



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 30, 2017 – 10:24 PM EDT

PDB ID : 4YLN
Title : E. coli Transcription Initiation Complex - 17-bp spacer and 4-nt RNA
Authors : Zuo, Y.; Steitz, T.A.
Deposited on : unknown
Resolution : 5.50 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20029824

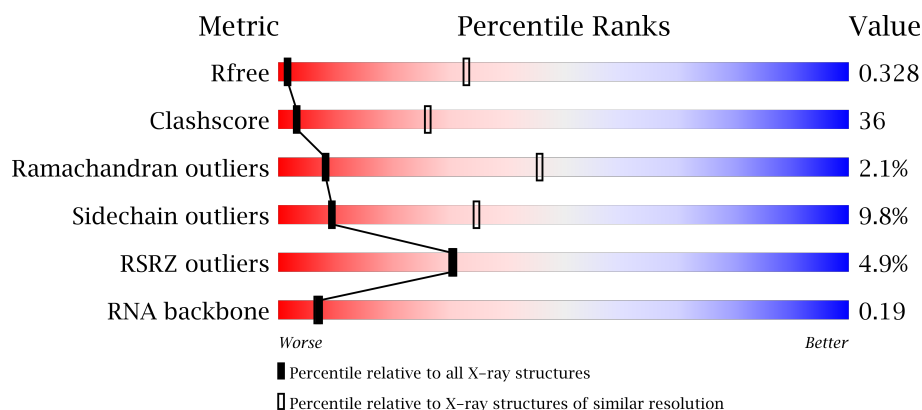
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.50 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.







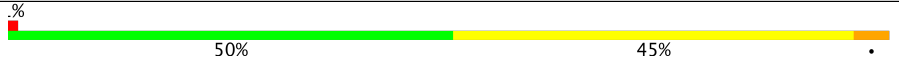
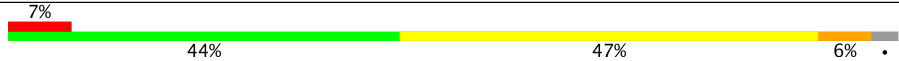
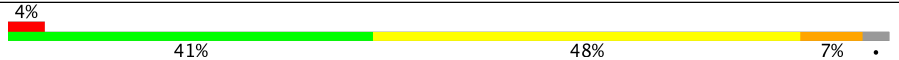
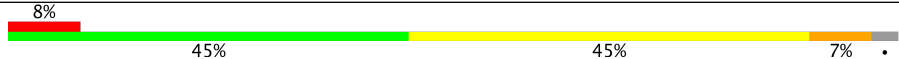
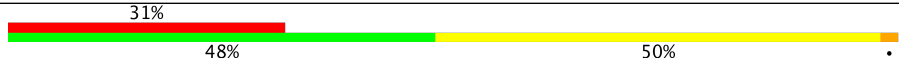
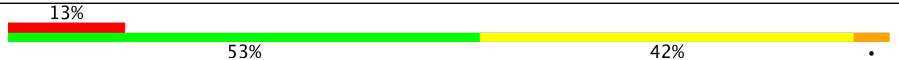
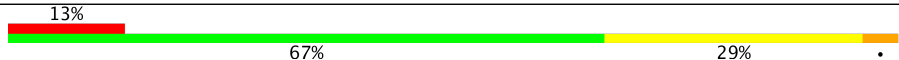
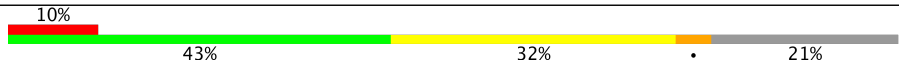
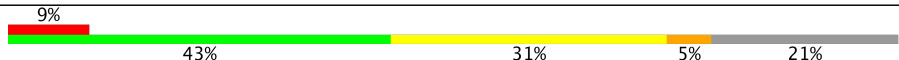
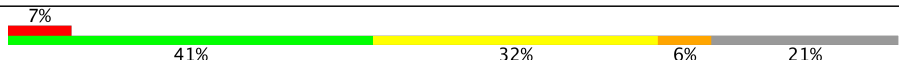
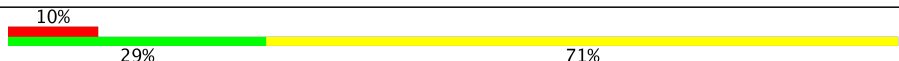
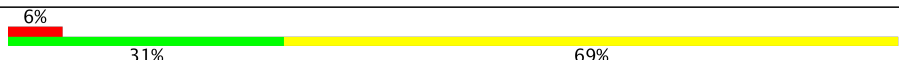
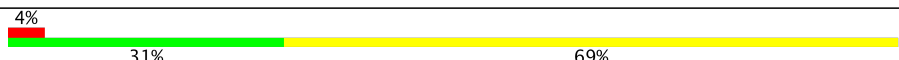
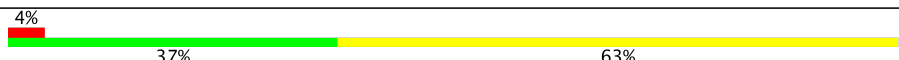
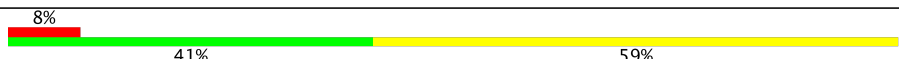
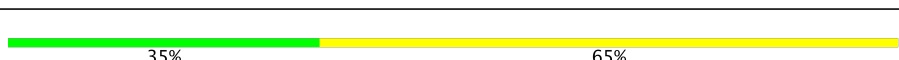
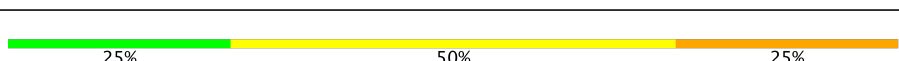

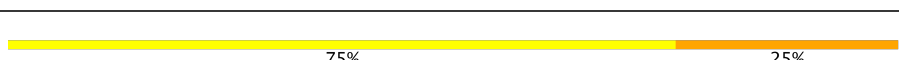
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1052 (7.20-3.70)
Clashscore	112137	1021 (7.20-3.76)
Ramachandran outliers	110173	1082 (7.20-3.70)
Sidechain outliers	110143	1055 (7.20-3.70)
RSRZ outliers	101464	1061 (7.20-3.70)
RNA backbone	2435	1049 (7.80-2.90)

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	242	<div> <div> <div>0.1%</div> <div>38%</div> <div>51%</div> <div>5%</div> <div>5%</div> </div> </div>
1	B	242	<div> <div>0.1%</div> <div>40%</div> <div>47%</div> <div>7%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	M	242	
1	N	242	
2	C	1342	
2	I	1342	
2	O	1342	
3	D	1407	
3	J	1407	
3	P	1407	
4	E	90	
4	K	90	
4	Q	90	
5	F	628	
5	L	628	
5	R	628	
6	1	49	
6	4	49	
6	7	49	
7	2	49	
7	5	49	
7	8	49	
8	3	4	
8	6	4	
8	9	4	

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
9	ZN	J	1502	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 94608 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 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1787	1112	317	352	6			
1	B	228	Total	C	N	O	S	0	0	0
			1767	1100	312	349	6			
1	G	230	Total	C	N	O	S	0	0	0
			1787	1112	317	352	6			
1	H	228	Total	C	N	O	S	0	0	0
			1767	1100	312	349	6			
1	M	230	Total	C	N	O	S	0	0	0
			1787	1112	317	352	6			
1	N	228	Total	C	N	O	S	0	0	0
			1767	1100	312	349	6			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ALA	-	expression tag	UNP A7ZSI4
A	-5	HIS	-	expression tag	UNP A7ZSI4
A	-4	HIS	-	expression tag	UNP A7ZSI4
A	-3	HIS	-	expression tag	UNP A7ZSI4
A	-2	HIS	-	expression tag	UNP A7ZSI4
A	-1	HIS	-	expression tag	UNP A7ZSI4
A	0	HIS	-	expression tag	UNP A7ZSI4
B	-6	ALA	-	expression tag	UNP A7ZSI4
B	-5	HIS	-	expression tag	UNP A7ZSI4
B	-4	HIS	-	expression tag	UNP A7ZSI4
B	-3	HIS	-	expression tag	UNP A7ZSI4
B	-2	HIS	-	expression tag	UNP A7ZSI4
B	-1	HIS	-	expression tag	UNP A7ZSI4
B	0	HIS	-	expression tag	UNP A7ZSI4
G	-6	ALA	-	expression tag	UNP A7ZSI4
G	-5	HIS	-	expression tag	UNP A7ZSI4
G	-4	HIS	-	expression tag	UNP A7ZSI4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	HIS	-	expression tag	UNP A7ZSI4
G	-2	HIS	-	expression tag	UNP A7ZSI4
G	-1	HIS	-	expression tag	UNP A7ZSI4
G	0	HIS	-	expression tag	UNP A7ZSI4
H	-6	ALA	-	expression tag	UNP A7ZSI4
H	-5	HIS	-	expression tag	UNP A7ZSI4
H	-4	HIS	-	expression tag	UNP A7ZSI4
H	-3	HIS	-	expression tag	UNP A7ZSI4
H	-2	HIS	-	expression tag	UNP A7ZSI4
H	-1	HIS	-	expression tag	UNP A7ZSI4
H	0	HIS	-	expression tag	UNP A7ZSI4
M	-6	ALA	-	expression tag	UNP A7ZSI4
M	-5	HIS	-	expression tag	UNP A7ZSI4
M	-4	HIS	-	expression tag	UNP A7ZSI4
M	-3	HIS	-	expression tag	UNP A7ZSI4
M	-2	HIS	-	expression tag	UNP A7ZSI4
M	-1	HIS	-	expression tag	UNP A7ZSI4
M	0	HIS	-	expression tag	UNP A7ZSI4
N	-6	ALA	-	expression tag	UNP A7ZSI4
N	-5	HIS	-	expression tag	UNP A7ZSI4
N	-4	HIS	-	expression tag	UNP A7ZSI4
N	-3	HIS	-	expression tag	UNP A7ZSI4
N	-2	HIS	-	expression tag	UNP A7ZSI4
N	-1	HIS	-	expression tag	UNP A7ZSI4
N	0	HIS	-	expression tag	UNP A7ZSI4

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1341	Total	C	N	O	S	0	0	0
			10576	6636	1842	2055	43			
2	I	1341	Total	C	N	O	S	0	0	0
			10576	6636	1842	2055	43			
2	O	1341	Total	C	N	O	S	0	0	0
			10576	6636	1842	2055	43			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1362	Total	C	N	O	S	0	0	0
			10568	6633	1887	1998	50			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	1362	Total	C	N	O	S	0	0	0
			10568	6633	1887	1998	50			
3	P	1362	Total	C	N	O	S	0	0	0
			10568	6633	1887	1998	50			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	90	Total	C	N	O	S	0	0	0
			708	430	136	141	1			
4	K	90	Total	C	N	O	S	0	0	0
			708	430	136	141	1			
4	Q	90	Total	C	N	O	S	0	0	0
			708	430	136	141	1			

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	497	Total	C	N	O	S	0	0	0
			4022	2512	719	768	23			
5	L	497	Total	C	N	O	S	0	0	0
			4022	2512	719	768	23			
5	R	497	Total	C	N	O	S	0	0	0
			4022	2512	719	768	23			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-14	MET	-	expression tag	UNP P00579
F	-13	ARG	-	expression tag	UNP P00579
F	-12	GLY	-	expression tag	UNP P00579
F	-11	SER	-	expression tag	UNP P00579
F	-10	HIS	-	expression tag	UNP P00579
F	-9	HIS	-	expression tag	UNP P00579
F	-8	HIS	-	expression tag	UNP P00579
F	-7	HIS	-	expression tag	UNP P00579
F	-6	HIS	-	expression tag	UNP P00579
F	-5	HIS	-	expression tag	UNP P00579
F	-4	THR	-	expression tag	UNP P00579
F	-3	ASP	-	expression tag	UNP P00579
F	-2	GLN	-	expression tag	UNP P00579
F	-1	PHE	-	expression tag	UNP P00579

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	THR	-	expression tag	UNP P00579
L	-14	MET	-	expression tag	UNP P00579
L	-13	ARG	-	expression tag	UNP P00579
L	-12	GLY	-	expression tag	UNP P00579
L	-11	SER	-	expression tag	UNP P00579
L	-10	HIS	-	expression tag	UNP P00579
L	-9	HIS	-	expression tag	UNP P00579
L	-8	HIS	-	expression tag	UNP P00579
L	-7	HIS	-	expression tag	UNP P00579
L	-6	HIS	-	expression tag	UNP P00579
L	-5	HIS	-	expression tag	UNP P00579
L	-4	THR	-	expression tag	UNP P00579
L	-3	ASP	-	expression tag	UNP P00579
L	-2	GLN	-	expression tag	UNP P00579
L	-1	PHE	-	expression tag	UNP P00579
L	0	THR	-	expression tag	UNP P00579
R	-14	MET	-	expression tag	UNP P00579
R	-13	ARG	-	expression tag	UNP P00579
R	-12	GLY	-	expression tag	UNP P00579
R	-11	SER	-	expression tag	UNP P00579
R	-10	HIS	-	expression tag	UNP P00579
R	-9	HIS	-	expression tag	UNP P00579
R	-8	HIS	-	expression tag	UNP P00579
R	-7	HIS	-	expression tag	UNP P00579
R	-6	HIS	-	expression tag	UNP P00579
R	-5	HIS	-	expression tag	UNP P00579
R	-4	THR	-	expression tag	UNP P00579
R	-3	ASP	-	expression tag	UNP P00579
R	-2	GLN	-	expression tag	UNP P00579
R	-1	PHE	-	expression tag	UNP P00579
R	0	THR	-	expression tag	UNP P00579

- Molecule 6 is a DNA chain called NT strand DNA (49-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1	49	Total	C	N	O	P	0	0	0
			996	476	178	294	48			
6	4	49	Total	C	N	O	P	0	0	0
			996	476	178	294	48			
6	7	49	Total	C	N	O	P	0	0	0
			996	476	178	294	48			

- Molecule 7 is a DNA chain called T strand DNA (49-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	2	49	Total	C	N	O	P	0	0	0
			1012	481	191	292	48			
7	5	49	Total	C	N	O	P	0	0	0
			1012	481	191	292	48			
7	8	49	Total	C	N	O	P	0	0	0
			1012	481	191	292	48			

- Molecule 8 is a RNA chain called RNA (5'-D*(GTP))-R(P*AP*GP*U)-3').

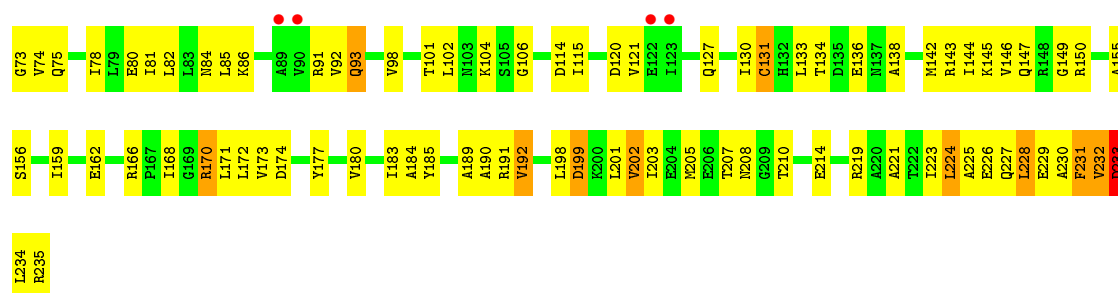
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	3	4	Total	C	N	O	P	0	0	0
			97	39	17	35	6			
8	6	4	Total	C	N	O	P	0	0	0
			97	39	17	35	6			
8	9	4	Total	C	N	O	P	0	0	0
			97	39	17	35	6			

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

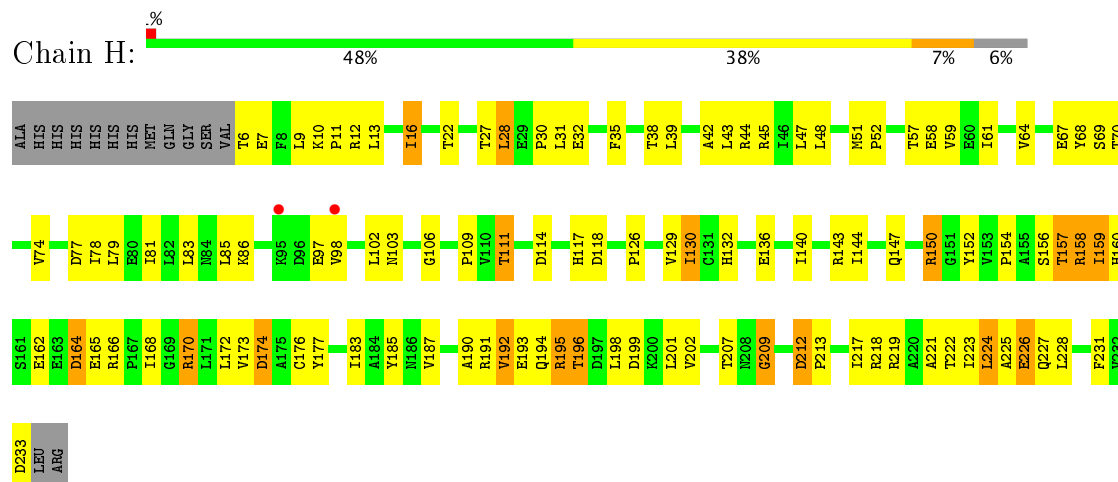
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	P	2	Total	Zn	0	0
			2	2		
9	J	2	Total	Zn	0	0
			2	2		
9	D	2	Total	Zn	0	0
			2	2		

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

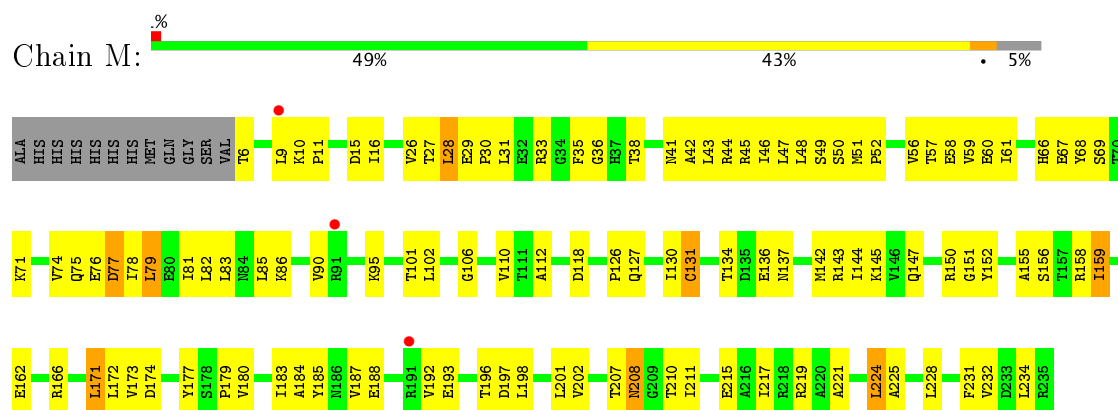
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	P	1	Total	Mg	0	0
			1	1		
10	D	1	Total	Mg	0	0
			1	1		
10	6	1	Total	Mg	0	0
			1	1		



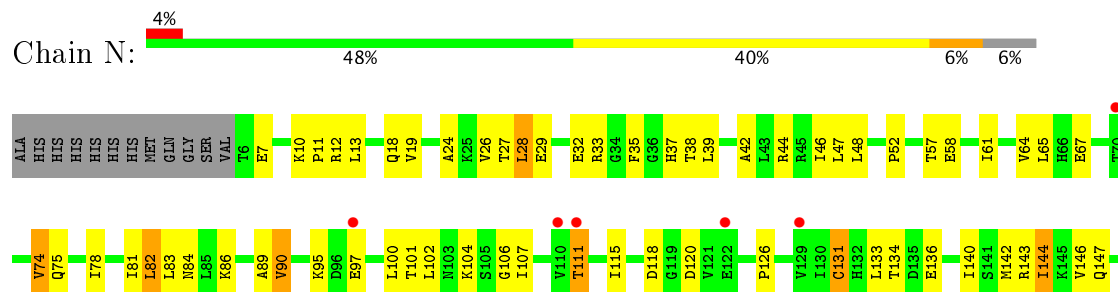
- Molecule 1: DNA-directed RNA polymerase subunit alpha

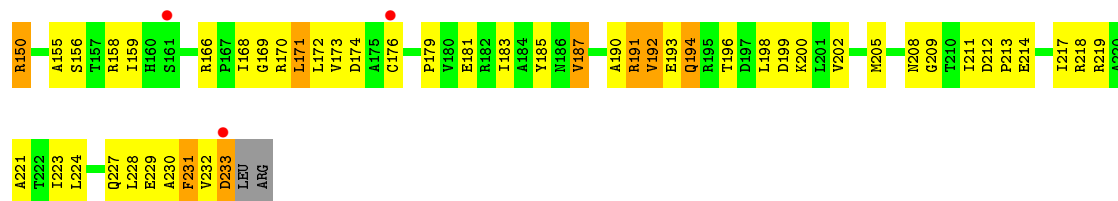


- Molecule 1: DNA-directed RNA polymerase subunit alpha

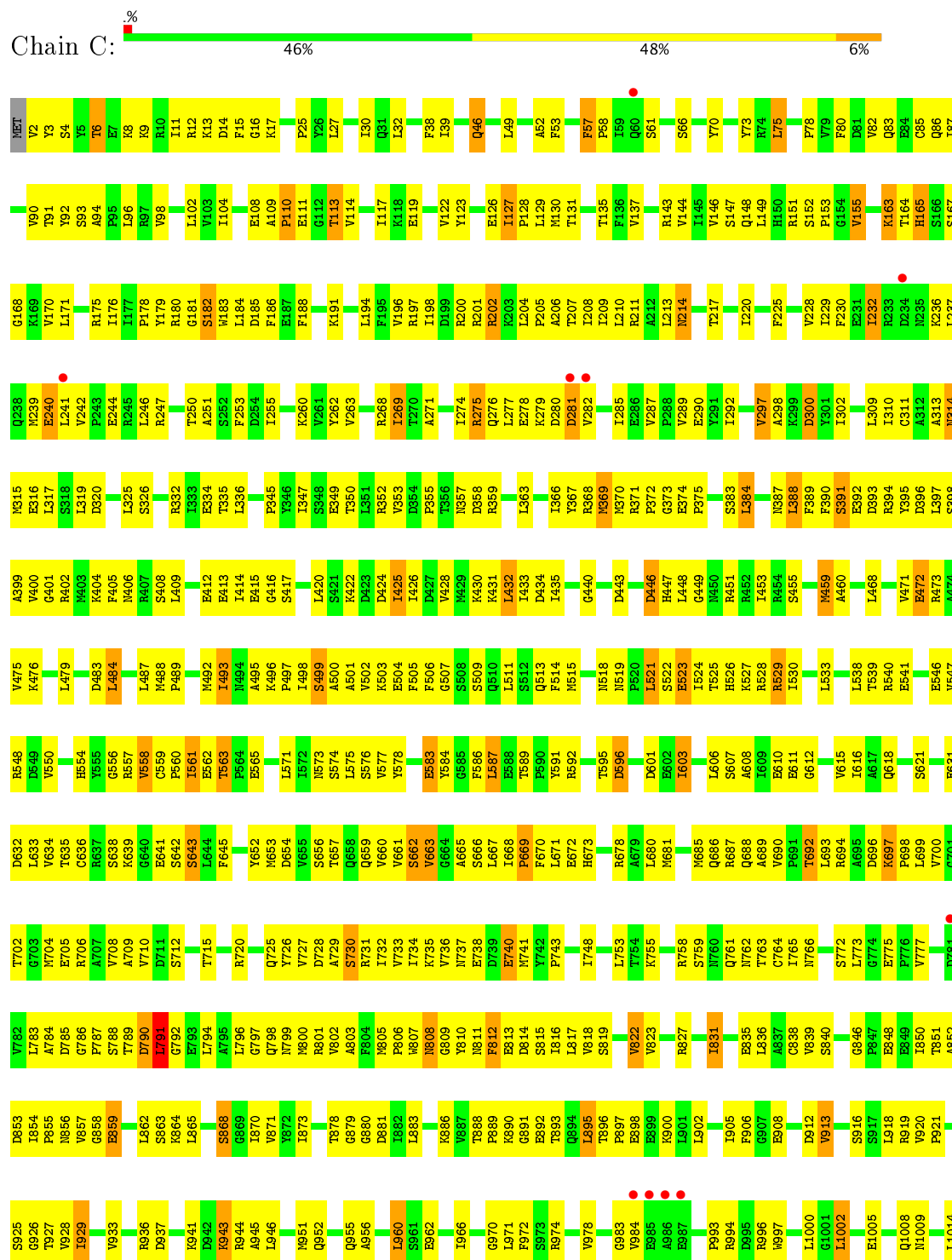


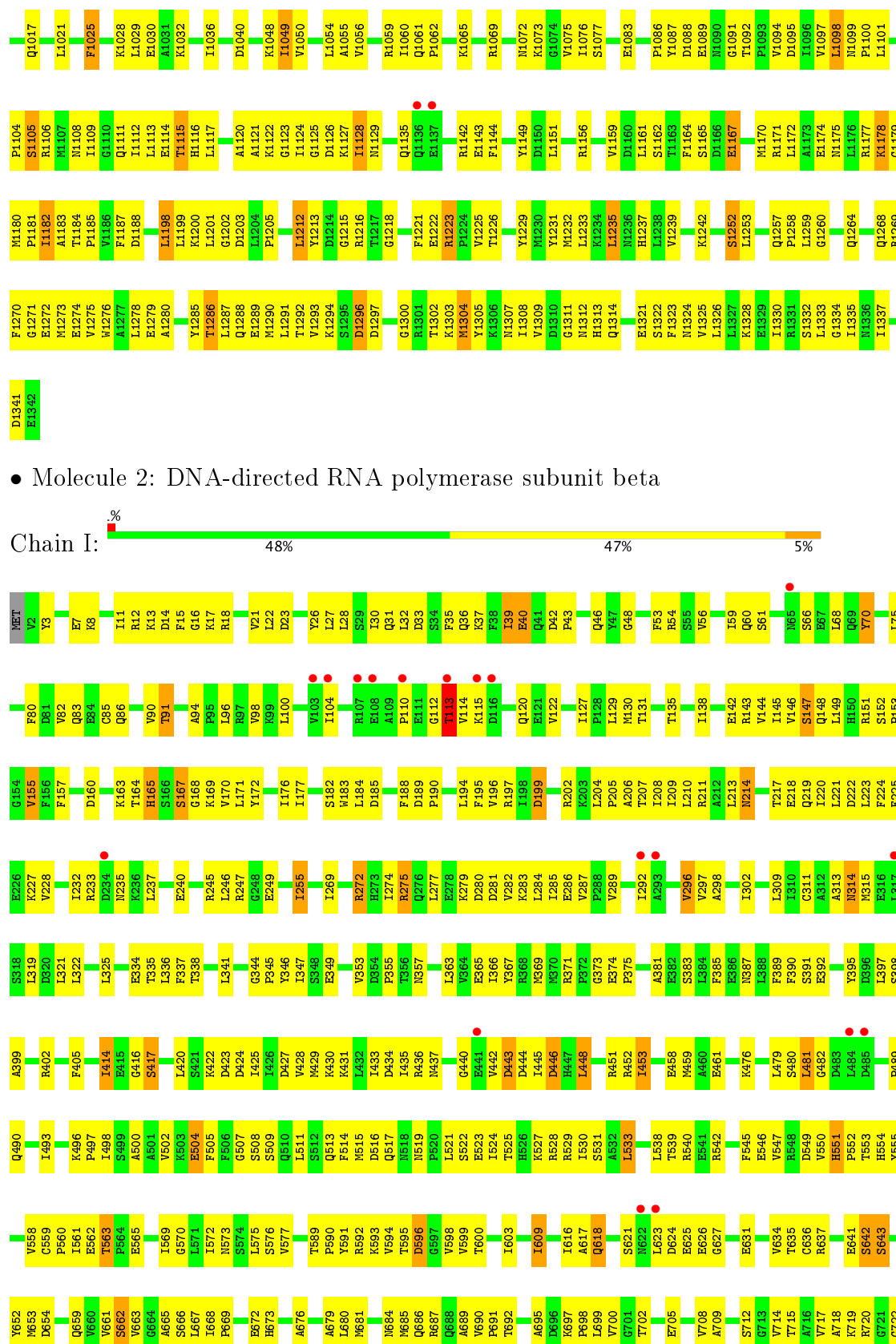
- Molecule 1: DNA-directed RNA polymerase subunit alpha





• Molecule 2: DNA-directed RNA polymerase subunit beta



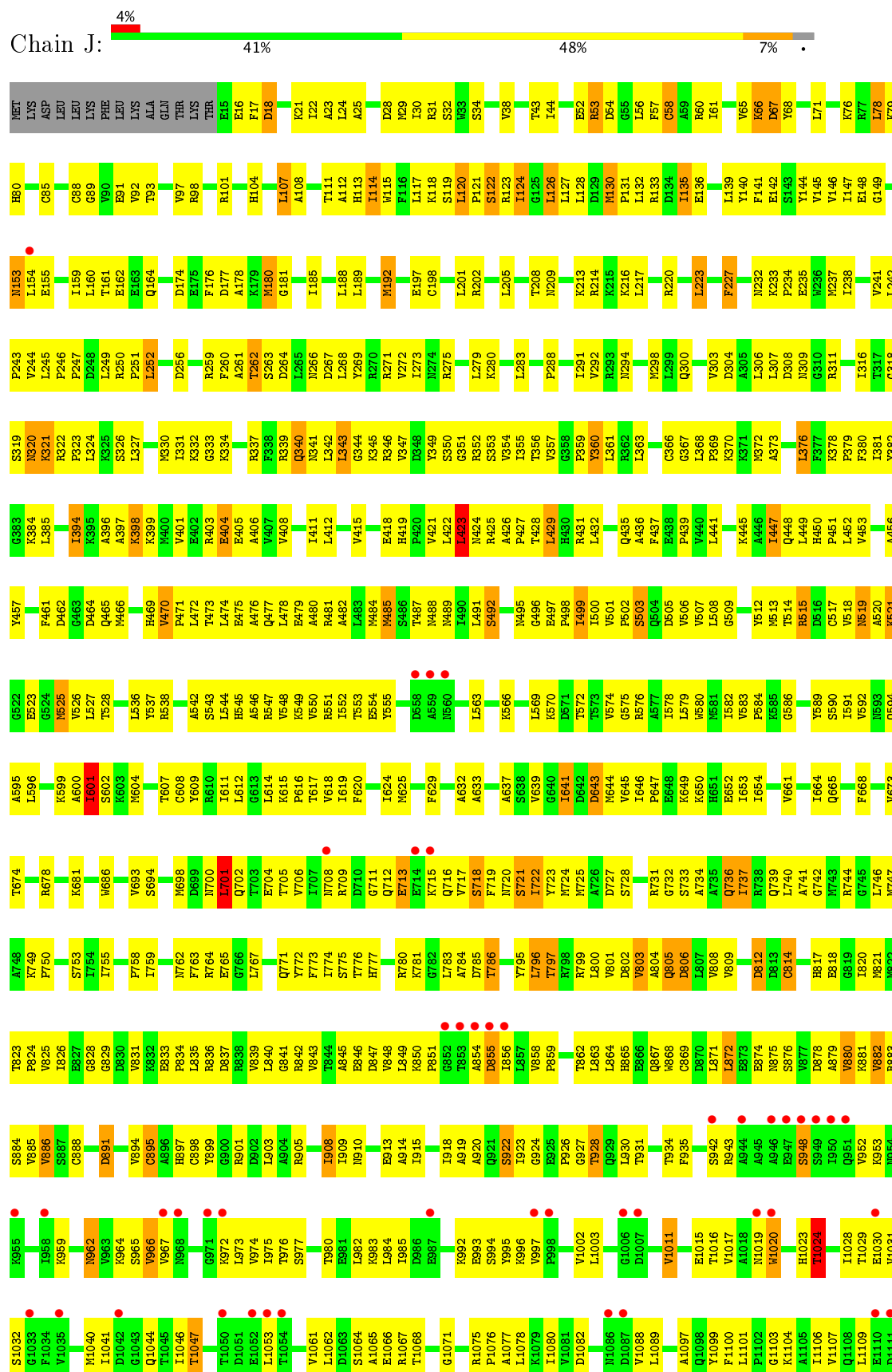


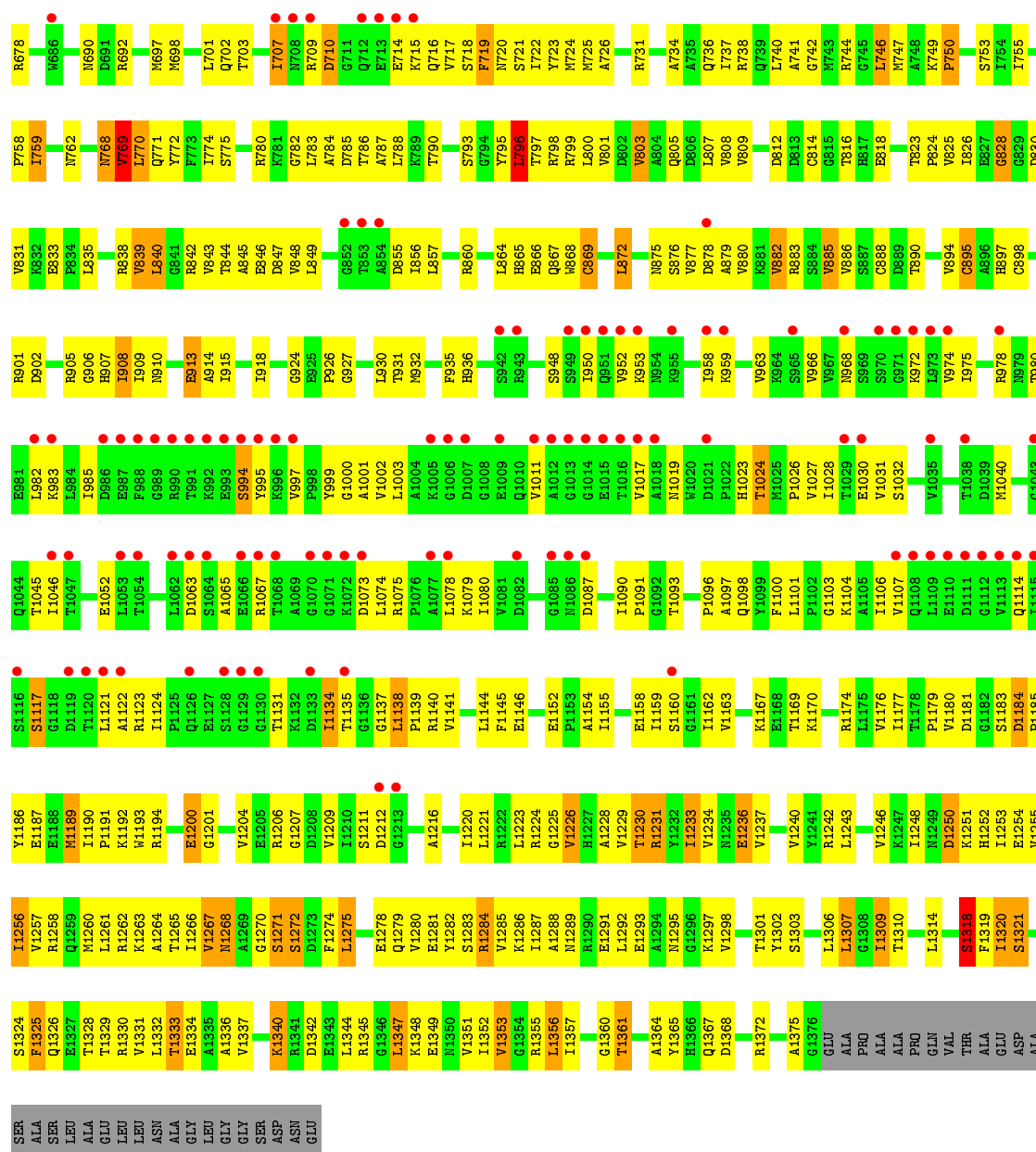




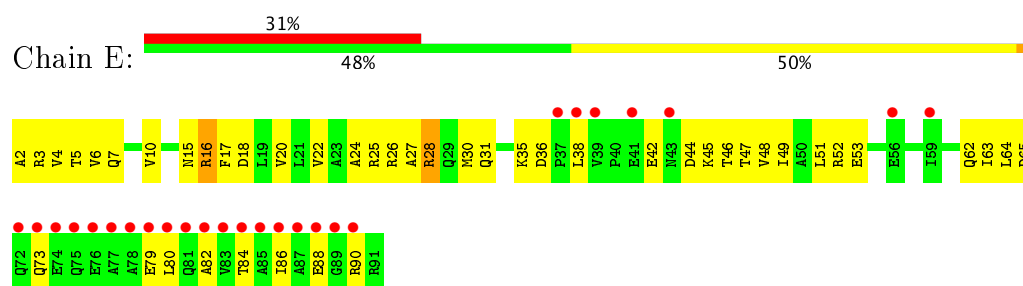
ALA	I1320	R1242	L1175	I1035	Y966	B311	M743	Q685	Y512	K445	F377	R309
GLY	S1321	L1243	V1176	R1036	Y967	D812	R744	Q688	M513	A446	K378	G310
LEU		Q1244	I1177	F1037	Y968	D813	G745	F688	T514	I447	P379	R311
GLY	S1324		T1178	I1106		C814	L746		R515	Q448	F380	R312
GLY				I1038		C815	M747	G671	R516	L449	I381	G313
SER	Q1325	I1248	P1179	D1039	K972	G815	M748	L672	V518	H450	Y382	R314
ASP	E1327		V1180	D1041	L973	T816	A748	L673	M519	P451	G383	A315
ASN	T1328		D1181	I1041	Y974	H817	K749	V673	A520	L452	K364	
GLU	R1250		G1182	D1042	Y975	B818	P750	T674	K598	L385	K385	G318
	K1251		S1183	G1043	T976	G819			T528	A456	E386	S319
	H1252		Q1044	Q1044	S977		S753	K681	G529	Y457	L387	N320
	I1253		T1045	I1045	R978	T823	I755	V682	P530		R388	K321
	V1255		Y1186	P1046	R979	R824	I756	L683		F461	G389	R322
	I1256		G1117	I1047	T980	V825	T757		E534	D464	L390	F253
	V1257		D1119	R1048	Y981	I826		W686	R535	Q465	K395	L324
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	R1259		L1121	L1050	R983	G828	T759		L536	A467	A397	
	M1260		R1122	L1051	L984	G829	T760		Y537	Y467	A397	
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			I1124	L1053	D986	B831	N762		S539	V468	K398	L331
	K1263		F1125	T1054	Y987	R832	T763		G540	H469	M400	K332
			Q1126		Y988	B833	R764		A542	V470	V401	G333
						E834			L544	T473	R403	K337
						R835	L767		R547	E474	E404	
						B836	T768		V548	E475	V407	L342
						R837	Q771		K549	A476	V408	L343
						R838	T772		R550	Q477	W409	K345
						R839	F773		V551	L478	D410	K346
						R840	T774		R552	E479	I411	V347
						R841	S775		T553	D480	L412	D348
						R842	T776		E594	A482	I416	
						R843	R777		Y555	L483		G351
						R844	T780		K556	N484	P420	R352
						R845			K557	N485	V421	S353
						R846	T786		D558	S486	L422	V354
						R847	A787		L563	T487	L423	L355
						R848	L788		V564	N488	N424	T356
						R849	K789		R425	N489	R425	V357
						R850	T790		K566	S492	A426	G358
						R851			L569	P493	P427	P359
						R852	S793		K570	L493	T428	Y360
						R853	T795		D571	N495	L429	L361
						R854	Y796		G496	R430	R362	
						R855	T797		T572	R431	L363	L363
						R856	R798		T573	P498	L432	H364
						R857	R799		V574	G433	G433	G365
						R858	R800		G575	I499	I434	G366
						R859	L801		V501	V500	Q435	G367
						R860	V801		A577	P502	A436	L368
						R861	D802		L578	S503	F437	P369
						R862	V803		L579	S504	E438	K370
						R863	Q805		W580	P439	P439	K371
						R864	D806		V505	D505	W440	K372
						R865	L807		I582	V507	L441	A373
						R866	V808		G586	L510	L442	E375
						R867	S887		L587	E443	E443	L374
						R868	T810			G444	G444	L376
						R869						
						R870						
						R871						
						R872						
						R873						
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						R978						
						R979						
						R980						
						R981						
						R982						
						R983						

● Molecule 3: DNA-directed RNA polymerase subunit beta'



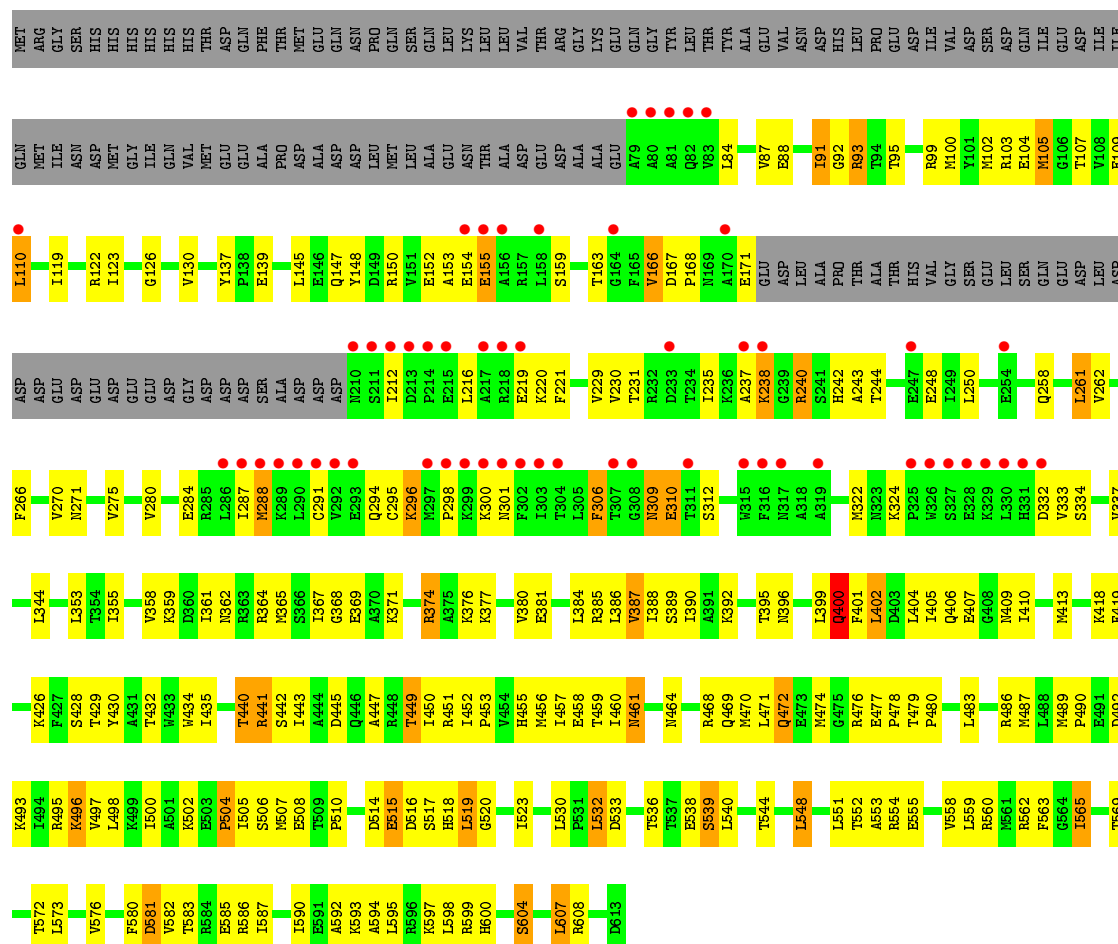


• Molecule 4: DNA-directed RNA polymerase subunit omega

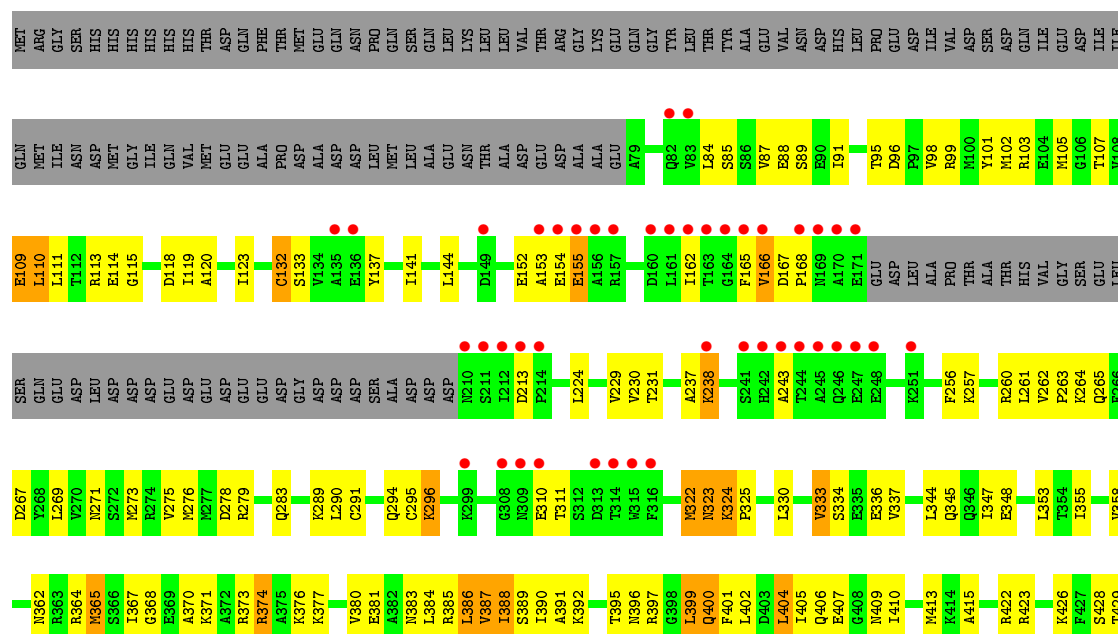
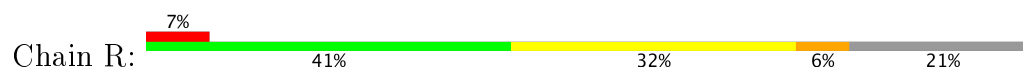


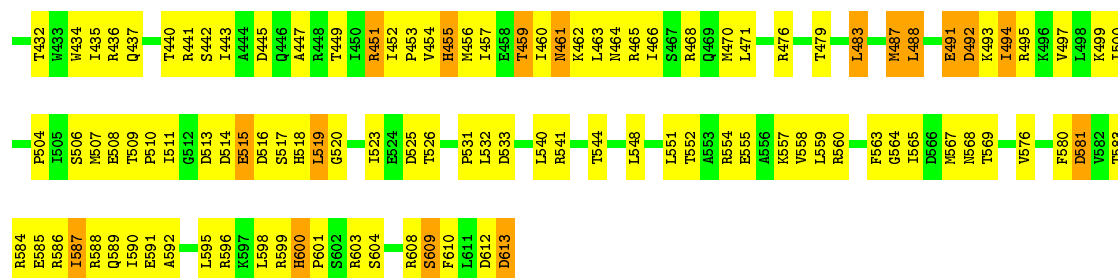
• Molecule 4: DNA-directed RNA polymerase subunit omega





● Molecule 5: RNA polymerase sigma factor RpoD





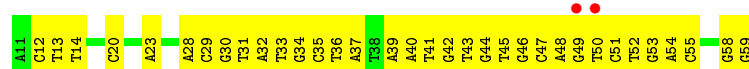
• Molecule 6: NT strand DNA (49-MER)



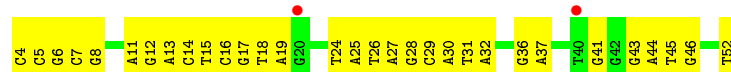
• Molecule 6: NT strand DNA (49-MER)

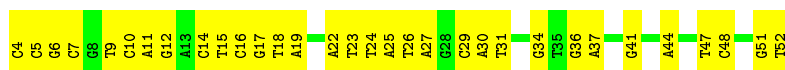


• Molecule 6: NT strand DNA (49-MER)

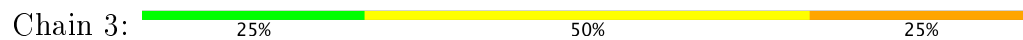


• Molecule 7: T strand DNA (49-MER)





- Molecule 8: RNA (5'-D*(GTP))-R(P*AP*GP*U)-3')



- Molecule 8: RNA (5'-D*(GTP))-R(P*AP*GP*U)-3')



- Molecule 8: RNA (5'-D*(GTP))-R(P*AP*GP*U)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	237.40Å 206.05Å 248.69Å 90.00° 116.55° 90.00°	Depositor
Resolution (Å)	39.90 – 5.50 39.90 – 5.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.90-5.50) 99.6 (39.90-5.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 5.37Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.245 , 0.328 0.244 , 0.328	Depositor DCC
R_{free} test set	3459 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	268.1	Xtriage
Anisotropy	0.597	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 203.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	94608	wwPDB-VP
Average B, all atoms (Å ²)	219.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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: GTP, 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	0.59	0/1809	0.84	1/2450 (0.0%)
1	B	0.54	0/1789	0.78	0/2425
1	G	0.56	0/1809	0.76	1/2450 (0.0%)
1	H	0.53	0/1789	0.76	0/2425
1	M	0.53	0/1809	0.74	0/2450
1	N	0.54	0/1789	0.79	2/2425 (0.1%)
2	C	0.54	0/10745	0.78	4/14499 (0.0%)
2	I	0.54	3/10745 (0.0%)	0.77	2/14499 (0.0%)
2	O	0.53	0/10745	0.75	3/14499 (0.0%)
3	D	0.54	0/10729	0.77	4/14487 (0.0%)
3	J	0.58	2/10729 (0.0%)	0.81	10/14487 (0.1%)
3	P	0.55	1/10729 (0.0%)	0.77	6/14487 (0.0%)
4	E	0.54	1/710 (0.1%)	0.72	0/956
4	K	0.53	0/710	0.73	0/956
4	Q	0.52	0/710	0.72	0/956
5	F	0.49	1/4076 (0.0%)	0.69	0/5482
5	L	0.51	0/4076	0.72	0/5482
5	R	0.55	2/4076 (0.0%)	0.74	1/5482 (0.0%)
6	1	0.41	0/1115	0.69	0/1718
6	4	0.33	0/1112	0.66	0/1706
6	7	0.37	0/1114	0.67	0/1714
7	2	0.37	0/1134	0.67	0/1744
7	5	0.35	0/1134	0.65	0/1744
7	8	0.38	0/1136	0.64	0/1752
8	3	0.44	0/72	0.62	0/110
8	6	0.40	0/72	0.61	0/110
8	9	0.36	0/72	0.59	0/110
All	All	0.53	10/96535 (0.0%)	0.76	34/131605 (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
3	D	0	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	1340	LYS	CB-CG	6.65	1.70	1.52
2	I	626	GLU	CD-OE2	6.62	1.32	1.25
2	I	626	GLU	CD-OE1	5.92	1.32	1.25
5	R	109	GLU	CD-OE1	5.75	1.31	1.25
5	F	491	GLU	CB-CG	5.70	1.62	1.52

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	737	ILE	CB-CA-C	-7.98	95.64	111.60
3	J	803	VAL	CB-CA-C	-7.38	97.38	111.40
5	R	488	LEU	CA-CB-CG	7.32	132.12	115.30
3	D	737	ILE	CB-CA-C	-7.15	97.30	111.60
2	O	57	PHE	C-N-CD	-7.09	105.00	120.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	671	GLY	Peptide

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	1787	0	1813	220	0
1	B	1767	0	1789	175	0
1	G	1787	0	1812	173	0
1	H	1767	0	1789	149	0
1	M	1787	0	1813	178	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	1767	0	1789	142	0
2	C	10576	0	10591	868	0
2	I	10576	0	10591	845	0
2	O	10576	0	10591	771	0
3	D	10568	0	10782	856	3
3	J	10568	0	10780	1069	2
3	P	10568	0	10780	901	0
4	E	708	0	719	42	0
4	K	708	0	719	48	0
4	Q	708	0	719	36	0
5	F	4022	0	4083	243	0
5	L	4022	0	4083	270	0
5	R	4022	0	4083	282	0
6	1	996	0	554	70	1
6	4	996	0	557	76	0
6	7	996	0	555	74	0
7	2	1012	0	556	62	0
7	5	1012	0	556	59	0
7	8	1012	0	554	64	0
8	3	97	0	44	7	0
8	6	97	0	44	8	0
8	9	97	0	44	4	0
9	D	2	0	0	0	0
9	J	2	0	0	2	0
9	P	2	0	0	0	0
10	6	1	0	0	0	0
10	D	1	0	0	0	0
10	P	1	0	0	0	0
All	All	94608	0	92790	6821	3

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 36.

The worst 5 of 6821 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)
3:D:608:CYS:SG	3:D:617:THR:HG22	1.31	1.67
3:D:501:VAL:CG1	3:D:502:PRO:HD2	1.33	1.55
3:J:349:TYR:O	3:J:470:VAL:HG23	1.24	1.30
3:D:645:VAL:CG2	3:D:701:LEU:HD13	1.59	1.30
5:L:573:LEU:HB2	7:5:46:DG:OP2	1.15	1.28

All (3) 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)
3:D:1169:THR:OG1	6:1:16:DA:OP1[2_657]	1.85	0.35
3:D:710:ASP:OD2	3:J:1282:TYR:OH[2_547]	1.93	0.27
3:D:710:ASP:CA	3:J:1302:TYR:OH[2_547]	2.07	0.13

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	228/242 (94%)	214 (94%)	11 (5%)	3 (1%)	14	56
1	B	226/242 (93%)	204 (90%)	17 (8%)	5 (2%)	8	45
1	G	228/242 (94%)	209 (92%)	16 (7%)	3 (1%)	14	56
1	H	226/242 (93%)	207 (92%)	13 (6%)	6 (3%)	6	40
1	M	228/242 (94%)	214 (94%)	14 (6%)	0	100	100
1	N	226/242 (93%)	209 (92%)	14 (6%)	3 (1%)	14	56
2	C	1339/1342 (100%)	1218 (91%)	98 (7%)	23 (2%)	11	51
2	I	1339/1342 (100%)	1214 (91%)	105 (8%)	20 (2%)	12	53
2	O	1339/1342 (100%)	1234 (92%)	90 (7%)	15 (1%)	17	60
3	D	1360/1407 (97%)	1220 (90%)	109 (8%)	31 (2%)	7	44
3	J	1360/1407 (97%)	1227 (90%)	99 (7%)	34 (2%)	6	41
3	P	1360/1407 (97%)	1226 (90%)	99 (7%)	35 (3%)	6	41
4	E	88/90 (98%)	83 (94%)	5 (6%)	0	100	100
4	K	88/90 (98%)	84 (96%)	3 (3%)	1 (1%)	17	60
4	Q	88/90 (98%)	84 (96%)	4 (4%)	0	100	100
5	F	493/628 (78%)	444 (90%)	27 (6%)	22 (4%)	3	29
5	L	493/628 (78%)	447 (91%)	28 (6%)	18 (4%)	4	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	R	493/628 (78%)	449 (91%)	30 (6%)	14 (3%)	6	40
All	All	11202/11853 (94%)	10187 (91%)	782 (7%)	233 (2%)	8	46

5 of 233 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	164	ASP
1	B	118	ASP
2	C	110	PRO
2	C	214	ASN
2	C	247	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	198/208 (95%)	181 (91%)	17 (9%)	12	42
1	B	196/208 (94%)	172 (88%)	24 (12%)	6	27
1	G	198/208 (95%)	178 (90%)	20 (10%)	9	33
1	H	196/208 (94%)	174 (89%)	22 (11%)	7	29
1	M	198/208 (95%)	178 (90%)	20 (10%)	9	33
1	N	196/208 (94%)	176 (90%)	20 (10%)	8	33
2	C	1156/1157 (100%)	1042 (90%)	114 (10%)	9	34
2	I	1156/1157 (100%)	1052 (91%)	104 (9%)	11	39
2	O	1156/1157 (100%)	1050 (91%)	106 (9%)	11	38
3	D	1135/1168 (97%)	1026 (90%)	109 (10%)	10	36
3	J	1135/1168 (97%)	1014 (89%)	121 (11%)	8	31
3	P	1135/1168 (97%)	1017 (90%)	118 (10%)	8	32
4	E	74/74 (100%)	70 (95%)	4 (5%)	26	59
4	K	74/74 (100%)	67 (90%)	7 (10%)	10	36
4	Q	74/74 (100%)	66 (89%)	8 (11%)	7	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	F	439/554 (79%)	406 (92%)	33 (8%)	16	48
5	L	439/554 (79%)	394 (90%)	45 (10%)	8	33
5	R	439/554 (79%)	393 (90%)	46 (10%)	8	32
All	All	9594/10107 (95%)	8656 (90%)	938 (10%)	9	35

5 of 938 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	1085	MET
3	J	882	VAL
3	P	1250	ASP
2	I	1255	THR
3	J	321	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 148 such sidechains are listed below:

Mol	Chain	Res	Type
3	J	419	HIS
3	J	979	ASN
3	P	1259	GLN
3	J	465	GLN
3	J	700	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	3	2/4 (50%)	1 (50%)	0
8	6	3/4 (75%)	1 (33%)	1 (33%)
8	9	3/4 (75%)	1 (33%)	1 (33%)
All	All	8/12 (66%)	3 (37%)	2 (25%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	3	15	G
8	6	15	G
8	9	15	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	6	13	GTP
8	9	13	GTP

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
7	2	3
6	4	3
7	5	3
7	8	1
6	7	1

The worst 5 of 11 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4	45:DT	O3'	46:DG	P	5.04
1	7	50:DT	O3'	51:DC	P	4.24
1	8	22:DA	O3'	23:DT	P	3.80
1	2	22:DA	O3'	23:DT	P	3.79
1	5	22:DA	O3'	23:DT	P	3.79

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	230/242 (95%)	-0.14	3 (1%) 77 71	153, 175, 210, 235	0
1	B	228/242 (94%)	-0.18	2 (0%) 84 79	162, 194, 217, 238	0
1	G	230/242 (95%)	0.04	6 (2%) 56 52	157, 185, 217, 248	0
1	H	228/242 (94%)	-0.14	2 (0%) 84 79	160, 191, 229, 261	0
1	M	230/242 (95%)	0.05	3 (1%) 77 71	166, 200, 233, 252	0
1	N	228/242 (94%)	0.25	9 (3%) 40 38	186, 233, 258, 273	0
2	C	1341/1342 (99%)	-0.10	12 (0%) 84 79	119, 186, 244, 277	0
2	I	1341/1342 (99%)	-0.10	20 (1%) 74 68	130, 195, 278, 377	0
2	O	1341/1342 (99%)	-0.10	13 (0%) 82 77	144, 183, 235, 270	0
3	D	1362/1407 (96%)	0.16	92 (6%) 18 21	128, 214, 296, 349	0
3	J	1362/1407 (96%)	0.08	56 (4%) 38 35	132, 194, 280, 314	0
3	P	1362/1407 (96%)	0.29	119 (8%) 11 15	148, 208, 292, 330	0
4	E	90/90 (100%)	1.11	28 (31%) 0 4	169, 206, 407, 461	0
4	K	90/90 (100%)	0.42	12 (13%) 4 8	144, 199, 394, 442	0
4	Q	90/90 (100%)	0.67	12 (13%) 4 8	167, 222, 416, 460	0
5	F	497/628 (79%)	0.37	61 (12%) 5 10	182, 294, 404, 418	0
5	L	497/628 (79%)	0.32	57 (11%) 5 10	169, 262, 400, 406	0
5	R	497/628 (79%)	0.25	44 (8%) 10 14	172, 259, 413, 444	0
6	1	49/49 (100%)	0.36	5 (10%) 7 12	201, 272, 311, 317	0
6	4	49/49 (100%)	0.16	3 (6%) 22 23	209, 264, 308, 350	0
6	7	49/49 (100%)	0.22	2 (4%) 38 35	211, 255, 278, 300	0
7	2	49/49 (100%)	0.24	2 (4%) 38 35	215, 278, 312, 343	0
7	5	49/49 (100%)	0.41	4 (8%) 12 16	198, 270, 339, 341	0
7	8	49/49 (100%)	0.22	0 100 100	195, 260, 296, 335	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
8	3	3/4 (75%)	0.55	0	100	100	255, 255, 281, 321	0
8	6	3/4 (75%)	0.39	0	100	100	263, 263, 272, 282	0
8	9	3/4 (75%)	0.74	0	100	100	262, 262, 277, 295	0
All	All	11547/12159 (94%)	0.09	567 (4%)	30	31	119, 203, 358, 461	0

The worst 5 of 567 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	L	210	ASN	8.7
3	P	1068	THR	8.4
3	P	1006	GLY	8.1
5	L	211	SER	8.0
3	D	961	SER	6.9

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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(Å ²)	Q<0.9
9	ZN	P	1502	1/1	0.98	0.17	-0.01	187,187,187,187	0
9	ZN	J	1501	1/1	0.88	0.15	-0.87	200,200,200,200	0
9	ZN	D	1502	1/1	0.94	0.11	-0.98	212,212,212,212	0
9	ZN	J	1502	1/1	0.98	0.12	-1.02	174,174,174,174	0
10	MG	D	1503	1/1	0.95	0.16	-1.22	176,176,176,176	0
9	ZN	D	1501	1/1	0.97	0.09	-1.41	228,228,228,228	0
9	ZN	P	1501	1/1	0.95	0.10	-2.02	214,214,214,214	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
10	MG	P	1503	1/1	0.91	0.15	-2.25	194,194,194,194	0
10	MG	6	101	1/1	0.88	0.34	-	189,189,189,189	0

6.5 Other polymers [i](#)

There are no such residues in this entry.