



## wwPDB EM Validation Summary Report ⓘ

May 26, 2025 – 10:14 AM EDT

PDB ID : 8TQW / pdb\_00008tqw  
EMDB ID : EMD-41565  
Title : Structure of human transcriptional Mediator complex  
Authors : Chen, S.F.; Chao, T.C.; Kim, H.J.; Tang, H.C.; Khadka, S.; Li, T.; Murakami, K.; Boyer, T.G.; Tsai, K.L.  
Deposited on : 2023-08-08  
Resolution : 8.20 Å(reported)

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 ⓘ 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 ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev118  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

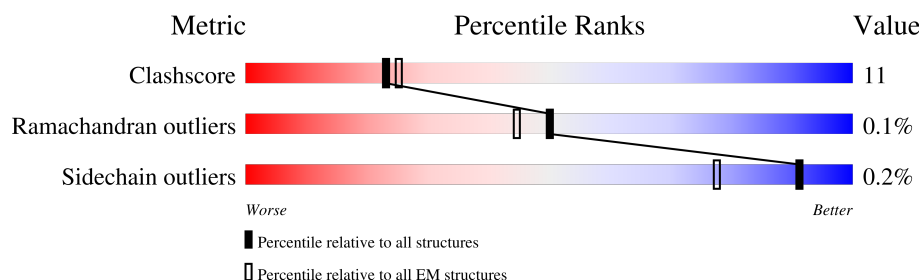
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.20 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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  $\leq 5\%$ . 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.

Mol	Chain	Length	Quality of chain
1	0	311	
2	1	178	
3	2	200	
4	3	178	
5	4	131	
6	A	1581	
7	B	20	
8	D	270	

*Continued on next page...*

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Mol	Chain	Length	Quality of chain
9	F	246	
10	G	233	
11	H	268	
12	I	146	
13	J	135	
14	K	117	
15	N	1454	
16	O	788	
17	P	877	
18	Q	651	
19	R	208	
20	S	244	
21	T	212	
22	U	144	
23	V	200	
24	W	1368	
25	X	989	
26	a	464	
27	b	283	
28	c	2177	
29	d	2174	

## 2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 83816 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 Mediator of RNA polymerase II transcription subunit 27.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	267	Total	C	N	O	S	0	0
			2159	1373	384	390	12		

- Molecule 2 is a protein called Mediator of RNA polymerase II transcription subunit 28.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	99	Total	C	N	O	S	0	0
			817	511	143	160	3		

- Molecule 3 is a protein called Mediator of RNA polymerase II transcription subunit 29.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	115	Total	C	N	O	S	0	0
			899	563	155	172	9		

- Molecule 4 is a protein called Mediator of RNA polymerase II transcription subunit 30.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	122	Total	C	N	O	S	0	0
			1022	639	187	189	7		

- Molecule 5 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	113	Total	C	N	O	S	0	0
			986	642	171	168	5		

- Molecule 6 is a protein called Mediator of RNA polymerase II transcription subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	467	Total	C	N	O	S	0	0
			3578	2278	613	663	24		

- Molecule 7 is a protein called Unknown Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	B	20	Total	C	N	O	0	0
			100	60	20	20		

- Molecule 8 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	158	Total	C	N	O	S	0	0
			1268	791	228	243	6		

- Molecule 9 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	166	Total	C	N	O	S	0	0
			1363	882	234	242	5		

- Molecule 10 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	161	Total	C	N	O	S	0	0
			1348	856	239	243	10		

- Molecule 11 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	181	Total	C	N	O	S	0	0
			1422	888	250	280	4		

- Molecule 12 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	73	Total	C	N	O	S	0	0
			605	382	107	110	6		

- Molecule 13 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	122	Total	C	N	O	S	0	0
			840	527	151	159	3		

- Molecule 14 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	112	Total	C	N	O	S	0	0
			879	537	163	175	4		

- Molecule 15 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	1017	Total	C	N	O	S	0	0
			7772	4958	1365	1407	42		

- Molecule 16 is a protein called Mediator of RNA polymerase II transcription subunit 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	157	Total	C	N	O	S	0	0
			1226	783	213	223	7		

- Molecule 17 is a protein called Mediator of RNA polymerase II transcription subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	753	Total	C	N	O	S	0	0
			5875	3742	1008	1077	48		

- Molecule 18 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	546	Total	C	N	O	S	0	0
			4319	2732	773	794	20		

- Molecule 19 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	191	Total	C	N	O	S	0	0
			1532	971	270	276	15		

- Molecule 20 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	75	Total	C	N	O	S	0	0
			517	328	87	100	2		

- Molecule 21 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	193	Total	C	N	O	S	0	0
			1499	955	247	280	17		

- Molecule 22 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	121	Total	C	N	O	S	0	0
			918	570	153	190	5		

- Molecule 23 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	130	Total	C	N	O	S	0	0
			1063	656	181	222	4		

- Molecule 24 is a protein called Mediator of RNA polymerase II transcription subunit 23.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	1334	Total	C	N	O	S	0	0
			10774	6967	1827	1909	71		

- Molecule 25 is a protein called Mediator of RNA polymerase II transcription subunit 24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	897	Total	C	N	O	S	0	0
			7061	4524	1190	1293	54		

- Molecule 26 is a protein called Cyclin-dependent kinase 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	313	Total	C	N	O	S	0	0
			2561	1663	439	442	17		

- Molecule 27 is a protein called Cyclin-C.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	262	Total	C	N	O	S	1	0
			2196	1442	358	379	17		

- Molecule 28 is a protein called Mediator of RNA polymerase II transcription subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	1452	Total	C	N	O	S	0	0
			11499	7270	2009	2147	73		

- Molecule 29 is a protein called Mediator of RNA polymerase II transcription subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	969	Total	C	N	O	S	0	0
			7714	4945	1310	1393	66		

- Molecule 30 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

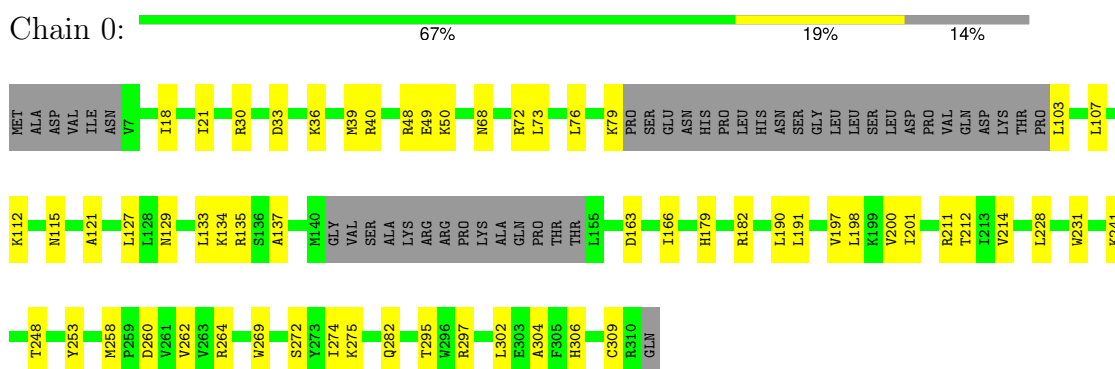
Mol	Chain	Residues	Atoms		AltConf
30	0	1	Total	Zn	0
			1	1	
30	P	1	Total	Zn	0
			1	1	
30	c	1	Total	Zn	0
			1	1	
30	d	1	Total	Zn	0
			1	1	



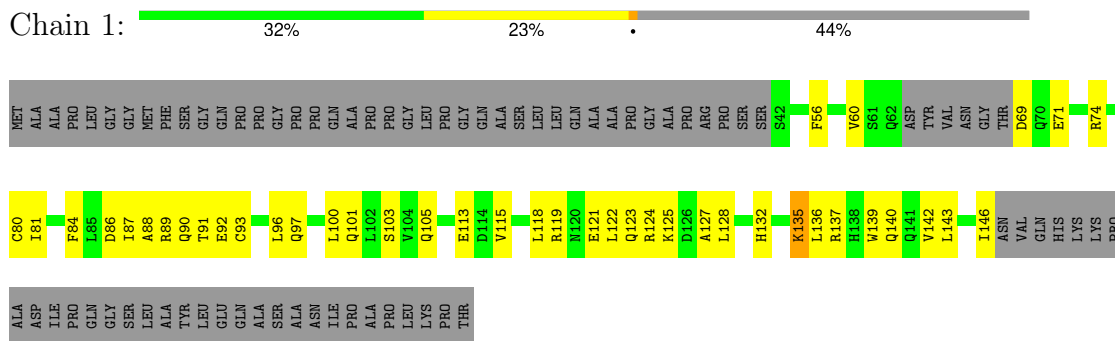
### 3 Residue-property plots [i](#)

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.

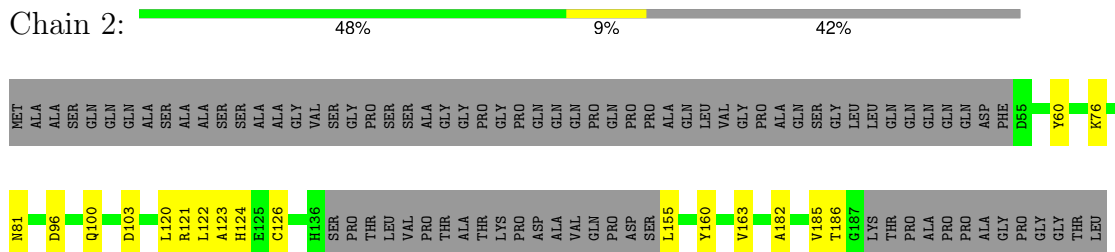
- Molecule 1: Mediator of RNA polymerase II transcription subunit 27



- Molecule 2: Mediator of RNA polymerase II transcription subunit 28



- Molecule 3: Mediator of RNA polymerase II transcription subunit 29



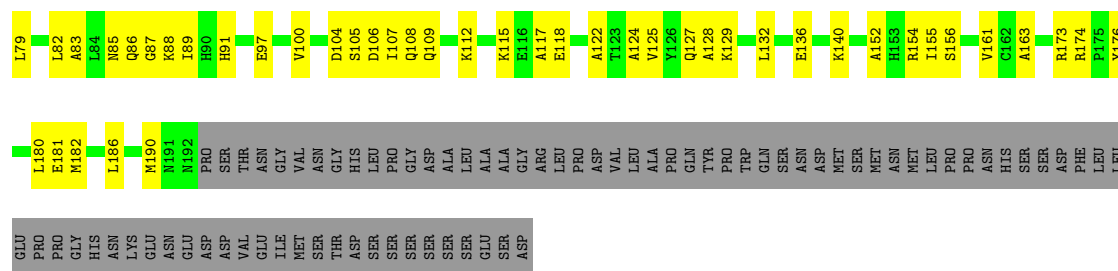
- Molecule 4: Mediator of RNA polymerase II transcription subunit 30

[illegible]

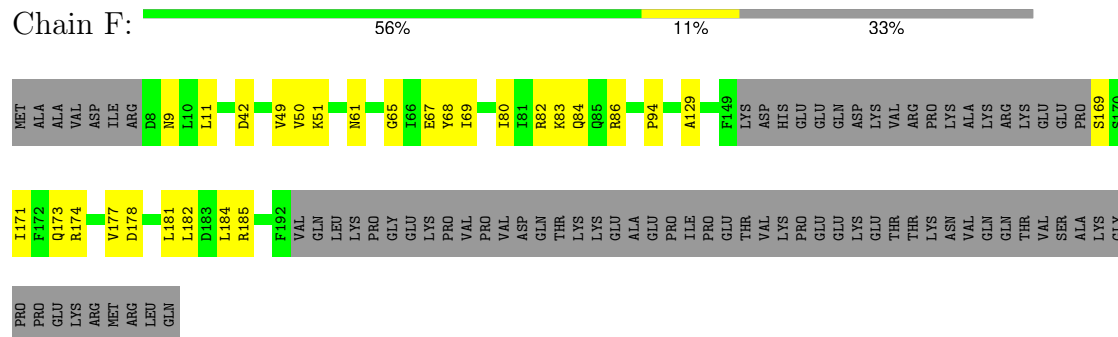
N90	A91	Q92	L103	H104	H107	Y108	S109	R110	R114	Q122	GLN	GLN	GLN	ASN	ASN	THR	SER	GLY	LYS	MET	ALA	ALA	ALA	VAL	ALA	GLU	THR	D10	R17	F18	Q19	L20	E21	L22	E23	Q26	C27	L28	A29	N30	L34	L37	R40	G41	Y42	F43	K46	V49	Y54	V58	K59	D60	P61	A64	K65	Y66	C72	L73	L76	E77	L78	L79	Q80	R85
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THR	GLN	GLN	GLY	D485	T397	P310	G206	PRO	LYS	MET
ASP	ASN	ILE	MET	I488	F398	P310	G207	GLY	ALA	LYS
THR	SER	THR	THR	C489	R403	V313	G208	GLN	GLN	ALA
LEU	SER	GLY	ASN	T490	V404	R314	G209	LEU	GLY	GLN
ASP	GLY	GLY	ASN	D491	R315	R315	G210	CYS	GLU	GLU
THR	SER	GLY	ASN	D492	I407	A316		ASP	THR	
PRO	PRO	THR	PRO	F493	L408	F317	L219	VAL	GLU	THR
PRO	PRO	THR	MET	N409	N409	V318	M220	LYS	GLU	THR
ILE	MET	THR	ILE	A495	L410	Q319	N221	VAL	GLU	THR
THR	GLU	GLY	GLY	K496	I411	K320	L222	ALA	GLU	THR
PRO	ILE	SER	THR	V497	R412	L321	K223	LYS	LYS	THR
ALA	CYS	SER	THR	V498	R413	Q322	G224	H127		
PRO	PRO	PRO	THR	Q499	Q414		G225	S14	L13	
SER	GLY	THR	PRO	R500	Q414		G225	S14	L142	
GLN	SER	PRO	THR	C501	L420	L329	G234	K145	K15	
ASN	ASN	PRO	ASN	M502	I421	P338	LYS	N148	L19	
LYS	THR	HIS	THR	S503	G422	L339	THR	F147	L19	
THR	HIS	HIS	PHE	I504		V340	ALA	D148	R22	
PRO	THR	THR	PRO	P505	V425	E341	ALA	E149		
PRO	PRO	GLY	GLY	V506	K426	L342	PRO	F150	F27	
THR	LYS	PRO	GLY	T507	R427	I343	GLY	S151	ASN	
THR	LYS	PRO	PRO	M508	T428	T344	GLY	K152	GLN	
TYR	SER	VAL	ILE	R509	I429	Q345	A255	K152	ASN	
PRO	SER	SER	THR	L430	F346	E256	ARG	G156	ASN	
GLN	THR	SER	THR	R513	E347	V257	GLY	G156	ARG	
LEU	LEU	MET	LEU	K514	L348	L348	T258	W33	PRO	
VAL	PRO	ALA	PHE	A515	G436		L259	L160	W33	
PRO	PRO	GLY	ASN		E441	P354		L160	G46	
HIS	GLU	ASN	MET	I518	V442	I355	T282	L163	ARG	
PRO	LYS	THR	SER	GLN	C443	P356	G283	L163	VAL	
GLN	PRO	LYS	MET	ALA	P444	L357	A284	K168	VAL	
PRO	LYS	ASN	ASN	ASP	L445		V285	L169	MET	
SER	HIS	HIS	ILE	THR	S446	M361		K170	SER	
ILE	GLN	PRO	LYS	THR	E447	R362	P269	T171	SER	
GLN	THR	MET	ASP	ALA	S448	F363	L270	K172	GLY	
ARG	GLU	LEU	ASP	LEU	N449	A271	M173	G173	GLY	
MET	ASP	MET	HIS	SER	F450	A365	HIS	Y174	GLY	
VAL	ASN	ASN	GLU	LEU	S451	A366	L273	L175	HIS	
ARG	PHE	LEU	SER	ILE	V452	L367		A176	Q56	
LEU	GLN	LEU	VAL	ALA	S453		G278	L177	Q56	
SER	ARG	LYS	GLY	GLU	F454	Q370	P279	Q176	V69	
SER	GLU	ASP	HIS	THR	Q455	Q371	V280	Q176	V69	
SER	LEU	ASN	GLY	VAL		H372		S179	T64	
ASP	PRO	PRO	GLU	GLU	N459	C373	F288	E181	L65	
SER	ALA	ALA	ASP	ASP	D460	Y374	SER	Q182	Q66	
ILE	MET	GLN	PHE	MET	S461	F375	SER	D183	K67	
ASP	ASP	ASP	SER	VAL	L462	L376	ILE	L184	W77	
PRO	VAL	PHE	LYS	LYS	V463	K377	THR	S185	W77	
ASP	ASP	SER	VAL	LYS	C464	K378	SER	K186	R80	
VAL	ASN	THR	ASN	ASN	D379	D379	ALA	M187	L81	
THR	GLN	LEU	GLN	LEU	S476	R386	G295	A188	L81	
ASN	TYR	TYR	ASN	PRO	C477	S387	G296	I189	I84	
ILE	PRO	GLY	PRO	PRO	K478	S387</				

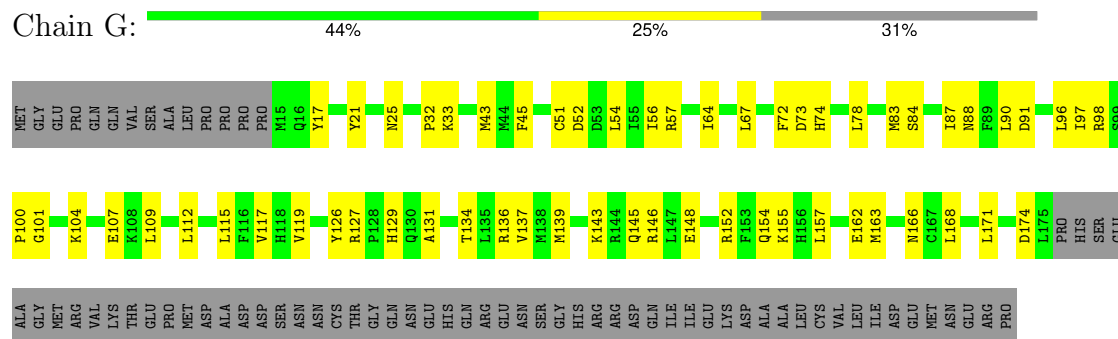




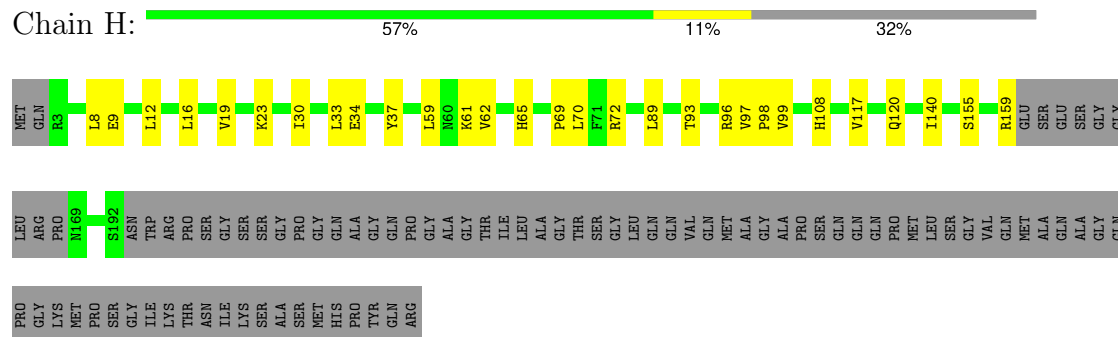
• Molecule 9: Mediator of RNA polymerase II transcription subunit 6



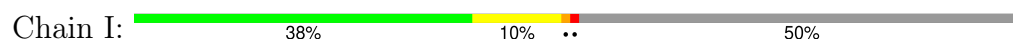
• Molecule 10: Mediator of RNA polymerase II transcription subunit 7



• Molecule 11: Mediator of RNA polymerase II transcription subunit 8

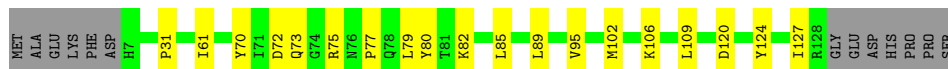


• Molecule 12: Mediator of RNA polymerase II transcription subunit 9

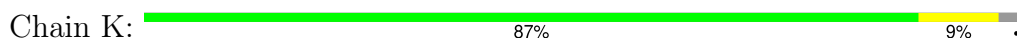




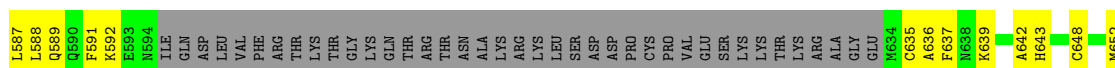
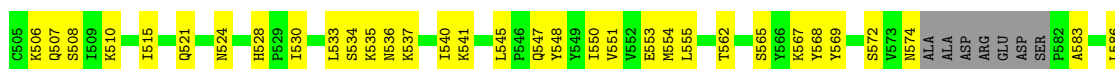
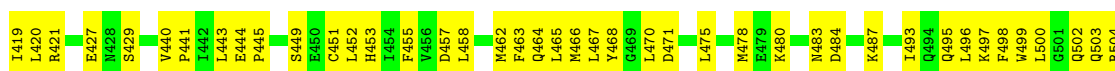
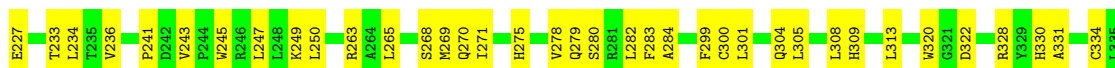
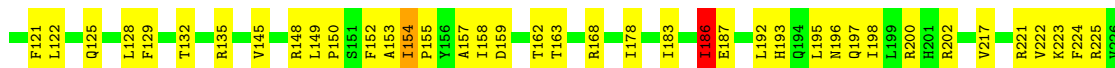
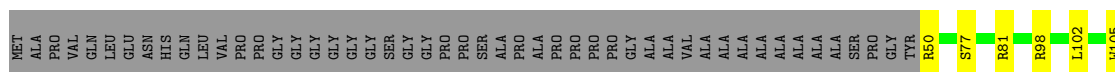
- Molecule 13: Mediator of RNA polymerase II transcription subunit 10



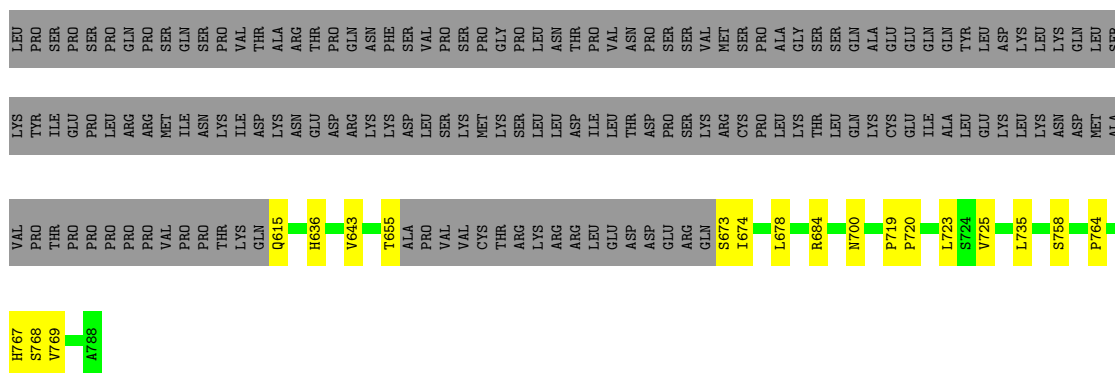
- Molecule 14: Mediator of RNA polymerase II transcription subunit 11



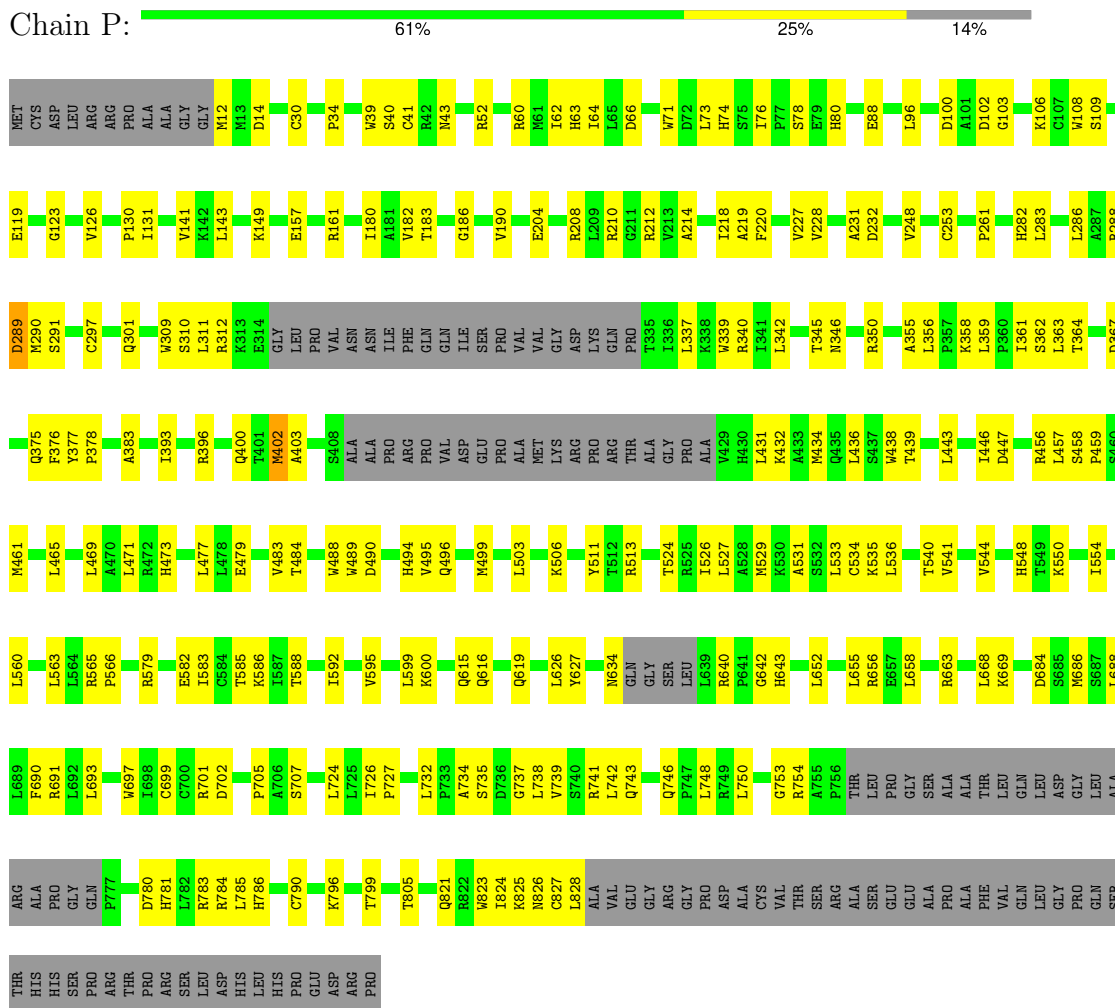
- Molecule 15: Mediator of RNA polymerase II transcription subunit 14



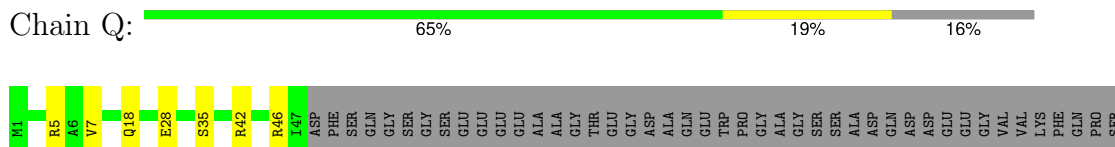


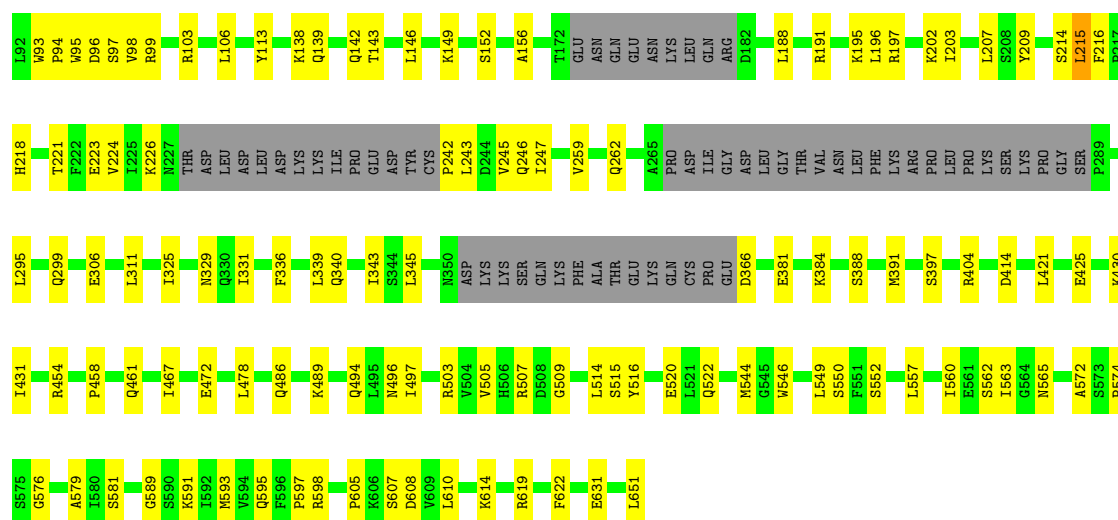


- Molecule 17: Mediator of RNA polymerase II transcription subunit 16



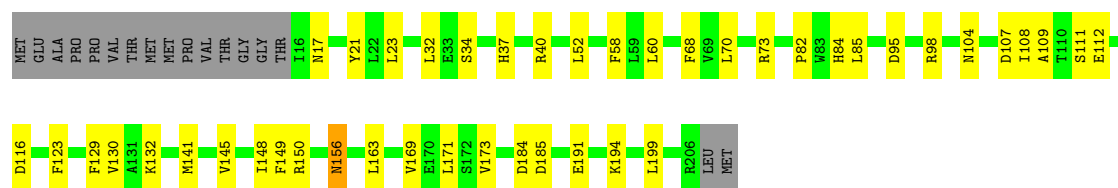
- Molecule 18: Mediator of RNA polymerase II transcription subunit 17





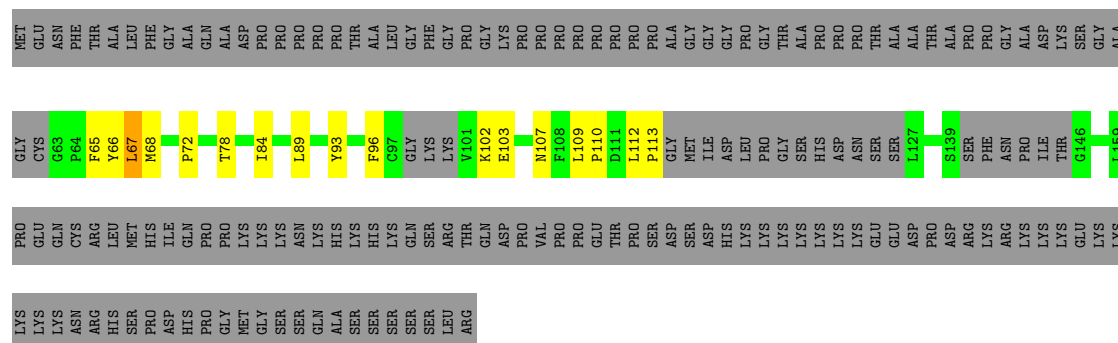
• Molecule 19: Mediator of RNA polymerase II transcription subunit 18

Chain R: 71% 21% 8%



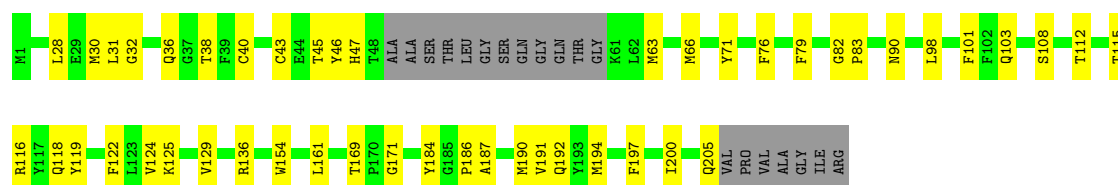
• Molecule 20: Mediator of RNA polymerase II transcription subunit 19

Chain S: 24% 7% 69%



• Molecule 21: Mediator of RNA polymerase II transcription subunit 20

Chain T: 69% 22% 9%





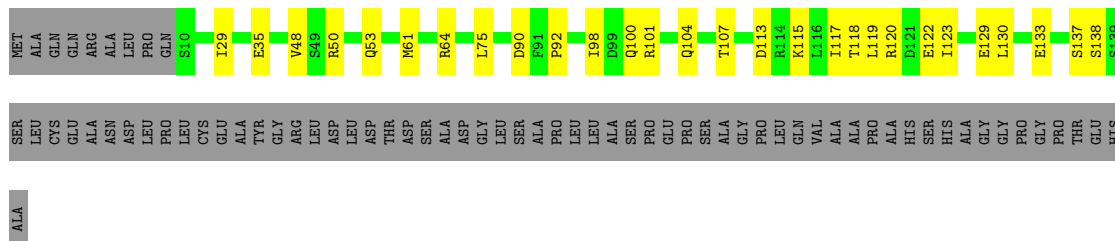
- Molecule 22: Mediator of RNA polymerase II transcription subunit 21

Chain U:  74% 10% 16%



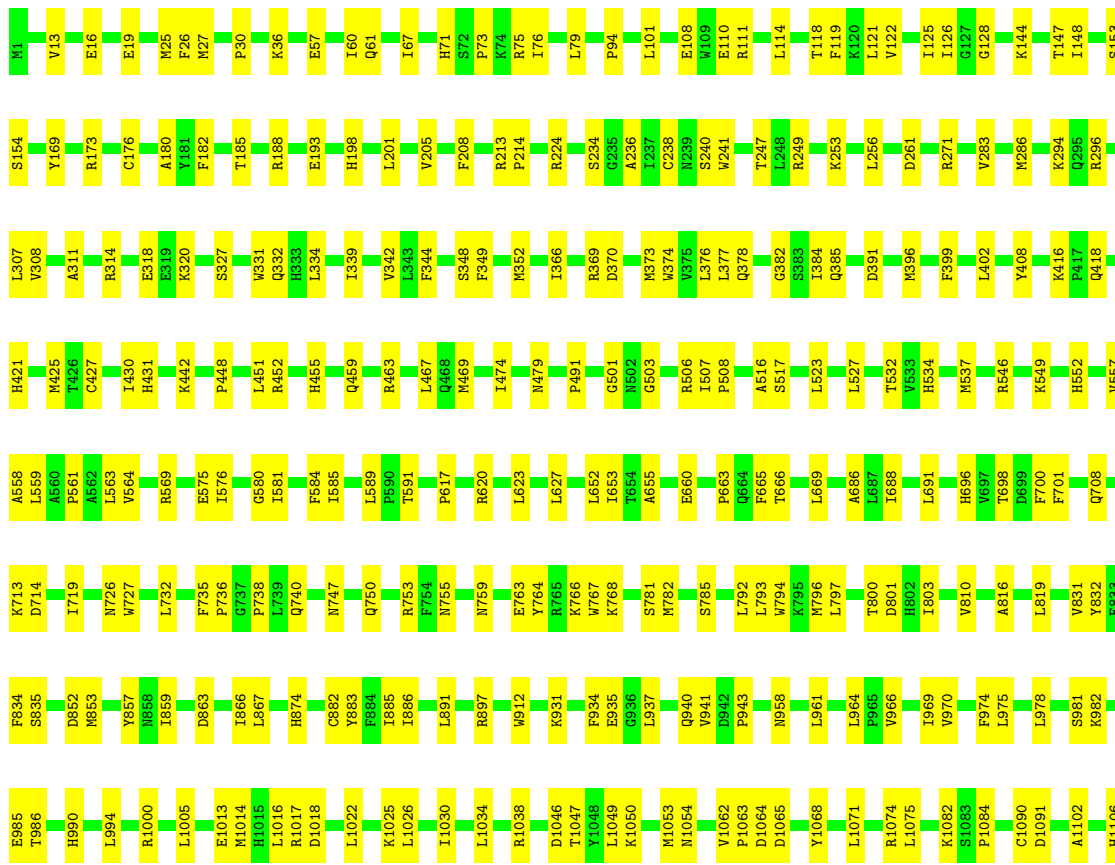
- Molecule 23: Mediator of RNA polymerase II transcription subunit 22

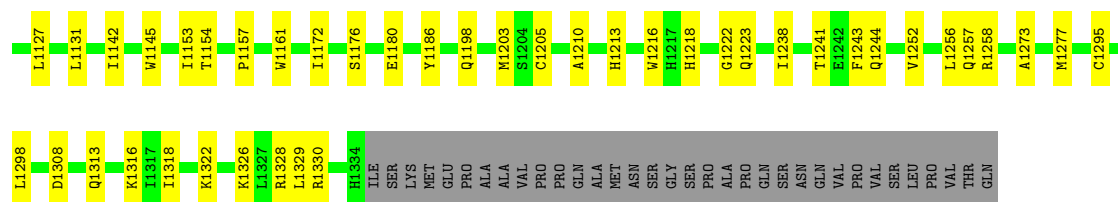
Chain V:  51% 14% 35%



- Molecule 24: Mediator of RNA polymerase II transcription subunit 23

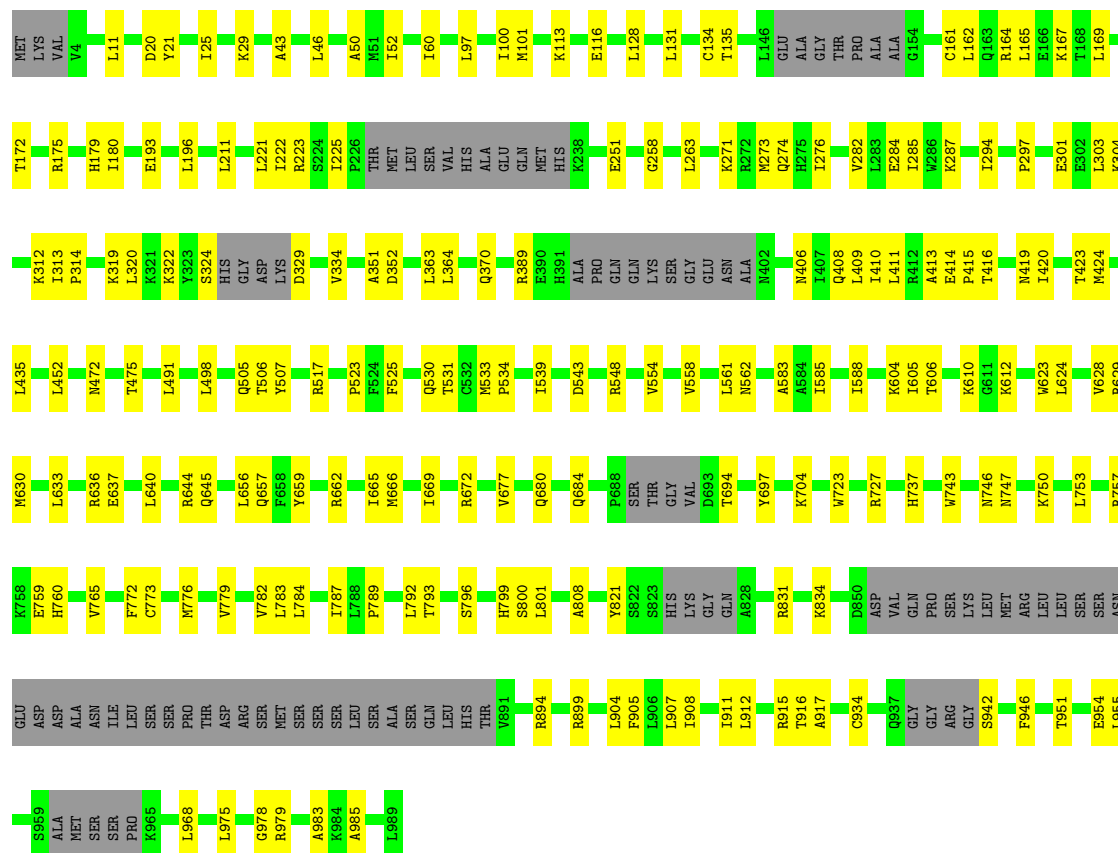
Chain W:  74% 23% 3%





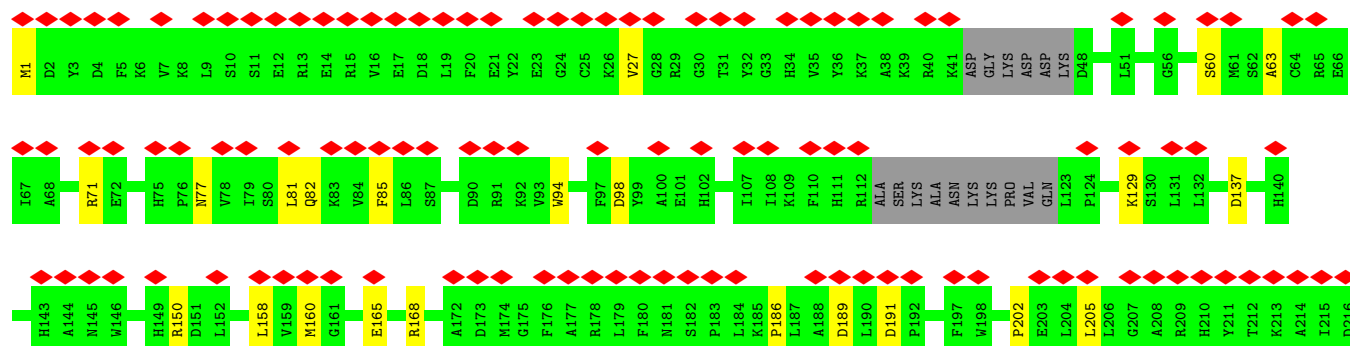
• Molecule 25: Mediator of RNA polymerase II transcription subunit 24

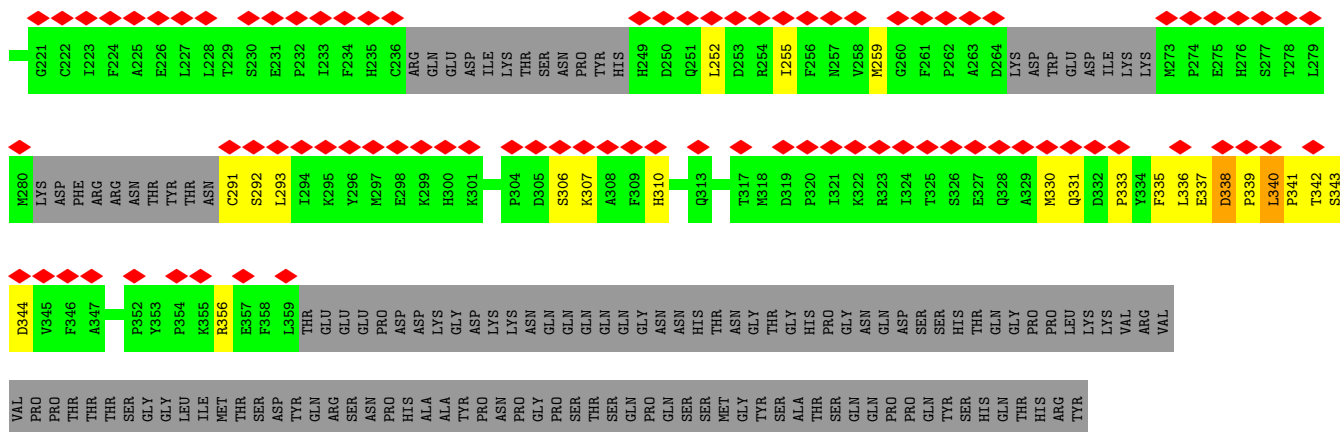
Chain X: 71% 19% 9%



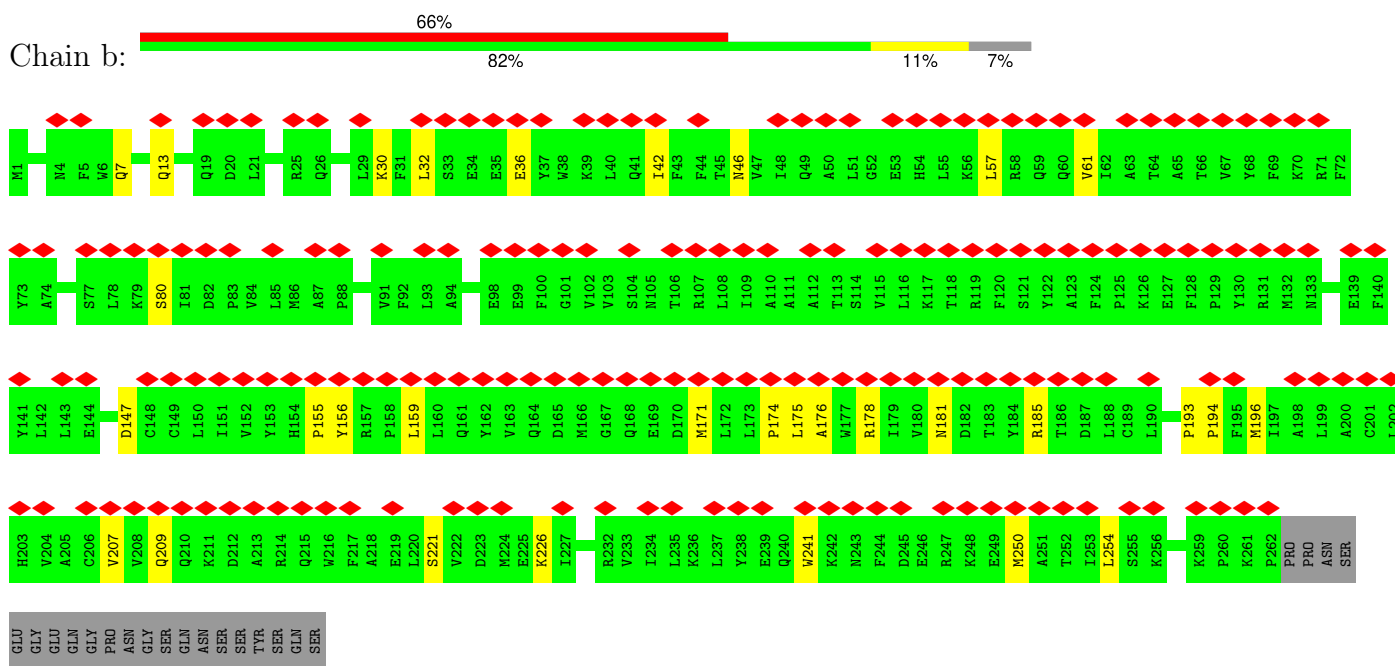
• Molecule 26: Cyclin-dependent kinase 8

Chain a: 43% 58% 9% 33%

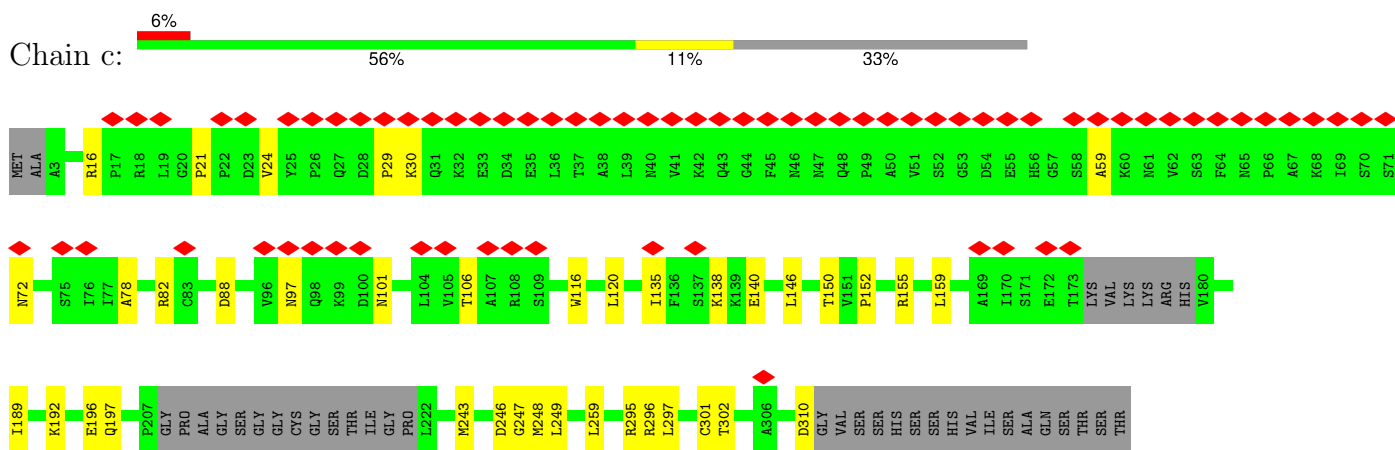




### • Molecule 27: Cyclin-C

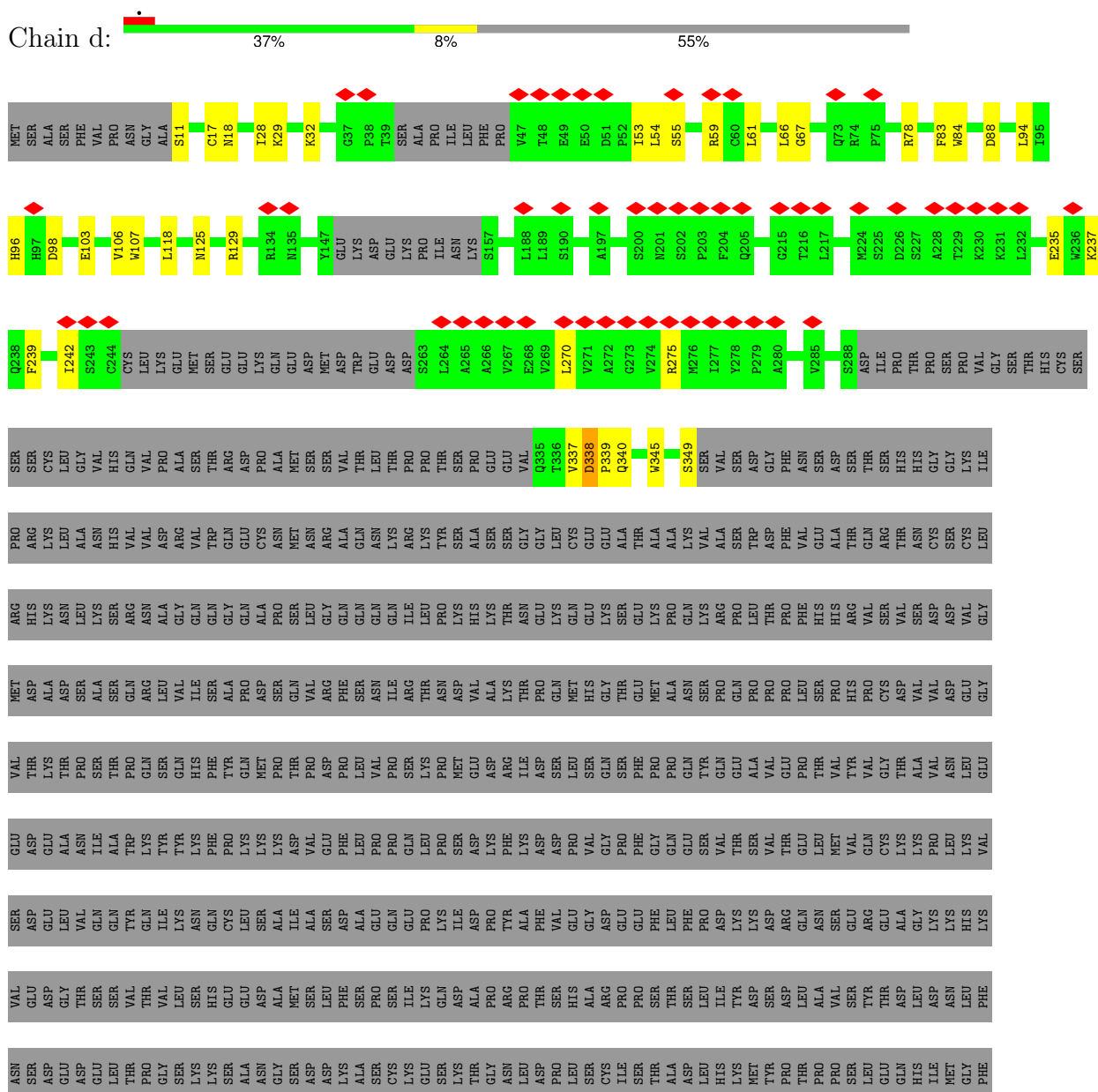


### • Molecule 28: Mediator of RNA polymerase II transcription subunit 12





- Molecule 29: Mediator of RNA polymerase II transcription subunit 13





F2132	F2133	L2134	E2135	Q2136	Y2137	N2138
S2141	C2145	D2146	P2147	R2152	S2153	S2154
C2155	L2156	H2159	N2173	L2174		

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6348	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	52	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.063	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.004	Depositor
Map size ( $\text{\AA}$ )	727.04004, 727.04004, 727.04004	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	2.272, 2.272, 2.272	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: 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	0	0.16	0/2201	0.48	1/2972 (0.0%)
2	1	0.30	0/825	0.61	1/1107 (0.1%)
3	2	0.20	0/911	0.49	0/1229
4	3	0.18	0/1029	0.48	0/1378
5	4	0.18	0/1013	0.44	0/1364
6	A	0.28	0/3653	0.55	0/4961
8	D	0.24	0/1281	0.53	0/1718
9	F	0.24	0/1400	0.54	0/1902
10	G	0.23	0/1374	0.59	1/1847 (0.1%)
11	H	0.19	0/1441	0.51	2/1946 (0.1%)
12	I	0.24	0/612	0.70	1/815 (0.1%)
13	J	0.21	0/849	0.50	0/1150
14	K	0.17	0/885	0.49	0/1190
15	N	0.27	0/7923	0.61	4/10761 (0.0%)
16	O	0.21	0/1261	0.55	0/1731
17	P	0.18	0/6001	0.48	1/8151 (0.0%)
18	Q	0.17	0/4400	0.47	1/5941 (0.0%)
19	R	0.17	0/1562	0.44	0/2101
20	S	0.23	0/524	0.59	0/709
21	T	0.18	0/1530	0.51	0/2066
22	U	0.18	0/927	0.43	0/1257
23	V	0.17	0/1072	0.44	0/1440
24	W	0.17	0/11056	0.42	0/15023
25	X	0.19	0/7191	0.48	0/9728
26	a	0.20	0/2627	0.50	2/3542 (0.1%)
27	b	0.18	0/2253	0.46	0/3051
28	c	0.18	0/11719	0.46	0/15850
29	d	0.19	0/7895	0.50	3/10703 (0.0%)
All	All	0.20	0/85415	0.50	17/115633 (0.0%)

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	368	LYS	CA-C-N	9.14	129.56	120.52
15	N	368	LYS	C-N-CA	9.14	129.56	120.52
29	d	337	VAL	N-CA-C	8.51	119.30	110.62
29	d	1136	ASN	N-CA-C	7.91	119.90	111.28
26	a	340	LEU	CA-C-N	6.60	128.09	119.84

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	0	2159	0	2176	39	0
2	1	817	0	818	72	0
3	2	899	0	908	14	0
4	3	1022	0	1054	28	0
5	4	986	0	965	28	0
6	A	3578	0	3522	149	0
7	B	100	0	23	4	0
8	D	1268	0	1305	59	0
9	F	1363	0	1344	22	0
10	G	1348	0	1373	77	0
11	H	1422	0	1440	22	0
12	I	605	0	628	33	0
13	J	840	0	718	39	0
14	K	879	0	886	7	0
15	N	7772	0	7557	353	0
16	O	1226	0	1217	21	0
17	P	5875	0	5968	150	0
18	Q	4319	0	4403	117	0
19	R	1532	0	1542	28	0
20	S	517	0	432	27	0
21	T	1499	0	1484	38	0
22	U	918	0	905	12	0
23	V	1063	0	1051	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	W	10774	0	10838	197	0
25	X	7061	0	7223	130	0
26	a	2561	0	2578	60	0
27	b	2196	0	2233	21	0
28	c	11499	0	11504	153	0
29	d	7714	0	7627	151	0
30	0	1	0	0	0	0
30	P	1	0	0	0	0
30	c	1	0	0	0	0
30	d	1	0	0	0	0
All	All	83816	0	83722	1828	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 11.

The worst 5 of 1828 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)
26:a:340:LEU:HD21	29:d:1622:VAL:CG2	1.33	1.53
26:a:340:LEU:CD2	29:d:1622:VAL:HG21	1.56	1.34
26:a:338:ASP:HB3	26:a:339:PRO:CD	1.62	1.29
15:N:375:ASP:CB	15:N:376:PRO:HD3	1.67	1.22
2:1:115:VAL:HG22	4:3:142:ILE:HD11	1.29	1.14

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	0	261/311 (84%)	250 (96%)	11 (4%)	0	100	100
2	1	95/178 (53%)	92 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	2	111/200 (56%)	107 (96%)	4 (4%)	0	100	100
4	3	114/178 (64%)	112 (98%)	2 (2%)	0	100	100
5	4	111/131 (85%)	106 (96%)	5 (4%)	0	100	100
6	A	455/1581 (29%)	427 (94%)	27 (6%)	1 (0%)	44	78
8	D	154/270 (57%)	148 (96%)	6 (4%)	0	100	100
9	F	162/246 (66%)	148 (91%)	14 (9%)	0	100	100
10	G	159/233 (68%)	152 (96%)	7 (4%)	0	100	100
11	H	177/268 (66%)	169 (96%)	7 (4%)	1 (1%)	22	60
12	I	69/146 (47%)	66 (96%)	3 (4%)	0	100	100
13	J	120/135 (89%)	119 (99%)	1 (1%)	0	100	100
14	K	110/117 (94%)	108 (98%)	2 (2%)	0	100	100
15	N	995/1454 (68%)	902 (91%)	89 (9%)	4 (0%)	30	68
16	O	153/788 (19%)	143 (94%)	10 (6%)	0	100	100
17	P	743/877 (85%)	689 (93%)	53 (7%)	1 (0%)	48	83
18	Q	534/651 (82%)	497 (93%)	36 (7%)	1 (0%)	44	78
19	R	189/208 (91%)	177 (94%)	12 (6%)	0	100	100
20	S	67/244 (28%)	65 (97%)	1 (2%)	1 (2%)	8	40
21	T	189/212 (89%)	166 (88%)	23 (12%)	0	100	100
22	U	117/144 (81%)	114 (97%)	3 (3%)	0	100	100
23	V	128/200 (64%)	122 (95%)	6 (5%)	0	100	100
24	W	1332/1368 (97%)	1278 (96%)	54 (4%)	0	100	100
25	X	877/989 (89%)	828 (94%)	49 (6%)	0	100	100
26	a	301/464 (65%)	292 (97%)	8 (3%)	1 (0%)	37	73
27	b	261/283 (92%)	258 (99%)	3 (1%)	0	100	100
28	c	1422/2177 (65%)	1359 (96%)	63 (4%)	0	100	100
29	d	923/2174 (42%)	874 (95%)	49 (5%)	0	100	100
All	All	10329/16227 (64%)	9768 (95%)	551 (5%)	10 (0%)	50	83

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	N	375	ASP
20	S	67	LEU

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Mol	Chain	Res	Type
26	a	338	ASP
11	H	99	VAL
17	P	362	SER

### 5.3.2 Protein sidechains ⓘ

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	0	241/280 (86%)	241 (100%)	0	100	100
2	1	94/152 (62%)	94 (100%)	0	100	100
3	2	102/163 (63%)	102 (100%)	0	100	100
4	3	116/155 (75%)	116 (100%)	0	100	100
5	4	102/115 (89%)	102 (100%)	0	100	100
6	A	394/1391 (28%)	391 (99%)	3 (1%)	79	85
8	D	139/230 (60%)	139 (100%)	0	100	100
9	F	150/223 (67%)	150 (100%)	0	100	100
10	G	153/216 (71%)	153 (100%)	0	100	100
11	H	161/225 (72%)	161 (100%)	0	100	100
12	I	71/133 (53%)	68 (96%)	3 (4%)	25	46
13	J	66/124 (53%)	66 (100%)	0	100	100
14	K	94/98 (96%)	94 (100%)	0	100	100
15	N	810/1271 (64%)	808 (100%)	2 (0%)	92	94
16	O	141/697 (20%)	141 (100%)	0	100	100
17	P	670/766 (88%)	669 (100%)	1 (0%)	92	95
18	Q	488/577 (85%)	487 (100%)	1 (0%)	92	94
19	R	169/183 (92%)	168 (99%)	1 (1%)	84	88
20	S	43/208 (21%)	43 (100%)	0	100	100
21	T	166/178 (93%)	166 (100%)	0	100	100
22	U	98/119 (82%)	98 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	V	122/173 (70%)	122 (100%)	0	100	100
24	W	1203/1232 (98%)	1203 (100%)	0	100	100
25	X	789/864 (91%)	789 (100%)	0	100	100
26	a	277/412 (67%)	277 (100%)	0	100	100
27	b	241/258 (93%)	241 (100%)	0	100	100
28	c	1282/1916 (67%)	1282 (100%)	0	100	100
29	d	869/1918 (45%)	863 (99%)	6 (1%)	81	87
All	All	9251/14277 (65%)	9234 (100%)	17 (0%)	91	94

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	d	1359	MET
29	d	1735	LEU
15	N	372	ILE
17	P	289	ASP
18	Q	215	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 117 such sidechains are listed below:

Mol	Chain	Res	Type
18	Q	565	ASN
29	d	287	GLN
24	W	345	GLN
29	d	184	GLN
28	c	458	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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.

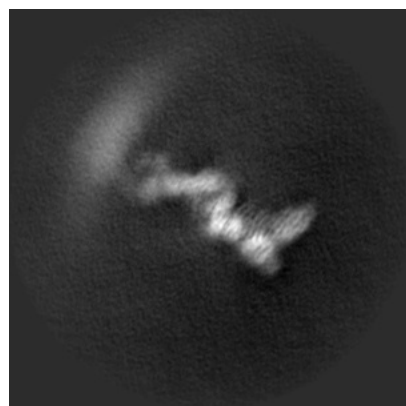
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41565. These allow visual inspection of the internal detail of the map and identification of artifacts.

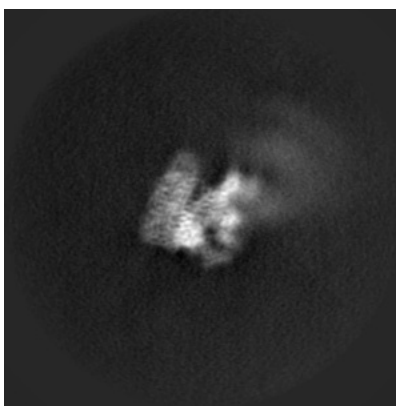
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

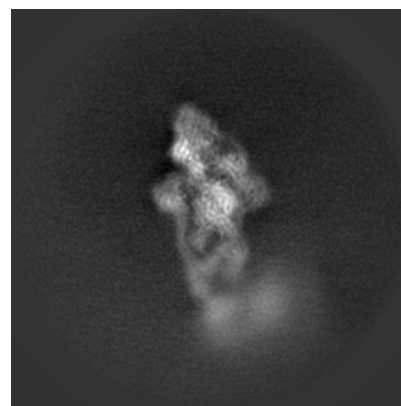
#### 6.1.1 Primary map



X

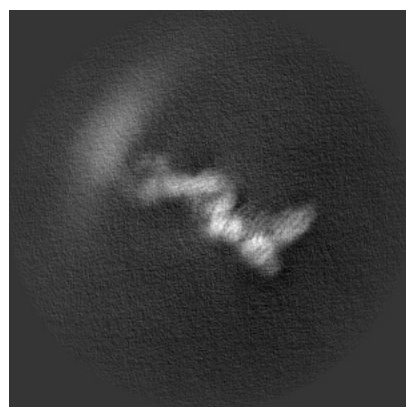


Y

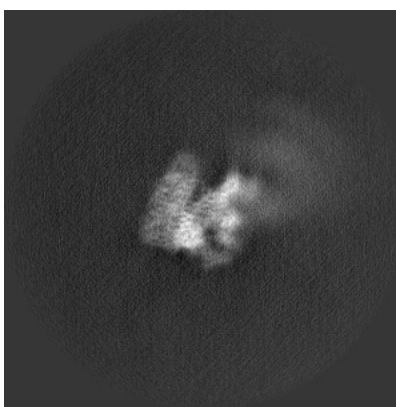


Z

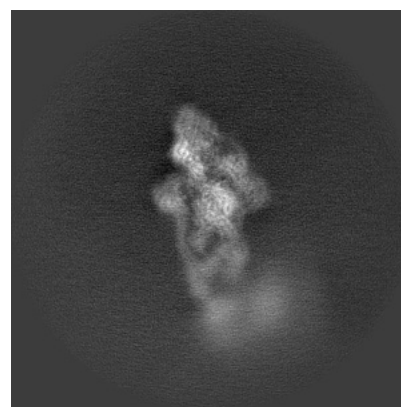
#### 6.1.2 Raw map



X



Y



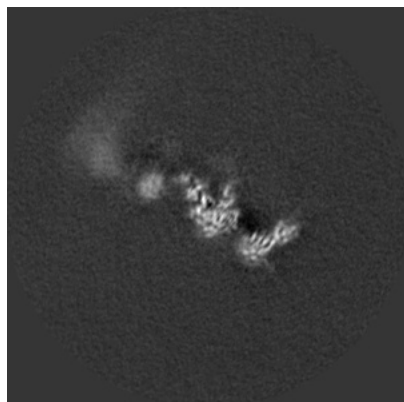
Z

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

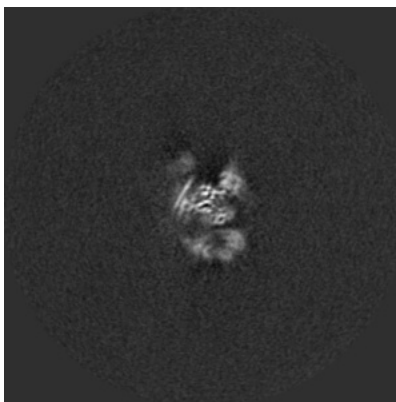


## 6.2 Central slices [i](#)

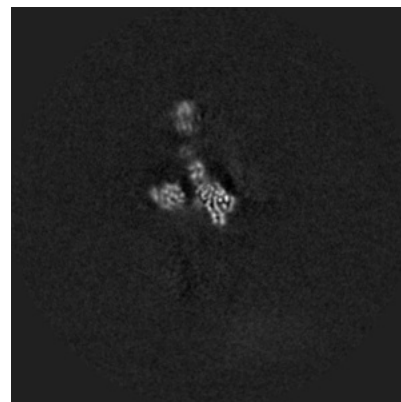
### 6.2.1 Primary map



X Index: 160

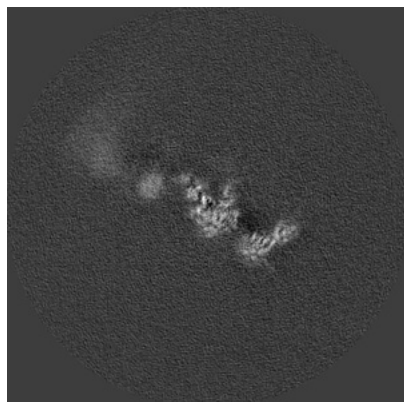


Y Index: 160

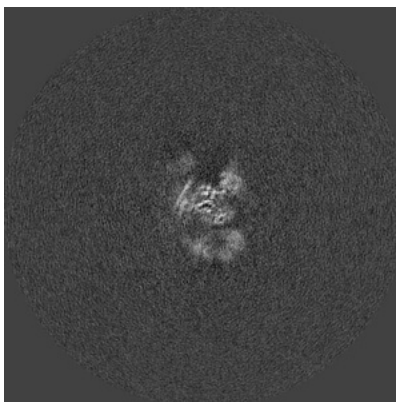


Z Index: 160

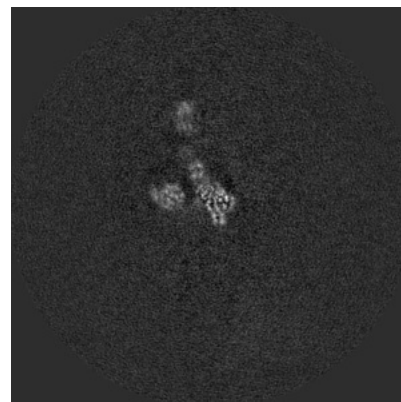
### 6.2.2 Raw map



X Index: 160



Y Index: 160

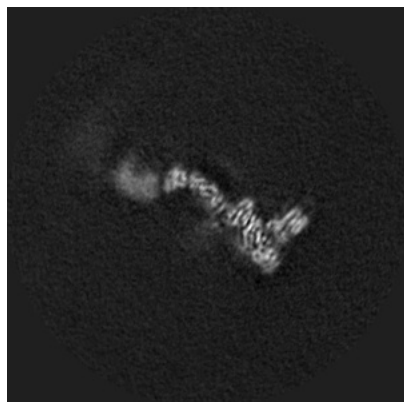


Z Index: 160

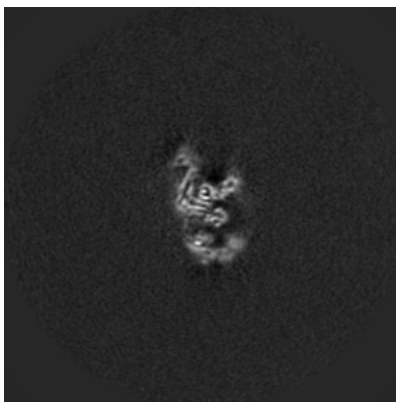
The images above show central slices of the map in three orthogonal directions.

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

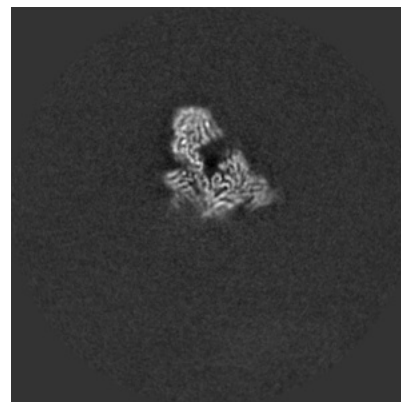
### 6.3.1 Primary map



X Index: 149

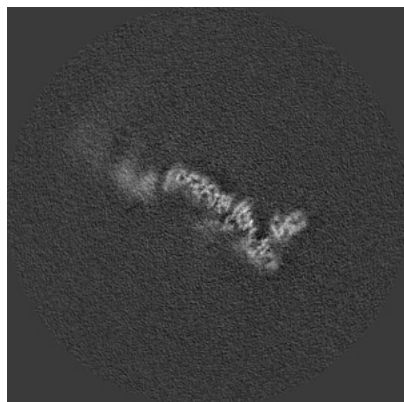


Y Index: 165



Z Index: 145

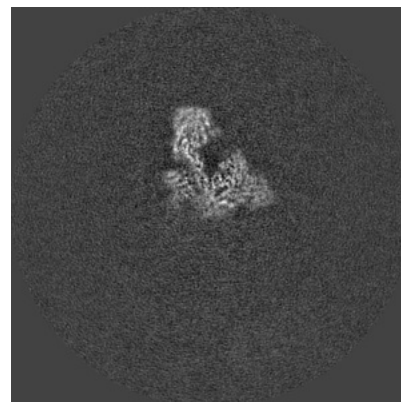
### 6.3.2 Raw map



X Index: 152



Y Index: 166



Z Index: 146

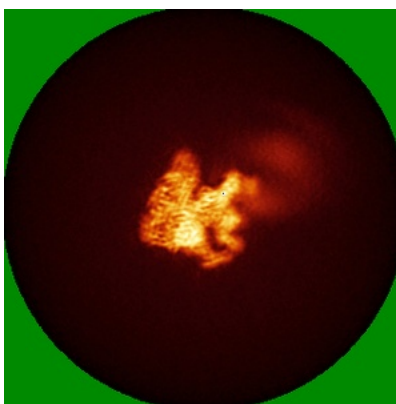
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

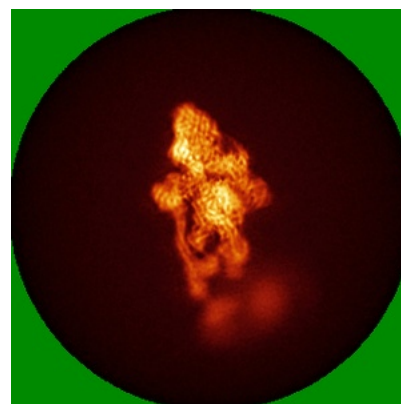
### 6.4.1 Primary map



X

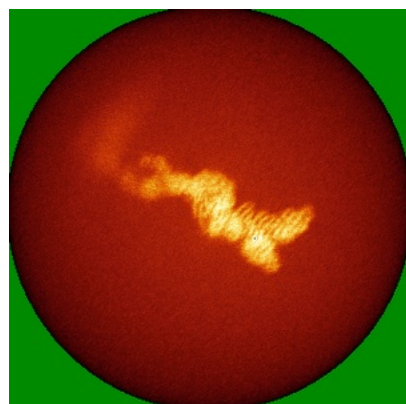


Y

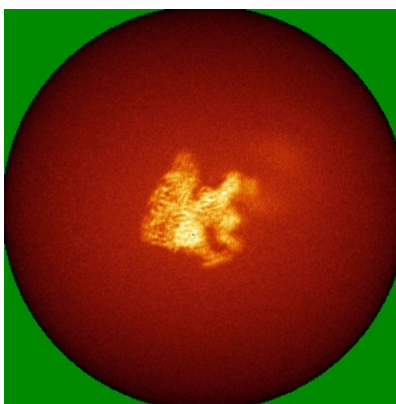


Z

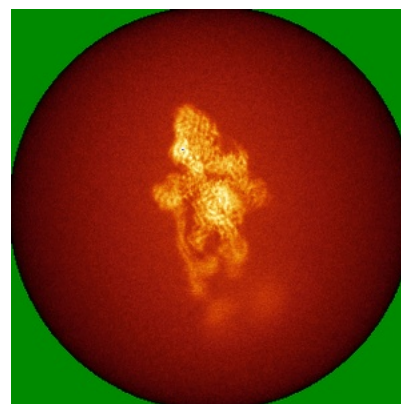
### 6.4.2 Raw map



X



Y

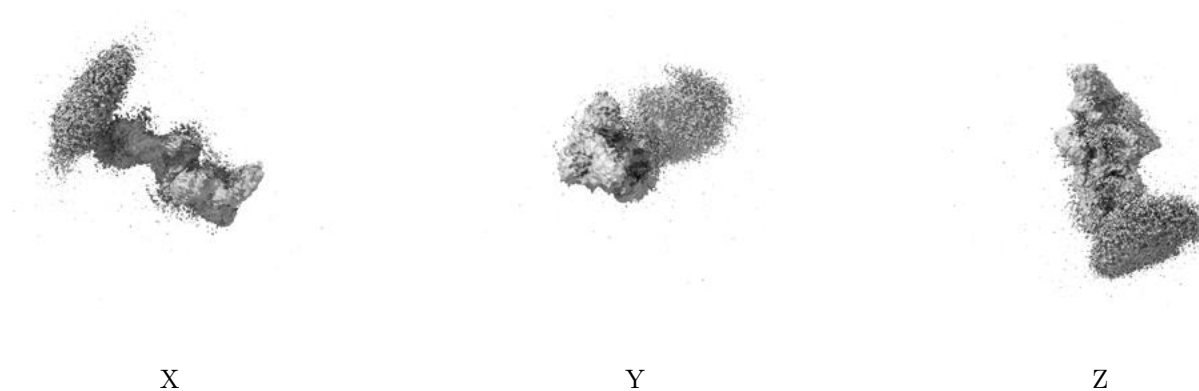


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

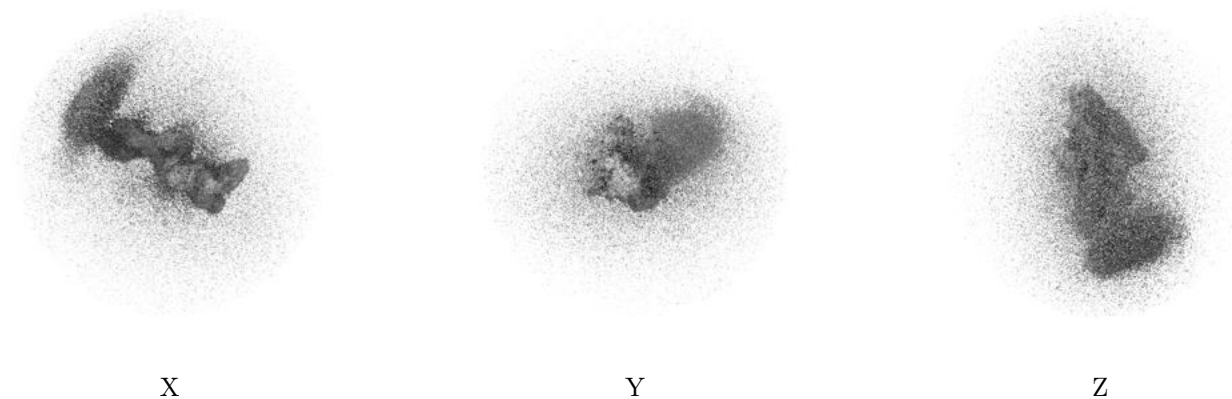
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

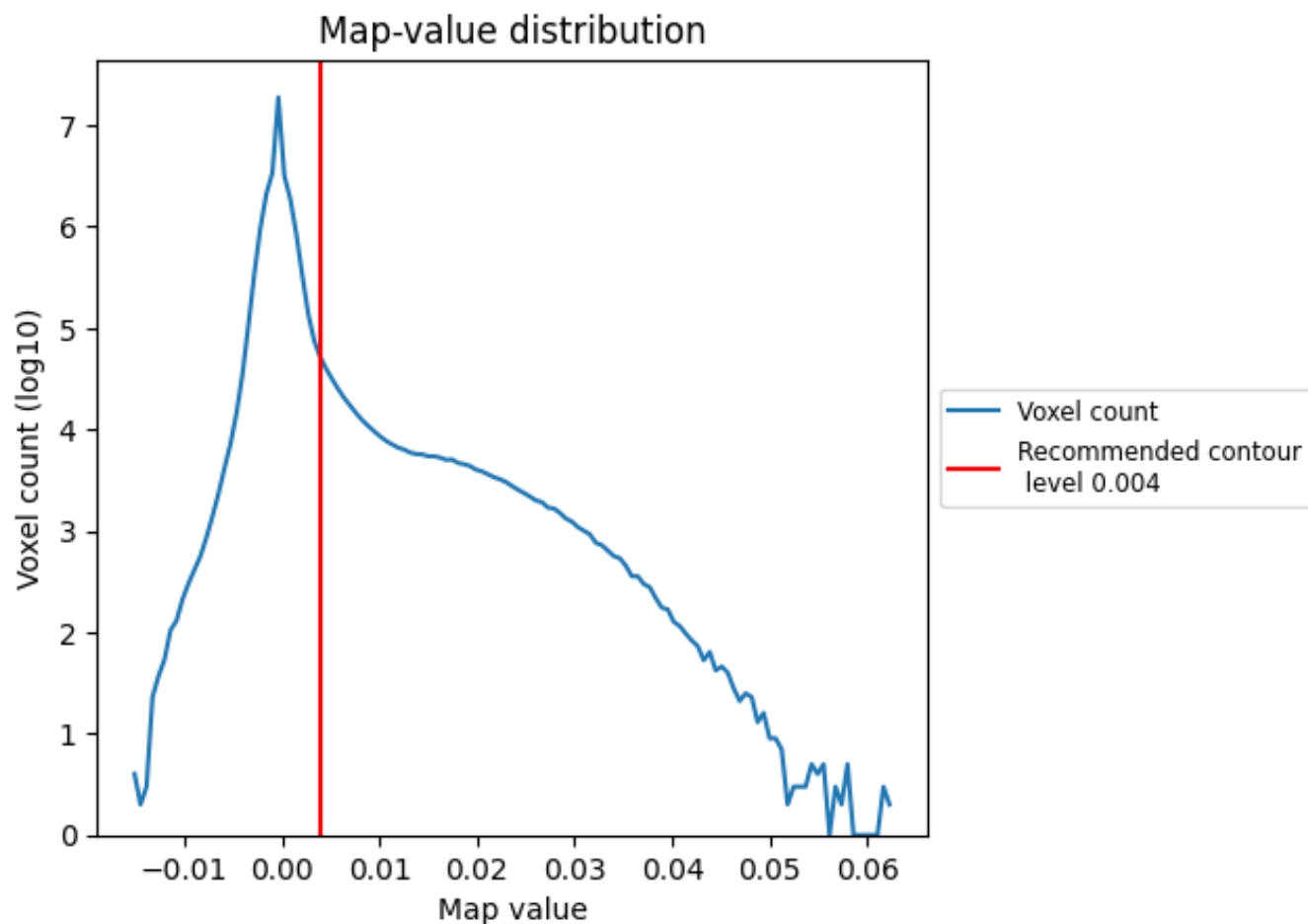
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

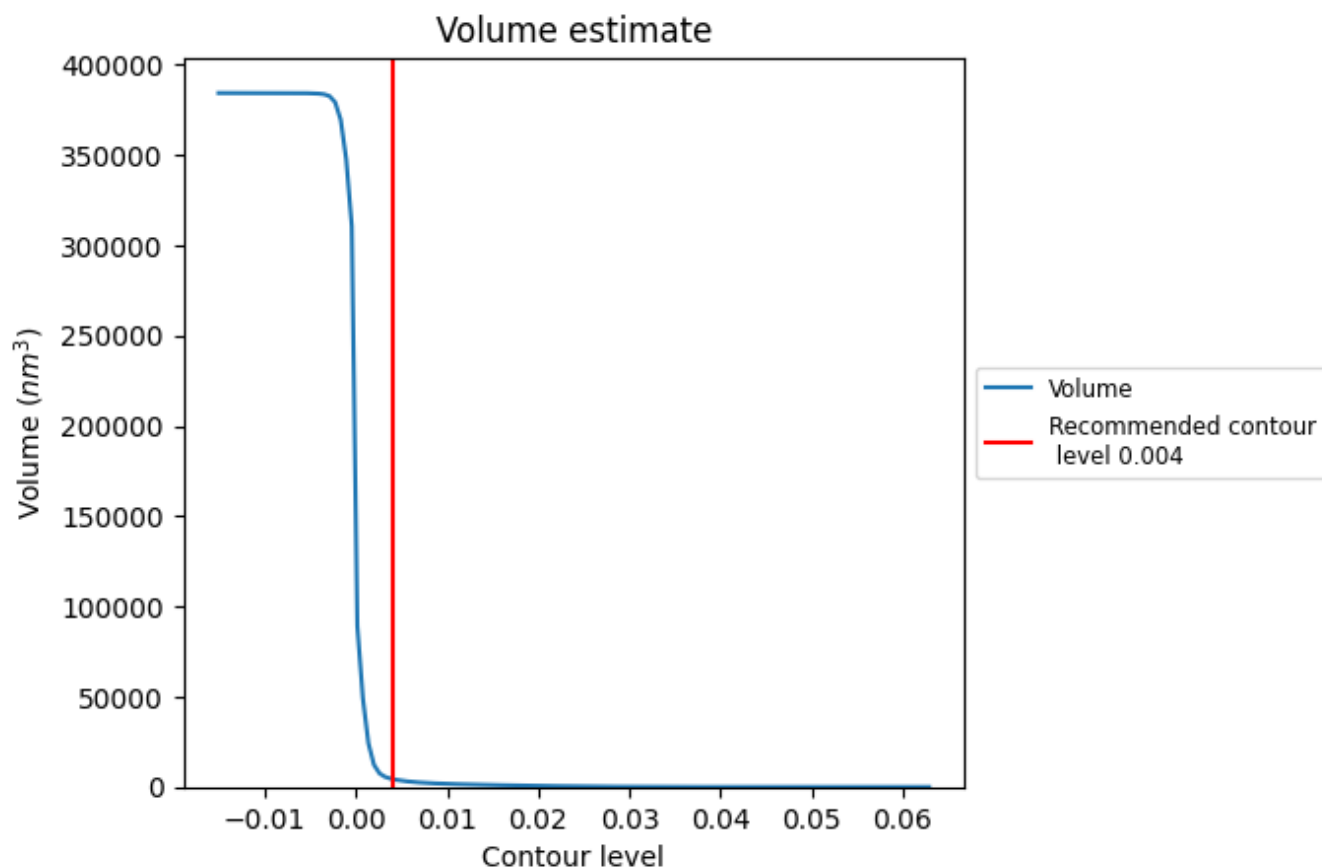
This section contains the results of statistical analysis of the map.

### 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.

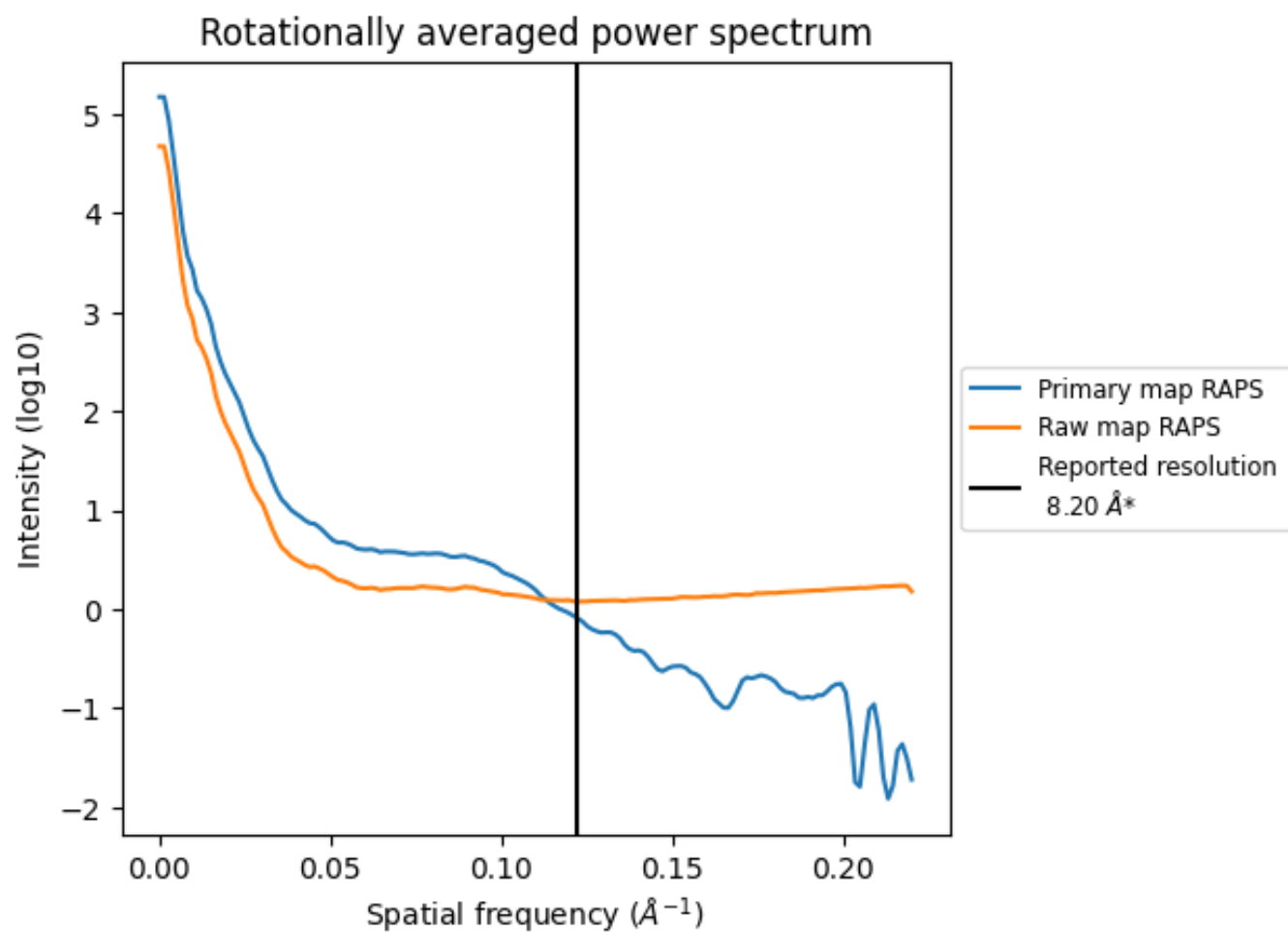
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4396  $\text{nm}^3$ ; this corresponds to an approximate mass of 3971 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 ⓘ



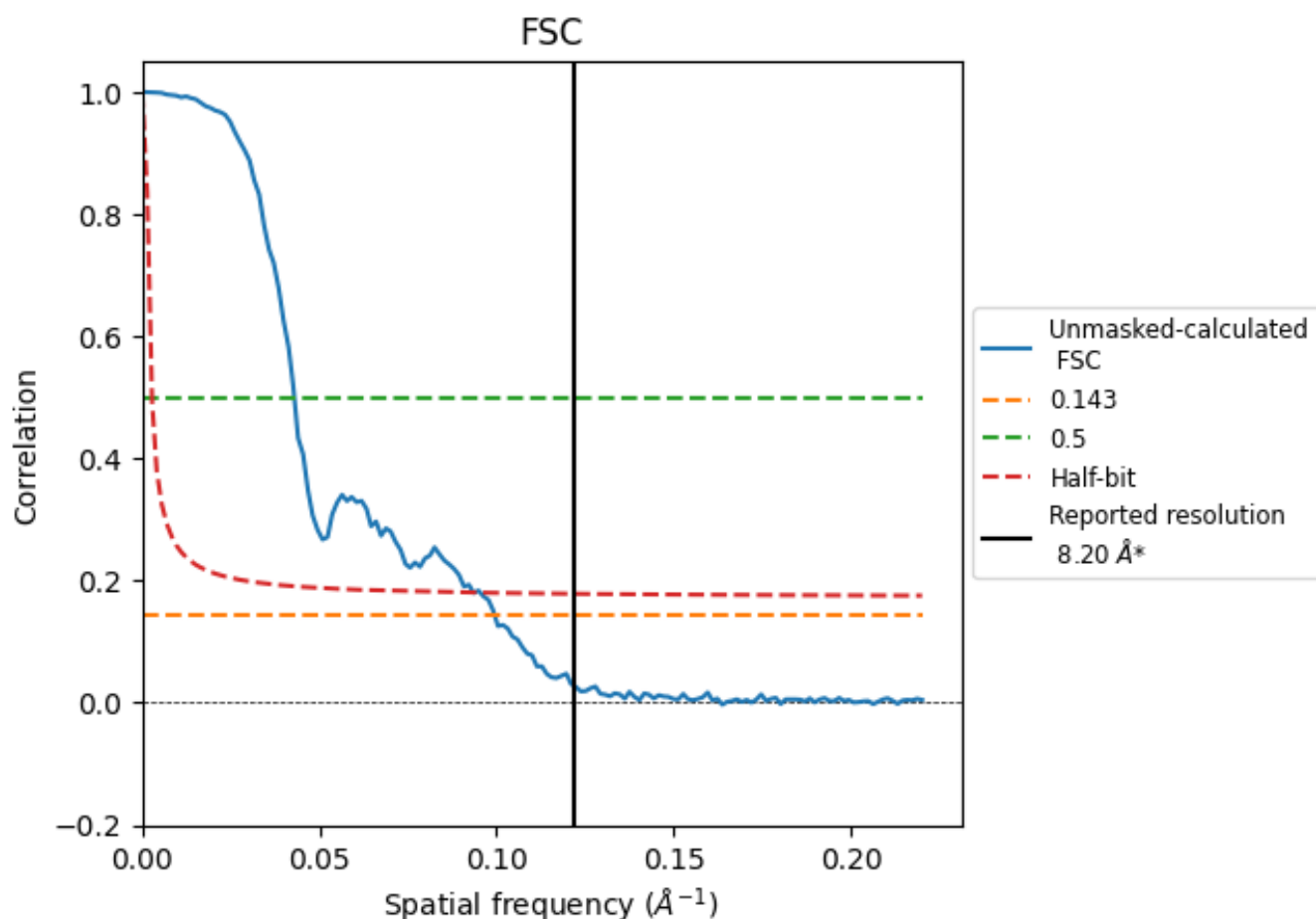
\*Reported resolution corresponds to spatial frequency of 0.122  $\text{\AA}^{-1}$



## 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 0.122 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

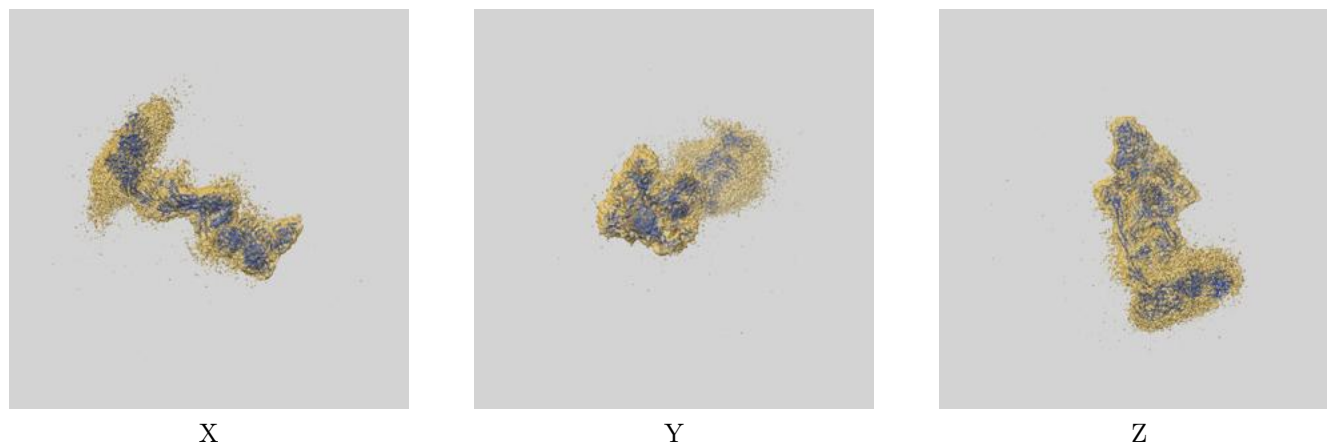
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	10.05	23.31	10.70

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 10.05 differs from the reported value 8.2 by more than 10 %

## 9 Map-model fit [i](#)

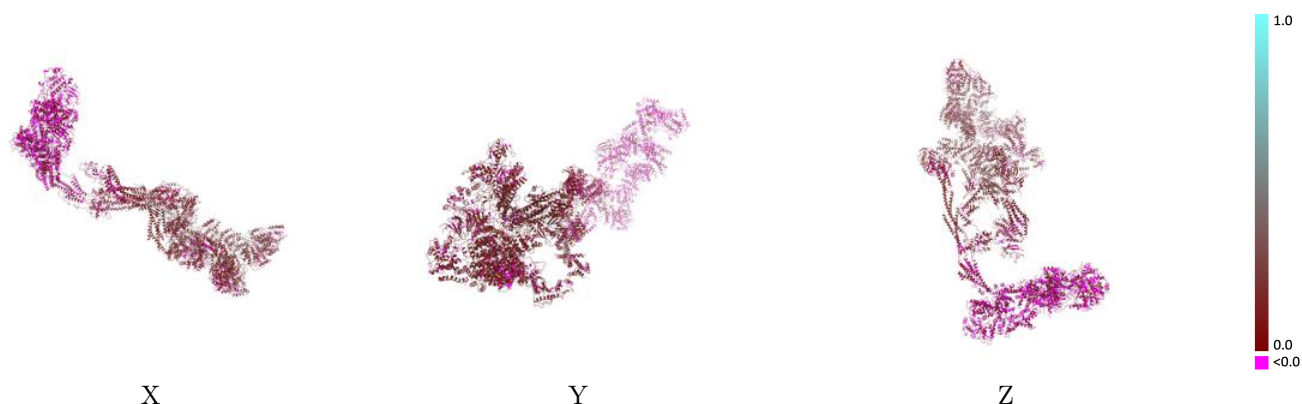
This section contains information regarding the fit between EMDB map EMD-41565 and PDB model 8TQW. Per-residue inclusion information can be found in section [3](#) on page [9](#).

### 9.1 Map-model overlay [i](#)



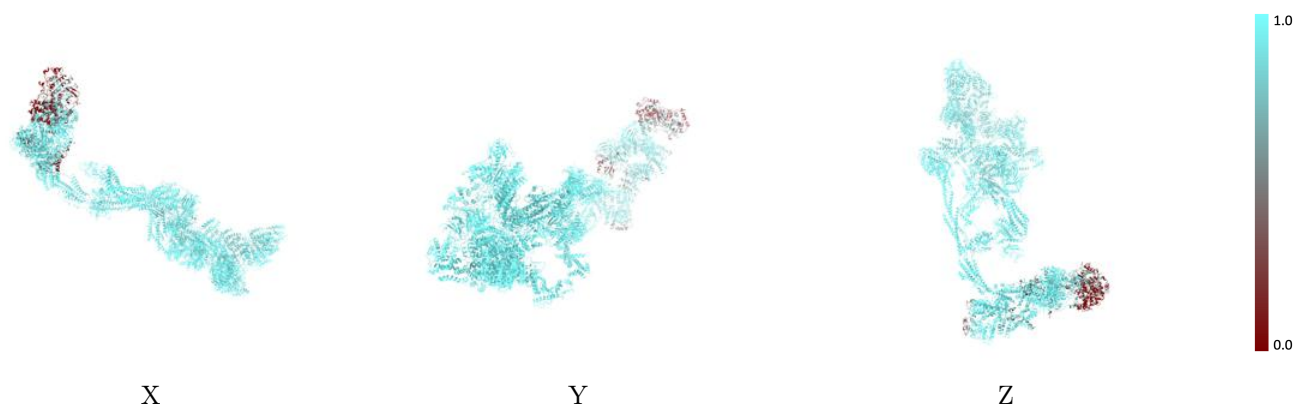
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



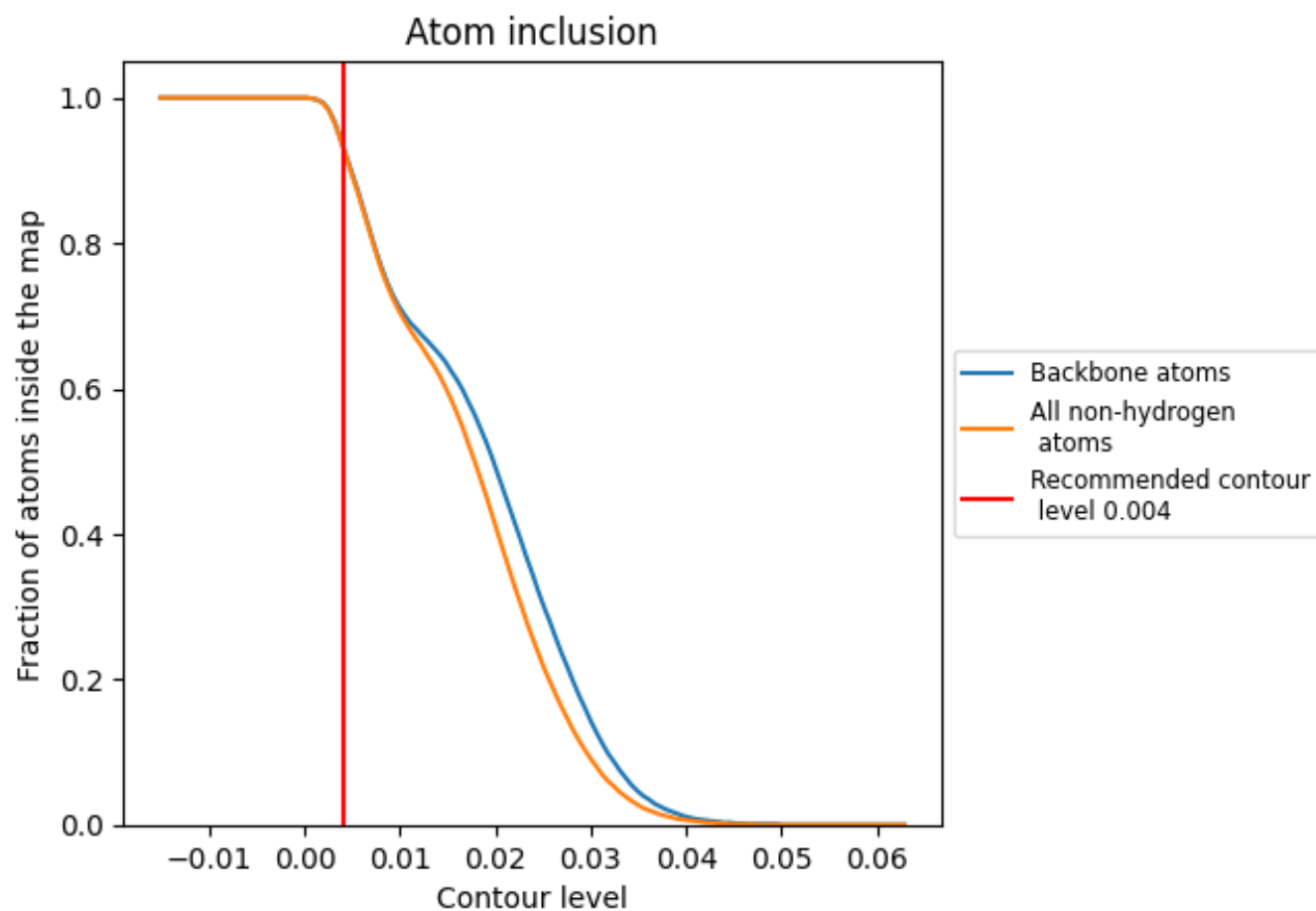
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.004).





























































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 94% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9340	 0.1110
0	 0.9980	 0.1790
1	 1.0000	 0.1670
2	 1.0000	 0.1470
3	 1.0000	 0.1610
4	 1.0000	 0.0940
A	 1.0000	 0.1290
B	 1.0000	 0.2460
D	 1.0000	 0.1340
F	 1.0000	 0.0940
G	 0.9990	 0.0980
H	 0.9950	 0.1220
I	 1.0000	 0.1670
J	 0.9960	 0.0370
K	 1.0000	 0.1270
N	 1.0000	 0.1720
O	 1.0000	 0.2010
P	 0.9990	 0.1450
Q	 1.0000	 0.1780
R	 1.0000	 0.1390
S	 1.0000	 0.0690
T	 1.0000	 0.1490
U	 0.9960	 0.0850
V	 1.0000	 0.1440
W	 1.0000	 0.1550
X	 0.9990	 0.1660
a	 0.3260	 0.0050
b	 0.2570	 0.0040
c	 0.8820	 0.0110
d	 0.8920	 0.0170

