wwPDB EM Validation Summary Report (i)

Nov 22, 2022 – 03:18 PM JST

PDB ID	:	7EMF
EMDB ID	:	EMD-31191
Title	:	Human Mediator (deletion of MED1-IDR) in a Tail-extended conformation
Authors	:	Yin, X.; Li, J.; Wu, Z.; Liu, W.; Xu, Y.
Deposited on	:	2021-04-13
Resolution	:	3.50 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*
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.

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

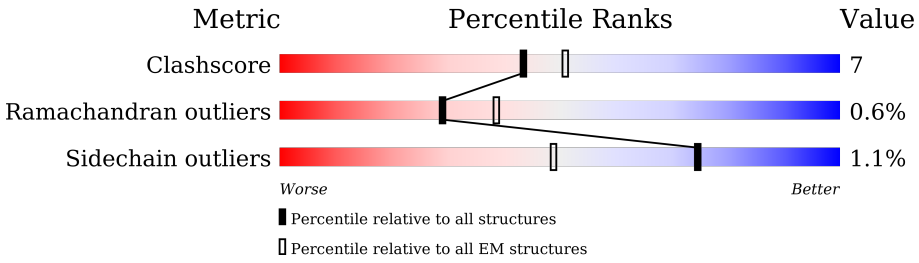
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.50 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.

Mol	Chain	Length	Quality of chain
1	A	1581	8% 24% 5% 70%
2	B	20	5% 100%
3	D	270	27% 49% 9% 41%
4	F	246	52% 50% 17% 32%
5	G	233	55% 54% 15% 31%
6	H	268	44% 59% 8% 32%
7	I	146	23% 42% 7% 50%
8	J	135	88% 82% 8% 10%

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Mol	Chain	Length	Quality of chain
9	K	117	25% 79% 17%
10	N	1454	10% 58% 11% 30%
11	O	788	16% 80%
12	P	841	73% 18% 9%
13	Q	651	15% 70% 14% 15%
14	R	208	8% 71% 21% 8%
15	S	244	31% 27% 69%
16	T	212	74% 17% 9%
17	U	144	58% 67% 15% 16%
18	V	200	10% 52% 12% 35%
19	W	1368	83% 14%
20	X	989	78% 13% 9%
21	Y	747	24% 72%
22	Z	600	13% 12% 84%
23	0	311	68% 16% 14%
24	1	178	48% 7% 44%
25	2	200	52% 5% 42%
26	3	178	60% 8% 31%
27	4	131	47% 66% 19% 14%

2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 62334 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 1.

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

- Molecule 2 is a protein called Unknown Chain (poly A).

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

- Molecule 3 is a protein called Mediator of RNA polymerase II transcription subunit 4.

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

- Molecule 4 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F	167	1374	888	238	243	5	0	0

- Molecule 5 is a protein called Mediator of RNA polymerase II transcription subunit 7.

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

- Molecule 6 is a protein called Isoform 2 of Mediator of RNA polymerase II transcription subunit 8.

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

- Molecule 7 is a protein called Mediator of RNA polymerase II transcription subunit 9.

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

- Molecule 8 is a protein called Mediator of RNA polymerase II transcription subunit 10.

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

- Molecule 9 is a protein called Mediator of RNA polymerase II transcription subunit 11.

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

- Molecule 10 is a protein called Mediator of RNA polymerase II transcription subunit 14.

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

- Molecule 11 is a protein called Mediator of RNA polymerase II transcription subunit 15.

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

- Molecule 12 is a protein called Isoform 2 of Mediator of RNA polymerase II transcription subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	766	Total	C	N	O	S	0	0
			5983	3816	1026	1092	49		

- Molecule 13 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	551	Total	C	N	O	S	0	0
			4361	2760	780	801	20		

- Molecule 14 is a protein called Mediator of RNA polymerase II transcription subunit 18.

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

- Molecule 15 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	75	Total	C	N	O	S	0	0
			476	295	85	94	2		

- Molecule 16 is a protein called Mediator of RNA polymerase II transcription subunit 20.

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

- Molecule 17 is a protein called Mediator of RNA polymerase II transcription subunit 21.

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

- Molecule 18 is a protein called Mediator of RNA polymerase II transcription subunit 22.

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

- Molecule 19 is a protein called Mediator of RNA polymerase II transcription subunit 23.

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

- Molecule 20 is a protein called Mediator of RNA polymerase II transcription subunit 24.

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

- Molecule 21 is a protein called Mediator of RNA polymerase II transcription subunit 25.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Y	210	Total	C	N	O	S	0	0
			1605	1030	264	302	9		

- Molecule 22 is a protein called Mediator of RNA polymerase II transcription subunit 26.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Z	97	Total	C	N	O	S	0	0
			765	472	136	154	3		

- Molecule 23 is a protein called Mediator of RNA polymerase II transcription subunit 27.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	0	267	Total	C	N	O	S	0	0
			2159	1373	384	390	12		

- Molecule 24 is a protein called Mediator of RNA polymerase II transcription subunit 28.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1	99	Total	C	N	O	S	0	0
			817	511	143	160	3		

- Molecule 25 is a protein called Mediator of RNA polymerase II transcription subunit 29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	2	115	Total	C	N	O	S	0	0
			899	563	155	172	9		

- Molecule 26 is a protein called Mediator of RNA polymerase II transcription subunit 30.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	3	122	Total	C	N	O	S	0	0
			1022	639	187	189	7		

- Molecule 27 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	4	113	Total	C	N	O	S	0	0
			986	642	171	168	5		

- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn).

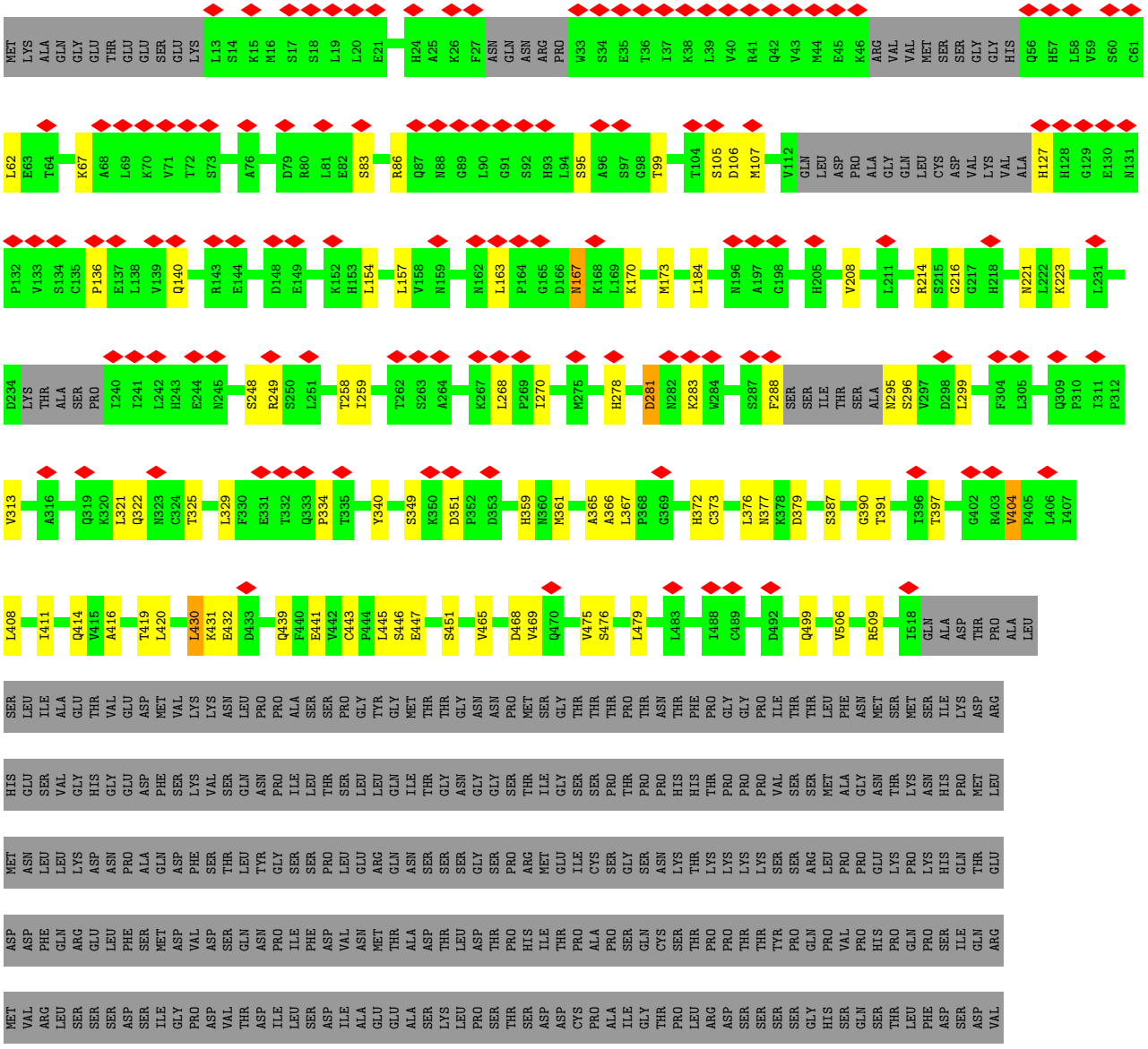
Mol	Chain	Residues	Atoms	AltConf
28	P	1	Total Zn 1 1	0
28	0	1	Total Zn 1 1	0

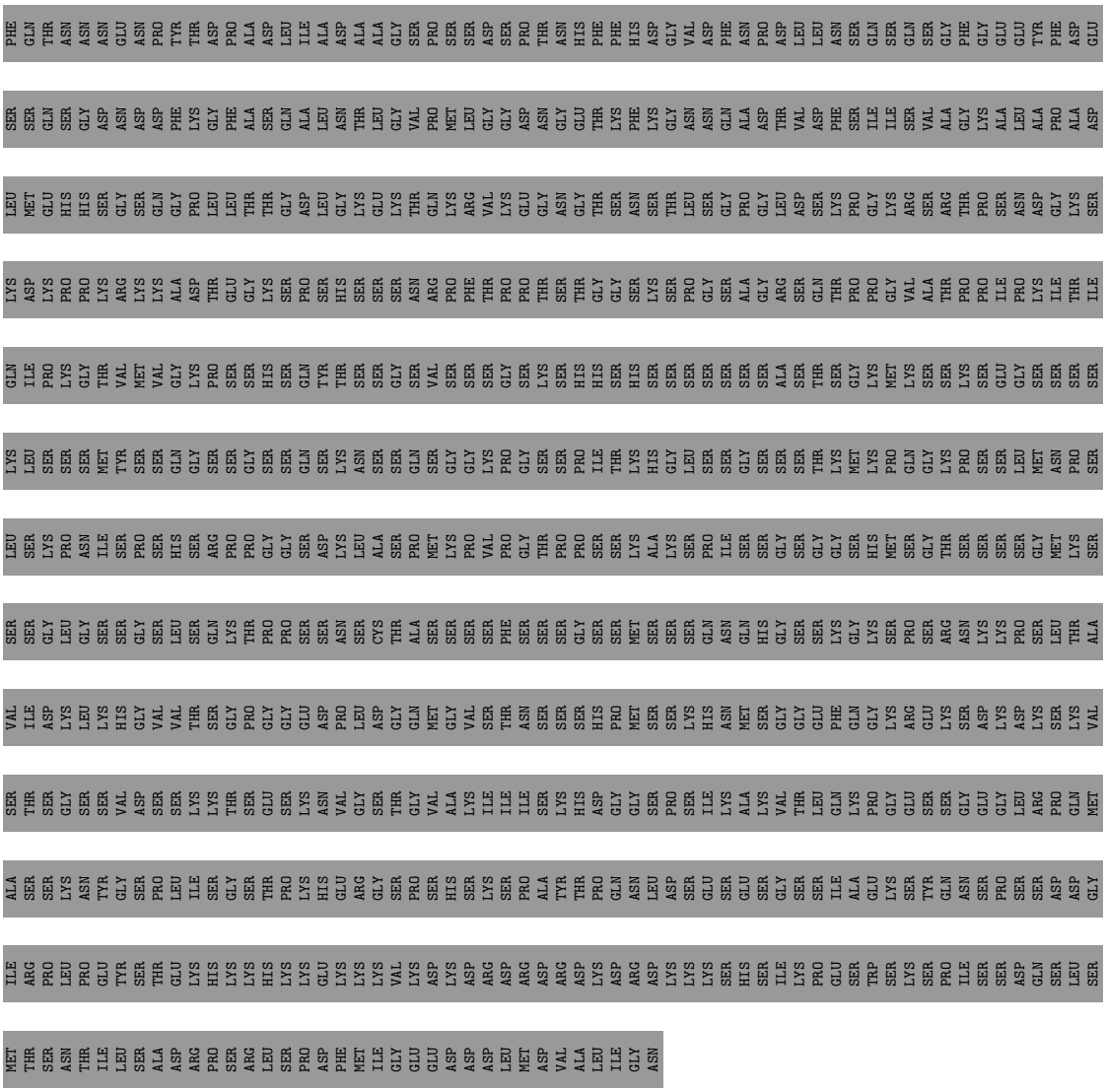
3 Residue-property plots (i)

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.

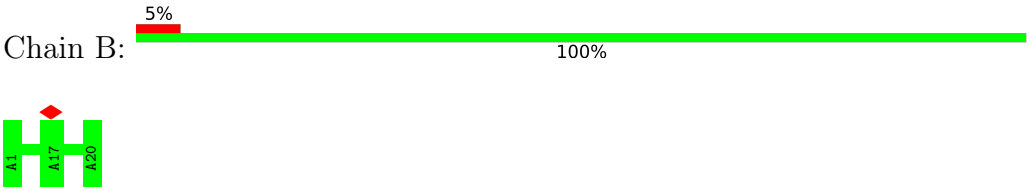
• Molecule 1: Mediator of RNA polymerase II transcription subunit 1

Chain A:

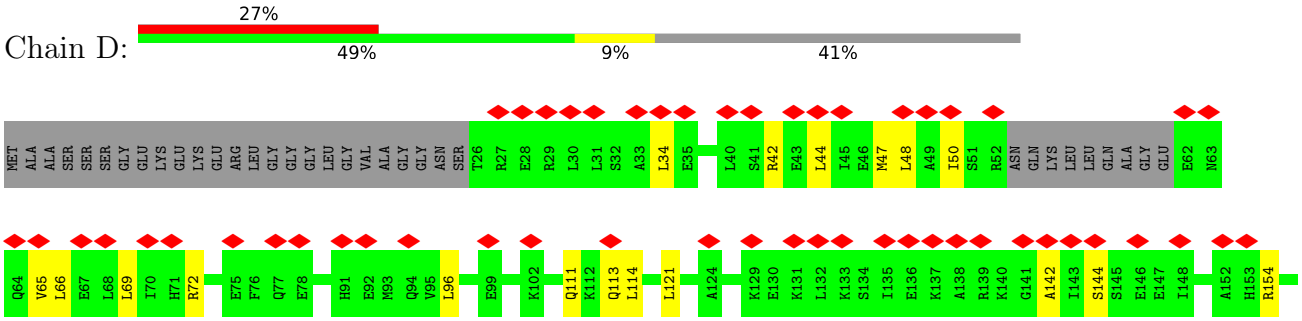


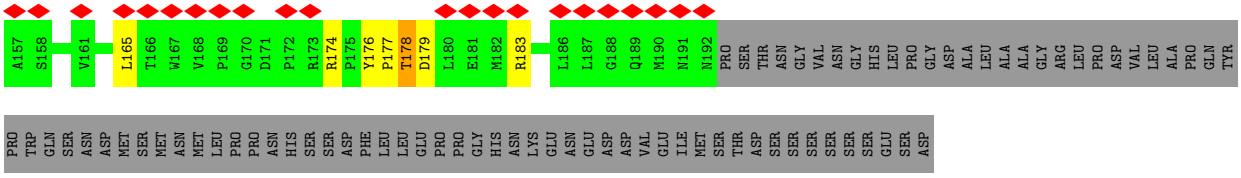


• Molecule 2: Unknown Chain (poly A)



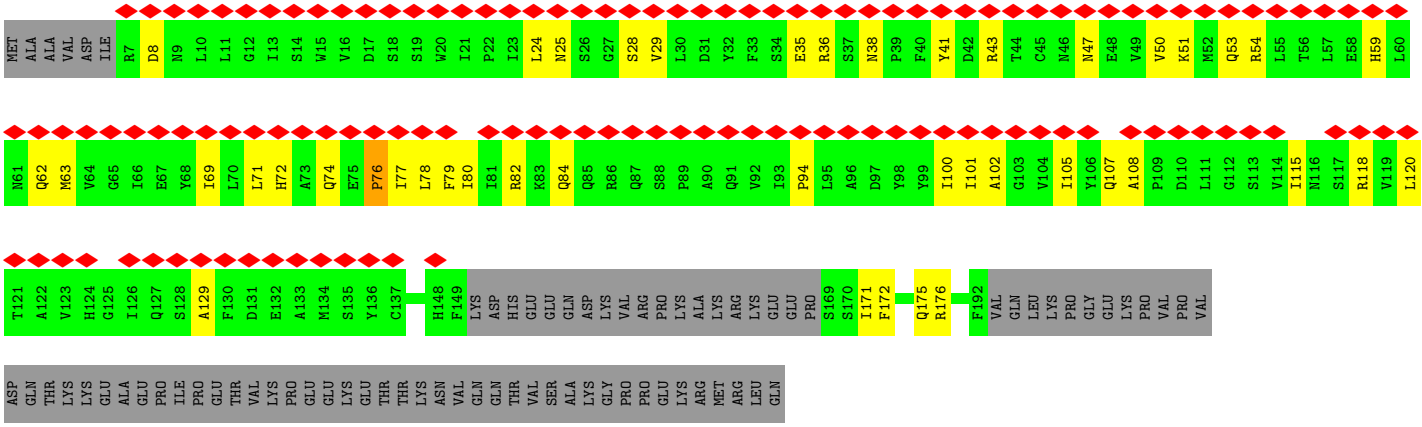
• Molecule 3: Mediator of RNA polymerase II transcription subunit 4





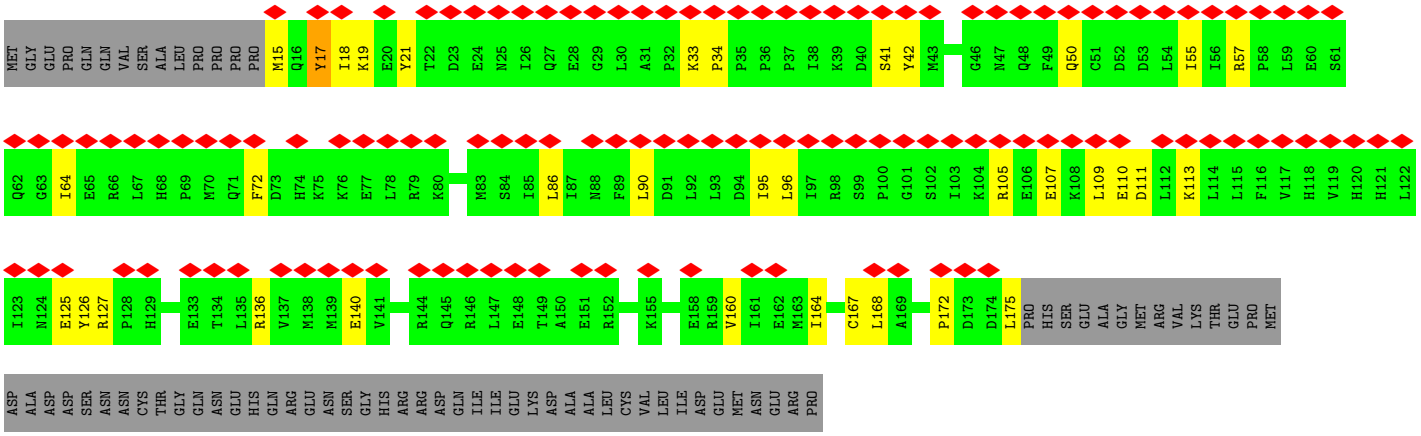
• Molecule 4: Mediator of RNA polymerase II transcription subunit 6

Chain F:



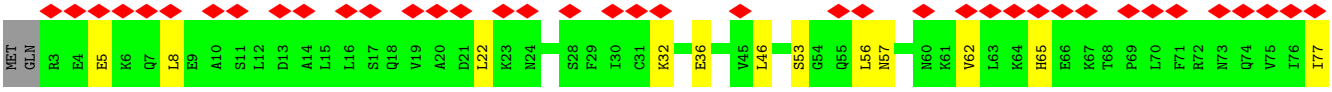
• Molecule 5: Mediator of RNA polymerase II transcription subunit 7

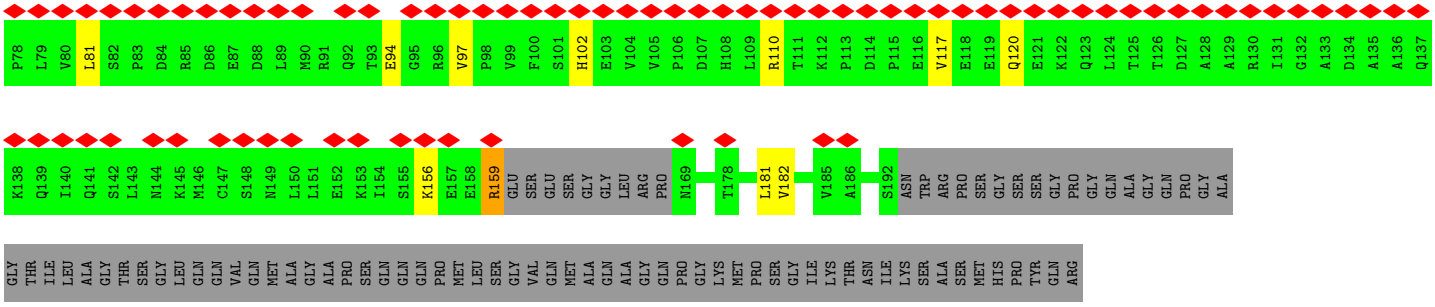
Chain G:



• Molecule 6: Isoform 2 of Mediator of RNA polymerase II transcription subunit 8

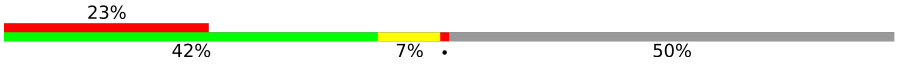
Chain H:

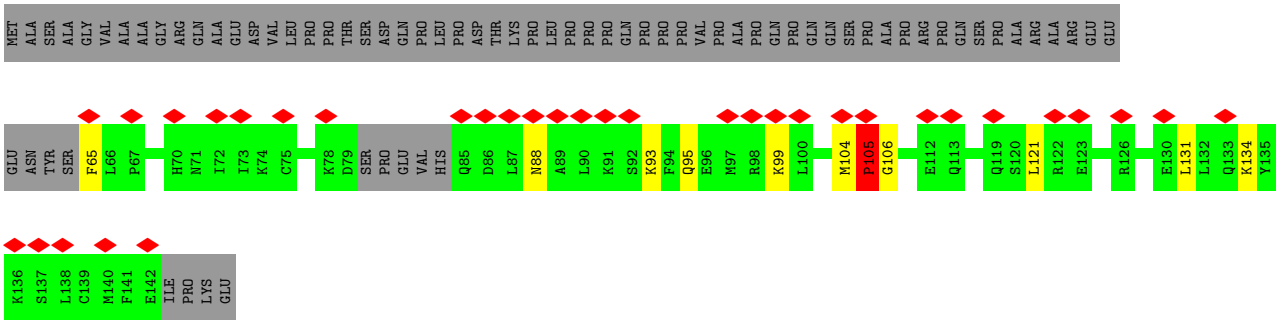




• Molecule 7: Mediator of RNA polymerase II transcription subunit 9

Chain I:



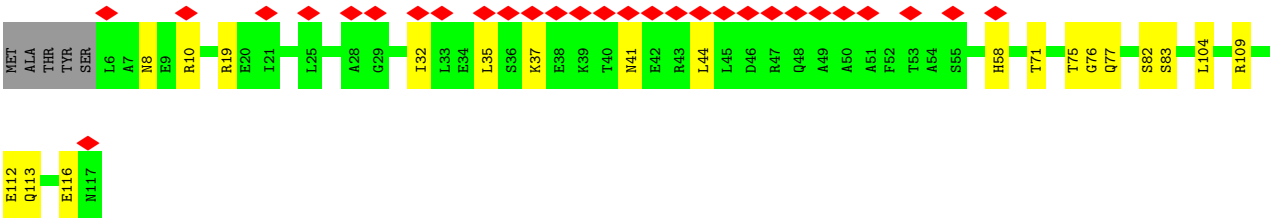


• Molecule 8: Mediator of RNA polymerase II transcription subunit 10

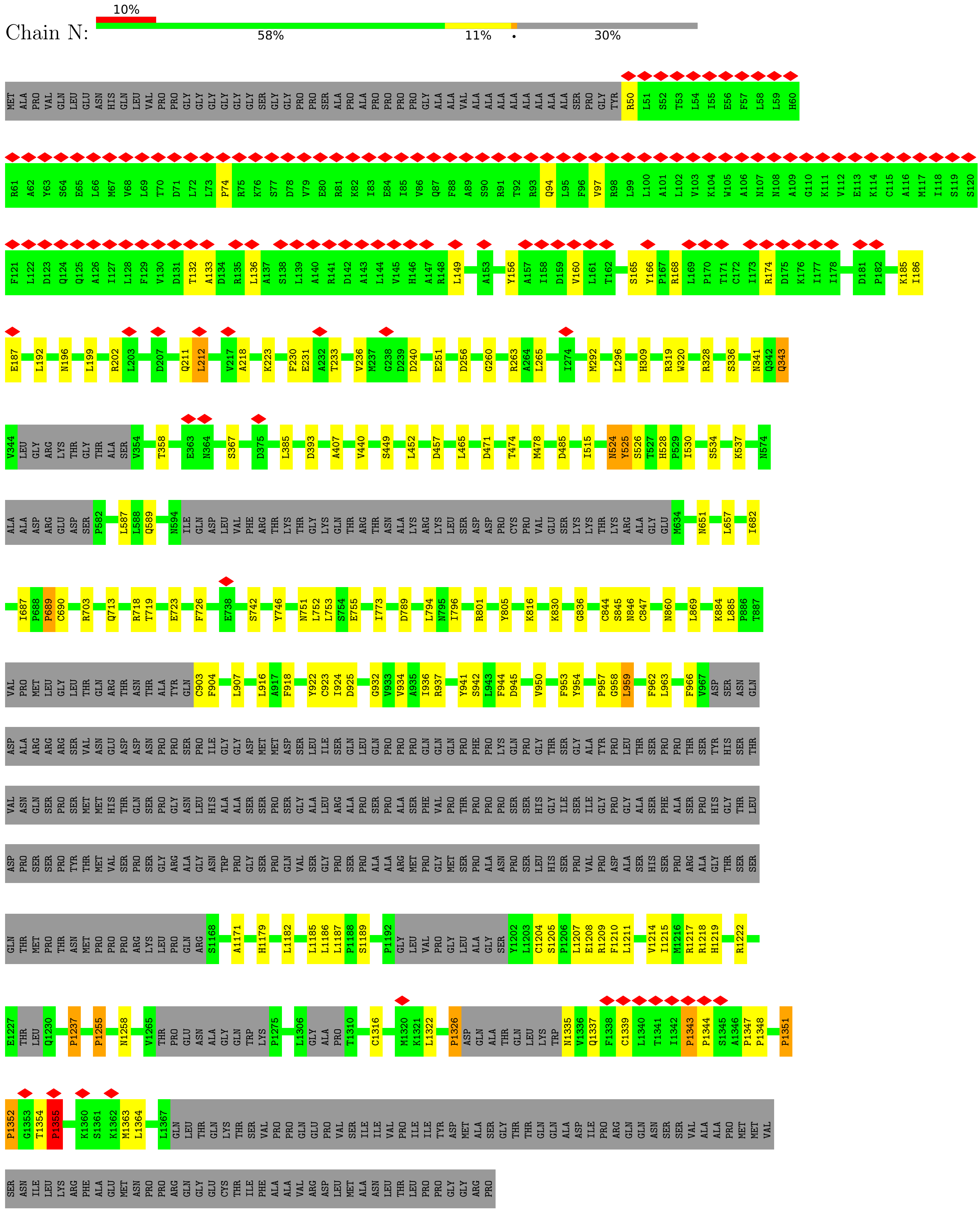
Chain J:

• Molecule 9: Mediator of RNA polymerase II transcription subunit 11

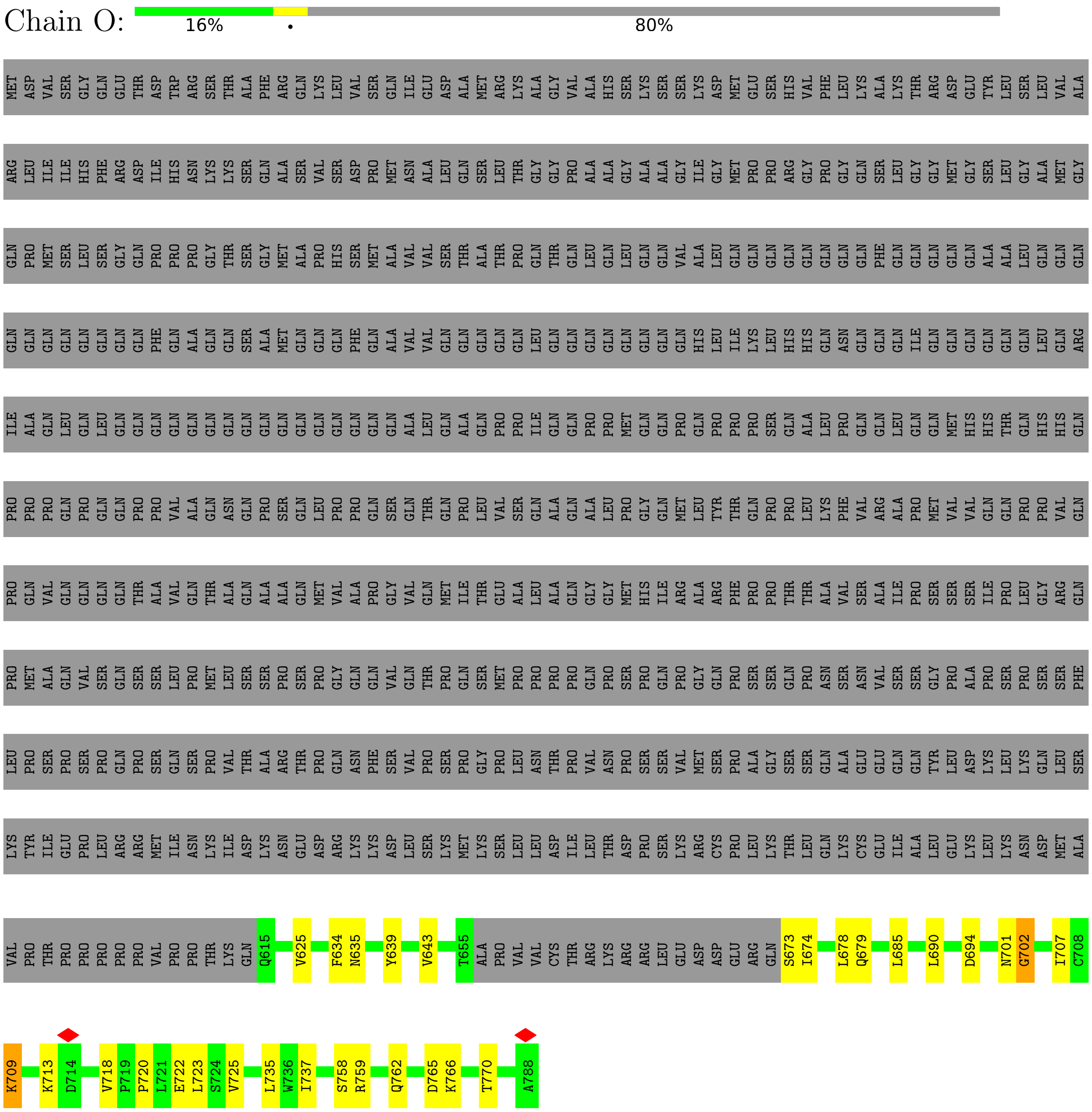
Chain K:



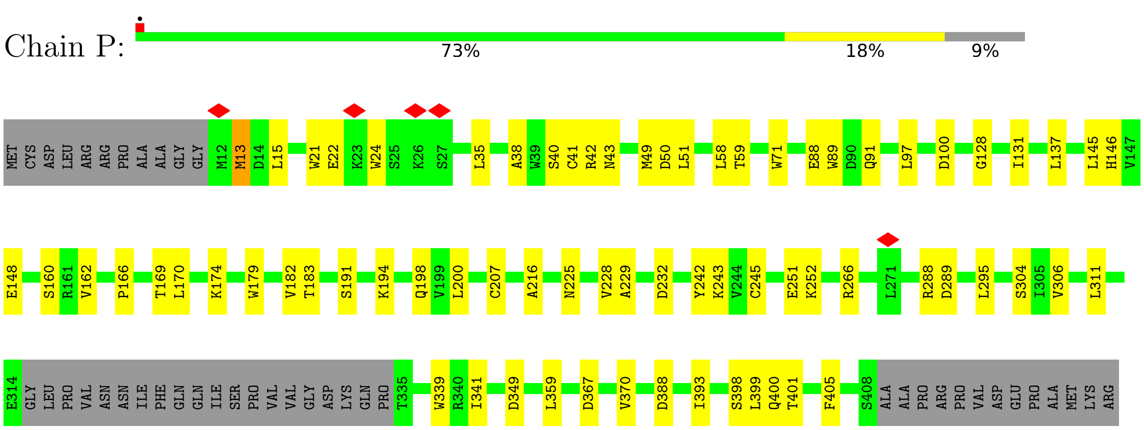
• Molecule 10: Mediator of RNA polymerase II transcription subunit 14

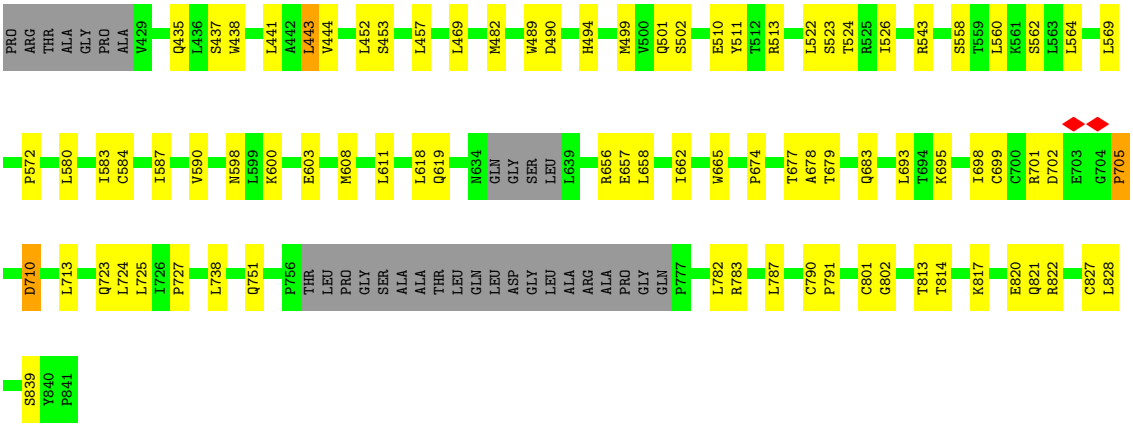

Chain N:
10%
58%
11%
30%
MET ALA PRO VAL GLN LEU GLU ASN HIS GLN LEU VAL PRO PRO GLY GLY GLY GLY GLY GLY SER GLY GLY PRO PRO SER ALA PRO ALA PRO PRO PRO PRO GLY ALA ALA VAL ALA ALA ALA ALA ALA ALA ALA ALA SER PRO GLY TYR R50 L51 S52 T53 L54 I55 E56 F57 L58 L59 H60
R61 A62 Y63 S64 E65 L66 M67 V68 L69 T70 D71 L72 L73 P74 R75 K76 S77 D78 V79 E80 R81 K82 I83 E84 I85 V86 Q87 F88 A89 S90 R91 T92 R93 Q94 L95 F96 V97 R98 L99 L100 A101 L102 V103 K104 W105 A106 N107 N108 A109 G110 K111 V112 E113 K114 C115 A116 M117 I118 S119 S120
F121 L122 D123 Q124 Q125 A126 I127 L128 F129 V130 D131 T132 A133 D134 R135 L136 A137 S138 L139 A140 R141 D142 A143 L144 V145 H146 A147 R148 L149 A153 Y156 A157 I158 D159 V160 L161 T162 S165 Y166 P167 R168 L169 P170 T171 C172 I173 R174 D175 K176 I177 I178 D181 P182 K185 I186
E187 L192 N196 L199 R202 L203 D207 Q211 L212 V217 A218 K223 F230 E231 A232 T233 V236 M237 G238 D239 D240 E251 D256 G260 R263 A264 L265 I274 M292 L296 H309 R319 W320 R328 S336 N341 Q342 Q343
V344 LEU GLY ARG LYS THR GLY THR ALA SER V354 T358 E363 N364 S367 D375 L385 D393 A407 V440 S449 L452 D457 L465 D471 T474 M478 D485 I515 N524 Y525 S526 T527 H528 P529 I530 S534 K537 N574
ALA ALA ASP ARG GLU ASP SER P582 L587 L588 Q589 N594 ILE GLN ASP LEU VAL PHE ARG THR LYS THR GLY LYS GLN THR ARG THR ASN ALA LYS ARG LYS LEU SER ASP ASP PRO CYS PRO VAL GLU SER LYS LYS THR LYS ARG ALA GLY GLU M634 N651 L657 I682
I687 P688 P689 C690 R703 Q713 R718 T719 E723 F726 E738 S742 Y746 N751 L752 L753 S754 E755 I773 D789 L794 N795 I796 R801 Y805 K816 K830 G836 C844 S845 N846 C847 N860 L869 K884 L885 P886 T887
VAL PRO MET LEU GLY LEU THR GLN ARG THR ASN THR ALA TYR GLN C903 F904 L907 L916 A917 F918 Y922 C923 I924 D925 G932 V933 V934 A935 I936 R937 Y941 S942 L943 F944 D945 V950 F953 Y954 P957 G958 L959 F962 L963 F966 V967 ASP SER ASN GLN
ASP ALA ARG ARG ARG SER VAL ASN GLU ASP ASP ASN PRO PRO SER PRO ILE GLY GLY ASP MET MET ASP SER LEU ILE SER GLN LEU GLN PRO PRO PRO GLN GLN GLN PRO PHE PRO LYS GLN PRO GLY THR SER GLY ALA TYR PRO LEU THR SER PRO PRO THR SER TYR HIS SER THR
VAL ASN GLN SER PRO SER MET MET HIS THR GLN SER PRO GLY ASN LEU HIS ALA ALA SER SER PRO SER GLY ALA LEU ARG ALA PRO SER PRO ALA SER PHE VAL PRO THR PRO PRO PRO SER SER HIS GLY ILE SER ILE GLY PRO GLY ALA SER PHE ALA SER PRO HIS GLY THR LEU
ASP PRO SER SER PRO TYR THR MET VAL SER PRO SER GLY ARG ALA GLY ASN TRP PRO GLY SER PRO GLN VAL SER GLY PRO SER PRO ALA ALA ARG MET PRO GLY MET SER PRO ALA ASN PRO SER LEU HIS SER PRO VAL PRO ASP ALA SER HIS SER PRO ARG ALA GLY THR SER SER
GLN THR MET PRO THR ASN MET PRO PRO PRO ARG LYS LEU PRO GLN ARG S1168 A1171 H1179 L1182 L1185 L1186 L1187 P1188 S1189 P1192 GLY LEU VAL PRO GLY LEU ALA GLY SER Y1202 L1203 C1204 S1205 P1206 L1207 E1208 R1209 F1210 L1211 V1214 I1215 M1216 R1217 R1218 H1219 R1222
E1227 THR LEU Q1230 P1237 P1255 N1258 V1265 THR PRO GLU ASN ALA GLY GLN TRP LYS P1275 L1306 GLY ALA PRO T1310 C1316 M1320 K1321 L1322 P1326 ASP GLN ALA THR GLN LEU LYS TRP N1335 V1336 Q1337 F1338 C1339 L1340 T1341 I1342 P1343 P1344 S1345 A1346 P1347 P1348 P1351
P1352 G1353 T1354 P1355 K1360 S1361 K1362 M1363 L1364 L1367 GLN LEU THR GLN LYS THR SER VAL PRO PRO GLN GLU PRO VAL SER ILE ILE VAL PRO ILE ILE TYR ASP MET ALA SER GLY THR THR GLN GLN ALA ASP ILE PRO ARG GLN GLN ASN SER SER VAL ALA ALA PRO MET MET VAL
SER ASN ILE LEU LYS ARG PHE ALA GLU MET ASN PRO PRO ARG GLN GLY GLU CYS THR ILE PHE ALA ALA VAL ARG ASP LEU MET ALA ASN LEU THR LEU PRO PRO GLY GLY ARG PRO

- Molecule 11: Mediator of RNA polymerase II transcription subunit 15



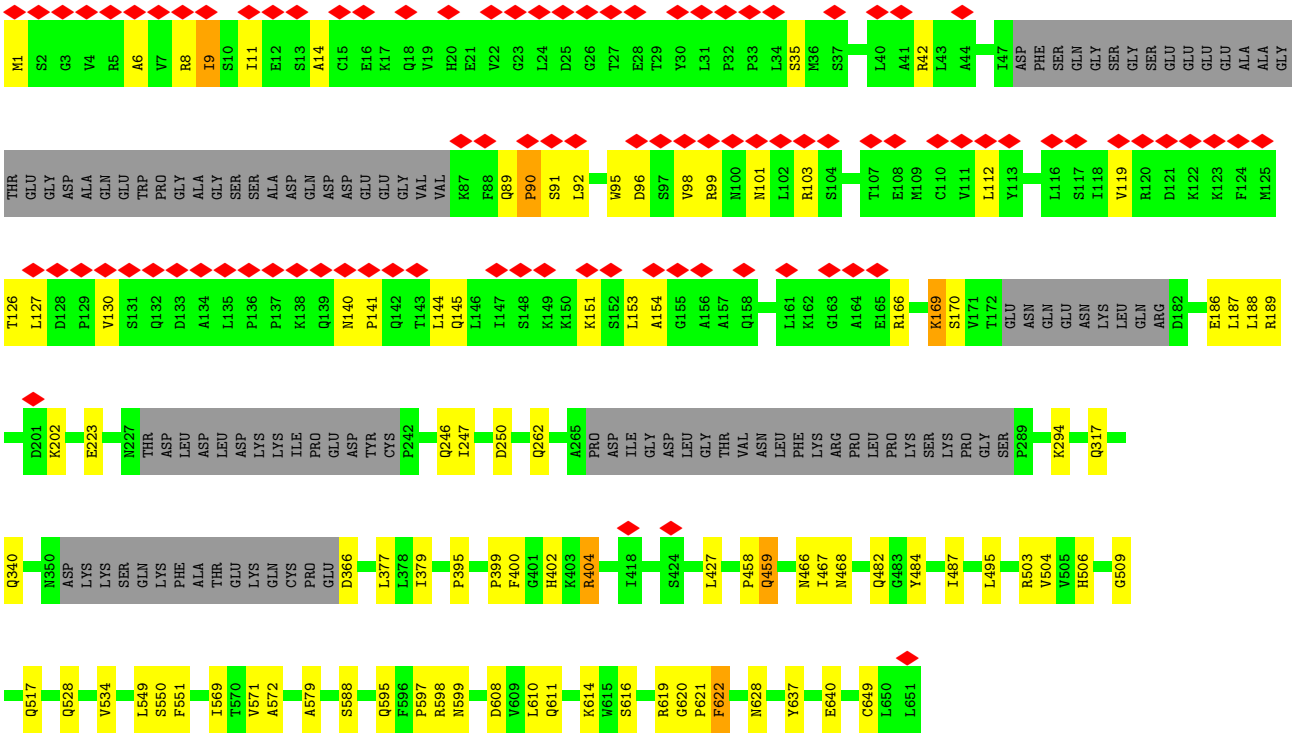
- Molecule 12: Isoform 2 of Mediator of RNA polymerase II transcription subunit 16





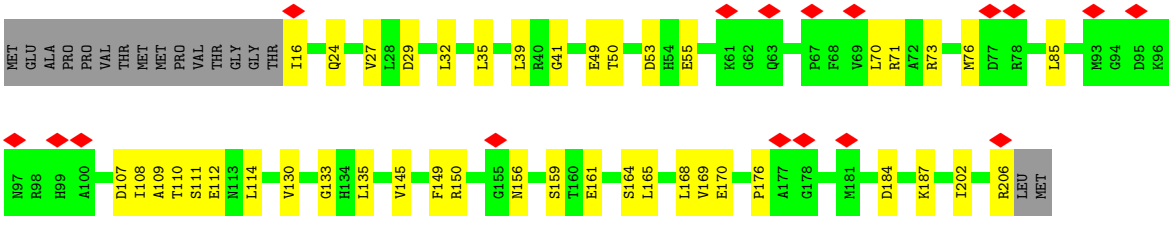
• Molecule 13: Mediator of RNA polymerase II transcription subunit 17

Chain Q:



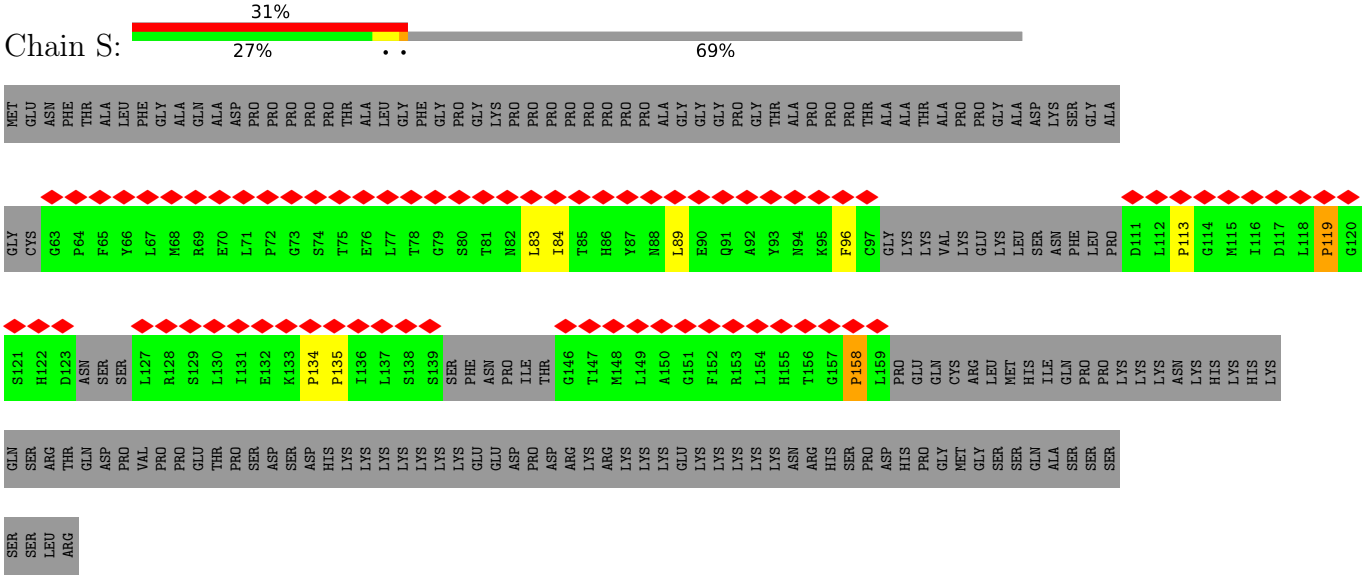
• Molecule 14: Mediator of RNA polymerase II transcription subunit 18

Chain R:



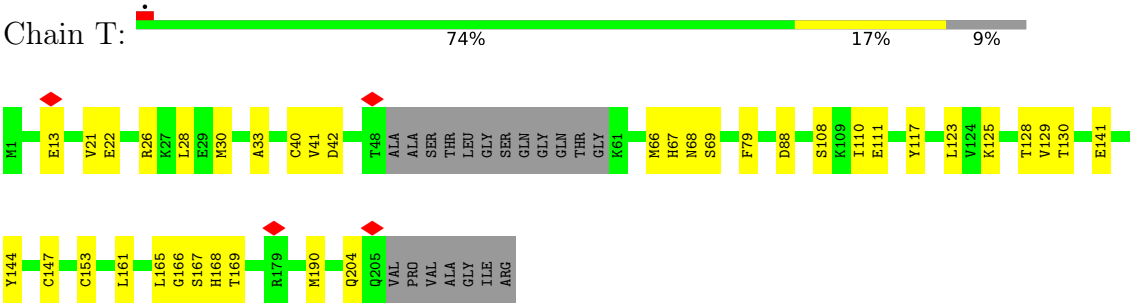
• Molecule 15: Mediator of RNA polymerase II transcription subunit 19

Chain S:



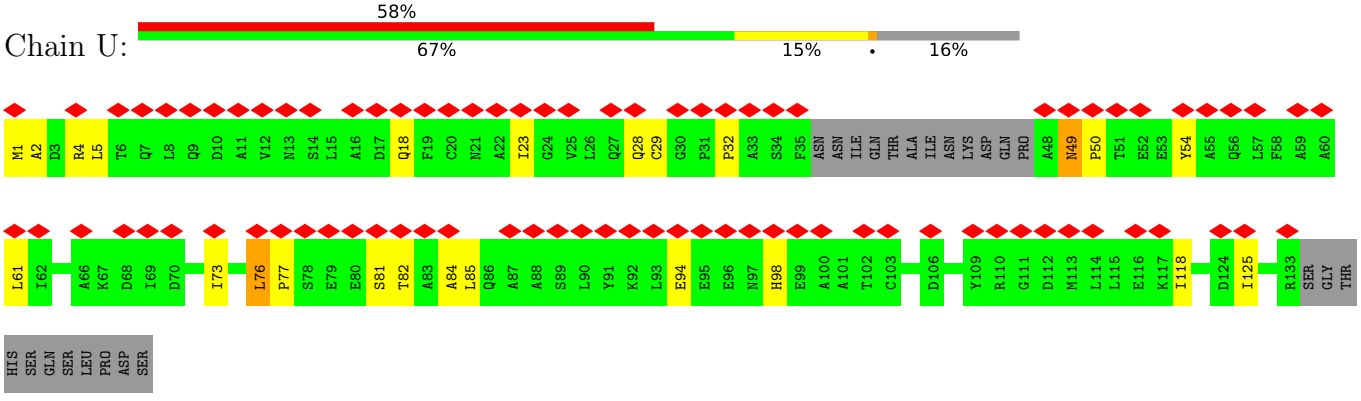
• Molecule 16: Mediator of RNA polymerase II transcription subunit 20

Chain T:



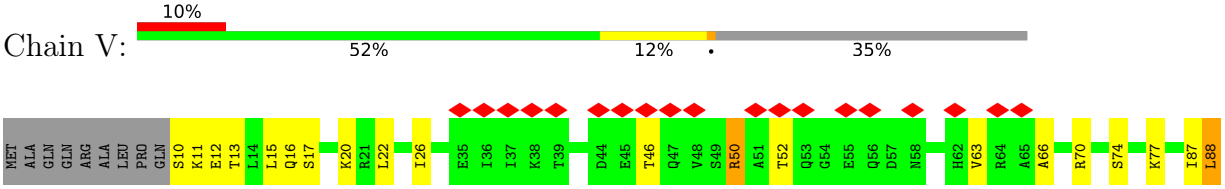
• Molecule 17: Mediator of RNA polymerase II transcription subunit 21

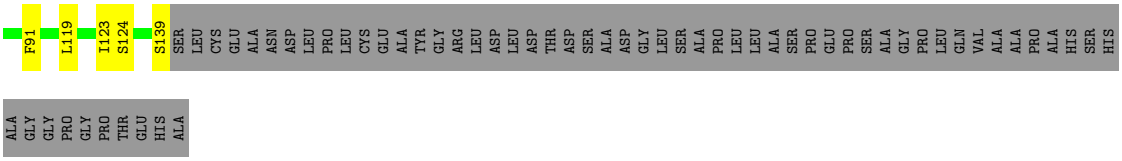
Chain U:



• Molecule 18: Mediator of RNA polymerase II transcription subunit 22

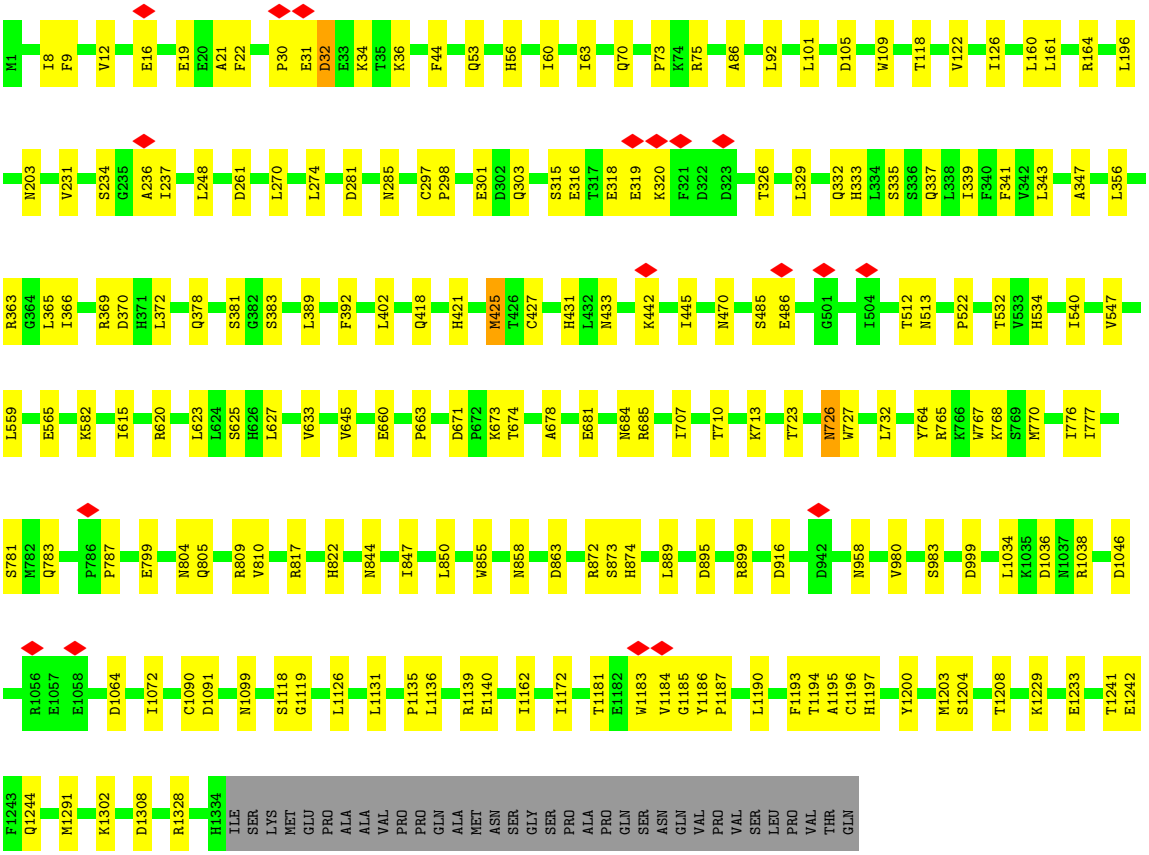
Chain V:





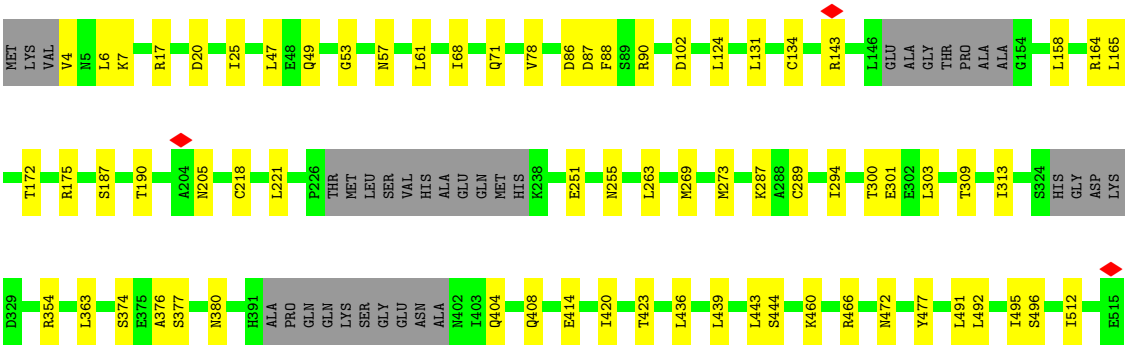
• Molecule 19: Mediator of RNA polymerase II transcription subunit 23

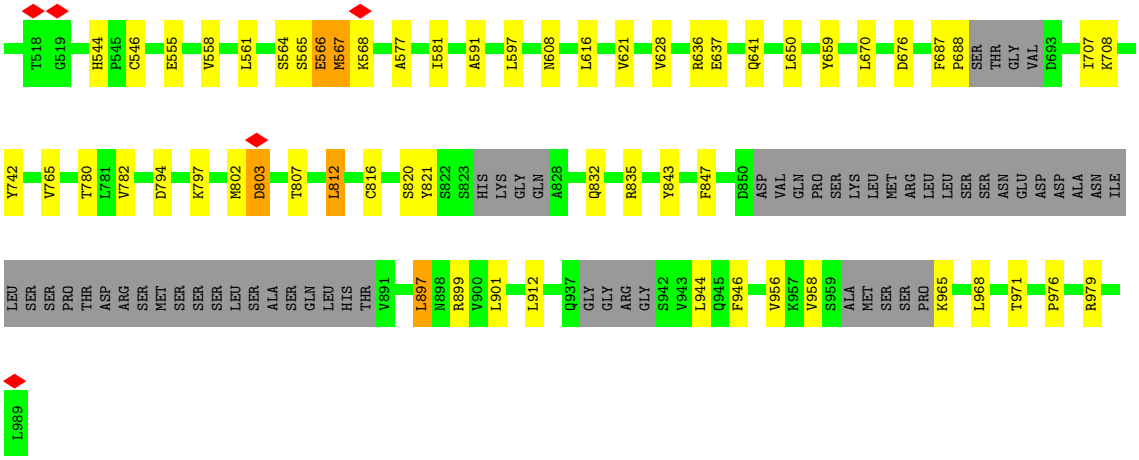
Chain W:



• Molecule 20: Mediator of RNA polymerase II transcription subunit 24

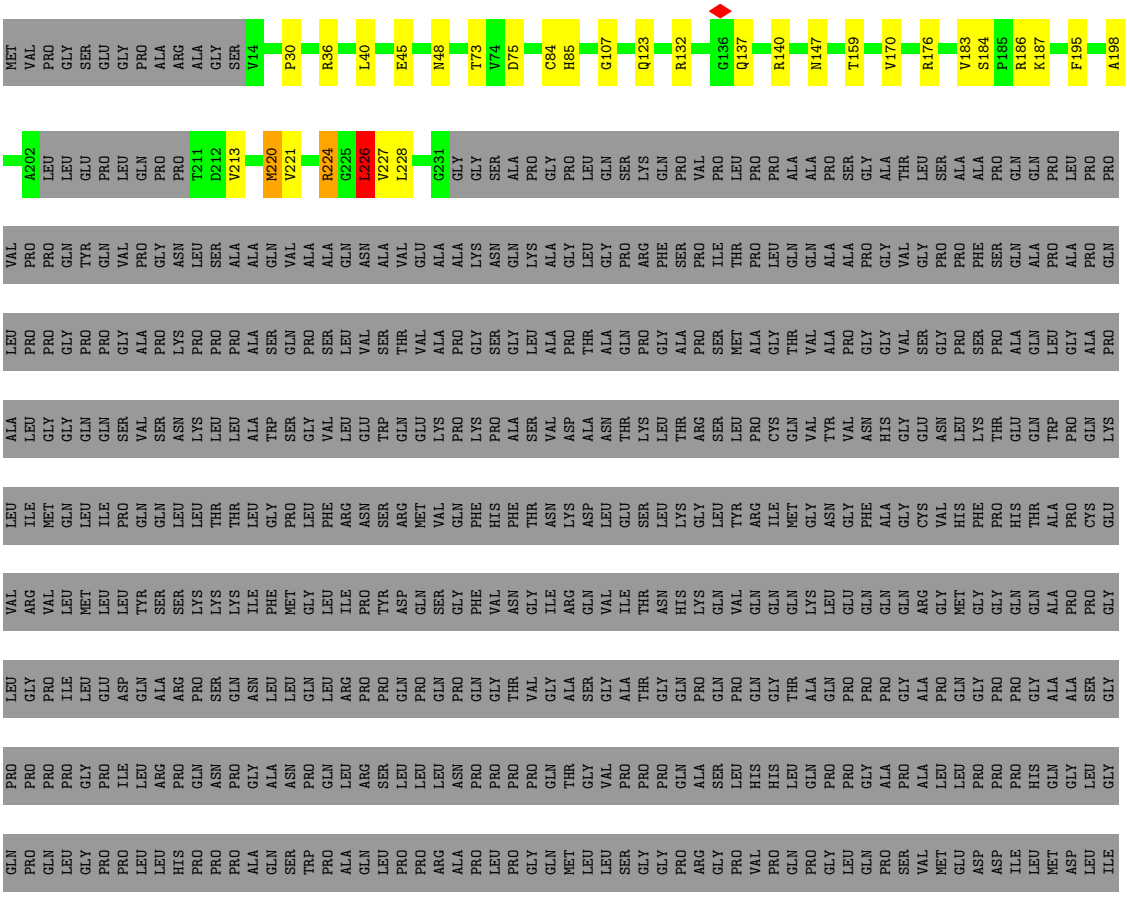
Chain X:





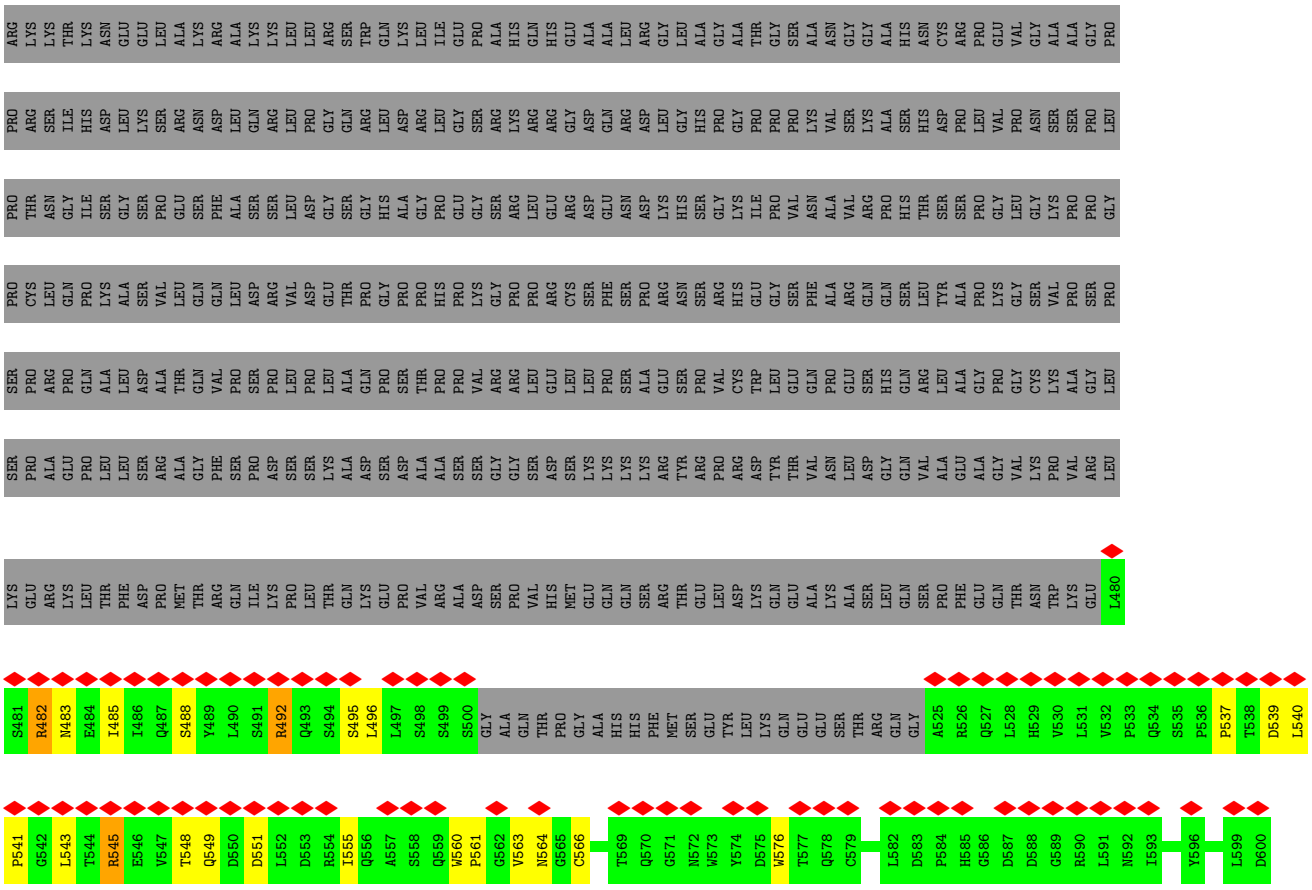
• Molecule 21: Mediator of RNA polymerase II transcription subunit 25

Chain Y: 24% 72%



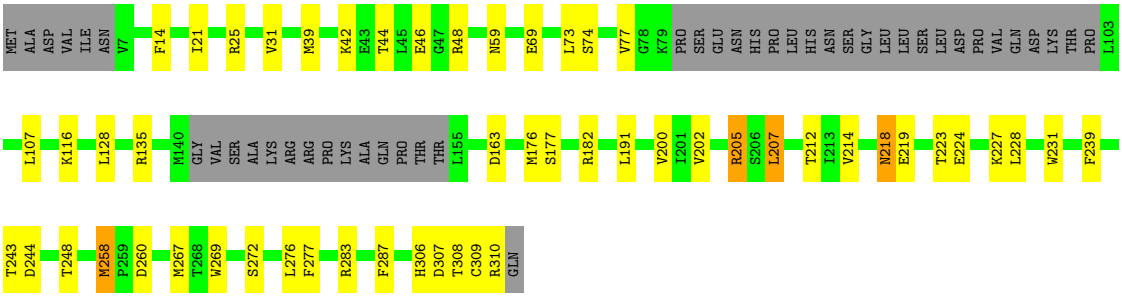
• Molecule 22: Mediator of RNA polymerase II transcription subunit 26

Chain Z: 13% 12% 84%



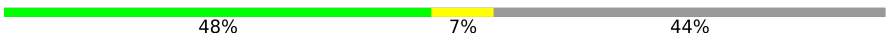
• Molecule 23: Mediator of RNA polymerase II transcription subunit 27

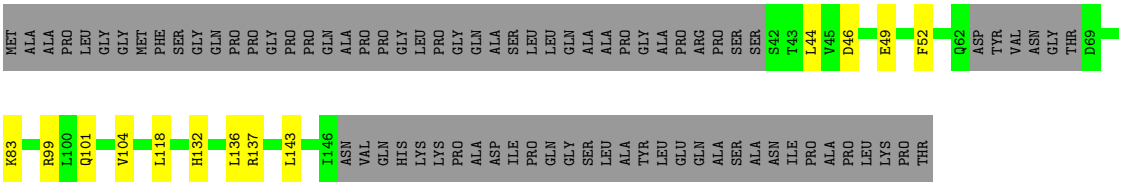
Chain 0:



• Molecule 24: Mediator of RNA polymerase II transcription subunit 28

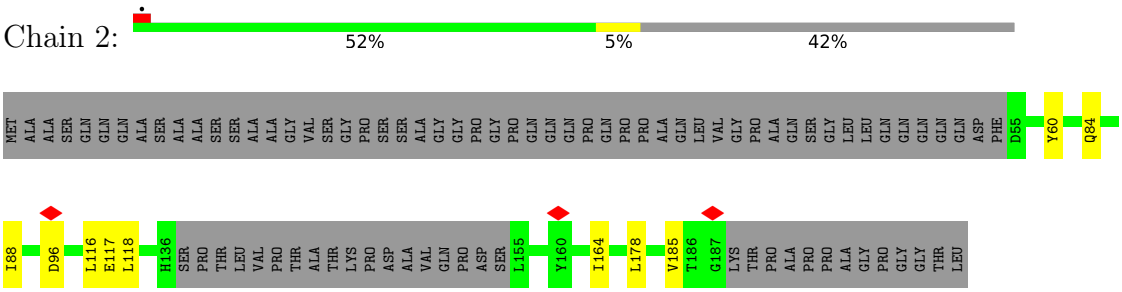
Chain 1:





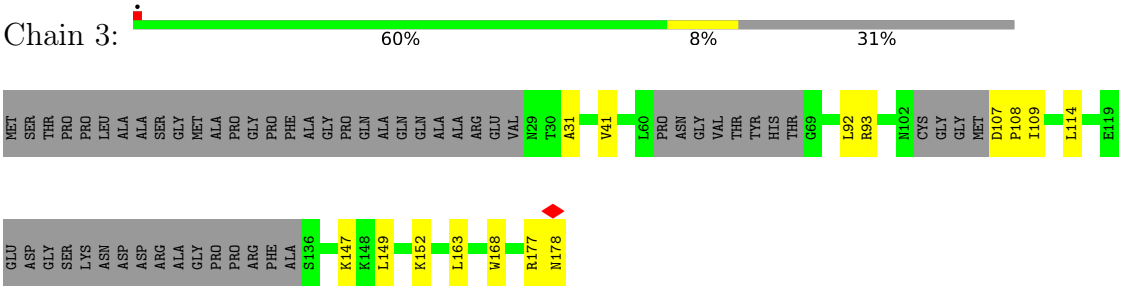
• Molecule 25: Mediator of RNA polymerase II transcription subunit 29

Chain 2:



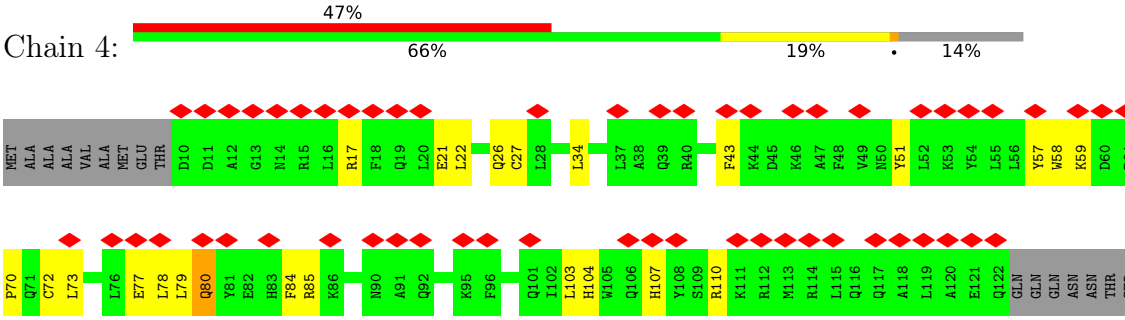
• Molecule 26: Mediator of RNA polymerase II transcription subunit 30

Chain 3:



• Molecule 27: Mediator of RNA polymerase II transcription subunit 31

Chain 4:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	95433	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 ($e^-/Å^2$)	50	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	0.114	Depositor
Minimum map value	-0.064	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	539.648, 539.648, 539.648	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.054, 1.054, 1.054	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

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	0.51	0/3653	0.62	0/4961
2	B	0.68	0/99	0.77	0/137
3	D	0.40	0/1281	0.56	0/1718
4	F	0.37	0/1411	0.63	0/1916
5	G	0.51	0/1374	0.61	0/1847
6	H	0.35	0/1441	0.56	0/1946
7	I	0.36	0/612	0.58	0/815
8	J	0.33	0/849	0.54	1/1150 (0.1%)
9	K	0.42	0/885	0.53	0/1190
10	N	0.50	0/7923	0.64	11/10761 (0.1%)
11	O	0.59	0/1261	0.69	0/1731
12	P	0.65	0/6116	0.69	0/8311
13	Q	0.52	0/4444	0.61	0/6000
14	R	0.49	0/1562	0.60	0/2101
15	S	0.37	0/480	0.74	5/651 (0.8%)
16	T	0.57	0/1530	0.64	0/2066
17	U	0.53	0/927	0.64	0/1257
18	V	0.56	0/1072	0.65	0/1440
19	W	0.56	0/11056	0.60	0/15023
20	X	0.58	0/7191	0.63	0/9728
21	Y	0.57	0/1645	0.64	0/2240
22	Z	0.51	0/781	0.64	0/1067
23	0	0.57	0/2201	0.60	0/2972
24	1	0.47	0/825	0.55	0/1107
25	2	0.47	0/911	0.56	0/1229
26	3	0.45	0/1029	0.54	0/1378
27	4	0.48	0/1013	0.61	0/1364
All	All	0.53	0/63572	0.62	17/86106 (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(^{o})	Ideal(^{o})
10	N	1351	PRO	N-CA-CB	7.37	112.14	103.30
10	N	1343	PRO	N-CA-CB	7.30	112.06	103.30
10	N	1355	PRO	N-CA-CB	6.88	111.56	103.30
8	J	31	PRO	N-CA-CB	6.61	111.23	103.30
10	N	1352	PRO	N-CA-CB	6.35	110.92	103.30

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	3578	0	3522	63	0
2	B	100	0	102	0	0
3	D	1268	0	1305	23	0
4	F	1374	0	1357	35	0
5	G	1348	0	1373	32	0
6	H	1422	0	1440	16	0
7	I	605	0	628	7	0
8	J	840	0	718	8	0
9	K	879	0	886	20	0
10	N	7772	0	7557	139	0
11	O	1226	0	1217	24	0
12	P	5983	0	6071	95	0
13	Q	4361	0	4445	71	0
14	R	1532	0	1542	25	0
15	S	476	0	347	3	0
16	T	1499	0	1484	24	0
17	U	918	0	905	26	0
18	V	1063	0	1051	25	0
19	W	10774	0	10838	130	0
20	X	7061	0	7223	84	0
21	Y	1605	0	1576	24	0
22	Z	765	0	728	16	0
23	0	2159	0	2176	45	0
24	1	817	0	818	13	0
25	2	899	0	908	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	3	1022	0	1054	14	0
27	4	986	0	965	27	0
28	0	1	0	0	0	0
28	P	1	0	0	0	0
All	All	62334	0	62236	874	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 7.

The worst 5 of 874 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:18:ILE:HD11	27:4:51:TYR:OH	1.35	1.26
10:N:922:TYR:CE2	10:N:1215:ILE:HD13	1.76	1.19
10:N:885:LEU:HD21	10:N:1186:LEU:HD22	1.31	1.10
10:N:962:PHE:HB2	10:N:1210:PHE:CE2	1.88	1.08
10:N:932:GLY:HA2	10:N:1179:HIS:CE1	1.90	1.06

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	455/1581 (29%)	429 (94%)	23 (5%)	3 (1%)	22 61
2	B	18/20 (90%)	18 (100%)	0	0	100 100
3	D	154/270 (57%)	150 (97%)	3 (2%)	1 (1%)	25 64
4	F	163/246 (66%)	153 (94%)	8 (5%)	2 (1%)	13 50
5	G	159/233 (68%)	151 (95%)	8 (5%)	0	100 100
6	H	177/268 (66%)	165 (93%)	12 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	I	69/146 (47%)	66 (96%)	1 (1%)	2 (3%)	4 31
8	J	120/135 (89%)	117 (98%)	2 (2%)	1 (1%)	19 58
9	K	110/117 (94%)	105 (96%)	5 (4%)	0	100 100
10	N	995/1454 (68%)	889 (89%)	95 (10%)	11 (1%)	14 52
11	O	153/788 (19%)	138 (90%)	13 (8%)	2 (1%)	12 48
12	P	756/841 (90%)	705 (93%)	49 (6%)	2 (0%)	41 75
13	Q	539/651 (83%)	505 (94%)	30 (6%)	4 (1%)	22 61
14	R	189/208 (91%)	180 (95%)	9 (5%)	0	100 100
15	S	67/244 (28%)	60 (90%)	5 (8%)	2 (3%)	4 30
16	T	189/212 (89%)	175 (93%)	13 (7%)	1 (0%)	29 68
17	U	117/144 (81%)	114 (97%)	2 (2%)	1 (1%)	17 56
18	V	128/200 (64%)	125 (98%)	2 (2%)	1 (1%)	19 58
19	W	1332/1368 (97%)	1262 (95%)	66 (5%)	4 (0%)	41 75
20	X	877/989 (89%)	829 (94%)	44 (5%)	4 (0%)	29 68
21	Y	206/747 (28%)	196 (95%)	9 (4%)	1 (0%)	29 68
22	Z	93/600 (16%)	83 (89%)	8 (9%)	2 (2%)	6 37
23	0	261/311 (84%)	245 (94%)	16 (6%)	0	100 100
24	1	95/178 (53%)	91 (96%)	3 (3%)	1 (1%)	14 52
25	2	111/200 (56%)	106 (96%)	5 (4%)	0	100 100
26	3	114/178 (64%)	111 (97%)	3 (3%)	0	100 100
27	4	111/131 (85%)	107 (96%)	3 (3%)	1 (1%)	17 56
All	All	7758/12460 (62%)	7275 (94%)	437 (6%)	46 (1%)	29 64

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	I	105	PRO
10	N	186	ILE
10	N	525	TYR
10	N	689	PRO
10	N	1351	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	394/1391 (28%)	392 (100%)	2 (0%)	88 94
3	D	139/230 (60%)	139 (100%)	0	100 100
4	F	151/223 (68%)	151 (100%)	0	100 100
5	G	153/216 (71%)	150 (98%)	3 (2%)	55 79
6	H	161/225 (72%)	160 (99%)	1 (1%)	86 94
7	I	71/133 (53%)	70 (99%)	1 (1%)	67 85
8	J	66/124 (53%)	66 (100%)	0	100 100
9	K	94/98 (96%)	94 (100%)	0	100 100
10	N	810/1271 (64%)	802 (99%)	8 (1%)	76 88
11	O	141/697 (20%)	140 (99%)	1 (1%)	84 93
12	P	681/736 (92%)	671 (98%)	10 (2%)	65 84
13	Q	493/577 (85%)	485 (98%)	8 (2%)	62 83
14	R	169/183 (92%)	166 (98%)	3 (2%)	59 81
15	S	31/208 (15%)	31 (100%)	0	100 100
16	T	166/178 (93%)	163 (98%)	3 (2%)	59 81
17	U	98/119 (82%)	96 (98%)	2 (2%)	55 79
18	V	122/173 (70%)	118 (97%)	4 (3%)	38 68
19	W	1203/1232 (98%)	1200 (100%)	3 (0%)	93 98
20	X	789/864 (91%)	780 (99%)	9 (1%)	73 88
21	Y	175/601 (29%)	172 (98%)	3 (2%)	60 82
22	Z	89/512 (17%)	84 (94%)	5 (6%)	21 54
23	0	241/280 (86%)	234 (97%)	7 (3%)	42 71
24	1	94/152 (62%)	94 (100%)	0	100 100
25	2	102/163 (63%)	102 (100%)	0	100 100
26	3	116/155 (75%)	116 (100%)	0	100 100
27	4	102/115 (89%)	101 (99%)	1 (1%)	76 88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	6851/10856 (63%)	6777 (99%)	74 (1%)	74 88

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	X	897	LEU
23	0	218	ASN
21	Y	224	ARG
22	Z	551	ASP
12	P	699	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 109 such sidechains are listed below:

Mol	Chain	Res	Type
13	Q	411	GLN
19	W	203	ASN
20	X	544	HIS
13	Q	468	ASN
17	U	28	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 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.

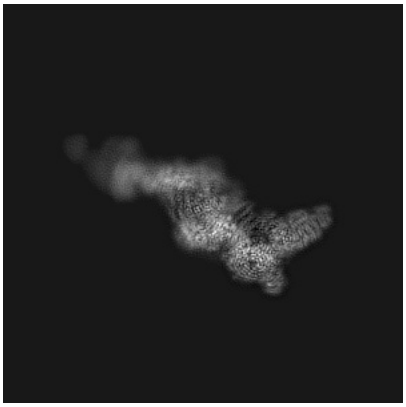
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31191. These allow visual inspection of the internal detail of the map and identification of artifacts.

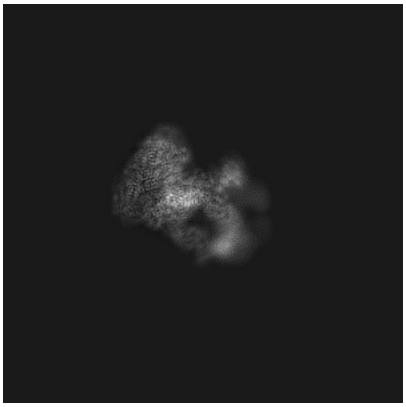
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

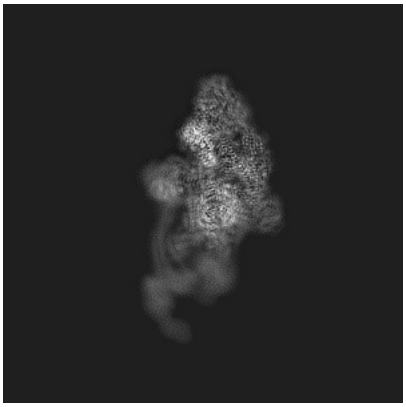
6.1.1 Primary map



X



Y

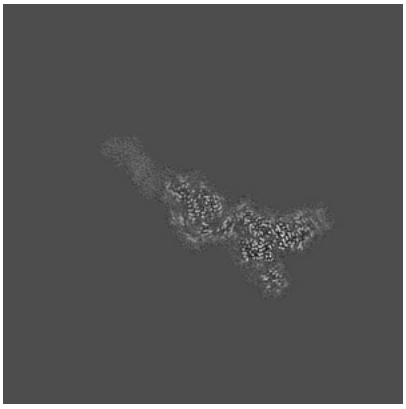


Z

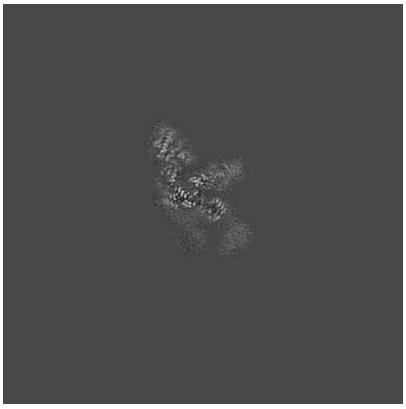
The images above show the map projected in three orthogonal directions.

6.2 Central slices

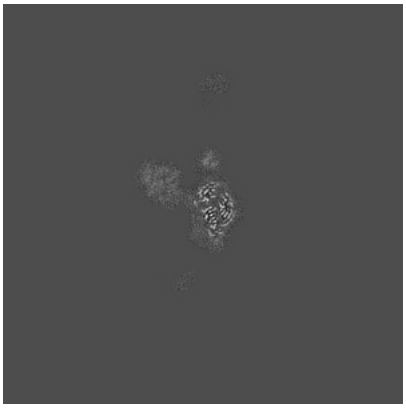
6.2.1 Primary map



X Index: 256



Y Index: 256

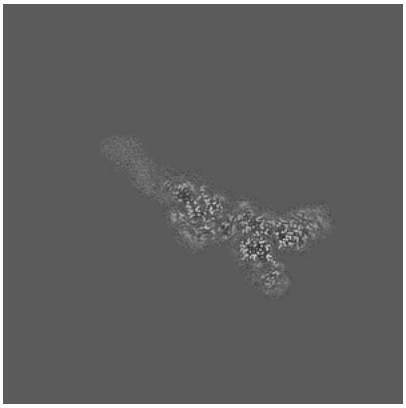


Z Index: 256

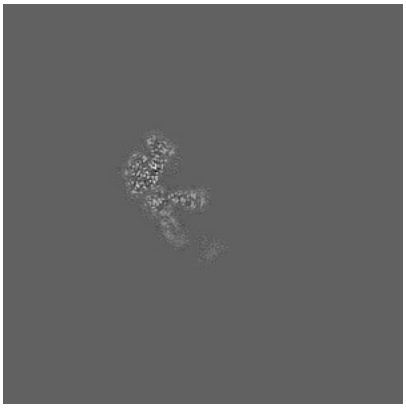
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

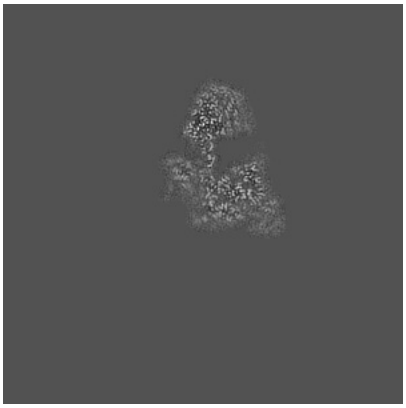
6.3.1 Primary map



X Index: 258



Y Index: 308



Z Index: 215

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

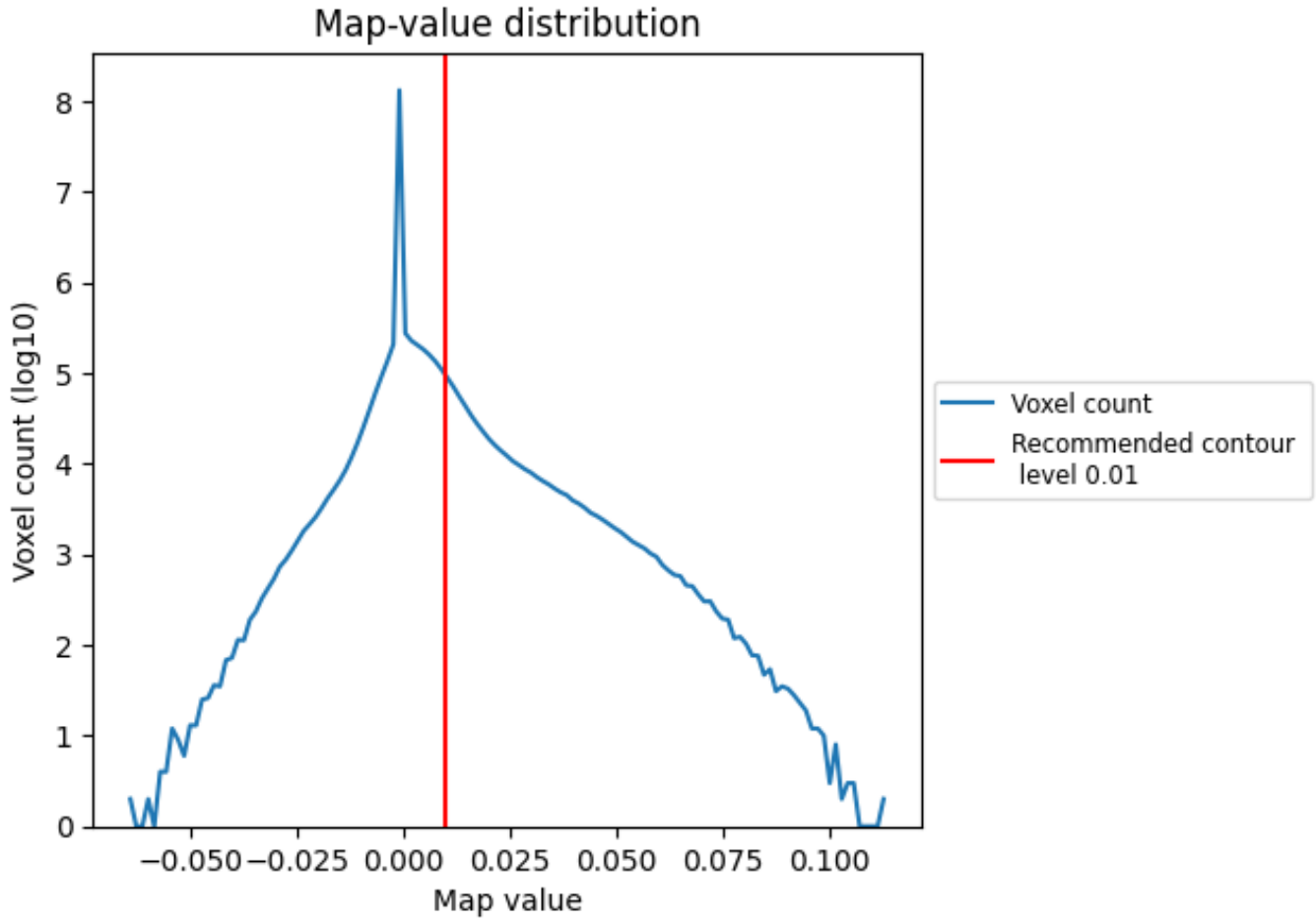
6.5 Mask visualisation (i)

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

7 Map analysis

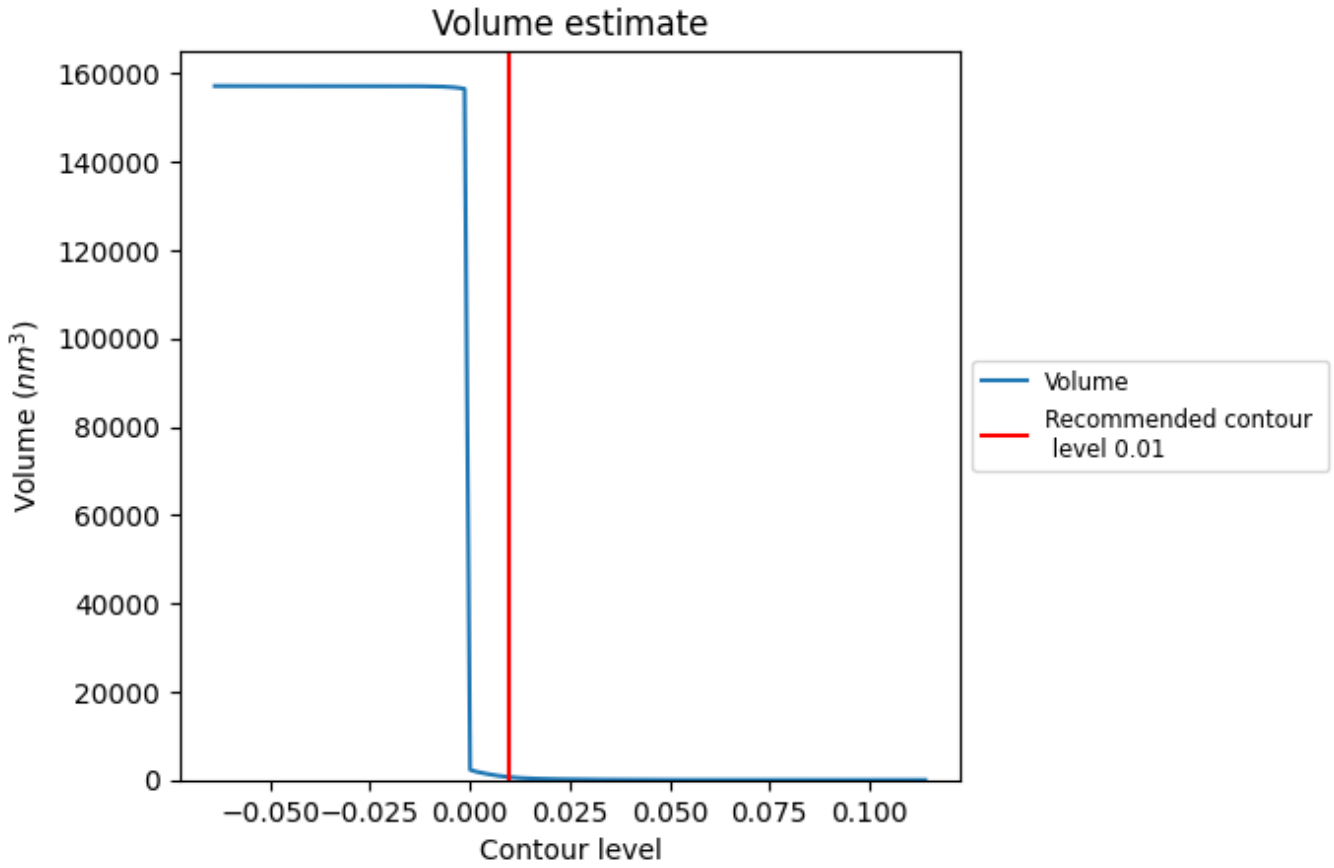
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

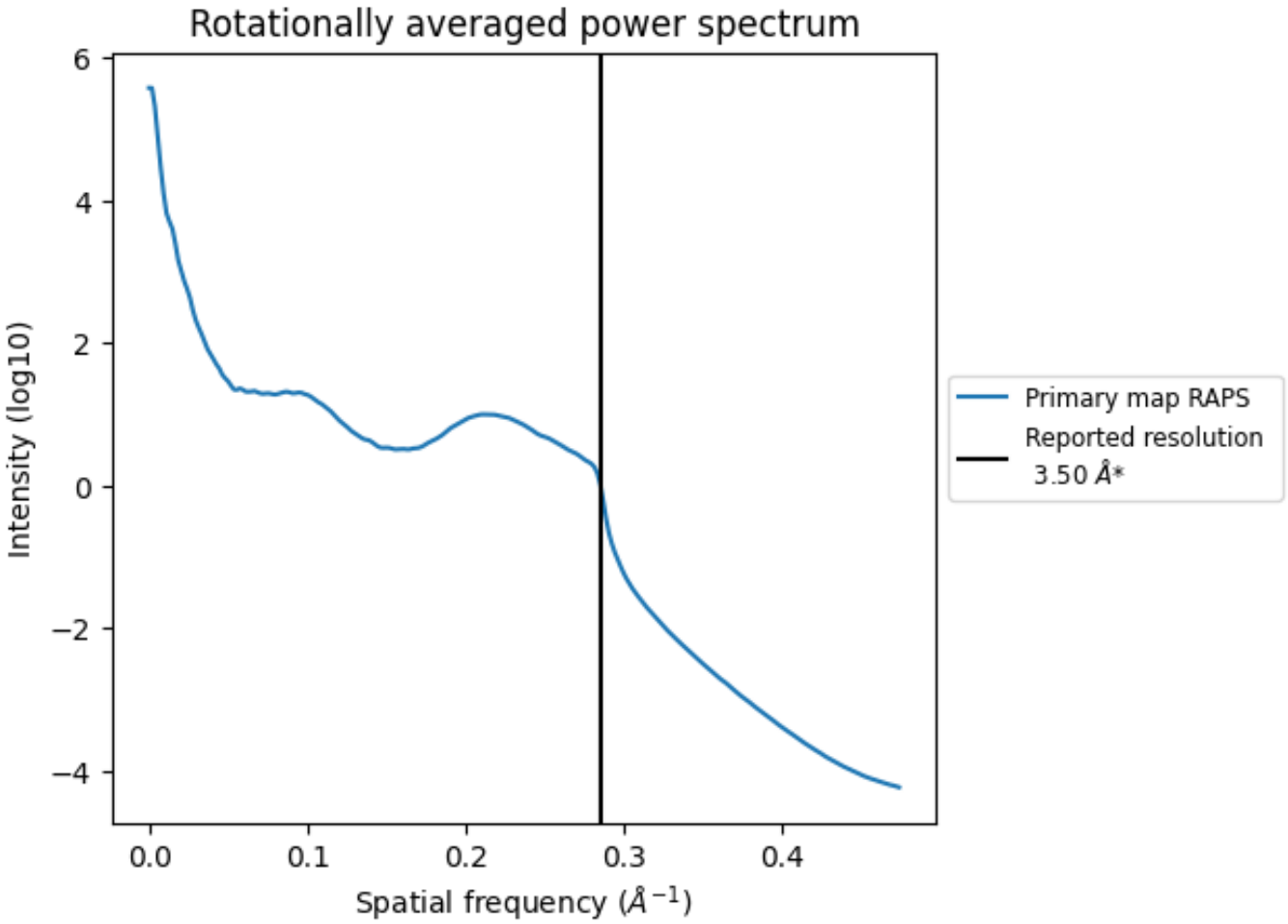
7.2 Volume estimate (i)



The volume at the recommended contour level is 635 nm^3; this corresponds to an approximate mass of 574 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 0.286 $Å^{-1}$

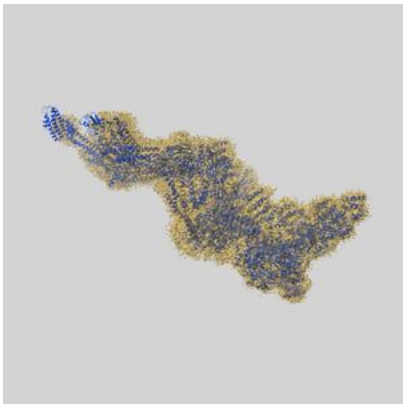
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

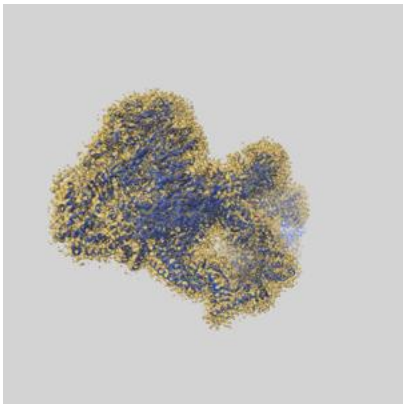
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31191 and PDB model 7EMF. Per-residue inclusion information can be found in section 3 on page 9.

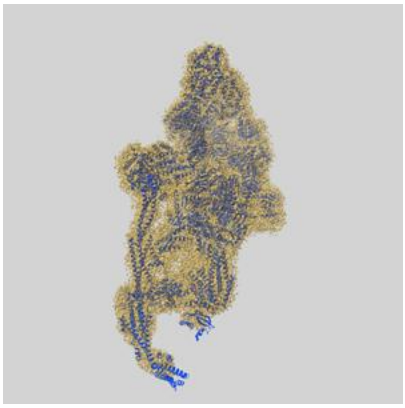
9.1 Map-model overlay



X



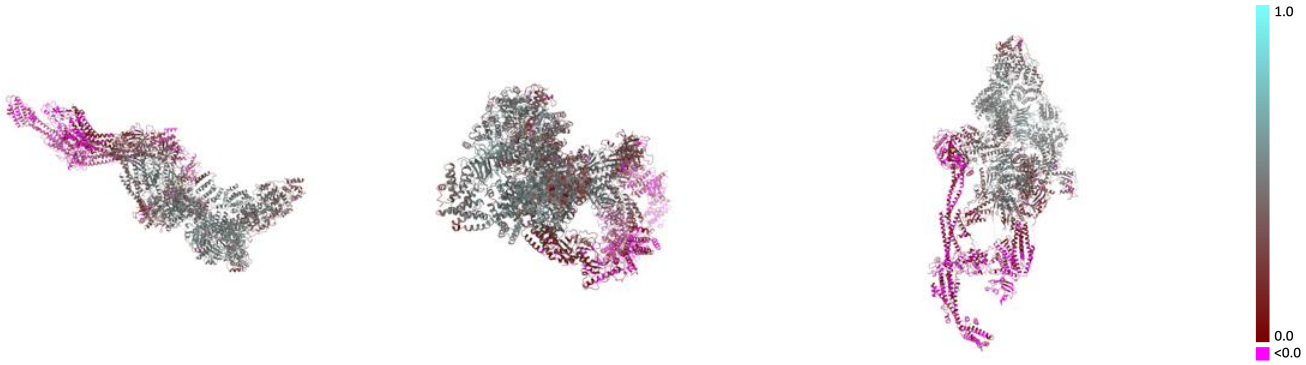
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

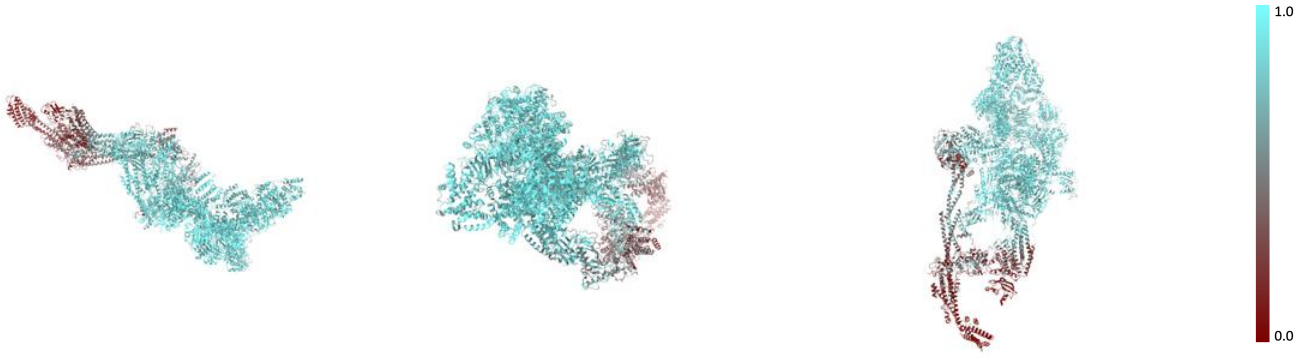
9.2 Q-score mapped to coordinate model



X Y Z

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.

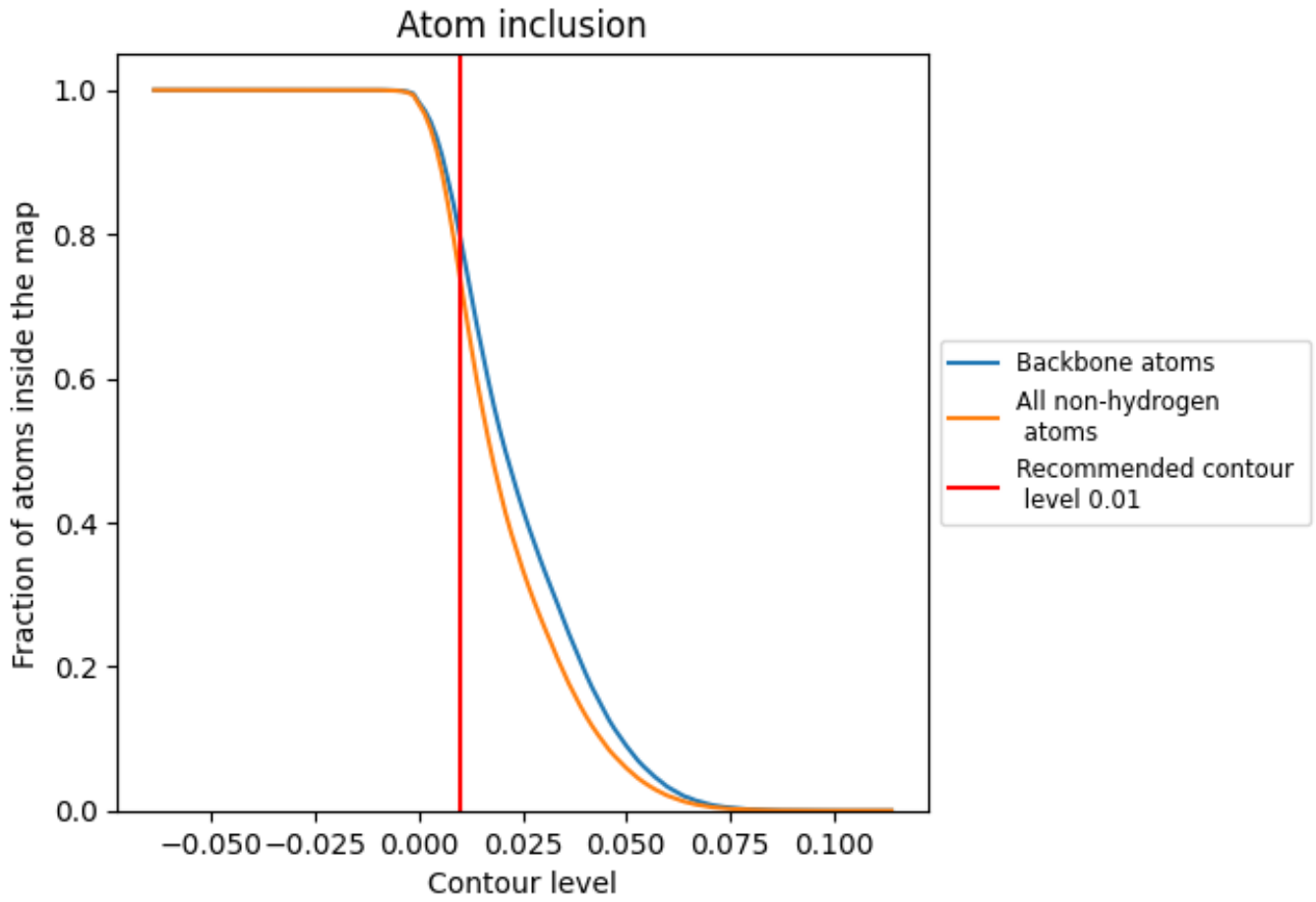
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 74% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7371	0.3310
0	0.8882	0.4600
1	0.8881	0.4270
2	0.8459	0.4080
3	0.8683	0.4040
4	0.3906	0.0260
A	0.5806	0.1230
B	0.8100	0.2100
D	0.4452	0.0670
F	0.2532	0.0420
G	0.2629	-0.0020
H	0.3374	0.0430
I	0.4716	0.0710
J	0.0989	0.0040
K	0.6262	0.2120
N	0.7703	0.3540
O	0.8898	0.4410
P	0.9089	0.5060
Q	0.7476	0.3540
R	0.7535	0.2470
S	0.0722	0.0080
T	0.8261	0.3300
U	0.3043	0.0120
V	0.6881	0.2070
W	0.8759	0.4390
X	0.8747	0.4380
Y	0.8980	0.4810
Z	0.2195	0.0280