



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 30, 2024 – 12:45 PM EST

PDB ID : 1I3Q
Title : RNA POLYMERASE II CRYSTAL FORM I AT 3.1 A RESOLUTION
Authors : Cramer, P.; Bushnell, D.A.; Kornberg, R.D.
Deposited on : 2001-02-15
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

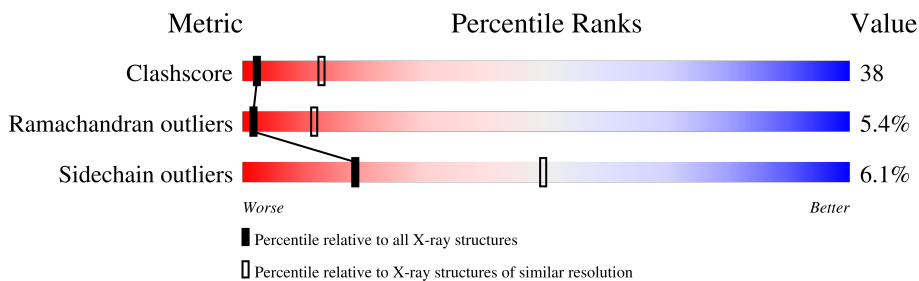
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)



The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1733	36% 40% 6% 18%
2	B	1224	37% 45% 6% 12%
3	C	318	34% 42% 8% 16%
4	E	215	52% 46% .
5	F	155	21% 29% 5% 46%
6	H	146	34% 46% 9% . 9%
7	I	122	45% 46% 9%
8	J	70	29% 56% 6% . 7%

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Mol	Chain	Length	Quality of chain
9	K	120	
10	L	70	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 28161 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
			Total	C	N	O	S			
1	A	1414	11114	7000	1947	2106	61	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1083	8624	5470	1501	1600	53	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	215	1760	1116	310	322	12	0	0	0

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

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

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

TIDE.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	L	46	364	224	72	64	4	0	0	0

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	2	Total	Zn	0	0
			2	2		
11	B	1	Total	Zn	0	0
			1	1		
11	C	1	Total	Zn	0	0
			1	1		
11	I	2	Total	Zn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	J	1	Total	Zn	0	0
			1	1		
11	L	1	Total	Zn	0	0
			1	1		

- Molecule 12 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

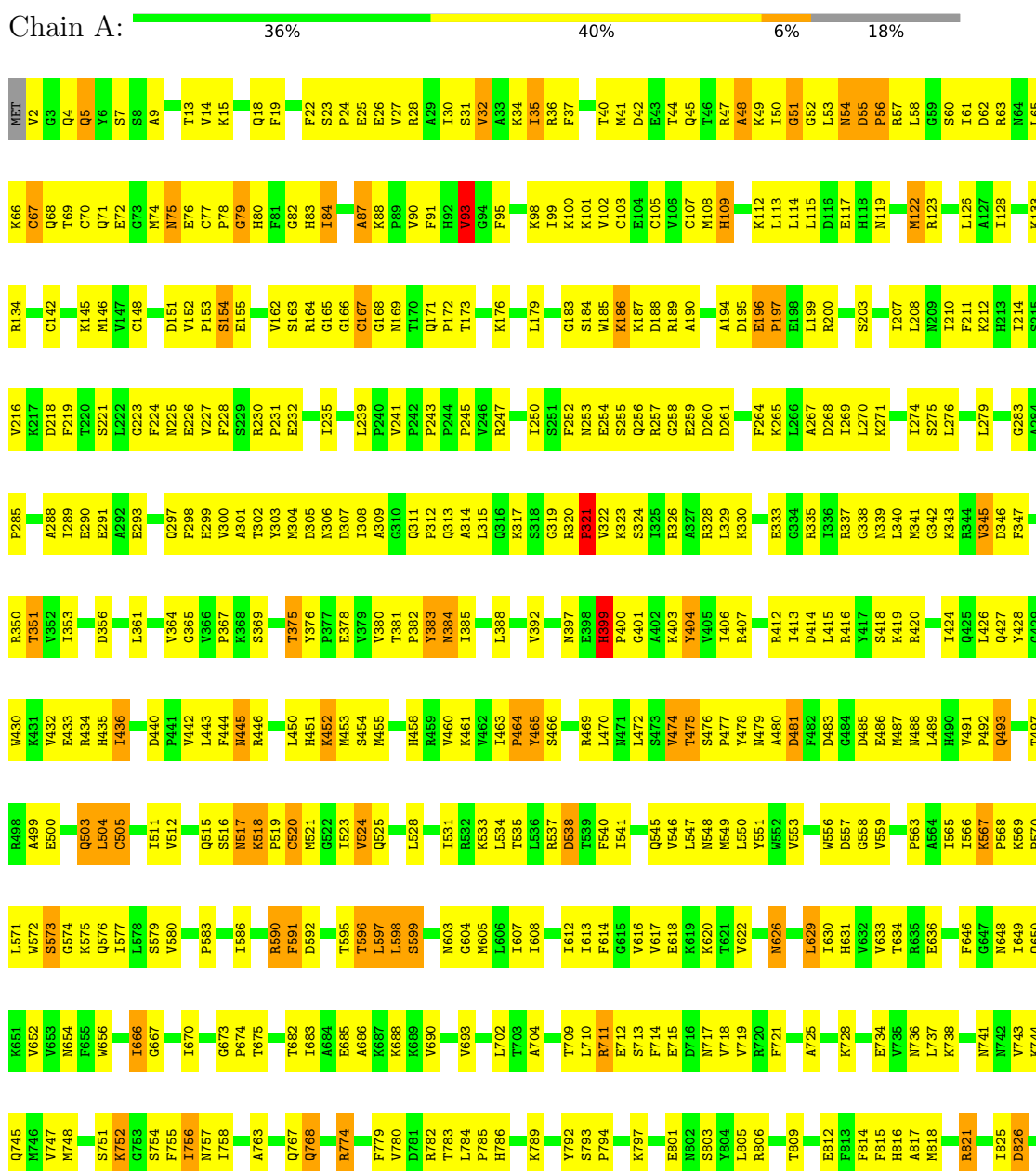
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	1	Total	Mg	0	0
			1	1		

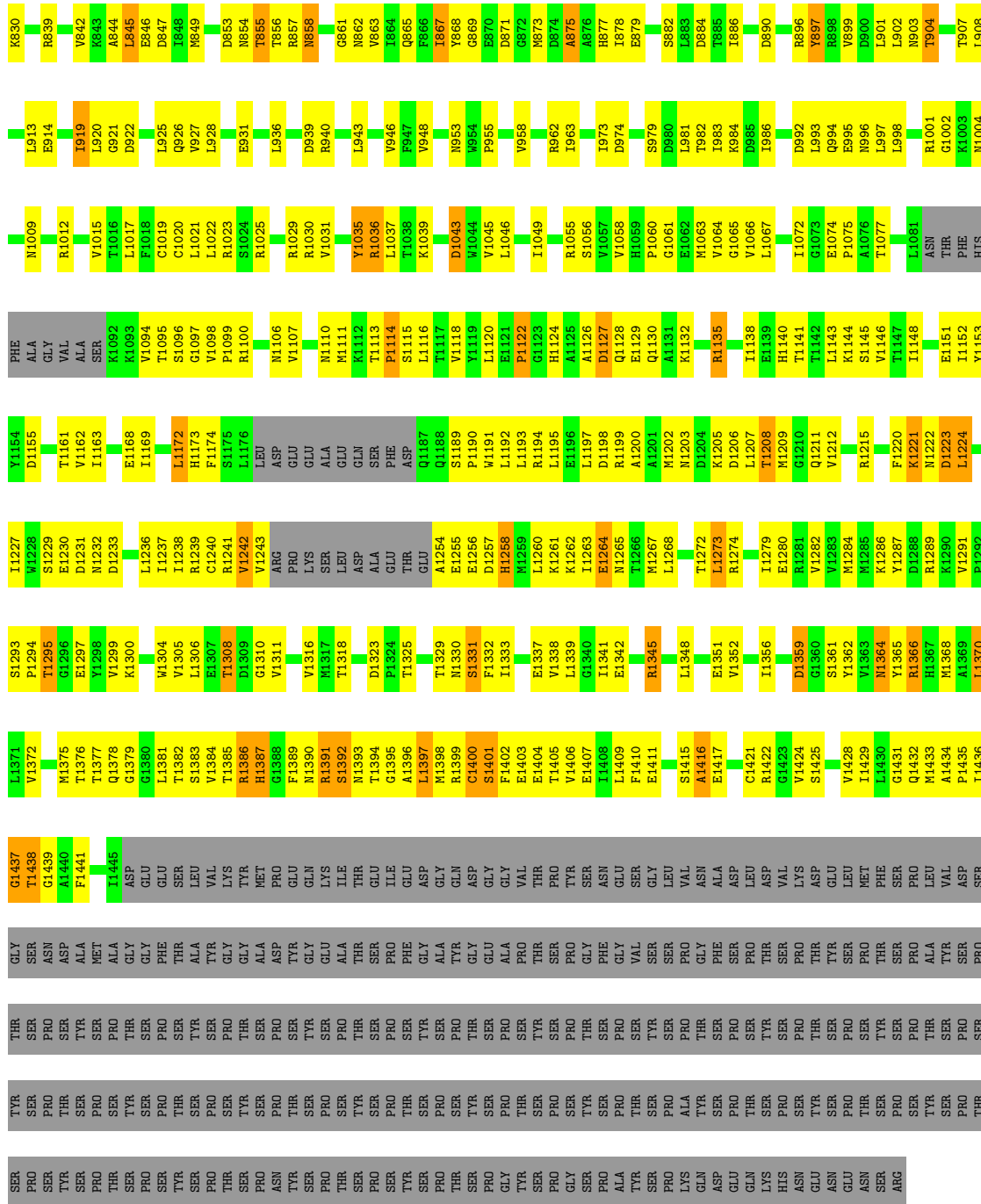
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

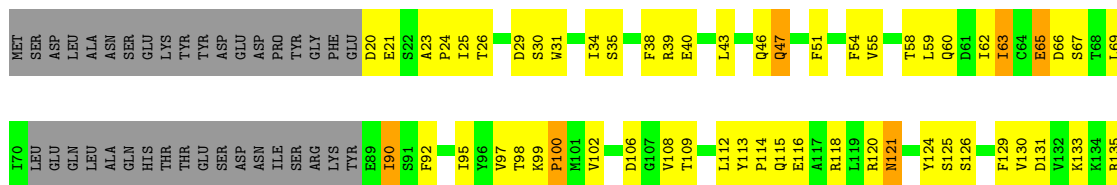
- Molecule 1: DNA-DIRECTED RNA POLYMERASE II LARGEST SUBUNIT



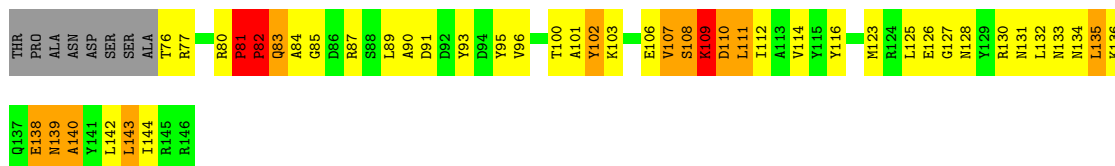


• Molecule 2: DNA-DIRECTED RNA POLYMERASE II 140KD POLYPEPTIDE

Chain B: 37% 45% 6% 12%

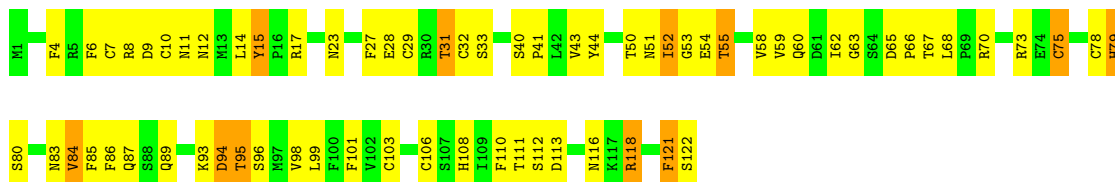


F1146	M1152	I1077	K934	Q862	L783	GLU	R654	B579	LYS	F437	Y351	I282	Y202	T136
L1147	M1153	T1077	R935	E863	N794	GLU	K655	V580	LEU	GLU	A352	V283	F203	Y137
K1148	E1154	G1078	D936	R864	L796	ASN	G656	F581	A509	ALA	K353	I284	I204	E138
	S1155	A937	A937		H657	ASP	H657		K510	HIS		I285	I205	ALA
M1152	E1154	Q1084	L941	T871	Y797	LEU	I658	V586	P511	ASP	E359	F286	G207	ILE
A1154	I1085	I1085	R942	T873	Y798	D722	A659	H587	R512	PHE	F360	G207	G206	ASP
S1155	F1086	F1087	F874	F874	Q800	A726	L661	G588	Q513	ASN	L361	S208	S208	VAL
A1157	F1098		R879	R879	R801		R662	V589	H515	LYS	P362	E209	R210	PRO
F1158	T944		R879	R879	P802		T663	H590	H515	LYS	H363	E209	K210	GLY
R1159	T944		R879	R879	P802		T663	H590	H515	LYS	H363	E209	K210	GLY
V1160	E945		R881	R881	T806		E665	L596	M516	ALA	I364	V211	V211	ARG
H1161	G947		T882	T882	T806		V666	M597	M449	ALA	I364	V211	V211	ARG
I1162	L948		L883	L883	R807		R687	E598	M449	ALA	L367	E216	E216	LEU
	V952		R884	R884	R808		D688	T599	A450	ALA	F370	G220	G220	TYR
	V1014		R887	R887	R809		I680	L600	I453	ALA	R373	L297	L297	LEU
I1165	L953		R887	R887	R809		I680	L600	I453	ALA	R373	L297	L297	LEU
C1166	V954		G888	G888	E810		T736	R601	T454	GLY	K374	L298	L298	LEU
G1167	T955		T889	T889	L812		F738	G603	T454	GLY	R374	L298	L298	LEU
L1168	T956		R890	R890	L812		F738	G603	T454	GLY	R374	L298	L298	LEU
M1169	R957		D891	D891	K813		H739	R605	S455	ALA	A375	V225	V225	ALA
T1170	Q958		R892	R892	F814		H740	R605	S455	ALA	F376	V225	V225	ALA
V1171	D959		L893	L893	R815		T743	R605	S455	ALA	F376	V225	V225	ALA
A1172	A107		R960	R960	E816		H744	V536	G464	ASP	L378	D307	D307	GLU
A1173	L961		D896	D896	L817		H744	V536	G464	ASP	L378	D307	D307	GLU
K1174	R962		G897	G897	L817		H744	V536	G464	ASP	L378	D307	D307	GLU
L1175	L898		L898	L898	F818		E678	E612	M538	ASP	I382	L311	L311	SER
H1176	F963		R899	R899	A819		V679	V613	M538	ASP	I382	L311	L311	SER
H1177	V964		Q820	Q820	M681		T616	T616	L541	GLN	L387	L314	L314	GLU
N1178	K965		R822	R822	M681		R617	R617	M542	GLN	L387	L314	L314	GLU
Q1179	V966		A823	A823	S683		D618	D618	T645	LYS	D391	K315	K315	SER
F1180	R969		R824	R824	L684		I619	I619	T645	LYS	D391	K315	K315	SER
E1181	R970		A826	A826	L684		R620	R620	S546	ALA	K393	C317	C317	GLY
K1183	R971		R827	R827	L686		E621	E621	S547	MET	D394	D320	D320	THR
G1184	R973		Y830	Y830	M686		E621	E621	S547	MET	D394	D320	D320	THR
C1185	R974		N834	N834	L688		E621	E621	S547	MET	D394	D320	D320	THR
D1186	Q975		Q835	Q835	L688		E621	E621	S547	MET	D394	D320	D320	THR
M1187	G977		R845	R845	L688		E621	E621	S547	MET	D394	D320	D320	THR
I1194	D977		D847	D847	L688		E621	E621	S547	MET	D394	D320	D320	THR
H1195	R979		N841	N841	L688		E621	E621	S547	MET	D394	D320	D320	THR
I1196	F980		N842	N842	L688		E621	E621	S547	MET	D394	D320	D320	THR
P1197	A981		Q843	Q843	L688		E621	E621	S547	MET	D394	D320	D320	THR
A1200	S982		S844	S844	L688		E621	E621	S547	MET	D394	D320	D320	THR
K1201	R983		R845	R845	L688		E621	E621	S547	MET	D394	D320	D320	THR
L1202	H984		D847	D847	L688		E621	E621	S547	MET	D394	D320	D320	THR
Q1205	G985		N850	N850	L688		E621	E621	S547	MET	D394	D320	D320	THR
E1206	R986		F851	F851	L688		E621	E621	S547	MET	D394	D320	D320	THR
L1207	G988		L854	L854	L688		E621	E621	S547	MET	D394	D320	D320	THR
M1210	R989		R854	R854	L688		E621	E621	S547	MET	D394	D320	D320	THR
N1211	G991		G138	G138	L688		E621	E621	S547	MET	D394	D320	D320	THR
I1212	Y1064		F855	F855	L688		E621	E621	S547	MET	D394	D320	D320	THR
R1215	Q1065		R992	R992	L688		E621	E621	S547	MET	D394	D320	D320	THR
	S1066		R1067	R1067	L688		E621	E621	S547	MET	D394	D320	D320	THR
	R1060		R995	R995	L688		E621	E621	S547	MET	D394	D320	D320	THR
	Y1064		R996	R996	L688		E621	E621	S547	MET	D394	D320	D320	THR
	Q1065		E997	E997	L688		E621	E621	S547	MET	D394	D320	D320	THR
	S1066		H1141	H1141	L688		E621	E621	S547	MET	D394	D320	D320	THR
	R1067		A1144	A1144	L688		E621	E621	S547	MET	D394	D320	D320	THR
	M1072		Y1073	Y1073	L688		E621	E621	S547	MET	D394	D320	D320	THR
	S1145				L688		E621	E621	S547	MET	D394	D320	D320	THR



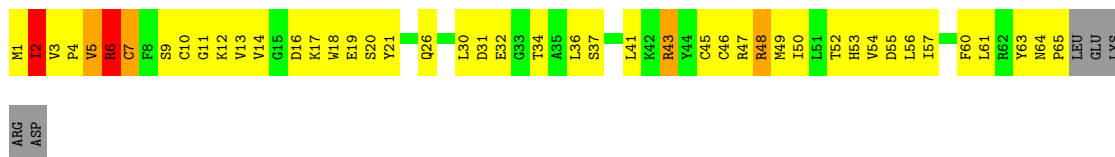
- Molecule 7: DNA-DIRECTED RNA POLYMERASE II 14.2KD POLYPEPTIDE

Chain I: 45% 46% 9%



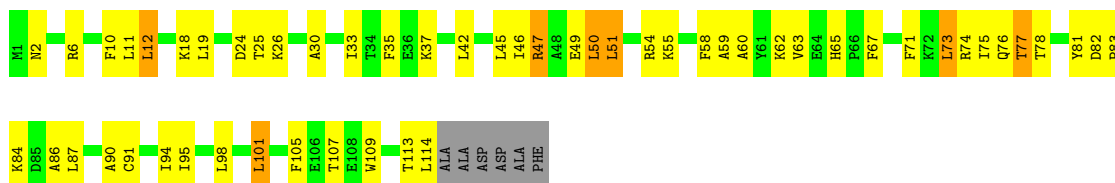
- Molecule 8: DNA-DIRECTED RNA POLYMERASE II 8.3KD POLYPEPTIDE

Chain J: 29% 56% 6% 7%



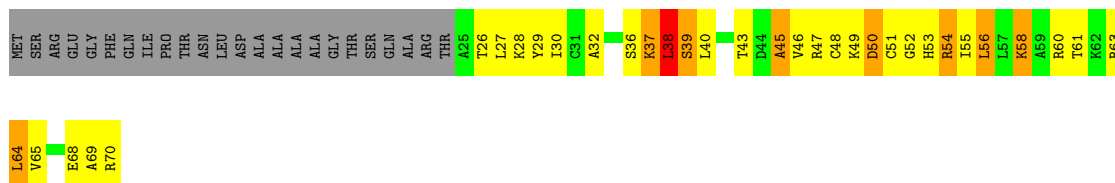
- Molecule 9: DNA-DIRECTED RNA POLYMERASE II 13.6KD POLYPEPTIDE

Chain K: 50% 39% 6% 5%



- Molecule 10: DNA-DIRECTED RNA POLYMERASE II 7.7KD POLYPEPTIDE

Chain L: 19% 34% 11% 34%



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	130.70Å 224.80Å 369.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-3.10)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	28161	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

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, 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	0.40	1/11312 (0.0%)	0.70	2/15298 (0.0%)
2	B	0.40	0/8793	0.68	3/11857 (0.0%)
3	C	0.42	0/2133	0.72	1/2891 (0.0%)
4	E	0.37	0/1796	0.63	0/2416
5	F	0.42	0/691	0.66	0/933
6	H	0.59	2/1086 (0.2%)	0.91	6/1470 (0.4%)
7	I	0.41	0/1016	0.70	0/1365
8	J	0.43	0/541	0.85	1/727 (0.1%)
9	K	0.42	0/937	0.61	0/1265
10	L	0.41	0/366	0.66	0/485
All	All	0.41	3/28671 (0.0%)	0.70	13/38707 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	109	LYS	CD-CE	7.54	1.70	1.51
6	H	109	LYS	CE-NZ	5.69	1.63	1.49
1	A	520	CYS	CB-SG	-5.67	1.72	1.81

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	109	LYS	N-CA-C	7.39	130.95	111.00
1	A	452	LYS	N-CA-C	-6.74	92.80	111.00
6	H	109	LYS	CA-CB-CG	6.68	128.09	113.40
6	H	80	ARG	NE-CZ-NH1	-6.09	117.25	120.30
6	H	80	ARG	NE-CZ-NH2	5.97	123.28	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11114	0	11193	945	0
2	B	8624	0	8642	736	1
3	C	2095	0	2051	177	0
4	E	1760	0	1788	103	0
5	F	679	0	701	56	0
6	H	1068	0	1040	93	0
7	I	997	0	955	71	0
8	J	532	0	542	78	0
9	K	919	0	929	62	0
10	L	364	0	388	47	0
11	A	2	0	0	0	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0
11	I	2	0	0	1	0
11	J	1	0	0	0	0
11	L	1	0	0	0	0
12	A	1	0	0	0	0
All	All	28161	0	28229	2150	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 38.

The worst 5 of 2150 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:1364:ASN:ND2	1:A:1366:ARG:HG2	1.59	1.17
7:I:111:THR:HG22	7:I:113:ASP:H	1.05	1.17
10:L:60:ARG:HG3	10:L:61:THR:H	1.04	1.12
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.32	1.11
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.06	1.10

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)
2:B:106:ASP:OD1	2:B:106:ASP:OD1[2_655]	2.08	0.12

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%)	1138 (81%)	203 (14%)	65 (5%)	2	15
2	B	1061/1224 (87%)	868 (82%)	128 (12%)	65 (6%)	1	9
3	C	264/318 (83%)	210 (80%)	35 (13%)	19 (7%)	1	6
4	E	213/215 (99%)	184 (86%)	27 (13%)	2 (1%)	17	52
5	F	82/155 (53%)	63 (77%)	15 (18%)	4 (5%)	2	14
6	H	129/146 (88%)	91 (70%)	22 (17%)	16 (12%)	0	1
7	I	120/122 (98%)	97 (81%)	17 (14%)	6 (5%)	2	13
8	J	63/70 (90%)	53 (84%)	7 (11%)	3 (5%)	2	14
9	K	112/120 (93%)	106 (95%)	5 (4%)	1 (1%)	17	52
10	L	44/70 (63%)	28 (64%)	9 (20%)	7 (16%)	0	0
All	All	3494/4173 (84%)	2838 (81%)	468 (13%)	188 (5%)	2	12

5 of 188 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	35	ILE
1	A	48	ALA
1	A	55	ASP
1	A	56	PRO

5.3.2 Protein sidechains [i](#)

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	1234/1520 (81%)	1165 (94%)	69 (6%)	21	52
2	B	942/1061 (89%)	884 (94%)	58 (6%)	18	49
3	C	234/274 (85%)	221 (94%)	13 (6%)	21	52
4	E	197/197 (100%)	193 (98%)	4 (2%)	55	80
5	F	74/137 (54%)	67 (90%)	7 (10%)	8	31
6	H	117/128 (91%)	108 (92%)	9 (8%)	13	41
7	I	116/116 (100%)	107 (92%)	9 (8%)	12	40
8	J	60/65 (92%)	54 (90%)	6 (10%)	7	28
9	K	99/102 (97%)	90 (91%)	9 (9%)	9	33
10	L	40/57 (70%)	35 (88%)	5 (12%)	4	18
All	All	3113/3657 (85%)	2924 (94%)	189 (6%)	18	49

5 of 189 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	976	ILE
4	E	204	THR
2	B	1028	GLU
3	C	57	VAL
5	F	140	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 81 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	102	GLN
6	H	11	GLN
3	C	123	ASN
4	E	101	GLN
7	I	12	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 monosaccharides 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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.