



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:41 AM UTC

PDB ID : 4YLO / pdb_00004ylo
Title : E. coli Transcription Initiation Complex - 16-bp spacer and 4-nt RNA
Authors : Zuo, Y.; Steitz, T.A.
Deposited on : 2015-03-05
Resolution : 6.00 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

<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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

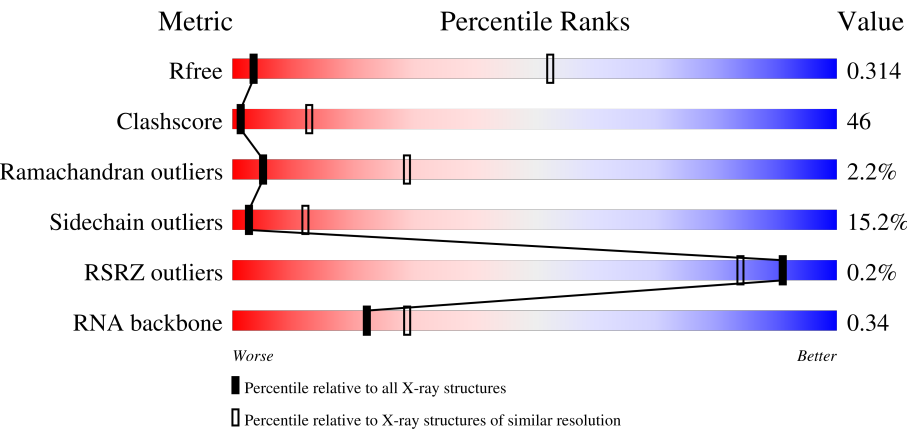
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.00 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))
R _{free}	180053	1143 (8.00-4.00)
Clashscore	190562	1210 (8.00-4.00)
Ramachandran outliers	187476	1034 (8.00-4.00)
Sidechain outliers	187428	1000 (8.00-4.00)
RSRZ outliers	180081	1136 (8.00-4.00)
RNA backbone	3983	1054 (8.70-3.10)

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 $\leq 5\%$. 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	45% 39% 10% • 5%
1	B	242	38% 45% 10% • 6%
1	G	242	39% 48% 7% • 5%
1	H	242	43% 43% 7% • 6%

Continued on next page...

Continued from previous page...

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
10	ZN	D	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

Continued on next page...

Continued from previous page...

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			

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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').

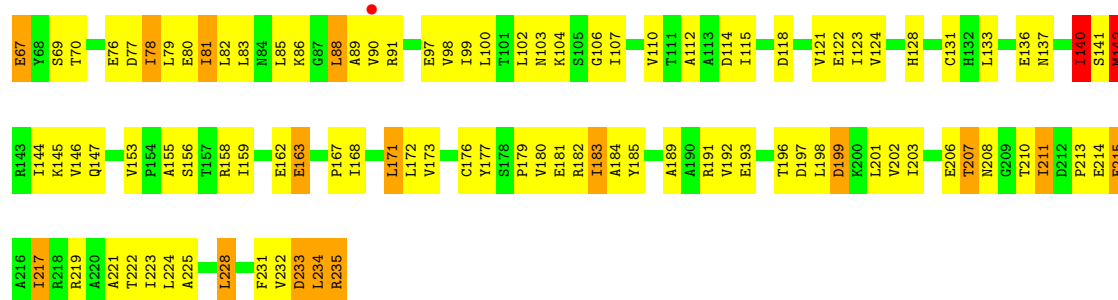
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	3	4	Total	C	N	O	P	0	0	0
			97	39	17	35	6			
8	6	4	Total	C	N	O	P	0	0	0
			97	39	17	35	6			
8	9	4	Total	C	N	O	P	0	0	0
			97	39	17	35	6			

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	1	Total	Mg	0	0
			1	1		
9	J	1	Total	Mg	0	0
			1	1		
9	P	1	Total	Mg	0	0
			1	1		

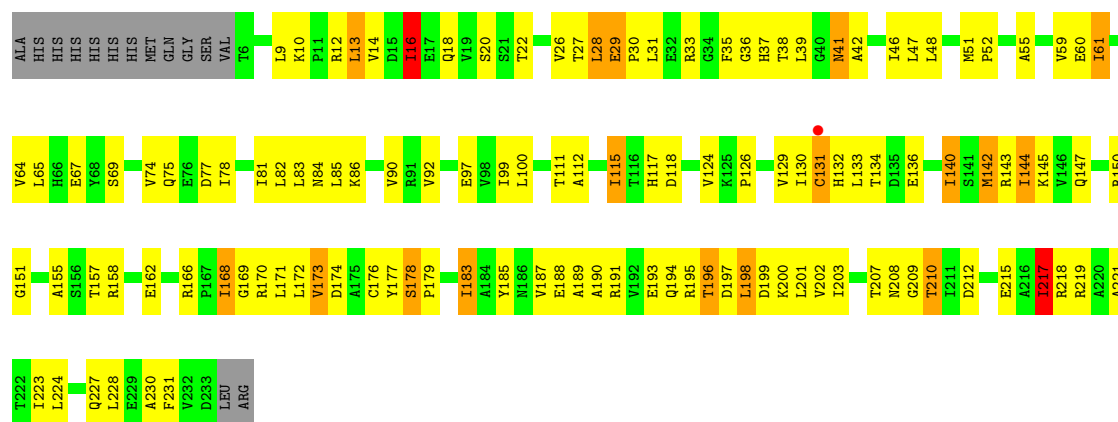
- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

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



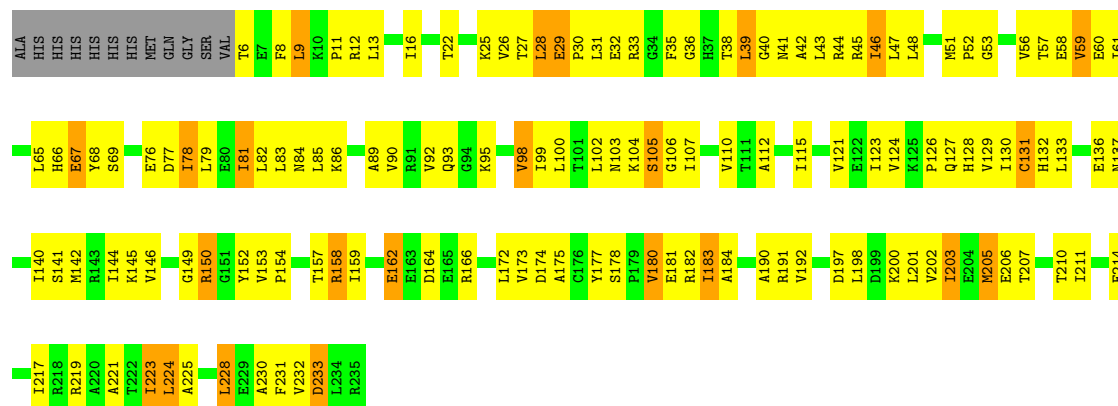
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain H: 43% 43% 7% 6%



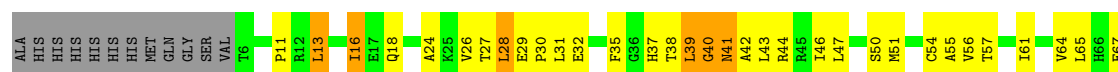
• Molecule 1: DNA-directed RNA polymerase subunit alpha

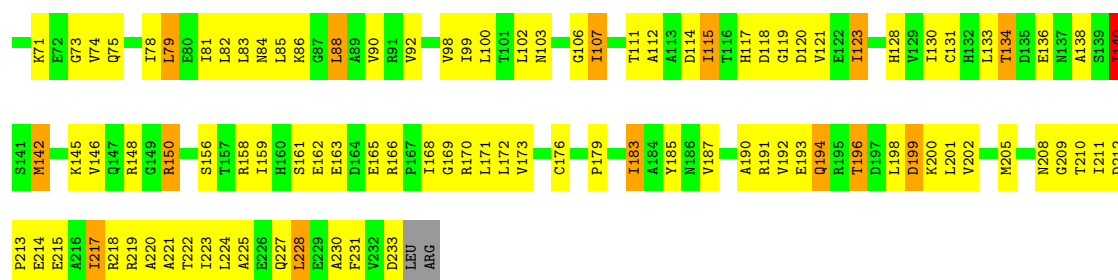
Chain M: 38% 48% 10% 5%



• Molecule 1: DNA-directed RNA polymerase subunit alpha

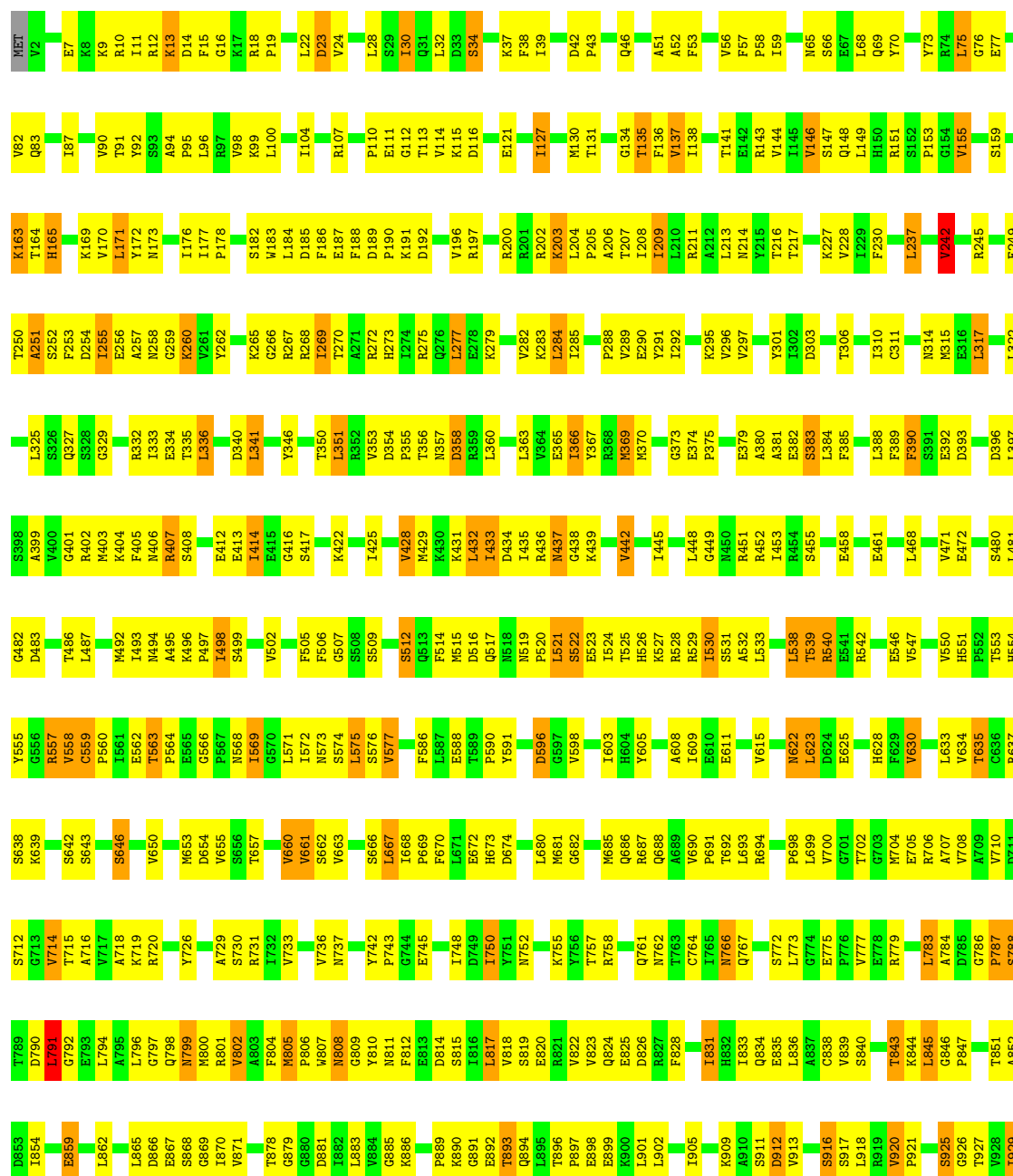
Chain N: 40% 45% 8% 6%

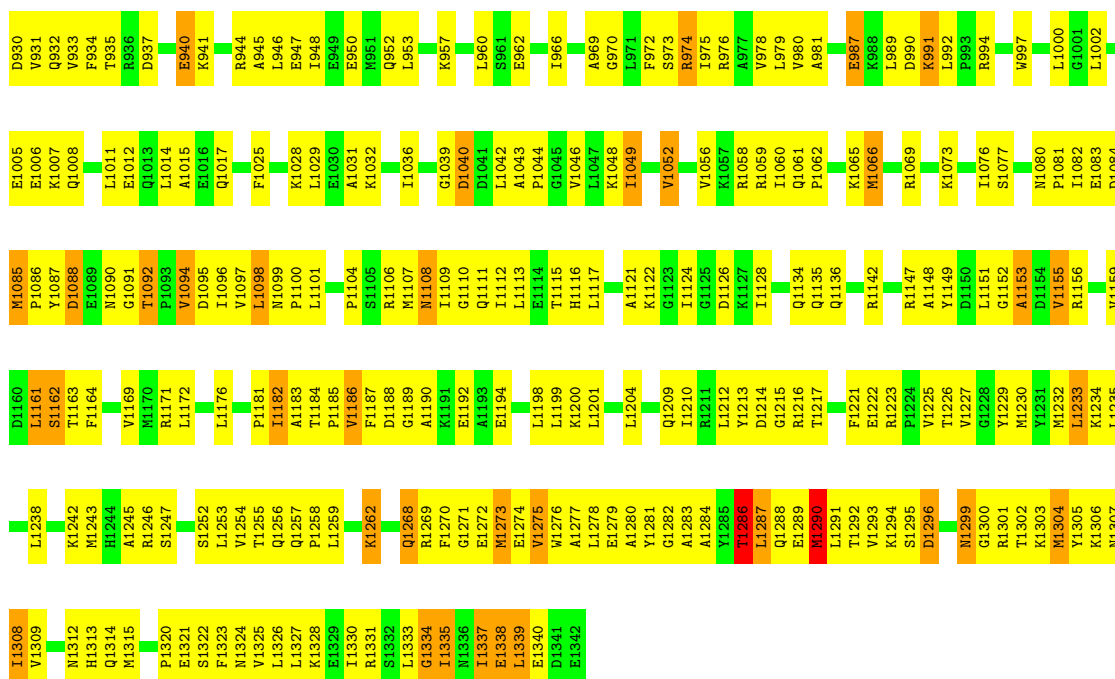




• Molecule 2: DNA-directed RNA polymerase subunit beta

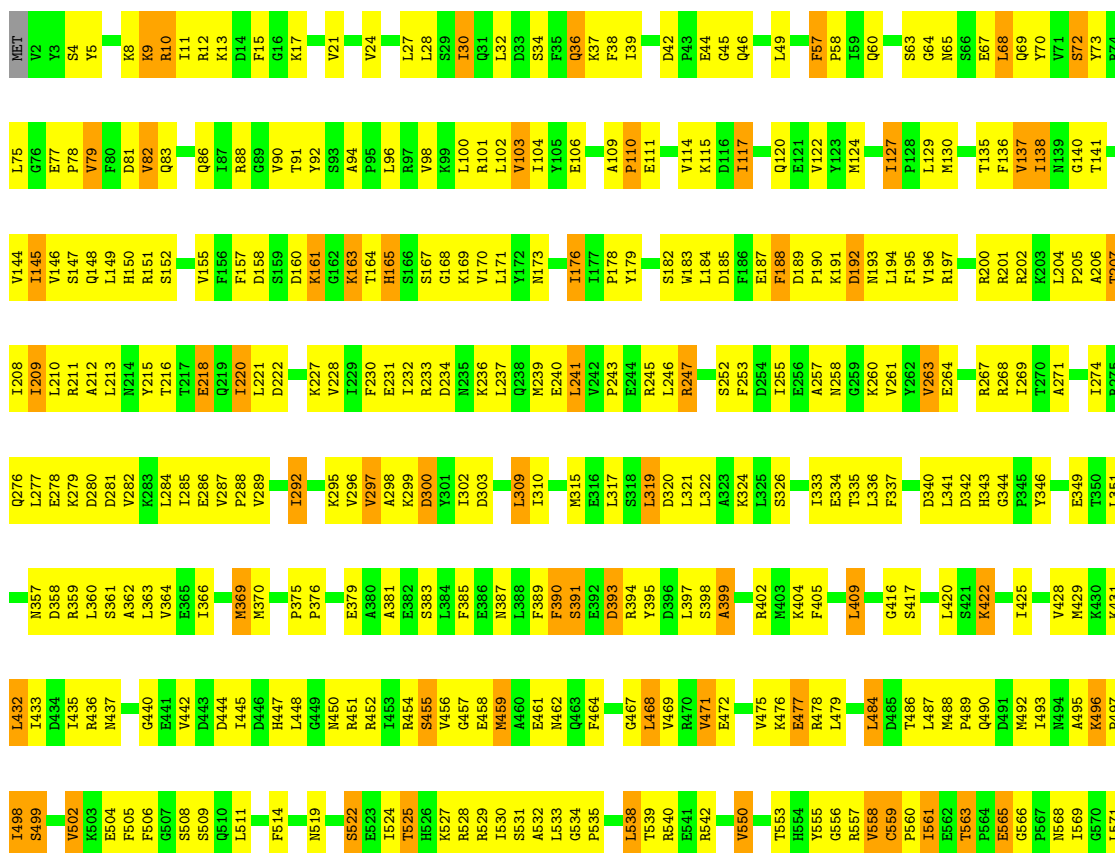
Chain C: 43% 48% 9%

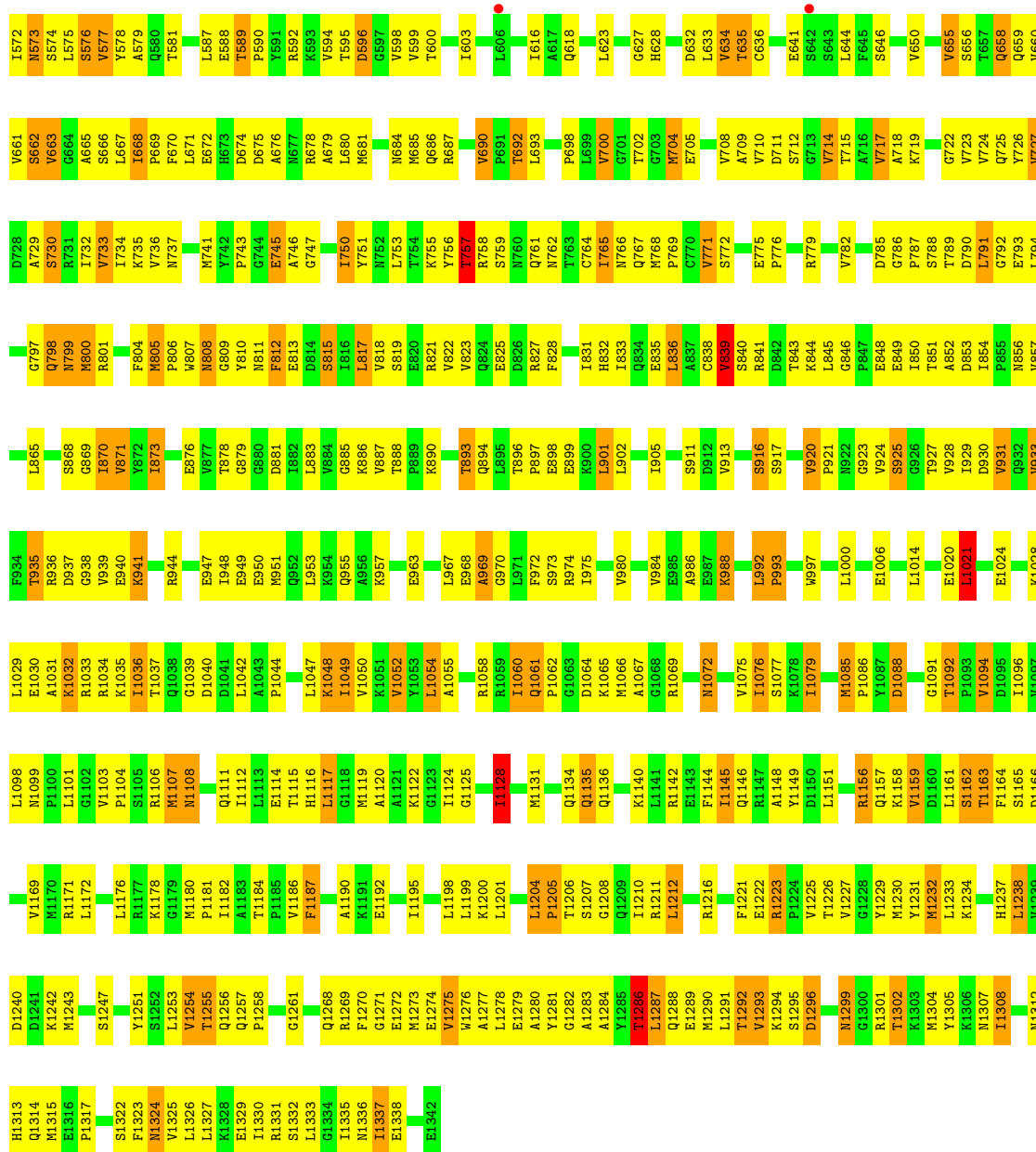




• Molecule 2: DNA-directed RNA polymerase subunit beta

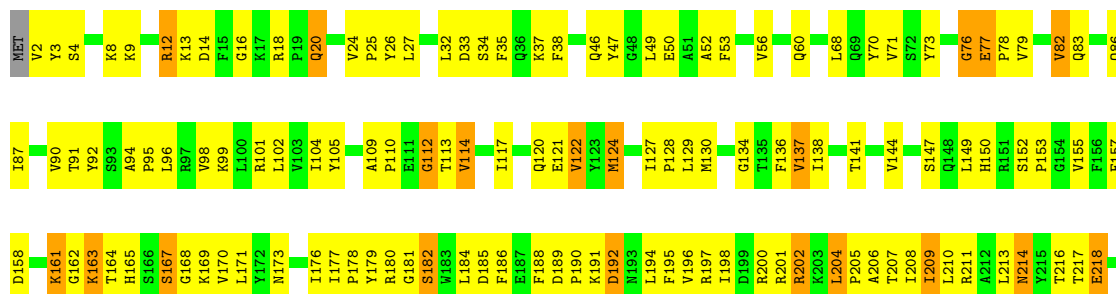
Chain I: 41% 47% 12%





● Molecule 2: DNA-directed RNA polymerase subunit beta

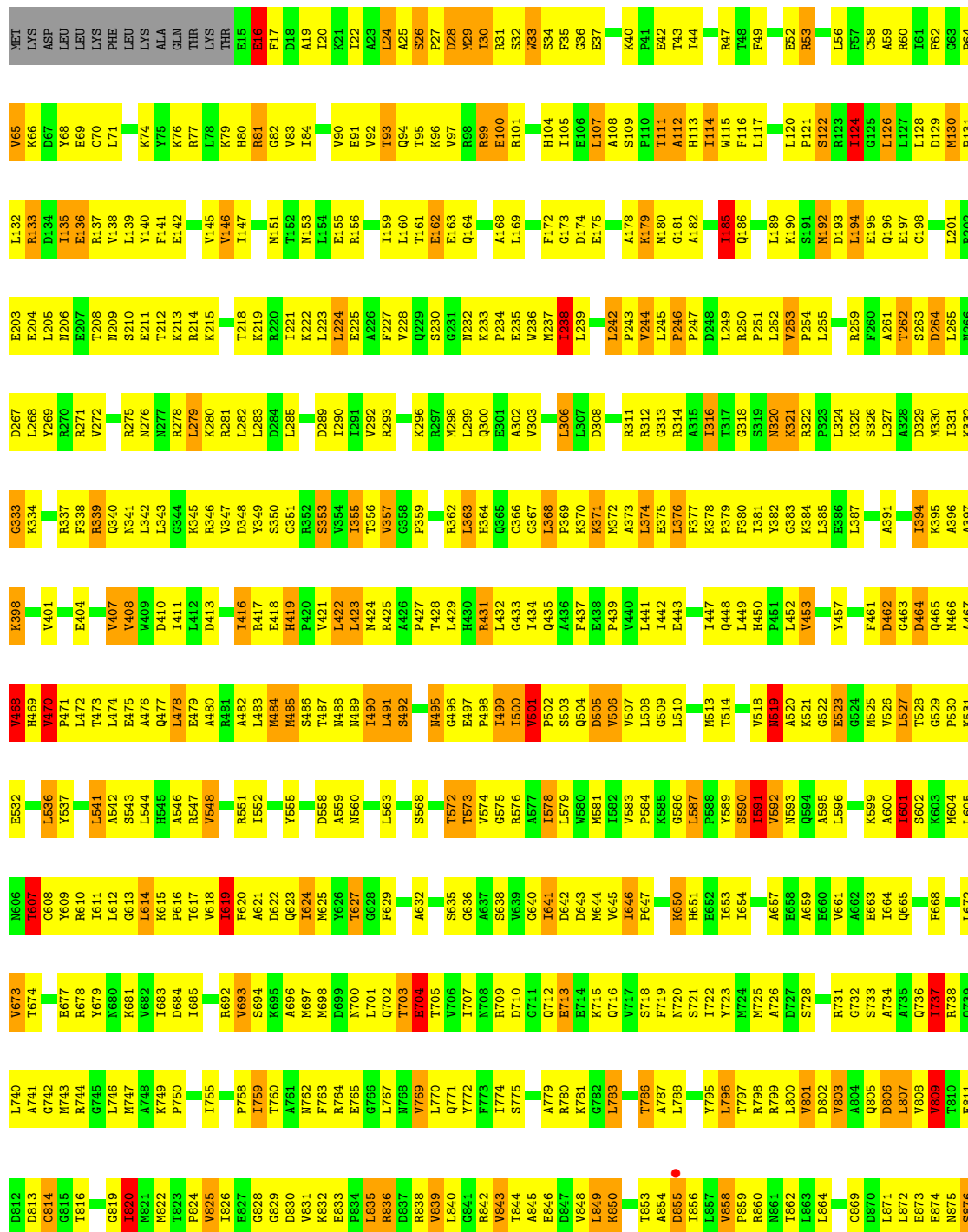
Chain O: 41% 49% 10%

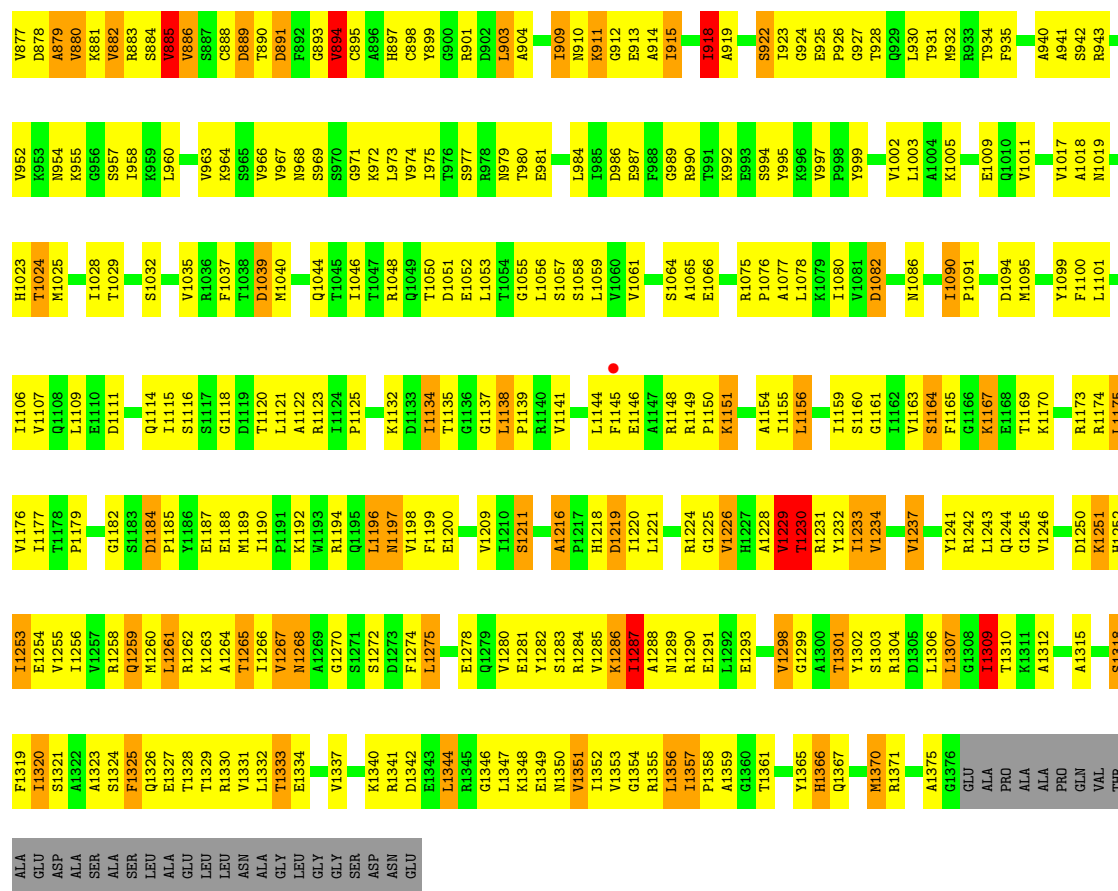




● Molecule 3: DNA-directed RNA polymerase subunit beta'

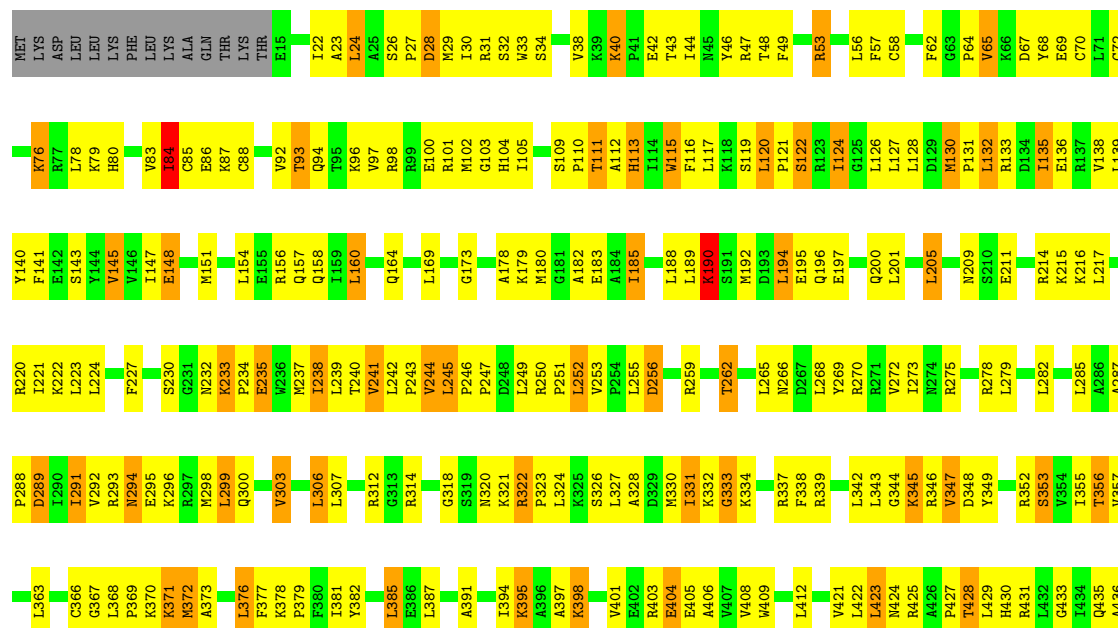
Chain D: 34% 50% 12% ..

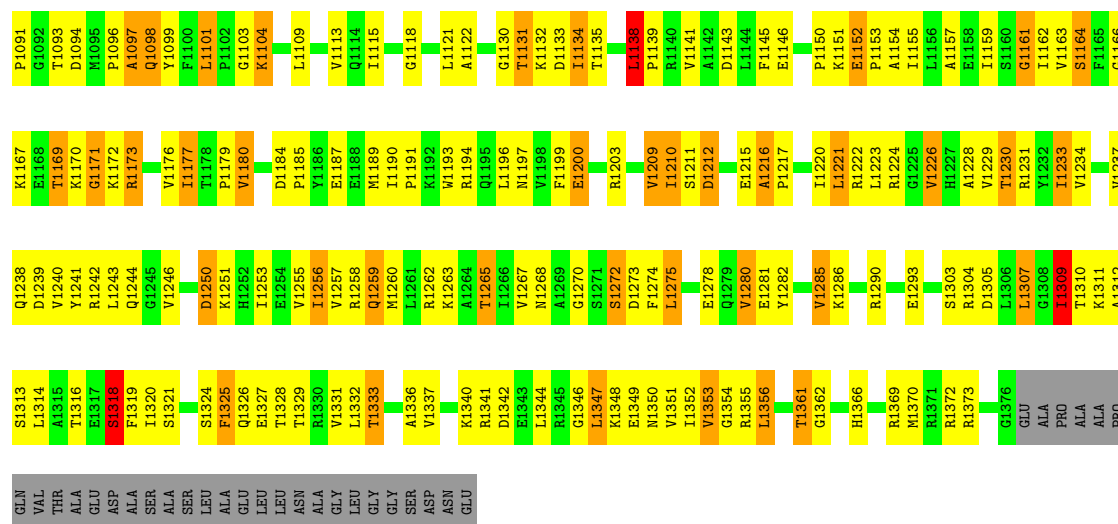




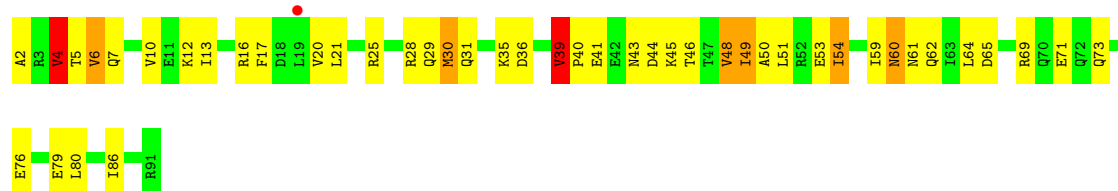
• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain J: 38% 47% 11% . .

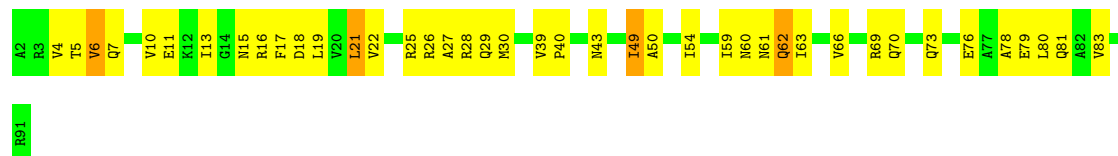




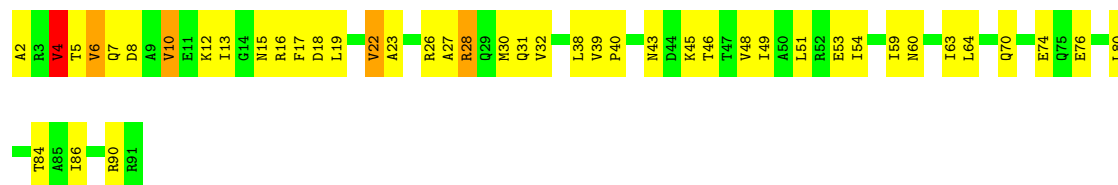
• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 4: DNA-directed RNA polymerase subunit omega

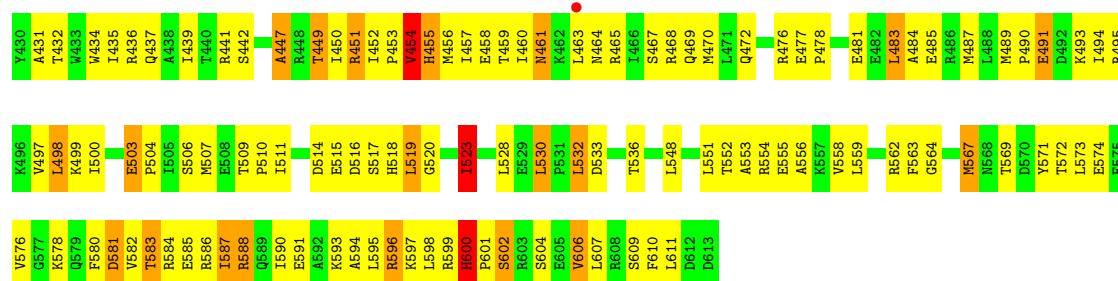


• Molecule 4: DNA-directed RNA polymerase subunit omega



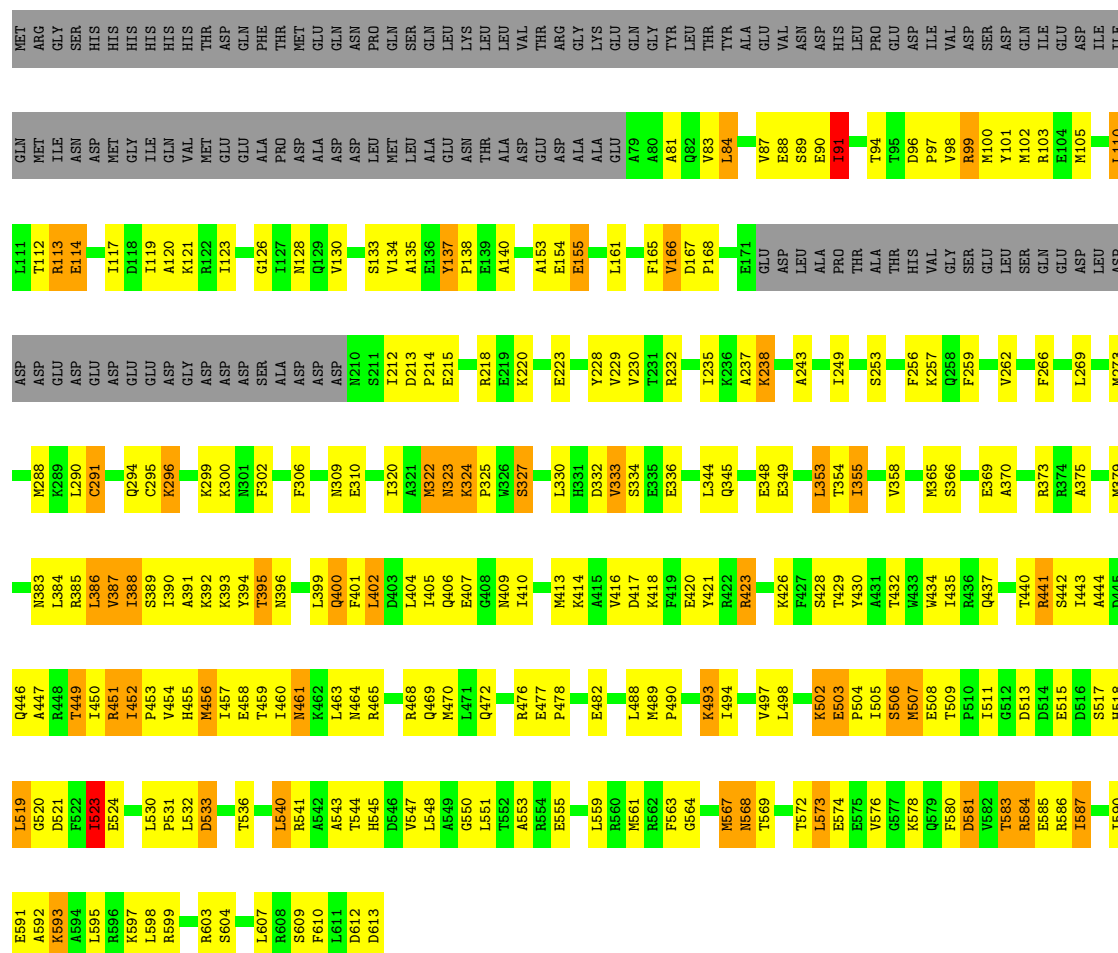
• Molecule 5: RNA polymerase sigma factor RpoD





• Molecule 5: RNA polymerase sigma factor RpoD

Chain R: 39% 32% 7% 21%

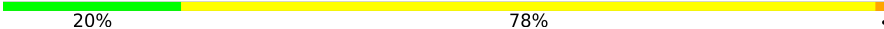


• Molecule 6: NT strand DNA (49-MER)

Chain 1: 24% 76%

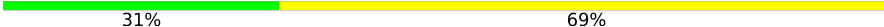


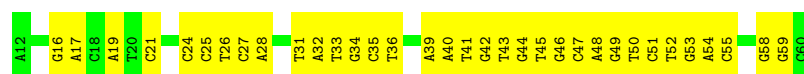
• Molecule 6: NT strand DNA (49-MER)

Chain 4:  20% 78% .

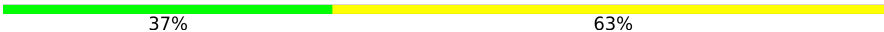


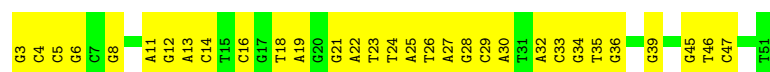
- Molecule 6: NT strand DNA (49-MER)

Chain 7:  31% 69%



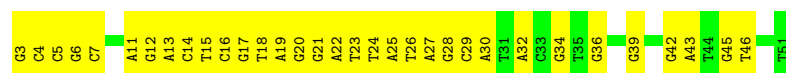
- Molecule 7: T strand DNA (49-MER)

Chain 2:  37% 63%



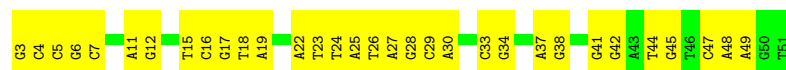
- Molecule 7: T strand DNA (49-MER)

Chain 5:  33% 67%



- Molecule 7: T strand DNA (49-MER)

Chain 8:  35% 65%



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

Chain 3:  50% 50%



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

Chain 6:  50% 50%



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

Chain 9:  25% 75%

G13
A14
G15
U16

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	240.89Å 208.17Å 256.32Å 90.00° 119.31° 90.00°	Depositor
Resolution (Å)	39.95 – 6.00 39.95 – 6.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.95-6.00) 99.6 (39.95-6.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 6.13Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.227 , 0.314 0.227 , 0.314	Depositor DCC
R_{free} test set	2938 reflections (5.31%)	wwPDB-VP
Wilson B-factor (Å ²)	343.5	Xtriage
Anisotropy	0.527	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 229.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	94608	wwPDB-VP
Average B, all atoms (Å ²)	238.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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, MG, ZN

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	0.84	0/1809	1.27	11/2450 (0.4%)
1	B	0.82	0/1789	1.31	9/2425 (0.4%)
1	G	0.84	1/1809 (0.1%)	1.24	3/2450 (0.1%)
1	H	0.82	0/1789	1.26	10/2425 (0.4%)
1	M	0.89	0/1809	1.27	7/2450 (0.3%)
1	N	0.87	0/1789	1.33	7/2425 (0.3%)
2	C	0.77	1/10745 (0.0%)	1.17	49/14499 (0.3%)
2	I	0.81	5/10745 (0.0%)	1.20	56/14499 (0.4%)
2	O	0.82	3/10745 (0.0%)	1.20	48/14499 (0.3%)
3	D	0.91	10/10729 (0.1%)	1.28	76/14487 (0.5%)
3	J	0.89	7/10729 (0.1%)	1.23	61/14487 (0.4%)
3	P	0.82	4/10729 (0.0%)	1.17	47/14487 (0.3%)
4	E	0.86	0/710	1.26	4/956 (0.4%)
4	K	0.72	0/710	1.06	0/956
4	Q	0.76	0/710	1.08	0/956
5	F	0.75	2/4076 (0.0%)	1.14	17/5482 (0.3%)
5	L	0.82	1/4076 (0.0%)	1.13	13/5482 (0.2%)
5	R	0.76	0/4076	1.11	13/5482 (0.2%)
6	1	0.38	0/1112	0.68	0/1706
6	4	0.45	1/1114 (0.1%)	0.72	0/1714
6	7	0.38	0/1115	0.70	0/1718
7	2	0.37	0/1136	0.63	0/1752
7	5	0.38	0/1137	0.68	0/1756
7	8	0.35	0/1137	0.62	0/1756
8	3	0.45	0/72	0.76	0/110
8	6	0.53	0/72	0.89	0/110
8	9	0.54	0/72	0.93	1/110 (0.9%)
All	All	0.81	35/96541 (0.0%)	1.17	432/131629 (0.3%)

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	J	0	1
3	P	0	1
All	All	0	2

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	943	ARG	CZ-NH1	11.29	1.48	1.32
3	D	431	ARG	CZ-NH1	10.94	1.48	1.32
3	D	484	MET	SD-CE	9.46	2.03	1.79
2	O	316	GLU	CD-OE2	7.77	1.40	1.25
2	I	565	GLU	CB-CG	6.47	1.71	1.52

The worst 5 of 432 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	359	LYS	CG-CD-CE	-11.40	85.08	111.30
2	O	1188	ASP	N-CA-C	-10.56	97.77	110.44
3	J	704	GLU	N-CA-C	10.34	123.94	111.02
3	D	185	ILE	CB-CA-C	-10.19	98.92	111.97
3	P	646	ILE	CA-C-N	10.15	132.53	119.84

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	J	943	ARG	Sidechain
3	P	210	SER	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	190	0
1	B	1767	0	1789	201	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1787	0	1813	183	0
1	H	1767	0	1789	145	0
1	M	1787	0	1813	264	0
1	N	1767	0	1789	215	0
2	C	10576	0	10591	961	0
2	I	10576	0	10591	1010	0
2	O	10576	0	10591	1030	1
3	D	10568	0	10781	1394	1
3	J	10568	0	10782	1204	0
3	P	10568	0	10780	1060	1
4	E	708	0	719	66	0
4	K	708	0	719	42	0
4	Q	708	0	719	45	0
5	F	4022	0	4083	377	1
5	L	4022	0	4083	373	0
5	R	4022	0	4083	354	0
6	1	996	0	557	71	0
6	4	996	0	555	103	1
6	7	996	0	554	70	0
7	2	1012	0	554	66	0
7	5	1012	0	553	62	0
7	8	1012	0	553	66	0
8	3	97	0	44	23	0
8	6	97	0	44	6	0
8	9	97	0	44	20	0
9	C	1	0	0	0	0
9	J	1	0	0	0	0
9	P	1	0	0	0	0
10	D	2	0	0	2	0
10	J	2	0	0	2	0
10	P	2	0	0	1	0
All	All	94608	0	92786	8533	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 46.

The worst 5 of 8533 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)
5:F:359:LYS:NZ	5:F:359:LYS:CE	1.67	1.54
3:D:484:MET:CE	3:D:484:MET:SD	2.03	1.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:139:LEU:CD2	3:P:185:ILE:HD11	1.49	1.43
3:J:367:GLY:O	3:J:447:ILE:CG2	1.68	1.38
1:G:25:LYS:NZ	1:G:202:VAL:HG11	1.34	1.37

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)
6:4:12:DA:O5'	6:4:60:DC:O5'[2_454]	1.86	0.34
5:F:482:GLU:OE2	2:O:275:ARG:NH2[2_455]	1.99	0.21
3:D:1282:TYR:OH	3:P:710:ASP:OD2[1_655]	2.08	0.12

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%)	210 (92%)	15 (7%)	3 (1%)	9	42
1	B	226/242 (93%)	207 (92%)	13 (6%)	6 (3%)	4	25
1	G	228/242 (94%)	211 (92%)	14 (6%)	3 (1%)	9	42
1	H	226/242 (93%)	207 (92%)	17 (8%)	2 (1%)	14	50
1	M	228/242 (94%)	209 (92%)	16 (7%)	3 (1%)	9	42
1	N	226/242 (93%)	207 (92%)	14 (6%)	5 (2%)	5	29
2	C	1339/1342 (100%)	1218 (91%)	98 (7%)	23 (2%)	7	36
2	I	1339/1342 (100%)	1210 (90%)	102 (8%)	27 (2%)	6	31
2	O	1339/1342 (100%)	1222 (91%)	87 (6%)	30 (2%)	5	29
3	D	1360/1407 (97%)	1210 (89%)	122 (9%)	28 (2%)	5	29
3	J	1360/1407 (97%)	1225 (90%)	110 (8%)	25 (2%)	6	34
3	P	1360/1407 (97%)	1208 (89%)	112 (8%)	40 (3%)	3	23

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	88/90 (98%)	82 (93%)	5 (6%)	1 (1%)	11	46
4	K	88/90 (98%)	83 (94%)	4 (4%)	1 (1%)	11	46
4	Q	88/90 (98%)	81 (92%)	6 (7%)	1 (1%)	11	46
5	F	493/628 (78%)	443 (90%)	34 (7%)	16 (3%)	3	21
5	L	493/628 (78%)	441 (90%)	36 (7%)	16 (3%)	3	21
5	R	493/628 (78%)	441 (90%)	36 (7%)	16 (3%)	3	21
All	All	11202/11853 (94%)	10115 (90%)	841 (8%)	246 (2%)	5	29

5 of 246 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	GLY
1	A	210	THR
2	C	113	THR
2	C	481	LEU
2	C	791	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	198/208 (95%)	163 (82%)	35 (18%)	2	9
1	B	196/208 (94%)	161 (82%)	35 (18%)	2	9
1	G	198/208 (95%)	164 (83%)	34 (17%)	2	10
1	H	196/208 (94%)	164 (84%)	32 (16%)	2	10
1	M	198/208 (95%)	166 (84%)	32 (16%)	2	11
1	N	196/208 (94%)	167 (85%)	29 (15%)	3	13
2	C	1156/1157 (100%)	988 (86%)	168 (14%)	3	13
2	I	1156/1157 (100%)	986 (85%)	170 (15%)	3	13
2	O	1156/1157 (100%)	1000 (86%)	156 (14%)	4	14
3	D	1135/1168 (97%)	934 (82%)	201 (18%)	2	9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	J	1135/1168 (97%)	948 (84%)	187 (16%)	2	10
3	P	1135/1168 (97%)	965 (85%)	170 (15%)	3	12
4	E	74/74 (100%)	59 (80%)	15 (20%)	1	7
4	K	74/74 (100%)	68 (92%)	6 (8%)	11	31
4	Q	74/74 (100%)	64 (86%)	10 (14%)	4	14
5	F	439/554 (79%)	383 (87%)	56 (13%)	4	15
5	L	439/554 (79%)	375 (85%)	64 (15%)	3	13
5	R	439/554 (79%)	385 (88%)	54 (12%)	4	17
All	All	9594/10107 (95%)	8140 (85%)	1454 (15%)	3	12

5 of 1454 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	1353	VAL
2	O	662	SER
5	L	166	VAL
3	J	1333	THR
1	N	61	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 185 such sidechains are listed below:

Mol	Chain	Res	Type
4	K	60	ASN
2	O	752	ASN
5	L	383	ASN
2	O	20	GLN
2	O	1116	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	3	3/4 (75%)	1 (33%)	1 (33%)
8	6	3/4 (75%)	1 (33%)	1 (33%)
8	9	3/4 (75%)	1 (33%)	1 (33%)
All	All	9/12 (75%)	3 (33%)	3 (33%)

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 (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	3	13	GTP
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 oligosaccharides 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
6	1	3
6	4	1
7	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4	51:DC	O3'	52:DT	P	3.86
1	1	51:DC	O3'	52:DT	P	3.85
1	1	46:DG	O3'	47:DC	P	3.49
1	2	12:DG	O3'	13:DA	P	2.97
1	1	36:DT	O3'	37:DA	P	2.64

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%)	-0.84	0 100 100	162, 207, 238, 299	0
1	B	228/242 (94%)	-0.76	1 (0%) 88 79	165, 211, 254, 284	0
1	G	230/242 (95%)	-0.79	1 (0%) 88 79	175, 216, 259, 292	0
1	H	228/242 (94%)	-0.73	1 (0%) 88 79	200, 264, 307, 325	0
1	M	230/242 (95%)	-0.78	0 100 100	155, 186, 230, 311	0
1	N	228/242 (94%)	-0.82	0 100 100	162, 205, 248, 280	0
2	C	1341/1342 (99%)	-0.86	0 100 100	126, 243, 333, 427	0
2	I	1341/1342 (99%)	-0.82	2 (0%) 92 87	142, 196, 276, 345	0
2	O	1341/1342 (99%)	-0.82	3 (0%) 91 84	126, 202, 287, 327	0
3	D	1362/1407 (96%)	-0.82	2 (0%) 92 87	129, 204, 384, 437	0
3	J	1362/1407 (96%)	-0.74	1 (0%) 92 87	145, 213, 344, 397	0
3	P	1362/1407 (96%)	-0.85	3 (0%) 91 84	133, 223, 391, 441	0
4	E	90/90 (100%)	-0.78	1 (1%) 78 66	138, 184, 398, 452	0
4	K	90/90 (100%)	-0.81	0 100 100	165, 213, 389, 436	0
4	Q	90/90 (100%)	-0.91	0 100 100	157, 202, 400, 463	0
5	F	497/628 (79%)	-0.75	4 (0%) 82 72	176, 304, 513, 589	0
5	L	497/628 (79%)	-0.79	1 (0%) 91 84	171, 277, 369, 399	0
5	R	497/628 (79%)	-0.78	0 100 100	170, 322, 414, 449	0
6	1	49/49 (100%)	-0.59	0 100 100	206, 263, 311, 333	0
6	4	49/49 (100%)	-0.53	0 100 100	50, 261, 289, 312	0
6	7	49/49 (100%)	-0.53	0 100 100	214, 295, 334, 336	0
7	2	49/49 (100%)	-0.57	0 100 100	183, 272, 334, 388	0
7	5	49/49 (100%)	-0.53	0 100 100	172, 257, 298, 371	0
7	8	49/49 (100%)	-0.47	0 100 100	228, 300, 347, 427	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
8	3	3/4 (75%)	-0.88	0 100 100	310, 310, 316, 331	0
8	6	3/4 (75%)	-0.94	0 100 100	242, 242, 251, 272	0
8	9	3/4 (75%)	-0.57	0 100 100	257, 257, 296, 373	0
All	All	11547/12159 (94%)	-0.80	20 (0%) 91 84	50, 219, 383, 589	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	1145	PHE	4.5
3	J	1145	PHE	3.4
3	P	285	LEU	3.1
2	O	492	MET	3.0
3	P	773	PHE	2.5

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 oligosaccharides 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. 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(Å ²)	Q<0.9
9	MG	C	1401	1/1	0.97	0.14	218,218,218,218	0
10	ZN	J	1501	1/1	0.97	0.04	218,218,218,218	0
10	ZN	D	1501	1/1	0.98	0.04	215,215,215,215	0
9	MG	J	1503	1/1	1.00	0.02	204,204,204,204	0
10	ZN	D	1502	1/1	1.00	0.05	172,172,172,172	0
9	MG	P	1503	1/1	1.00	0.01	187,187,187,187	0
10	ZN	J	1502	1/1	1.00	0.02	196,196,196,196	0
10	ZN	P	1501	1/1	1.00	0.01	252,252,252,252	0
10	ZN	P	1502	1/1	1.00	0.01	204,204,204,204	0

6.5 Other polymers [i](#)

There are no such residues in this entry.