wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 09:07 AM GMT

PDB ID	:	3H0G
Title	:	RNA Polymerase II from Schizosaccharomyces pombe
Authors	:	Spahr, H.; Calero, G.; Bushnell, D.A.; Kornberg, R.D.
Deposited on	:	2009-04-09
Resolution	:	3.65 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:

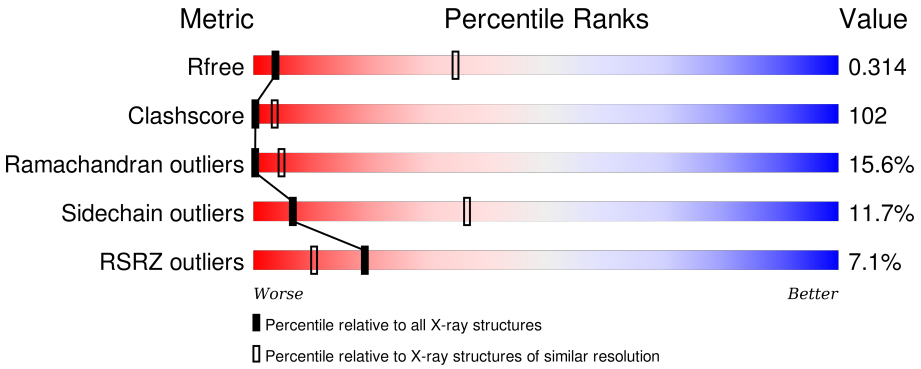
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.65 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	1010 (3.82-3.50)
Clashscore	102246	1125 (3.82-3.50)
Ramachandran outliers	100387	1079 (3.82-3.50)
Sidechain outliers	100360	1078 (3.82-3.50)
RSRZ outliers	91569	1017 (3.82-3.50)

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	1752	5% 19% 45% 18% • 15%
1	M	1752	10% 19% 45% 17% • 16%
2	B	1210	2% 25% 54% 14% • 5%
2	N	1210	10% 25% 54% 14% • 5%
3	C	297	30% 48% 10% • 11%

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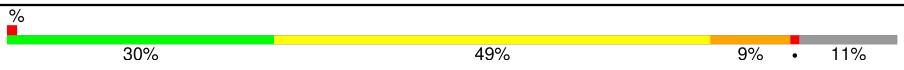
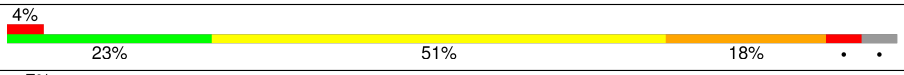
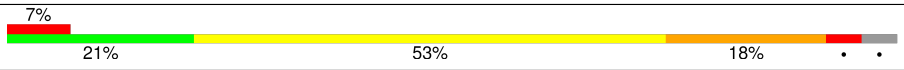
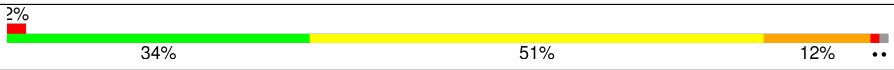
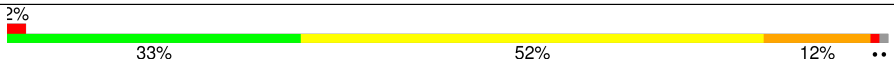
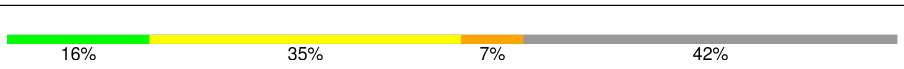
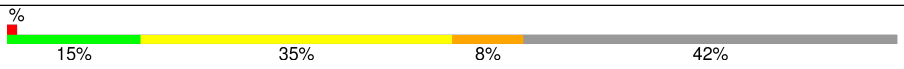
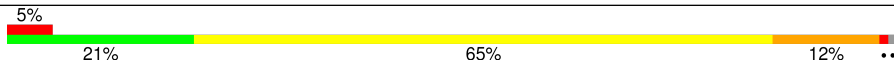
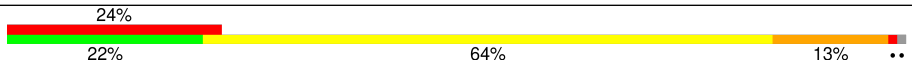
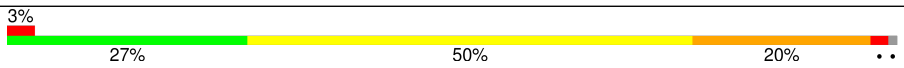
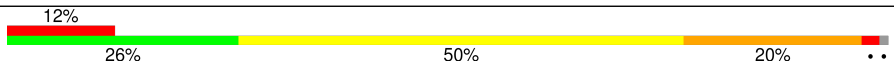
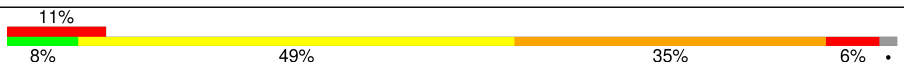
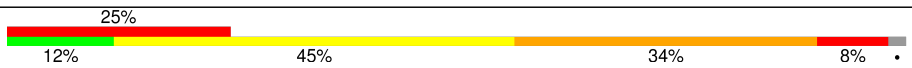
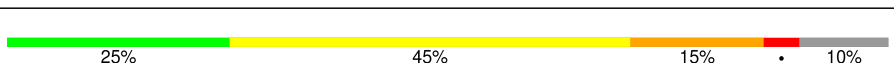
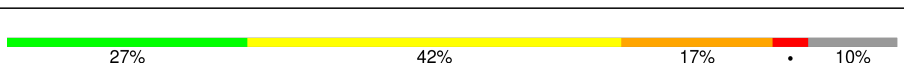
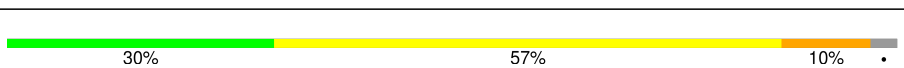
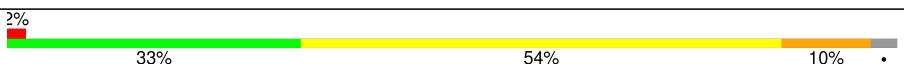
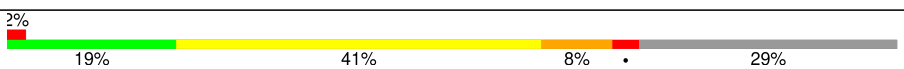
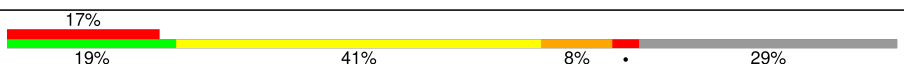
Mol	Chain	Length	Quality of chain
3	O	297	
4	D	135	
4	P	135	
5	E	210	
5	Q	210	
6	F	142	
6	R	142	
7	G	172	
7	S	172	
8	H	125	
8	T	125	
9	I	113	
9	U	113	
10	J	71	
10	V	71	
11	K	123	
11	W	123	
12	L	63	
12	X	63	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 62870 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 II subunit rpb1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1496	Total	C	N	O	S	0	0	0
			11802	7415	2071	2246	70			
1	M	1476	Total	C	N	O	S	0	0	0
			11666	7334	2047	2216	69			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1150	Total	C	N	O	S	0	0	0
			9180	5772	1630	1716	62			
2	N	1150	Total	C	N	O	S	0	0	0
			9180	5772	1630	1716	62			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	263	Total	C	N	O	S	0	0	0
			2088	1315	355	406	12			
3	O	263	Total	C	N	O	S	0	0	0
			2088	1315	355	406	12			

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit rpb4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	130	Total	C	N	O	S	0	0	0
			1036	649	176	205	6			
4	P	130	Total	C	N	O	S	0	0	0
			1036	649	176	205	6			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	207	Total	C	N	O	S	0	0	0
			1663	1050	301	306	6			
5	Q	207	Total	C	N	O	S	0	0	0
			1663	1050	301	306	6			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	83	Total	C	N	O	S	0	0	0
			656	416	112	125	3			
6	R	83	Total	C	N	O	S	0	0	0
			656	416	112	125	3			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit rpb7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	170	Total	C	N	O	S	0	0	0
			1330	860	217	247	6			
7	S	170	Total	C	N	O	S	0	0	0
			1330	860	217	247	6			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	124	Total	C	N	O	S	0	0	0
			996	631	167	195	3			
8	T	124	Total	C	N	O	S	0	0	0
			996	631	167	195	3			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	111	Total	C	N	O	S	0	0	0
			902	551	164	176	11			
9	U	111	Total	C	N	O	S	0	0	0
			902	551	164	176	11			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	64	Total	C	N	O	S	0	0	0
			518	330	87	94	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	V	64	Total	C	N	O	S	0	0	0
			518	330	87	94	7			

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	119	Total	C	N	O	S	0	0	0
			955	608	159	182	6			
11	W	119	Total	C	N	O	S	0	0	0
			955	608	159	182	6			

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	45	Total	C	N	O	S	0	0	0
			368	225	74	61	8			
12	X	45	Total	C	N	O	S	0	0	0
			368	225	74	61	8			

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	J	1	Total	Zn	0	0
			1	1		
13	B	1	Total	Zn	0	0
			1	1		
13	I	2	Total	Zn	0	0
			2	2		
13	C	1	Total	Zn	0	0
			1	1		
13	V	1	Total	Zn	0	0
			1	1		
13	A	2	Total	Zn	0	0
			2	2		
13	N	1	Total	Zn	0	0
			1	1		
13	U	2	Total	Zn	0	0
			2	2		
13	X	1	Total	Zn	0	0
			1	1		
13	O	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	L	1	Total Zn 1 1	0	0
13	M	2	Total Zn 2 2	0	0

- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

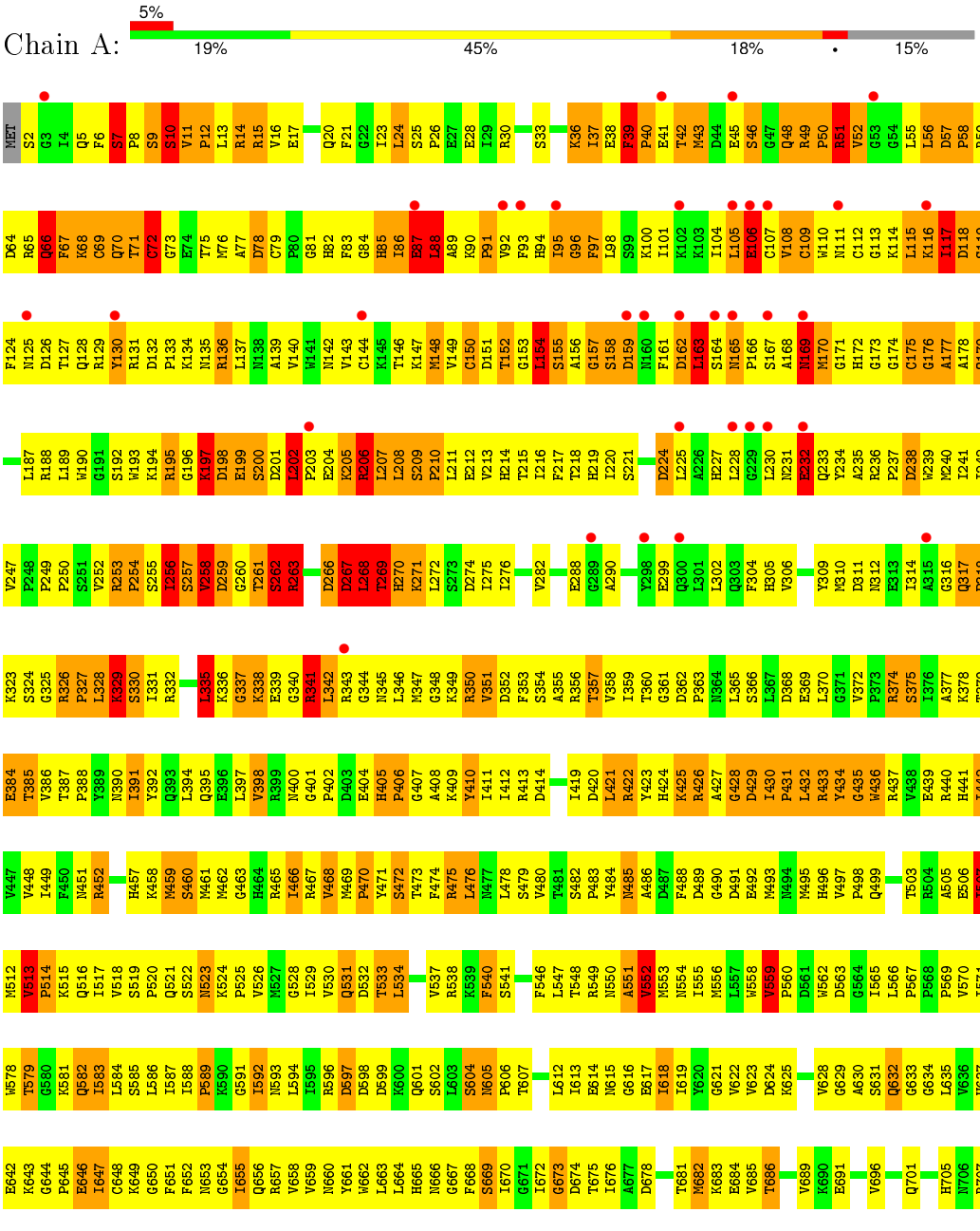
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	1	Total Mg 1 1	0	0
14	M	1	Total Mg 1 1	0	0

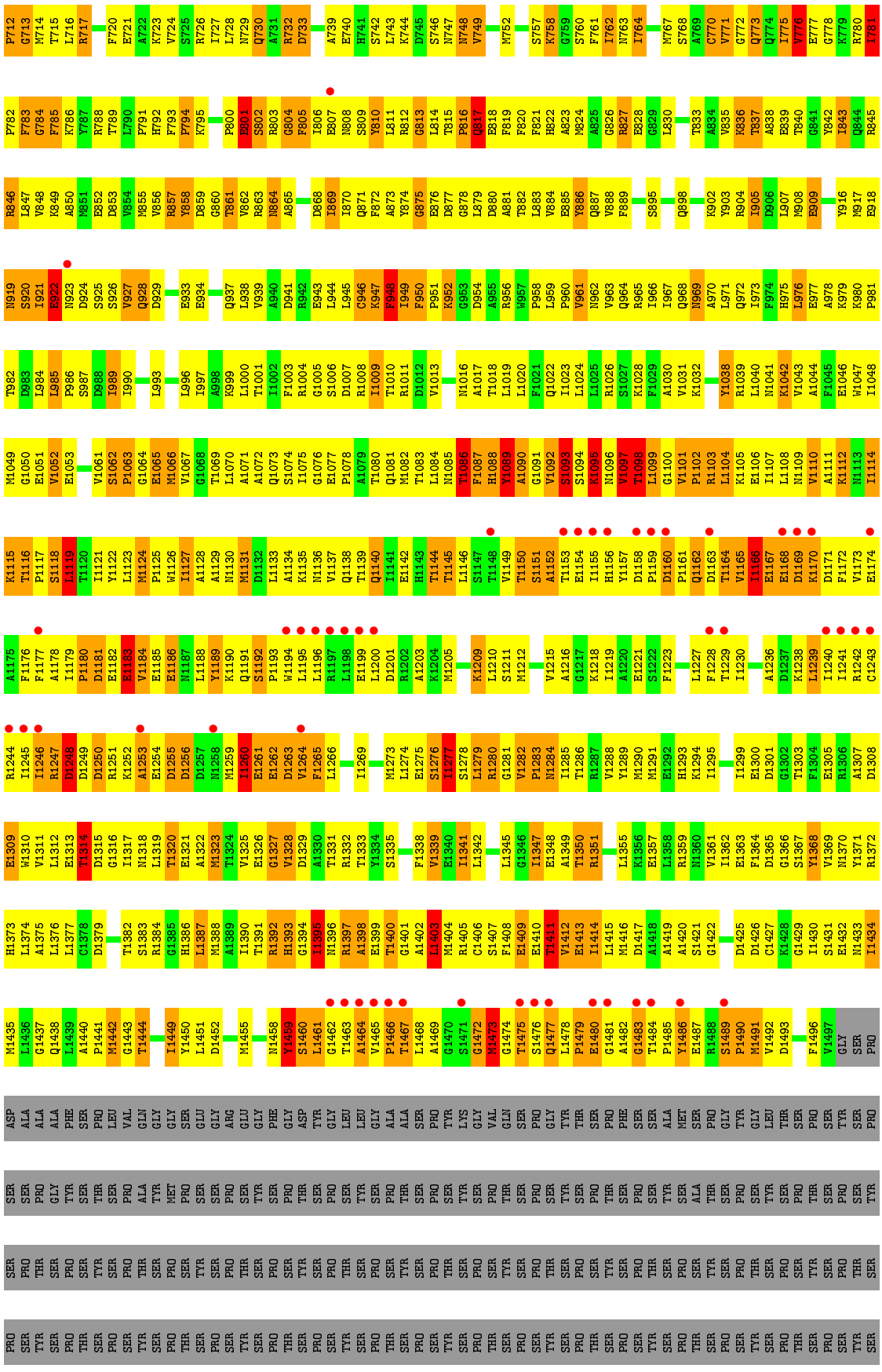
3 Residue-property plots (i)

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 II subunit rpb1

Chain A:

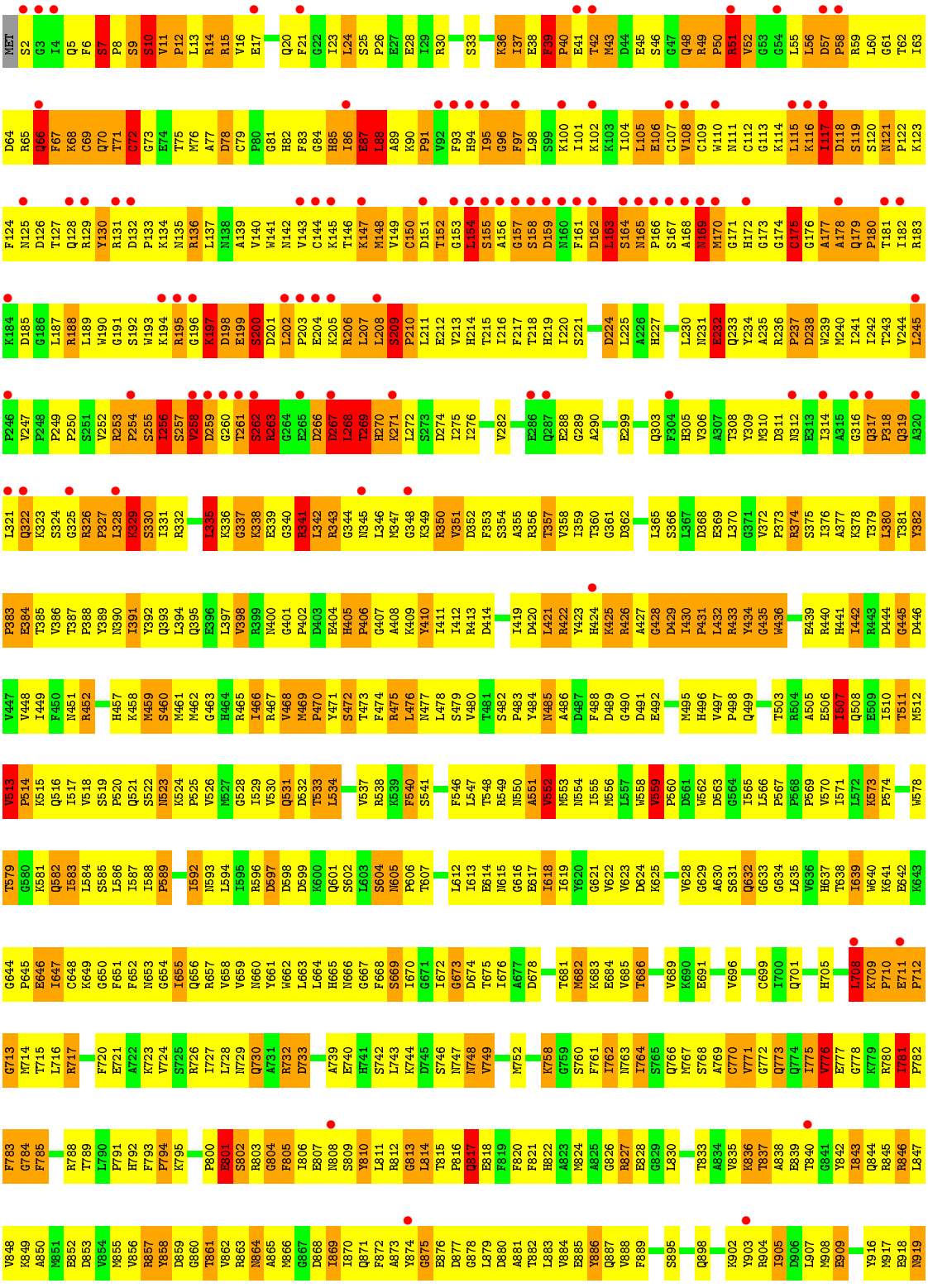


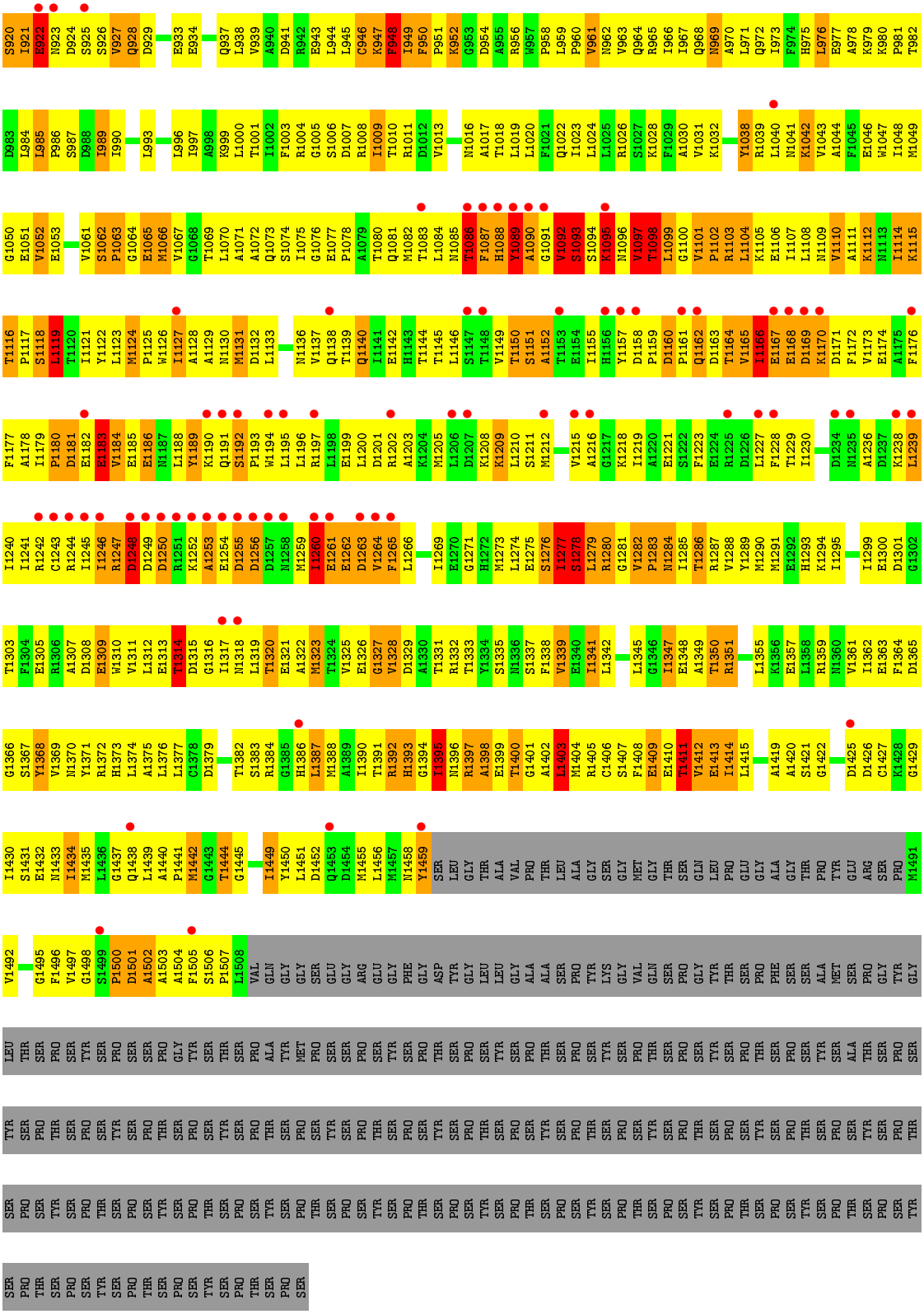


PRO THR SER PRO SER TYR SER PRO THR SER PRO SER

- Molecule 1: DNA-directed RNA polymerase II subunit rpb1

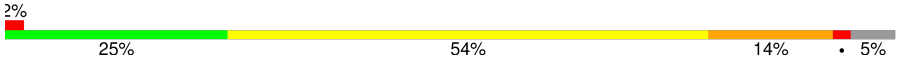
Chain M:

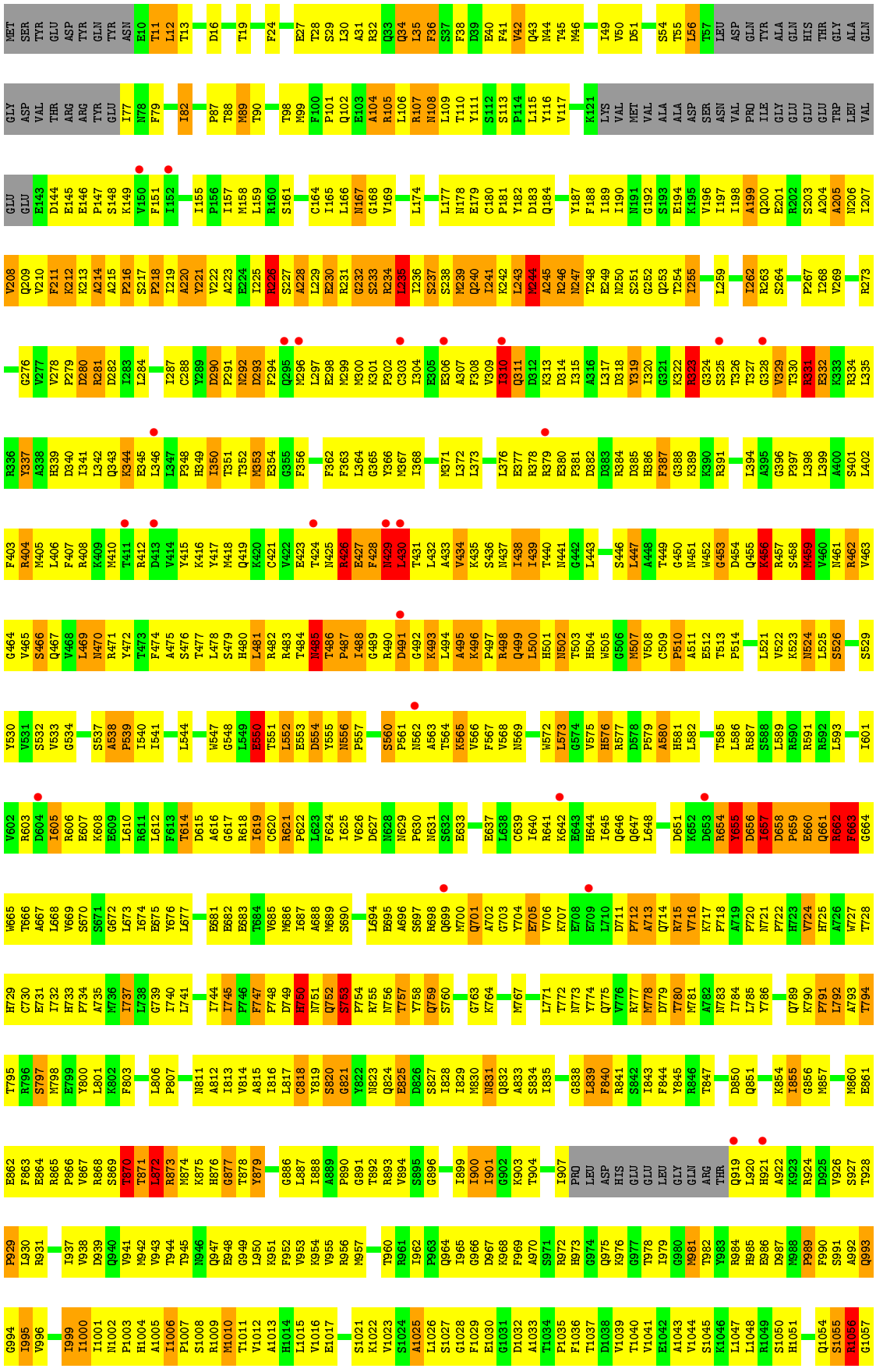


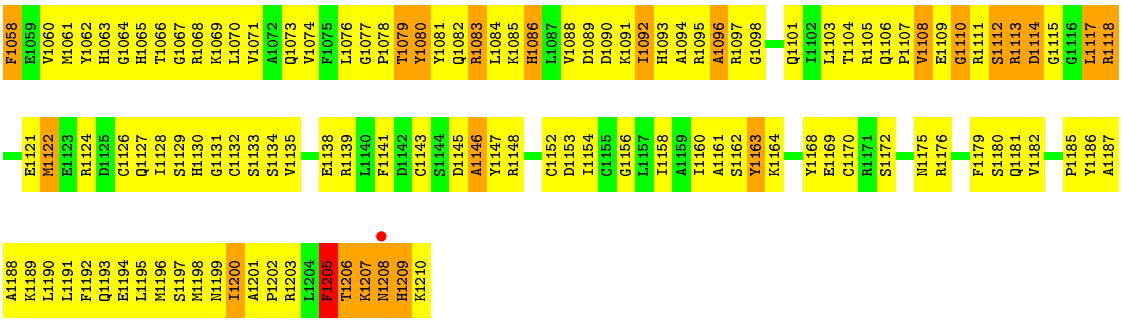


• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

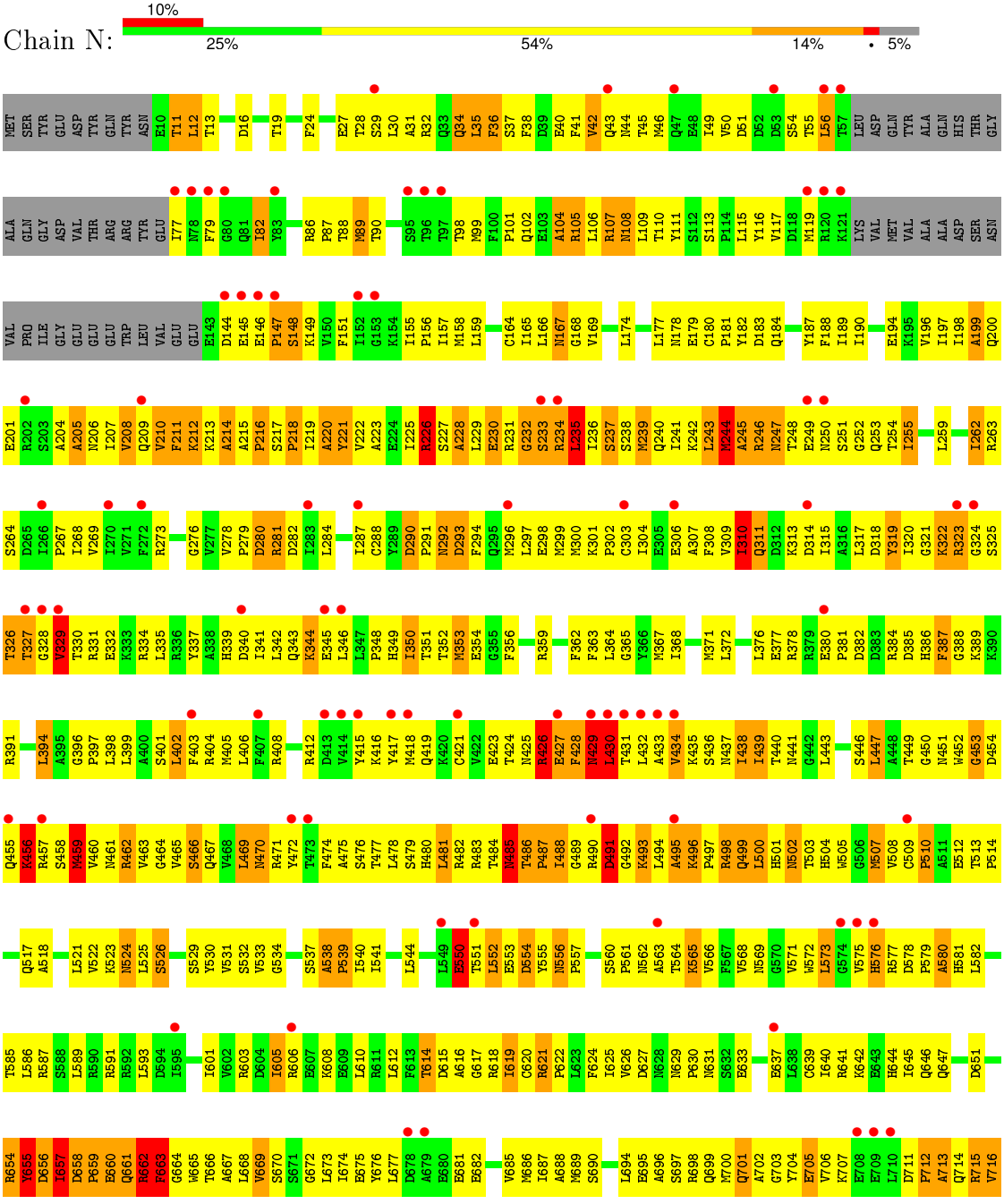
Chain B:

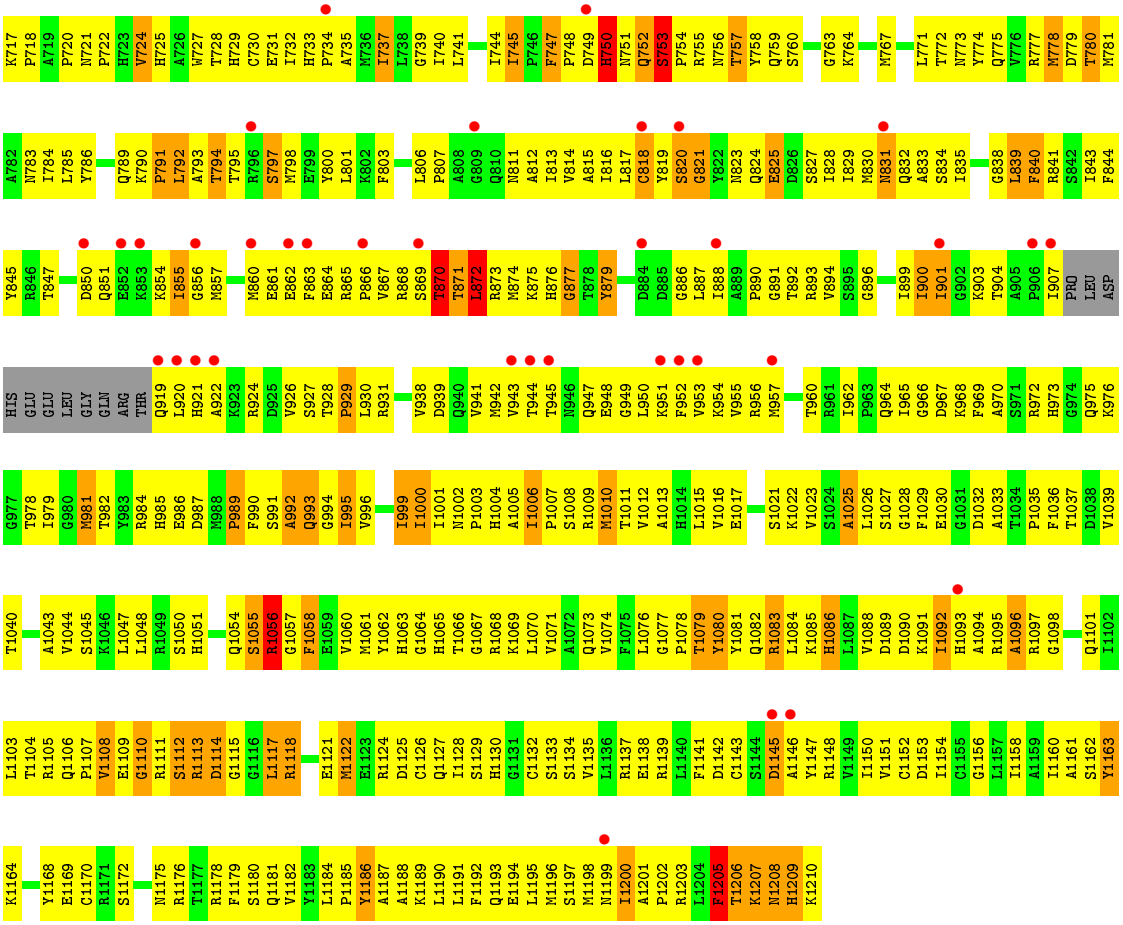






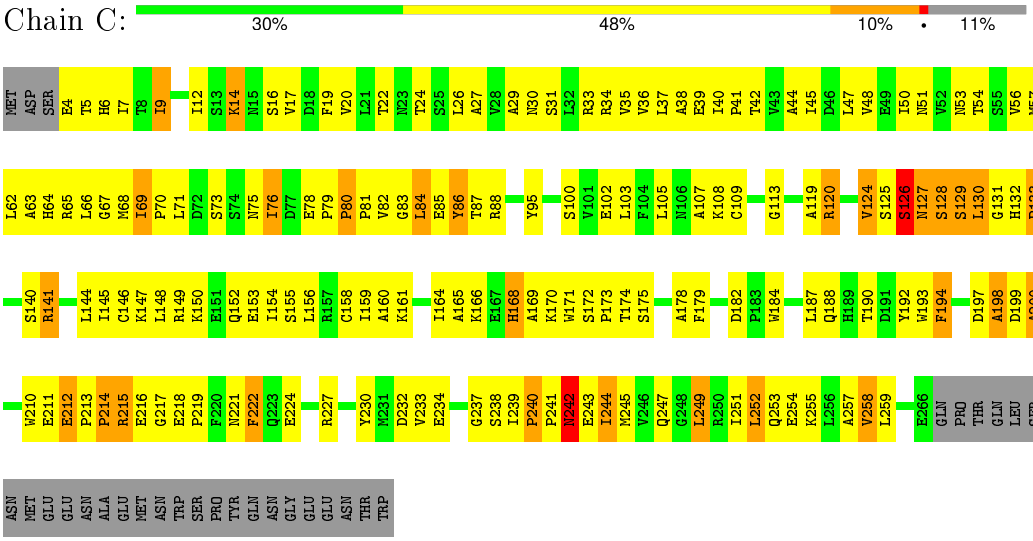
• Molecule 2: DNA-directed RNA polymerase II subunit RPB2





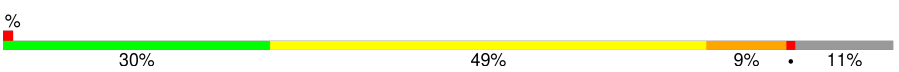
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

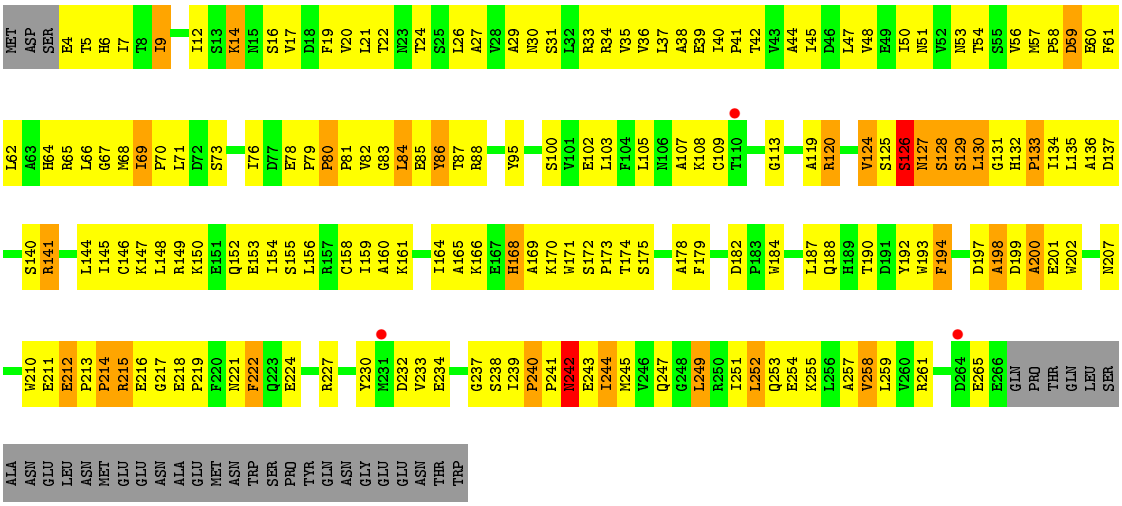
Chain C:



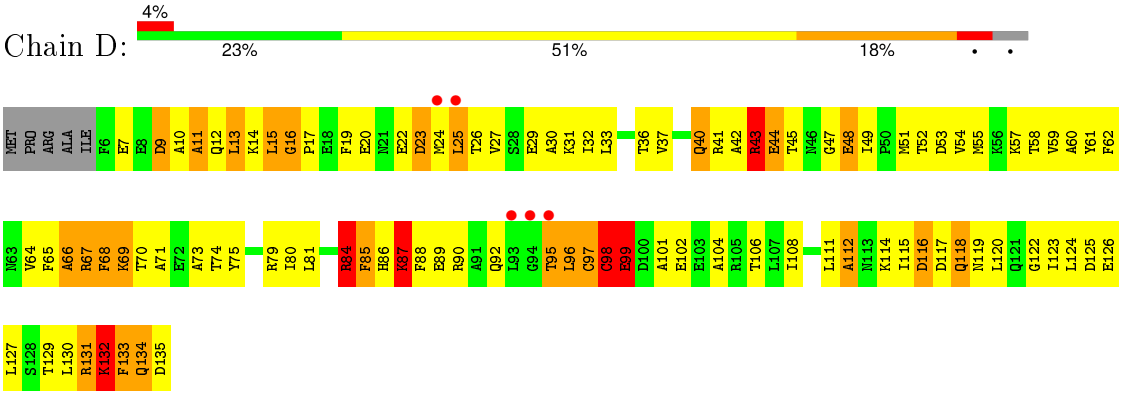
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain O:

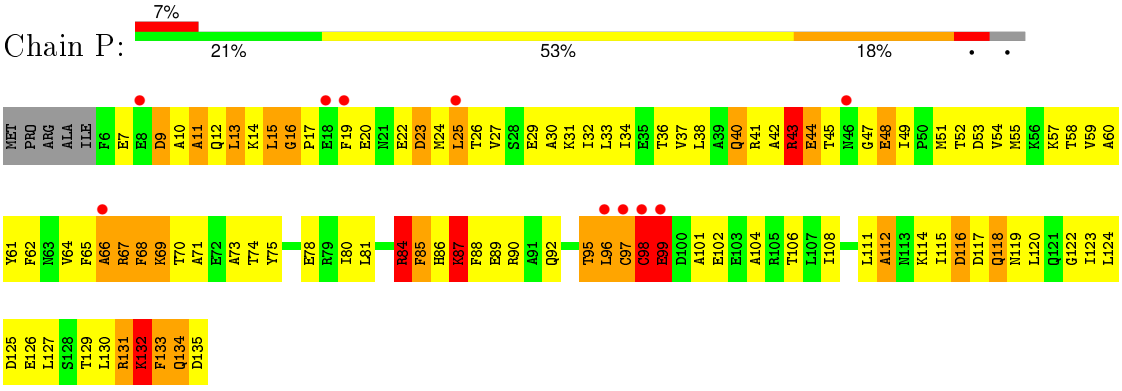




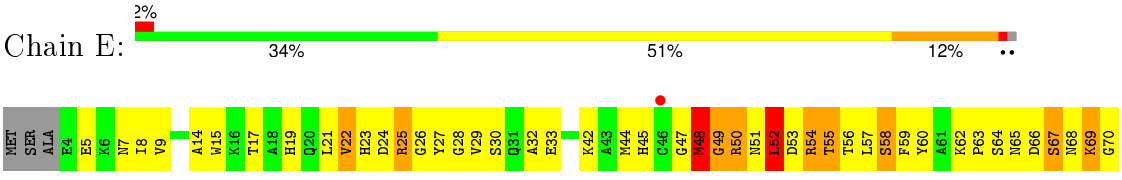
• Molecule 4: DNA-directed RNA polymerase II subunit rpb4

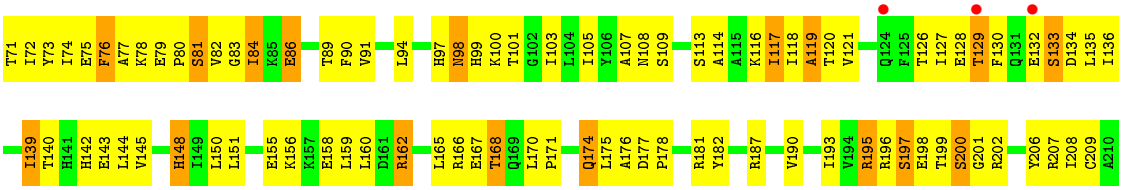


• Molecule 4: DNA-directed RNA polymerase II subunit rpb4



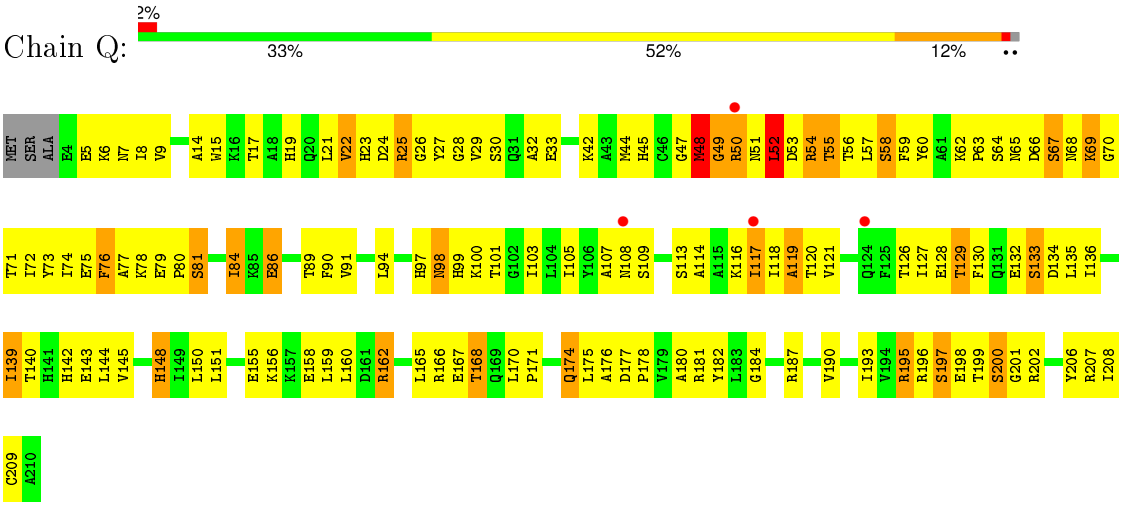
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1





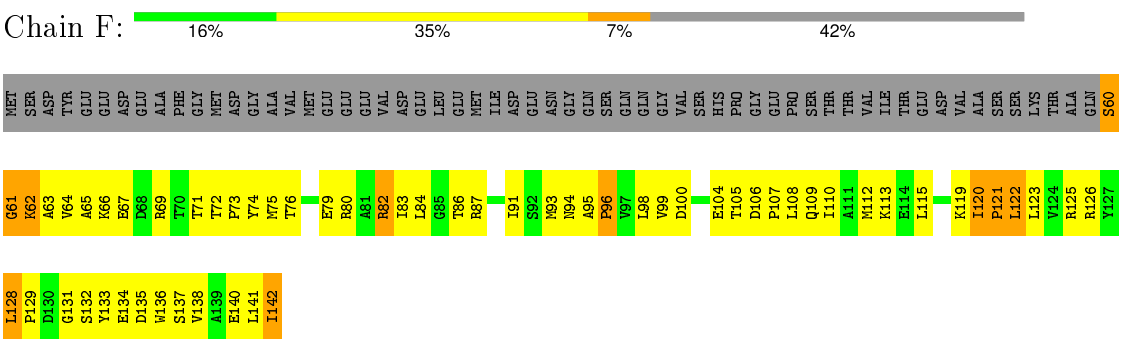
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain Q:



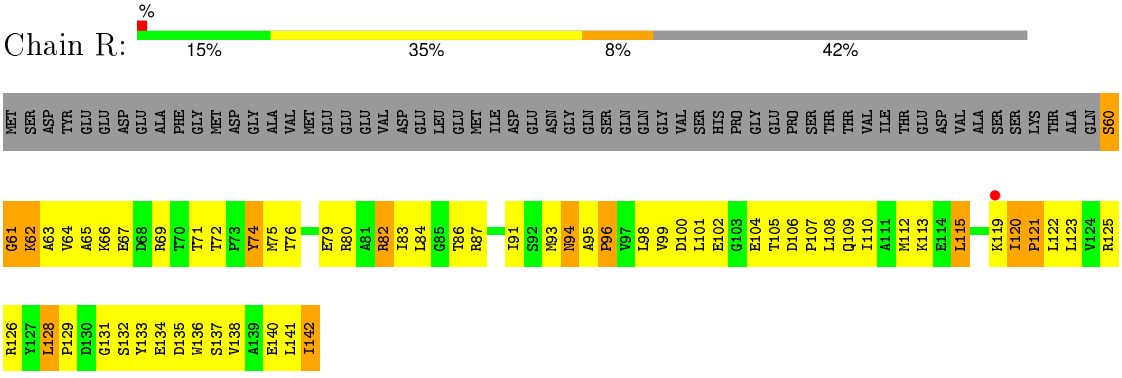
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



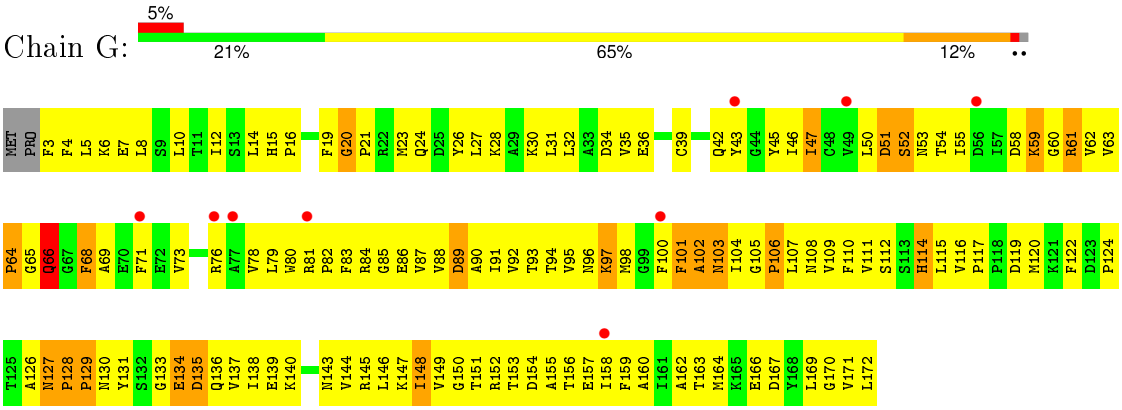
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain R:



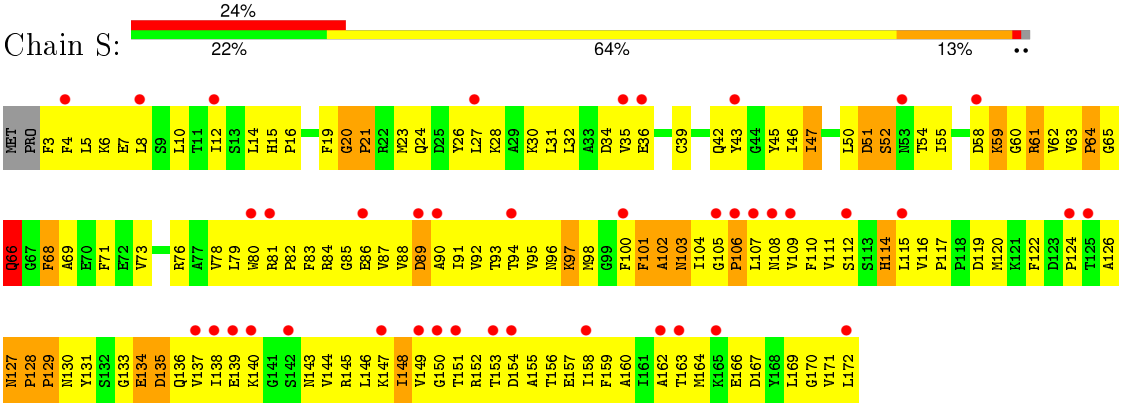
• Molecule 7: DNA-directed RNA polymerase II subunit rpb7

Chain G:



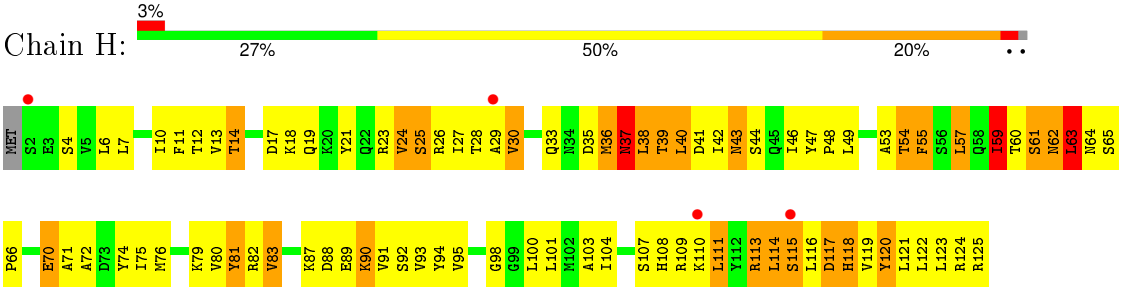
• Molecule 7: DNA-directed RNA polymerase II subunit rpb7

Chain S:



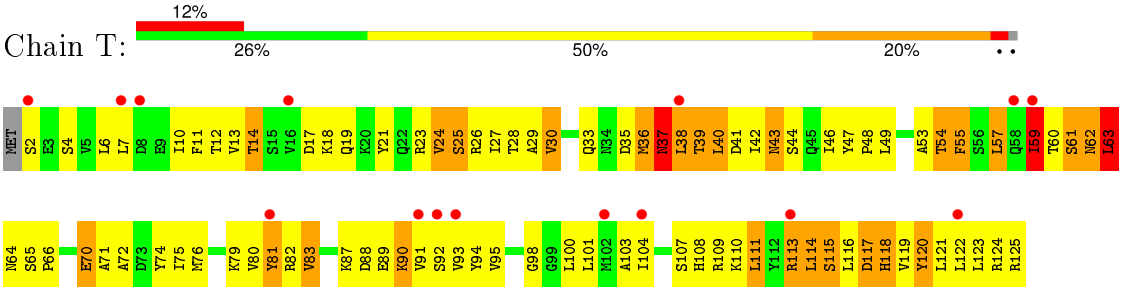
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



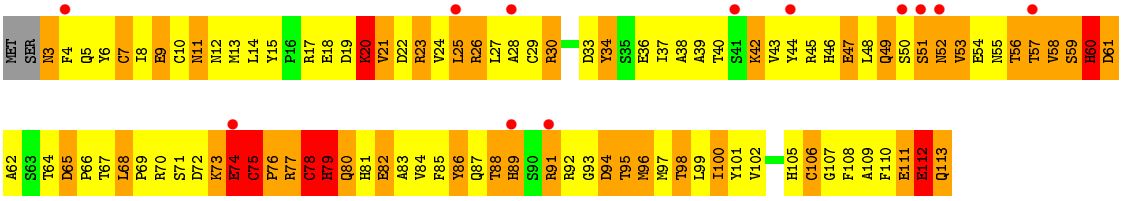
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

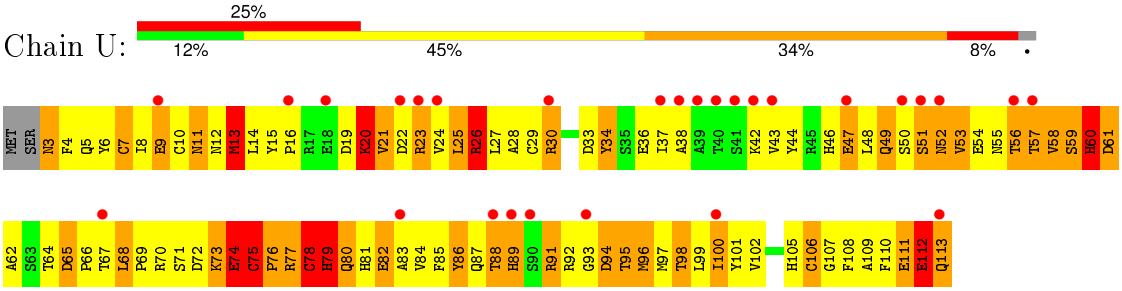
Chain T:



• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:



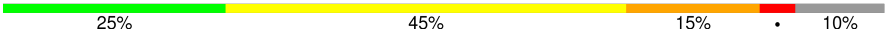


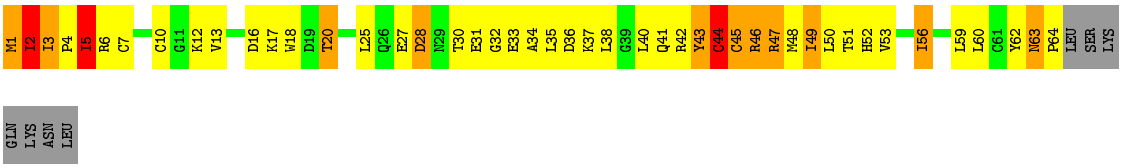
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain U:

• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

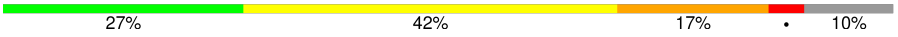
Chain J:

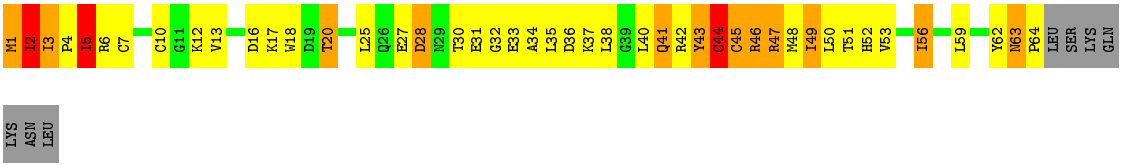




• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

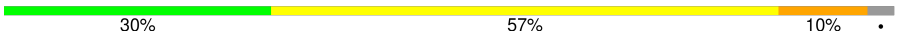
Chain V:

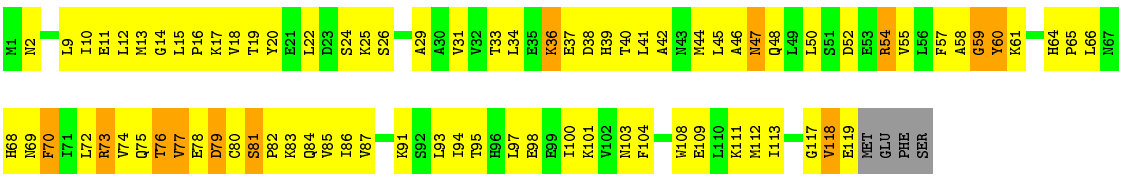




• Molecule 11: DNA-directed RNA polymerase II subunit RPB11

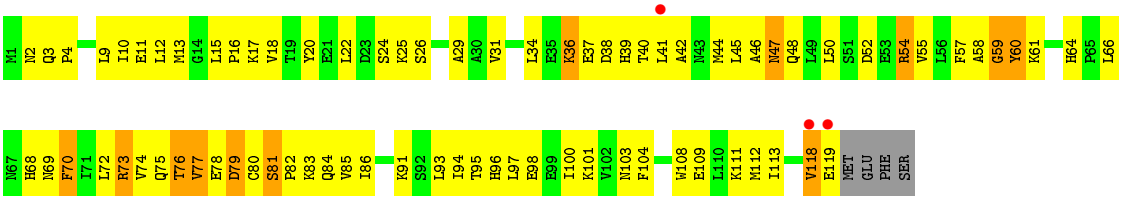
Chain K:





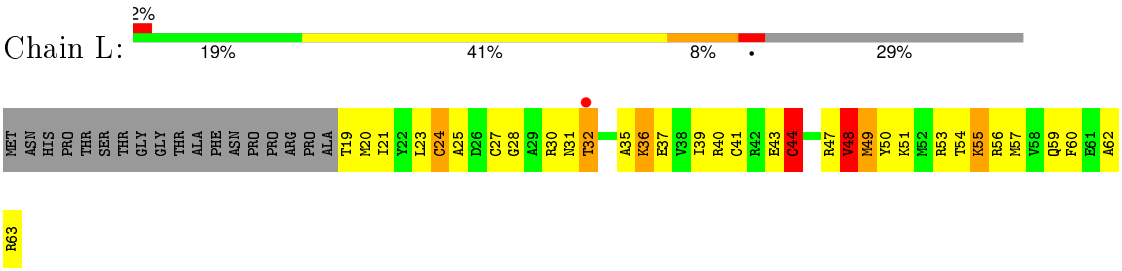
• Molecule 11: DNA-directed RNA polymerase II subunit RPB11

Chain W:



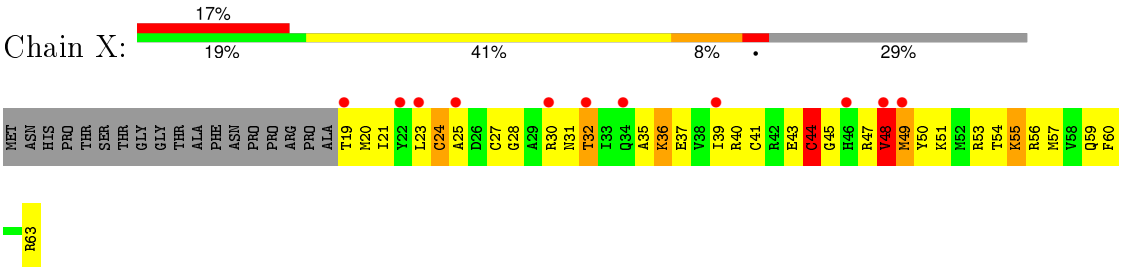
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:



• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	163.03Å 202.68Å 391.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.70 – 3.65 48.69 – 3.65	Depositor EDS
% Data completeness (in resolution range)	92.8 (48.70-3.65) 96.2 (48.69-3.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.297 , 0.321 0.308 , 0.314	Depositor DCC
R_{free} test set	6932 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	125.6	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 140.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Outliers	1 of 138803 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	62870	wwPDB-VP
Average B, all atoms (Å^2)	203.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.85% 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	0.41	0/12026	0.57	1/16260 (0.0%)
1	M	0.42	0/11887	0.56	1/16069 (0.0%)
2	B	0.44	0/9360	0.60	5/12643 (0.0%)
2	N	0.43	0/9360	0.59	5/12643 (0.0%)
3	C	0.44	0/2135	0.60	0/2904
3	O	0.44	0/2135	0.59	0/2904
4	D	0.24	0/1049	0.38	0/1412
4	P	0.24	0/1049	0.38	0/1412
5	E	0.38	0/1695	0.60	0/2287
5	Q	0.39	0/1695	0.60	0/2287
6	F	0.50	0/666	0.67	0/901
6	R	0.50	0/666	0.67	0/901
7	G	0.26	0/1361	0.57	3/1847 (0.2%)
7	S	0.26	0/1361	0.57	3/1847 (0.2%)
8	H	0.42	0/1010	0.65	0/1363
8	T	0.42	0/1010	0.65	0/1363
9	I	0.22	0/921	0.37	0/1246
9	U	0.24	0/921	0.37	0/1246
10	J	0.57	0/526	0.77	0/709
10	V	0.57	0/526	0.76	0/709
11	K	0.47	0/972	0.61	0/1317
11	W	0.47	0/972	0.61	0/1317
12	L	0.36	0/371	0.57	0/491
12	X	0.37	0/371	0.57	0/491
All	All	0.41	0/64045	0.58	18/86569 (0.0%)

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	992	ALA	N-CA-C	-5.71	95.59	111.00
2	N	992	ALA	N-CA-C	-5.69	95.65	111.00
7	G	167	ASP	CB-CG-OD2	5.38	123.14	118.30
7	S	167	ASP	CB-CG-OD2	5.35	123.12	118.30
2	N	711	ASP	CB-CG-OD2	5.30	123.07	118.30

There are no chirality outliers.

There are no planarity outliers.

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	11802	0	11784	3283	0
1	M	11666	0	11647	3212	0
2	B	9180	0	9163	1630	0
2	N	9180	0	9164	1653	0
3	C	2088	0	2045	267	0
3	O	2088	0	2045	269	0
4	D	1036	0	1025	349	0
4	P	1036	0	1025	318	0
5	E	1663	0	1684	205	0
5	Q	1663	0	1684	209	0
6	F	656	0	679	75	0
6	R	656	0	679	82	0
7	G	1330	0	1329	424	0
7	S	1330	0	1329	425	0
8	H	996	0	1006	168	0
8	T	996	0	1006	178	0
9	I	902	0	840	282	0
9	U	902	0	839	268	0
10	J	518	0	529	90	0
10	V	518	0	529	90	0
11	K	955	0	968	120	0
11	W	955	0	968	113	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	368	0	380	38	0
12	X	368	0	380	38	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
13	M	2	0	0	0	0
13	N	1	0	0	0	0
13	O	1	0	0	0	0
13	U	2	0	0	0	0
13	V	1	0	0	0	0
13	X	1	0	0	0	0
14	A	1	0	0	0	0
14	M	1	0	0	0	0
All	All	62870	0	62727	12749	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 102.

The worst 5 of 12749 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:M:1161:PRO:HG2	1:M:1190:LYS:CG	1.29	1.62
1:A:1161:PRO:HG2	1:A:1190:LYS:CG	1.29	1.58
1:M:1161:PRO:CG	1:M:1190:LYS:HG2	1.33	1.57
1:M:1091:GLY:HA3	1:M:1092:VAL:CG1	1.35	1.56
1:M:267:ASP:CB	1:M:268:LEU:HB2	1.35	1.54

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	1494/1752 (85%)	939 (63%)	280 (19%)	275 (18%)	0 3
1	M	1472/1752 (84%)	932 (63%)	281 (19%)	259 (18%)	0 3
2	B	1142/1210 (94%)	735 (64%)	245 (22%)	162 (14%)	0 6
2	N	1142/1210 (94%)	738 (65%)	243 (21%)	161 (14%)	0 6
3	C	261/297 (88%)	178 (68%)	56 (22%)	27 (10%)	1 12
3	O	261/297 (88%)	178 (68%)	56 (22%)	27 (10%)	1 12
4	D	128/135 (95%)	86 (67%)	20 (16%)	22 (17%)	0 4
4	P	128/135 (95%)	86 (67%)	20 (16%)	22 (17%)	0 4
5	E	205/210 (98%)	137 (67%)	43 (21%)	25 (12%)	0 8
5	Q	205/210 (98%)	137 (67%)	43 (21%)	25 (12%)	0 8
6	F	81/142 (57%)	58 (72%)	15 (18%)	8 (10%)	1 13
6	R	81/142 (57%)	57 (70%)	16 (20%)	8 (10%)	1 13
7	G	168/172 (98%)	128 (76%)	24 (14%)	16 (10%)	1 14
7	S	168/172 (98%)	128 (76%)	24 (14%)	16 (10%)	1 14
8	H	122/125 (98%)	73 (60%)	27 (22%)	22 (18%)	0 3
8	T	122/125 (98%)	73 (60%)	27 (22%)	22 (18%)	0 3
9	I	109/113 (96%)	46 (42%)	27 (25%)	36 (33%)	0 0
9	U	109/113 (96%)	45 (41%)	25 (23%)	39 (36%)	0 0
10	J	62/71 (87%)	41 (66%)	15 (24%)	6 (10%)	1 13
10	V	62/71 (87%)	41 (66%)	15 (24%)	6 (10%)	1 13
11	K	117/123 (95%)	80 (68%)	24 (20%)	13 (11%)	0 10
11	W	117/123 (95%)	80 (68%)	24 (20%)	13 (11%)	0 10
12	L	43/63 (68%)	23 (54%)	12 (28%)	8 (19%)	0 3
12	X	43/63 (68%)	23 (54%)	12 (28%)	8 (19%)	0 3
All	All	7842/8826 (89%)	5042 (64%)	1574 (20%)	1226 (16%)	0 5

5 of 1226 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	12	PRO
1	A	37	ILE

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Mol	Chain	Res	Type
1	A	42	THR
1	A	50	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	1301/1536 (85%)	1113 (86%)	188 (14%)	4 27
1	M	1286/1536 (84%)	1097 (85%)	189 (15%)	4 26
2	B	1012/1064 (95%)	914 (90%)	98 (10%)	10 46
2	N	1012/1064 (95%)	914 (90%)	98 (10%)	10 46
3	C	236/267 (88%)	220 (93%)	16 (7%)	20 62
3	O	236/267 (88%)	220 (93%)	16 (7%)	20 62
4	D	111/115 (96%)	94 (85%)	17 (15%)	3 24
4	P	111/115 (96%)	94 (85%)	17 (15%)	3 24
5	E	182/184 (99%)	169 (93%)	13 (7%)	18 60
5	Q	182/184 (99%)	169 (93%)	13 (7%)	18 60
6	F	71/121 (59%)	64 (90%)	7 (10%)	10 45
6	R	71/121 (59%)	64 (90%)	7 (10%)	10 45
7	G	146/148 (99%)	139 (95%)	7 (5%)	31 72
7	S	146/148 (99%)	139 (95%)	7 (5%)	31 72
8	H	113/114 (99%)	99 (88%)	14 (12%)	6 33
8	T	113/114 (99%)	99 (88%)	14 (12%)	6 33
9	I	103/105 (98%)	80 (78%)	23 (22%)	1 9
9	U	103/105 (98%)	80 (78%)	23 (22%)	1 9
10	J	59/66 (89%)	46 (78%)	13 (22%)	1 9
10	V	59/66 (89%)	46 (78%)	13 (22%)	1 9
11	K	109/113 (96%)	104 (95%)	5 (5%)	33 73
11	W	109/113 (96%)	103 (94%)	6 (6%)	27 69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
12	L	39/53 (74%)	34 (87%)	5 (13%)	5 32
12	X	39/53 (74%)	34 (87%)	5 (13%)	5 32
All	All	6949/7772 (89%)	6135 (88%)	814 (12%)	7 36

5 of 814 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	I	47	GLU
1	M	262	SER
7	S	114	HIS
9	I	94	ASP
1	M	48	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 225 such sidechains are listed below:

Mol	Chain	Res	Type
8	H	33	GLN
1	M	395	GLN
6	R	94	ASN
9	I	55	ASN
1	M	48	GLN

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 (i)

Of 18 ligands modelled in this entry, 18 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	1496/1752 (85%)	0.19	87 (5%) 26 15	51, 150, 385, 628	0
1	M	1476/1752 (84%)	0.56	175 (11%) 6 4	83, 199, 449, 672	0
2	B	1150/1210 (95%)	0.08	26 (2%) 64 46	69, 143, 314, 580	0
2	N	1150/1210 (95%)	0.58	119 (10%) 9 5	85, 222, 419, 618	0
3	C	263/297 (88%)	-0.15	0 100 100	80, 126, 252, 477	0
3	O	263/297 (88%)	0.11	3 (1%) 82 68	125, 190, 350, 511	0
4	D	130/135 (96%)	0.35	5 (3%) 44 28	128, 240, 360, 596	0
4	P	130/135 (96%)	0.58	10 (7%) 16 9	152, 287, 414, 545	0
5	E	207/210 (98%)	-0.12	4 (1%) 70 53	70, 164, 293, 516	0
5	Q	207/210 (98%)	-0.02	4 (1%) 70 53	119, 181, 373, 501	0
6	F	83/142 (58%)	-0.46	0 100 100	70, 97, 170, 232	0
6	R	83/142 (58%)	-0.32	1 (1%) 81 66	111, 126, 200, 335	0
7	G	170/172 (98%)	0.38	9 (5%) 30 18	92, 199, 323, 514	0
7	S	170/172 (98%)	1.10	41 (24%) 1 1	122, 240, 388, 494	0
8	H	124/125 (99%)	0.17	4 (3%) 51 34	82, 138, 298, 408	0
8	T	124/125 (99%)	0.63	15 (12%) 6 4	115, 197, 344, 429	0
9	I	111/113 (98%)	0.53	12 (10%) 8 5	98, 239, 367, 549	0
9	U	111/113 (98%)	1.67	28 (25%) 1 1	151, 330, 482, 585	0
10	J	64/71 (90%)	-0.17	0 100 100	85, 108, 220, 304	0
10	V	64/71 (90%)	0.07	0 100 100	137, 203, 326, 373	0
11	K	119/123 (96%)	-0.30	0 100 100	60, 126, 221, 319	0
11	W	119/123 (96%)	0.18	3 (2%) 61 43	76, 168, 295, 470	0
12	L	45/63 (71%)	0.01	1 (2%) 65 47	93, 177, 299, 481	0
12	X	45/63 (71%)	1.02	11 (24%) 1 1	153, 277, 425, 580	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	7904/8826 (89%)	0.32	558 (7%)	19	10	51, 181, 397, 672	0

The worst 5 of 558 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	U	41	SER	22.0
9	U	40	THR	16.1
9	U	39	ALA	14.8
11	W	119	GLU	14.7
1	A	107	CYS	12.6

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

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
13	ZN	A	2457	1/1	0.94	0.20	-0.36	122,122,122,122	0
13	ZN	N	2225	1/1	0.80	0.22	-0.77	180,180,180,180	0
13	ZN	M	2456	1/1	0.64	0.25	-0.85	432,432,432,432	0
13	ZN	B	2225	1/1	0.94	0.17	-0.94	149,149,149,149	0
13	ZN	I	1122	1/1	0.83	0.10	-1.26	126,126,126,126	0
13	ZN	C	1269	1/1	0.91	0.07	-1.33	122,122,122,122	0
13	ZN	M	2457	1/1	0.83	0.14	-1.39	172,172,172,172	0
13	ZN	L	1071	1/1	0.87	0.09	-1.39	123,123,123,123	0
13	ZN	J	1066	1/1	0.97	0.23	-1.44	87,87,87,87	0
13	ZN	X	1071	1/1	0.84	0.05	-1.81	195,195,195,195	0
13	ZN	A	2456	1/1	0.68	0.06	-1.92	245,245,245,245	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
13	ZN	V	1066	1/1	0.95	0.20	-1.97	155,155,155,155	0
13	ZN	I	1121	1/1	0.83	0.06	-2.20	160,160,160,160	0
13	ZN	O	1269	1/1	0.69	0.11	-2.22	189,189,189,189	0
13	ZN	U	1121	1/1	0.89	0.06	-2.56	284,284,284,284	0
13	ZN	U	1122	1/1	0.80	0.05	-3.17	240,240,240,240	0
14	MG	A	2458	1/1	0.55	1.80	-	109,109,109,109	0
14	MG	M	2458	1/1	0.28	0.39	-	197,197,197,197	0

6.5 Other polymers

There are no such residues in this entry.