wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 12:25 AM GMT

PDB ID	:	2A6E
Title	:	Crystal structure of the T. Thermophilus RNA polymerase holoenzyme
Authors	:	Artsimovitch, I.; Vassylyeva, M.N.; Svetlov, D.; Svetlov, V.; Perederina, A.; Igarashi, N.; Matsugaki, N.; Wakatsuki, S.; Tahirov, T.H.; Vassylyev, D.G.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2005-07-02
Resolution	:	2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

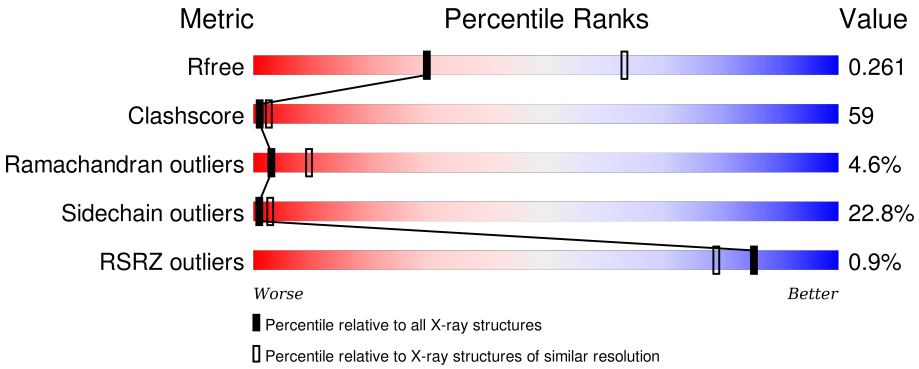
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 <=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	315	17% 40% 16% 27%
1	B	315	3% 17% 45% 11% 27%
1	K	315	14% 47% 11% 27%
1	L	315	% 18% 44% 10% 27%
2	C	1119	% 22% 60% 17%

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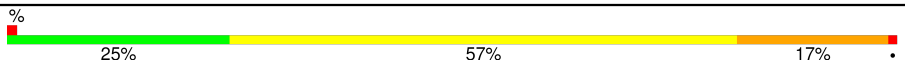
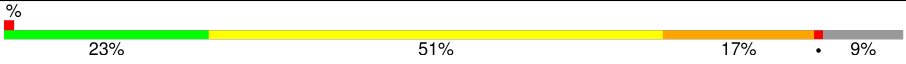
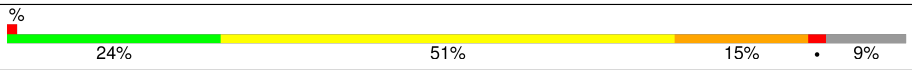
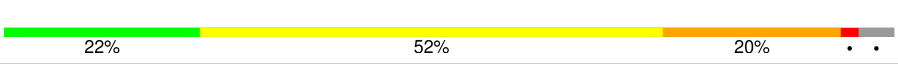
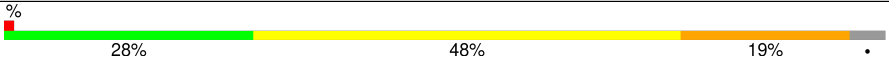
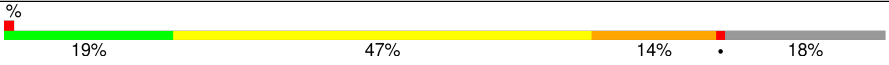
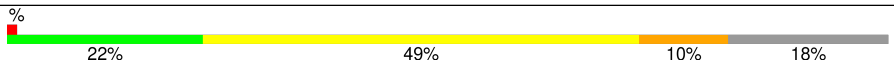
Mol	Chain	Length	Quality of chain
2	M	1119	
3	D	1524	
3	N	1524	
4	E	99	
4	O	99	
5	F	423	
5	P	423	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 58679 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 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	B	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	K	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	L	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	24			
2	M	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1392	Total	C	N	O	S	0	0	0
			10797	6819	1925	2020	33			
3	N	1392	Total	C	N	O	S	0	0	0
			10797	6819	1925	2020	33			

- Molecule 4 is a protein called RNA polymerase omega chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	95	Total	C	N	O	S	0	0	0
			769	488	133	144	4			
4	O	95	Total	C	N	O	S	0	0	0
			769	488	133	144	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	345	Total	C	N	O	S	0	0	0
			2771	1744	504	519	4			
5	P	345	Total	C	N	O	S	0	0	0
			2771	1744	504	519	4			

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	2	Total	Zn	0	0
			2	2		
6	N	2	Total	Zn	0	0
			2	2		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	Mg	0	0
			1	1		
7	N	1	Total	Mg	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	191	Total	O	0	0
			191	191		
8	B	181	Total	O	0	0
			181	181		
8	C	767	Total	O	0	0
			767	767		
8	D	1100	Total	O	0	0
			1100	1100		
8	E	93	Total	O	0	0
			93	93		
8	F	333	Total	O	0	0
			333	333		
8	K	151	Total	O	0	0
			151	151		
8	L	179	Total	O	0	0
			179	179		
8	M	739	Total	O	0	0
			739	739		

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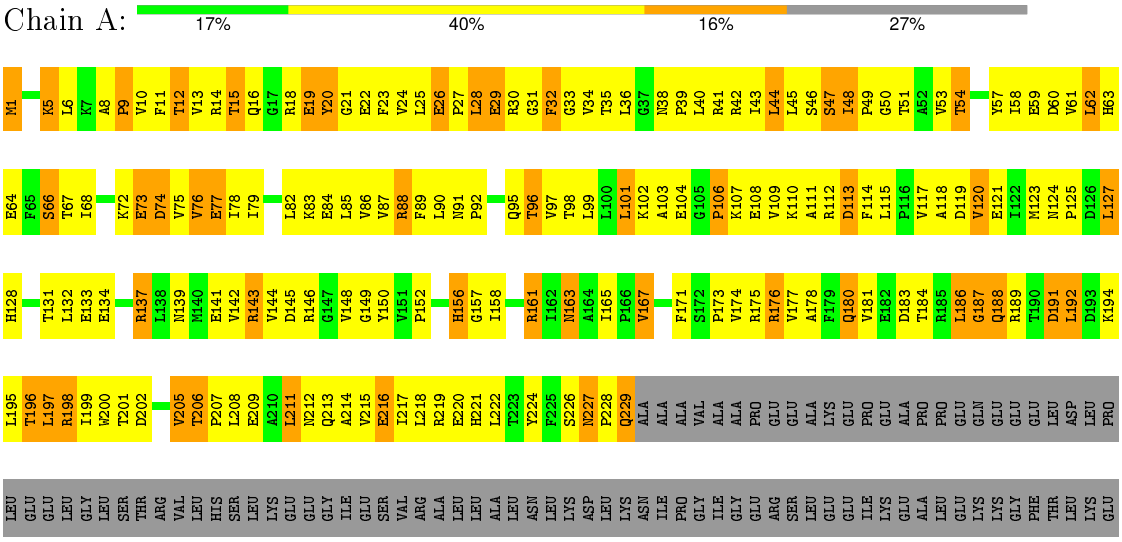
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	N	1038	Total O 1038 1038	0	0
8	O	78	Total O 78 78	0	0
8	P	267	Total O 267 267	0	0

3 Residue-property plots (i)

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.

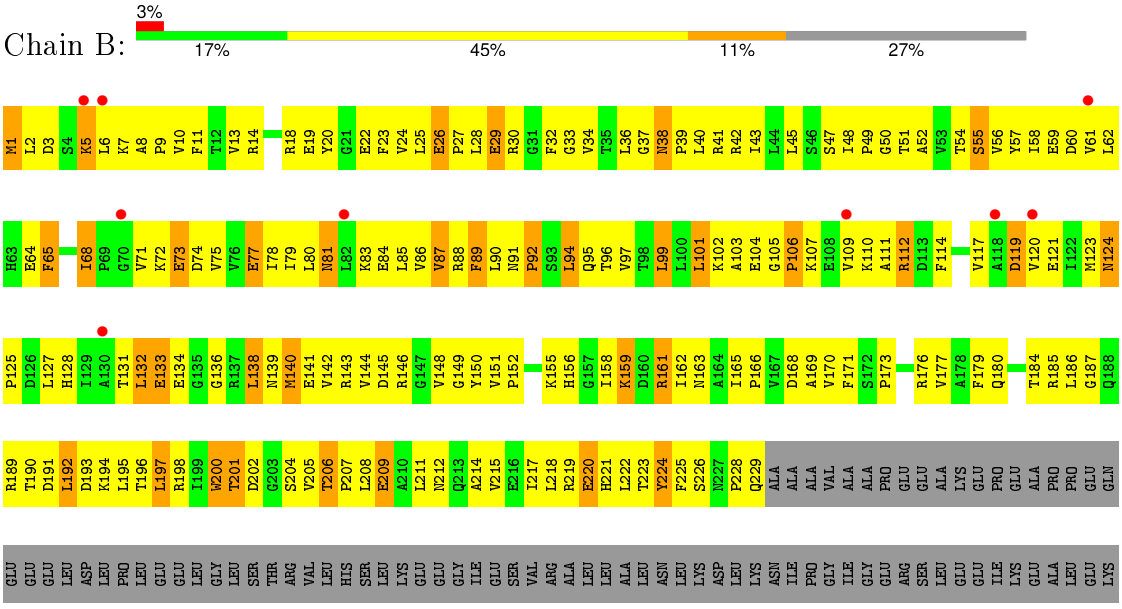
- Molecule 1: DNA-directed RNA polymerase alpha chain

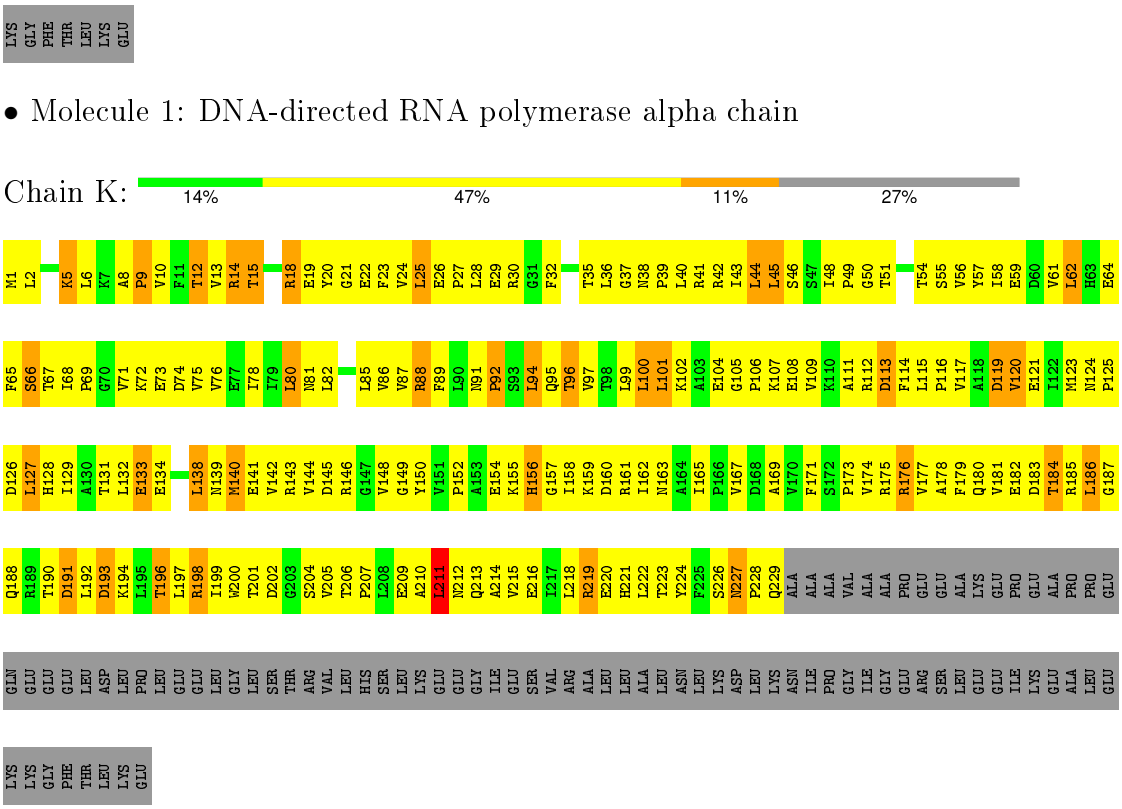
Chain A:



- Molecule 1: DNA-directed RNA polymerase alpha chain

Chain B:



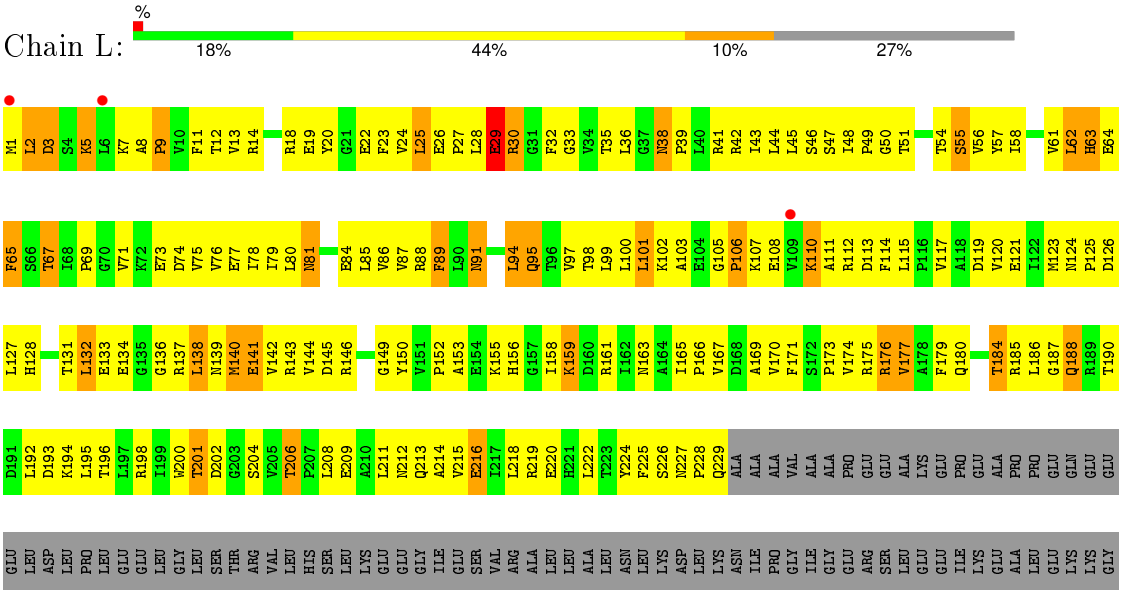


• Molecule 1: DNA-directed RNA polymerase alpha chain

Chain K:

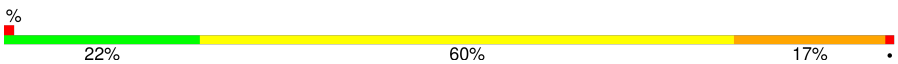
• Molecule 1: DNA-directed RNA polymerase alpha chain

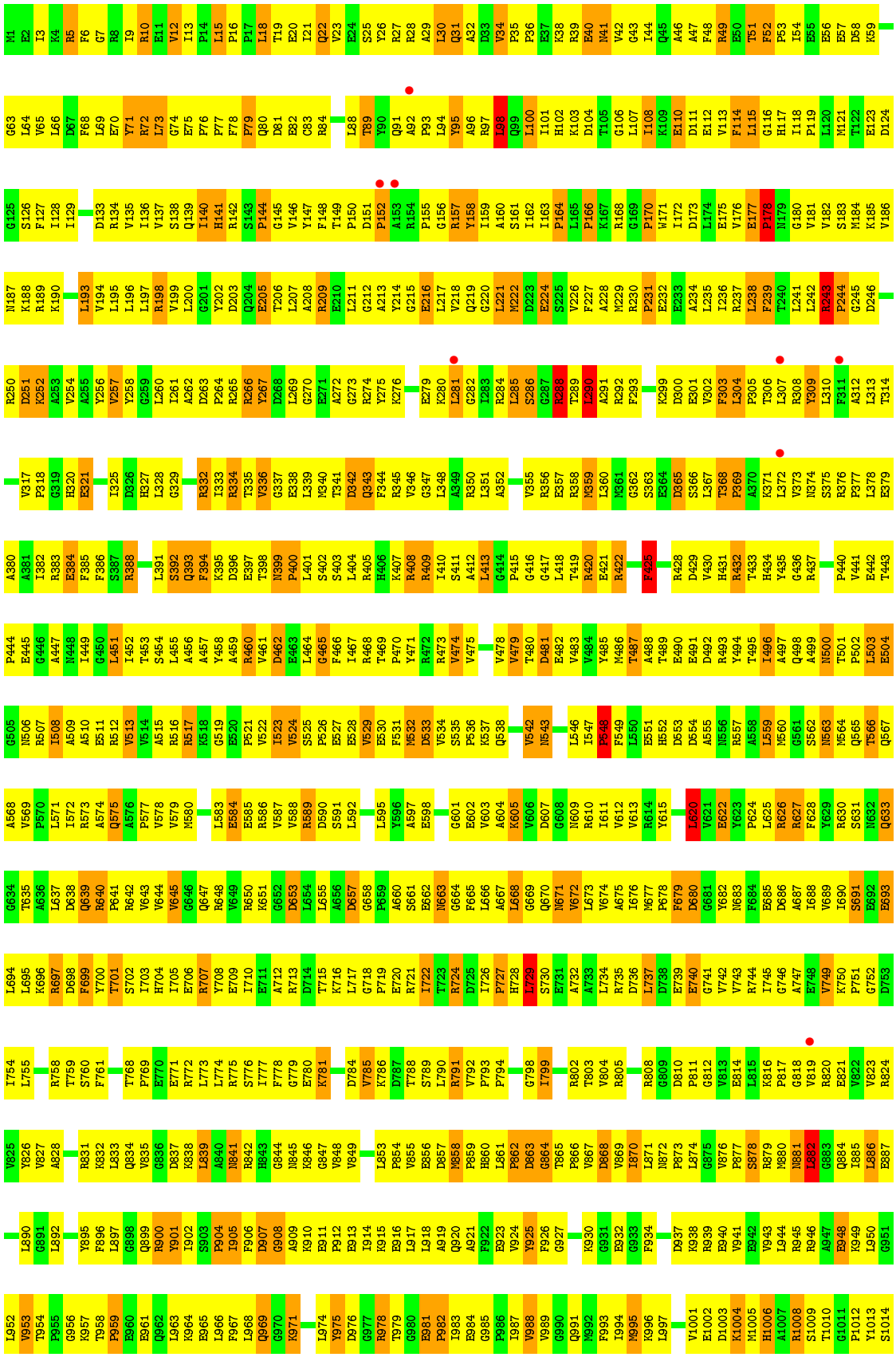
Chain L:

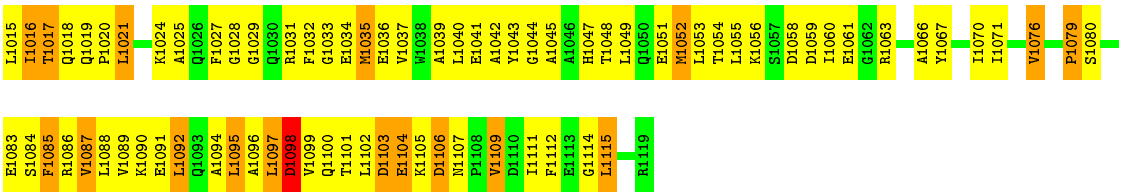


• Molecule 2: DNA-directed RNA polymerase beta chain

Chain C:

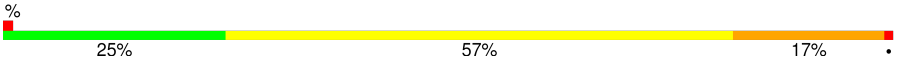


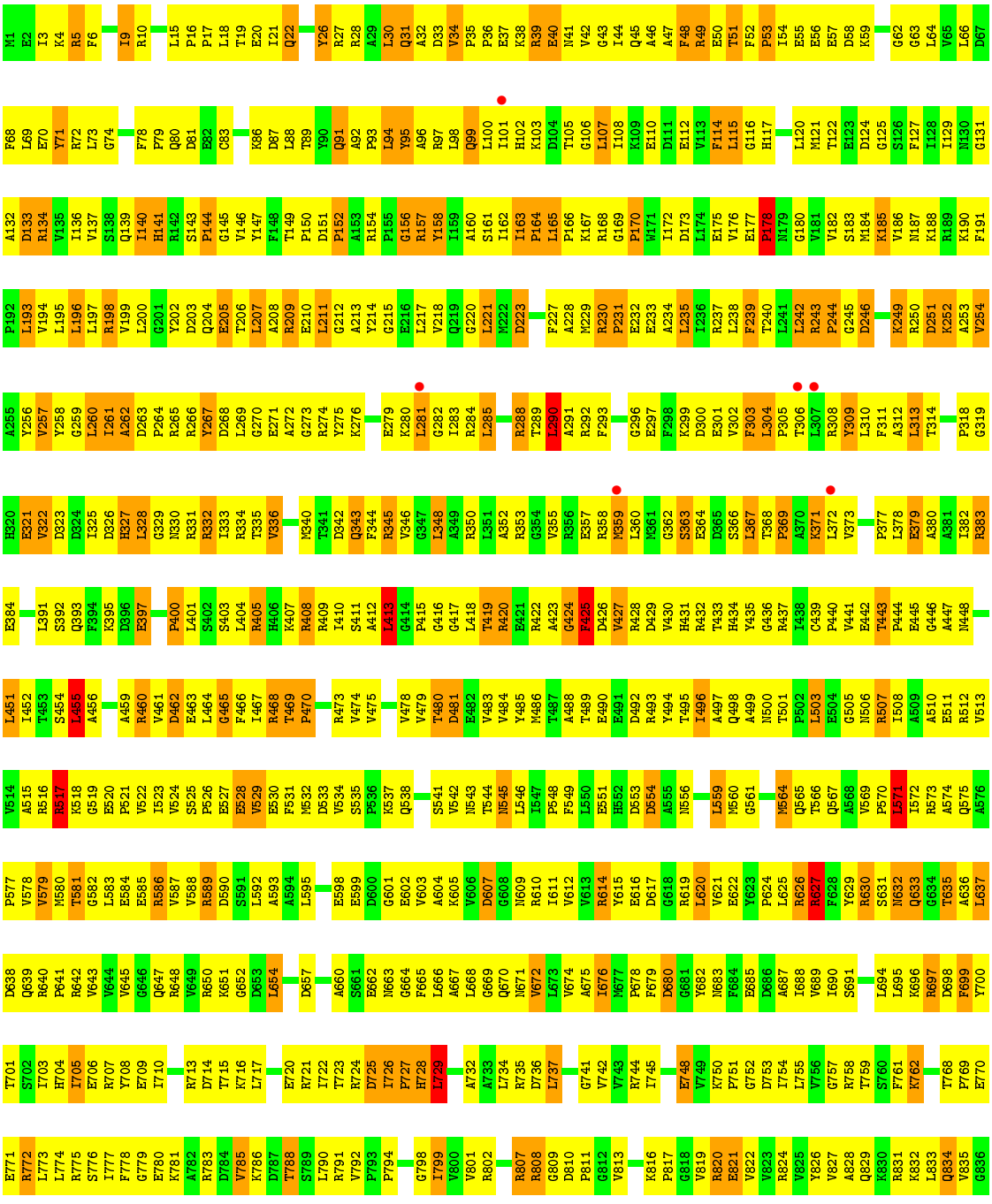


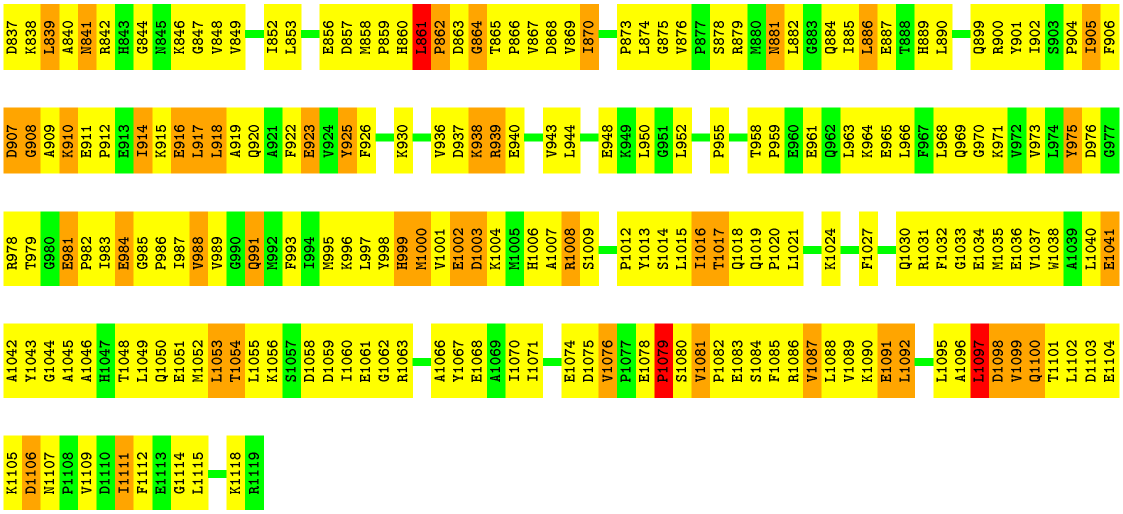


• Molecule 2: DNA-directed RNA polymerase beta chain

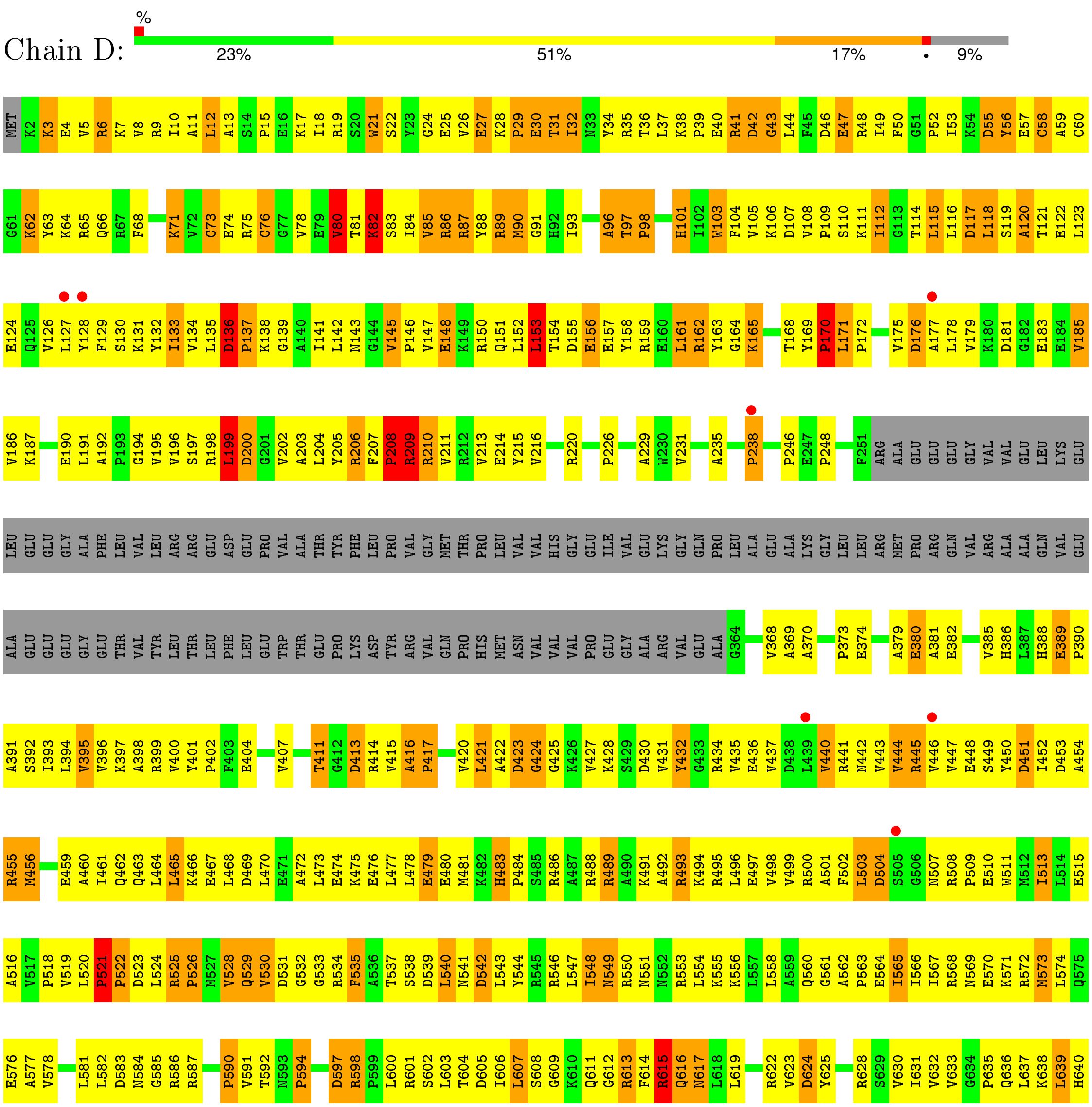
Chain M:

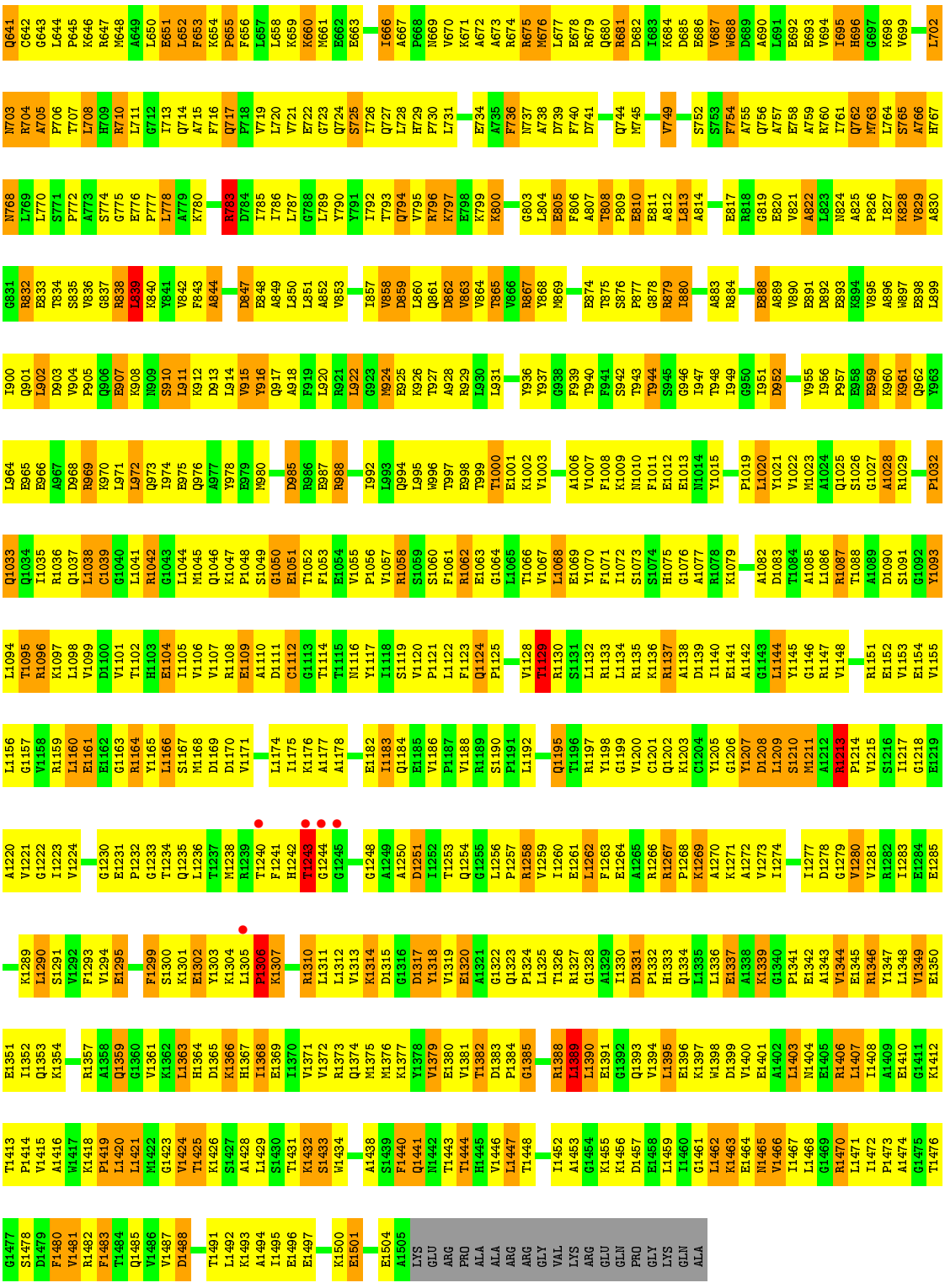




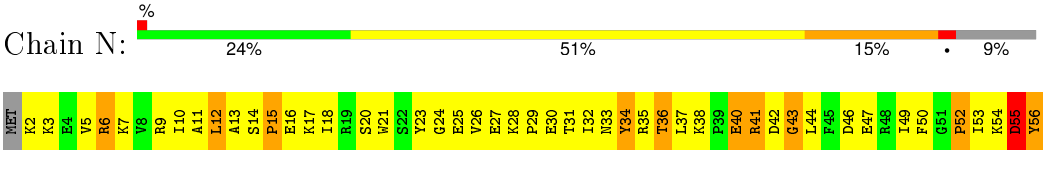


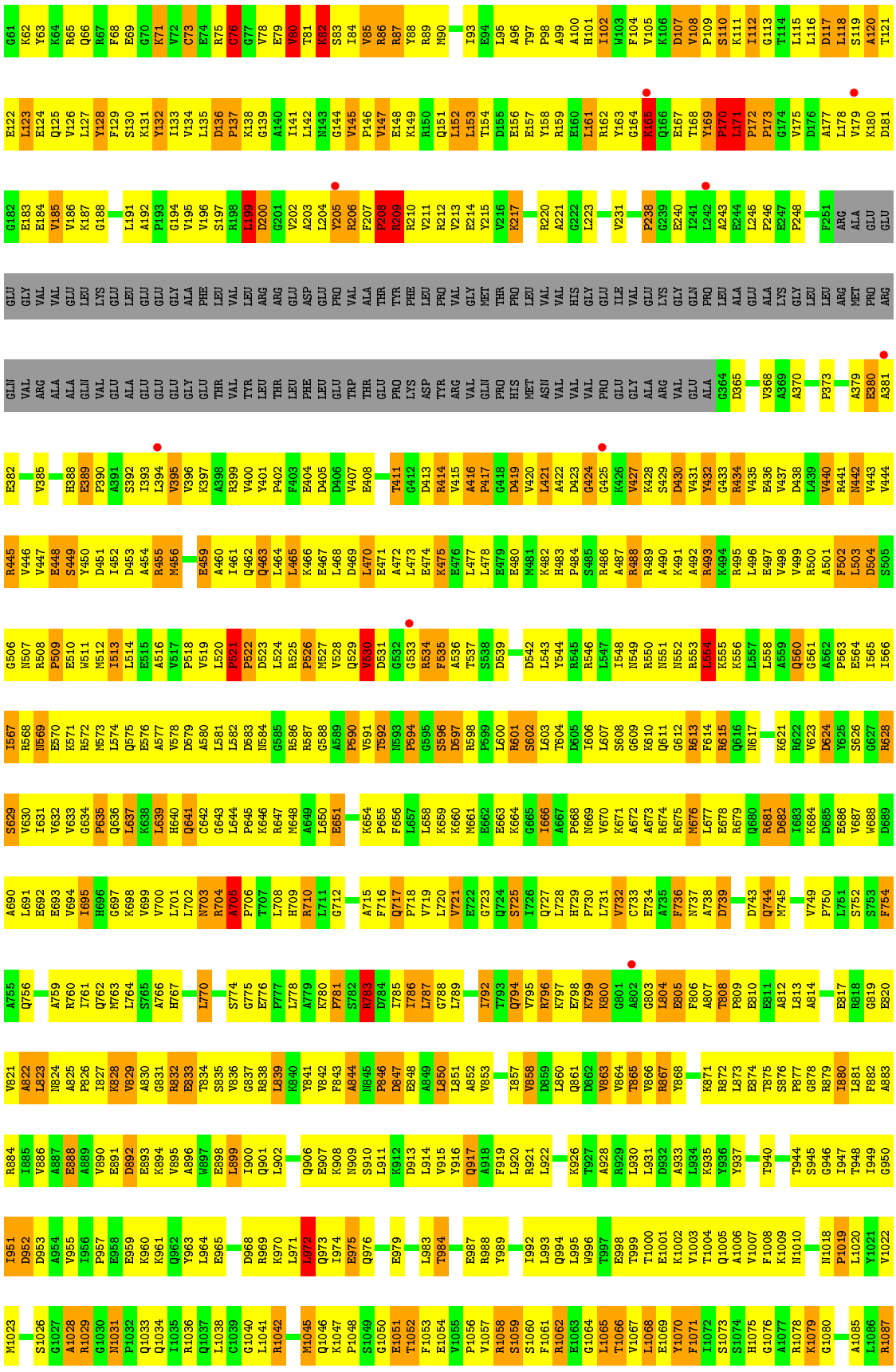
• Molecule 3: DNA-directed RNA polymerase beta' chain

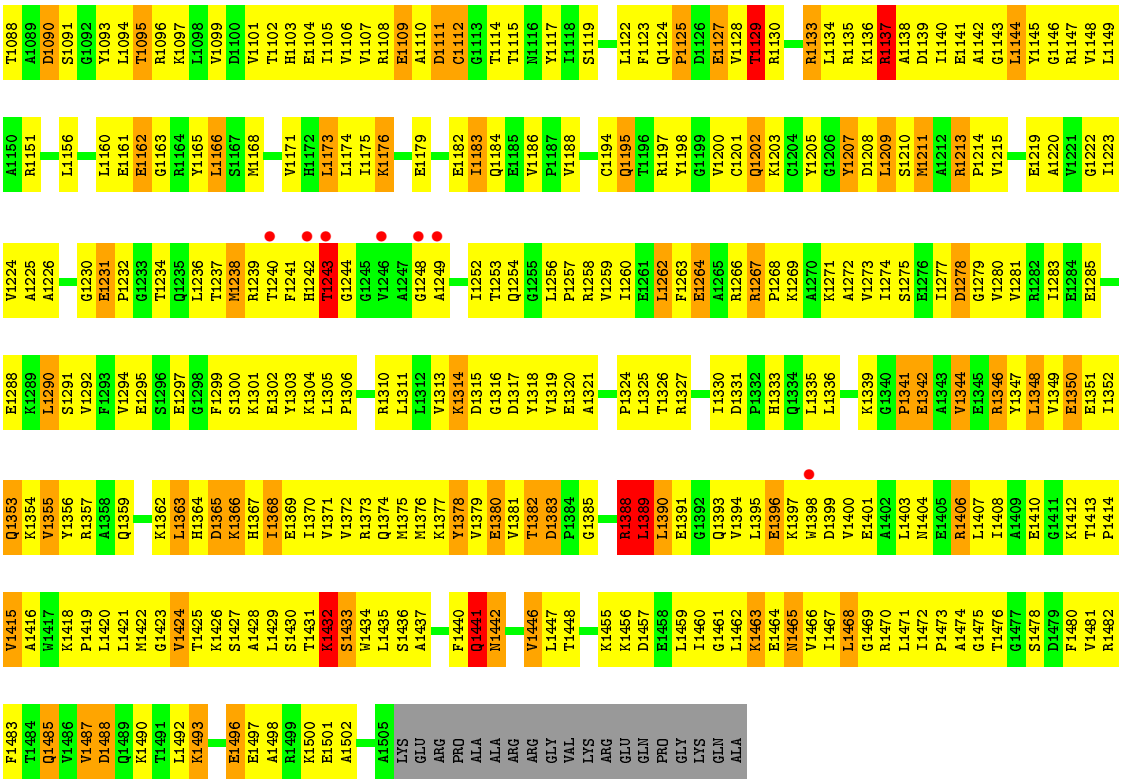




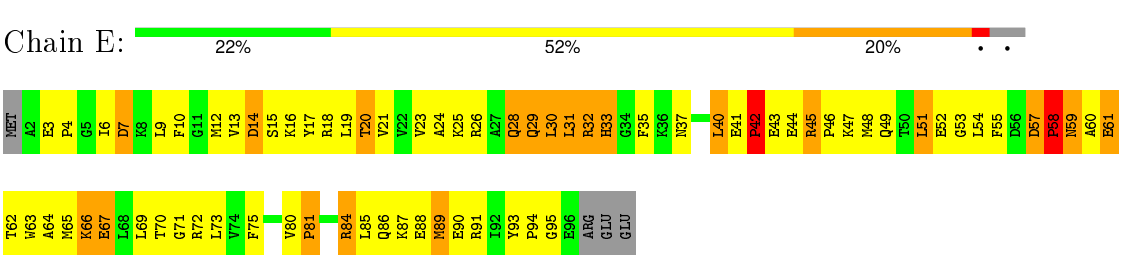
• Molecule 3: DNA-directed RNA polymerase beta' chain



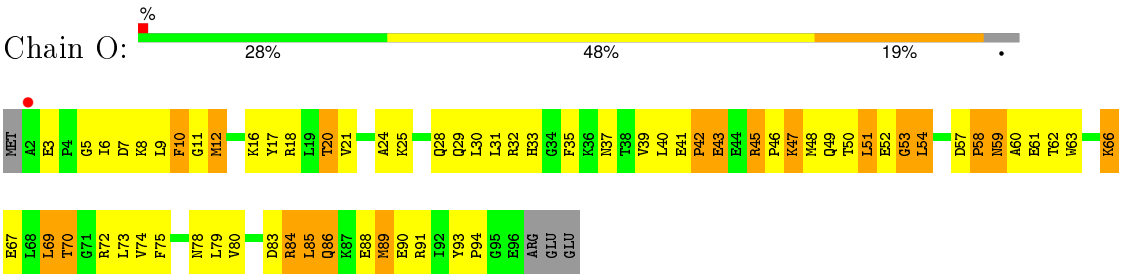




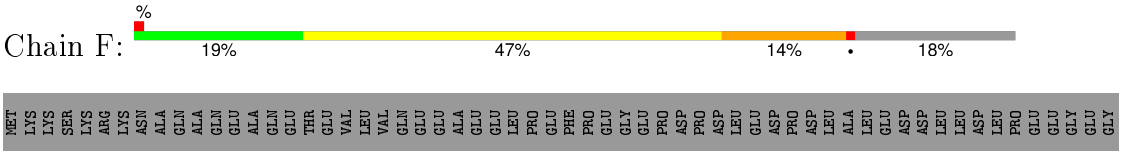
• Molecule 4: RNA polymerase omega chain

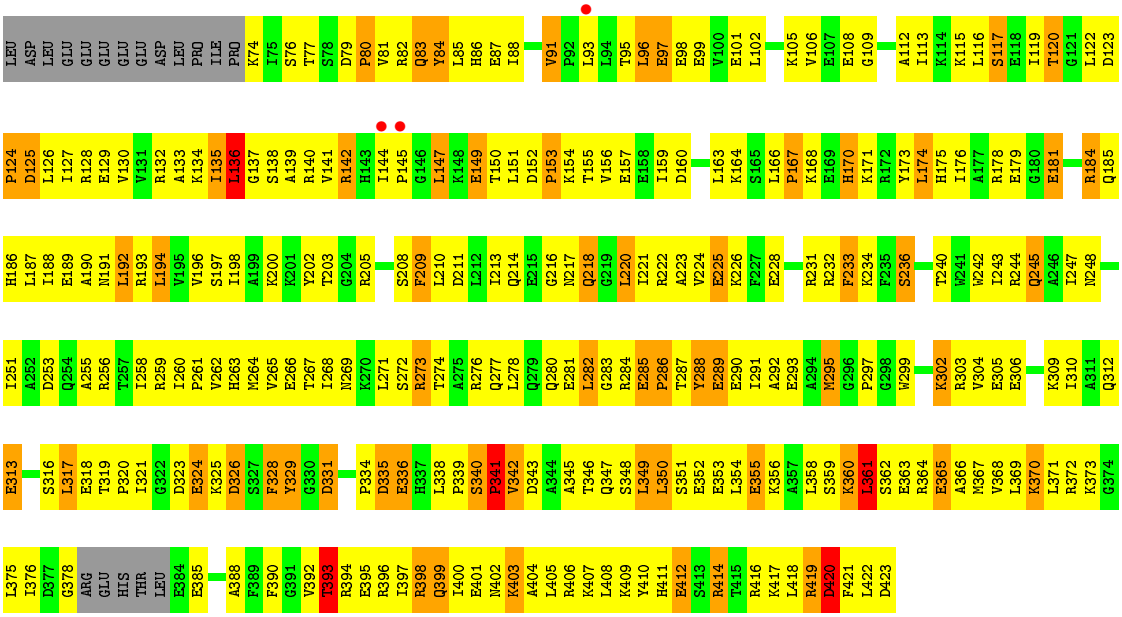


• Molecule 4: RNA polymerase omega chain



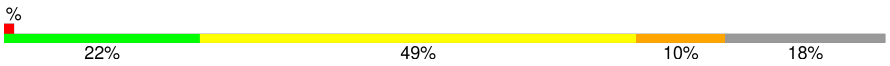
• Molecule 5: RNA polymerase sigma factor rpoD

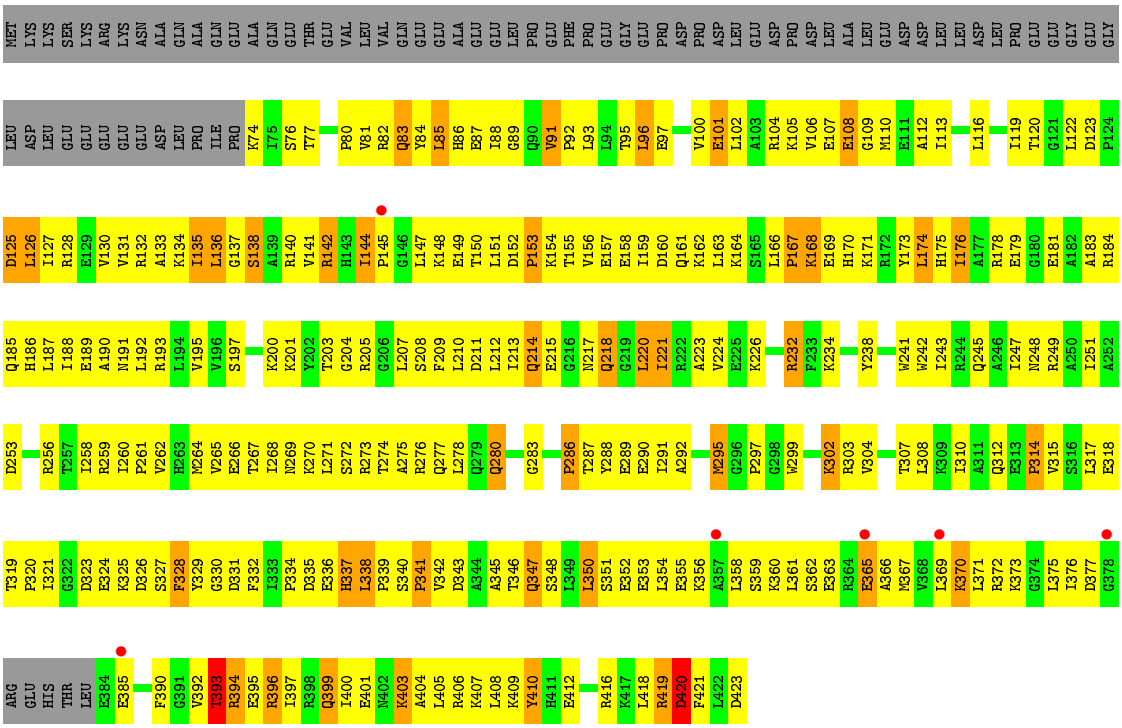




• Molecule 5: RNA polymerase sigma factor rpoD

Chain P:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	239.50Å 239.50Å 253.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.80 24.96 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.80) 92.0 (24.96-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.231 , 0.268 0.226 , 0.261	Depositor DCC
R_{free} test set	21166 reflections (6.13%)	DCC
Wilson B-factor (Å^2)	58.9	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 80.0	EDS
Estimated twinning fraction	0.499 for -h,-k,l 0.068 for h,-h-k,-l 0.068 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Outliers	0 of 366401 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	58679	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.80	1/1838 (0.1%)	0.88	1/2498 (0.0%)
1	B	0.75	0/1838	0.82	2/2498 (0.1%)
1	K	0.75	0/1838	0.86	2/2498 (0.1%)
1	L	0.72	0/1838	0.78	1/2498 (0.0%)
2	C	0.84	0/8997	0.90	8/12164 (0.1%)
2	M	0.82	0/8997	0.89	7/12164 (0.1%)
3	D	0.84	0/10975	0.94	20/14836 (0.1%)
3	N	0.83	0/10975	0.93	18/14836 (0.1%)
4	E	0.84	0/783	0.97	0/1054
4	O	0.88	0/783	1.00	1/1054 (0.1%)
5	F	0.75	0/2812	0.82	3/3781 (0.1%)
5	P	0.75	0/2812	0.80	1/3781 (0.0%)
All	All	0.82	1/54486 (0.0%)	0.90	64/73662 (0.1%)

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	N	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	ILE	C-N	5.57	1.44	1.34

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	199	LEU	CA-CB-CG	-8.69	95.30	115.30
1	B	138	LEU	CA-CB-CG	8.01	133.72	115.30
3	N	1389	LEU	CA-CB-CG	7.77	133.18	115.30
5	P	136	LEU	CA-CB-CG	7.49	132.51	115.30
3	N	76	CYS	CA-CB-SG	6.73	126.11	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	N	132	TYR	Sidechain

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	1806	0	1861	216	0
1	B	1806	0	1861	199	0
1	K	1806	0	1861	208	0
1	L	1806	0	1861	206	0
2	C	8829	0	8933	1184	0
2	M	8829	0	8933	1106	0
3	D	10797	0	10873	1450	0
3	N	10797	0	10873	1345	0
4	E	769	0	775	97	0
4	O	769	0	775	108	0
5	F	2771	0	2844	336	0
5	P	2771	0	2844	342	0
6	D	2	0	0	0	0
6	N	2	0	0	0	0
7	D	1	0	0	0	0
7	N	1	0	0	0	0
8	A	191	0	0	37	0
8	B	181	0	0	34	0
8	C	767	0	0	174	0
8	D	1100	0	0	234	0
8	E	93	0	0	14	0
8	F	333	0	0	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	K	151	0	0	30	0
8	L	179	0	0	49	0
8	M	739	0	0	195	0
8	N	1038	0	0	225	0
8	O	78	0	0	24	0
8	P	267	0	0	61	0
All	All	58679	0	54294	6401	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 59.

The worst 5 of 6401 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)
2:M:1054:THR:HG21	2:M:1079:PRO:HB3	1.28	1.11
1:A:95:GLN:HA	1:A:146:ARG:HH12	1.12	1.08
2:C:135:VAL:HG11	2:C:407:LYS:HA	1.36	1.04
3:N:1036:ARG:HH21	3:N:1042:ARG:HA	1.20	1.04
1:A:42:ARG:HH12	2:C:857:ASP:HB3	1.14	1.04

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	227/315 (72%)	202 (89%)	21 (9%)	4 (2%)	11	34
1	B	227/315 (72%)	202 (89%)	21 (9%)	4 (2%)	11	34
1	K	227/315 (72%)	200 (88%)	23 (10%)	4 (2%)	11	34
1	L	227/315 (72%)	204 (90%)	19 (8%)	4 (2%)	11	34
2	C	1117/1119 (100%)	917 (82%)	150 (13%)	50 (4%)	3	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	M	1117/1119 (100%)	907 (81%)	159 (14%)	51 (5%)	3 9
3	D	1388/1524 (91%)	1123 (81%)	191 (14%)	74 (5%)	2 7
3	N	1388/1524 (91%)	1110 (80%)	195 (14%)	83 (6%)	2 5
4	E	93/99 (94%)	74 (80%)	16 (17%)	3 (3%)	5 17
4	O	93/99 (94%)	75 (81%)	15 (16%)	3 (3%)	5 17
5	F	341/423 (81%)	283 (83%)	42 (12%)	16 (5%)	3 9
5	P	341/423 (81%)	285 (84%)	40 (12%)	16 (5%)	3 9
All	All	6786/7590 (89%)	5582 (82%)	892 (13%)	312 (5%)	3 9

5 of 312 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	B	29	GLU
1	B	48	ILE
2	C	152	PRO
2	C	178	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	202/273 (74%)	147 (73%)	55 (27%)	0 1
1	B	202/273 (74%)	163 (81%)	39 (19%)	2 5
1	K	202/273 (74%)	152 (75%)	50 (25%)	1 2
1	L	202/273 (74%)	158 (78%)	44 (22%)	1 3
2	C	941/941 (100%)	734 (78%)	207 (22%)	1 3
2	M	941/941 (100%)	730 (78%)	211 (22%)	1 3
3	D	1123/1279 (88%)	846 (75%)	277 (25%)	1 2
3	N	1123/1279 (88%)	866 (77%)	257 (23%)	1 3
4	E	83/87 (95%)	58 (70%)	25 (30%)	0 1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	O	83/87 (95%)	64 (77%)	19 (23%)	1 3
5	F	295/370 (80%)	228 (77%)	67 (23%)	1 3
5	P	295/370 (80%)	249 (84%)	46 (16%)	3 9
All	All	5692/6446 (88%)	4395 (77%)	1297 (23%)	1 3

5 of 1297 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	30	LEU
1	L	25	LEU
3	N	1353	GLN
5	F	80	PRO
5	F	361	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 179 such sidechains are listed below:

Mol	Chain	Res	Type
4	E	86	GLN
1	L	212	ASN
3	N	1374	GLN
5	F	337	HIS
1	K	156	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 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

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, 95^{th} 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	229/315 (72%)	-0.37	0 100 100	38, 65, 92, 117	0
1	B	229/315 (72%)	-0.26	9 (3%) 43 31	53, 95, 115, 121	0
1	K	229/315 (72%)	-0.36	0 100 100	41, 66, 93, 122	0
1	L	229/315 (72%)	-0.38	3 (1%) 79 71	52, 94, 114, 127	0
2	C	1119/1119 (100%)	-0.34	8 (0%) 89 84	23, 81, 110, 119	0
2	M	1119/1119 (100%)	-0.38	6 (0%) 91 88	27, 79, 109, 122	0
3	D	1392/1524 (91%)	-0.32	12 (0%) 85 79	17, 68, 113, 130	0
3	N	1392/1524 (91%)	-0.34	16 (1%) 82 74	27, 69, 110, 138	0
4	E	95/99 (95%)	-0.34	0 100 100	47, 85, 115, 133	0
4	O	95/99 (95%)	-0.48	1 (1%) 82 74	40, 76, 97, 111	0
5	F	345/423 (81%)	-0.39	3 (0%) 85 79	46, 84, 112, 131	0
5	P	345/423 (81%)	-0.38	6 (1%) 73 63	54, 87, 112, 125	0
All	All	6818/7590 (89%)	-0.35	64 (0%) 85 79	17, 77, 111, 138	0

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	130	ALA	5.1
3	D	1240	THR	4.9
3	N	1243	THR	4.8
3	D	1243	THR	4.6
5	F	145	PRO	4.6

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 (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 95^{th} 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
6	ZN	D	7112	1/1	0.99	0.14	0.51	75,75,75,75	0
6	ZN	N	7059	1/1	0.99	0.11	-0.82	100,100,100,100	0
7	MG	N	9002	1/1	0.94	0.13	-0.83	64,64,64,64	0
6	ZN	N	7113	1/1	0.98	0.10	-1.18	87,87,87,87	0
6	ZN	D	7058	1/1	0.98	0.07	-1.71	109,109,109,109	0
7	MG	D	9001	1/1	0.97	0.15	-	67,67,67,67	0

6.5 Other polymers (i)

There are no such residues in this entry.