wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 04:54 PM GMT

PDB ID	:	4G7Z
Title	:	Crystal structure of Thermus thermophilus transcription initiation complex containing 5-BrU at template-strand position +1
Authors	:	Zhang, Y.; Ebright, R.H.
Deposited on	:	2012-07-20
Resolution	:	3.81 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:

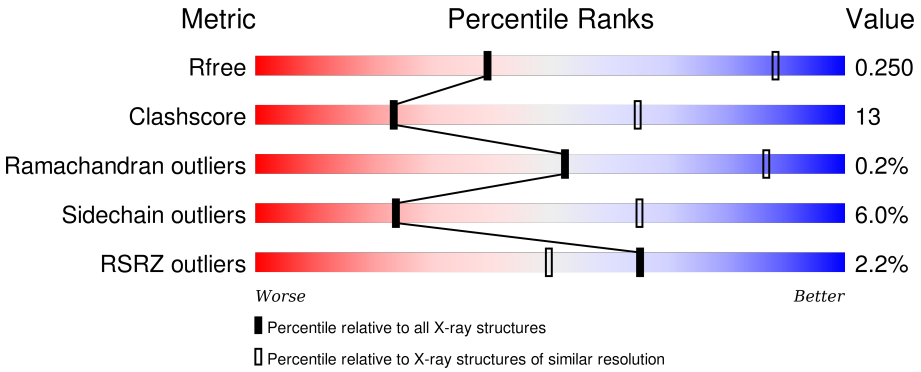
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.81 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	315	42% 27% • 28%
1	B	315	43% 26% • 30%
1	K	315	% 55% 16% • 28%
1	L	315	54% 17% • 29%
2	C	1119	% 60% 36% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	M	1119	5% 70% 27%
3	D	1524	% 58% 35%
3	N	1524	2% 72% 24%
4	E	99	% 60% 31% 5%
4	O	99	4% 74% 19% 5%
5	F	443	5% 56% 21% 22%
5	P	443	5% 58% 17% 22%
6	H	27	19% 48% 22% 11%
6	R	27	7% 67% 15% 11%
7	G	21	5% 29% 43% 5% 24%
7	Q	21	29% 38% 10% 24%

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
7	BRU	Q	15	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 56872 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	226	Total	C	N	O	S	0	0	0
			1782	1138	310	332	2			
1	B	222	Total	C	N	O	S	0	0	0
			1750	1118	304	326	2			
1	K	226	Total	C	N	O	S	0	0	0
			1782	1138	310	332	2			
1	L	225	Total	C	N	O	S	0	0	0
			1773	1133	308	330	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0	0
			8770	5548	1564	1634	24			
2	M	1111	Total	C	N	O	S	0	0	0
			8770	5548	1564	1634	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1482	Total	C	N	O	S	0	0	0
			11704	7421	2059	2189	35			
3	N	1489	Total	C	N	O	S	0	0	0
			11746	7446	2066	2198	36			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			
4	O	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total	C	N	O	S	0	0	0
			2807	1770	509	524	4			
5	P	347	Total	C	N	O	S	0	0	0
			2814	1774	510	526	4			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	EXPRESSION TAG	UNP Q5SKW1
F	-18	GLY	-	EXPRESSION TAG	UNP Q5SKW1
F	-17	SER	-	EXPRESSION TAG	UNP Q5SKW1
F	-16	SER	-	EXPRESSION TAG	UNP Q5SKW1
F	-15	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-14	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-13	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-12	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-11	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-10	HIS	-	EXPRESSION TAG	UNP Q5SKW1
F	-9	SER	-	EXPRESSION TAG	UNP Q5SKW1
F	-8	SER	-	EXPRESSION TAG	UNP Q5SKW1
F	-7	GLY	-	EXPRESSION TAG	UNP Q5SKW1
F	-6	LEU	-	EXPRESSION TAG	UNP Q5SKW1
F	-5	VAL	-	EXPRESSION TAG	UNP Q5SKW1
F	-4	PRO	-	EXPRESSION TAG	UNP Q5SKW1
F	-3	ARG	-	EXPRESSION TAG	UNP Q5SKW1
F	-2	GLY	-	EXPRESSION TAG	UNP Q5SKW1
F	-1	SER	-	EXPRESSION TAG	UNP Q5SKW1
F	0	HIS	-	EXPRESSION TAG	UNP Q5SKW1
P	-19	MET	-	EXPRESSION TAG	UNP Q5SKW1
P	-18	GLY	-	EXPRESSION TAG	UNP Q5SKW1
P	-17	SER	-	EXPRESSION TAG	UNP Q5SKW1
P	-16	SER	-	EXPRESSION TAG	UNP Q5SKW1
P	-15	HIS	-	EXPRESSION TAG	UNP Q5SKW1
P	-14	HIS	-	EXPRESSION TAG	UNP Q5SKW1
P	-13	HIS	-	EXPRESSION TAG	UNP Q5SKW1
P	-12	HIS	-	EXPRESSION TAG	UNP Q5SKW1
P	-11	HIS	-	EXPRESSION TAG	UNP Q5SKW1
P	-10	HIS	-	EXPRESSION TAG	UNP Q5SKW1
P	-9	SER	-	EXPRESSION TAG	UNP Q5SKW1
P	-8	SER	-	EXPRESSION TAG	UNP Q5SKW1
P	-7	GLY	-	EXPRESSION TAG	UNP Q5SKW1
P	-6	LEU	-	EXPRESSION TAG	UNP Q5SKW1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
P	-5	VAL	-	EXPRESSION TAG	UNP Q5SKW1
P	-4	PRO	-	EXPRESSION TAG	UNP Q5SKW1
P	-3	ARG	-	EXPRESSION TAG	UNP Q5SKW1
P	-2	GLY	-	EXPRESSION TAG	UNP Q5SKW1
P	-1	SER	-	EXPRESSION TAG	UNP Q5SKW1
P	0	HIS	-	EXPRESSION TAG	UNP Q5SKW1

- Molecule 6 is a DNA chain called 5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	24	Total	C	N	O	P	0	0	0
			495	236	94	142	23			
6	R	24	Total	C	N	O	P	0	0	0
			495	236	94	142	23			

- Molecule 7 is a DNA chain called 5'-D(*CP*CP*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*(BRU)P*CP*GP*AP*GP*GP*G)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	G	16	Total	Br	C	N	O	P	0	0	0
			328	1	155	63	94	15			
7	Q	16	Total	Br	C	N	O	P	0	0	0
			328	1	155	63	94	15			

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

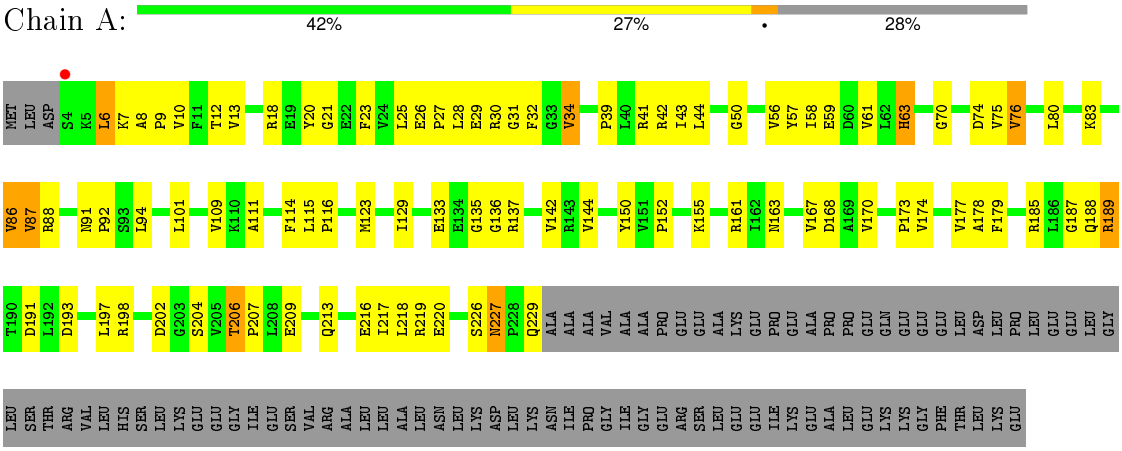
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	1	Total	Mg	0	0
			1	1		
9	N	1	Total	Mg	0	0
			1	1		

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.

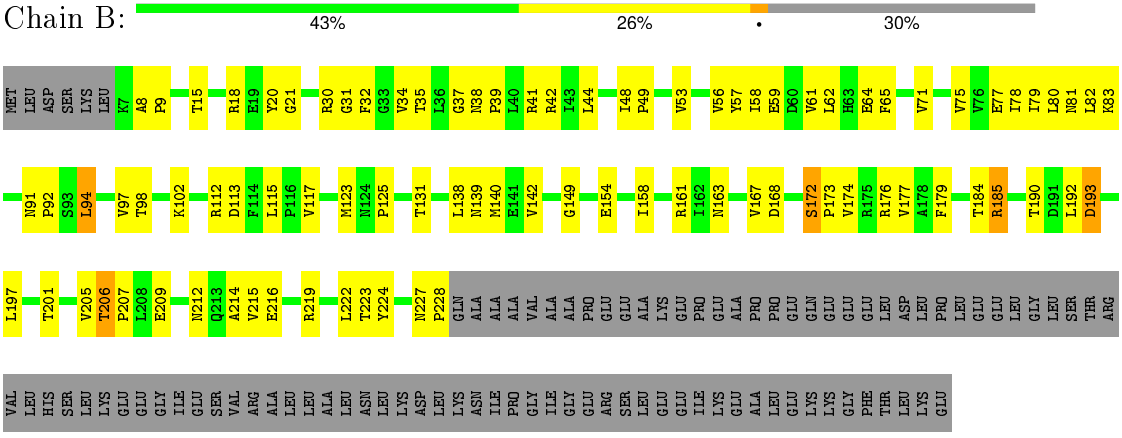
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



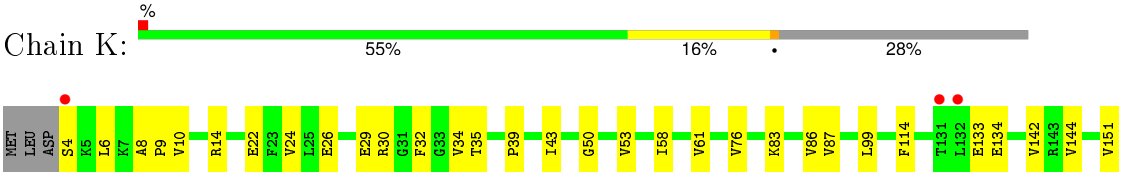
- Molecule 1: DNA-directed RNA polymerase subunit alpha

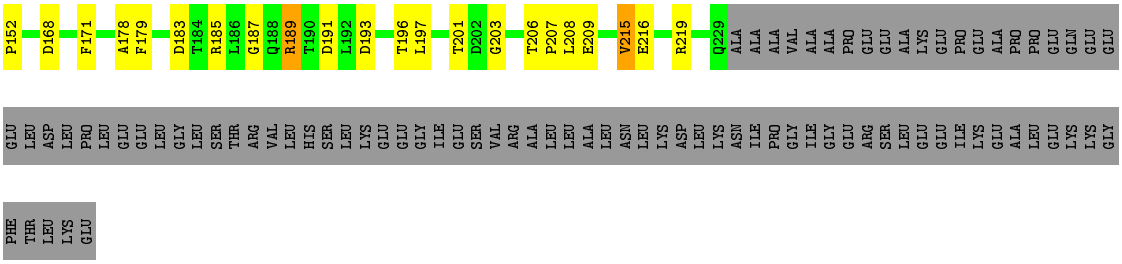
Chain B:

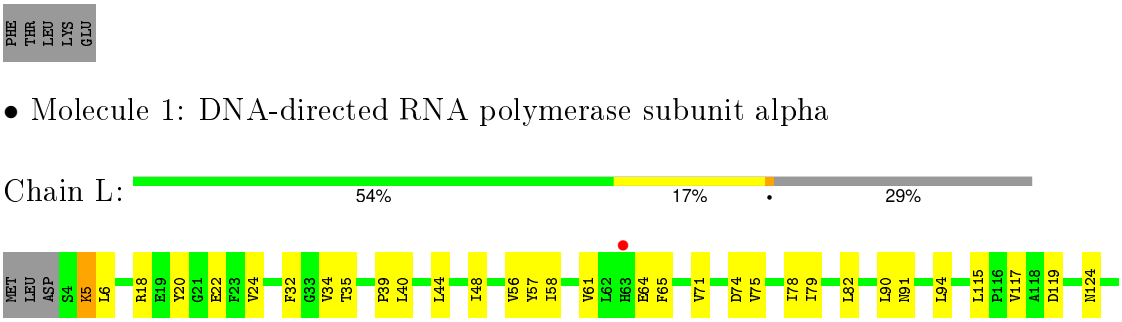


- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain K:

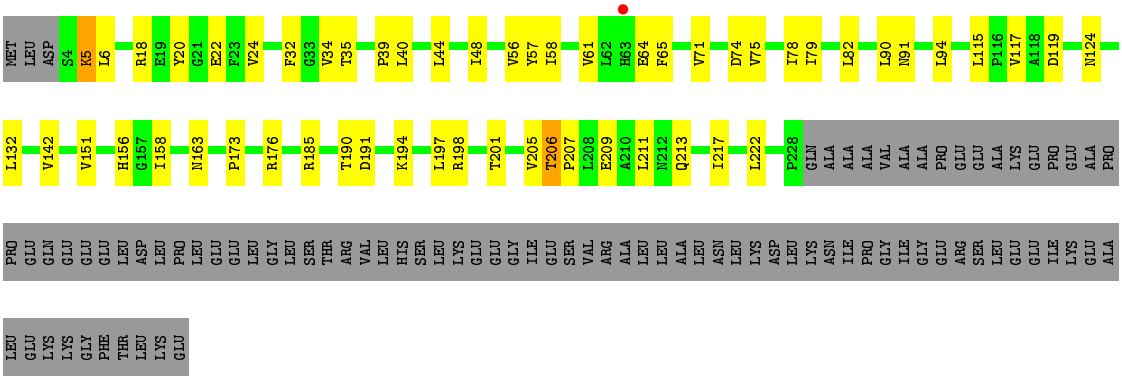






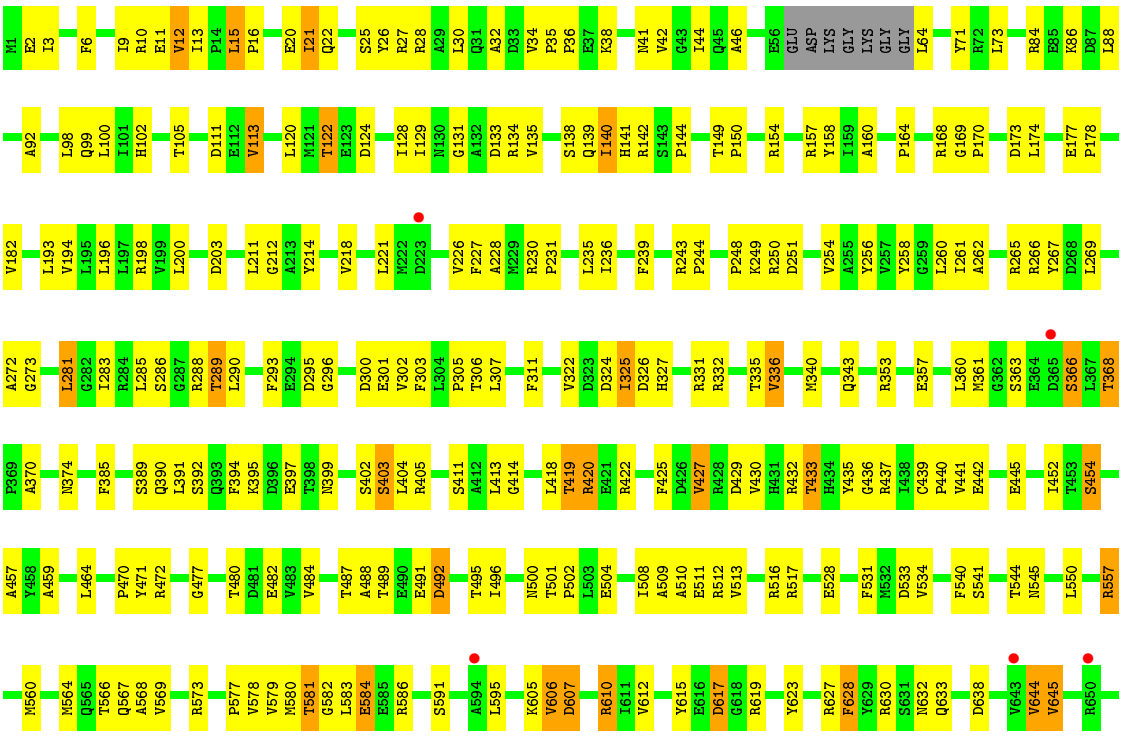
• Molecule 1: DNA-directed RNA polymerase subunit alpha

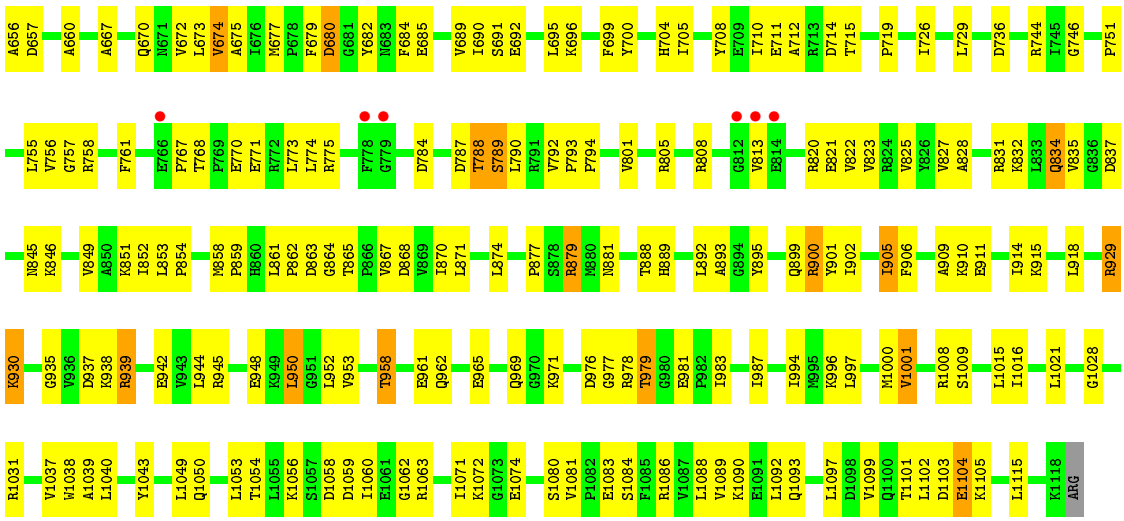
Chain L:



• Molecule 2: DNA-directed RNA polymerase subunit beta

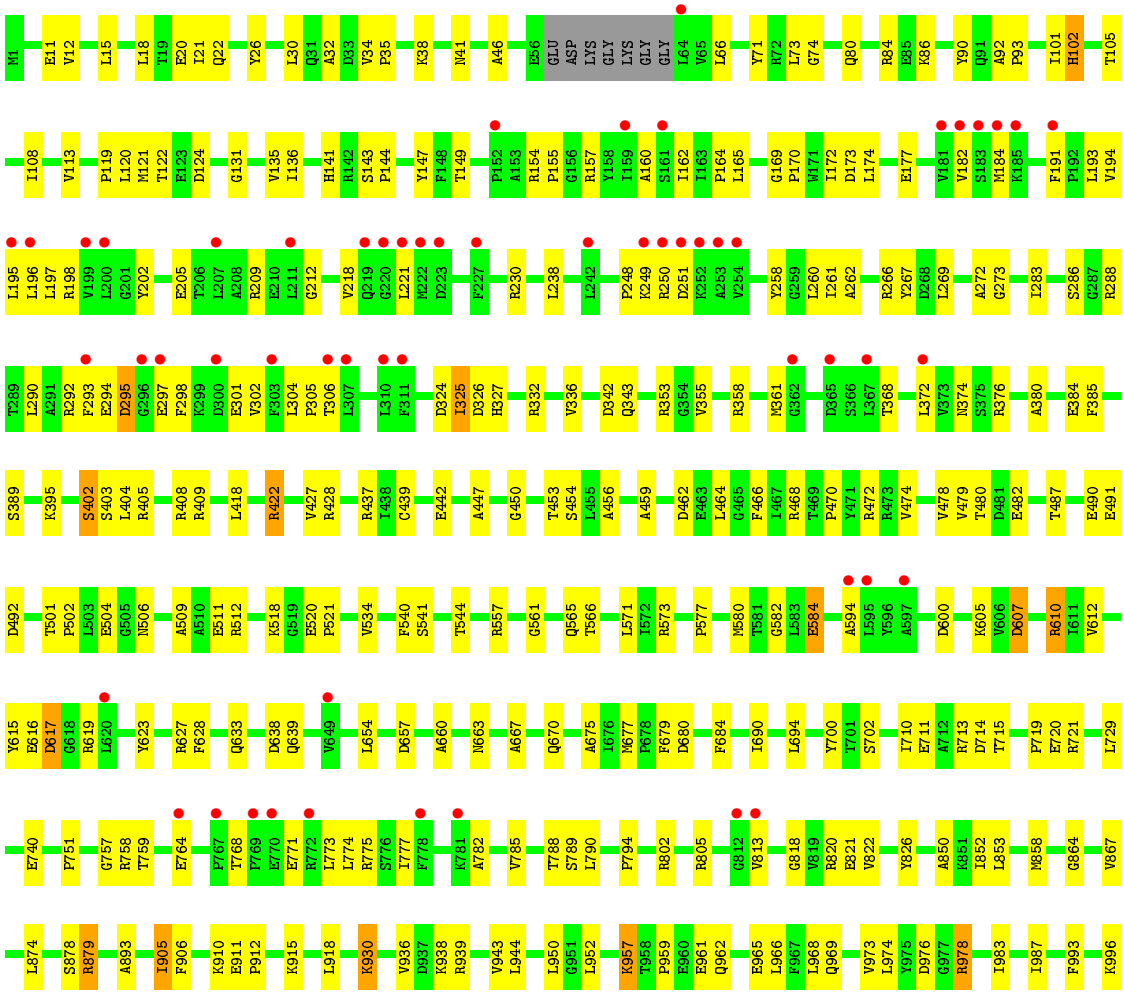
Chain C:

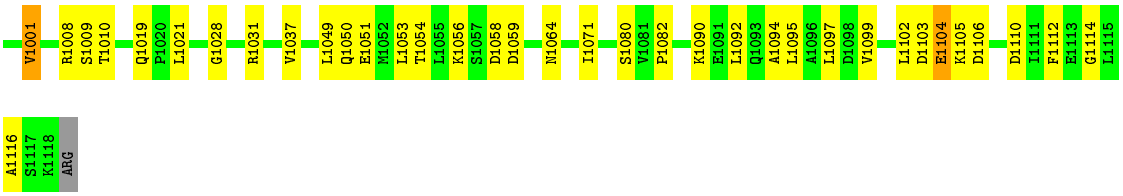




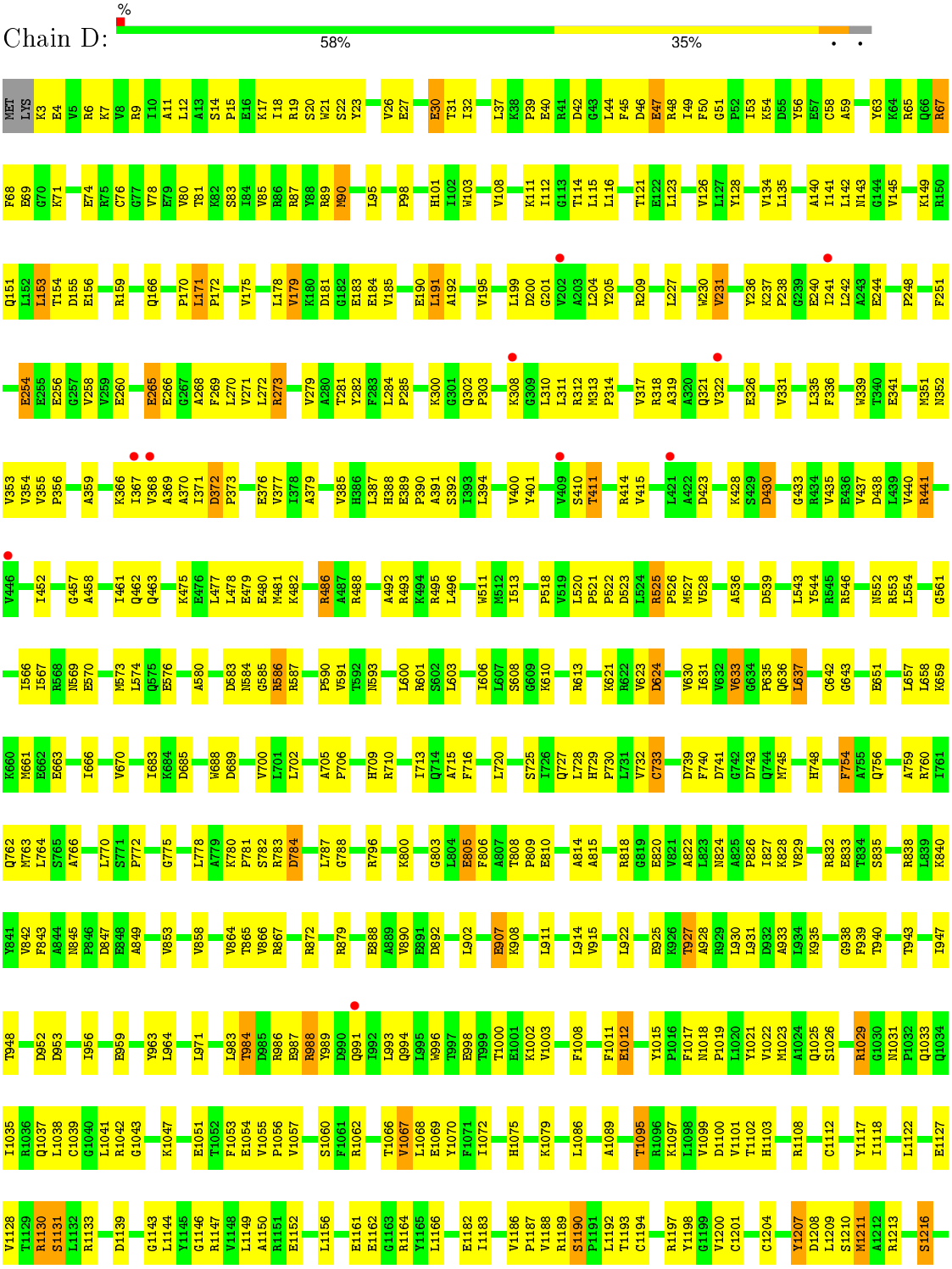
• Molecule 2: DNA-directed RNA polymerase subunit beta

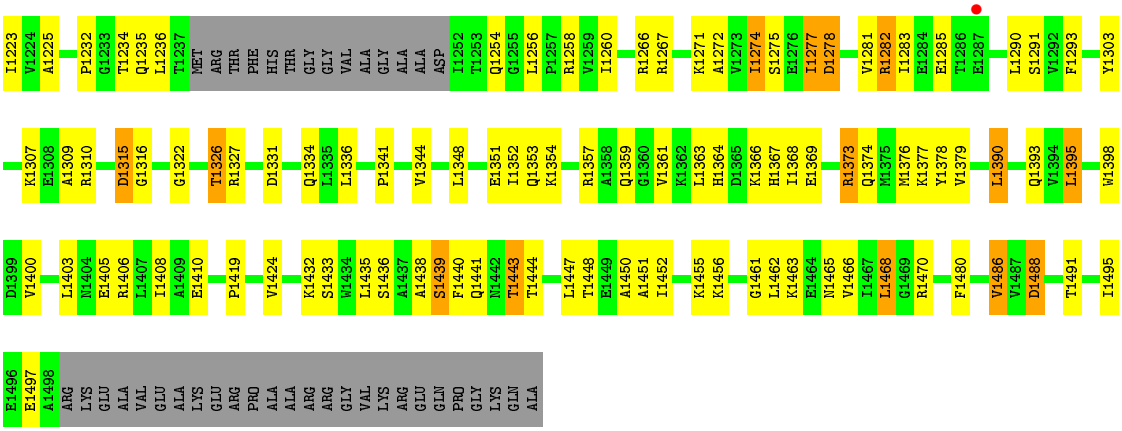
Chain M:





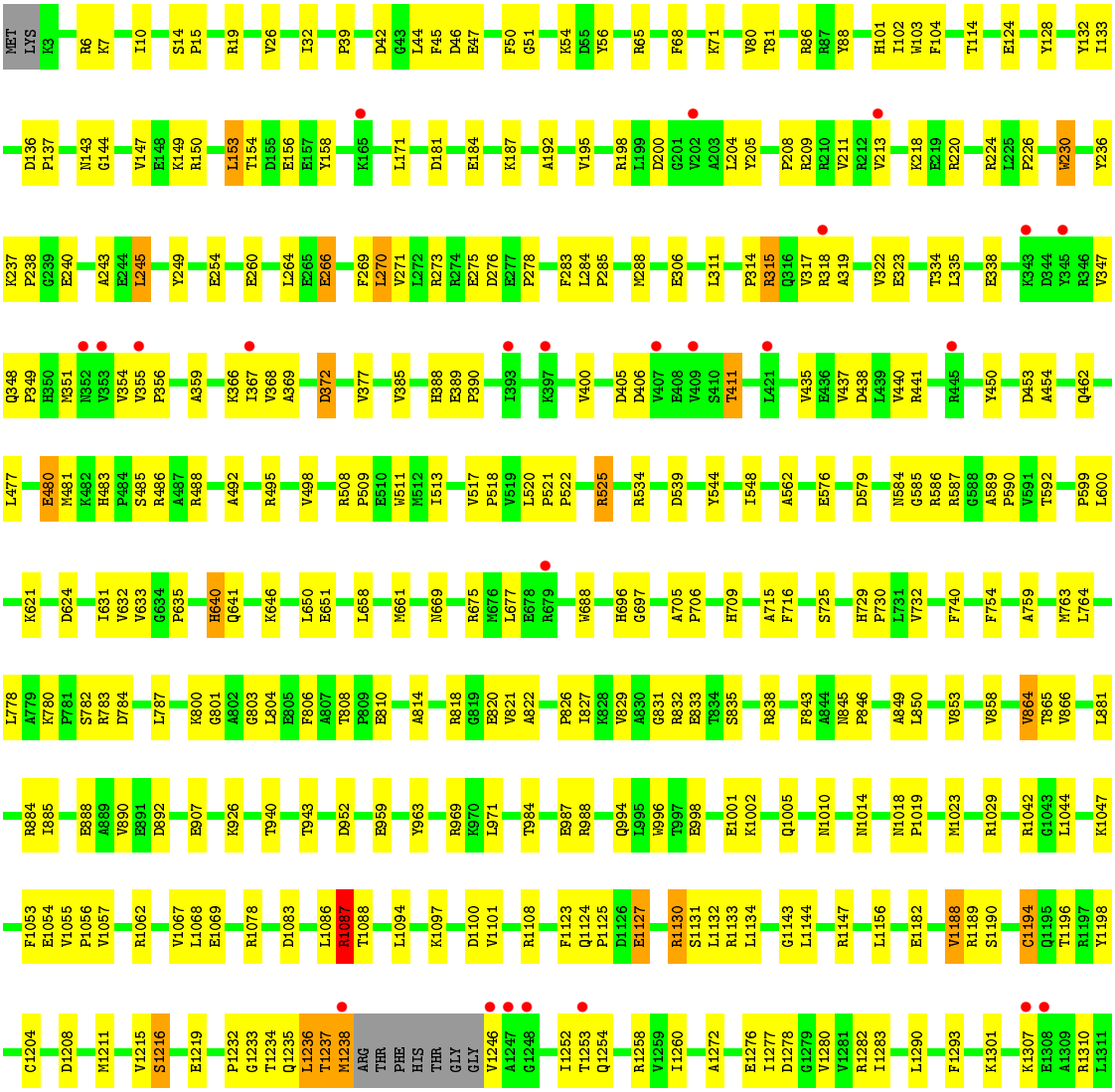
• Molecule 3: DNA-directed RNA polymerase subunit beta'

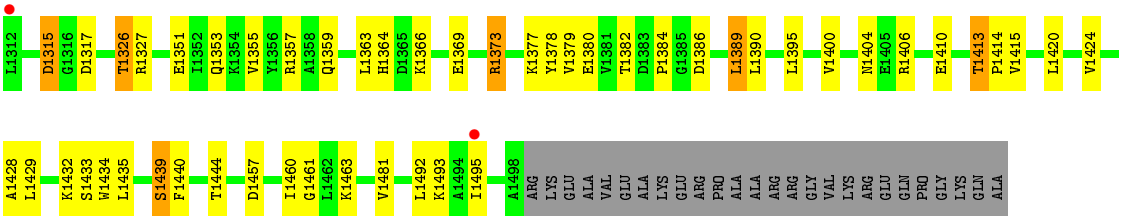




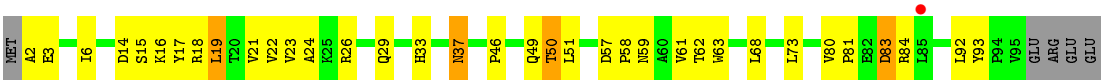
• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain N:

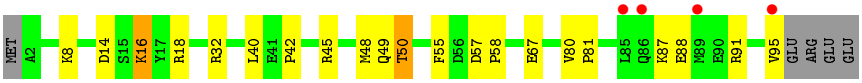




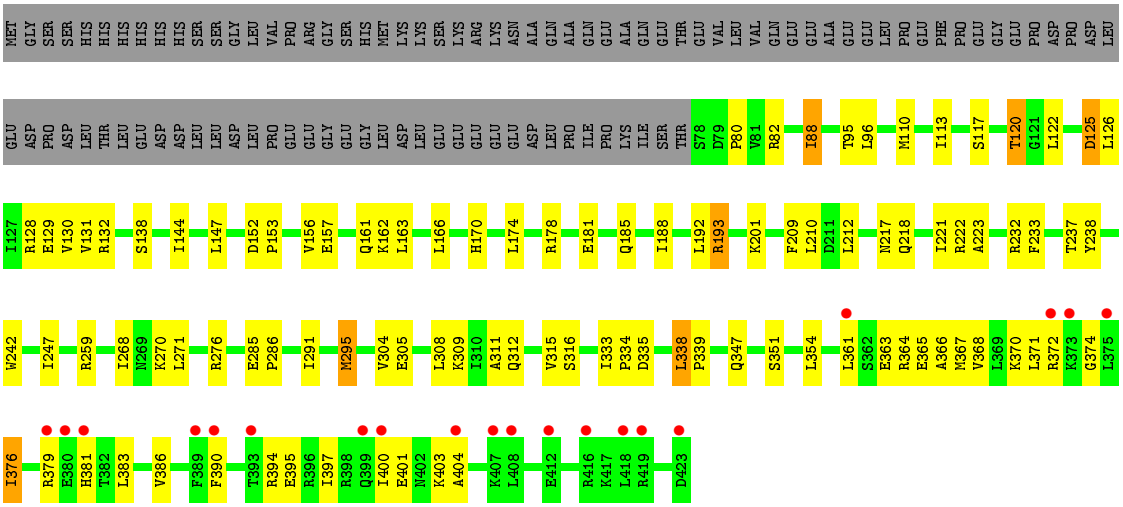
• Molecule 4: DNA-directed RNA polymerase subunit omega



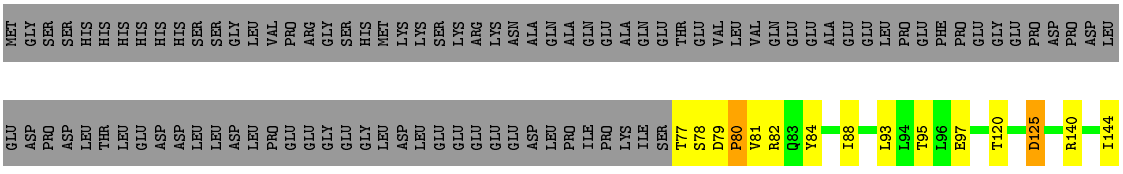
• Molecule 4: DNA-directed RNA polymerase subunit omega

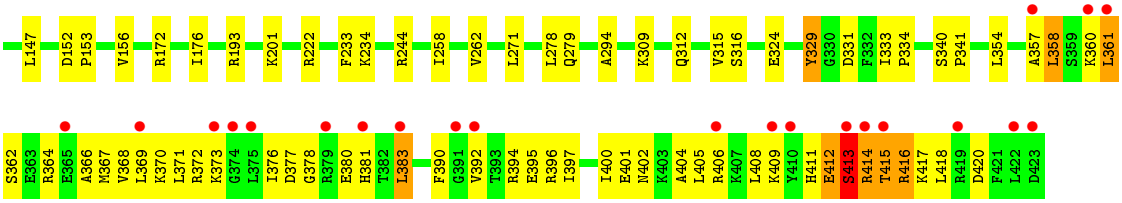


• Molecule 5: RNA polymerase sigma factor



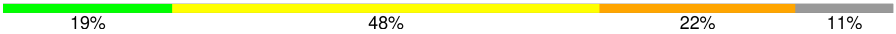
• Molecule 5: RNA polymerase sigma factor

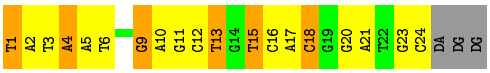




• Molecule 6: 5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*GP*G)-3'

Chain H:



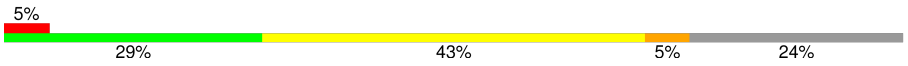


• Molecule 6: 5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*GP*G)-3'

Chain R:

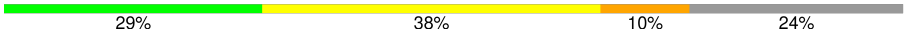
• Molecule 7: 5'-D(*CP*CP*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*(BRU)P*CP*GP*AP*GP*GP*G)-3'

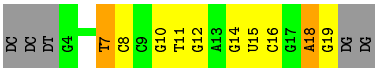
Chain G:



• Molecule 7: 5'-D(*CP*CP*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*(BRU)P*CP*GP*AP*GP*GP*G)-3'

Chain Q:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	185.47Å 103.59Å 296.51Å 90.00° 98.53° 90.00°	Depositor
Resolution (Å)	49.85 – 3.81 49.85 – 3.81	Depositor EDS
% Data completeness (in resolution range)	51.6 (49.85-3.81) 82.2 (49.85-3.81)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	3.44 (at 3.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.176 , 0.232 0.197 , 0.250	Depositor DCC
R_{free} test set	1776 reflections (2.02%)	DCC
Wilson B-factor (Å^2)	120.0	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 99.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	5 of 97591 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	56872	wwPDB-VP
Average B, all atoms (Å^2)	151.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.98 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.5249e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: MG, ZN, BRU

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	0.46	0/1814	0.66	0/2466
1	B	0.45	0/1782	0.67	0/2424
1	K	0.26	0/1814	0.45	0/2466
1	L	0.26	0/1805	0.47	0/2454
2	C	0.47	0/8937	0.70	0/12087
2	M	0.26	0/8937	0.48	1/12087 (0.0%)
3	D	0.48	0/11910	0.69	1/16105 (0.0%)
3	N	0.25	0/11952	0.47	0/16162
4	E	0.45	0/775	0.66	0/1045
4	O	0.24	0/775	0.43	0/1045
5	F	0.25	0/2852	0.44	0/3837
5	P	0.26	0/2859	0.45	0/3847
6	H	0.89	0/556	1.73	20/858 (2.3%)
6	R	1.00	2/556 (0.4%)	1.66	15/858 (1.7%)
7	G	0.82	0/345	1.34	4/529 (0.8%)
7	Q	0.79	0/345	1.37	6/529 (1.1%)
All	All	0.39	2/58014 (0.0%)	0.64	47/78799 (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
2	M	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	5	DA	N9-C4	5.04	1.40	1.37
6	R	12	DC	C1'-N1	5.01	1.55	1.49

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	12	DC	O4'-C1'-N1	10.39	115.27	108.00
6	R	17	DA	O4'-C1'-N9	9.91	114.94	108.00
6	H	18	DC	O4'-C4'-C3'	-9.12	100.53	106.00
2	M	422	ARG	NE-CZ-NH2	-8.82	115.89	120.30
6	R	23	DG	O4'-C1'-N9	8.35	113.84	108.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	M	294	GLU	Peptide

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	1782	0	1834	69	0
1	B	1750	0	1797	63	0
1	K	1782	0	1834	32	0
1	L	1773	0	1826	35	0
2	C	8770	0	8874	308	0
2	M	8770	0	8874	214	0
3	D	11704	0	11934	397	0
3	N	11746	0	11974	270	0
4	E	761	0	778	31	0
4	O	761	0	778	18	0
5	F	2807	0	2882	74	0
5	P	2814	0	2889	120	0
6	H	495	0	272	18	0
6	R	495	0	272	15	0
7	G	328	0	178	7	0
7	Q	328	0	178	13	0
8	D	2	0	0	0	0
8	N	2	0	0	0	0
9	D	1	0	0	0	0
9	N	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	56872	0	57174	1519	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 13.

The worst 5 of 1519 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:408:LEU:O	5:P:412:GLU:CB	1.72	1.37
5:P:408:LEU:O	5:P:412:GLU:HB2	1.07	1.23
5:P:408:LEU:HD23	5:P:412:GLU:CG	1.69	1.21
7:Q:14:DG:H2"	7:Q:15:BRU:O5'	1.43	1.15
3:N:1238:MET:SD	3:N:1359:GLN:OE1	2.07	1.12

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	224/315 (71%)	219 (98%)	3 (1%)	2 (1%)	21 67
1	B	220/315 (70%)	209 (95%)	11 (5%)	0	100 100
1	K	224/315 (71%)	220 (98%)	4 (2%)	0	100 100
1	L	223/315 (71%)	214 (96%)	9 (4%)	0	100 100
2	C	1107/1119 (99%)	1066 (96%)	40 (4%)	1 (0%)	56 90
2	M	1107/1119 (99%)	1065 (96%)	40 (4%)	2 (0%)	52 86
3	D	1478/1524 (97%)	1418 (96%)	59 (4%)	1 (0%)	56 90
3	N	1485/1524 (97%)	1423 (96%)	59 (4%)	3 (0%)	52 86
4	E	92/99 (93%)	88 (96%)	4 (4%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	O	92/99 (93%)	88 (96%)	4 (4%)	0	100	100
5	F	344/443 (78%)	337 (98%)	7 (2%)	0	100	100
5	P	345/443 (78%)	331 (96%)	12 (4%)	2 (1%)	30	74
All	All	6941/7630 (91%)	6678 (96%)	252 (4%)	11 (0%)	52	86

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	325	ILE
2	M	295	ASP
2	M	325	ILE
5	P	413	SER
3	N	1234	THR

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	199/273 (73%)	185 (93%)	14 (7%)	19	60
1	B	195/273 (71%)	182 (93%)	13 (7%)	20	61
1	K	199/273 (73%)	191 (96%)	8 (4%)	38	75
1	L	198/273 (72%)	192 (97%)	6 (3%)	48	80
2	C	936/941 (100%)	854 (91%)	82 (9%)	12	50
2	M	936/941 (100%)	903 (96%)	33 (4%)	43	78
3	D	1250/1279 (98%)	1139 (91%)	111 (9%)	12	50
3	N	1253/1279 (98%)	1197 (96%)	56 (4%)	34	73
4	E	83/88 (94%)	76 (92%)	7 (8%)	14	52
4	O	83/88 (94%)	81 (98%)	2 (2%)	57	84
5	F	301/388 (78%)	291 (97%)	10 (3%)	45	79
5	P	302/388 (78%)	285 (94%)	17 (6%)	26	67
All	All	5935/6484 (92%)	5576 (94%)	359 (6%)	24	65

5 of 359 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	754	PHE
3	D	1274	ILE
3	N	1315	ASP
3	D	805	GLU
3	D	1029	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	1172	HIS
3	D	1353	GLN
2	M	704	HIS
3	D	824	ASN
4	E	33	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)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
7	BRU	G	15	7	13,21,22	3.95	6 (46%)	16,30,33	1.71	2 (12%)
7	BRU	Q	15	7	13,21,22	3.95	5 (38%)	16,30,33	1.75	2 (12%)

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
7	BRU	G	15	7	-	0/3/21/22	0/2/2/2
7	BRU	Q	15	7	-	0/3/21/22	0/2/2/2

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	15	BRU	O4'-C4'	-2.74	1.38	1.45
7	Q	15	BRU	O4'-C4'	-2.71	1.38	1.45
7	G	15	BRU	C2'-C3'	-2.00	1.47	1.52
7	Q	15	BRU	C4-N3	4.58	1.41	1.33
7	G	15	BRU	C4-N3	4.59	1.41	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	Q	15	BRU	C5-C4-N3	-3.79	119.95	124.00
7	G	15	BRU	C5-C4-N3	-3.70	120.05	124.00
7	G	15	BRU	C4-N3-C2	5.43	119.94	115.25
7	Q	15	BRU	C4-N3-C2	5.52	120.02	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	15	BRU	1	0
7	Q	15	BRU	10	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	226/315 (71%)	-0.25	1 (0%) 93 87	112, 138, 163, 174	0
1	B	222/315 (70%)	-0.31	0 100 100	111, 145, 190, 215	0
1	K	226/315 (71%)	-0.20	3 (1%) 79 65	114, 145, 171, 193	0
1	L	225/315 (71%)	-0.21	1 (0%) 93 87	114, 150, 198, 222	0
2	C	1111/1119 (99%)	-0.15	11 (0%) 84 72	89, 136, 212, 240	0
2	M	1111/1119 (99%)	0.07	56 (5%) 32 21	98, 154, 239, 269	0
3	D	1482/1524 (97%)	-0.18	11 (0%) 89 80	86, 136, 196, 258	1 (0%)
3	N	1489/1524 (97%)	-0.10	26 (1%) 73 58	84, 139, 199, 263	1 (0%)
4	E	94/99 (94%)	-0.06	1 (1%) 82 69	107, 138, 175, 185	0
4	O	94/99 (94%)	0.05	4 (4%) 39 25	109, 141, 191, 201	0
5	F	346/443 (78%)	-0.00	20 (5%) 26 16	112, 152, 238, 251	0
5	P	347/443 (78%)	0.00	22 (6%) 23 14	117, 161, 253, 290	0
6	H	24/27 (88%)	-0.34	0 100 100	144, 191, 241, 247	0
6	R	24/27 (88%)	-0.35	0 100 100	142, 204, 241, 254	0
7	G	15/21 (71%)	-0.27	1 (6%) 21 12	146, 181, 229, 233	0
7	Q	15/21 (71%)	-0.33	0 100 100	160, 197, 234, 235	0
All	All	7051/7726 (91%)	-0.11	157 (2%) 65 50	84, 144, 219, 290	2 (0%)

The worst 5 of 157 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	1247	ALA	5.2
2	M	207	LEU	5.0
5	P	413	SER	5.0
3	N	1238	MET	4.9
2	M	221	LEU	4.9

6.2 Non-standard residues in protein, DNA, RNA chains (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	BRU	G	15	20/21	0.89	0.25	-	138,145,192,257	1
7	BRU	Q	15	20/21	0.83	0.24	-	177,196,247,303	1

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	ZN	N	2001	1/1	0.99	0.22	0.68	166,166,166,166	0
8	ZN	D	2001	1/1	1.00	0.17	-0.31	168,168,168,168	0
8	ZN	N	2002	1/1	0.99	0.06	-1.39	138,138,138,138	0
8	ZN	D	2002	1/1	0.99	0.09	-2.11	164,164,164,164	0
9	MG	N	2003	1/1	0.98	0.22	-	127,127,127,127	0
9	MG	D	2003	1/1	0.94	0.23	-	111,111,111,111	0

6.5 Other polymers (i)

There are no such residues in this entry.