



# wwPDB EM Validation Summary Report i

Jan 31, 2023 – 08:47 pm GMT

PDB ID : 7Q4U  
EMDB ID : EMD-13817  
Title : Cryo-EM structure of Mycobacterium tuberculosis RNA polymerase holoenzyme octamer comprising sigma factor SigB  
Authors : Brodolin, K.  
Deposited on : 2021-11-02  
Resolution : 4.39 Å(reported)  
Based on initial model : 7PP4

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the i symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

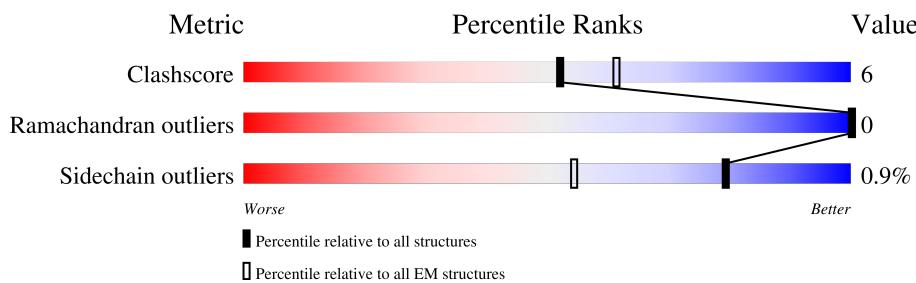
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.32.1

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
**ELECTRON MICROSCOPY**

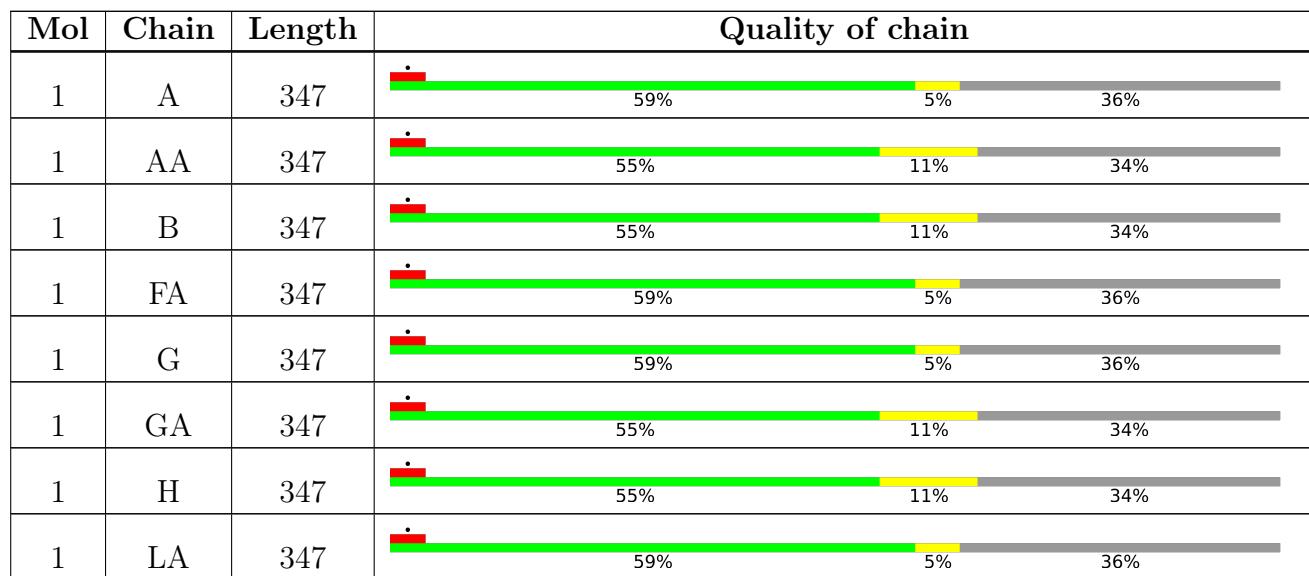
The reported resolution of this entry is 4.39 Å.

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.



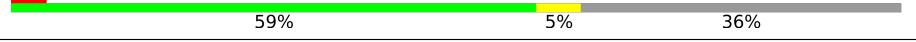
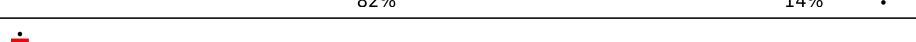
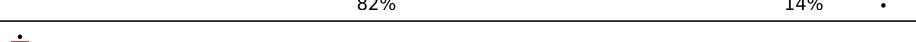
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.



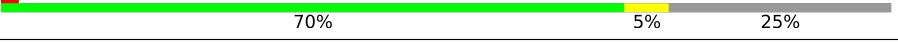
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Mol	Chain	Length	Quality of chain			
1	M	347		59%	5%	36%
1	MA	347		55%	11%	34%
1	N	347		55%	11%	34%
1	RA	347		59%	5%	36%
1	S	347		59%	5%	36%
1	SA	347		55%	11%	34%
1	T	347		55%	11%	34%
1	Z	347		59%	5%	36%
2	BA	1174		83%	11%	5%
2	C	1174		84%	11%	5%
2	HA	1174		84%	11%	5%
2	I	1174		84%	11%	5%
2	NA	1174		84%	11%	5%
2	O	1174		83%	11%	5%
2	TA	1174		83%	11%	5%
2	V	1174		83%	11%	5%
3	CA	1319		82%	14%	.
3	D	1319		82%	14%	.
3	IA	1319		82%	14%	.
3	J	1319		82%	14%	.
3	OA	1319		82%	14%	.
3	P	1319		82%	14%	.
3	UA	1319		81%	14%	.
3	W	1319		81%	15%	.
4	DA	110		70%	5%	25%

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Mol	Chain	Length	Quality of chain			
4	E	110		70%	5%	25%
4	JA	110		70%	5%	25%
4	K	110		70%	5%	25%
4	PA	110		70%	5%	25%
4	Q	110		70%	5%	25%
4	VA	110		70%	5%	25%
4	X	110		70%	5%	25%
5	EA	343		29%	13%	59%
5	F	343		29%	12%	59%
5	KA	343		30%	11%	59%
5	L	343		30%	11%	59%
5	QA	343		28%	13%	59%
5	R	343		29%	13%	59%
5	WA	343		29%	13%	59%
5	Y	343		29%	13%	59%

## 2 Entry composition [\(i\)](#)

There are 7 unique types of molecules in this entry. The entry contains 190528 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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					AltConf	Trace
1	A	223	Total	C	N	O	S	0	0
			1700	1068	294	336	2		
1	B	230	Total	C	N	O	S	0	0
			1749	1099	301	347	2		
1	G	223	Total	C	N	O	S	0	0
			1700	1068	294	336	2		
1	H	230	Total	C	N	O	S	0	0
			1749	1099	301	347	2		
1	M	223	Total	C	N	O	S	0	0
			1700	1068	294	336	2		
1	N	230	Total	C	N	O	S	0	0
			1749	1099	301	347	2		
1	S	223	Total	C	N	O	S	0	0
			1700	1068	294	336	2		
1	T	230	Total	C	N	O	S	0	0
			1749	1099	301	347	2		
1	Z	223	Total	C	N	O	S	0	0
			1700	1068	294	336	2		
1	AA	230	Total	C	N	O	S	0	0
			1749	1099	301	347	2		
1	FA	223	Total	C	N	O	S	0	0
			1700	1068	294	336	2		
1	GA	230	Total	C	N	O	S	0	0
			1749	1099	301	347	2		
1	LA	223	Total	C	N	O	S	0	0
			1700	1068	294	336	2		
1	MA	230	Total	C	N	O	S	0	0
			1749	1099	301	347	2		
1	RA	223	Total	C	N	O	S	0	0
			1700	1068	294	336	2		
1	SA	230	Total	C	N	O	S	0	0
			1749	1099	301	347	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1112	Total	C	N	O	S	0	0
			8640	5408	1515	1678	39		
2	I	1112	Total	C	N	O	S	0	0
			8640	5408	1515	1678	39		
2	O	1112	Total	C	N	O	S	0	0
			8640	5408	1515	1678	39		
2	V	1112	Total	C	N	O	S	0	0
			8640	5408	1515	1678	39		
2	BA	1112	Total	C	N	O	S	0	0
			8640	5408	1515	1678	39		
2	HA	1112	Total	C	N	O	S	0	0
			8640	5408	1515	1678	39		
2	NA	1112	Total	C	N	O	S	0	0
			8640	5408	1515	1678	39		
2	TA	1112	Total	C	N	O	S	0	0
			8640	5408	1515	1678	39		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	5	MET	-	initiating methionine	UNP P9WGY9
C	6	VAL	ILE	conflict	UNP P9WGY9
I	5	MET	-	initiating methionine	UNP P9WGY9
I	6	VAL	ILE	conflict	UNP P9WGY9
O	5	MET	-	initiating methionine	UNP P9WGY9
O	6	VAL	ILE	conflict	UNP P9WGY9
V	5	MET	-	initiating methionine	UNP P9WGY9
V	6	VAL	ILE	conflict	UNP P9WGY9
BA	5	MET	-	initiating methionine	UNP P9WGY9
BA	6	VAL	ILE	conflict	UNP P9WGY9
HA	5	MET	-	initiating methionine	UNP P9WGY9
HA	6	VAL	ILE	conflict	UNP P9WGY9
NA	5	MET	-	initiating methionine	UNP P9WGY9
NA	6	VAL	ILE	conflict	UNP P9WGY9
TA	5	MET	-	initiating methionine	UNP P9WGY9
TA	6	VAL	ILE	conflict	UNP P9WGY9

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1269	Total	C	N	O	S	0	0
			9951	6231	1805	1874	41		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	1269	Total	C 9951	N 6231	O 1805	S 1874	41	0
3	P	1269	Total	C 9951	N 6231	O 1805	S 1874	41	0
3	W	1269	Total	C 9951	N 6231	O 1805	S 1874	41	0
3	CA	1269	Total	C 9951	N 6231	O 1805	S 1874	41	0
3	IA	1269	Total	C 9951	N 6231	O 1805	S 1874	41	0
3	OA	1269	Total	C 9951	N 6231	O 1805	S 1874	41	0
3	UA	1269	Total	C 9951	N 6231	O 1805	S 1874	41	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1317	HIS	-	expression tag	UNP P9WGY7
D	1318	HIS	-	expression tag	UNP P9WGY7
D	1319	HIS	-	expression tag	UNP P9WGY7
D	1320	HIS	-	expression tag	UNP P9WGY7
D	1321	HIS	-	expression tag	UNP P9WGY7
D	1322	HIS	-	expression tag	UNP P9WGY7
J	1317	HIS	-	expression tag	UNP P9WGY7
J	1318	HIS	-	expression tag	UNP P9WGY7
J	1319	HIS	-	expression tag	UNP P9WGY7
J	1320	HIS	-	expression tag	UNP P9WGY7
J	1321	HIS	-	expression tag	UNP P9WGY7
J	1322	HIS	-	expression tag	UNP P9WGY7
P	1317	HIS	-	expression tag	UNP P9WGY7
P	1318	HIS	-	expression tag	UNP P9WGY7
P	1319	HIS	-	expression tag	UNP P9WGY7
P	1320	HIS	-	expression tag	UNP P9WGY7
P	1321	HIS	-	expression tag	UNP P9WGY7
P	1322	HIS	-	expression tag	UNP P9WGY7
W	1317	HIS	-	expression tag	UNP P9WGY7
W	1318	HIS	-	expression tag	UNP P9WGY7
W	1319	HIS	-	expression tag	UNP P9WGY7
W	1320	HIS	-	expression tag	UNP P9WGY7
W	1321	HIS	-	expression tag	UNP P9WGY7
W	1322	HIS	-	expression tag	UNP P9WGY7
CA	1317	HIS	-	expression tag	UNP P9WGY7

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Chain	Residue	Modelled	Actual	Comment	Reference
CA	1318	HIS	-	expression tag	UNP P9WGY7
CA	1319	HIS	-	expression tag	UNP P9WGY7
CA	1320	HIS	-	expression tag	UNP P9WGY7
CA	1321	HIS	-	expression tag	UNP P9WGY7
CA	1322	HIS	-	expression tag	UNP P9WGY7
IA	1317	HIS	-	expression tag	UNP P9WGY7
IA	1318	HIS	-	expression tag	UNP P9WGY7
IA	1319	HIS	-	expression tag	UNP P9WGY7
IA	1320	HIS	-	expression tag	UNP P9WGY7
IA	1321	HIS	-	expression tag	UNP P9WGY7
IA	1322	HIS	-	expression tag	UNP P9WGY7
OA	1317	HIS	-	expression tag	UNP P9WGY7
OA	1318	HIS	-	expression tag	UNP P9WGY7
OA	1319	HIS	-	expression tag	UNP P9WGY7
OA	1320	HIS	-	expression tag	UNP P9WGY7
OA	1321	HIS	-	expression tag	UNP P9WGY7
OA	1322	HIS	-	expression tag	UNP P9WGY7
UA	1317	HIS	-	expression tag	UNP P9WGY7
UA	1318	HIS	-	expression tag	UNP P9WGY7
UA	1319	HIS	-	expression tag	UNP P9WGY7
UA	1320	HIS	-	expression tag	UNP P9WGY7
UA	1321	HIS	-	expression tag	UNP P9WGY7
UA	1322	HIS	-	expression tag	UNP P9WGY7

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	83	Total	C	N	O	0	0
			654	417	108	129		
4	K	83	Total	C	N	O	0	0
			654	417	108	129		
4	Q	83	Total	C	N	O	0	0
			654	417	108	129		
4	X	83	Total	C	N	O	0	0
			654	417	108	129		
4	DA	83	Total	C	N	O	0	0
			654	417	108	129		
4	JA	83	Total	C	N	O	0	0
			654	417	108	129		
4	PA	83	Total	C	N	O	0	0
			654	417	108	129		
4	VA	83	Total	C	N	O	0	0
			654	417	108	129		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	142	Total	C	N	O	S		
			1119	705	210	201	3	0	0
5	L	142	Total	C	N	O	S		
			1119	705	210	201	3	0	0
5	R	142	Total	C	N	O	S		
			1119	705	210	201	3	0	0
5	Y	142	Total	C	N	O	S		
			1119	705	210	201	3	0	0
5	EA	142	Total	C	N	O	S		
			1119	705	210	201	3	0	0
5	KA	142	Total	C	N	O	S		
			1119	705	210	201	3	0	0
5	QA	142	Total	C	N	O	S		
			1119	705	210	201	3	0	0
5	WA	142	Total	C	N	O	S		
			1119	705	210	201	3	0	0

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	initiating methionine	UNP P9WGI5
F	-18	GLY	-	expression tag	UNP P9WGI5
F	-17	SER	-	expression tag	UNP P9WGI5
F	-16	SER	-	expression tag	UNP P9WGI5
F	-15	HIS	-	expression tag	UNP P9WGI5
F	-14	HIS	-	expression tag	UNP P9WGI5
F	-13	HIS	-	expression tag	UNP P9WGI5
F	-12	HIS	-	expression tag	UNP P9WGI5
F	-11	HIS	-	expression tag	UNP P9WGI5
F	-10	HIS	-	expression tag	UNP P9WGI5
F	-9	SER	-	expression tag	UNP P9WGI5
F	-8	SER	-	expression tag	UNP P9WGI5
F	-7	GLY	-	expression tag	UNP P9WGI5
F	-6	LEU	-	expression tag	UNP P9WGI5
F	-5	VAL	-	expression tag	UNP P9WGI5
F	-4	PRO	-	expression tag	UNP P9WGI5
F	-3	ARG	-	expression tag	UNP P9WGI5
F	-2	GLY	-	expression tag	UNP P9WGI5
F	-1	SER	-	expression tag	UNP P9WGI5
F	0	HIS	-	expression tag	UNP P9WGI5
L	-19	MET	-	initiating methionine	UNP P9WGI5
L	-18	GLY	-	expression tag	UNP P9WGI5

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-17	SER	-	expression tag	UNP P9WGI5
L	-16	SER	-	expression tag	UNP P9WGI5
L	-15	HIS	-	expression tag	UNP P9WGI5
L	-14	HIS	-	expression tag	UNP P9WGI5
L	-13	HIS	-	expression tag	UNP P9WGI5
L	-12	HIS	-	expression tag	UNP P9WGI5
L	-11	HIS	-	expression tag	UNP P9WGI5
L	-10	HIS	-	expression tag	UNP P9WGI5
L	-9	SER	-	expression tag	UNP P9WGI5
L	-8	SER	-	expression tag	UNP P9WGI5
L	-7	GLY	-	expression tag	UNP P9WGI5
L	-6	LEU	-	expression tag	UNP P9WGI5
L	-5	VAL	-	expression tag	UNP P9WGI5
L	-4	PRO	-	expression tag	UNP P9WGI5
L	-3	ARG	-	expression tag	UNP P9WGI5
L	-2	GLY	-	expression tag	UNP P9WGI5
L	-1	SER	-	expression tag	UNP P9WGI5
L	0	HIS	-	expression tag	UNP P9WGI5
R	-19	MET	-	initiating methionine	UNP P9WGI5
R	-18	GLY	-	expression tag	UNP P9WGI5
R	-17	SER	-	expression tag	UNP P9WGI5
R	-16	SER	-	expression tag	UNP P9WGI5
R	-15	HIS	-	expression tag	UNP P9WGI5
R	-14	HIS	-	expression tag	UNP P9WGI5
R	-13	HIS	-	expression tag	UNP P9WGI5
R	-12	HIS	-	expression tag	UNP P9WGI5
R	-11	HIS	-	expression tag	UNP P9WGI5
R	-10	HIS	-	expression tag	UNP P9WGI5
R	-9	SER	-	expression tag	UNP P9WGI5
R	-8	SER	-	expression tag	UNP P9WGI5
R	-7	GLY	-	expression tag	UNP P9WGI5
R	-6	LEU	-	expression tag	UNP P9WGI5
R	-5	VAL	-	expression tag	UNP P9WGI5
R	-4	PRO	-	expression tag	UNP P9WGI5
R	-3	ARG	-	expression tag	UNP P9WGI5
R	-2	GLY	-	expression tag	UNP P9WGI5
R	-1	SER	-	expression tag	UNP P9WGI5
R	0	HIS	-	expression tag	UNP P9WGI5
Y	-19	MET	-	initiating methionine	UNP P9WGI5
Y	-18	GLY	-	expression tag	UNP P9WGI5
Y	-17	SER	-	expression tag	UNP P9WGI5
Y	-16	SER	-	expression tag	UNP P9WGI5

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	-15	HIS	-	expression tag	UNP P9WGI5
Y	-14	HIS	-	expression tag	UNP P9WGI5
Y	-13	HIS	-	expression tag	UNP P9WGI5
Y	-12	HIS	-	expression tag	UNP P9WGI5
Y	-11	HIS	-	expression tag	UNP P9WGI5
Y	-10	HIS	-	expression tag	UNP P9WGI5
Y	-9	SER	-	expression tag	UNP P9WGI5
Y	-8	SER	-	expression tag	UNP P9WGI5
Y	-7	GLY	-	expression tag	UNP P9WGI5
Y	-6	LEU	-	expression tag	UNP P9WGI5
Y	-5	VAL	-	expression tag	UNP P9WGI5
Y	-4	PRO	-	expression tag	UNP P9WGI5
Y	-3	ARG	-	expression tag	UNP P9WGI5
Y	-2	GLY	-	expression tag	UNP P9WGI5
Y	-1	SER	-	expression tag	UNP P9WGI5
Y	0	HIS	-	expression tag	UNP P9WGI5
EA	-19	MET	-	initiating methionine	UNP P9WGI5
EA	-18	GLY	-	expression tag	UNP P9WGI5
EA	-17	SER	-	expression tag	UNP P9WGI5
EA	-16	SER	-	expression tag	UNP P9WGI5
EA	-15	HIS	-	expression tag	UNP P9WGI5
EA	-14	HIS	-	expression tag	UNP P9WGI5
EA	-13	HIS	-	expression tag	UNP P9WGI5
EA	-12	HIS	-	expression tag	UNP P9WGI5
EA	-11	HIS	-	expression tag	UNP P9WGI5
EA	-10	HIS	-	expression tag	UNP P9WGI5
EA	-9	SER	-	expression tag	UNP P9WGI5
EA	-8	SER	-	expression tag	UNP P9WGI5
EA	-7	GLY	-	expression tag	UNP P9WGI5
EA	-6	LEU	-	expression tag	UNP P9WGI5
EA	-5	VAL	-	expression tag	UNP P9WGI5
EA	-4	PRO	-	expression tag	UNP P9WGI5
EA	-3	ARG	-	expression tag	UNP P9WGI5
EA	-2	GLY	-	expression tag	UNP P9WGI5
EA	-1	SER	-	expression tag	UNP P9WGI5
EA	0	HIS	-	expression tag	UNP P9WGI5
KA	-19	MET	-	initiating methionine	UNP P9WGI5
KA	-18	GLY	-	expression tag	UNP P9WGI5
KA	-17	SER	-	expression tag	UNP P9WGI5
KA	-16	SER	-	expression tag	UNP P9WGI5
KA	-15	HIS	-	expression tag	UNP P9WGI5
KA	-14	HIS	-	expression tag	UNP P9WGI5

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Chain	Residue	Modelled	Actual	Comment	Reference
KA	-13	HIS	-	expression tag	UNP P9WGI5
KA	-12	HIS	-	expression tag	UNP P9WGI5
KA	-11	HIS	-	expression tag	UNP P9WGI5
KA	-10	HIS	-	expression tag	UNP P9WGI5
KA	-9	SER	-	expression tag	UNP P9WGI5
KA	-8	SER	-	expression tag	UNP P9WGI5
KA	-7	GLY	-	expression tag	UNP P9WGI5
KA	-6	LEU	-	expression tag	UNP P9WGI5
KA	-5	VAL	-	expression tag	UNP P9WGI5
KA	-4	PRO	-	expression tag	UNP P9WGI5
KA	-3	ARG	-	expression tag	UNP P9WGI5
KA	-2	GLY	-	expression tag	UNP P9WGI5
KA	-1	SER	-	expression tag	UNP P9WGI5
KA	0	HIS	-	expression tag	UNP P9WGI5
QA	-19	MET	-	initiating methionine	UNP P9WGI5
QA	-18	GLY	-	expression tag	UNP P9WGI5
QA	-17	SER	-	expression tag	UNP P9WGI5
QA	-16	SER	-	expression tag	UNP P9WGI5
QA	-15	HIS	-	expression tag	UNP P9WGI5
QA	-14	HIS	-	expression tag	UNP P9WGI5
QA	-13	HIS	-	expression tag	UNP P9WGI5
QA	-12	HIS	-	expression tag	UNP P9WGI5
QA	-11	HIS	-	expression tag	UNP P9WGI5
QA	-10	HIS	-	expression tag	UNP P9WGI5
QA	-9	SER	-	expression tag	UNP P9WGI5
QA	-8	SER	-	expression tag	UNP P9WGI5
QA	-7	GLY	-	expression tag	UNP P9WGI5
QA	-6	LEU	-	expression tag	UNP P9WGI5
QA	-5	VAL	-	expression tag	UNP P9WGI5
QA	-4	PRO	-	expression tag	UNP P9WGI5
QA	-3	ARG	-	expression tag	UNP P9WGI5
QA	-2	GLY	-	expression tag	UNP P9WGI5
QA	-1	SER	-	expression tag	UNP P9WGI5
QA	0	HIS	-	expression tag	UNP P9WGI5
WA	-19	MET	-	initiating methionine	UNP P9WGI5
WA	-18	GLY	-	expression tag	UNP P9WGI5
WA	-17	SER	-	expression tag	UNP P9WGI5
WA	-16	SER	-	expression tag	UNP P9WGI5
WA	-15	HIS	-	expression tag	UNP P9WGI5
WA	-14	HIS	-	expression tag	UNP P9WGI5
WA	-13	HIS	-	expression tag	UNP P9WGI5
WA	-12	HIS	-	expression tag	UNP P9WGI5

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
WA	-11	HIS	-	expression tag	UNP P9WGI5
WA	-10	HIS	-	expression tag	UNP P9WGI5
WA	-9	SER	-	expression tag	UNP P9WGI5
WA	-8	SER	-	expression tag	UNP P9WGI5
WA	-7	GLY	-	expression tag	UNP P9WGI5
WA	-6	LEU	-	expression tag	UNP P9WGI5
WA	-5	VAL	-	expression tag	UNP P9WGI5
WA	-4	PRO	-	expression tag	UNP P9WGI5
WA	-3	ARG	-	expression tag	UNP P9WGI5
WA	-2	GLY	-	expression tag	UNP P9WGI5
WA	-1	SER	-	expression tag	UNP P9WGI5
WA	0	HIS	-	expression tag	UNP P9WGI5

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
6	D	2	Total Zn 2 2	0
6	J	2	Total Zn 2 2	0
6	P	2	Total Zn 2 2	0
6	W	2	Total Zn 2 2	0
6	CA	2	Total Zn 2 2	0
6	IA	2	Total Zn 2 2	0
6	OA	2	Total Zn 2 2	0
6	UA	2	Total Zn 2 2	0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
7	D	1	Total Mg 1 1	0
7	J	1	Total Mg 1 1	0

*Continued on next page...*

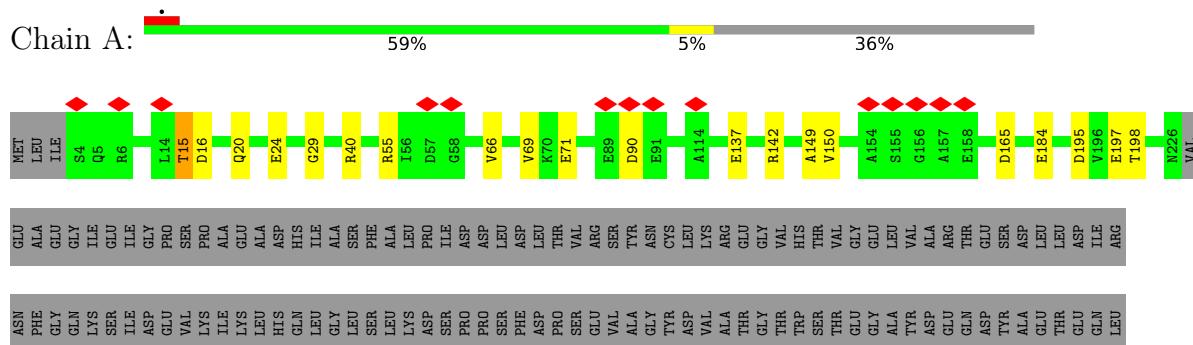
*Continued from previous page...*

Mol	Chain	Residues	Atoms	AltConf
7	P	1	Total Mg 1 1	0
7	W	1	Total Mg 1 1	0
7	CA	1	Total Mg 1 1	0
7	IA	1	Total Mg 1 1	0
7	OA	1	Total Mg 1 1	0
7	UA	1	Total Mg 1 1	0

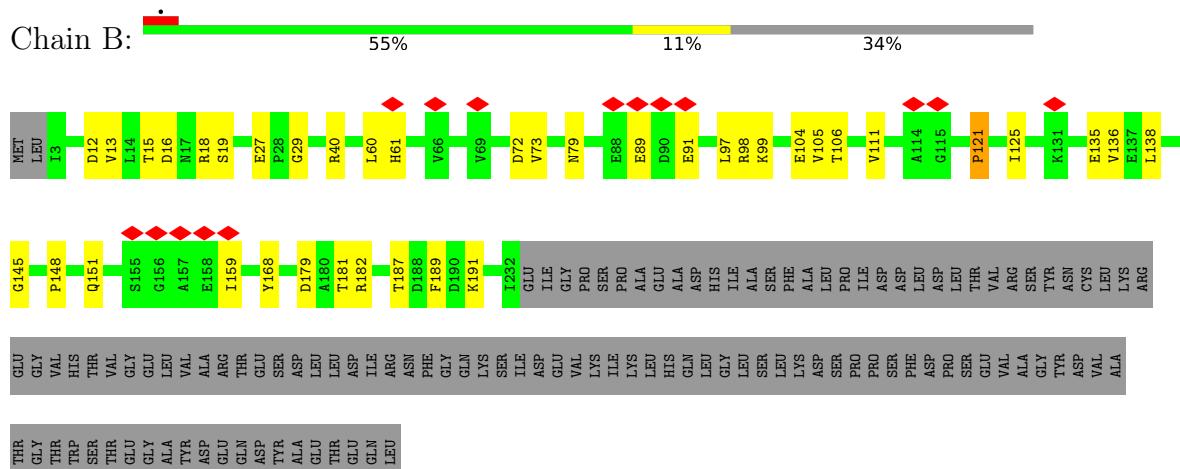
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

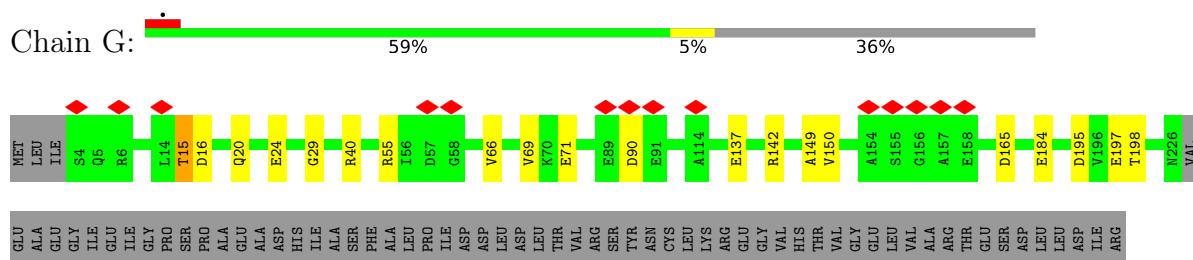
- Molecule 1: DNA-directed RNA polymerase subunit alpha

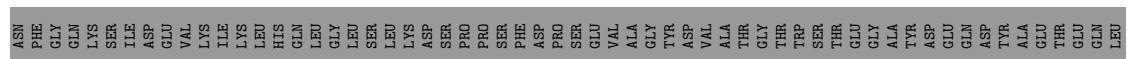


- Molecule 1: DNA-directed RNA polymerase subunit alpha

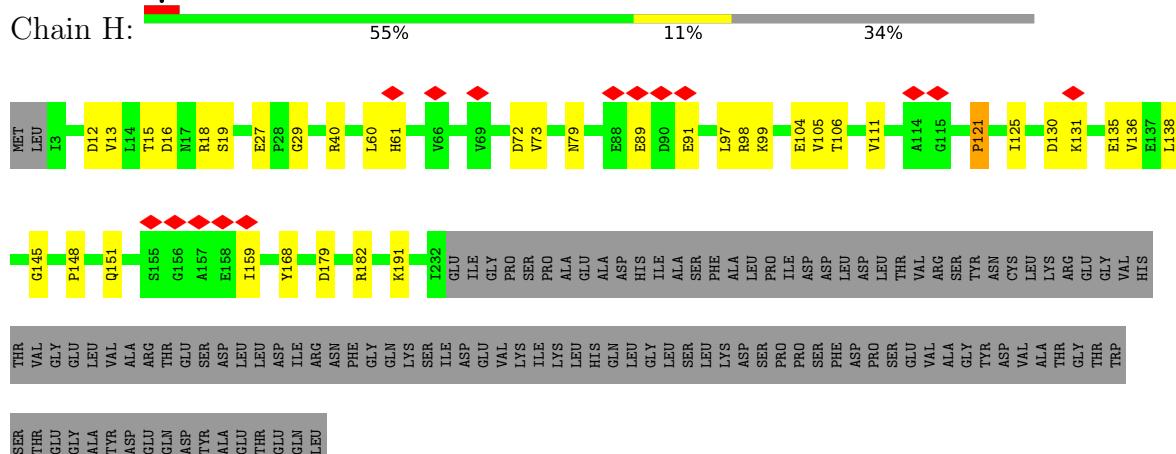


- Molecule 1: DNA-directed RNA polymerase subunit alpha

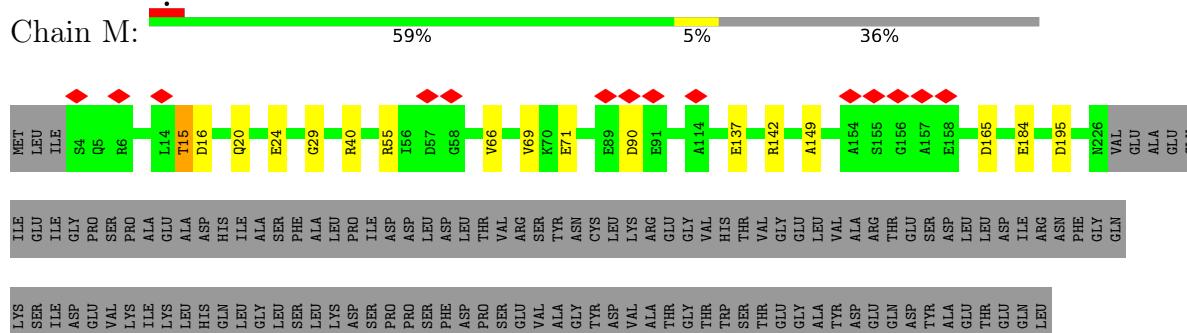




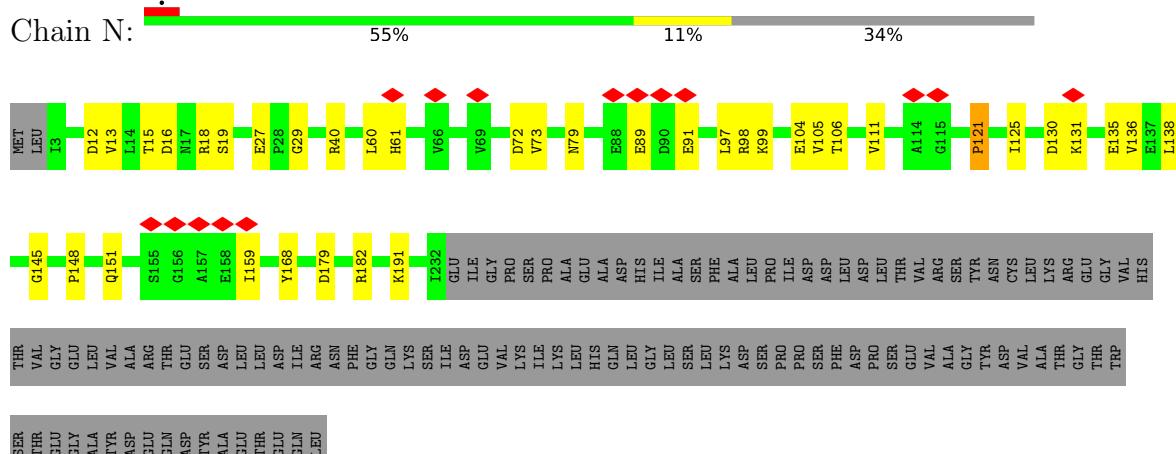
- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha

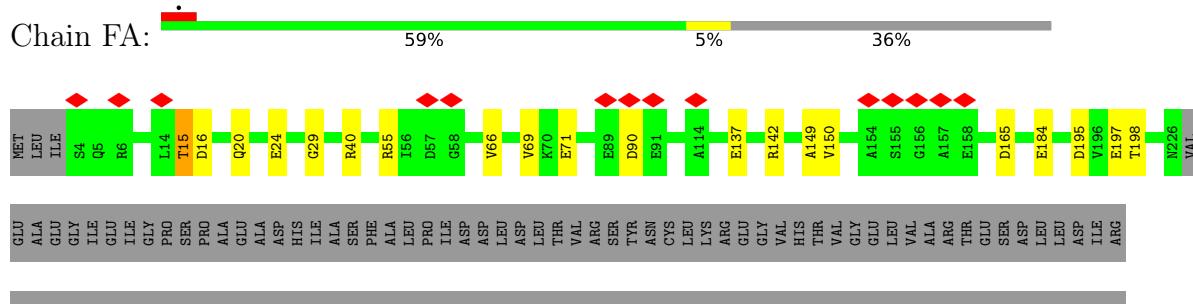


- Molecule 1: DNA-directed RNA polymerase subunit alpha

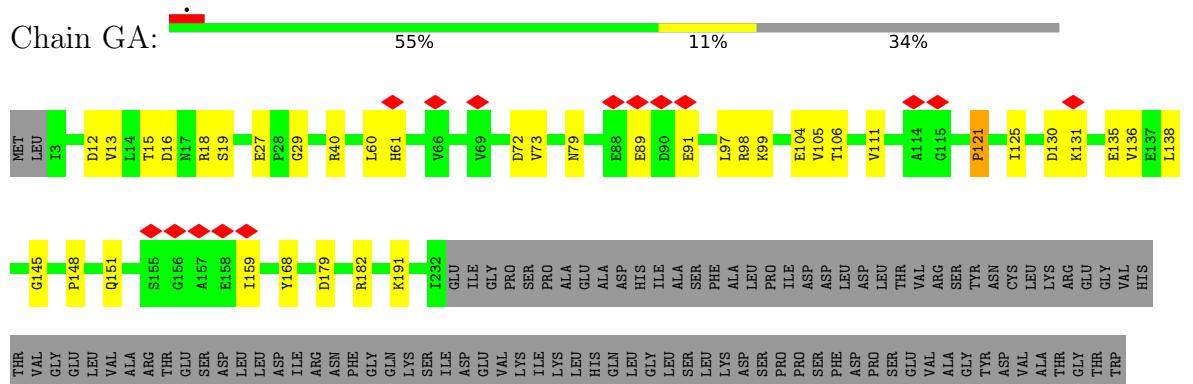




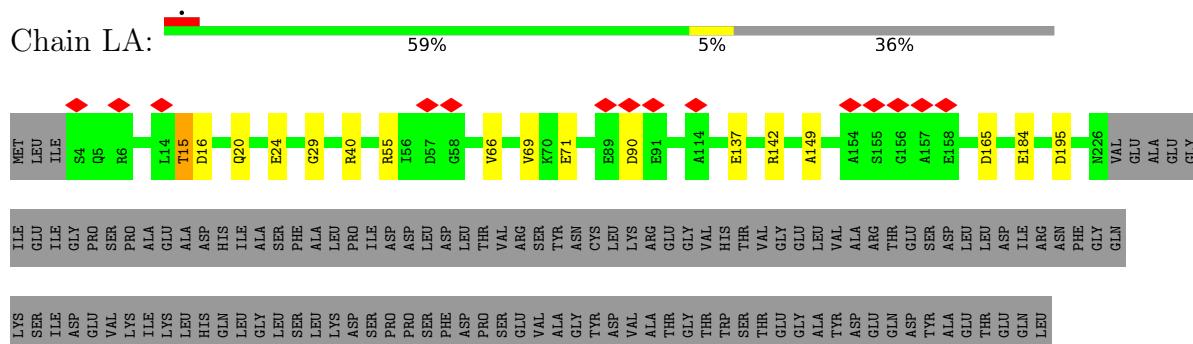
- Molecule 1: DNA-directed RNA polymerase subunit alpha



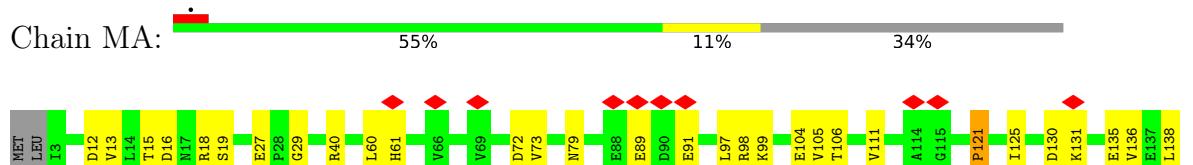
- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha



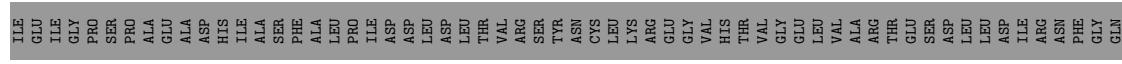
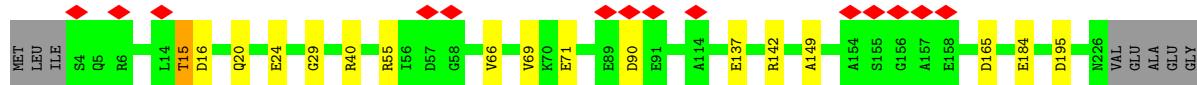
- Molecule 1: DNA-directed RNA polymerase subunit alpha



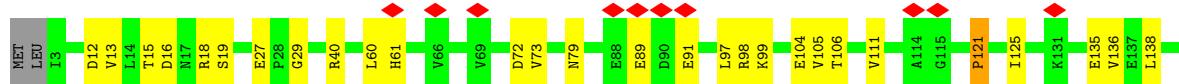


THR VAL GLY GLU LEU VAL ALA ARG THR GLU SER ASP PHE GLY GLN LYS SER ASN ASP GLU VAL LYS ILE LYS LYS SER SER LEU HIS GLN LEU GLY LEU SER PRO SER PHE ASP PRO SER GLU VAL ALA GLY TYR ASP VAL ALA THR GLY THR TRP

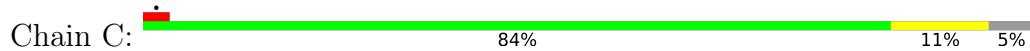
- Molecule 1: DNA-directed RNA polymerase subunit alpha

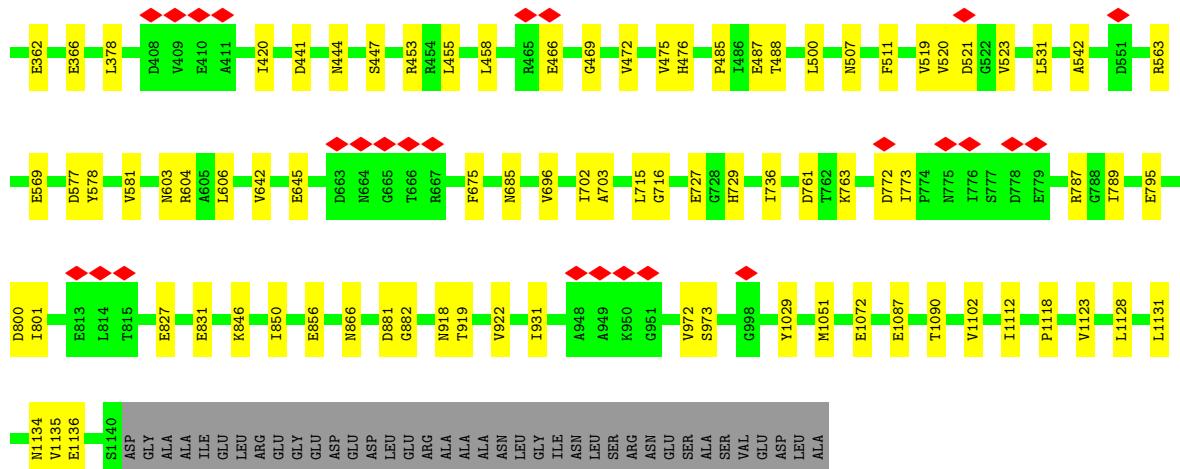


- Molecule 1: DNA-directed RNA polymerase subunit alpha



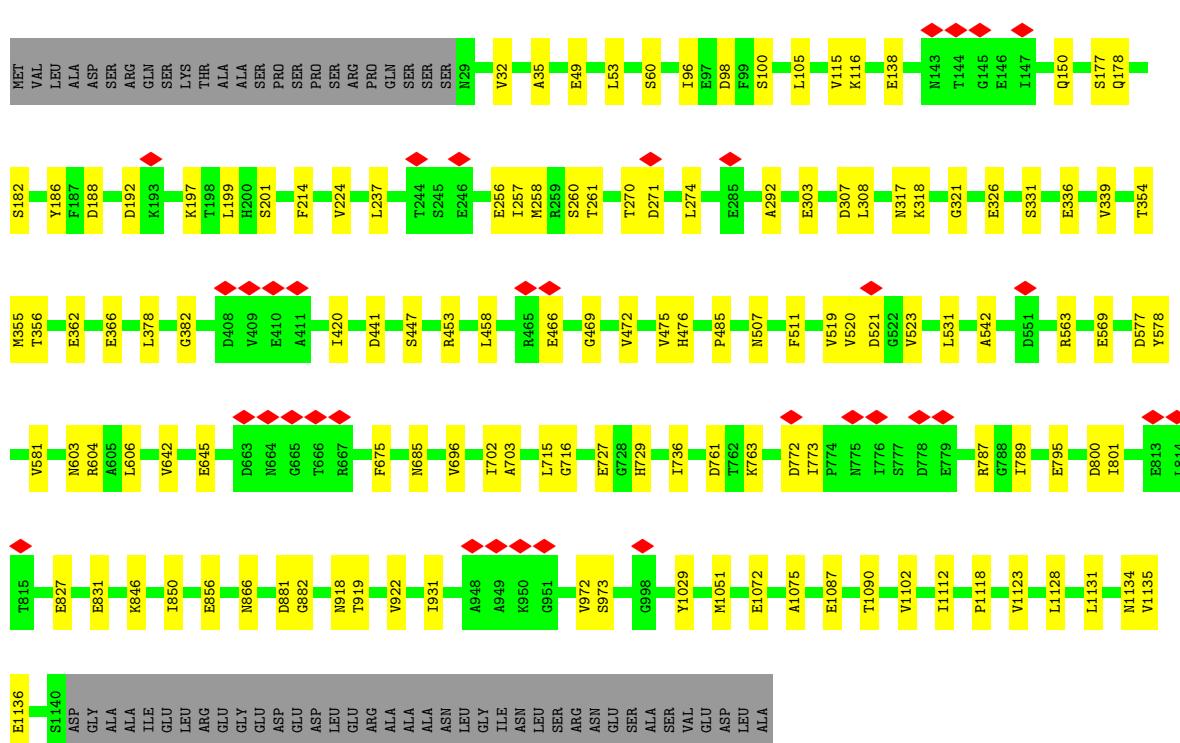
- Molecule 2: DNA-directed RNA polymerase subunit beta





- Molecule 2: DNA-directed RNA polymerase subunit beta

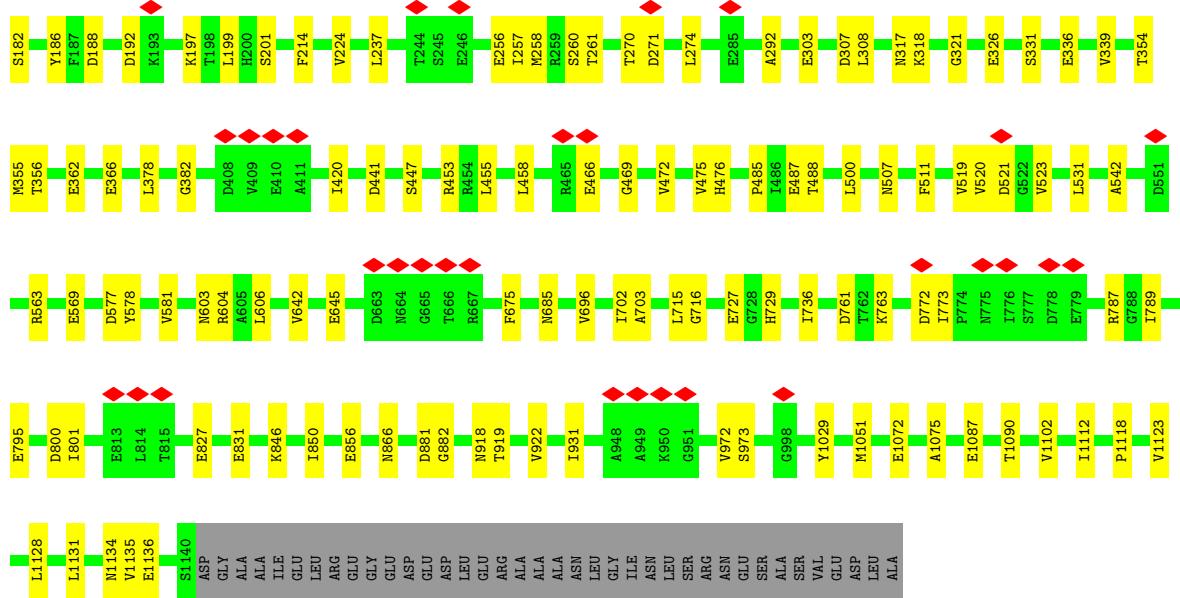
Chain I:



- Molecule 2: DNA-directed RNA polymerase subunit beta

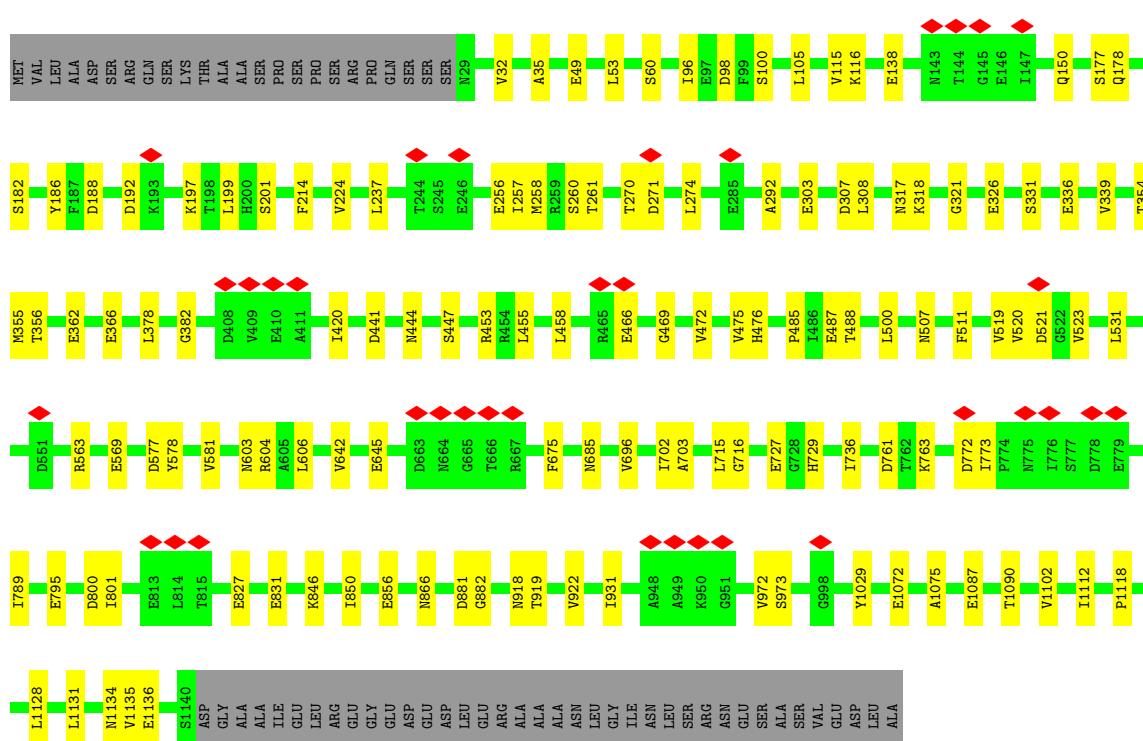
### Chain C





- Molecule 2: DNA-directed RNA polymerase subunit beta

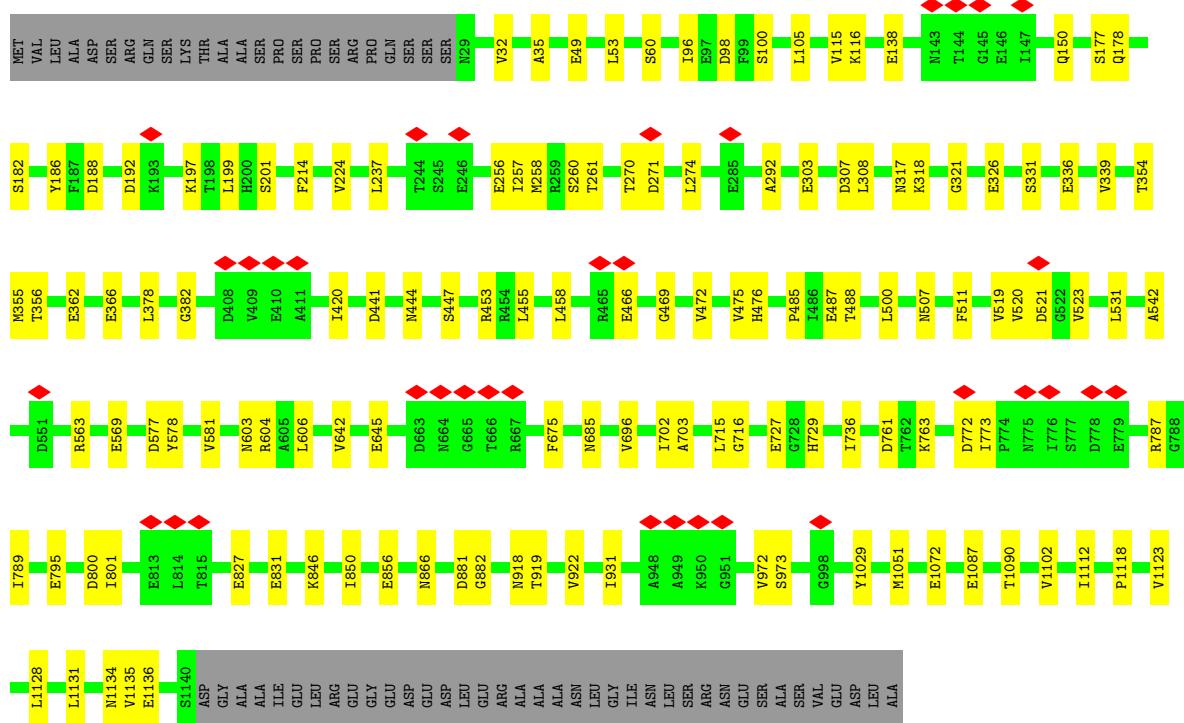
### Chain V:



- Molecule 2: DNA-directed RNA polymerase subunit beta

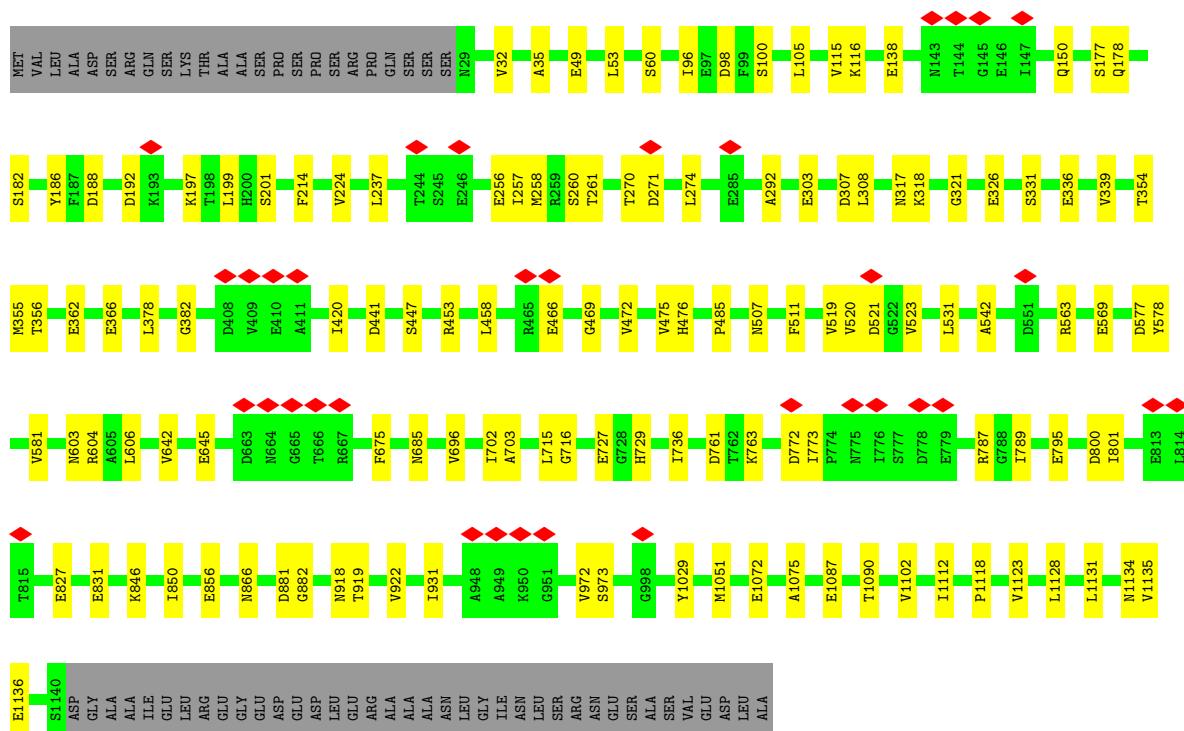
Chain BA:





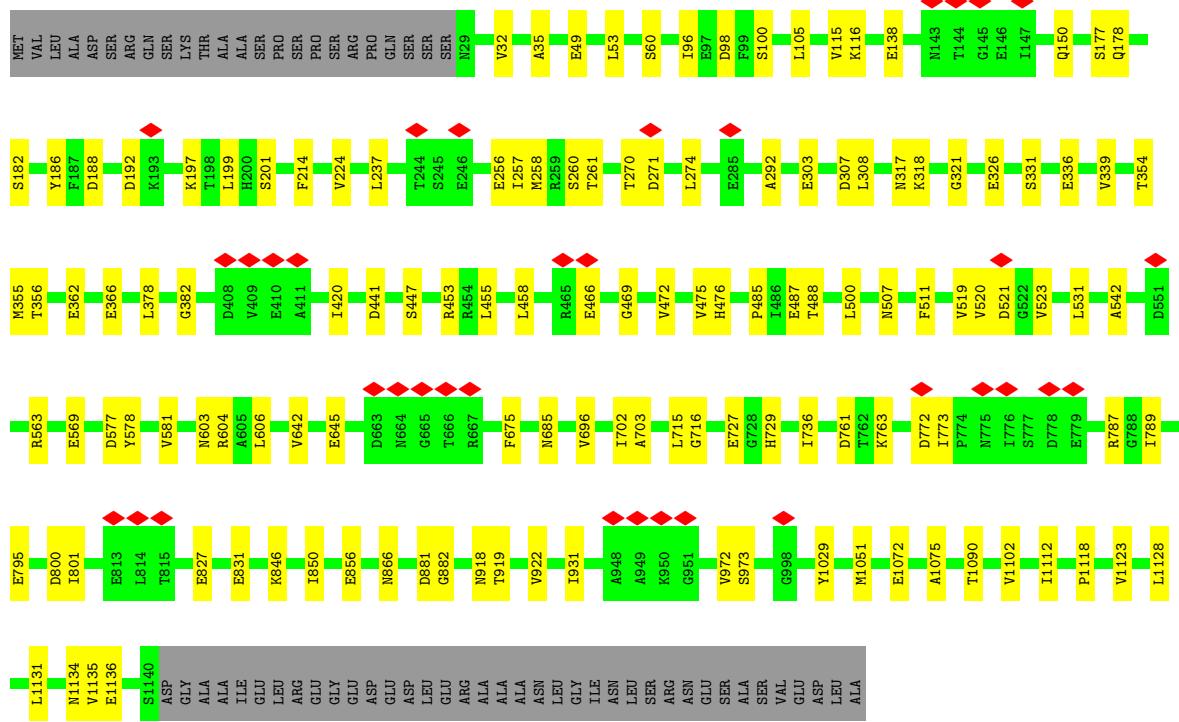
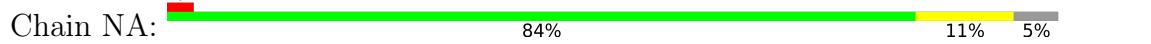
- Molecule 2: DNA-directed RNA polymerase subunit beta

Chain HA:



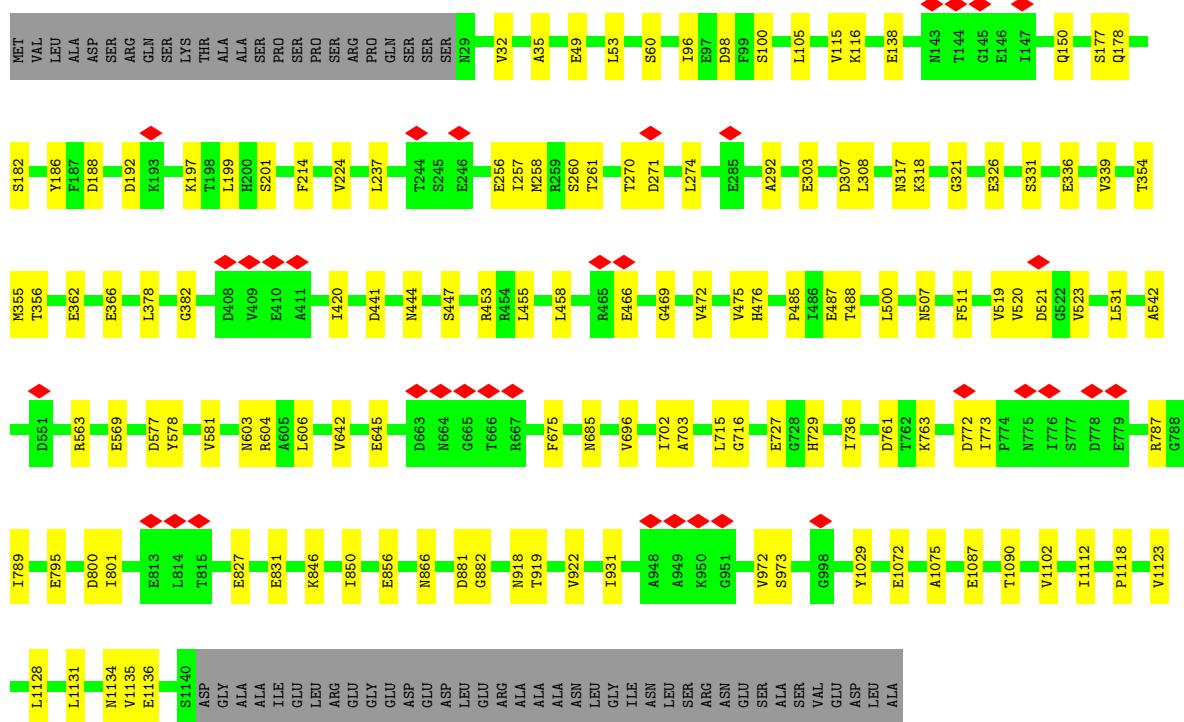
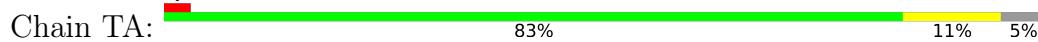
- Molecule 2: DNA-directed RNA polymerase subunit beta

Chain NA:

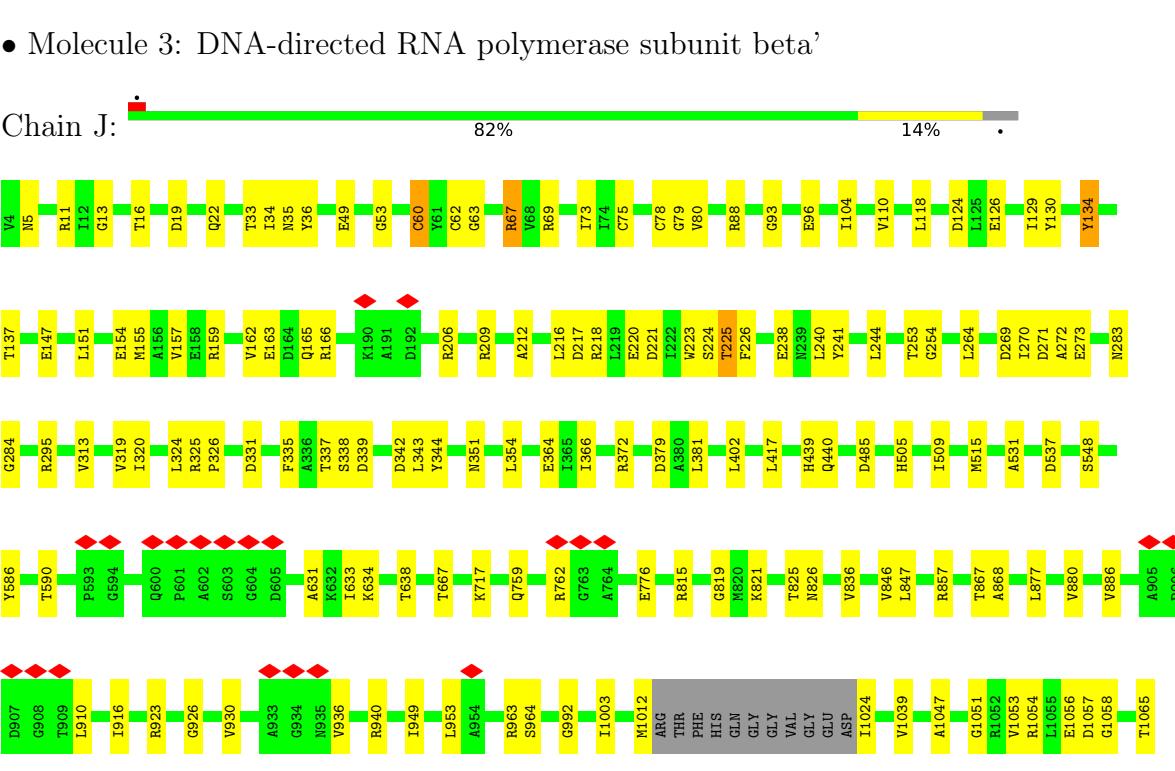
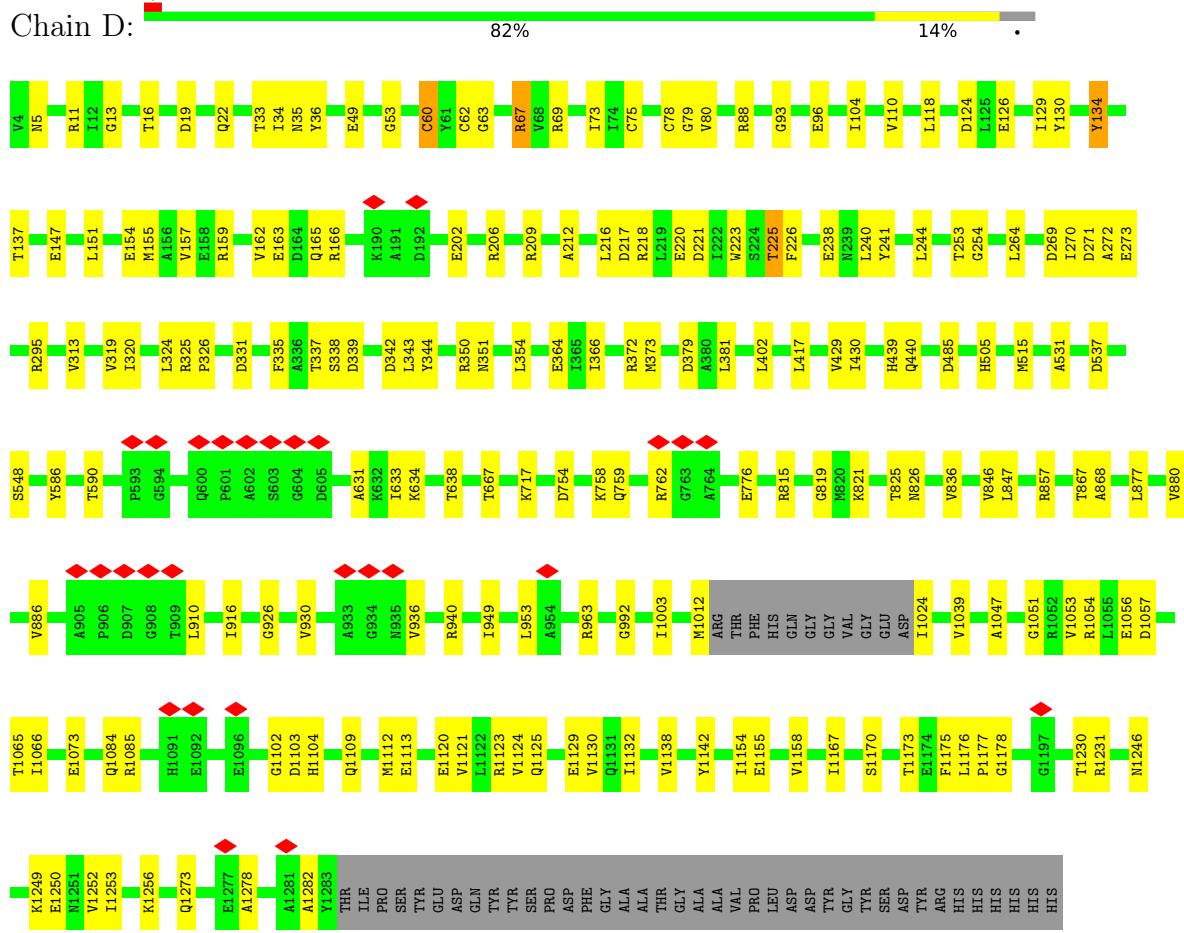


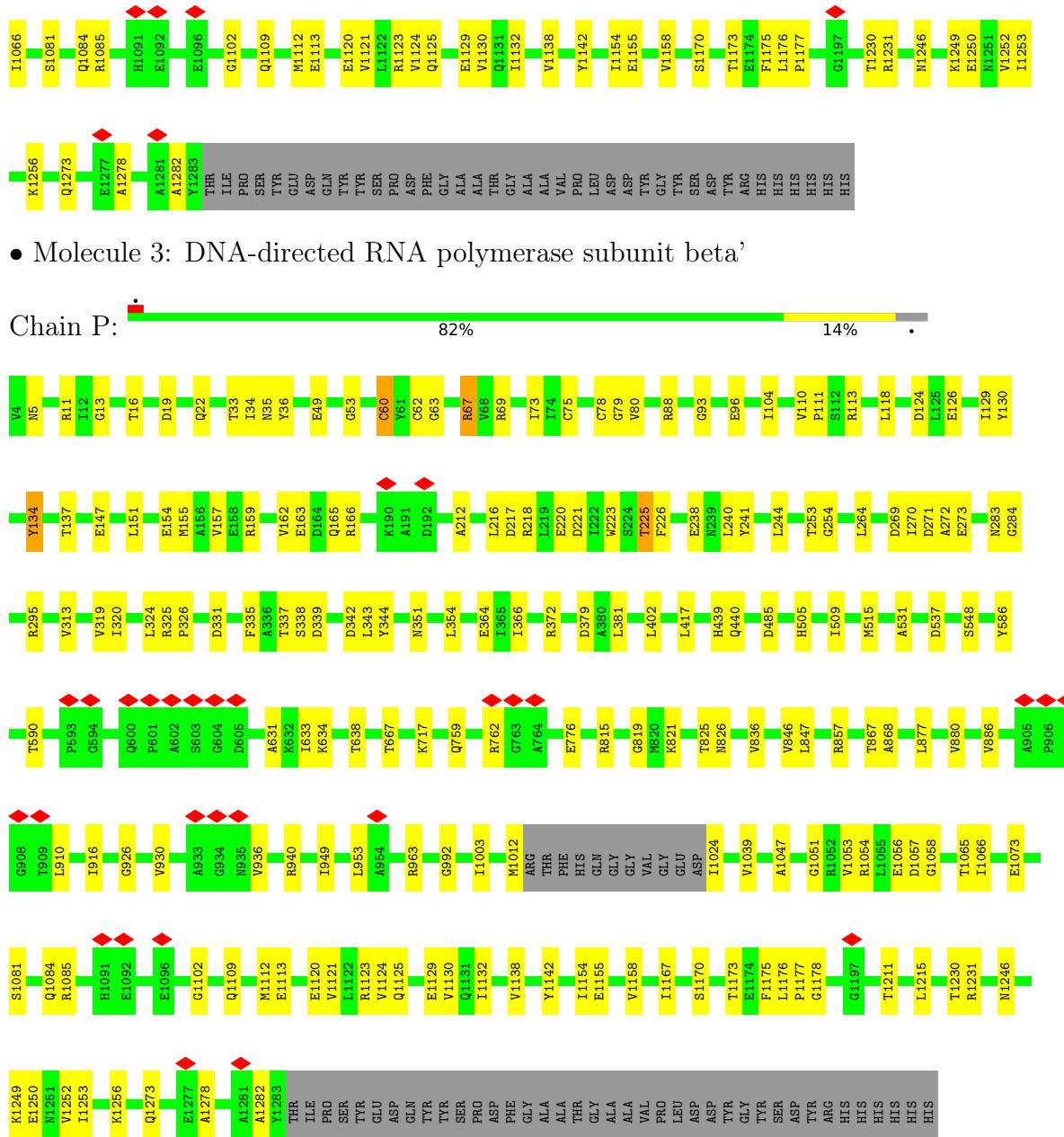
- Molecule 2: DNA-directed RNA polymerase subunit beta

Chain TA:



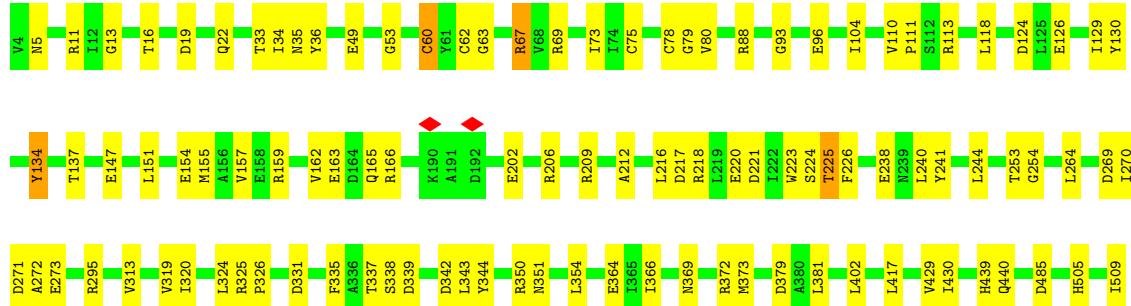
- Molecule 3: DNA-directed RNA polymerase subunit beta'

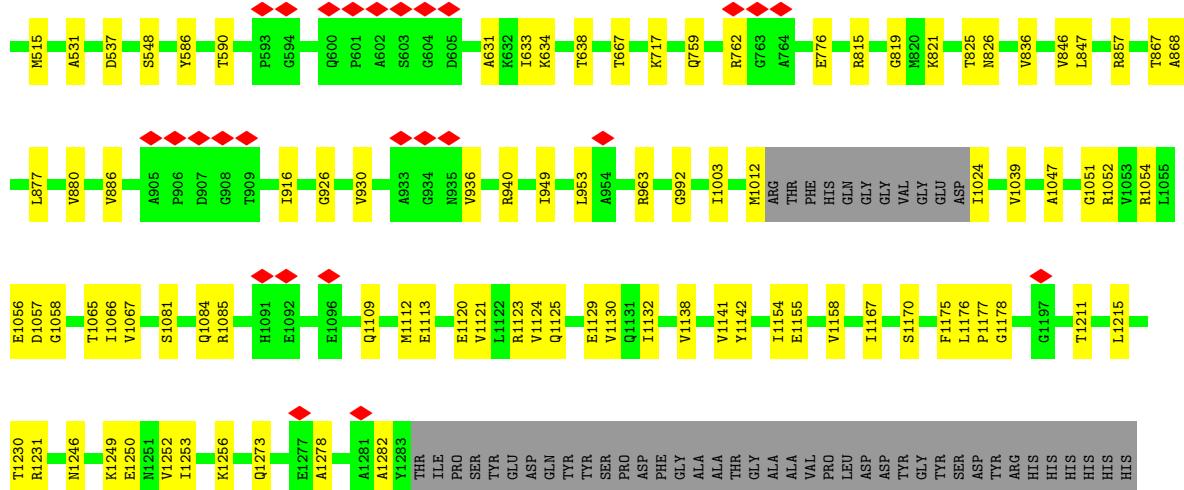




- Molecule 3: DNA-directed RNA polymerase subunit beta'

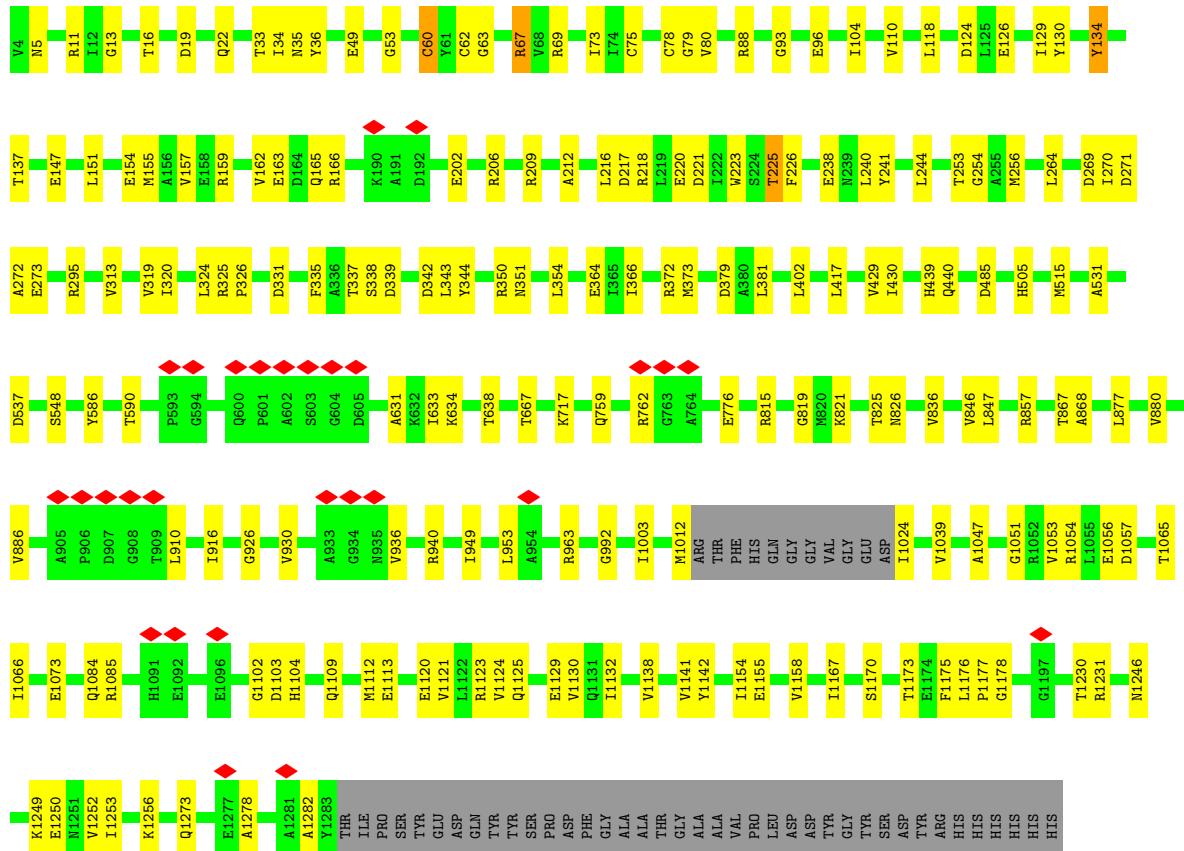
Chain W:  81%  15%





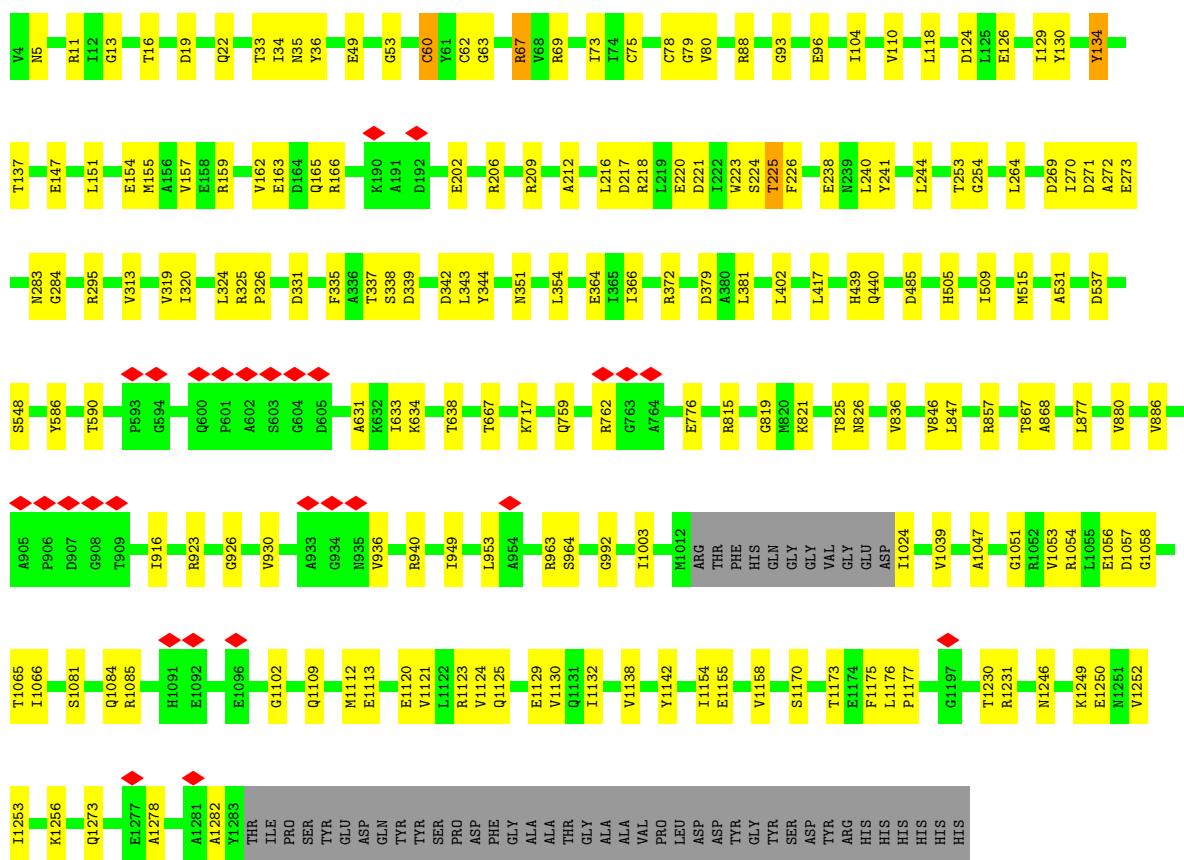
- Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain CA: 82% 14%



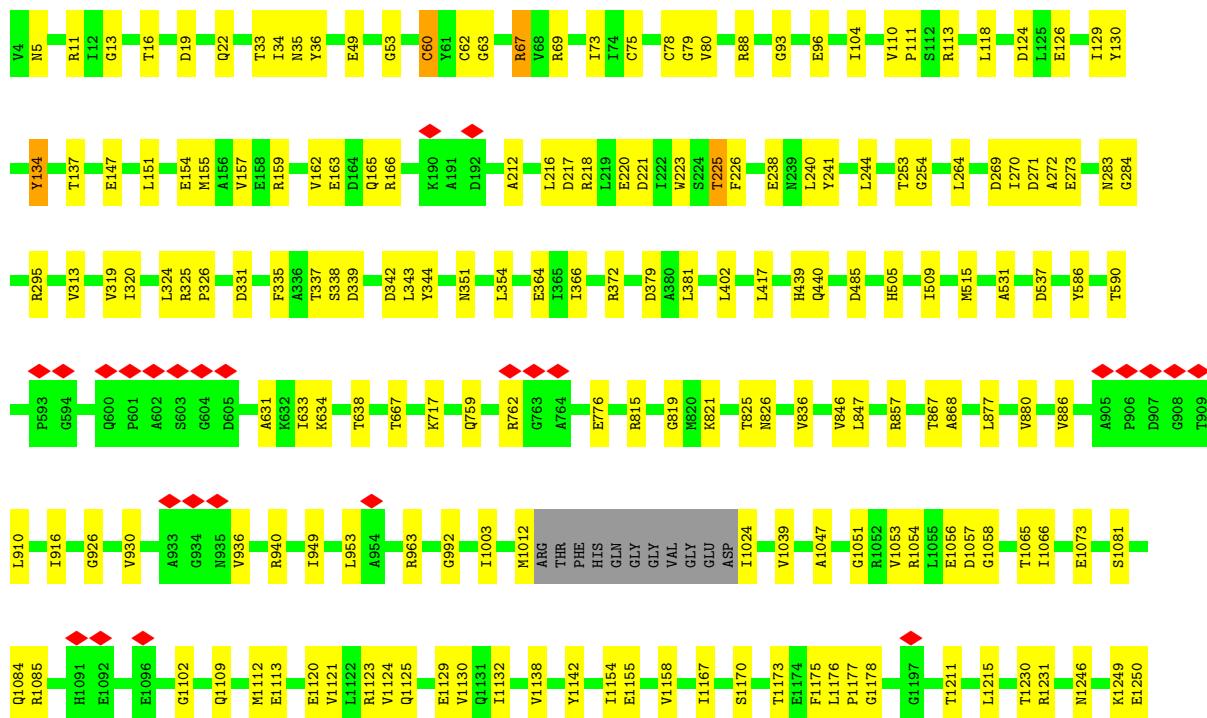
- Molecule 3: DNA-directed RNA polymerase subunit beta'

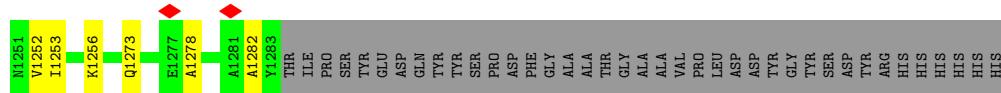
Chain IA: 82% 14%



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

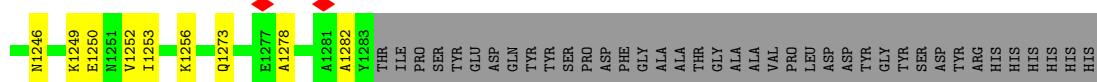
Chain OA:





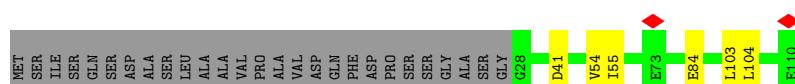
- Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain UA:



- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:



- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain K:



- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain Q: 70%

A horizontal progress bar with a green segment representing 70% completion. The bar is labeled "Chain Q:" at the start and has percentage markers at 5% and 25%.



- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain X: 70%

A horizontal progress bar consisting of three colored segments: green, yellow, and grey. The green segment on the left represents 70% completion. The yellow segment to its right represents 5% completion, and the grey segment on the far right represents 25% completion. The total length of the bar is 100%.



- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain DA: 70%

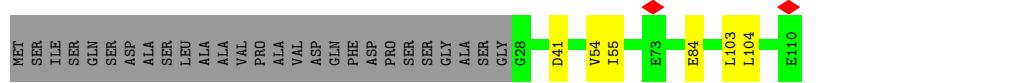
A horizontal progress bar consisting of a red dot at the start, followed by a green segment representing 70% completion, a grey segment representing 5%, and a black segment representing 25%.



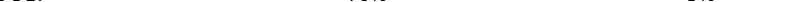
- Molecule 4: DNA-directed RNA polymerase subunit omega

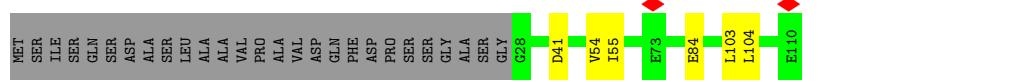
Chain JA: 70%

A horizontal progress bar consisting of a red dot at the start, followed by a green segment representing 70% completion, a grey segment representing 5%, and a yellow segment representing 25%.

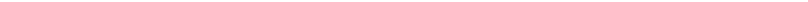


- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain PA:  70% 5% 25%



- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain VA:  70% 5% 25%

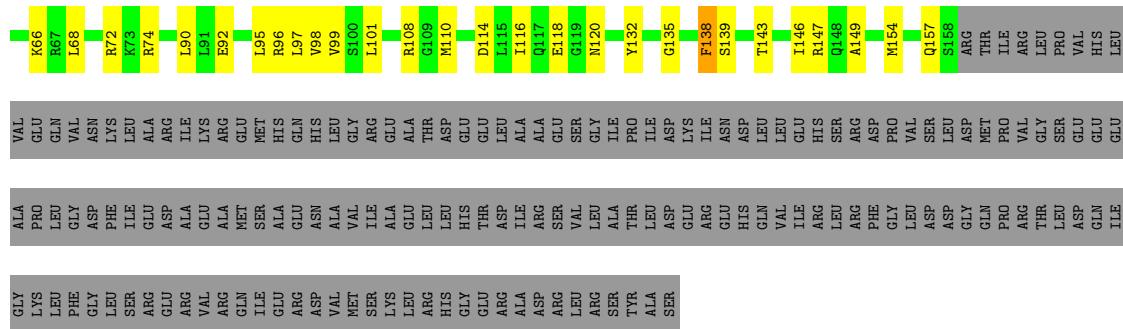


- Molecule 5: RNA polymerase sigma factor SigB

Chain F: 29% 12% 59%

A horizontal progress bar divided into three segments. The first segment is green and labeled '29%'. The second segment is yellow and labeled '12%'. The third segment is grey and labeled '59%'. The total length of the bar is 100%, indicated by the cumulative percentage labels.

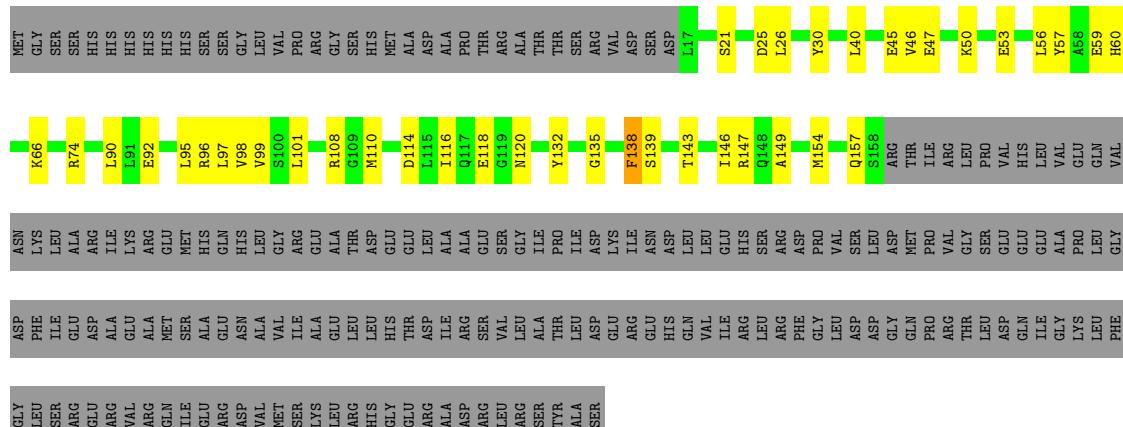




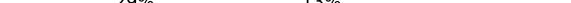
- Molecule 5: RNA polymerase sigma factor SigB

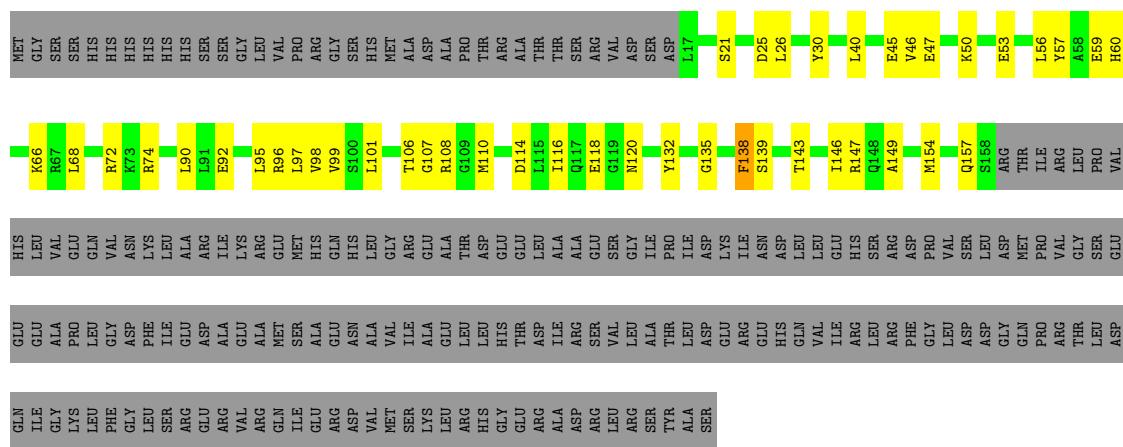
Chain L: 30% 11% 59%

A horizontal progress bar divided into three segments: green (30%), yellow (11%), and grey (59%). The segments are separated by thin black lines.



- Molecule 5: RNA polymerase sigma factor SigB

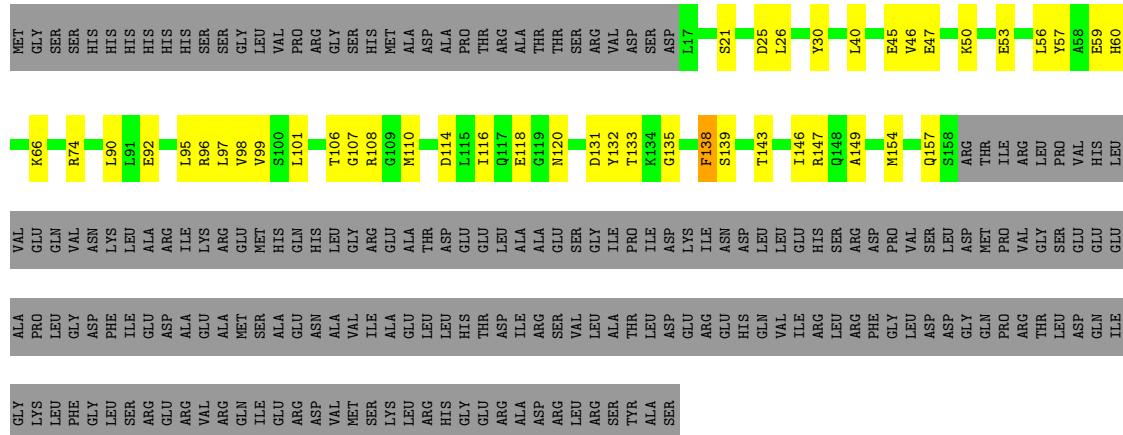
Chain R:  29% 13% 59%



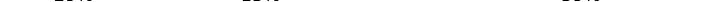
- Molecule 5: RNA polymerase sigma factor SigB

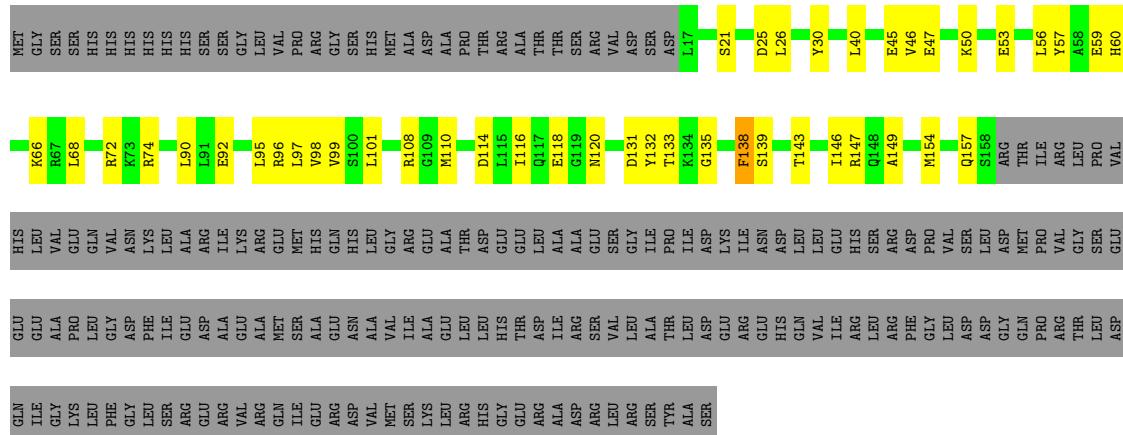
Chain Y: 59%

A horizontal progress bar for 'Chain Y' is shown. The bar is divided into three segments: a green segment on the left labeled '29%', a yellow segment in the middle labeled '13%', and a grey segment on the right labeled '59%'. The total length of the bar represents 100% completion.

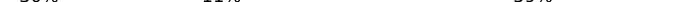


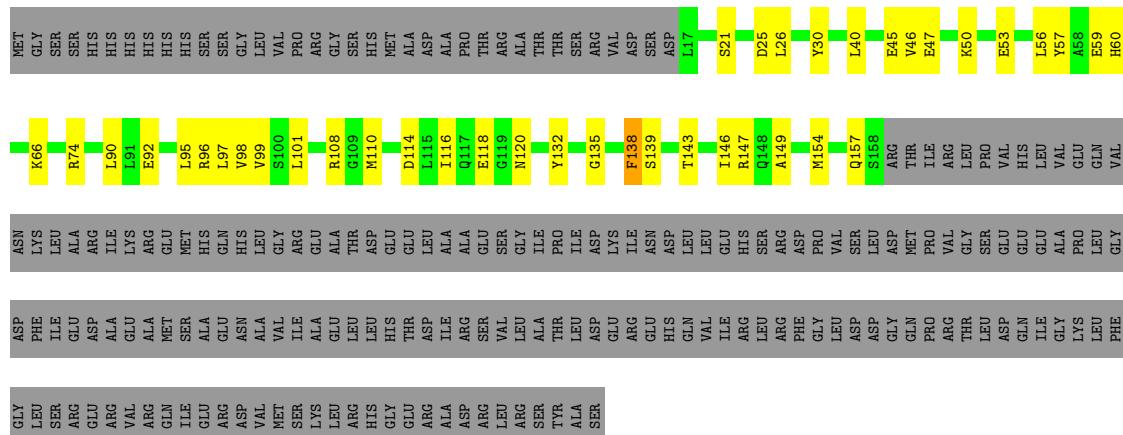
- Molecule 5: RNA polymerase sigma factor SigB

Chain EA:  29% 13% 59%



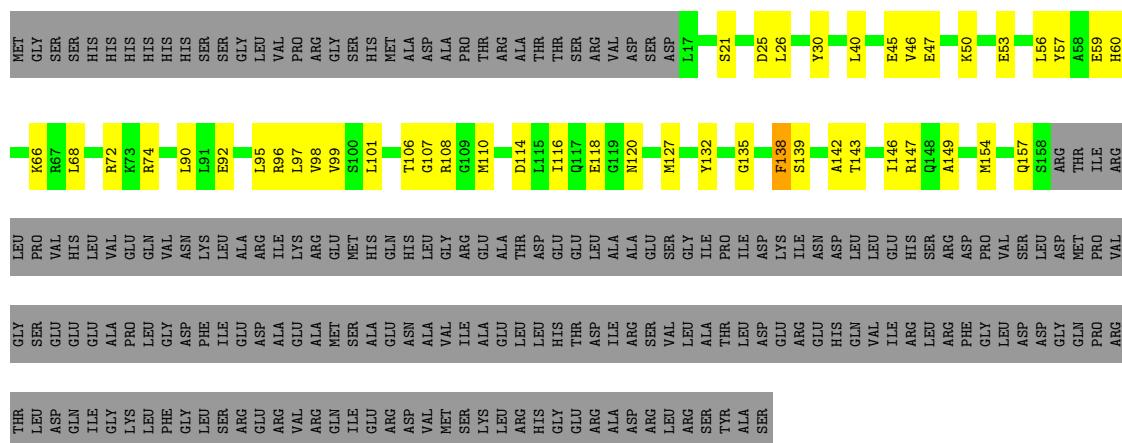
- Molecule 5: RNA polymerase sigma factor SigB

Chain KA:  30% 11% 59%



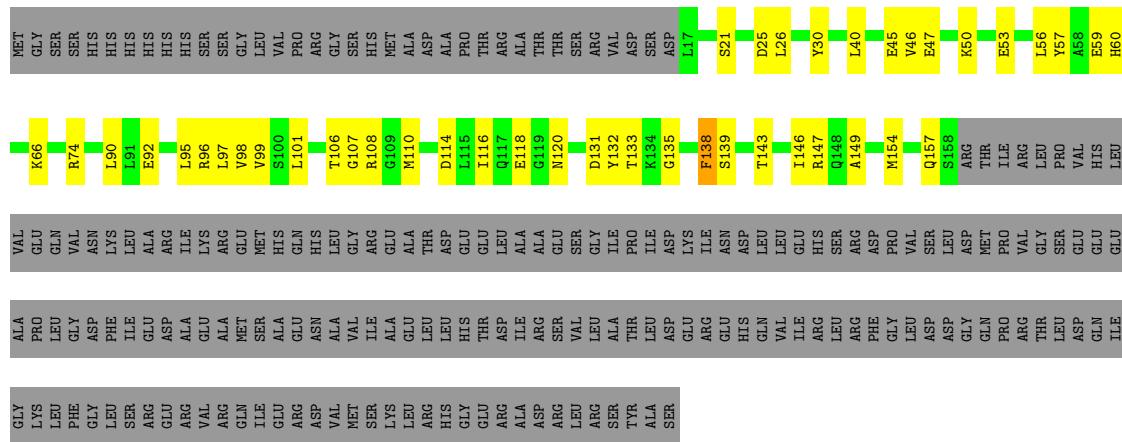
- Molecule 5: RNA polymerase sigma factor SigB

Chain QA:



- Molecule 5: RNA polymerase sigma factor SigB

Chain WA



## 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D4	Depositor
Number of particles used	115457	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	49.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.457	Depositor
Minimum map value	-0.959	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	495.0, 495.0, 495.0	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

## 5 Model quality [\(i\)](#)

### 5.1 Standard geometry [\(i\)](#)

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

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	0.24	0/1726	0.51	0/2348
1	AA	0.25	0/1775	0.51	0/2414
1	B	0.25	0/1775	0.51	0/2414
1	FA	0.24	0/1726	0.51	0/2348
1	G	0.24	0/1726	0.51	0/2348
1	GA	0.25	0/1775	0.51	0/2414
1	H	0.25	0/1775	0.51	0/2414
1	LA	0.24	0/1726	0.51	0/2348
1	M	0.24	0/1726	0.51	0/2348
1	MA	0.25	0/1775	0.51	0/2414
1	N	0.25	0/1775	0.51	0/2414
1	RA	0.24	0/1726	0.51	0/2348
1	S	0.24	0/1726	0.51	0/2348
1	SA	0.25	0/1775	0.51	0/2414
1	T	0.25	0/1775	0.51	0/2414
1	Z	0.24	0/1726	0.51	0/2348
2	BA	0.24	0/8799	0.50	0/11929
2	C	0.24	0/8799	0.50	0/11929
2	HA	0.24	0/8799	0.50	0/11929
2	I	0.24	0/8799	0.50	0/11929
2	NA	0.24	0/8799	0.50	0/11929
2	O	0.24	0/8799	0.50	0/11929
2	TA	0.24	0/8799	0.50	0/11929
2	V	0.24	0/8799	0.50	0/11929
3	CA	0.27	0/10118	0.53	0/13675
3	D	0.27	0/10118	0.53	0/13675
3	IA	0.27	0/10118	0.53	0/13675
3	J	0.27	0/10118	0.53	0/13675
3	OA	0.27	0/10118	0.53	0/13675
3	P	0.27	0/10118	0.53	0/13675
3	UA	0.27	0/10118	0.53	0/13675
3	W	0.27	0/10118	0.53	0/13675

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
4	DA	0.24	0/667	0.44	0/908
4	E	0.24	0/667	0.44	0/908
4	JA	0.24	0/667	0.44	0/908
4	K	0.24	0/667	0.44	0/908
4	PA	0.24	0/667	0.44	0/908
4	Q	0.24	0/667	0.44	0/908
4	VA	0.24	0/667	0.44	0/908
4	X	0.24	0/667	0.44	0/908
5	EA	0.39	0/1134	0.67	0/1525
5	F	0.39	0/1134	0.67	0/1525
5	KA	0.39	0/1134	0.67	0/1525
5	L	0.39	0/1134	0.67	0/1525
5	QA	0.39	0/1134	0.67	0/1525
5	R	0.39	0/1134	0.67	0/1525
5	WA	0.39	0/1134	0.67	0/1525
5	Y	0.39	0/1134	0.67	0/1525
All	All	0.26	0/193752	0.52	0/262392

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1700	0	1734	13	0
1	AA	1749	0	1781	25	0
1	B	1749	0	1781	25	0
1	FA	1700	0	1734	13	0
1	G	1700	0	1734	13	0
1	GA	1749	0	1781	24	0
1	H	1749	0	1781	24	0
1	LA	1700	0	1734	12	0
1	M	1700	0	1734	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	MA	1749	0	1781	24	0
1	N	1749	0	1781	24	0
1	RA	1700	0	1734	12	0
1	S	1700	0	1734	12	0
1	SA	1749	0	1781	24	0
1	T	1749	0	1781	24	0
1	Z	1700	0	1734	13	0
2	BA	8640	0	8584	87	0
2	C	8640	0	8584	86	0
2	HA	8640	0	8584	84	0
2	I	8640	0	8584	84	0
2	NA	8640	0	8584	86	0
2	O	8640	0	8584	87	0
2	TA	8640	0	8584	87	0
2	V	8640	0	8584	87	0
3	CA	9951	0	10035	136	0
3	D	9951	0	10035	135	0
3	IA	9951	0	10035	131	0
3	J	9951	0	10035	132	0
3	OA	9951	0	10035	134	0
3	P	9951	0	10035	135	0
3	UA	9951	0	10035	138	0
3	W	9951	0	10035	139	0
4	DA	654	0	648	4	0
4	E	654	0	648	4	0
4	JA	654	0	648	4	0
4	K	654	0	648	4	0
4	PA	654	0	648	4	0
4	Q	654	0	648	4	0
4	VA	654	0	648	4	0
4	X	654	0	648	4	0
5	EA	1119	0	1155	31	0
5	F	1119	0	1155	30	0
5	KA	1119	0	1155	31	0
5	L	1119	0	1155	30	0
5	QA	1119	0	1155	33	0
5	R	1119	0	1155	31	0
5	WA	1119	0	1155	31	0
5	Y	1119	0	1155	31	0
6	CA	2	0	0	0	0
6	D	2	0	0	0	0
6	IA	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	J	2	0	0	0	0
6	OA	2	0	0	0	0
6	P	2	0	0	0	0
6	UA	2	0	0	0	0
6	W	2	0	0	0	0
7	CA	1	0	0	0	0
7	D	1	0	0	0	0
7	IA	1	0	0	0	0
7	J	1	0	0	0	0
7	OA	1	0	0	0	0
7	P	1	0	0	0	0
7	UA	1	0	0	0	0
7	W	1	0	0	0	0
All	All	190528	0	191496	2187	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 6.

The worst 5 of 2187 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)
3:W:326:PRO:O	3:W:337:THR:OG1	1.93	0.87
3:UA:326:PRO:O	3:UA:337:THR:OG1	1.93	0.87
3:OA:326:PRO:O	3:OA:337:THR:OG1	1.93	0.87
3:P:326:PRO:O	3:P:337:THR:OG1	1.93	0.87
3:J:326:PRO:O	3:J:337:THR:OG1	1.93	0.85

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 PDB entries followed by that with respect to all EM entries.

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	221/347 (64%)	212 (96%)	9 (4%)	0	100 100
1	AA	228/347 (66%)	222 (97%)	6 (3%)	0	100 100
1	B	228/347 (66%)	222 (97%)	6 (3%)	0	100 100
1	FA	221/347 (64%)	212 (96%)	9 (4%)	0	100 100
1	G	221/347 (64%)	212 (96%)	9 (4%)	0	100 100
1	GA	228/347 (66%)	222 (97%)	6 (3%)	0	100 100
1	H	228/347 (66%)	222 (97%)	6 (3%)	0	100 100
1	LA	221/347 (64%)	212 (96%)	9 (4%)	0	100 100
1	M	221/347 (64%)	212 (96%)	9 (4%)	0	100 100
1	MA	228/347 (66%)	222 (97%)	6 (3%)	0	100 100
1	N	228/347 (66%)	222 (97%)	6 (3%)	0	100 100
1	RA	221/347 (64%)	212 (96%)	9 (4%)	0	100 100
1	S	221/347 (64%)	212 (96%)	9 (4%)	0	100 100
1	SA	228/347 (66%)	222 (97%)	6 (3%)	0	100 100
1	T	228/347 (66%)	222 (97%)	6 (3%)	0	100 100
1	Z	221/347 (64%)	212 (96%)	9 (4%)	0	100 100
2	BA	1110/1174 (94%)	1076 (97%)	34 (3%)	0	100 100
2	C	1110/1174 (94%)	1076 (97%)	34 (3%)	0	100 100
2	HA	1110/1174 (94%)	1076 (97%)	34 (3%)	0	100 100
2	I	1110/1174 (94%)	1076 (97%)	34 (3%)	0	100 100
2	NA	1110/1174 (94%)	1076 (97%)	34 (3%)	0	100 100
2	O	1110/1174 (94%)	1076 (97%)	34 (3%)	0	100 100
2	TA	1110/1174 (94%)	1076 (97%)	34 (3%)	0	100 100
2	V	1110/1174 (94%)	1076 (97%)	34 (3%)	0	100 100
3	CA	1265/1319 (96%)	1216 (96%)	49 (4%)	0	100 100
3	D	1265/1319 (96%)	1216 (96%)	49 (4%)	0	100 100
3	IA	1265/1319 (96%)	1216 (96%)	49 (4%)	0	100 100
3	J	1265/1319 (96%)	1216 (96%)	49 (4%)	0	100 100
3	OA	1265/1319 (96%)	1216 (96%)	49 (4%)	0	100 100
3	P	1265/1319 (96%)	1216 (96%)	49 (4%)	0	100 100
3	UA	1265/1319 (96%)	1216 (96%)	49 (4%)	0	100 100
3	W	1265/1319 (96%)	1216 (96%)	49 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	DA	81/110 (74%)	75 (93%)	6 (7%)	0	100 100
4	E	81/110 (74%)	75 (93%)	6 (7%)	0	100 100
4	JA	81/110 (74%)	75 (93%)	6 (7%)	0	100 100
4	K	81/110 (74%)	75 (93%)	6 (7%)	0	100 100
4	PA	81/110 (74%)	75 (93%)	6 (7%)	0	100 100
4	Q	81/110 (74%)	75 (93%)	6 (7%)	0	100 100
4	VA	81/110 (74%)	75 (93%)	6 (7%)	0	100 100
4	X	81/110 (74%)	75 (93%)	6 (7%)	0	100 100
5	EA	140/343 (41%)	136 (97%)	4 (3%)	0	100 100
5	F	140/343 (41%)	136 (97%)	4 (3%)	0	100 100
5	KA	140/343 (41%)	136 (97%)	4 (3%)	0	100 100
5	L	140/343 (41%)	136 (97%)	4 (3%)	0	100 100
5	QA	140/343 (41%)	136 (97%)	4 (3%)	0	100 100
5	R	140/343 (41%)	136 (97%)	4 (3%)	0	100 100
5	WA	140/343 (41%)	136 (97%)	4 (3%)	0	100 100
5	Y	140/343 (41%)	136 (97%)	4 (3%)	0	100 100
All	All	24360/29120 (84%)	23496 (96%)	864 (4%)	0	100 100

There are no Ramachandran outliers to report.

### 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 PDB entries followed by that with respect to all EM entries.

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	192/297 (65%)	191 (100%)	1 (0%)	88 93
1	AA	197/297 (66%)	195 (99%)	2 (1%)	76 86
1	B	197/297 (66%)	195 (99%)	2 (1%)	76 86
1	FA	192/297 (65%)	191 (100%)	1 (0%)	88 93
1	G	192/297 (65%)	191 (100%)	1 (0%)	88 93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	GA	197/297 (66%)	195 (99%)	2 (1%)	76 86
1	H	197/297 (66%)	195 (99%)	2 (1%)	76 86
1	LA	192/297 (65%)	191 (100%)	1 (0%)	88 93
1	M	192/297 (65%)	191 (100%)	1 (0%)	88 93
1	MA	197/297 (66%)	195 (99%)	2 (1%)	76 86
1	N	197/297 (66%)	195 (99%)	2 (1%)	76 86
1	RA	192/297 (65%)	191 (100%)	1 (0%)	88 93
1	S	192/297 (65%)	191 (100%)	1 (0%)	88 93
1	SA	197/297 (66%)	195 (99%)	2 (1%)	76 86
1	T	197/297 (66%)	195 (99%)	2 (1%)	76 86
1	Z	192/297 (65%)	191 (100%)	1 (0%)	88 93
2	BA	946/995 (95%)	944 (100%)	2 (0%)	93 96
2	C	946/995 (95%)	944 (100%)	2 (0%)	93 96
2	HA	946/995 (95%)	944 (100%)	2 (0%)	93 96
2	I	946/995 (95%)	944 (100%)	2 (0%)	93 96
2	NA	946/995 (95%)	944 (100%)	2 (0%)	93 96
2	O	946/995 (95%)	944 (100%)	2 (0%)	93 96
2	TA	946/995 (95%)	944 (100%)	2 (0%)	93 96
2	V	946/995 (95%)	944 (100%)	2 (0%)	93 96
3	CA	1058/1098 (96%)	1048 (99%)	10 (1%)	78 88
3	D	1058/1098 (96%)	1048 (99%)	10 (1%)	78 88
3	IA	1058/1098 (96%)	1048 (99%)	10 (1%)	78 88
3	J	1058/1098 (96%)	1048 (99%)	10 (1%)	78 88
3	OA	1058/1098 (96%)	1048 (99%)	10 (1%)	78 88
3	P	1058/1098 (96%)	1048 (99%)	10 (1%)	78 88
3	UA	1058/1098 (96%)	1048 (99%)	10 (1%)	78 88
3	W	1058/1098 (96%)	1048 (99%)	10 (1%)	78 88
4	DA	70/90 (78%)	70 (100%)	0	100 100
4	E	70/90 (78%)	70 (100%)	0	100 100
4	JA	70/90 (78%)	70 (100%)	0	100 100
4	K	70/90 (78%)	70 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	PA	70/90 (78%)	70 (100%)	0	100 100
4	Q	70/90 (78%)	70 (100%)	0	100 100
4	VA	70/90 (78%)	70 (100%)	0	100 100
4	X	70/90 (78%)	70 (100%)	0	100 100
5	EA	111/284 (39%)	104 (94%)	7 (6%)	18 44
5	F	111/284 (39%)	104 (94%)	7 (6%)	18 44
5	KA	111/284 (39%)	104 (94%)	7 (6%)	18 44
5	L	111/284 (39%)	104 (94%)	7 (6%)	18 44
5	QA	111/284 (39%)	104 (94%)	7 (6%)	18 44
5	R	111/284 (39%)	104 (94%)	7 (6%)	18 44
5	WA	111/284 (39%)	104 (94%)	7 (6%)	18 44
5	Y	111/284 (39%)	104 (94%)	7 (6%)	18 44
All	All	20592/24488 (84%)	20416 (99%)	176 (1%)	79 88

5 of 176 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	IA	60	CYS
3	OA	537	ASP
3	IA	225	THR
5	KA	114	ASP
5	QA	74	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
3	UA	369	ASN
3	OA	369	ASN
3	CA	369	ASN
3	W	369	ASN
3	IA	369	ASN

### 5.3.3 RNA

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 monosaccharides in this entry.

## 5.6 Ligand geometry [\(i\)](#)

Of 24 ligands modelled in this entry, 24 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 [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

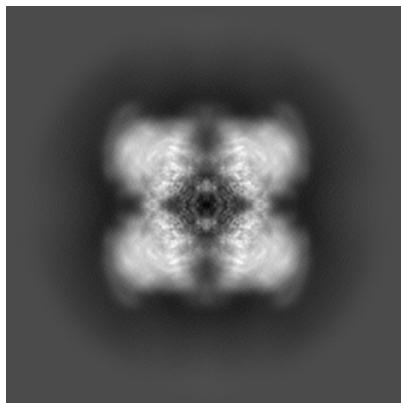
## 6 Map visualisation i

This section contains visualisations of the EMDB entry EMD-13817. These allow visual inspection of the internal detail of the map and identification of artifacts.

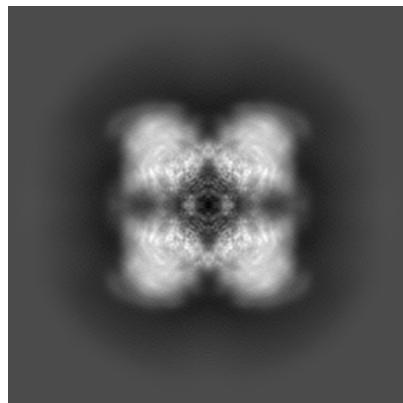
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections i

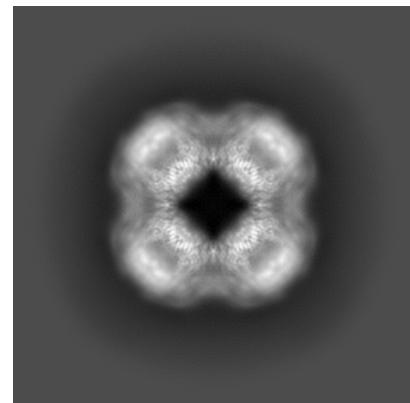
#### 6.1.1 Primary map



X



Y

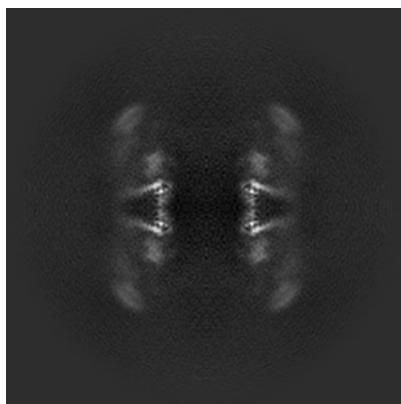


Z

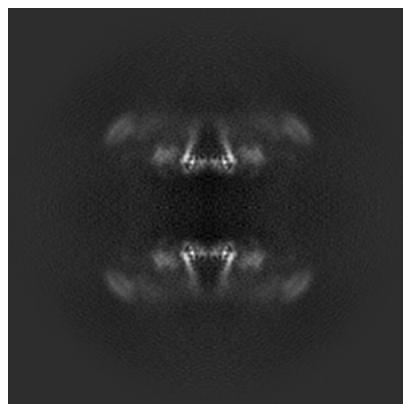
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices i

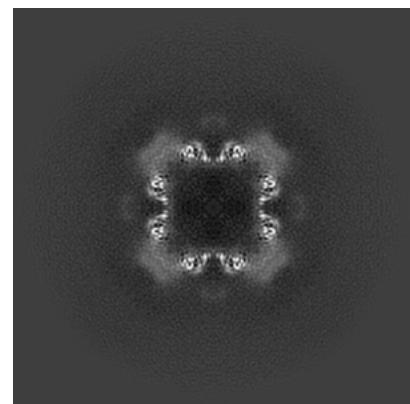
#### 6.2.1 Primary map



X Index: 225



Y Index: 225

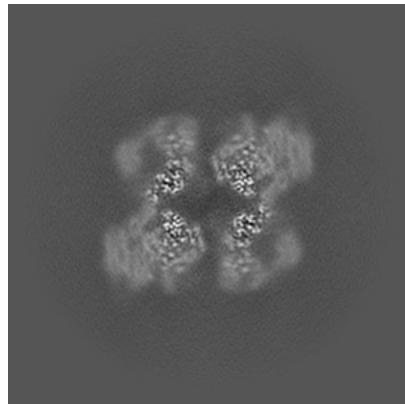


Z Index: 225

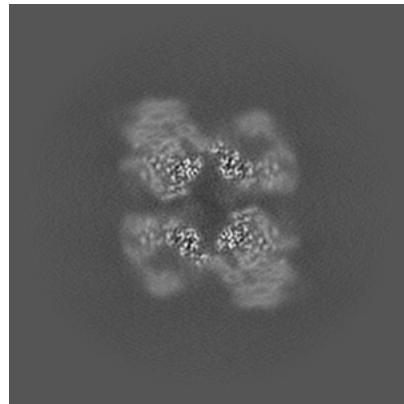
The images above show central slices of the map in three orthogonal directions.

### 6.3 Largest variance slices [\(i\)](#)

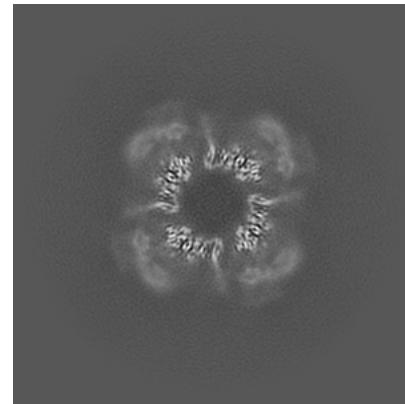
#### 6.3.1 Primary map



X Index: 262



Y Index: 262



Z Index: 201

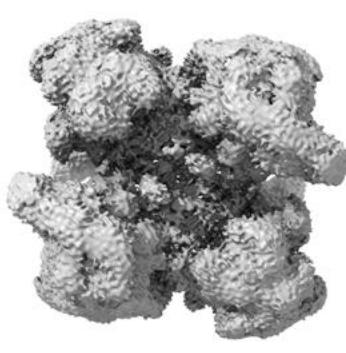
The images above show the largest variance slices of the map in three orthogonal directions.

### 6.4 Orthogonal surface views [\(i\)](#)

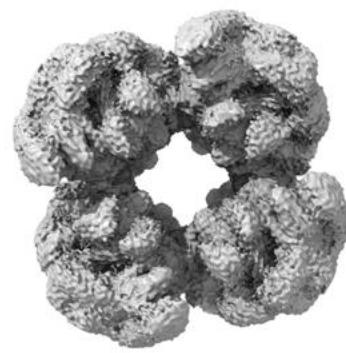
#### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

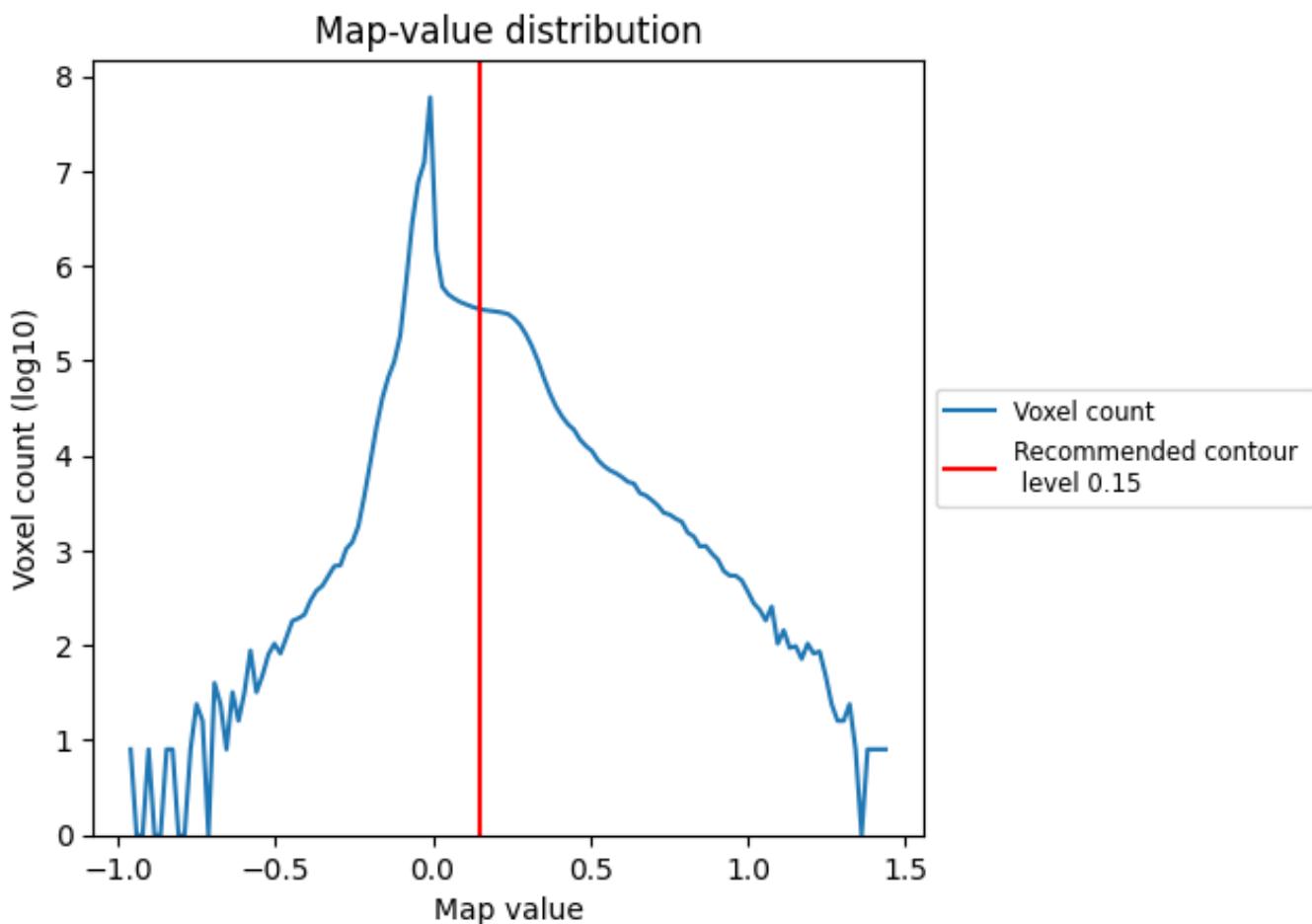
## 6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis (i)

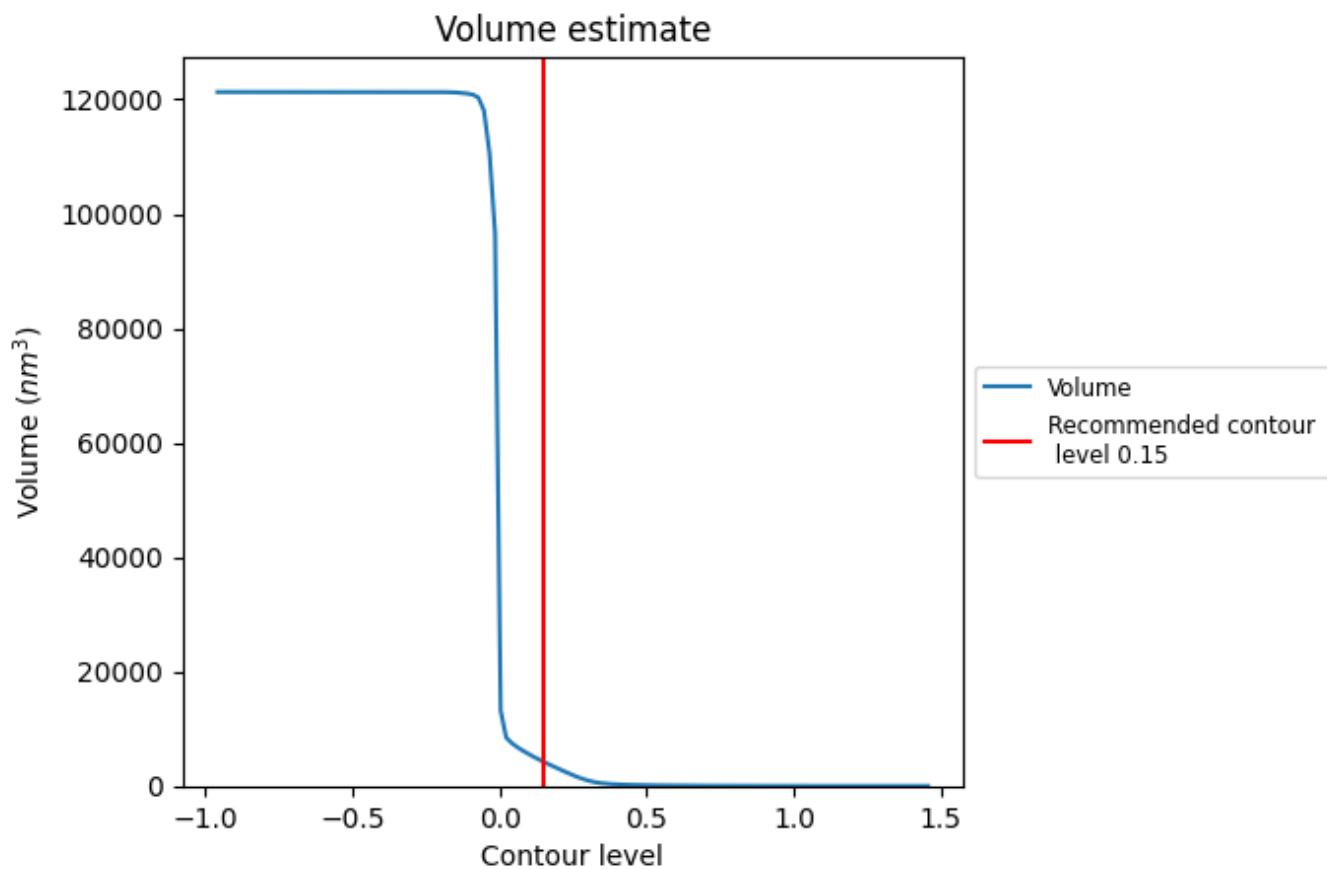
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

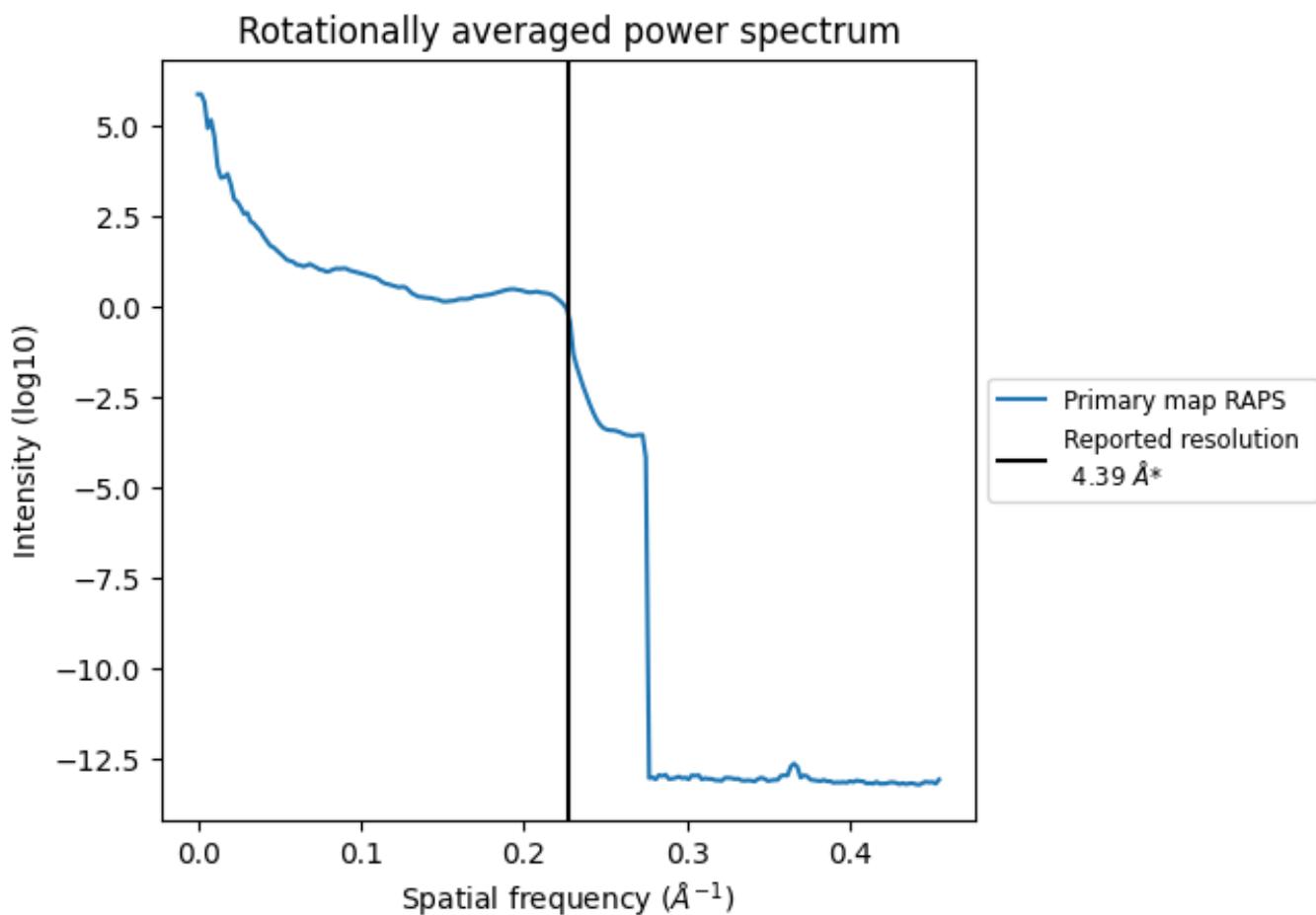
## 7.2 Volume estimate (i)



The volume at the recommended contour level is 4205 nm<sup>3</sup>; this corresponds to an approximate mass of 3799 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [\(i\)](#)

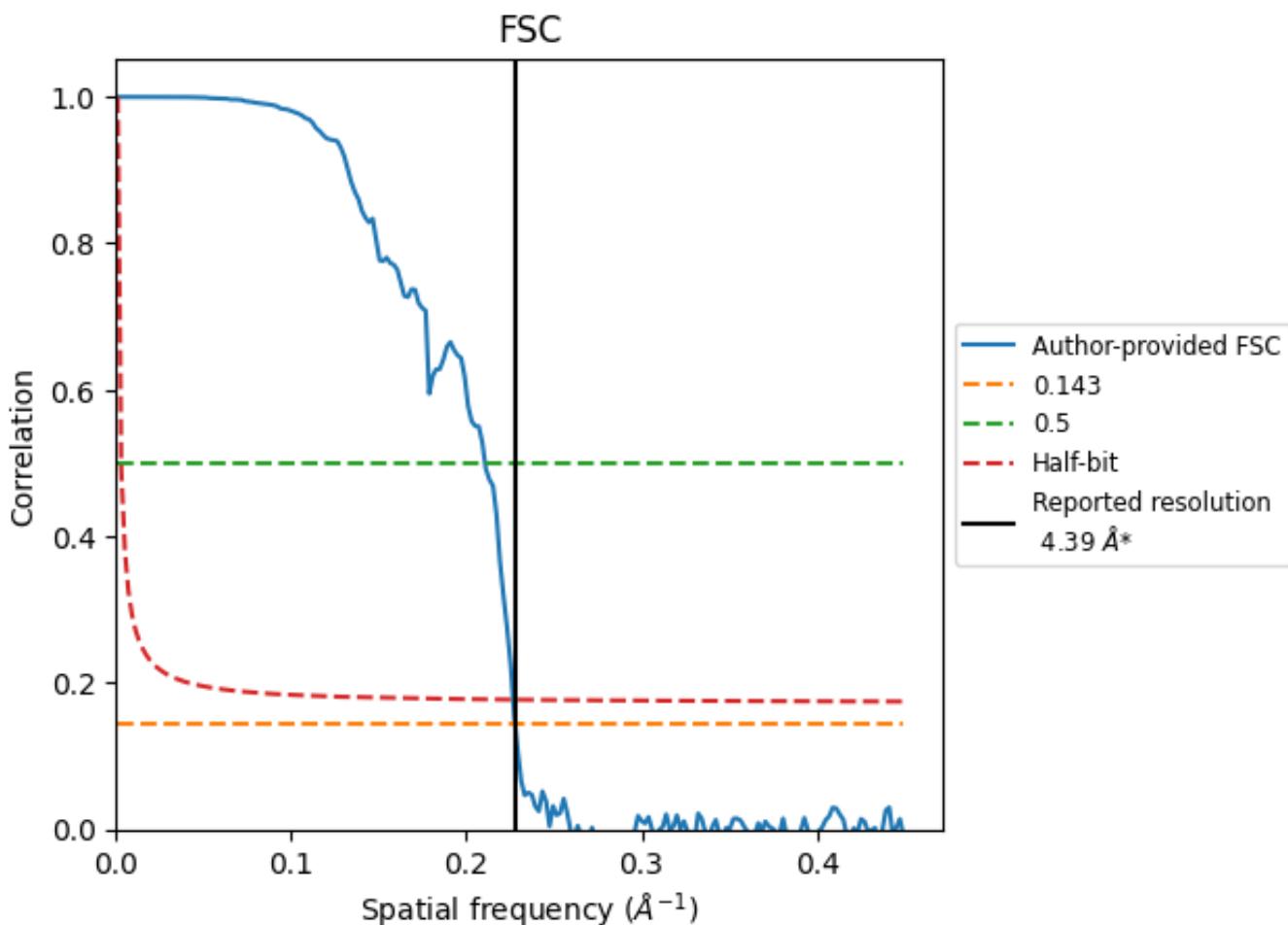


\*Reported resolution corresponds to spatial frequency of  $0.228 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation [\(i\)](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [\(i\)](#)



\*Reported resolution corresponds to spatial frequency of  $0.228 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [\(i\)](#)

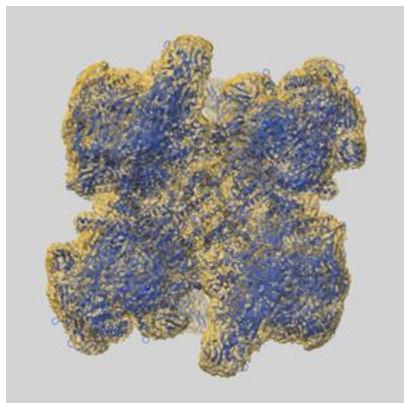
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.39	-	-
Author-provided FSC curve	4.39	4.75	4.41
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

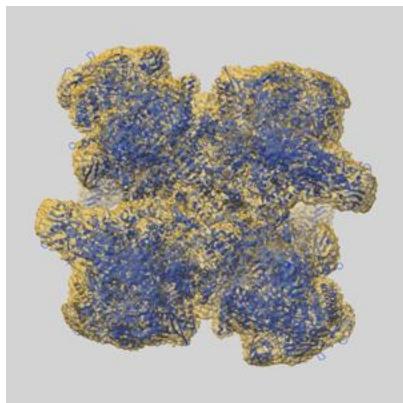
## 9 Map-model fit i

This section contains information regarding the fit between EMDB map EMD-13817 and PDB model 7Q4U. Per-residue inclusion information can be found in section 3 on page 15.

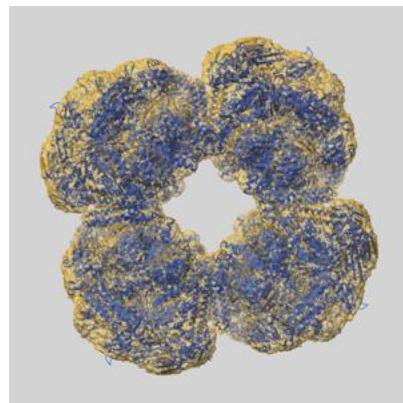
### 9.1 Map-model overlay i



X



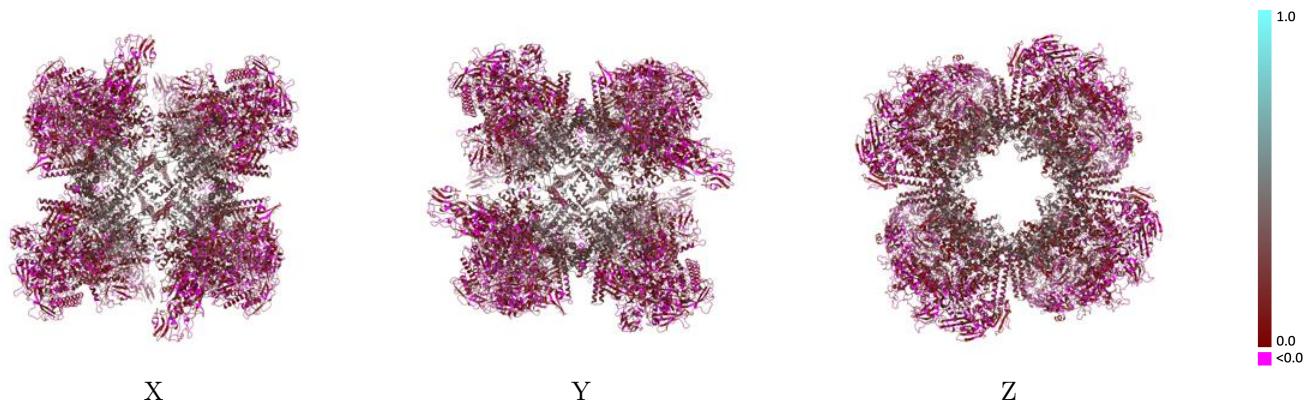
Y



Z

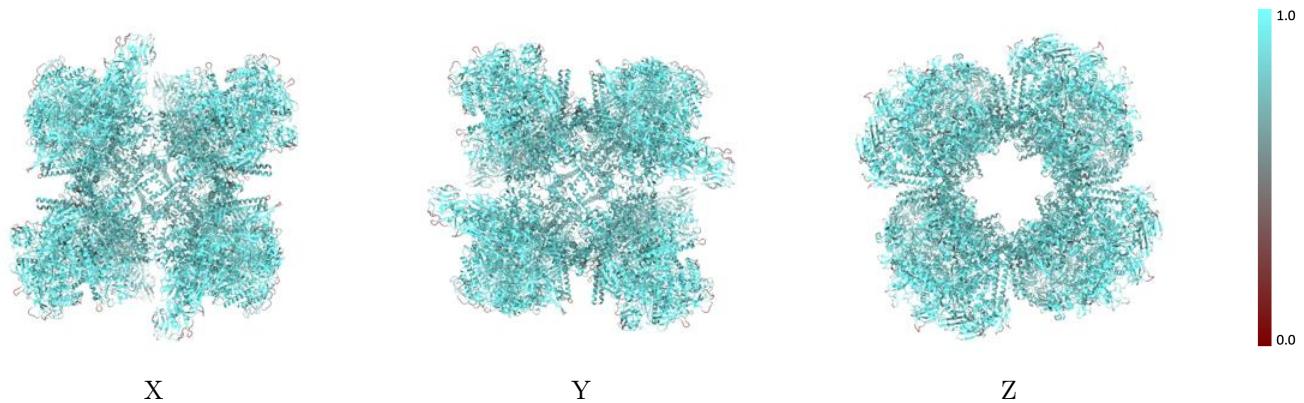
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [\(i\)](#)



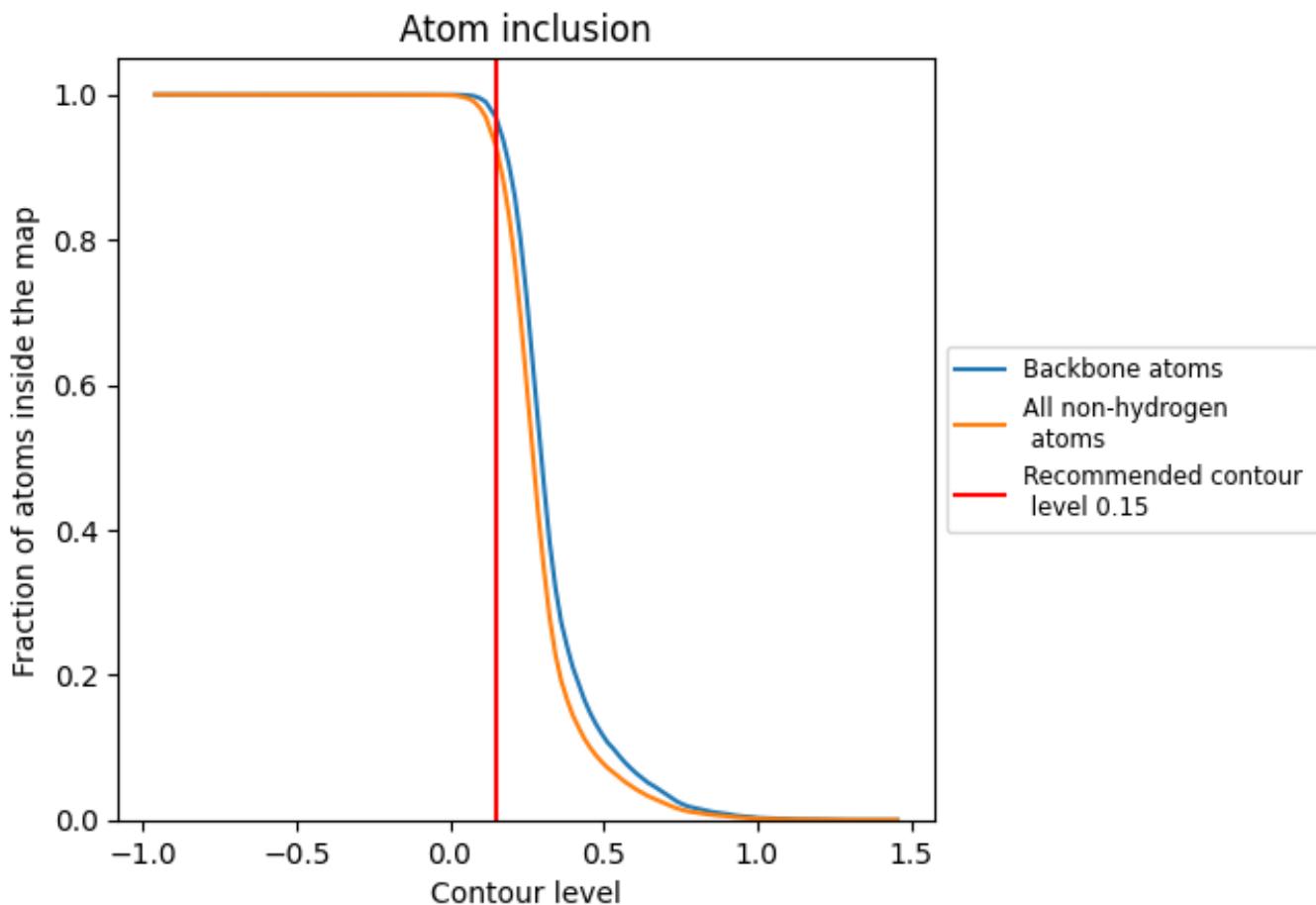
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

## 9.4 Atom inclusion [\(i\)](#)



At the recommended contour level, 97% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9286	0.1610
A	0.9028	0.0800
AA	0.8765	0.1040
B	0.8770	0.1050
BA	0.9395	0.1120
C	0.9395	0.1110
CA	0.9313	0.2080
D	0.9316	0.2070
DA	0.9219	0.1880
E	0.9219	0.1880
EA	0.9445	0.3340
F	0.9445	0.3330
FA	0.9028	0.0790
G	0.9028	0.0800
GA	0.8765	0.1010
H	0.8765	0.1040
HA	0.9395	0.1110
I	0.9394	0.1110
IA	0.9313	0.2080
J	0.9314	0.2080
JA	0.9203	0.1880
K	0.9219	0.1900
KA	0.9445	0.3350
L	0.9445	0.3350
LA	0.9028	0.0780
M	0.9028	0.0770
MA	0.8776	0.1010
N	0.8765	0.1030
NA	0.9394	0.1110
O	0.9395	0.1110
OA	0.9314	0.2070
P	0.9315	0.2080
PA	0.9219	0.1880
Q	0.9219	0.1920
QA	0.9445	0.3340



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Chain	Atom inclusion	Q-score
R	0.9445	0.3350
RA	0.9028	0.0800
S	0.9028	0.0780
SA	0.8770	0.1050
T	0.8770	0.1020
TA	0.9395	0.1120
UA	0.9313	0.2070
V	0.9395	0.1110
VA	0.9219	0.1880
W	0.9313	0.2070
WA	0.9445	0.3320
X	0.9203	0.1900
Y	0.9445	0.3340
Z	0.9028	0.0820