



wwPDB EM Validation Summary Report ⓘ

Aug 5, 2026 – 08:24 AM EDT

PDB ID : 7ML1 / pdb_00007ml1
EMDB ID : EMD-23905
Title : RNA polymerase II pre-initiation complex (PIC2)
Authors : Yang, C.; Fujiwara, R.; Kim, H.J.; Gorbea Colon, J.J.; Steimle, S.; Garcia, B.A.; Murakami, K.
Deposited on : 2021-04-27
Resolution : 4.00 Å(reported)
Based on initial model : 5OQJ

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

We welcome your comments at 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>.

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

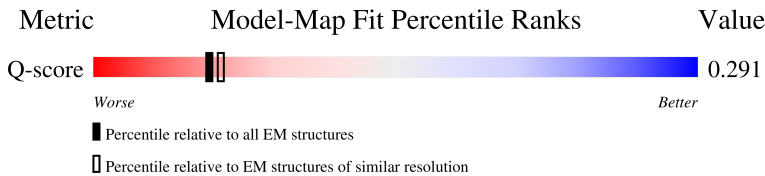
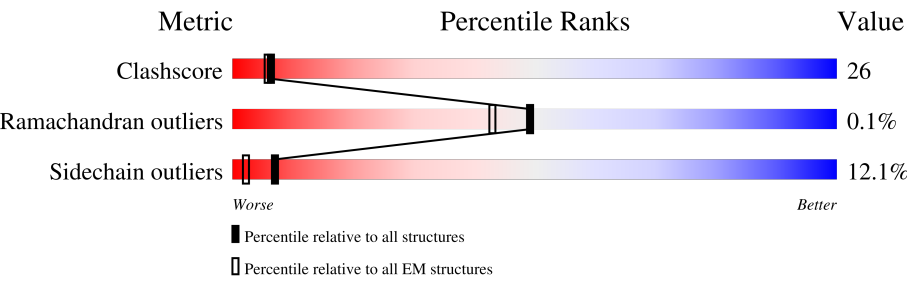
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

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 $\leq 5\%$. 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	1	542	 17% 37% 27% 32%
2	4	338	 9% 39% 39% 6% 16%
3	0	778	 20% 32% 58% 8%
4	6	461	 7% 29% 40% 7% 24%

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Mol	Chain	Length	Quality of chain
5	2	513	
6	5	72	
7	7	843	
8	3	321	
9	O	240	
10	N	57	
11	T	57	
12	A	1733	
13	B	1224	
14	C	318	
15	D	221	
16	E	215	
17	F	155	
18	G	171	
19	H	146	
20	I	122	
21	J	70	
22	K	120	
23	L	70	
24	M	345	
25	Q	735	
26	R	400	
27	U	286	
28	V	122	
29	W	482	

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Mol	Chain	Length	Quality of chain
30	X	328	25% 38% 9% 52%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	SF4	0	801	-	-	X	-

2 Entry composition [i](#)

There are 33 unique types of molecules in this entry. The entry contains 64538 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 Tfb1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	367	Total	C	N	O	S	0	0
			2411	1536	438	430	7		

- Molecule 2 is a protein called General transcription and DNA repair factor IIH subunit TFB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4	284	Total	C	N	O	S	0	0
			2041	1310	343	376	12		

- Molecule 3 is a protein called General transcription and DNA repair factor IIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	0	754	Total	C	N	O	S	0	0
			6108	3891	1032	1147	38		

- Molecule 4 is a protein called General transcription and DNA repair factor IIH subunit SSL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	351	Total	C	N	O	S	0	0
			2527	1590	454	456	27		

- Molecule 5 is a protein called RNA polymerase II transcription factor B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	2	460	Total	C	N	O	S	0	0
			3011	1856	562	584	9		

- Molecule 6 is a protein called General transcription and DNA repair factor IIH subunit TFB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	66	Total	C	N	O	S	0	0
			498	314	89	93	2		

- Molecule 7 is a protein called General transcription and DNA repair factor IIIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	634	Total	C	N	O	S	0	0
			4447	2722	827	874	24		

- Molecule 8 is a protein called BJ4_G0050160.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	3	138	Total	C	N	O	S	0	0
			860	533	160	160	7		

- Molecule 9 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	O	180	Total	C	N	O	S	0	0
			1416	921	242	247	6		

- Molecule 10 is a DNA chain called non-template strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	57	Total	C	N	O	P	0	0
			1178	562	227	332	57		

- Molecule 11 is a DNA chain called template strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	T	57	Total	C	N	O	P	0	0
			1159	559	191	352	57		

- Molecule 12 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A	1398	Total	C	N	O	S	0	0
			10997	6931	1927	2078	61		

- Molecule 13 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	B	1147	Total	C	N	O	S	0	0
			9132	5775	1602	1700	55		

- Molecule 14 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	C	262	Total	C	N	O	S	0	0
			2061	1299	343	406	13		

- Molecule 15 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	D	157	Total	C	N	O	S	0	0
			1253	779	220	252	2		

- Molecule 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	E	213	Total	C	N	O	S	0	0
			1744	1107	308	318	11		

- Molecule 17 is a protein called DNA-directed RNA polymerases I,II,and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	F	83	Total	C	N	O	S	0	0
			670	428	114	125	3		

- Molecule 18 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

- Molecule 19 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	H	136	Total	C	N	O	S	0	0
			1089	686	184	215	4		

- Molecule 20 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	I	116	Total	C	N	O	S	0	0
			944	581	172	181	10		

- Molecule 21 is a protein called DNA-directed RNA polymerases II subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	J	65	Total	C	N	O	S	0	0
			532	339	93	94	6		

- Molecule 22 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	K	112	Total	C	N	O	S	0	0
			904	580	154	168	2		

- Molecule 23 is a protein called DNA-directed RNA polymerases II subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	L	45	Total	C	N	O	S	0	0
			358	221	71	62	4		

- Molecule 24 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	M	279	Total	C	N	O	S	0	0
			2175	1382	373	403	17		

- Molecule 25 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	148	Total	C	N	O	S	0	0
			1144	733	195	212	4		

- Molecule 26 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	190	Total	C	N	O	S	0	0
			1303	812	238	246	7		

- Molecule 27 is a protein called Transcription initiation factor IIA large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	44	Total	C	N	O	S	0	0
			366	233	64	66	3		

- Molecule 28 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	50	Total	C	N	O	S	0	0
			389	245	65	76	3		

- Molecule 29 is a protein called Transcription initiation factor IIE subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	191	Total	C	N	O	S	0	0
			1469	932	254	277	6		

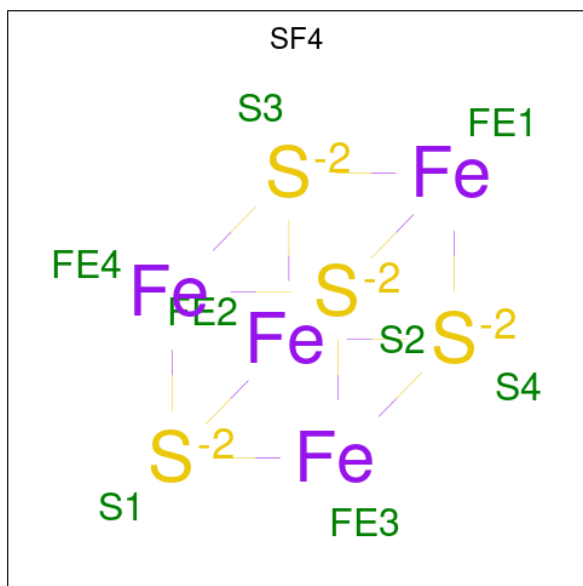
- Molecule 30 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	156	Total	C	N	O	S	0	0
			984	608	180	192	4		

- Molecule 31 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
31	4	1	Total	Zn	0
			1	1	
31	6	4	Total	Zn	0
			4	4	
31	3	2	Total	Zn	0
			2	2	
31	A	3	Total	Zn	0
			3	3	
31	B	1	Total	Zn	0
			1	1	
31	C	1	Total	Zn	0
			1	1	
31	I	2	Total	Zn	0
			2	2	
31	J	1	Total	Zn	0
			1	1	
31	L	1	Total	Zn	0
			1	1	
31	M	1	Total	Zn	0
			1	1	
31	W	1	Total	Zn	0
			1	1	
31	X	1	Total	Zn	0
			1	1	

- Molecule 32 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
32	0	1	Total	Fe	S	0
			8	4	4	

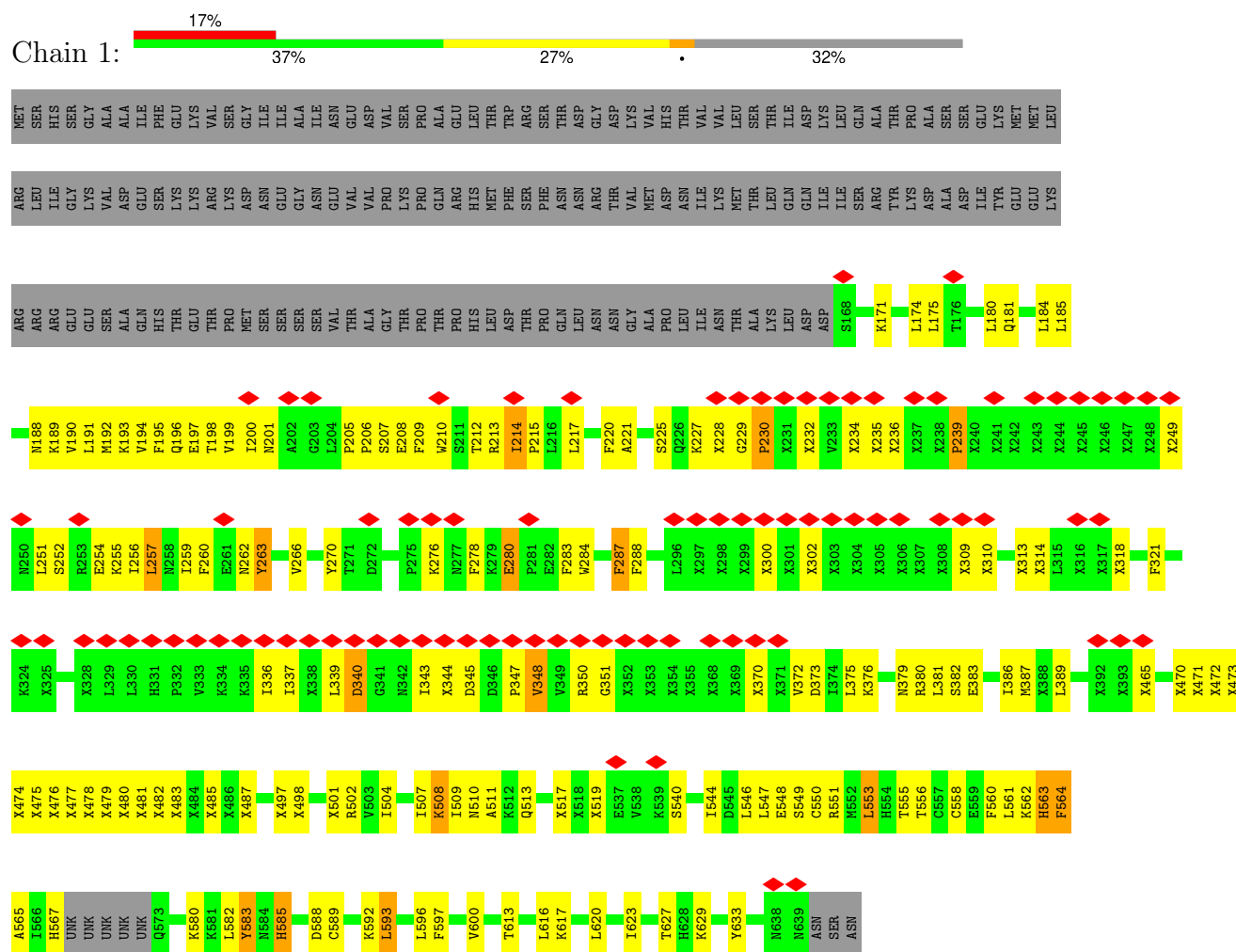
- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
33	A	1	Total	Mg	0
			1	1	

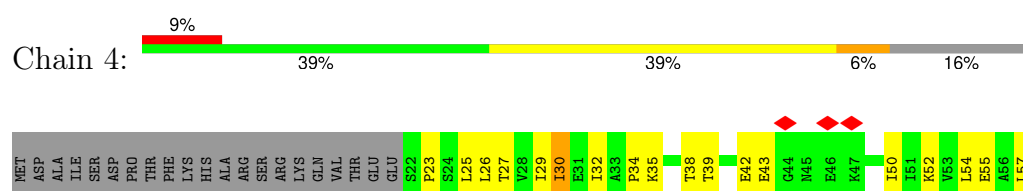
3 Residue-property plots

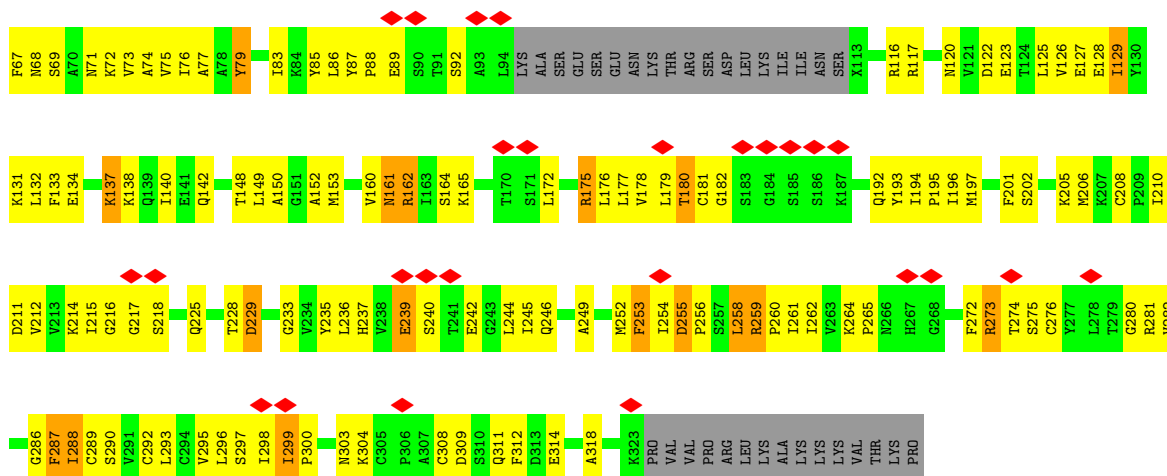
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Tfb1

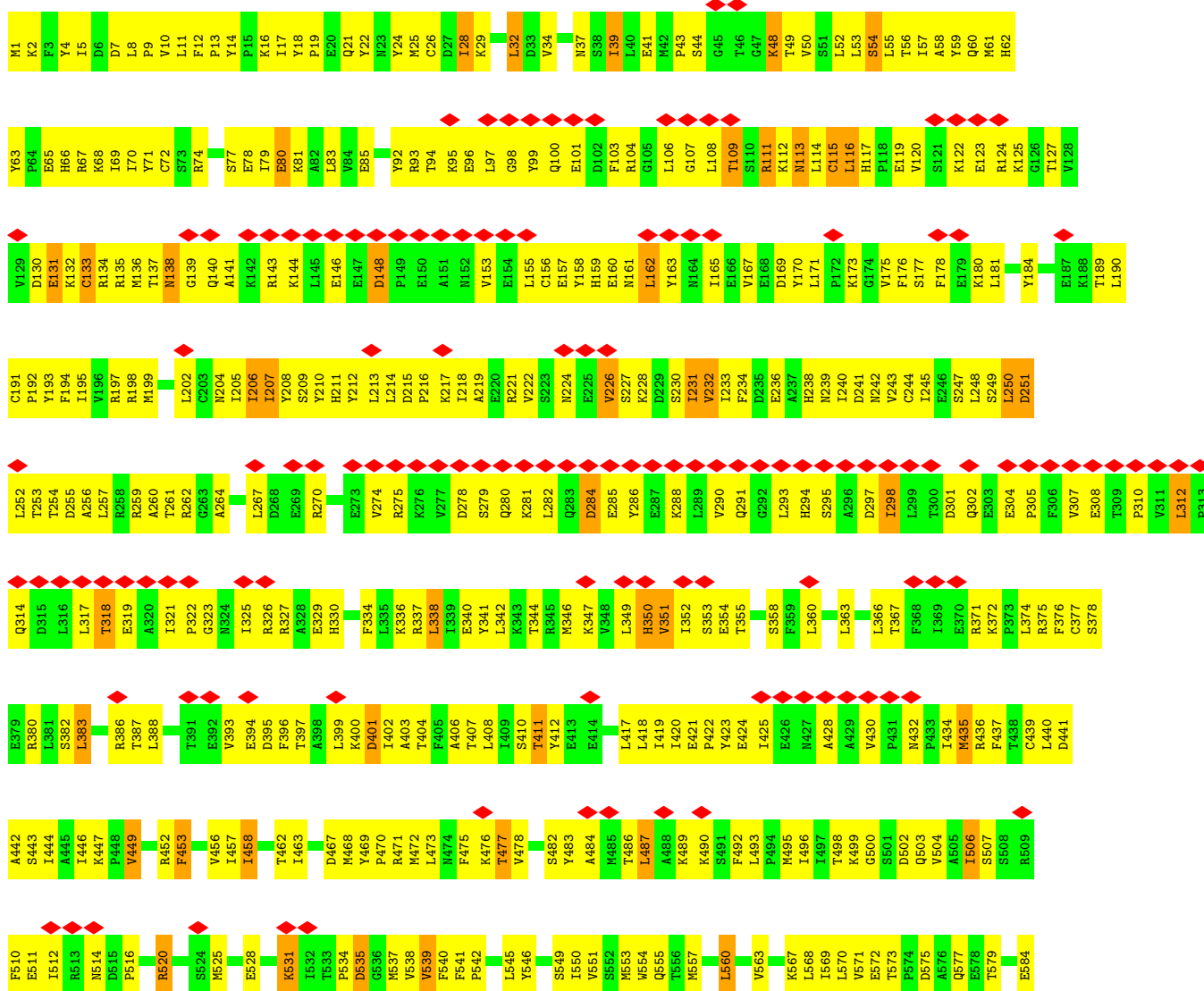


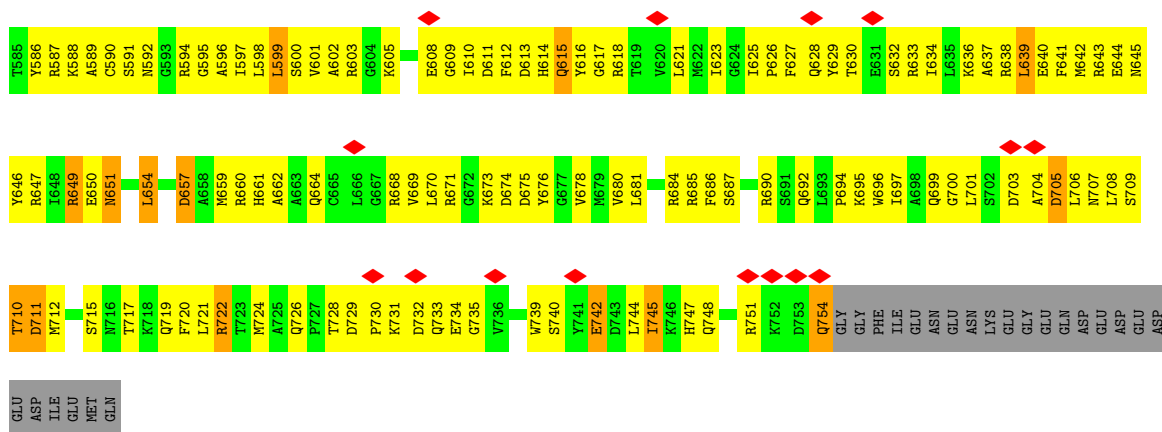
• Molecule 2: General transcription and DNA repair factor IIH subunit TFB4



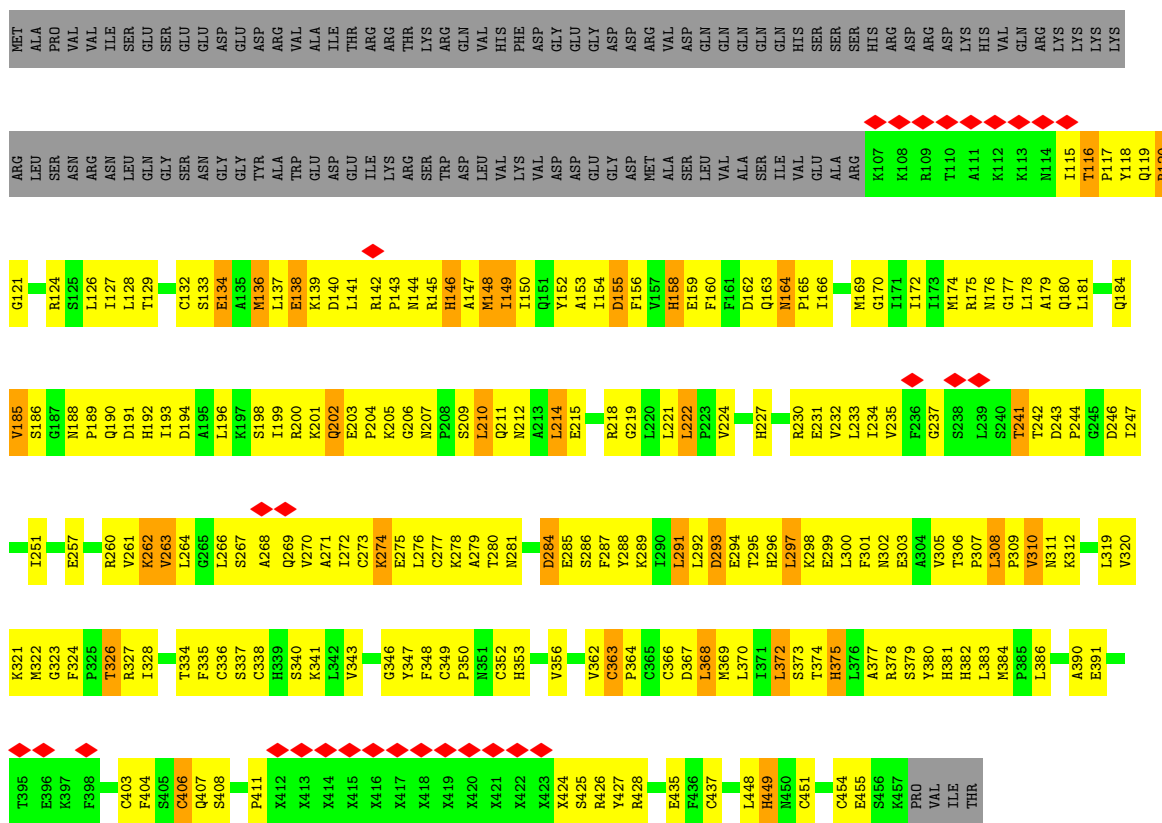


• Molecule 3: General transcription and DNA repair factor IIH helicase subunit XPD

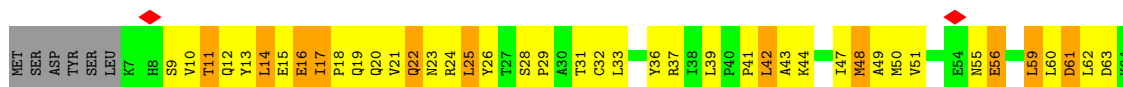


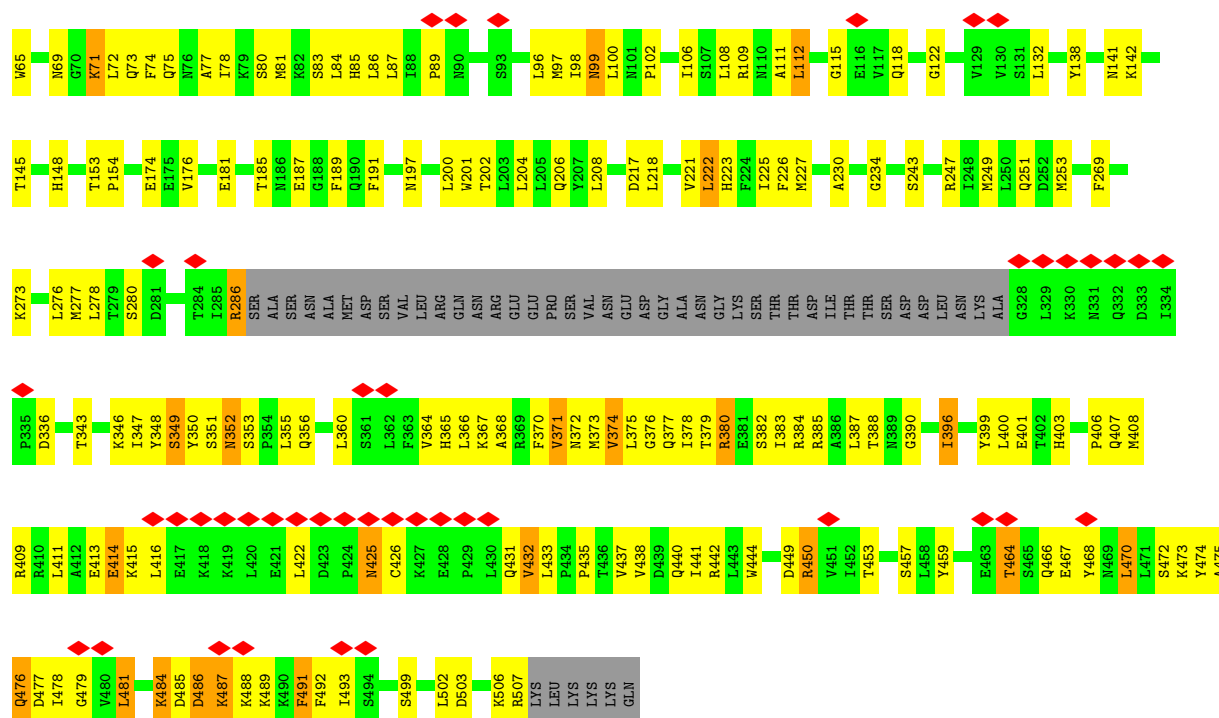


• Molecule 4: General transcription and DNA repair factor IIH subunit SSL1

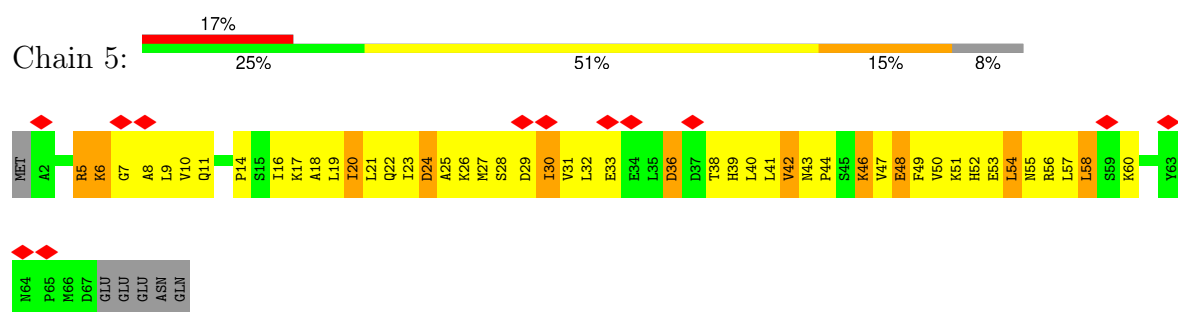


• Molecule 5: RNA polymerase II transcription factor B subunit 2

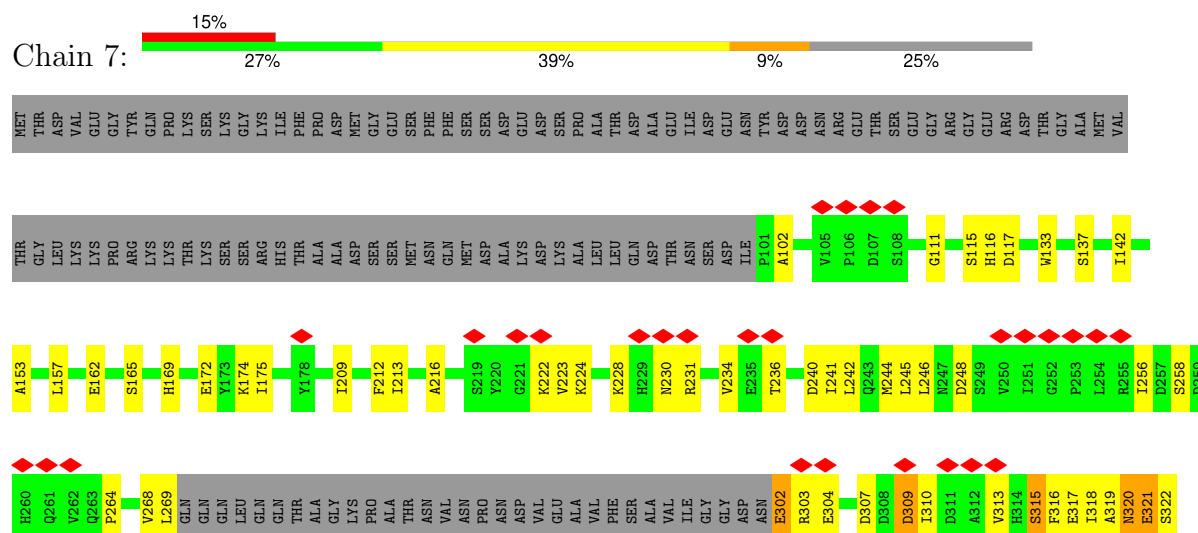




• Molecule 6: General transcription and DNA repair factor IIH subunit TFB5



• Molecule 7: General transcription and DNA repair factor IIH helicase subunit XPB



THR
GLU
ALA
PHE
MET
GLY
LEU
GLY
CYS
VAL
ILE
SER
GLU
LEU

• Molecule 9: TATA-box-binding protein

Chain O: 

MET
ALA
ASP
GLU
GLU
ARG
LEU
LYS
PHE
PHE
LYS
GLU
ASN
ALA
ASN
LYS
ILE
VAL
PHE
ASP
PRO
ASN
THR
ARG
GLN
VAL
TRP
GLU
ASN
GLN
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ARG
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PRO
GLU
SER
GLU
LYS
ASP
THR
SER
ALA
THR

S61
G62
I63
V64
P65
T66
L67
Q68
N69
I70
V71
A72
T73
Y74
T75
L76
G77
C78
R79
L80
D81
L82
K83
T84
V85
A86
L87
H88
A89
R90
N91
A92
E93
Y94
N95
P96
K97
R98
A101
V102
I103
M104
I105
I106
I107
E108
K109
K110
T111
T112
A113
L114
I115
F116
A117
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G119
K120
M121

V122
V123
T124
G125
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K127
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D131
S132
K133
L134
A135
S136
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K138
Y139
A140
R141
I142
I143
Q144
K145
I146
F147
G148
A149
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K151
F152
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K156
I157
Q158
N159
I160
V161
G162
S163
C164
D165
V166
D167
F168
P169
I170
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S178
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R220
E221
E222
I223
Y224
Q225
A226
F227
E228
A229
I230
V231
P232
V233
L234
S235
E236
F237
R238
K239
M240

• Molecule 10: non-template strand DNA

Chain N: 

A2
A3
A4
A5
A6
A7
A8
A9
A10
A11
G12
G13
C14
G15
C16
G17
T20
A21
A22
A23
A24
A25
A26
G27
T28
T29
C30
G31
A32
A33
G34
G35
C36
C37
G38
C39
G40
A41
A42
T43
T44
C45
G46
G47
G50
T51
T55
A56
C57
A58

• Molecule 11: template strand DNA

Chain T: 

T108
C120
T124
A130
C132
T133
T134
G135
A136
A137
A138
A144
T145
G150
C151
G152
C153
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T160
T161
T162
T163
T164

• Molecule 12: DNA-directed RNA polymerase subunit

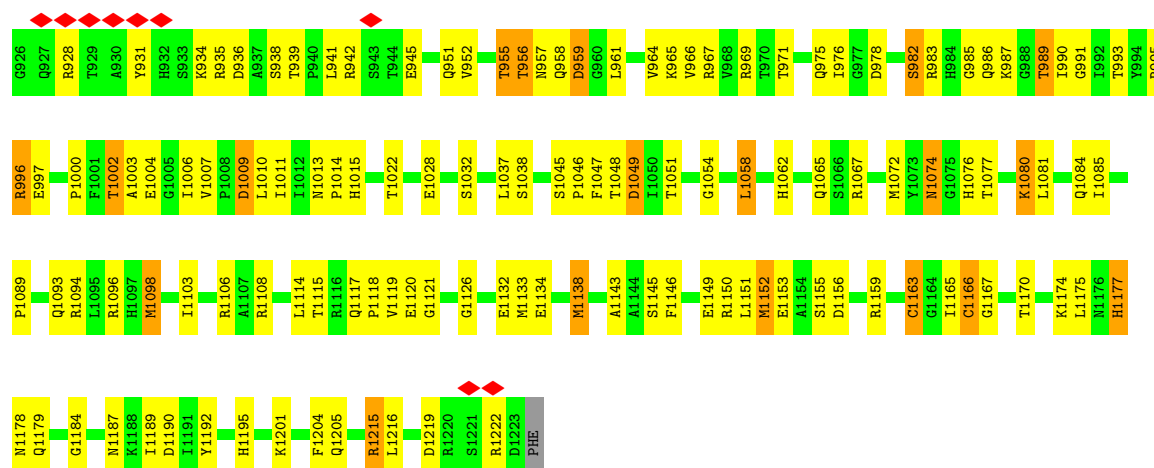
Chain A: 

MET
VAL
G3
Q4
V14
K15
E16
S23
P24
E25
E26
V27
R28
A29
I30
I35
M41
D42
T46
R47
A48
K49
L53
N54
D55
L58
G59
S60
I61
D62
L65
K66
T69
C70
Q71
E72
G73
M74
N75
E76
C77
P78
G79
H80
F81
I84
K88
P89
V90

F91
F95
V106
G107
M108
H109
L114
E120
R123
Q124
I128
K129
D130
S131
K132
R133
R134
T140
L141
C142
K143
T144
K145
M146
V147
C148
E149
T150
D151
V152
P153
S154
ASP
T200
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L222
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R230
P231
E232
V233
M234
L236
I237
K176

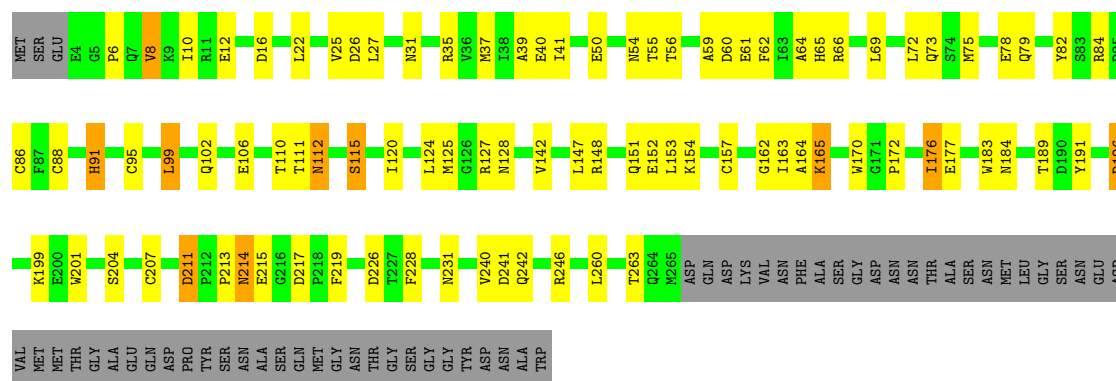
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L181
V182
G183
S184
H185
K186
K187
ASP
ARG
ALA
THR
GLY
ASP
ALA
ASP
GLU
P197
E198
L199
R200
V201
L202
S203
E205
E206
I207
L208
N209
I210
K211
K212
H213
V216
K217
D218
F219
S221
L222
G223
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R230
P231
E232
V233
M234
L236
I237
K176





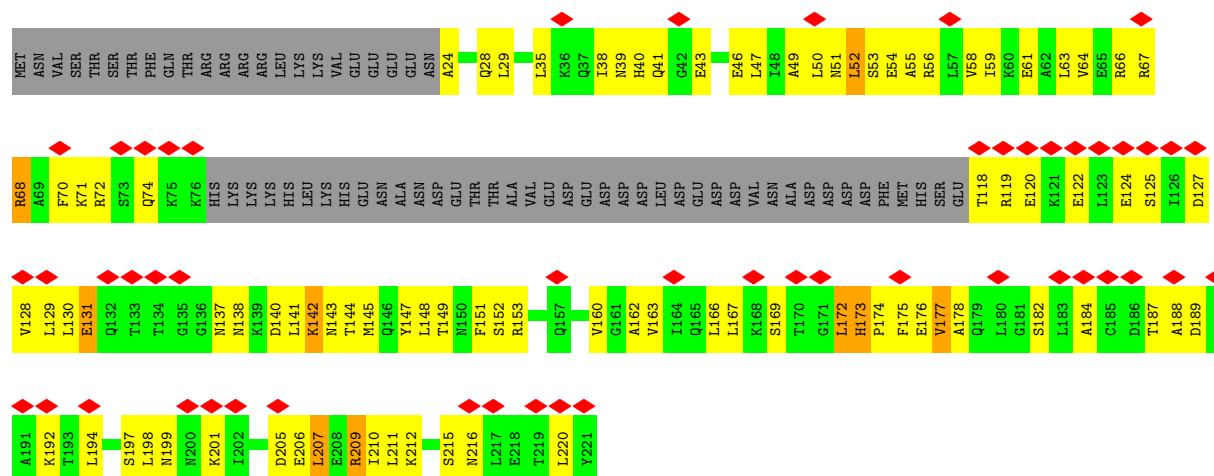
• Molecule 14: DNA-directed RNA polymerase II subunit RPB3

Chain C: 54% 25% 18%



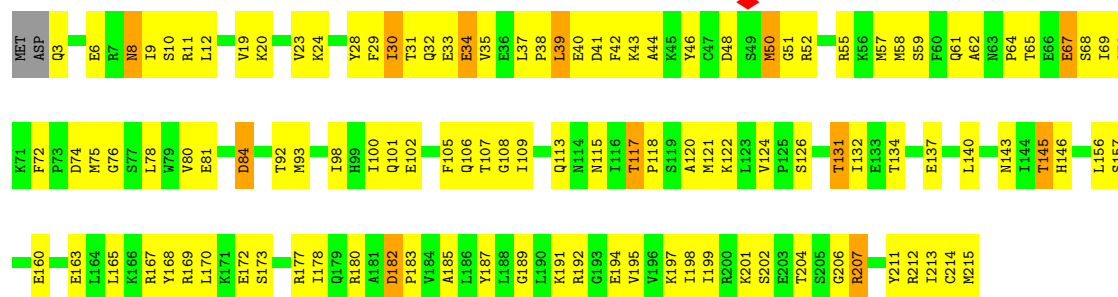
• Molecule 15: DNA-directed RNA polymerase II subunit RPB4

Chain D: 23% 30% 37% 29%



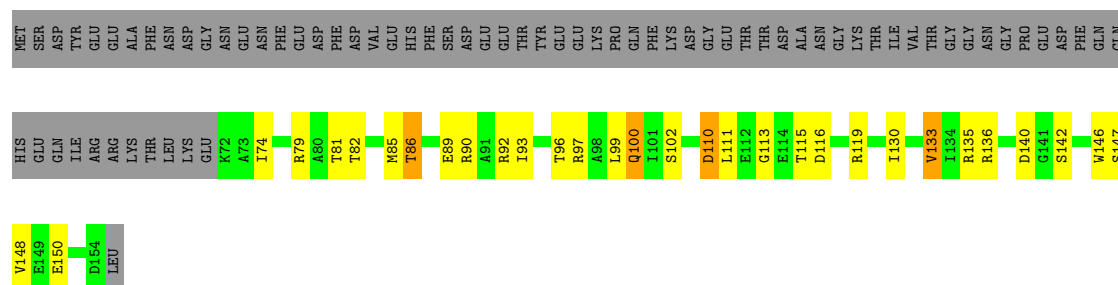
• Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 



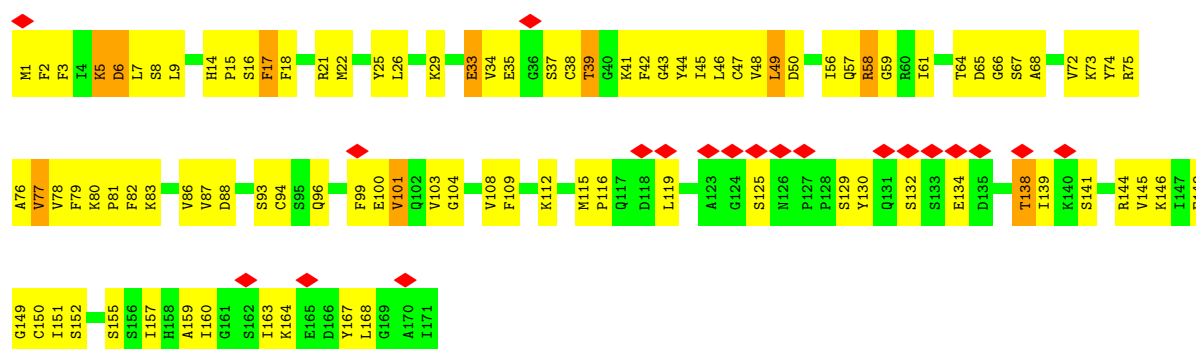
- Molecule 17: DNA-directed RNA polymerases I,II,and III subunit RPABC2

Chain F: 



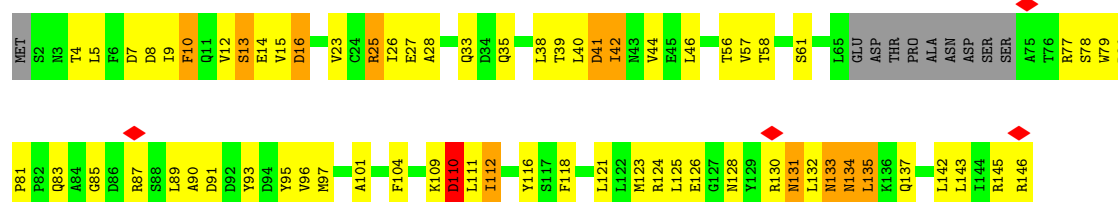
- Molecule 18: DNA-directed RNA polymerase II subunit RPB7

Chain G: 

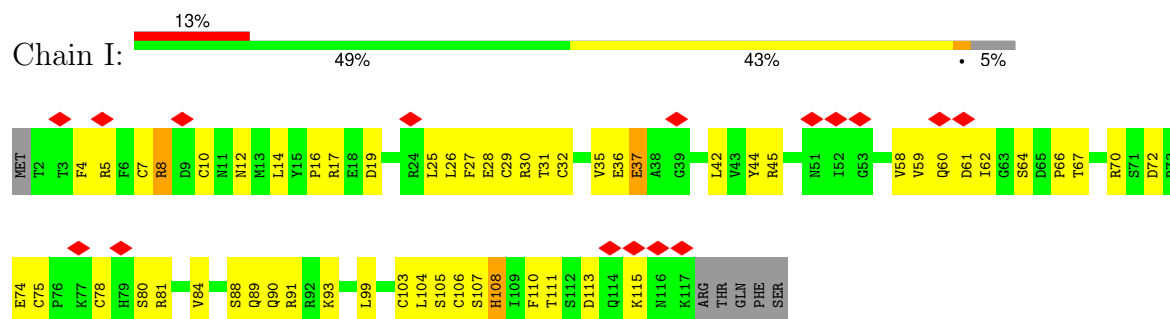


- Molecule 19: DNA-directed RNA polymerases I, II, and III subunit RPABC3

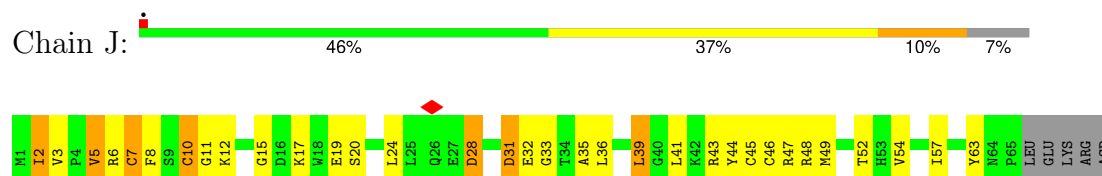
Chain H: 



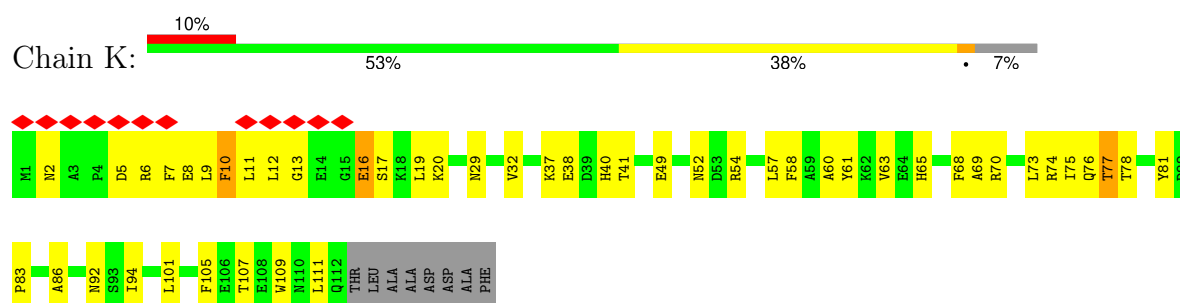
- Molecule 20: DNA-directed RNA polymerase II subunit RPB9



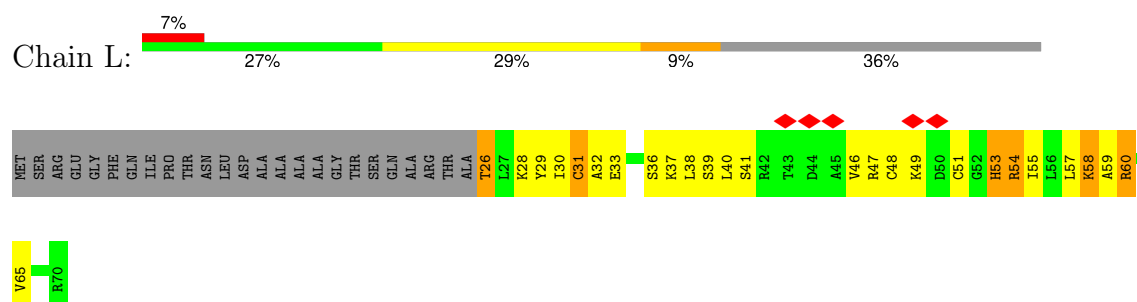
- Molecule 21: DNA-directed RNA polymerases II subunit RPABC5



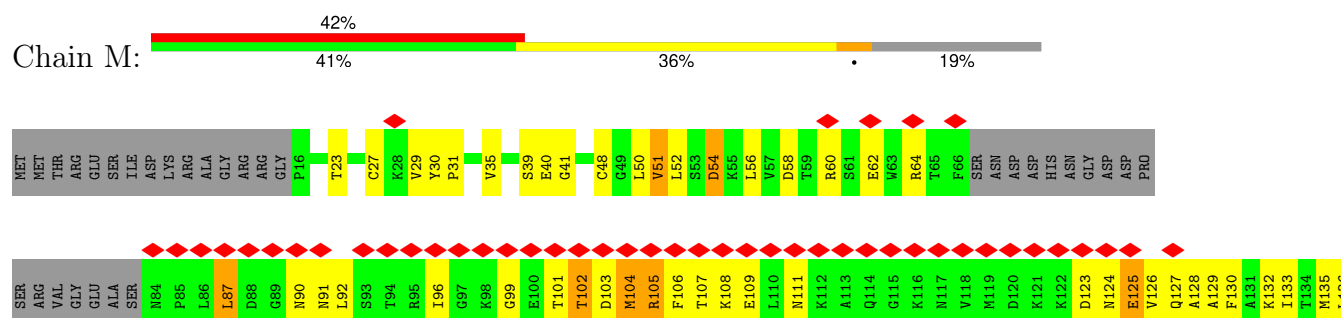
- Molecule 22: DNA-directed RNA polymerase II subunit RPB11

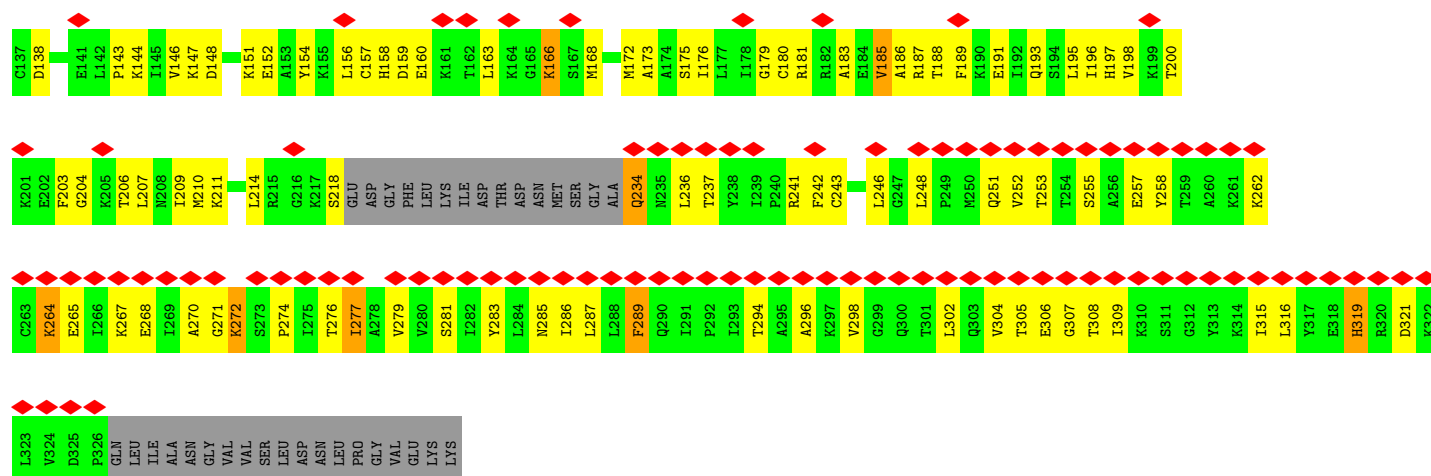


- Molecule 23: DNA-directed RNA polymerases II subunit RPABC4



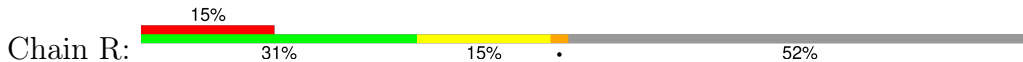
- Molecule 24: Transcription initiation factor IIB





GLU PHE GLY LYS PHE ILE ARG ARG LYS TYR PRO GLY ALA GLU ASN LYS LYS LEU MET PHE ALA ILE VAL LYS LYS LEU CYS ARG LYS VAL VAL GLY ASN ASP HIS MET GLU LEU LYS LYS GLU

- Molecule 26: Transcription initiation factor IIF subunit beta



WET	SER	GLY	ALA	GLY	ALA	PRO	ALA	ALA	LEU	ASN	ASN	SER	THR	ASN	SER	VAL	ALA	LYS	GLU	LYS	SER	GLY	ASN	ASP	GLU	TYR	LEU	SER	GLN	GLU	GLU	VAL	PHE	ASP	GLY	ASN	ASP	ILE	GLU	LYS	VAL	TYR	GLU	GLU	SER	LEU	D58	363
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S64		L70		R82	ASP	L92		X93		X103		I104		L106		L107		L108		L109		F110		ASN		ASN		ASN		ASP		ASP		SER		SER		L1F		L1F		P117		H118		E119		E120		D121		L122		E123		L124		L125	
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[illegible]

ASN	HIS	ARG	VAL	MET	THR	ASP	ARG	GLY	ARG	ASP	ARG	TYR	ILE	PRO	TYR	VAL	LYS	T207	T208	P209	K210	K211	I214	V215	G216	H220	E221	C222	Q223	V224	M225	P226	SER	NET	ASN	ASP	PRO	ASP	ASN	V238	M248	K249	E250	P251	L252	D256	E257	T258	V259	G260	V261	T262	W263
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T266	G287	M268	S269	M270	S271	D272	D273	M274	S275	M276	F277	L278	K279	V280	GLY	GLU	GLY	LYS	ALA	LYS	SER	ASN	ILE	LYS	SER	ILE	ARG	M284	P285	K286	K287	E288	I289	L290	D301	F302	D308	E309	D311	F312	M313	S314	L315	K316	G317
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E326	A327	H328	L329	K330	E331	D334	L339	V340	K341	K342	G343	P344	V345	A346	F347	T350	L351	PRO	GLU	GLY	TYR	LYS	LYS	LEU	LEU	LYS	GLU	GLU	GLY	ARG	LYS	ALA	ALA	THR	ASP	GLY	GLN	GLY	GLY	GLU	LEU	ALA	ALA	ALA	GLN	GLN	GLY	ASP	ASN	ASP	ASP
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GLU
ASP
GLU
ILE
GLU
MET
GLU
ASP
VAL
VAL

- Molecule 27: Transcription initiation factor IIA large subunit



MET	SER	ASN	ALA	GLU	ALA	SER	ARG	VAL	TYR	GLU	ILE	VAL	GLU	GLU	ASN	GLU	VAL	ARG	GLU	PHE	ASP	ILE	ASP	GLU	GLN	THR	LEU	LEU	ASP	LYS	ASN	ILE	TRP	GLN	LYS	LEU	LEU	THR	VAL	THR	THR	PHE	SER	TRP	ASP	ASN	ASN	GLN	PHE
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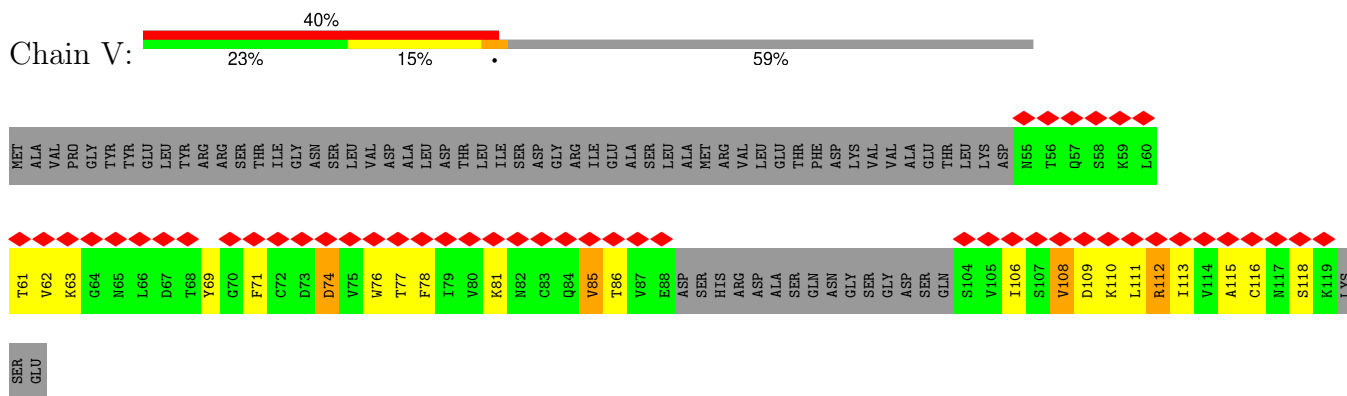
ASN	GLY	GLY	ASN	ASN	GLN	VAL	GLY	ASN	ASP	LEU	ASN	PHE	ASN	ASN	THR	ALA	PRO	GLY	VAL	ASN	SER	SER	GLU	GLU	ASN	ASN	THR	GLY	THR	GLY	ASN	GLY	GLU	GLU	ILE	LEU	LEU	PRO	ASN	ASN	ILE	ASN	ASN	THR	GLU	THR	ASN	ASN	ASN	ASN	ASN
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[illegible]

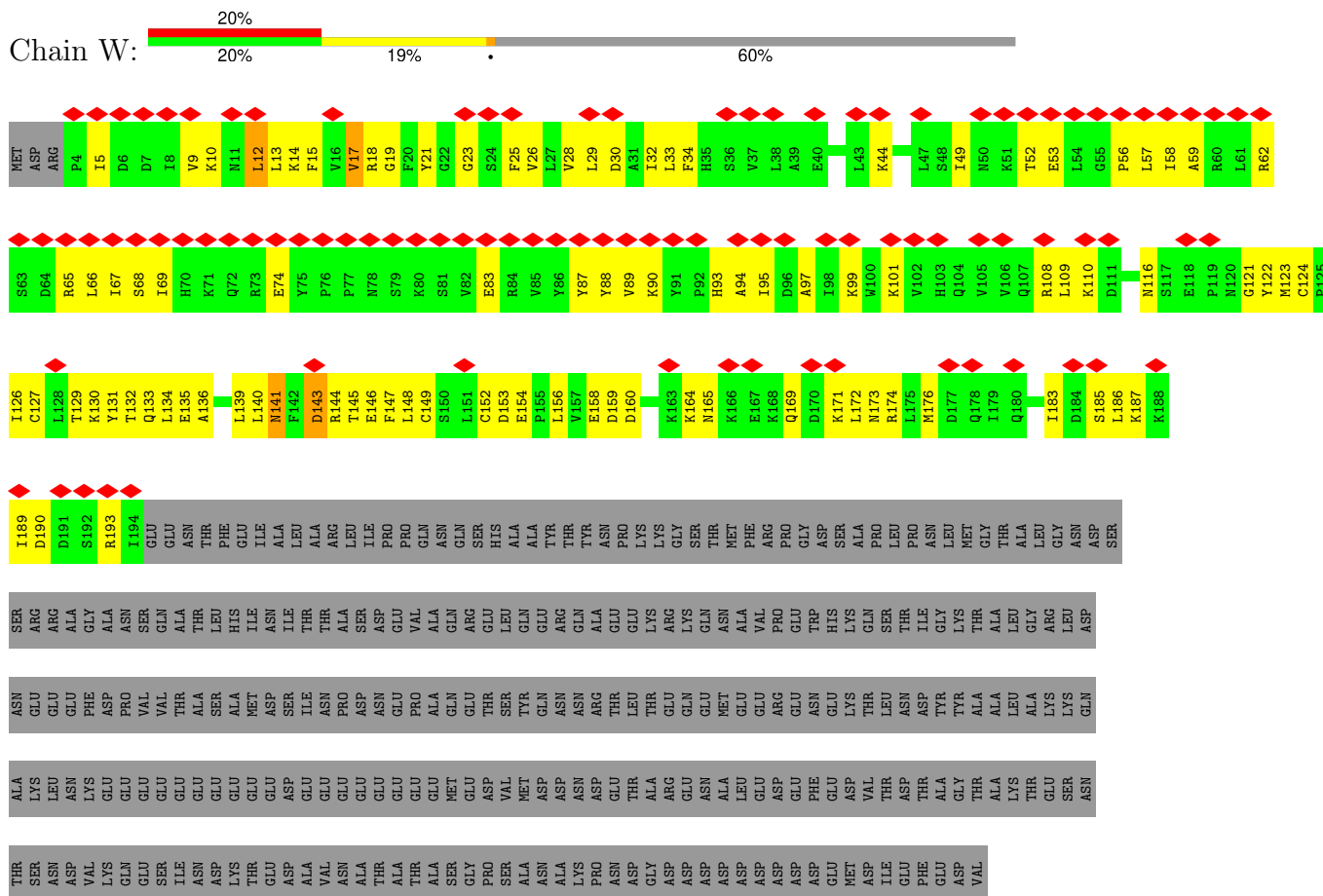
GLU	GLU	LYS	GLU	GLU	ASP	VAL	GLU	LYS	LYS	THR	ARG	LYS	GLU	LYS	ILE	GLU	GLU	GLN	VAL	LYS	LEU	LYS	GLN	LYS	LYS	GLU	GLU	ASP	ASP	THR	GLU	GLU	GLY	VAL	GLU	ASP	ASP	ASP	ASP	TYR	LEU	ILE	GLY	SER	GLU	GLY	GLY	GLU	GLU	ASP	ASP	PRO	ASP
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GLU	ASN	L243	H244	L245	C246	L247	L248	D249	K250	V251	T252	R253	T254	K255	A256	R257	K258	K259	C260	S261	L262	K263	D264	C265	V266	V267	T268	T269	N270	R271	N272	D273	V274	T275	F276	Q277	K278	A279	Q280	V281	E282	A283	E284	V285	V286
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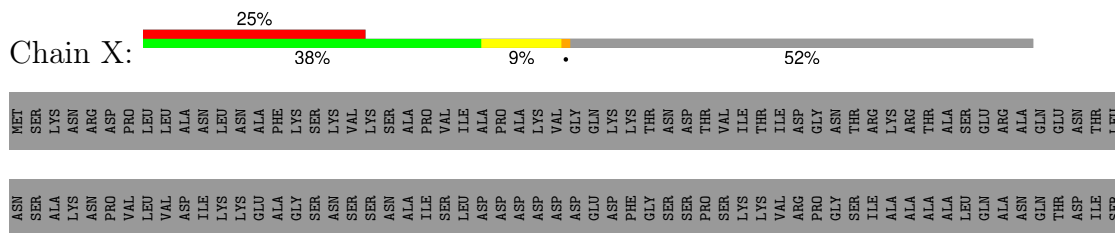
- Molecule 28: Transcription initiation factor IIA subunit 2



- Molecule 29: Transcription initiation factor IIE subunit alpha



- Molecule 30: Transcription initiation factor IIE subunit beta



A272	E273	L274	P275	R276	K277	L278	Q279	D280	L281	G282	L283	LYS	PRO	ALA	SER	VAL	ASP	PRO	ALA	THR	ILE	LYS	ARG	GLN	THR	LYS	ARG	VAL	GLU	VAL	LYS	LYS	ARG	GLN	ARG	LYS	GLY	GLY	LYS	ILE	THR	ASN	THR	HIS	MET	THR	GLY	ILE	LEU	LYS	ASP	TYR	SER	HIS	ARG	VAL	L196	R197	S198	T201	G204	I205	S206	C207	K208	D209	L210	K211	D212	G213	W214	P215	Q216	C217	D218	E219	T220	I221	N222	L233	R234	T235	K236	K237	D238	K239	T240	W245	Y246	N247	N251	L252	K253	C254	I255	D256	E257	E258	F259	V260	K261	M262	W263	E264	N265	V266	Q267	L268	P269	Q270	F271	LYS	SER	H123	D124	E133	Y134	K137	L143	V144	N145	E146	L147	L148	S152	M153	K154	K155	D156	D157	K158	E161	L162	L163	K164	K165	L166	D167	R168	I169	E170	F171	D172	P173	K174	K175	G176	T177	F178	K179	Y180	L181	SER	THR	TYR	ASP	VAL	H187	S188	P189	S190	E191	L192	L193	K194	L195

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33150	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.048	Depositor
Minimum map value	0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0135	Depositor
Map size (Å)	453.67996, 405.97998, 419.75998	wwPDB
Map dimensions	428, 383, 396	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SF4, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.14	0/1896	0.35	1/2543 (0.0%)
2	4	0.17	0/2062	0.46	3/2805 (0.1%)
3	0	0.14	0/6226	0.38	0/8407
4	6	0.16	0/2506	0.41	0/3402
5	2	0.16	0/3057	0.39	0/4071
6	5	0.18	0/502	0.46	0/677
7	7	0.19	0/4521	0.47	0/6036
8	3	0.13	0/870	0.36	0/1190
9	O	0.12	0/1443	0.31	0/1942
10	N	0.24	0/1326	0.48	0/2045
11	T	0.21	0/1294	0.42	0/1994
12	A	0.27	0/11192	0.39	0/15128
13	B	0.29	0/9311	0.38	0/12558
14	C	0.31	0/2099	0.39	0/2845
15	D	0.15	0/1262	0.37	0/1693
16	E	0.26	0/1780	0.37	0/2395
17	F	0.30	0/682	0.41	0/922
18	G	0.18	0/1368	0.36	0/1844
19	H	0.26	0/1107	0.42	0/1499
20	I	0.20	0/962	0.41	0/1295
21	J	0.34	0/541	0.51	0/727
22	K	0.28	0/922	0.40	0/1244
23	L	0.25	0/360	0.55	0/478
24	M	0.16	0/2204	0.42	0/2963
25	Q	0.20	0/1168	0.37	0/1579
26	R	0.17	0/1312	0.37	0/1777
27	U	0.12	0/372	0.33	0/500
28	V	0.11	0/392	0.27	0/529
29	W	0.11	0/1490	0.28	0/2014
30	X	0.10	0/993	0.31	0/1357
All	All	0.22	0/65220	0.40	4/88459 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	4	0	1
4	6	0	1
7	7	0	1
12	A	0	2
13	B	0	2
24	M	0	1
All	All	0	8

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	4	298	ILE	CA-C-N	8.43	125.55	120.24
2	4	298	ILE	C-N-CA	8.43	125.55	120.24
1	1	336	ILE	N-CA-C	-5.28	107.45	111.62
2	4	299	ILE	CB-CA-C	-5.14	108.90	114.35

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	4	255	ASP	Peptide
4	6	116	THR	Peptide
7	7	321	GLU	Peptide
12	A	465	TYR	Peptide
12	A	71	GLN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2411	0	1880	132	0
2	4	2041	0	1954	120	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	0	6108	0	6168	433	0
4	6	2527	0	2322	187	0
5	2	3011	0	2600	184	0
6	5	498	0	506	49	0
7	7	4447	0	3905	440	0
8	3	860	0	622	34	0
9	O	1416	0	1493	79	0
10	N	1178	0	642	52	0
11	T	1159	0	652	17	0
12	A	10997	0	11081	434	0
13	B	9132	0	9146	346	0
14	C	2061	0	2029	63	0
15	D	1253	0	1275	67	0
16	E	1744	0	1772	83	0
17	F	670	0	690	21	0
18	G	1340	0	1357	79	0
19	H	1089	0	1062	58	0
20	I	944	0	899	45	0
21	J	532	0	542	34	0
22	K	904	0	911	34	0
23	L	358	0	381	29	0
24	M	2175	0	2283	98	0
25	Q	1144	0	1034	65	0
26	R	1303	0	1110	60	0
27	U	366	0	372	41	0
28	V	389	0	394	31	0
29	W	1469	0	1432	78	0
30	X	984	0	722	27	0
31	3	2	0	0	0	0
31	4	1	0	0	0	0
31	6	4	0	0	0	0
31	A	3	0	0	0	0
31	B	1	0	0	0	0
31	C	1	0	0	0	0
31	I	2	0	0	0	0
31	J	1	0	0	0	0
31	L	1	0	0	0	0
31	M	1	0	0	0	0
31	W	1	0	0	0	0
31	X	1	0	0	0	0
32	0	8	0	0	3	0
33	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	64538	0	61236	3180	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 26.

The worst 5 of 3180 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)
3:0:133:CYS:HB2	32:0:801:SF4:S4	1.97	1.03
7:7:303:ARG:H	7:7:323:VAL:HG13	1.29	0.97
7:7:477:LEU:HA	7:7:482:TRP:HE1	1.36	0.91
7:7:592:GLN:HE22	7:7:747:ASN:HB3	1.38	0.89
7:7:234:VAL:H	7:7:316:PHE:H	1.20	0.88

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	1	256/542 (47%)	236 (92%)	18 (7%)	2 (1%)	16	52
2	4	279/338 (82%)	237 (85%)	42 (15%)	0	100	100
3	0	752/778 (97%)	677 (90%)	75 (10%)	0	100	100
4	6	336/461 (73%)	297 (88%)	37 (11%)	2 (1%)	21	57
5	2	456/513 (89%)	406 (89%)	50 (11%)	0	100	100
6	5	64/72 (89%)	54 (84%)	10 (16%)	0	100	100
7	7	630/843 (75%)	541 (86%)	89 (14%)	0	100	100
8	3	136/321 (42%)	122 (90%)	14 (10%)	0	100	100
9	O	178/240 (74%)	173 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	A	1386/1733 (80%)	1269 (92%)	115 (8%)	2 (0%)	48	81
13	B	1133/1224 (93%)	1057 (93%)	74 (6%)	2 (0%)	43	75
14	C	260/318 (82%)	243 (94%)	17 (6%)	0	100	100
15	D	153/221 (69%)	142 (93%)	11 (7%)	0	100	100
16	E	211/215 (98%)	205 (97%)	6 (3%)	0	100	100
17	F	81/155 (52%)	78 (96%)	3 (4%)	0	100	100
18	G	169/171 (99%)	156 (92%)	13 (8%)	0	100	100
19	H	132/146 (90%)	118 (89%)	13 (10%)	1 (1%)	16	52
20	I	114/122 (93%)	101 (89%)	13 (11%)	0	100	100
21	J	63/70 (90%)	54 (86%)	9 (14%)	0	100	100
22	K	110/120 (92%)	105 (96%)	5 (4%)	0	100	100
23	L	43/70 (61%)	33 (77%)	10 (23%)	0	100	100
24	M	273/345 (79%)	243 (89%)	30 (11%)	0	100	100
25	Q	140/735 (19%)	130 (93%)	10 (7%)	0	100	100
26	R	176/400 (44%)	167 (95%)	9 (5%)	0	100	100
27	U	42/286 (15%)	38 (90%)	4 (10%)	0	100	100
28	V	46/122 (38%)	44 (96%)	2 (4%)	0	100	100
29	W	189/482 (39%)	183 (97%)	6 (3%)	0	100	100
30	X	152/328 (46%)	139 (91%)	12 (8%)	1 (1%)	18	54
All	All	7960/11371 (70%)	7248 (91%)	702 (9%)	10 (0%)	49	81

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	6	411	PRO
13	B	364	ILE
1	1	230	PRO
4	6	425	SER
13	B	363	HIS

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	1	169/395 (43%)	151 (89%)	18 (11%)	6	24
2	4	198/298 (66%)	169 (85%)	29 (15%)	3	16
3	0	686/707 (97%)	601 (88%)	85 (12%)	4	20
4	6	247/406 (61%)	201 (81%)	46 (19%)	1	11
5	2	258/468 (55%)	212 (82%)	46 (18%)	2	12
6	5	53/66 (80%)	40 (76%)	13 (24%)	1	5
7	7	414/737 (56%)	316 (76%)	98 (24%)	1	5
8	3	53/303 (18%)	49 (92%)	4 (8%)	12	36
9	O	152/205 (74%)	145 (95%)	7 (5%)	24	47
12	A	1221/1520 (80%)	1085 (89%)	136 (11%)	6	23
13	B	995/1061 (94%)	890 (89%)	105 (11%)	6	24
14	C	230/274 (84%)	208 (90%)	22 (10%)	8	28
15	D	139/200 (70%)	120 (86%)	19 (14%)	3	17
16	E	195/197 (99%)	174 (89%)	21 (11%)	6	24
17	F	73/137 (53%)	67 (92%)	6 (8%)	10	34
18	G	152/152 (100%)	140 (92%)	12 (8%)	11	35
19	H	119/128 (93%)	102 (86%)	17 (14%)	3	17
20	I	110/116 (95%)	101 (92%)	9 (8%)	10	34
21	J	60/65 (92%)	52 (87%)	8 (13%)	4	18
22	K	97/102 (95%)	87 (90%)	10 (10%)	7	25
23	L	40/57 (70%)	31 (78%)	9 (22%)	1	6
24	M	245/299 (82%)	216 (88%)	29 (12%)	5	21
25	Q	109/641 (17%)	101 (93%)	8 (7%)	13	37
26	R	107/363 (30%)	97 (91%)	10 (9%)	8	29
27	U	40/260 (15%)	39 (98%)	1 (2%)	42	62
28	V	47/108 (44%)	43 (92%)	4 (8%)	10	33
29	W	155/429 (36%)	148 (96%)	7 (4%)	24	47
30	X	62/295 (21%)	61 (98%)	1 (2%)	55	70
All	All	6426/9989 (64%)	5646 (88%)	780 (12%)	7	21

5 of 780 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	A	1266	THR
13	B	1115	THR
12	A	1404	GLU
12	A	1256	GLU
13	B	555	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
15	D	34	GLN
24	M	127	GLN
16	E	63	ASN
20	I	90	GLN
30	X	199	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 20 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	SF4	0	801	3	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	SF4	0	801	3	-	-	0/6/5/5

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.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	0	801	SF4	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	393:UNK	C	465:UNK	N	84.64
1	1	355:UNK	C	368:UNK	N	13.08
1	1	519:UNK	C	537:GLU	N	12.00

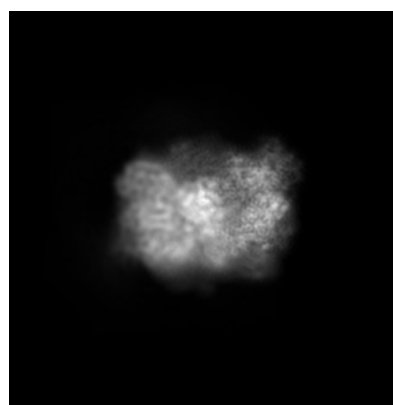
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23905. These allow visual inspection of the internal detail of the map and identification of artifacts.

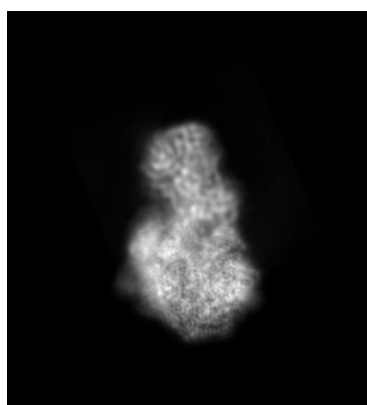
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

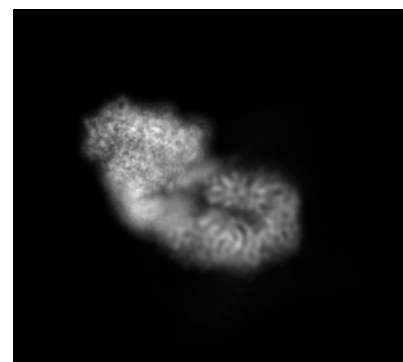
6.1.1 Primary map



X



Y

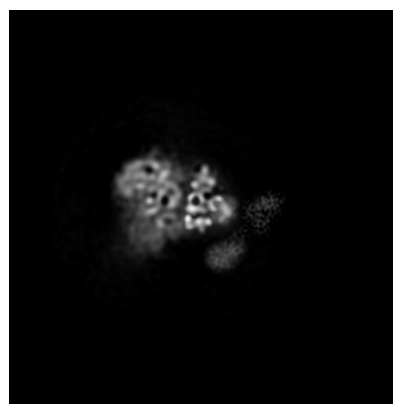


Z

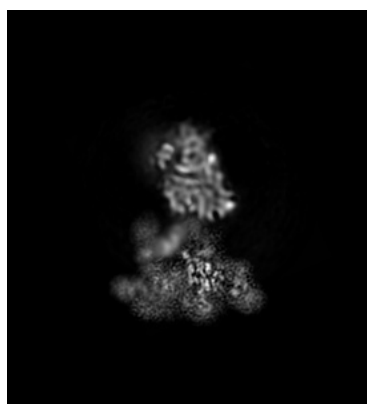
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

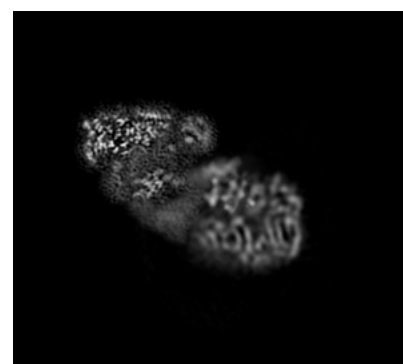
6.2.1 Primary map



X Index: 214



Y Index: 191

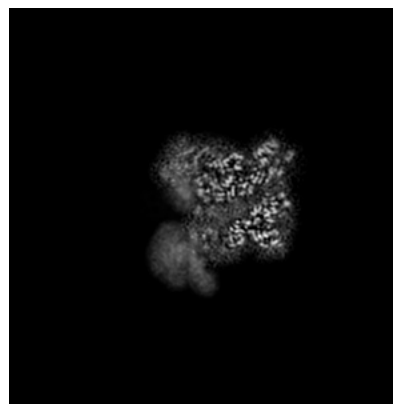


Z Index: 198

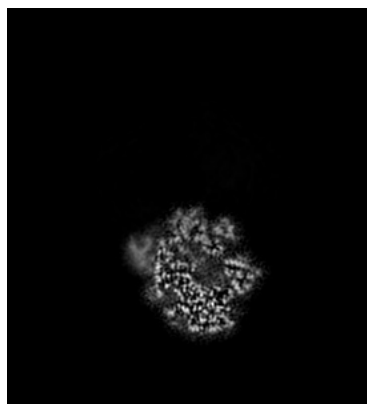
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

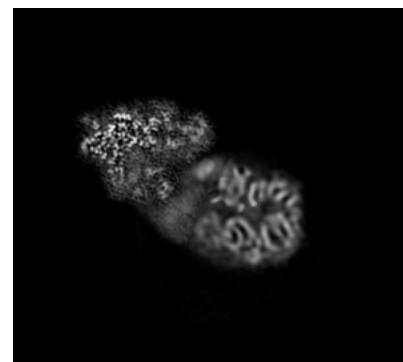
6.3.1 Primary map



X Index: 131



Y Index: 252

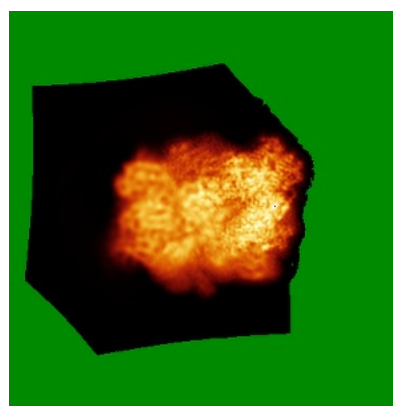


Z Index: 192

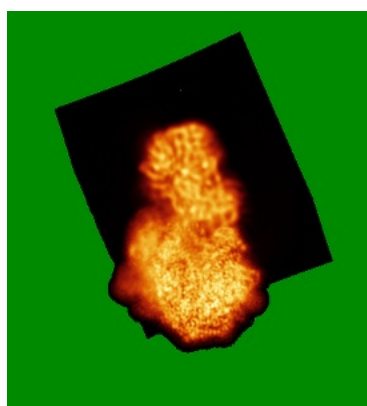
The images above show the largest variance slices of the map in three orthogonal directions.

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

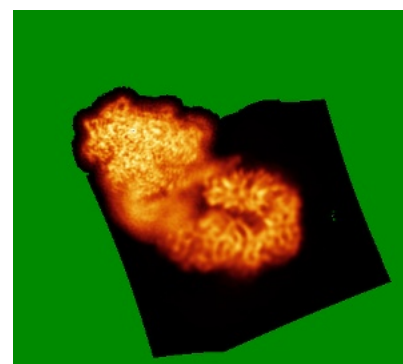
6.4.1 Primary map



X



Y

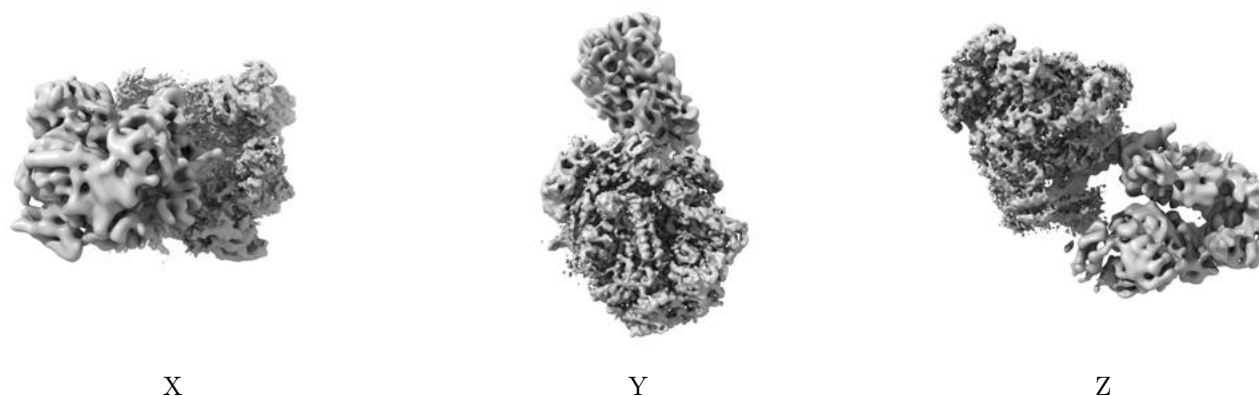


Z

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 0.0135. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

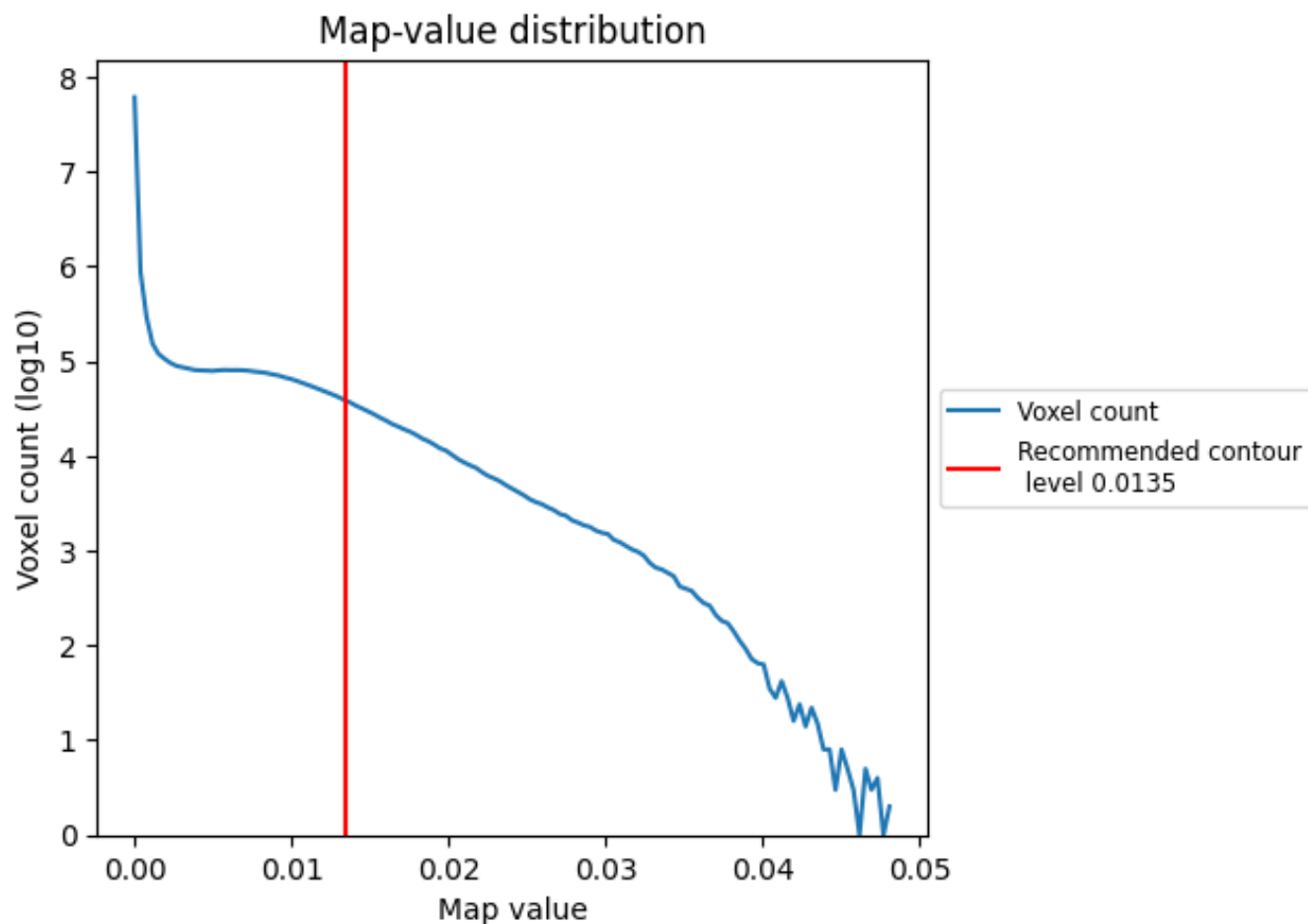
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

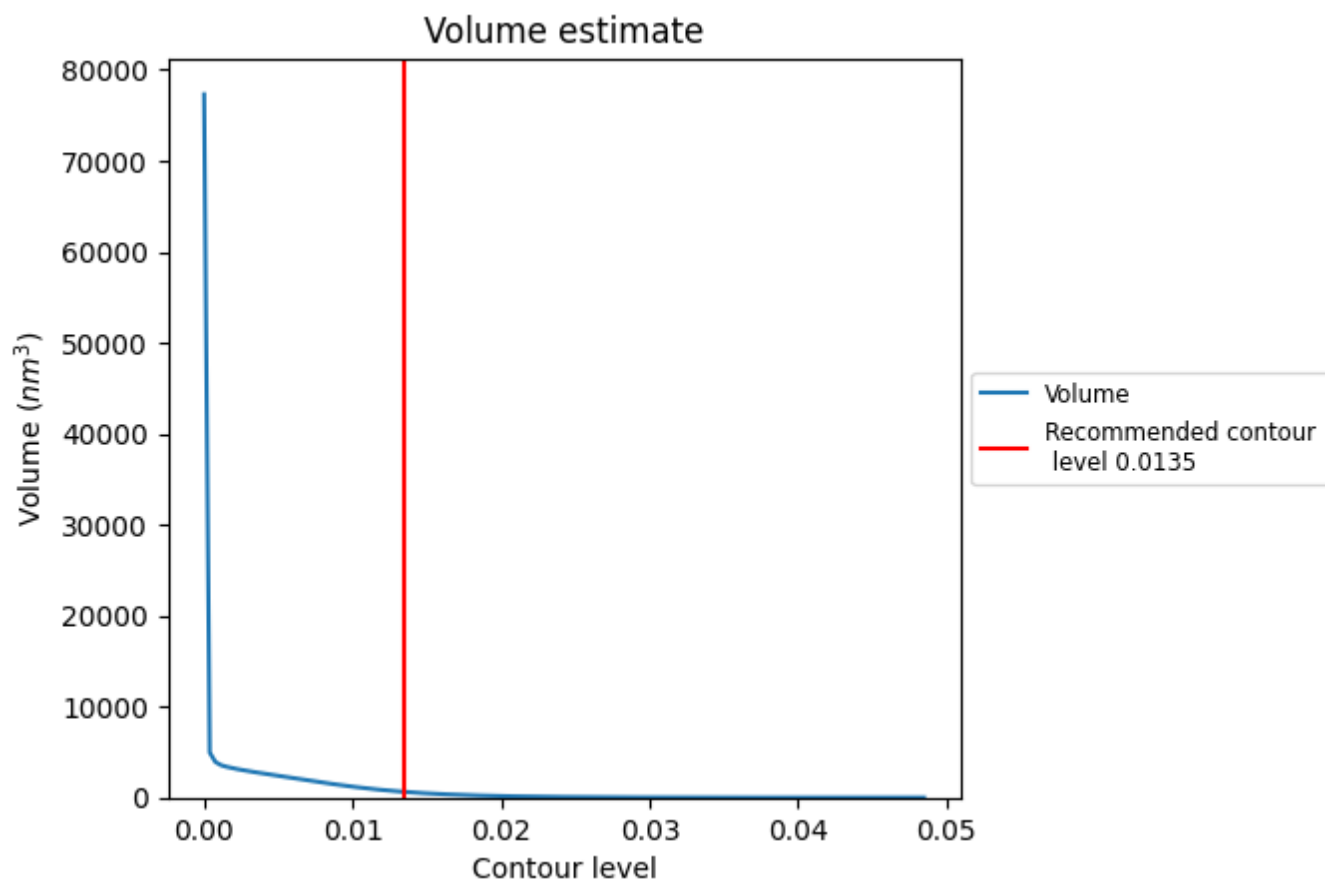
This section contains the results of statistical analysis of the map.

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 626 nm³; this corresponds to an approximate mass of 565 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.

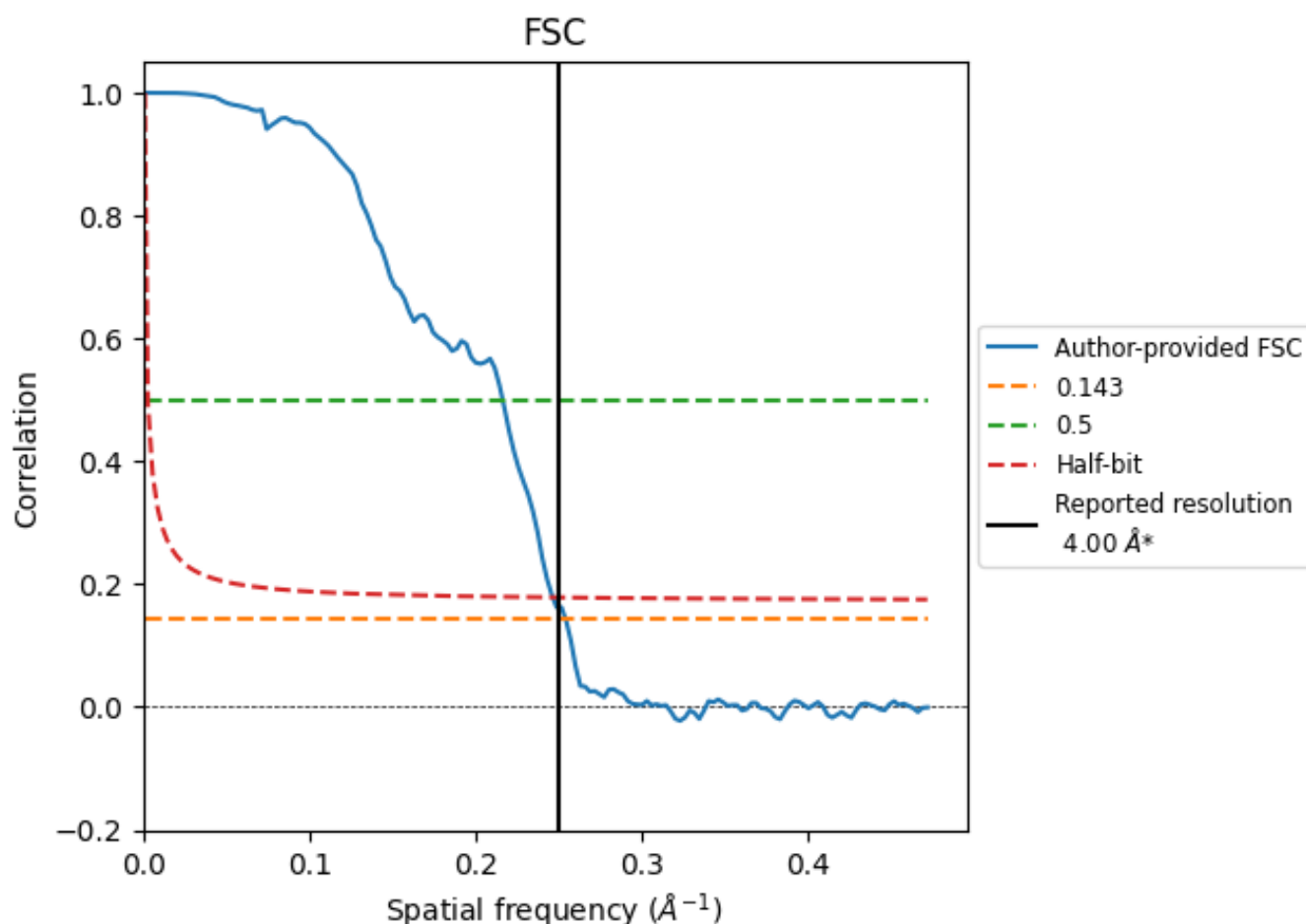
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.250 Å⁻¹

8.2 Resolution estimates [i](#)

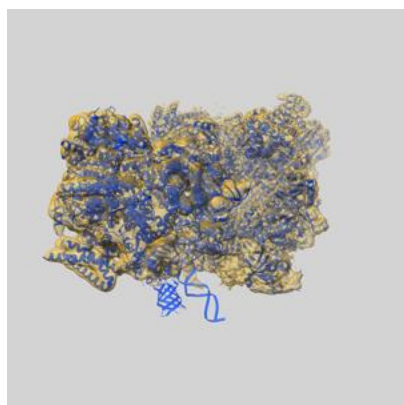
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.94	4.63	4.06
Unmasked-calculated*	-	-	-

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

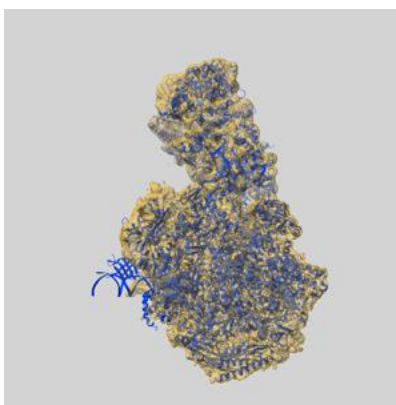
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23905 and PDB model 7ML1. Per-residue inclusion information can be found in section [3](#) on page [11](#).

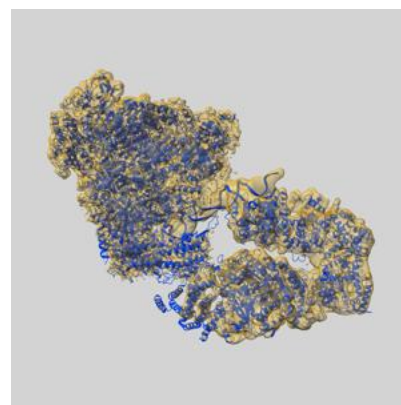
9.1 Map-model overlay [i](#)



X



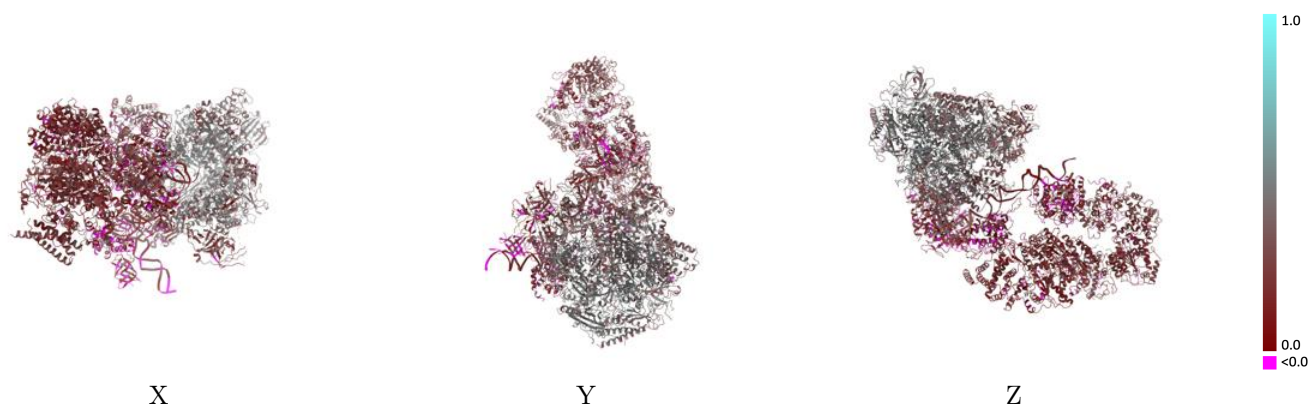
Y



Z

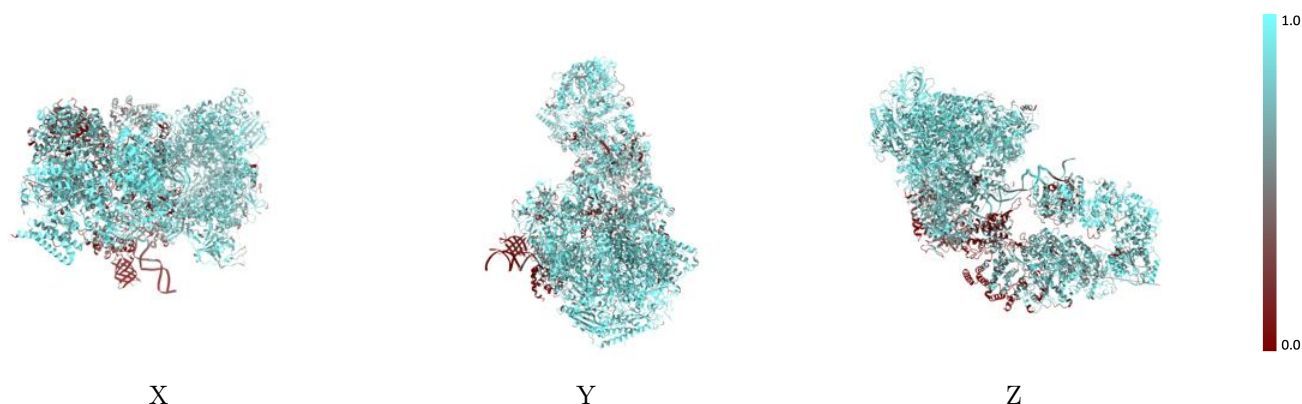
The images above show the 3D surface view of the map at the recommended contour level 0.0135 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



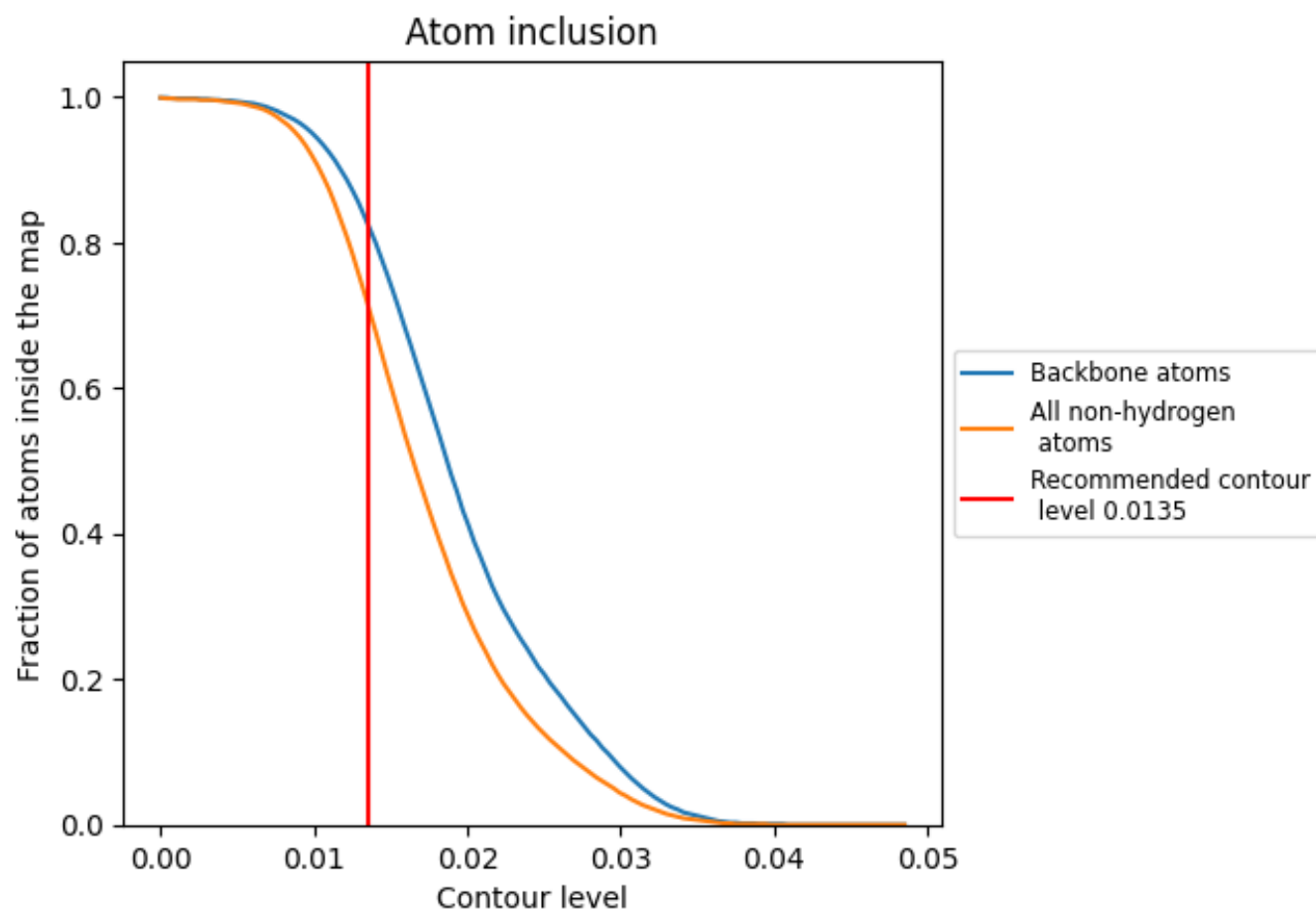
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0135).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 72% 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 (0.0135) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7160	 0.2910
0	 0.6340	 0.1760
1	 0.6450	 0.2160
2	 0.8020	 0.1990
3	 0.0820	 0.1450
4	 0.7700	 0.1940
5	 0.7150	 0.1830
6	 0.7740	 0.2030
7	 0.7140	 0.1470
A	 0.8460	 0.4220
B	 0.8510	 0.4330
C	 0.8900	 0.4570
D	 0.5210	 0.2800
E	 0.8380	 0.4000
F	 0.8800	 0.4500
G	 0.7240	 0.3180
H	 0.8460	 0.4070
I	 0.7490	 0.3410
J	 0.8670	 0.4430
K	 0.7820	 0.3930
L	 0.8010	 0.3570
M	 0.3860	 0.2450
N	 0.6130	 0.1410
O	 0.3700	 0.0900
Q	 0.7420	 0.2460
R	 0.6120	 0.2190
T	 0.6550	 0.1440
U	 0.0060	 0.0650
V	 0.0180	 0.0760
W	 0.4290	 0.1480
X	 0.4160	 0.1520

