wwPDB X-ray Structure Validation Summary Report (i)

Jan 5, 2017 – 03:53 AM EST

PDB ID	:	5UAQ
Title	:	Escherichia coli RNA polymerase RpoB H526Y mutant
Authors	:	Molodtsov, V.; Scharf, N.T.; Stefan, M.A.; Garcia, G.A.; Murakami, K.S.
Deposited on	:	2016-12-19
Resolution	:	3.60 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:

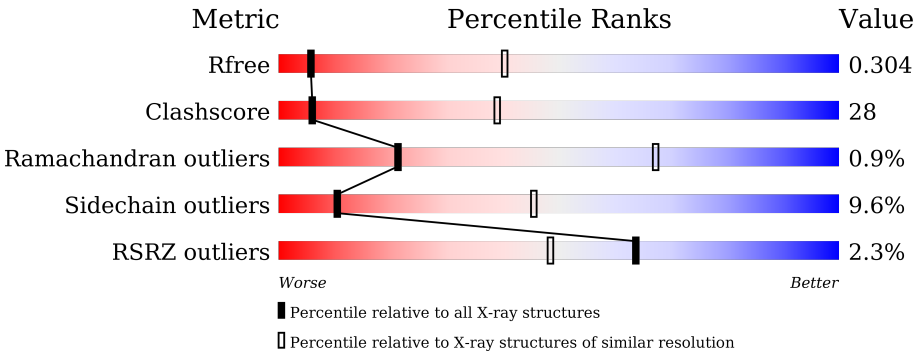
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 3.60 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.



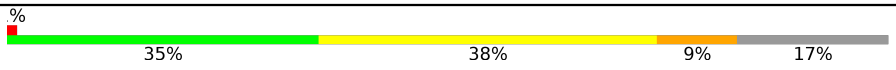
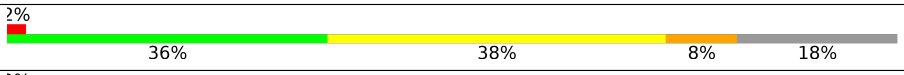
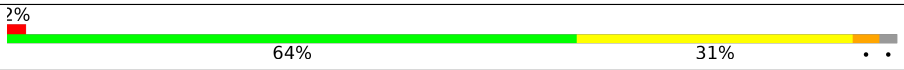
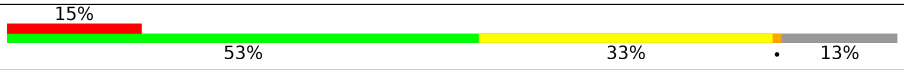
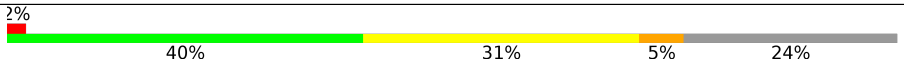
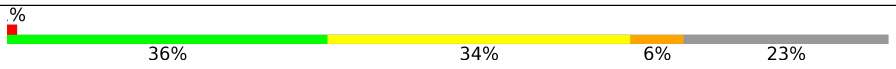
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

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	42% 42% 9% 6%
1	B	329	29% 33% 34%
1	G	329	29% 31% 6% 32%
1	H	329	4% 27% 35% 34%
2	C	1342	44% 47% 9%
2	I	1342	4% 50% 44% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	D	1407	
3	J	1407	
4	E	91	
4	K	91	
5	F	613	
5	L	613	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 55699 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	309	Total	C	N	O	S	0	0	0
			2403	1505	421	469	8			
1	B	217	Total	C	N	O	S	0	0	0
			1672	1044	295	327	6			
1	G	224	Total	C	N	O	S	0	0	0
			1730	1076	308	340	6			
1	H	217	Total	C	N	O	S	0	0	0
			1667	1041	293	327	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
			10572	6634	1839	2056	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10568	6632	1838	2055	43			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	526	TYR	HIS	engineered mutation	UNP P0A8V2
I	526	TYR	HIS	engineered mutation	UNP P0A8V2

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1166	Total	C	N	O	S	0	0	0
			9107	5723	1634	1704	46			
3	J	1155	Total	C	N	O	S	0	0	0
			9029	5676	1620	1687	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	467	Total	C	N	O	S	0	0	0
			3806	2385	677	721	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).

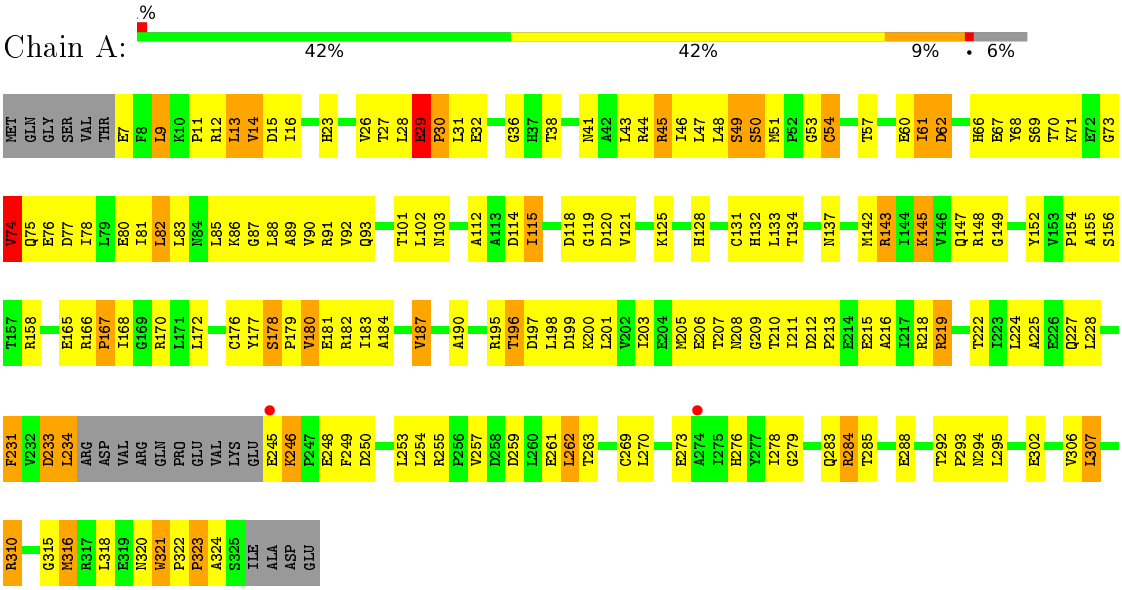
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	2	Total	Zn	0	0
			2	2		
7	D	2	Total	Zn	0	0
			2	2		

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.

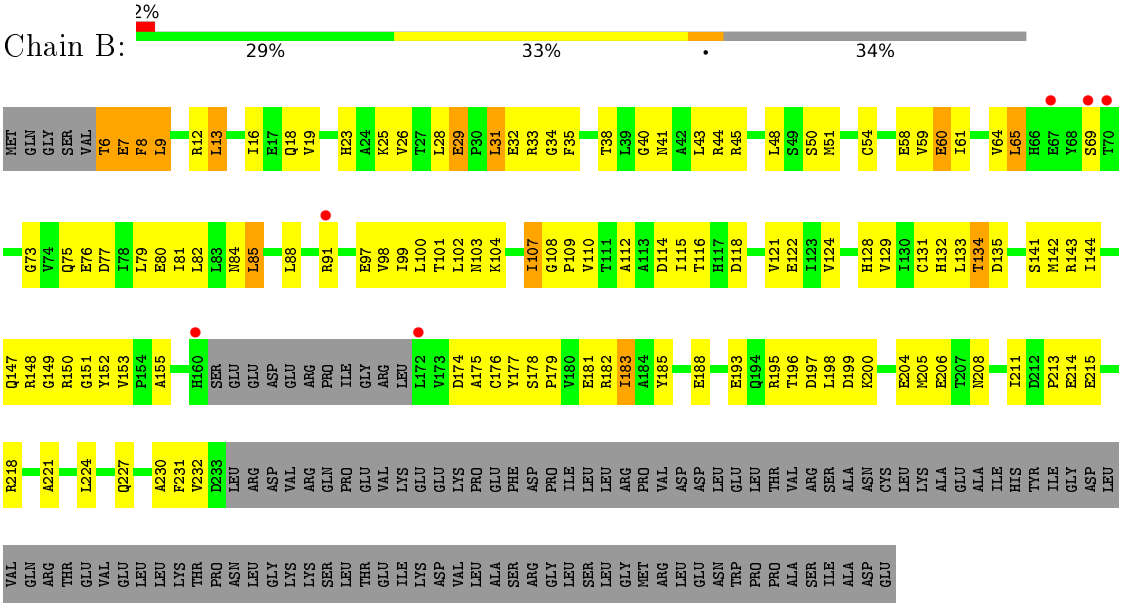
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



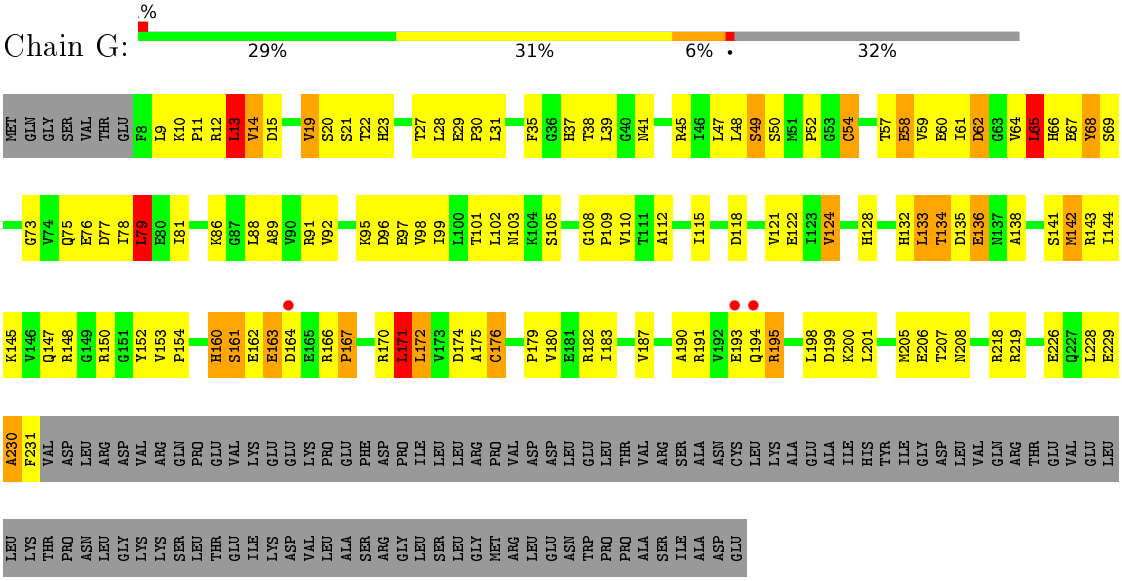
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:



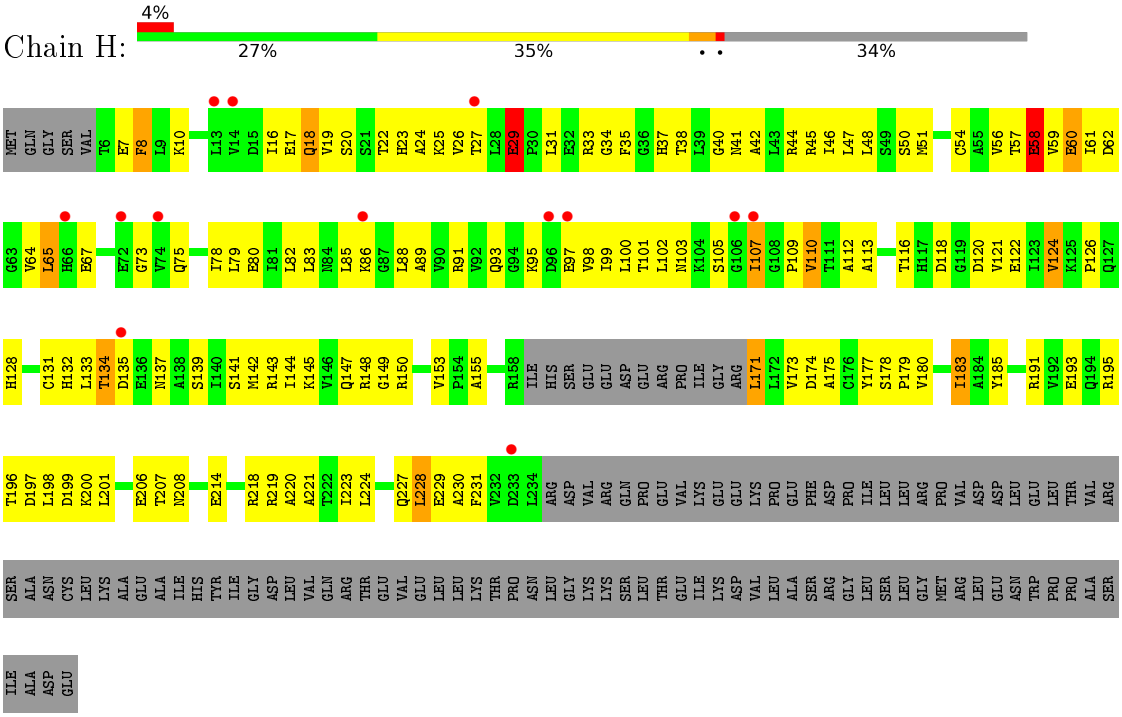
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain G:



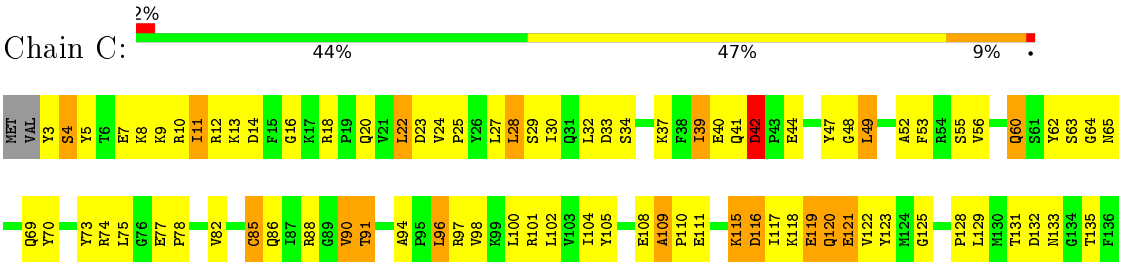
- Molecule 1: DNA-directed RNA polymerase subunit alpha

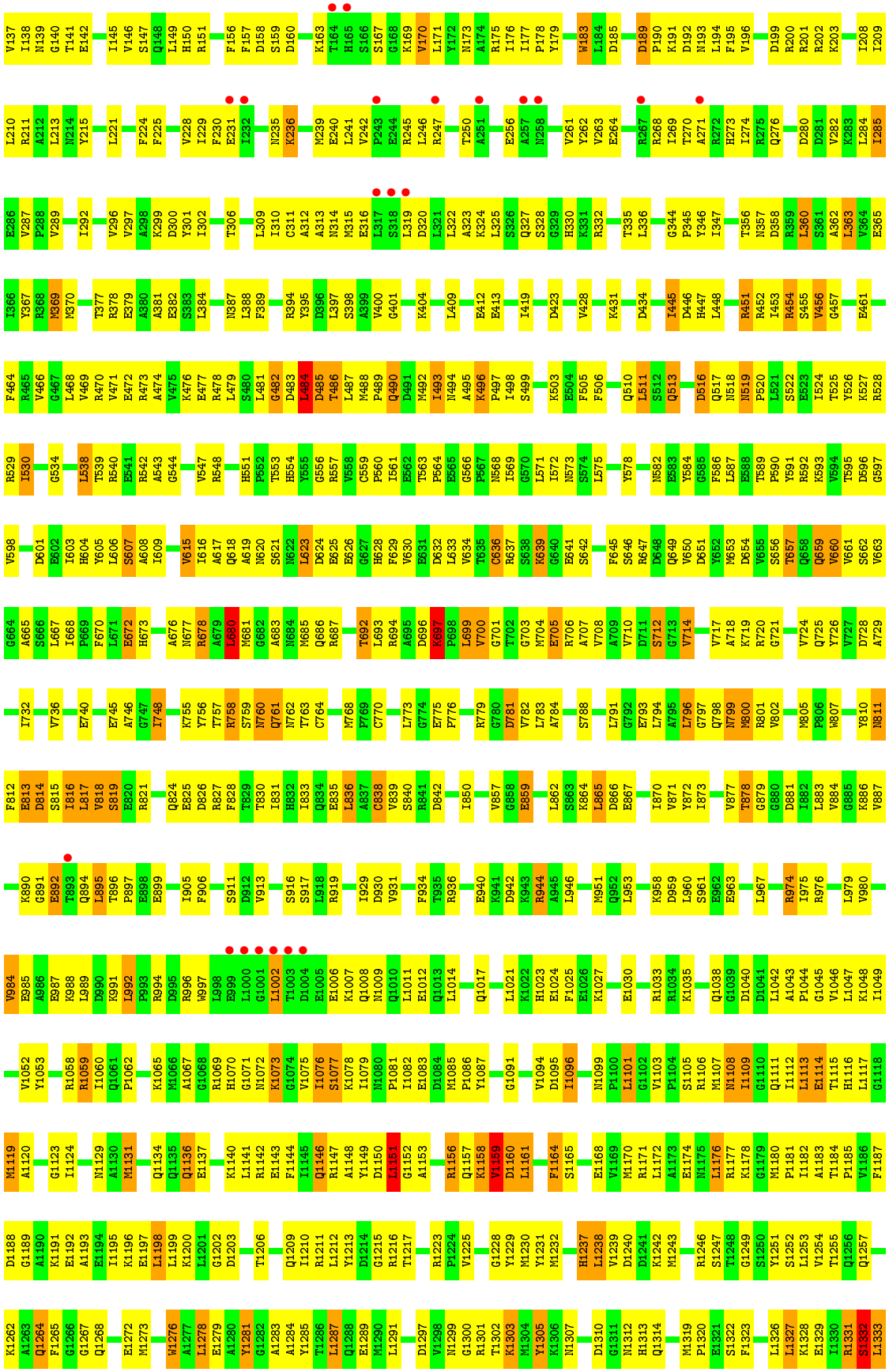
Chain H:



- Molecule 2: DNA-directed RNA polymerase subunit beta

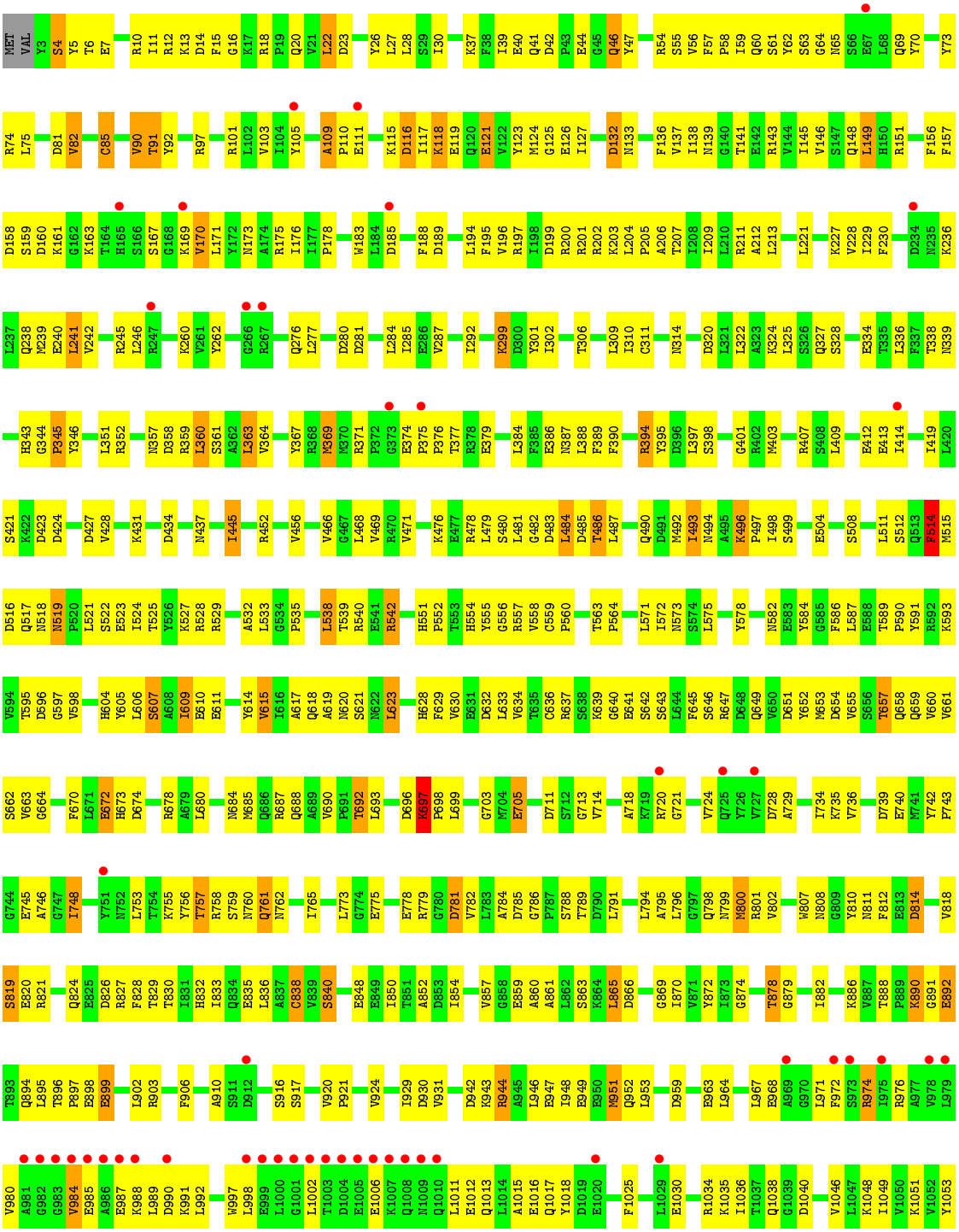
Chain C:

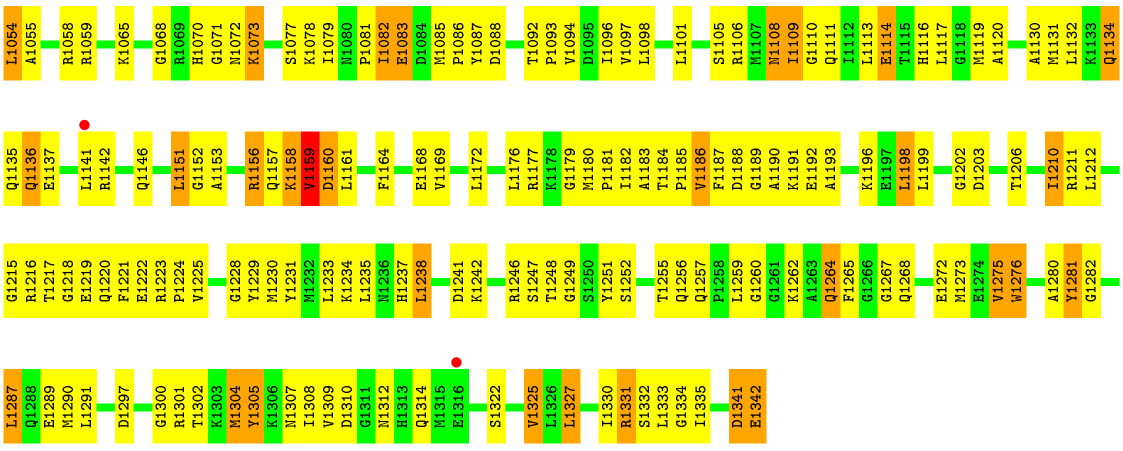




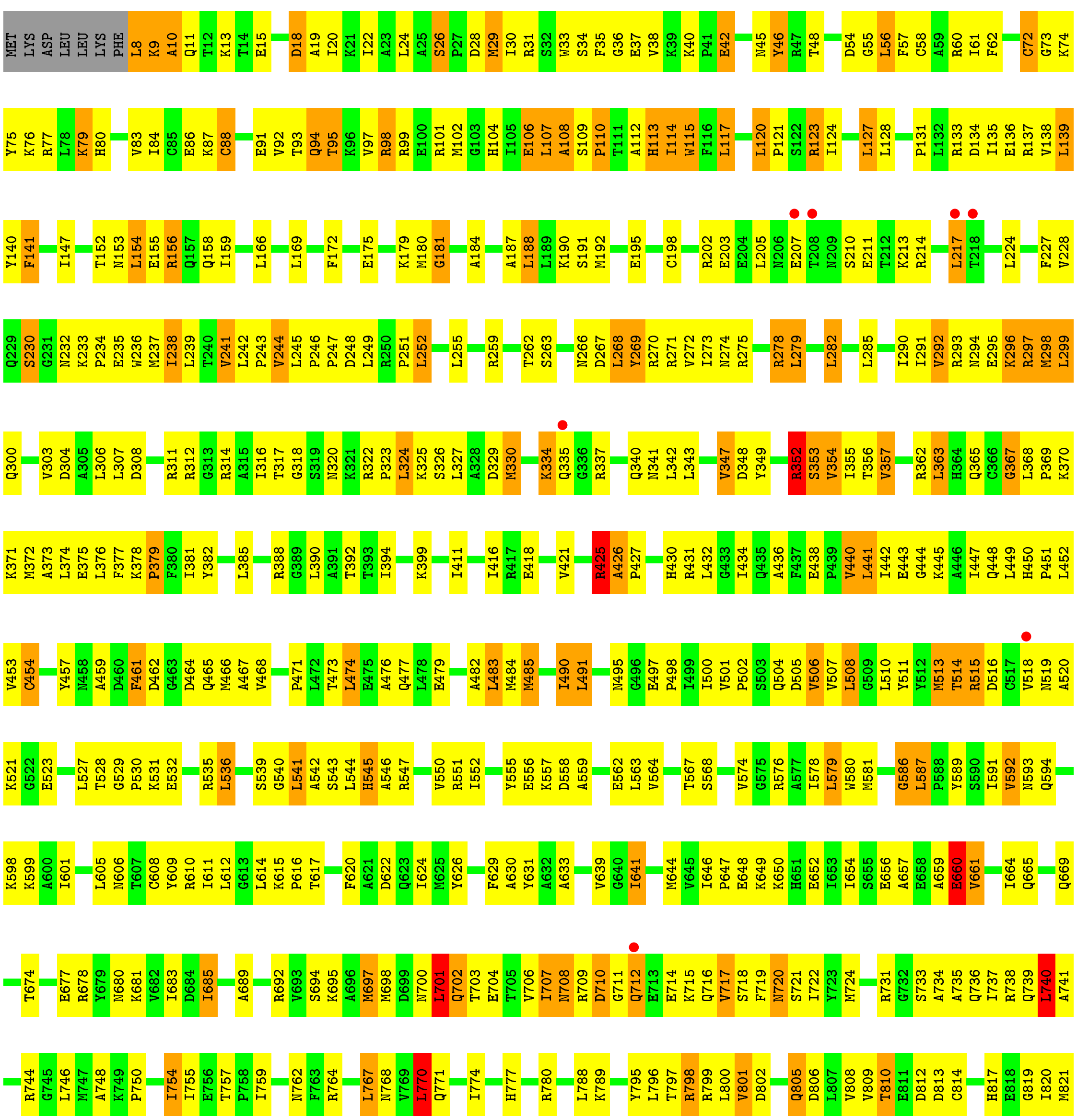
• Molecule 2: DNA-directed RNA polymerase subunit beta

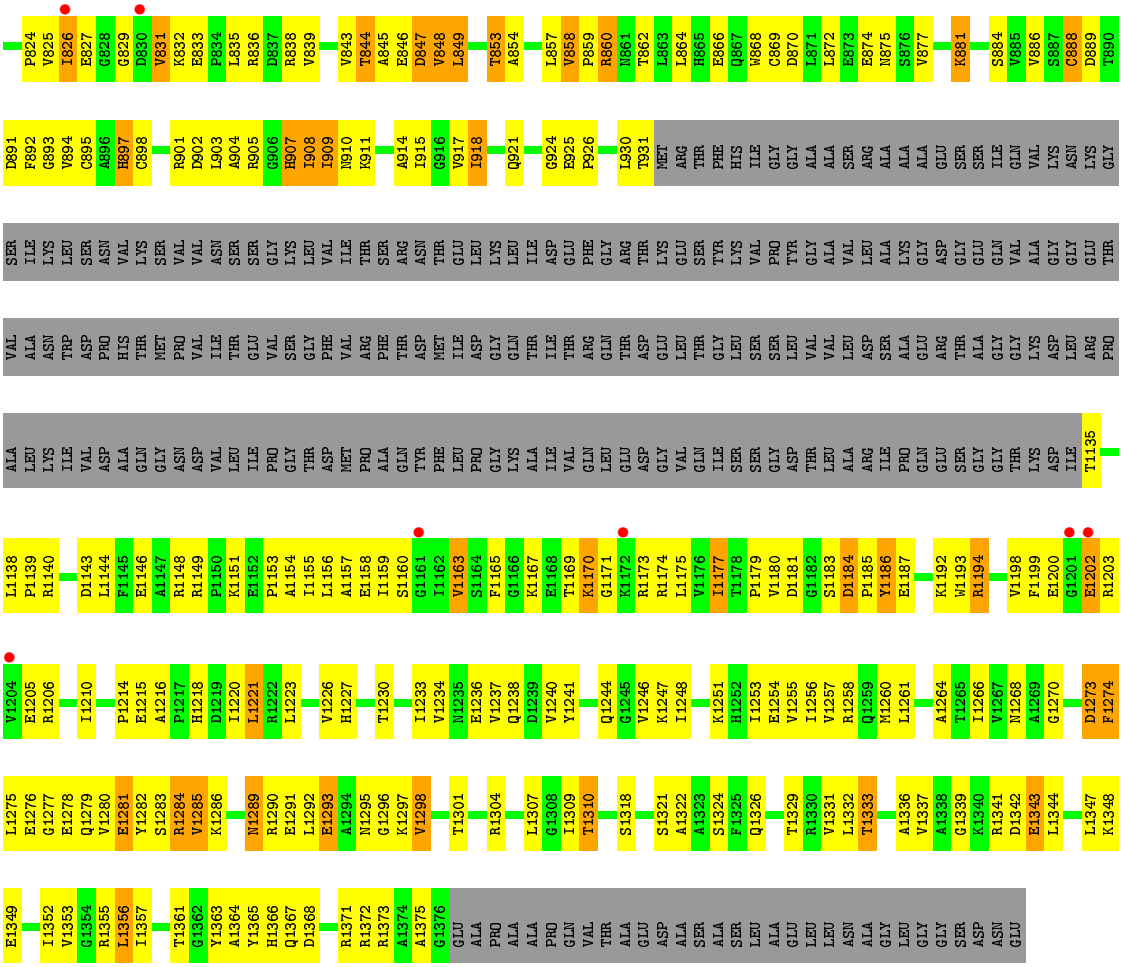
Chain I:



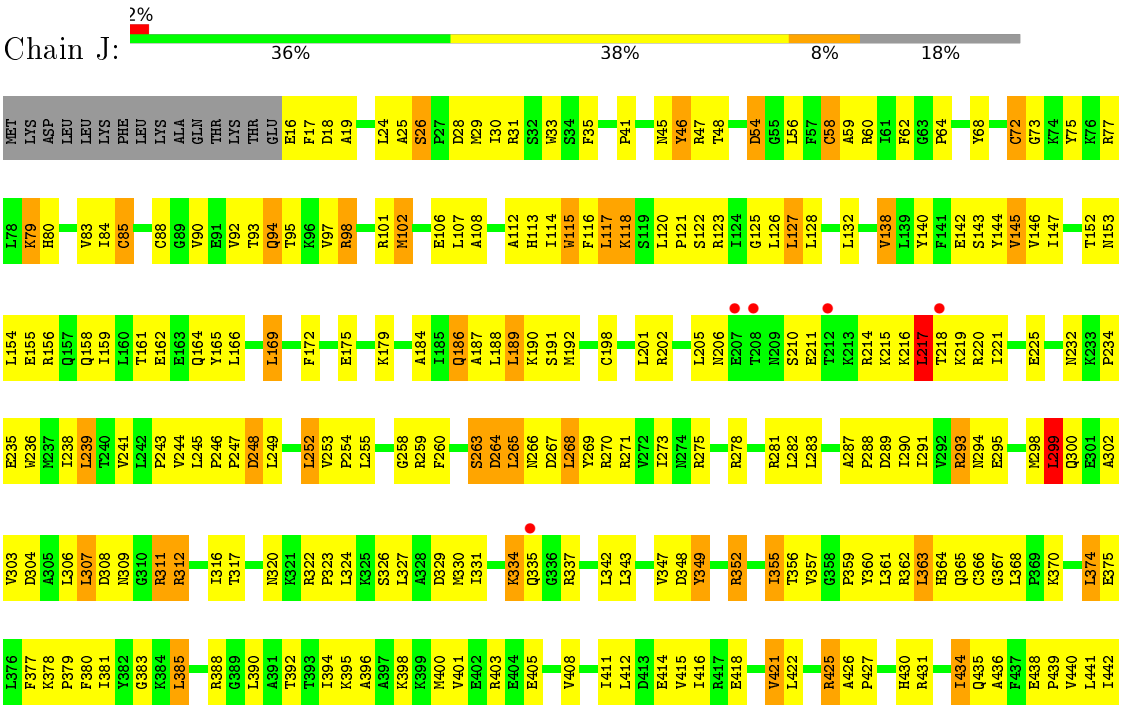


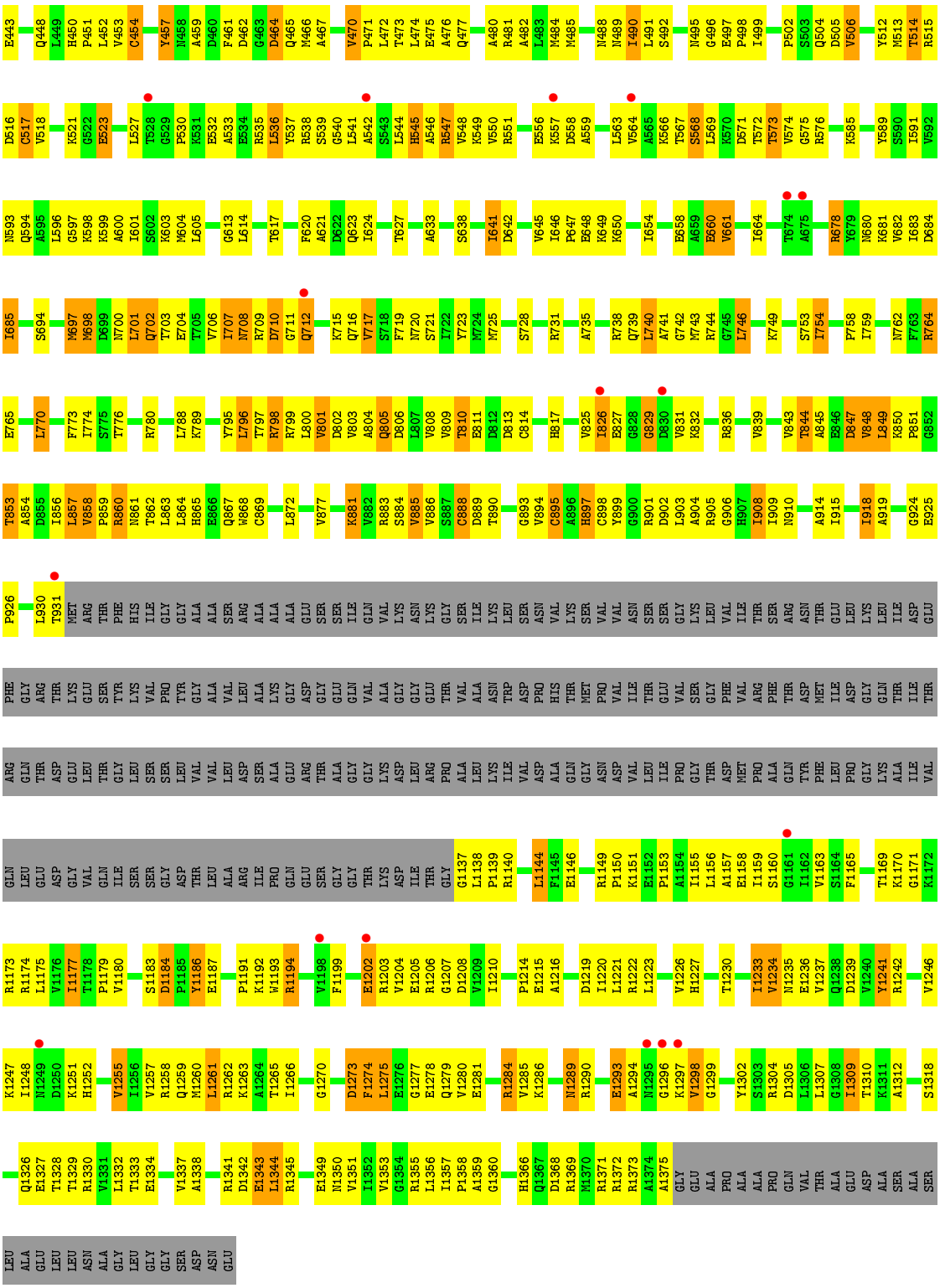
• Molecule 3: DNA-directed RNA polymerase subunit beta'



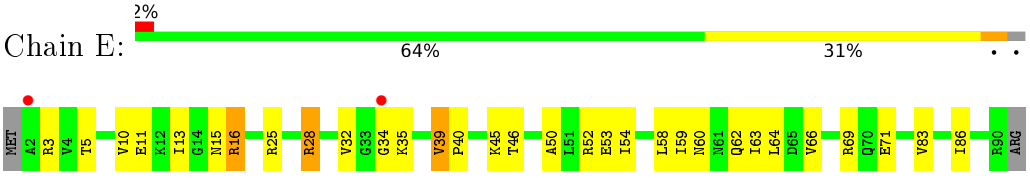


• Molecule 3: DNA-directed RNA polymerase subunit beta'



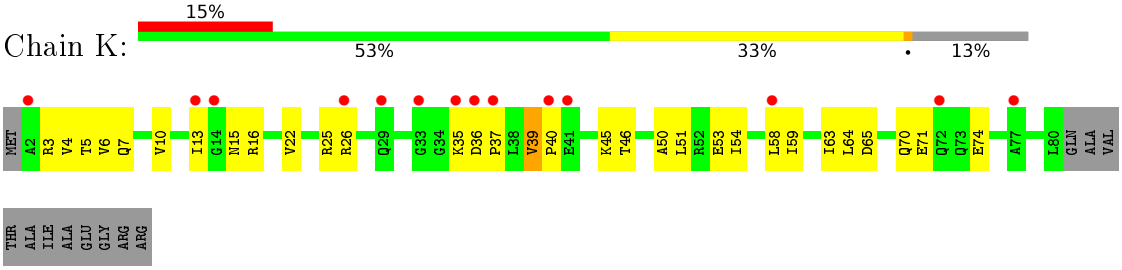


• Molecule 4: DNA-directed RNA polymerase subunit omega



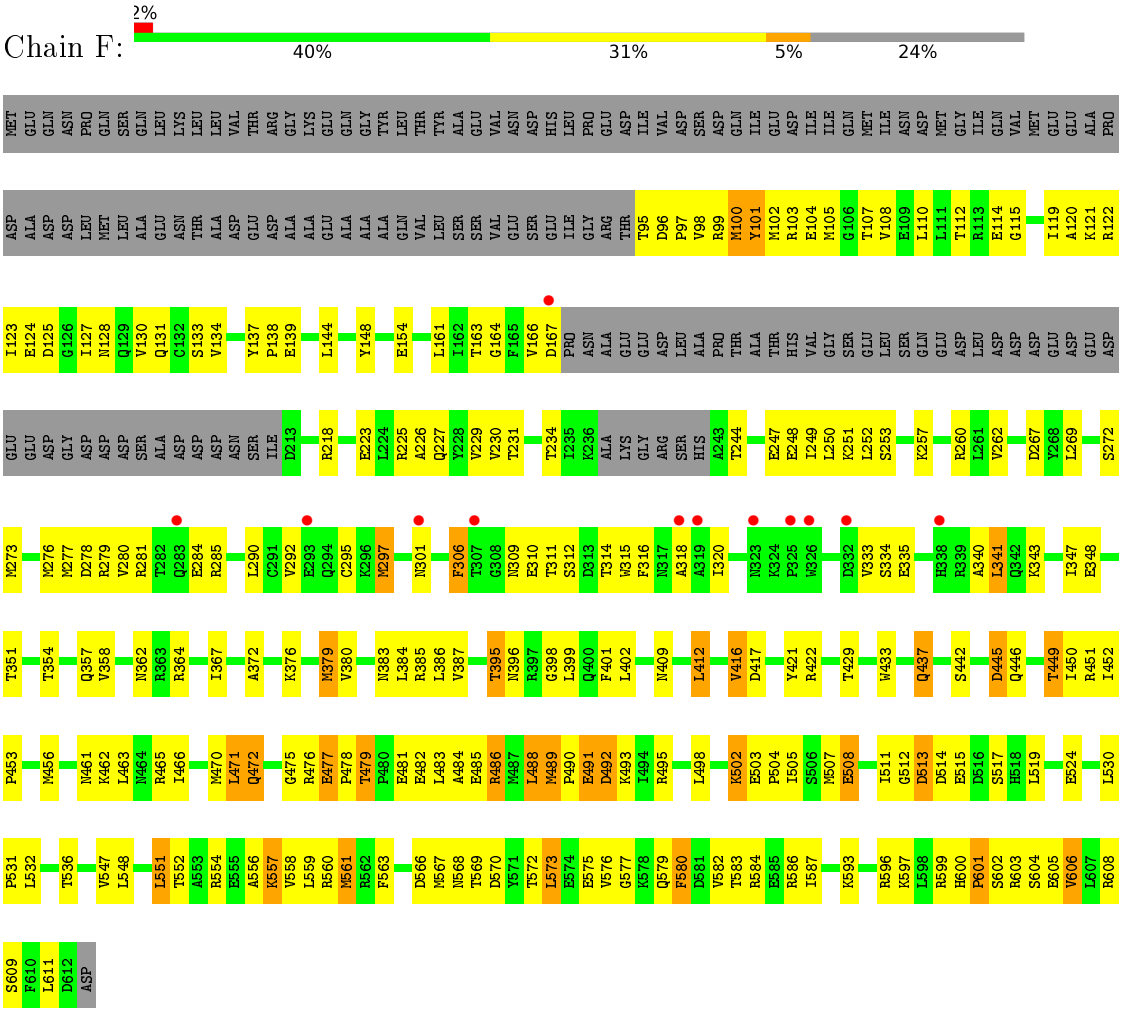
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain K:



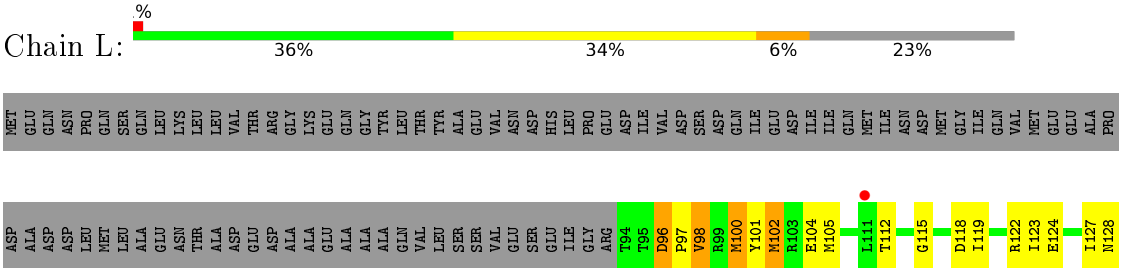
• Molecule 5: RNA polymerase sigma factor RpoD

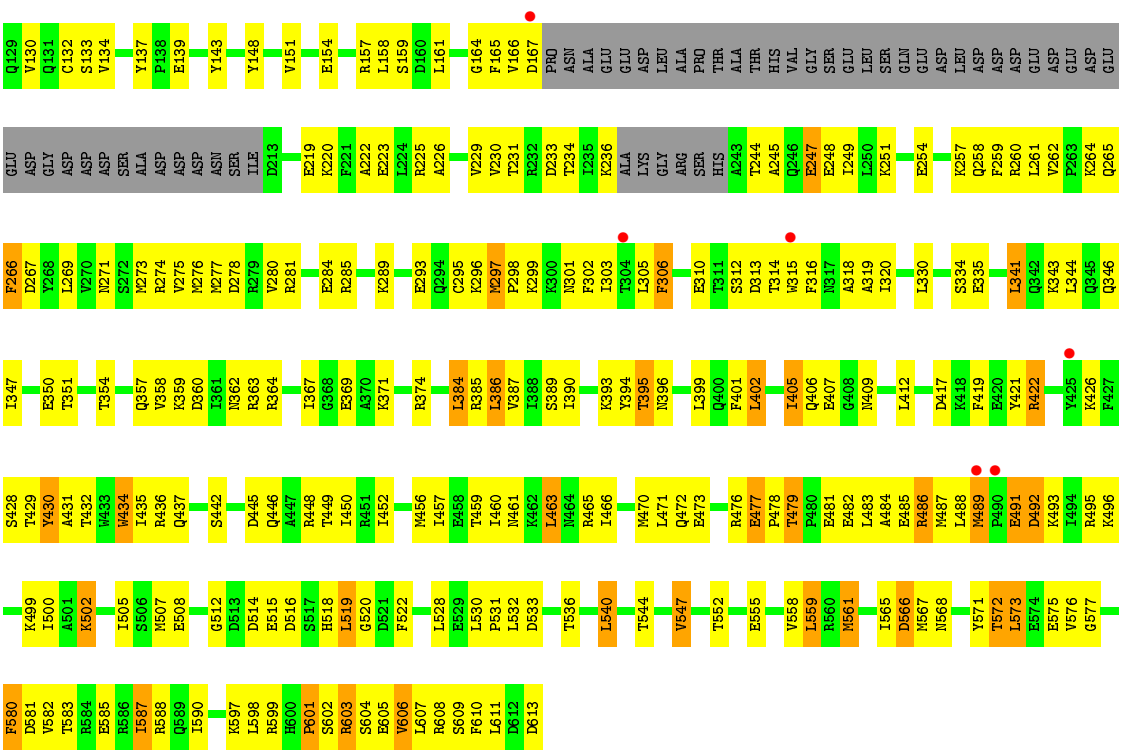
Chain F:



• Molecule 5: RNA polymerase sigma factor RpoD

Chain L:




Q129 V130 Q131 C132 S133 V134 Y137 P138 E139 Y143 Y148 V151 E154 R157 L158 S159 D160 L161 G164 F165 V166 D167 PRO ASN ALA GLU GLU ASP LEU ALA PRO THR ALA THR HIS VAL GLY SER GLU LEU SER GLN GLU ASP LEU ASP ASP ASP GLU ASP GLU ASP GLU
GLU ASP GLY ASP ASP SER ALA ASP ASP ASP ASN SER ILE D213 E219 K220 F221 A222 E223 L224 R225 A226 V229 V230 T231 R232 D233 T234 T235 K236 ALA LYS GLY ARG SER HIS A243 T244 A245 Q246 E247 E248 I249 L250 K251 E254 K257 Q258 F259 R260 L261 V262 P263 K264 Q265
F266 D267 Y268 L269 V270 N271 S272 M273 R274 V275 M276 M277 D278 R279 V280 R281 E284 R285 K289 E293 Q294 C295 K296 M297 P298 K299 K300 N301 F302 I303 T304 L305 F306 E310 T311 S312 D313 T314 W315 F316 N317 A318 A319 I320 L330 S334 E335 I341 Q342 K343 L344 Q345 Q346
I347 E350 T351 T354 Q357 V358 K359 D360 I361 N362 R363 R364 I367 G368 E369 A370 K371 R374 L384 R385 L386 V387 I388 S389 I390 K393 Y394 T395 N396 L399 Q400 F401 L402 T405 Q406 E407 G408 N409 L412 D417 K418 F419 E420 Y421 R422 Y425 K426 F427
S428 T429 Y430 A431 T432 W433 W434 I435 R436 Q437 S442 D445 Q446 A447 R448 T449 I450 R451 I452 M456 I457 E458 T459 I460 N461 K462 L463 N464 R465 I466 M470 L471 Q472 E473 R476 E477 P478 T479 P480 E481 E482 L483 A484 E485 R486 M487 L488 M489 P490 E491 D492 K493 I494 R495 K496
K499 I500 A501 K502 I505 S506 M507 E508 G512 D513 D514 E515 D516 S517 H518 L519 G520 D521 F522 L528 E529 L530 P531 L532 D533 T536 L540 T544 V547 T552 E555 V558 L559 R560 M561 I565 D566 M567 N568 Y571 T572 L573 E574 E575 V576 G577
P580 D581 V582 T583 R584 E585 R586 I587 R588 Q589 I590 K597 L598 R599 H600 P601 S602 R603 S604 E605 V606 L607 R608 S609 F610 L611 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	185.36Å 206.28Å 308.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 3.60 29.90 – 3.60	Depositor EDS
% Data completeness (in resolution range)	93.7 (29.90-3.60) 93.7 (29.90-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 3.56Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.246 , 0.305 0.245 , 0.304	Depositor DCC
R_{free} test set	1937 reflections (1.51%)	DCC
Wilson B-factor (Å^2)	142.2	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 91.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	55699	wwPDB-VP
Average B, all atoms (Å^2)	157.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% 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, 0.333 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: 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	0.84	4/2435 (0.2%)	1.07	12/3300 (0.4%)
1	B	0.75	1/1692 (0.1%)	1.01	5/2293 (0.2%)
1	G	0.58	0/1751	1.05	9/2373 (0.4%)
1	H	0.59	0/1686	0.91	4/2285 (0.2%)
2	C	1.17	37/10741 (0.3%)	1.21	65/14492 (0.4%)
2	I	0.80	7/10737 (0.1%)	0.97	15/14487 (0.1%)
3	D	1.21	60/9246 (0.6%)	1.24	74/12478 (0.6%)
3	J	1.02	27/9168 (0.3%)	1.13	52/12374 (0.4%)
4	E	0.65	0/693	0.83	0/935
4	K	0.38	0/629	0.61	0/847
5	F	0.82	2/3857 (0.1%)	1.05	10/5184 (0.2%)
5	L	0.77	3/3872 (0.1%)	0.99	12/5205 (0.2%)
All	All	0.98	141/56507 (0.2%)	1.10	258/76253 (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
1	A	0	2
1	G	0	1
2	C	0	11
2	I	0	2
3	D	0	12
3	J	0	9
5	F	0	1
5	L	0	1
All	All	0	39

The worst 5 of 141 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	811	ASN	CB-CG	-9.14	1.30	1.51
1	A	131	CYS	CB-SG	-8.93	1.67	1.82
3	J	145	VAL	CB-CG2	-8.81	1.34	1.52
2	C	636	CYS	CB-SG	-8.52	1.67	1.82
3	J	72	CYS	CB-SG	-7.87	1.68	1.82

The worst 5 of 258 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1287	LEU	CB-CG-CD2	-14.16	86.92	111.00
3	D	376	LEU	CB-CG-CD2	-10.83	92.59	111.00
3	D	114	ILE	CG1-CB-CG2	-10.71	87.84	111.40
2	C	796	LEU	CB-CG-CD2	-9.94	94.10	111.00
3	D	188	LEU	CB-CG-CD2	-9.88	94.20	111.00

There are no chirality outliers.

5 of 39 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	321	TRP	Peptide
1	A	49	SER	Mainchain
2	C	109	ALA	Peptide
2	C	236	LYS	Peptide
2	C	473	ARG	Mainchain

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	2403	0	2453	197	0
1	B	1672	0	1693	112	0
1	G	1730	0	1756	145	0
1	H	1667	0	1689	123	1
2	C	10572	0	10584	657	3
2	I	10568	0	10578	602	0
3	D	9107	0	9308	612	0
3	J	9029	0	9225	587	0
4	E	691	0	695	22	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	627	0	634	26	0
5	F	3806	0	3873	199	2
5	L	3821	0	3884	190	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
All	All	55699	0	56372	3190	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 28.

The worst 5 of 3190 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:THR:O	1:A:28:LEU:HD12	1.10	1.23
2:I:27:LEU:O	2:I:528:ARG:NH1	1.78	1.17
1:A:27:THR:O	1:A:28:LEU:CD1	1.93	1.17
3:D:1280:VAL:HG11	3:D:1304:ARG:HH21	1.16	1.08
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.36	1.08

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)
2:C:33:ASP:OD1	5:F:554:ARG:NH2[4_455]	1.99	0.21
2:C:44:GLU:OE1	5:F:596:ARG:NH1[4_455]	2.05	0.15
2:C:940:GLU:OE1	1:H:139:SER:OG[4_455]	2.05	0.15

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	305/329 (93%)	271 (89%)	25 (8%)	9 (3%)	5 44
1	B	213/329 (65%)	191 (90%)	20 (9%)	2 (1%)	21 67
1	G	222/329 (68%)	182 (82%)	28 (13%)	12 (5%)	2 27
1	H	213/329 (65%)	193 (91%)	20 (9%)	0	100 100
2	C	1338/1342 (100%)	1225 (92%)	103 (8%)	10 (1%)	26 72
2	I	1338/1342 (100%)	1226 (92%)	100 (8%)	12 (1%)	21 67
3	D	1162/1407 (83%)	1074 (92%)	79 (7%)	9 (1%)	24 69
3	J	1151/1407 (82%)	1064 (92%)	82 (7%)	5 (0%)	39 80
4	E	87/91 (96%)	79 (91%)	8 (9%)	0	100 100
4	K	77/91 (85%)	74 (96%)	3 (4%)	0	100 100
5	F	461/613 (75%)	422 (92%)	37 (8%)	2 (0%)	39 80
5	L	463/613 (76%)	423 (91%)	39 (8%)	1 (0%)	52 87
All	All	7030/8222 (86%)	6424 (91%)	544 (8%)	62 (1%)	21 67

5 of 62 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	A	30	PRO
1	A	324	ALA
1	B	232	VAL
2	C	345	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	268/286 (94%)	249 (93%)	19 (7%)	18 59
1	B	184/286 (64%)	166 (90%)	18 (10%)	10 44
1	G	191/286 (67%)	179 (94%)	12 (6%)	22 64
1	H	183/286 (64%)	165 (90%)	18 (10%)	10 44

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	C	1155/1157 (100%)	1046 (91%)	109 (9%)	11 47
2	I	1154/1157 (100%)	1046 (91%)	108 (9%)	11 47
3	D	975/1168 (84%)	875 (90%)	100 (10%)	9 42
3	J	967/1168 (83%)	869 (90%)	98 (10%)	9 43
4	E	72/75 (96%)	64 (89%)	8 (11%)	8 38
4	K	67/75 (89%)	63 (94%)	4 (6%)	24 65
5	F	416/540 (77%)	373 (90%)	43 (10%)	9 42
5	L	418/540 (77%)	372 (89%)	46 (11%)	8 39
All	All	6050/7024 (86%)	5467 (90%)	583 (10%)	10 45

5 of 583 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	335	GLU
1	H	193	GLU
5	L	100	MET
5	F	445	ASP
5	F	606	VAL

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	396	ASN
2	I	343	HIS
5	L	129	GLN
5	F	406	GLN
5	F	518	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

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	309/329 (93%)	-0.32	2 (0%) 90 83	99, 147, 225, 245	0
1	B	217/329 (65%)	-0.02	6 (2%) 56 42	112, 194, 254, 272	0
1	G	224/329 (68%)	-0.07	3 (1%) 79 66	163, 206, 241, 270	0
1	H	217/329 (65%)	0.07	13 (5%) 25 17	146, 213, 252, 285	0
2	C	1340/1342 (99%)	-0.35	21 (1%) 74 61	74, 121, 234, 285	0
2	I	1340/1342 (99%)	-0.16	50 (3%) 45 32	86, 159, 261, 388	0
3	D	1166/1407 (82%)	-0.30	14 (1%) 81 69	72, 112, 215, 264	0
3	J	1155/1407 (82%)	-0.22	22 (1%) 70 56	86, 138, 229, 274	0
4	E	89/91 (97%)	-0.02	2 (2%) 65 50	147, 183, 216, 241	0
4	K	79/91 (86%)	0.78	14 (17%) 2 2	202, 277, 319, 350	0
5	F	467/613 (76%)	-0.23	12 (2%) 59 44	93, 165, 290, 340	0
5	L	469/613 (76%)	-0.30	7 (1%) 76 64	116, 178, 288, 353	0
All	All	7072/8222 (86%)	-0.22	166 (2%) 64 48	72, 147, 251, 388	0

The worst 5 of 166 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	982	GLY	8.9
3	D	335	GLN	6.3
2	I	1001	GLY	5.3
1	B	160	HIS	5.1
2	I	1000	LEU	4.9

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 (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
7	ZN	D	1502	1/1	0.81	0.13	-0.94	134,134,134,134	0
7	ZN	D	1503	1/1	0.99	0.06	-0.97	51,51,51,51	0
7	ZN	J	1503	1/1	0.95	0.09	-1.43	97,97,97,97	0
7	ZN	J	1502	1/1	0.97	0.02	-1.80	131,131,131,131	0
6	MG	D	1501	1/1	0.94	0.54	-	87,87,87,87	0
6	MG	J	1501	1/1	0.92	0.35	-	94,94,94,94	0

6.5 Other polymers (i)

There are no such residues in this entry.