wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 10:39 PM GMT

PDB ID	:	4YFN
Title	:	Escherichia coli RNA polymerase in complex with squaramide compound 14 (N-[3,4-dioxo-2-(4-{[4-(trifluoromethyl)benzyl]amino}piperidin-1-yl)cyclobut-1 -en-1-yl]-3,5-dimethyl-1,2-oxazole-4-sulfonamide)
Authors	:	Molodtsov, V.; Fleming, P.R.; Eyermann, C.J.; Ferguson, A.D.; Foulk, M.A.; McKinney, D.C.; Masse, C.E.; Buurman, E.T.; Murakami, K.S.
Deposited on	:	2015-02-25
Resolution	:	3.82 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:

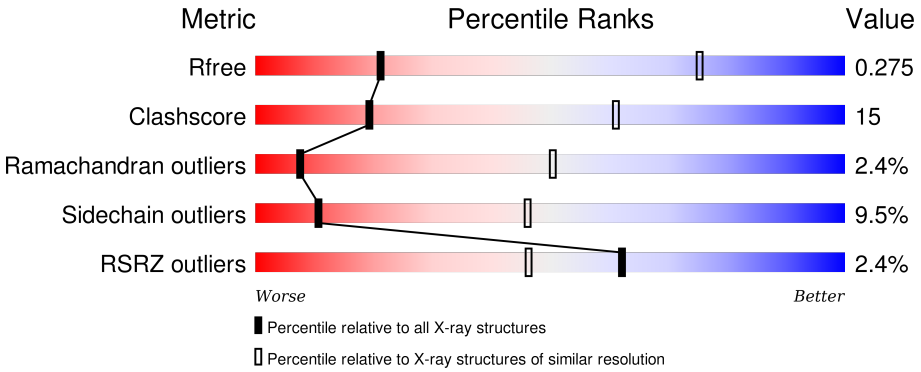
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.82 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	1324 (4.14-3.50)
Clashscore	102246	1028 (4.12-3.52)
Ramachandran outliers	100387	1404 (4.14-3.50)
Sidechain outliers	100360	1399 (4.14-3.50)
RSRZ outliers	91569	1332 (4.14-3.50)

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	329	43% 23% 5% 29%
1	B	329	47% 35% 5% 12%
1	G	329	41% 26% • 31%
1	H	329	4% 36% 27% • 34%
2	C	1342	64% 31% •

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Mol	Chain	Length	Quality of chain
2	I	1342	2% 65% 30%
3	D	1407	% 49% 28% 5% 17%
3	J	1407	2% 49% 28% 5% 18%
4	E	91	78% 15%
4	K	91	22% 53% 31% 13%
5	F	613	4% 51% 23% 24%
5	L	613	4% 53% 20% 23%

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
8	4C2	D	2004	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 55638 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	235	Total	C	N	O	S	0	0	0
			1820	1132	323	358	7			
1	B	289	Total	C	N	O	S	0	0	0
			2234	1400	393	433	8			
1	G	227	Total	C	N	O	S	0	0	0
			1755	1093	311	345	6			
1	H	216	Total	C	N	O	S	0	0	0
			1662	1038	292	326	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0	0
			10570	6631	1841	2055	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10560	6626	1837	2054	43			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1163	Total	C	N	O	S	0	0	0
			9029	5678	1613	1692	46			
3	J	1152	Total	C	N	O	S	0	0	0
			8980	5648	1605	1681	46			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	S	0	0	0
			691	421	129	140	1			
4	K	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	468	Total	C	N	O	S	0	0	0
			3813	2389	678	723	23			
5	L	469	Total	C	N	O	S	0	0	0
			3821	2393	679	726	23			

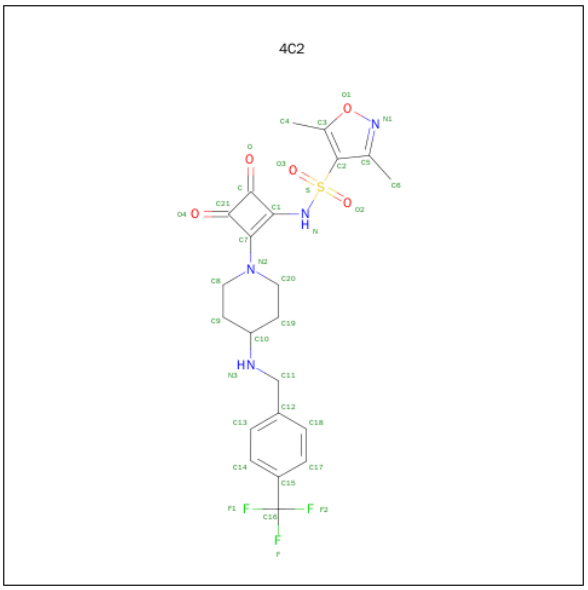
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 8 is N-[3,4-dioxo-2-(4-{[4-(trifluoromethyl)benzyl]amino}piperidin-1-yl)cyclobut-1-en-1-yl]-3,5-dimethyl-1,2-oxazole-4-sulfonamide (three-letter code: 4C2) (formula: $C_{22}H_{23}F_3N_4O_5S$).



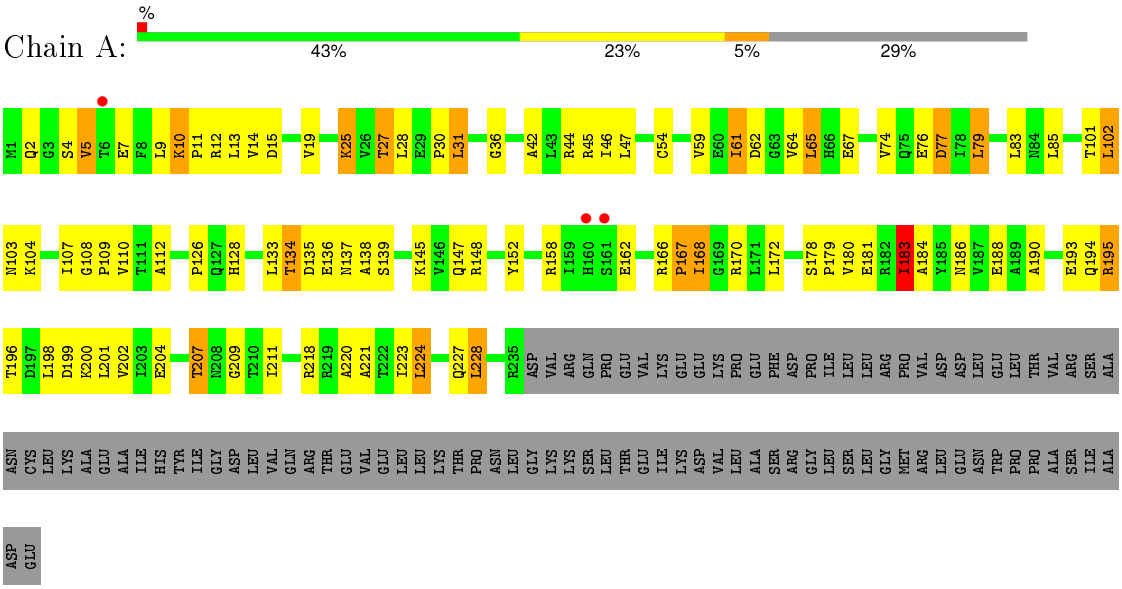
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	D	1	Total	C	F	N	O	S	0	0
			35	22	3	4	5	1		
8	J	1	Total	C	F	N	O	S	0	0
			35	22	3	4	5	1		

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.

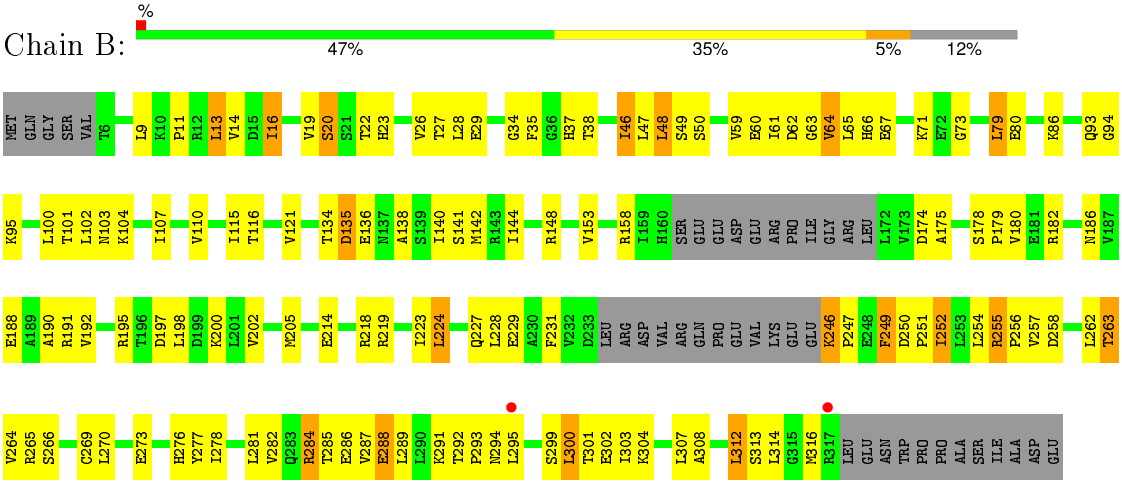
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



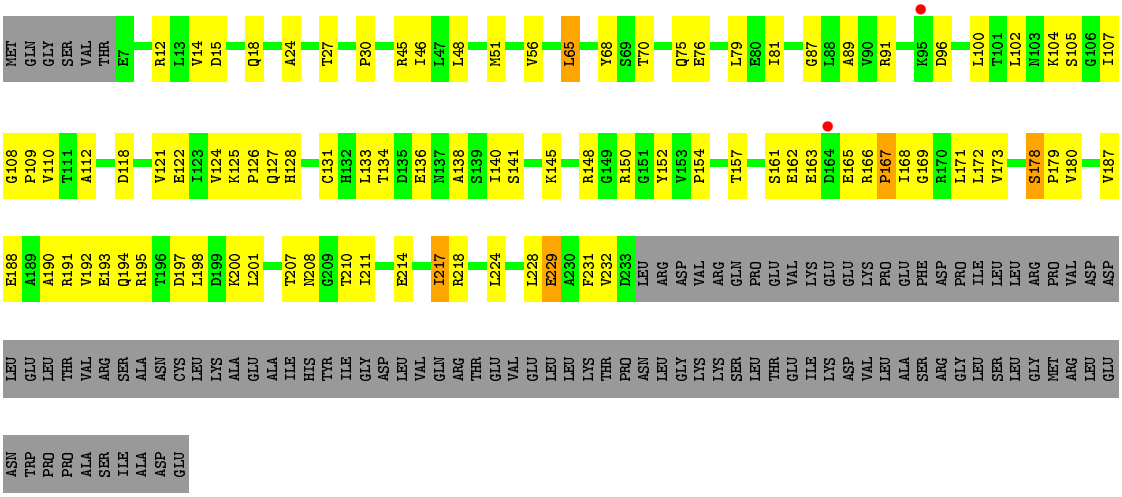
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:



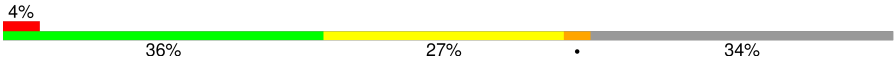
- Molecule 1: DNA-directed RNA polymerase subunit alpha

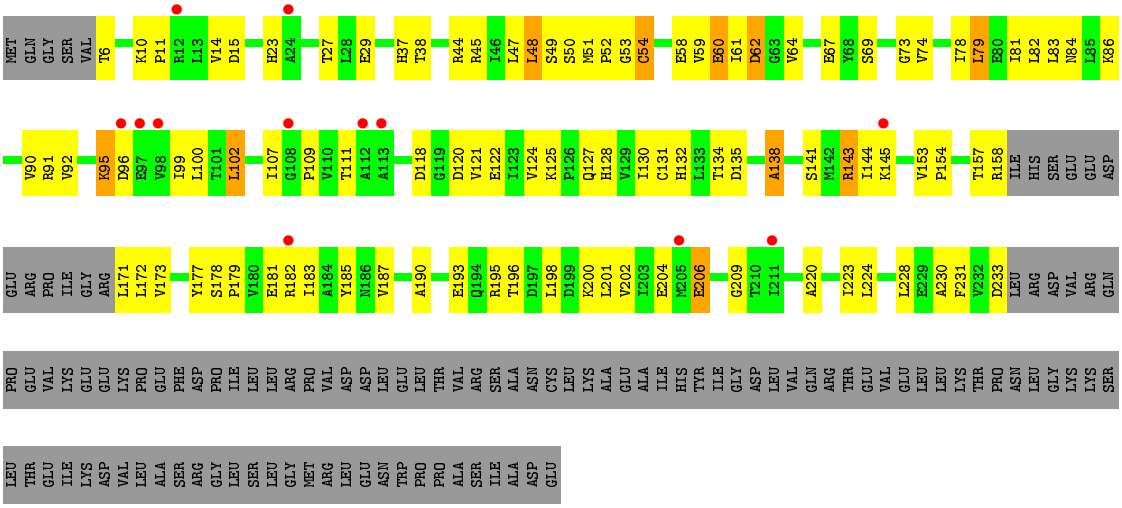
Chain G:



• Molecule 1: DNA-directed RNA polymerase subunit alpha

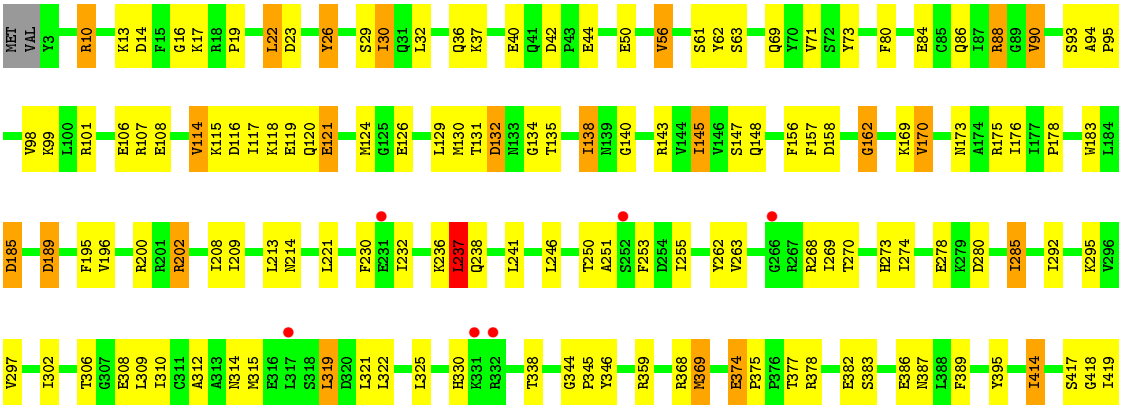
Chain H:

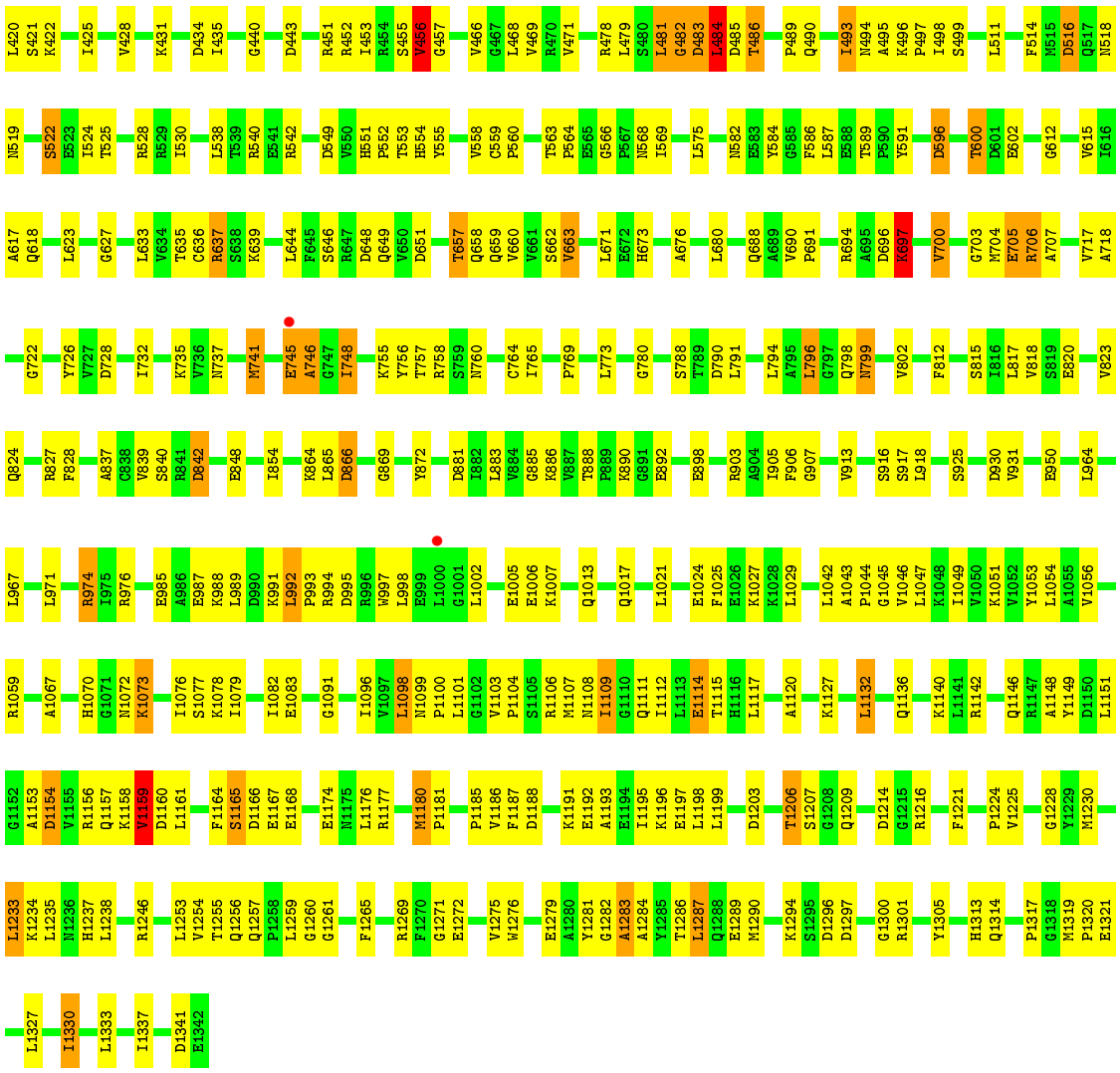




• Molecule 2: DNA-directed RNA polymerase subunit beta

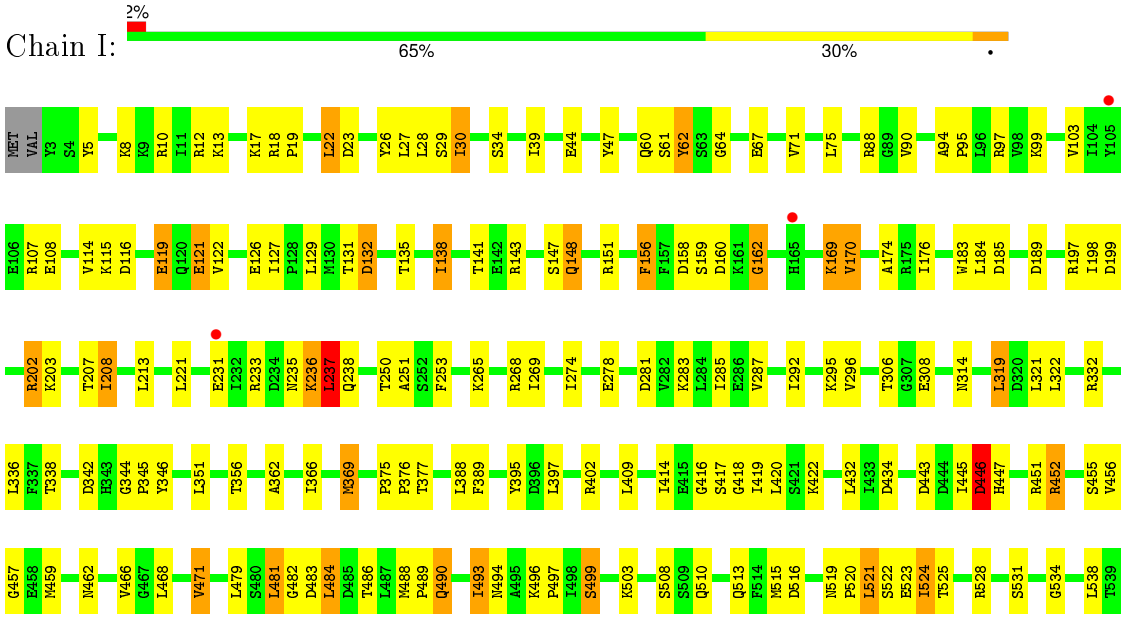
Chain C:

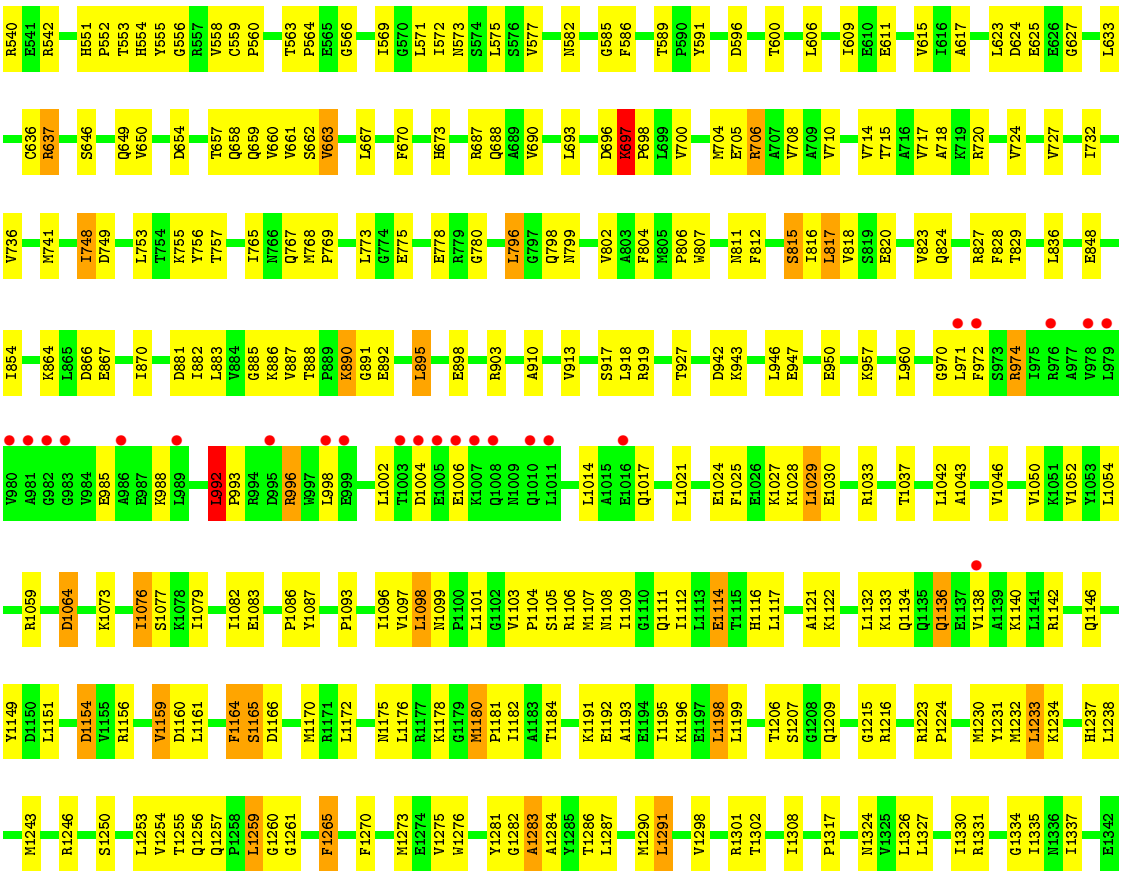




• Molecule 2: DNA-directed RNA polymerase subunit beta

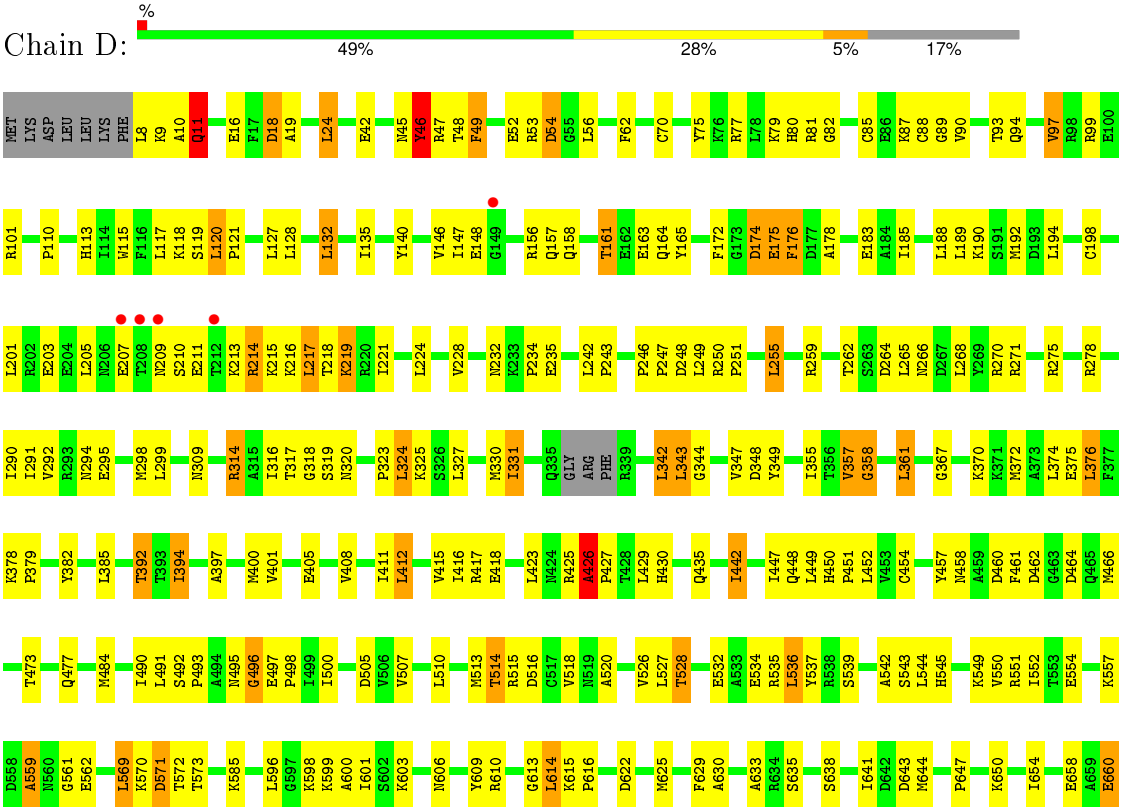
Chain I:

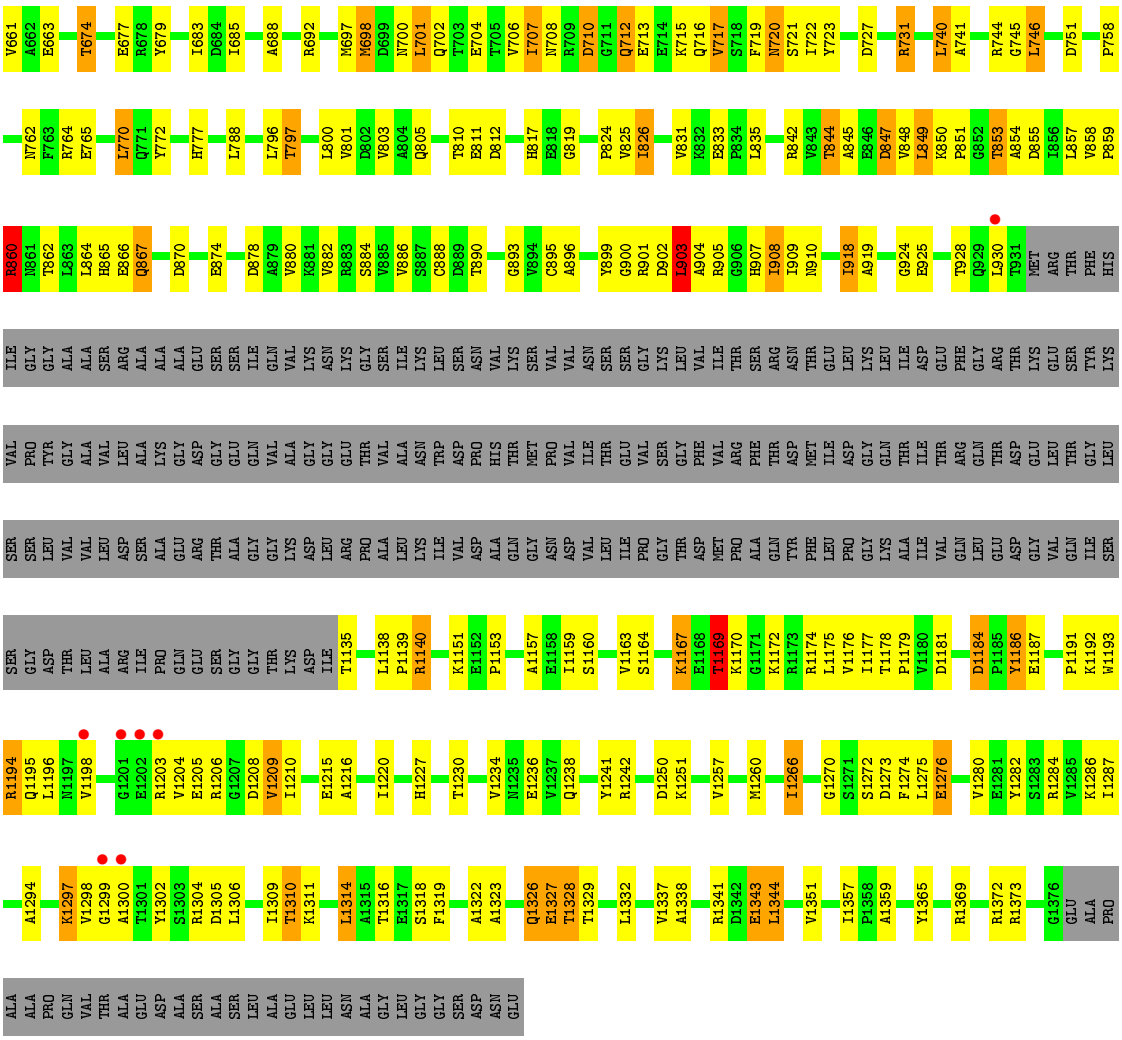




- Molecule 3: DNA-directed RNA polymerase subunit beta'

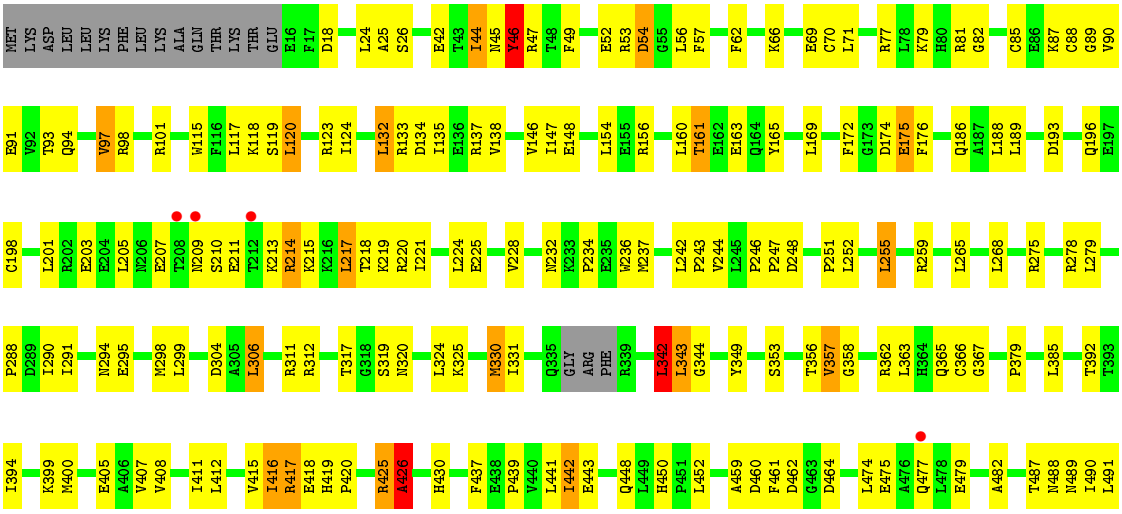
Chain D:

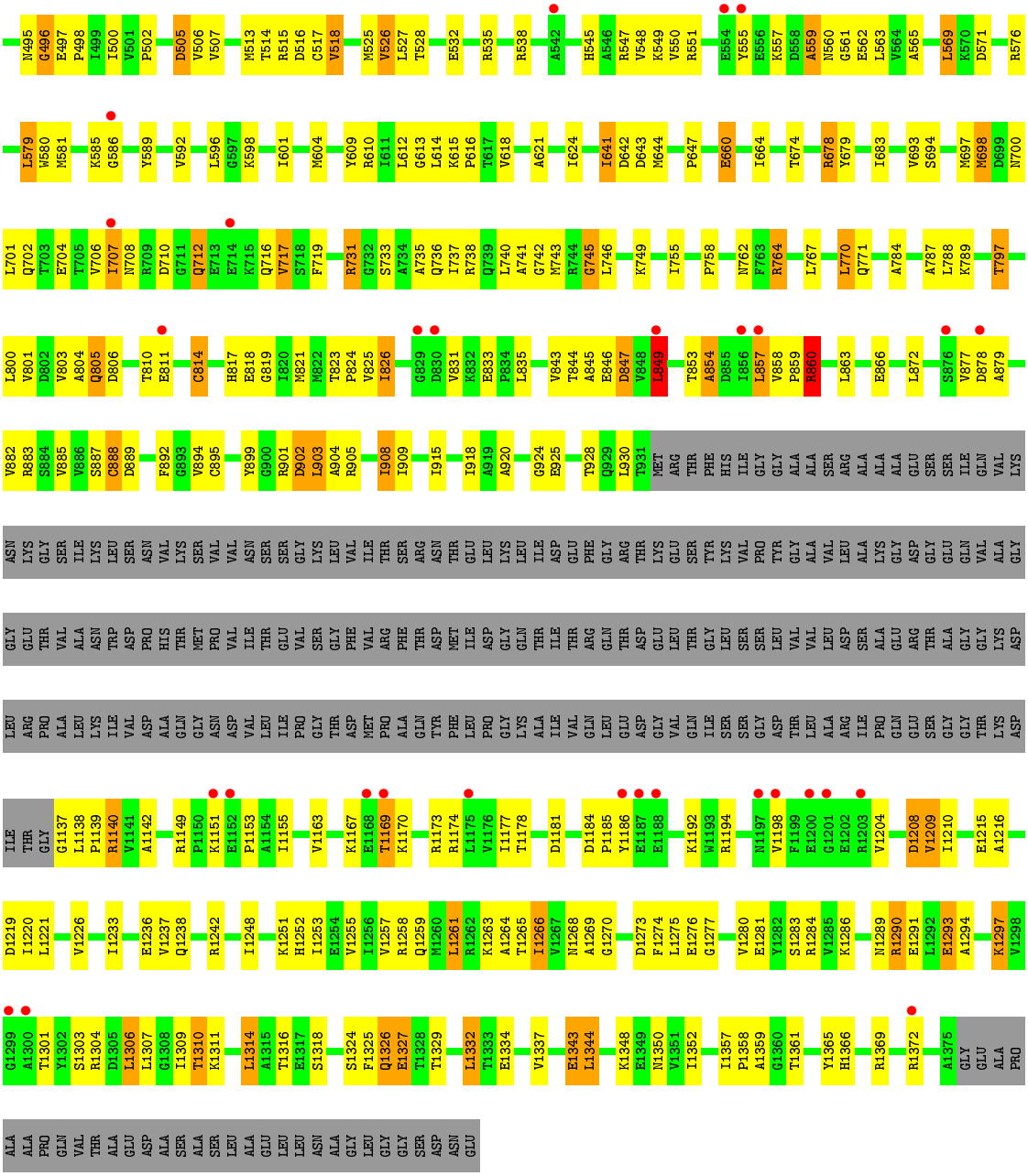




• Molecule 3: DNA-directed RNA polymerase subunit beta'

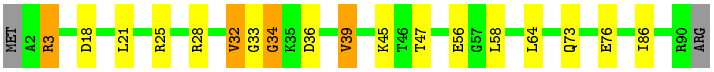
Chain J:





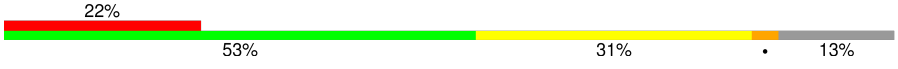
• Molecule 4: DNA-directed RNA polymerase subunit omega

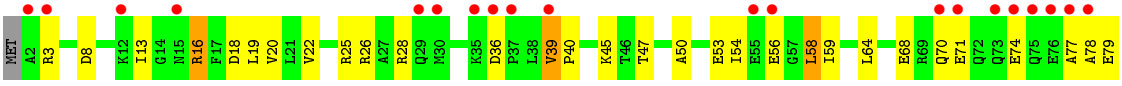
Chain E:



• Molecule 4: DNA-directed RNA polymerase subunit omega

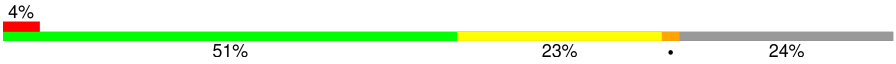
Chain K:

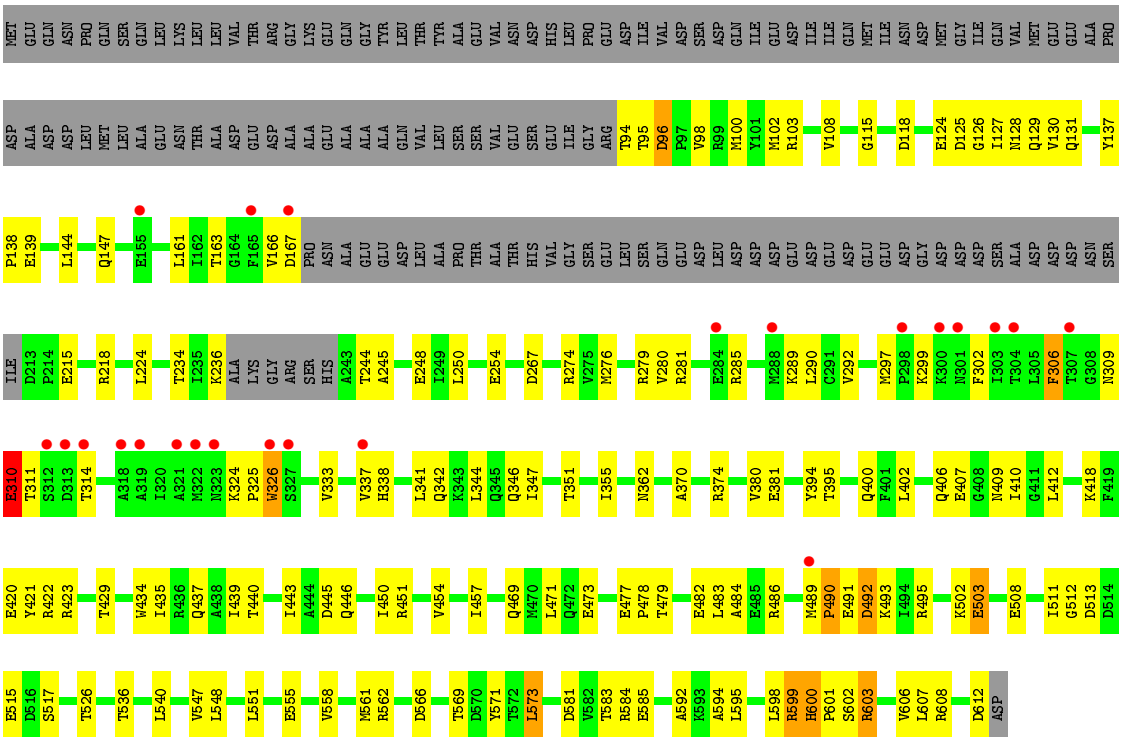




- Molecule 5: RNA polymerase sigma factor RpoD

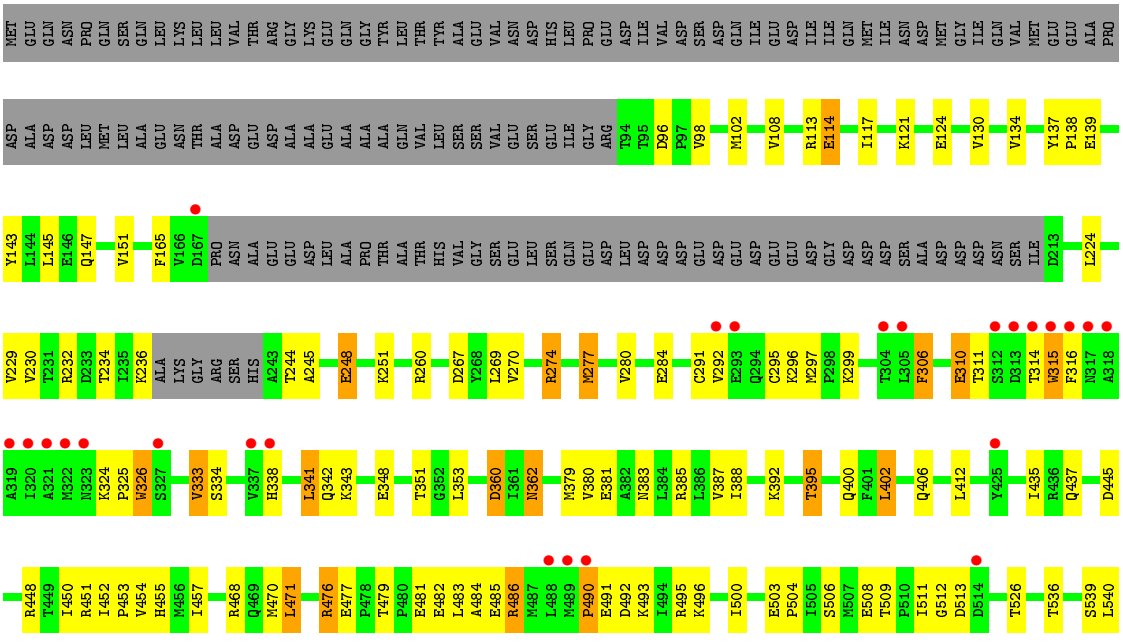
Chain F:





- Molecule 5: RNA polymerase sigma factor RpoD

Chain L:




V547
L551
E555
V558
M561
D566
M567
N568
T569
D570
Y571
T572
L573
G577
D581
V582
T583
R584
I587
A594
L598
R599
H600
P601
S602
R603
S604
R608
D612
D613

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	191.25Å 206.57Å 312.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 3.82 30.16 – 3.82	Depositor EDS
% Data completeness (in resolution range)	88.9 (29.96-3.82) 77.9 (30.16-3.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 3.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.222 , 0.270 0.241 , 0.275	Depositor DCC
R_{free} test set	2003 reflections (2.18%)	DCC
Wilson B-factor (Å^2)	141.4	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 114.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 107055 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	55638	wwPDB-VP
Average B, all atoms (Å^2)	188.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% 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, 4C2, 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	0.77	0/1842	0.98	5/2495 (0.2%)
1	B	0.82	2/2260 (0.1%)	0.87	0/3059
1	G	0.82	0/1777	0.89	1/2408 (0.0%)
1	H	1.03	1/1681 (0.1%)	0.97	2/2278 (0.1%)
2	C	0.83	5/10739 (0.0%)	0.90	3/14489 (0.0%)
2	I	0.76	1/10729 (0.0%)	0.86	10/14477 (0.1%)
3	D	0.86	1/9167 (0.0%)	0.92	10/12380 (0.1%)
3	J	0.79	0/9118	0.89	9/12312 (0.1%)
4	E	0.76	0/693	0.78	0/935
4	K	1.14	0/629	0.96	3/847 (0.4%)
5	F	0.90	2/3864 (0.1%)	0.86	0/5194
5	L	0.89	3/3872 (0.1%)	0.84	0/5205
All	All	0.83	15/56371 (0.0%)	0.89	43/76079 (0.1%)

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	291	CYS	CB-SG	10.11	1.99	1.82
3	D	454	CYS	CB-SG	-7.01	1.70	1.82
5	L	315	TRP	CB-CG	6.64	1.62	1.50
5	F	326	TRP	CB-CG	6.03	1.61	1.50
5	F	337	VAL	CA-CB	6.00	1.67	1.54

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	849	LEU	CA-CB-CG	9.21	136.48	115.30
3	D	426	ALA	C-N-CD	7.92	145.02	128.40
2	I	521	LEU	CA-CB-CG	7.53	132.62	115.30
1	H	54	CYS	CA-CB-SG	7.17	126.91	114.00
3	D	376	LEU	CA-CB-CG	-6.83	99.59	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1820	0	1850	62	0
1	B	2234	0	2291	90	0
1	G	1755	0	1773	63	0
1	H	1662	0	1687	81	0
2	C	10570	0	10582	318	0
2	I	10560	0	10565	296	0
3	D	9029	0	9175	334	0
3	J	8980	0	9148	338	0
4	E	691	0	695	7	0
4	K	627	0	634	20	0
5	F	3813	0	3880	101	0
5	L	3821	0	3884	92	0
6	D	1	0	0	0	0
6	J	1	0	0	0	0
7	D	2	0	0	0	0
7	J	2	0	0	0	0
8	D	35	0	23	1	0
8	J	35	0	23	2	0
All	All	55638	0	56210	1683	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 15.

The worst 5 of 1683 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:ARG:HG3	1:B:255:ARG:HH11	1.24	1.03
3:J:1215:GLU:HG3	3:J:1220:ILE:HD11	1.39	1.01
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.46	0.94
2:C:1160:ASP:HB2	2:C:1161:LEU:HA	1.48	0.93
2:I:1160:ASP:HB2	2:I:1161:LEU:HA	1.52	0.91

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	233/329 (71%)	211 (91%)	16 (7%)	6 (3%)	7 48
1	B	283/329 (86%)	247 (87%)	28 (10%)	8 (3%)	6 47
1	G	225/329 (68%)	205 (91%)	15 (7%)	5 (2%)	8 52
1	H	212/329 (64%)	196 (92%)	14 (7%)	2 (1%)	21 67
2	C	1338/1342 (100%)	1194 (89%)	112 (8%)	32 (2%)	7 50
2	I	1338/1342 (100%)	1185 (89%)	122 (9%)	31 (2%)	8 51
3	D	1157/1407 (82%)	1036 (90%)	91 (8%)	30 (3%)	7 48
3	J	1146/1407 (81%)	1030 (90%)	85 (7%)	31 (3%)	6 48
4	E	87/91 (96%)	77 (88%)	6 (7%)	4 (5%)	3 33
4	K	77/91 (85%)	69 (90%)	7 (9%)	1 (1%)	15 61
5	F	462/613 (75%)	419 (91%)	34 (7%)	9 (2%)	10 54
5	L	463/613 (76%)	425 (92%)	30 (6%)	8 (2%)	11 56
All	All	7021/8222 (85%)	6294 (90%)	560 (8%)	167 (2%)	7 50

5 of 167 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	196	THR
1	B	13	LEU
1	B	50	SER
1	B	135	ASP

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	202/286 (71%)	175 (87%)	27 (13%)	5 30
1	B	248/286 (87%)	215 (87%)	33 (13%)	5 31
1	G	193/286 (68%)	181 (94%)	12 (6%)	23 64
1	H	183/286 (64%)	169 (92%)	14 (8%)	16 56
2	C	1155/1157 (100%)	1053 (91%)	102 (9%)	12 50
2	I	1153/1157 (100%)	1058 (92%)	95 (8%)	14 53
3	D	959/1168 (82%)	849 (88%)	110 (12%)	7 37
3	J	959/1168 (82%)	861 (90%)	98 (10%)	9 42
4	E	72/75 (96%)	65 (90%)	7 (10%)	10 45
4	K	67/75 (89%)	58 (87%)	9 (13%)	5 30
5	F	417/540 (77%)	386 (93%)	31 (7%)	17 57
5	L	418/540 (77%)	385 (92%)	33 (8%)	15 55
All	All	6026/7024 (86%)	5455 (90%)	571 (10%)	11 46

5 of 571 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	1208	ASP
1	G	178	SER
3	J	1365	TYR
3	D	1306	LEU
5	F	314	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	258	GLN
1	H	128	HIS
3	J	1366	HIS
5	F	362	ASN

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Mol	Chain	Res	Type
5	F	600	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	4C2	D	2004	-	35,38,38	1.10	4 (11%)	45,58,58	1.91	9 (20%)
8	4C2	J	2004	-	35,38,38	0.80	1 (2%)	45,58,58	1.48	5 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	4C2	D	2004	-	-	0/14/52/52	0/3/4/4
8	4C2	J	2004	-	-	0/14/52/52	0/3/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	2004	4C2	C7-N2	-3.11	1.25	1.37
8	D	2004	4C2	O-C	-2.49	1.17	1.23
8	D	2004	4C2	C1-C7	-2.33	1.37	1.41
8	D	2004	4C2	C1-N	3.34	1.46	1.42
8	J	2004	4C2	C2-C3	3.52	1.42	1.38

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	J	2004	4C2	C19-C10-N3	-6.05	85.95	111.10
8	D	2004	4C2	C19-C10-N3	-5.99	86.20	111.10
8	J	2004	4C2	C3-C2-C5	-4.99	103.79	107.52
8	D	2004	4C2	C1-C-C21	-4.86	84.47	88.49
8	D	2004	4C2	O2-S-C2	-4.50	102.00	108.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	2004	4C2	1	0
8	J	2004	4C2	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	235/329 (71%)	-0.31	3 (1%) 79 65	140, 166, 193, 222	0
1	B	289/329 (87%)	-0.11	2 (0%) 89 80	146, 203, 247, 259	0
1	G	227/329 (68%)	-0.19	2 (0%) 85 74	189, 214, 238, 246	0
1	H	216/329 (65%)	0.21	12 (5%) 28 18	201, 246, 255, 259	0
2	C	1340/1342 (99%)	-0.31	8 (0%) 90 82	115, 159, 222, 268	0
2	I	1340/1342 (99%)	-0.13	27 (2%) 68 53	153, 185, 240, 340	0
3	D	1163/1407 (82%)	-0.20	12 (1%) 84 72	121, 156, 213, 257	0
3	J	1152/1407 (81%)	-0.06	34 (2%) 54 37	151, 192, 247, 273	0
4	E	89/91 (97%)	-0.05	0 100 100	174, 192, 209, 216	0
4	K	79/91 (86%)	1.30	20 (25%) 1 1	262, 289, 297, 302	0
5	F	468/613 (76%)	0.02	23 (4%) 33 22	150, 211, 305, 326	0
5	L	469/613 (76%)	0.04	25 (5%) 30 20	163, 215, 294, 309	0
All	All	7067/8222 (85%)	-0.12	168 (2%) 62 46	115, 183, 255, 340	0

The worst 5 of 168 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	L	318	ALA	6.7
5	L	321	ALA	6.6
2	I	1004	ASP	6.6
5	F	323	ASN	6.1
5	F	301	ASN	5.6

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
8	4C2	D	2004	35/35	0.92	0.39	2.54	166,166,166,175	0
8	4C2	J	2004	35/35	0.94	0.29	0.63	166,166,171,175	0
7	ZN	D	2003	1/1	1.00	0.24	-0.26	166,166,166,166	0
6	MG	D	2001	1/1	0.95	0.16	-0.64	166,166,166,166	0
7	ZN	D	2002	1/1	0.98	0.13	-0.72	166,166,166,166	0
7	ZN	J	2003	1/1	0.99	0.13	-1.06	217,217,217,217	0
7	ZN	J	2002	1/1	0.94	0.08	-1.11	201,201,201,201	0
6	MG	J	2001	1/1	0.94	0.28	-	166,166,166,166	0

6.5 Other polymers (i)

There are no such residues in this entry.