.90	111.92	116.82
15	T	17	TT	C5-C5T-C6T	-4.17	83.09	88.37
15	T	17	TT	C3R-C2R-C1R	-3.64	93.64	102.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	T	17	TT	22	0
15	T	22	BRU	4	0

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.