



# wwPDB EM Validation Summary Report ⓘ

Feb 25, 2023 – 04:11 PM EST

PDB ID : 7UIO  
EMDB ID : EMD-26551  
Title : Mediator-PIC Early (Composite Model)  
Authors : Gorbea Colon, J.J.; Chen, S.-F.; Tsai, K.L.; Murakami, K.  
Deposited on : 2022-03-29  
Resolution : 3.30 Å(reported)  
Based on initial models : 7UIL, 7UI9, 7UIK

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:

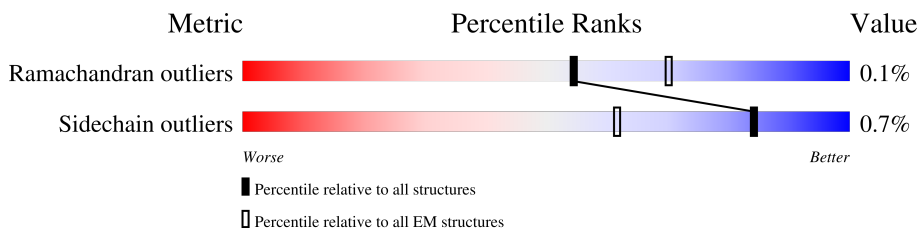
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.32.1

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 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.



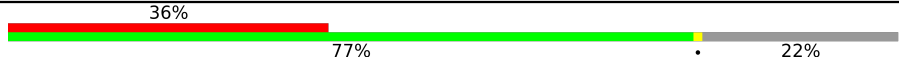
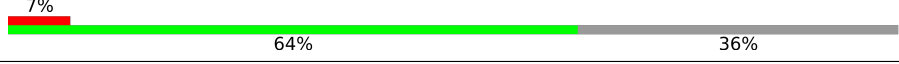
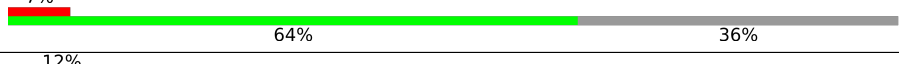
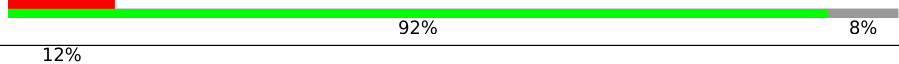
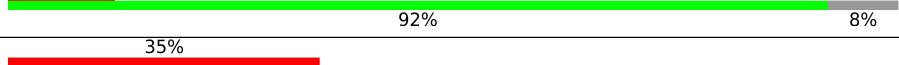
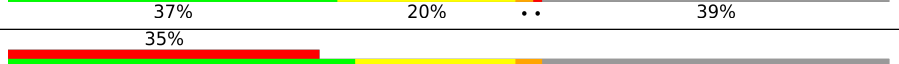
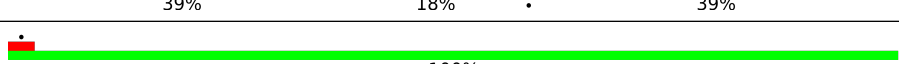
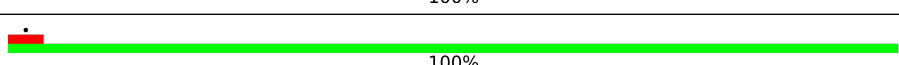
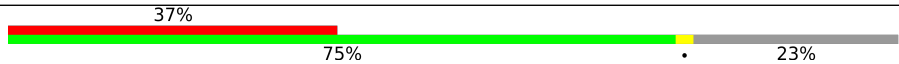


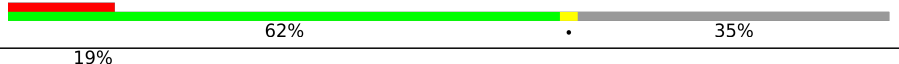
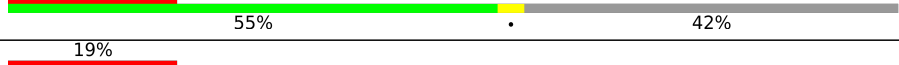

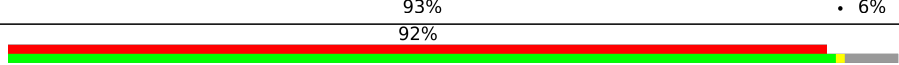
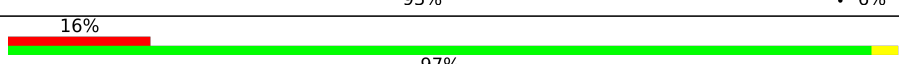
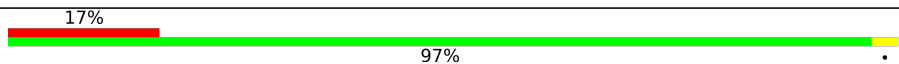








Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	A	38	
2	B	37	
3	Ao	1081	
3	Bo	1081	
4	Ab	431	
4	Bb	431	
5	Ac	397	
5	Bc	397	
6	An	1082	

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Mol	Chain	Length	Quality of chain
6	Bn	1082	
7	Ae	1132	
7	Be	1132	
8	Ap	974	
8	Bp	974	
9	GA	147	
9	GB	147	
10	At	210	
10	Bt	210	
11	Ag	222	
11	Bg	222	
12	Ah	223	
12	Bh	223	
13	Ai	149	
13	Bi	149	
14	Aj	157	
14	Bj	157	
15	Ak	115	
15	Bk	115	
16	Aq	687	
16	Bq	687	
17	Ar	307	
17	Br	307	
18	As	220	
18	Bs	220	

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Mol	Chain	Length	Quality of chain
19	Au	140	36% 84% 13%
19	Bu	140	35% 84% 13%
20	Av	120	17% 90% 9%
20	Bv	120	16% 90% 9%
21	Aw	127	14% 81% 19%
21	Bw	127	13% 81% 19%
22	Az	25	40% 96% .
22	Bz	25	40% 96% .
23	AA	1453	6% 100%
23	BA	1453	5% 100%
24	AB	1224	11% 96% .
24	BB	1224	10% 96% .
25	AC	318	. 85% 15%
25	BC	318	. 85% 15%
26	AD	221	48% 76% 24%
26	BD	221	48% 76% 24%
27	AE	215	. 100%
27	BE	215	. 100%
28	AF	155	. 55% 45%
28	BF	155	. 55% 45%
29	AG	171	42% 99% .
29	BG	171	41% 99% .
30	AH	146	5% 97% .
30	BH	146	5% 97% .
31	AI	122	10% 95% 5%

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Mol	Chain	Length	Quality of chain
31	BI	122	
32	AJ	70	
32	BJ	70	
33	AK	120	
33	BK	120	
34	AL	70	
34	BL	70	
35	AM	345	
35	BM	345	
36	AP	735	
36	BP	735	
37	AQ	400	
37	BQ	400	
38	AS	309	
38	BS	309	
39	Aa	566	
39	Ba	566	
40	Ad	284	
40	Bd	284	
41	Af	295	
41	Bf	295	

## 2 Entry composition [i](#)

There are 45 unique types of molecules in this entry. The entry contains 164116 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 DNA chain called DNA (38-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	38	774	367	146	224	37	0	0

- Molecule 2 is a DNA chain called DNA (37-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	37	761	359	142	223	37	0	0

- Molecule 3 is a protein called Mediator of RNA polymerase II transcription subunit 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	Ao	111	894	558	161	169	6	0	0
3	Bo	111	894	558	161	169	6	0	0

- Molecule 4 is a protein called Mediator of RNA polymerase II transcription subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	Ab	65	516	328	82	102	4	0	0
4	Bb	65	516	328	82	102	4	0	0

- Molecule 5 is a protein called Mediator of RNA polymerase II transcription subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	Ac	110	891	560	155	172	4	0	0
5	Bc	107	871	549	152	166	4	0	0

- Molecule 6 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	An	846	Total	C	N	O	S	0	0
			6927	4460	1187	1247	33		
6	Bn	846	Total	C	N	O	S	0	0
			6927	4460	1187	1247	33		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	Ae	729	Total	C	N	O	S	0	0
			5916	3826	956	1120	14		
7	Be	729	Total	C	N	O	S	0	0
			5916	3826	956	1120	14		

- Molecule 8 is a protein called Mediator of RNA polymerase II transcription subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	Ap	895	Total	C	N	O	S	0	0
			7247	4668	1202	1342	35		
8	Bp	895	Total	C	N	O	S	0	0
			7247	4668	1202	1342	35		

- Molecule 9 is a protein called Regulatory protein GAL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	GA	89	Total	C	N	O	S	0	0
			727	459	130	130	8		
9	GB	89	Total	C	N	O	S	0	0
			727	459	130	130	8		

- Molecule 10 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	At	210	Total	C	N	O	S	0	0
			1609	1016	270	317	6		
10	Bt	210	Total	C	N	O	S	0	0
			1609	1016	270	317	6		

- Molecule 11 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Ag	171	Total	C	N	O	S	0	0
			1426	914	242	265	5		
11	Bg	171	Total	C	N	O	S	0	0
			1426	914	242	265	5		

- Molecule 12 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Ah	144	Total	C	N	O	S	0	0
			1185	747	208	227	3		
12	Bh	144	Total	C	N	O	S	0	0
			1185	747	208	227	3		

- Molecule 13 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Ai	86	Total	C	N	O	S	0	0
			730	456	134	139	1		
13	Bi	86	Total	C	N	O	S	0	0
			730	456	134	139	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Aj	148	Total	C	N	O	S	0	0
			1189	736	209	241	3		
14	Bj	148	Total	C	N	O	S	0	0
			1189	736	209	241	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Ak	115	Total	C	N	O	S	0	0
			933	584	160	185	4		
15	Bk	115	Total	C	N	O	S	0	0
			933	584	160	185	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Aq	515	Total	C	N	O	S	0	0
			4182	2674	707	788	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Bq	515	Total	C	N	O	S	0	0
			4182	2674	707	788	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Ar	253	Total	C	N	O	S	0	0
			1995	1271	331	383	10		
17	Br	253	Total	C	N	O	S	0	0
			1995	1271	331	383	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	As	81	Total	C	N	O	S	0	0
			657	415	109	132	1		
18	Bs	81	Total	C	N	O	S	0	0
			657	415	109	132	1		

- Molecule 19 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	Au	122	Total	C	N	O	S	0	0
			978	611	163	199	5		
19	Bu	122	Total	C	N	O	S	0	0
			978	611	163	199	5		

- Molecule 20 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	Av	109	Total	C	N	O	S	0	0
			869	540	143	180	6		
20	Bv	109	Total	C	N	O	S	0	0
			869	540	143	180	6		

- Molecule 21 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	Aw	103	Total	C	N	O	S	0	0
			871	575	135	155	6		
21	Bw	103	Total	C	N	O	S	0	0
			871	575	135	155	6		

- Molecule 22 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	Az	25	Total	C	N	O	0	0
			185	116	25	44		
22	Bz	25	Total	C	N	O	0	0
			185	116	25	44		

- Molecule 23 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	AA	1453	Total	C	N	O	S	0	0
			11426	7192	1995	2177	62		
23	BA	1453	Total	C	N	O	S	0	0
			11426	7192	1995	2177	62		

- Molecule 24 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	AB	1172	Total	C	N	O	S	0	0
			9336	5895	1637	1748	56		
24	BB	1172	Total	C	N	O	S	0	0
			9336	5895	1637	1748	56		

- Molecule 25 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	AC	271	Total	C	N	O	S	0	0
			2133	1340	355	424	14		
25	BC	271	Total	C	N	O	S	0	0
			2133	1340	355	424	14		

- Molecule 26 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	AD	169	Total	C	N	O	S	0	0
			1353	838	237	275	3		
26	BD	169	Total	C	N	O	S	0	0
			1353	838	237	275	3		

- Molecule 27 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	AE	215	1760	1116	310	322	12	0	0
27	BE	215	1760	1116	310	322	12	0	0

- Molecule 28 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	AF	86	697	445	118	131	3	0	0
28	BF	86	697	445	118	131	3	0	0

- Molecule 29 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	AG	171	1340	861	222	249	8	0	0
29	BG	171	1340	861	222	249	8	0	0

- Molecule 30 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	AH	141	1126	706	189	226	5	0	0
30	BH	141	1126	706	189	226	5	0	0

- Molecule 31 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	AI	116	943	580	171	181	11	0	0
31	BI	116	943	580	171	181	11	0	0

- Molecule 32 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	AJ	70	578	366	102	104	6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
32	BJ	70	Total	C	N	O	S	0	0
			578	366	102	104	6		

- Molecule 33 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	AK	116	Total	C	N	O	S	0	0
			929	596	158	173	2		
33	BK	116	Total	C	N	O	S	0	0
			929	596	158	173	2		

- Molecule 34 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	AL	43	Total	C	N	O	S	0	0
			344	211	69	60	4		
34	BL	43	Total	C	N	O	S	0	0
			344	211	69	60	4		

- Molecule 35 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	AM	35	Total	C	N	O	S	0	0
			263	169	41	49	4		
35	BM	35	Total	C	N	O	S	0	0
			263	169	41	49	4		

- Molecule 36 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	AP	103	Total	C	N	O	S	0	0
			861	554	142	162	3		
36	BP	103	Total	C	N	O	S	0	0
			861	554	142	162	3		

- Molecule 37 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	AQ	125	Total	C	N	O	S	0	0
			1033	644	189	195	5		
37	BQ	125	Total	C	N	O	S	0	0
			1033	644	189	195	5		

- Molecule 38 is a protein called Transcription elongation factor S-II.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	AS	181	Total	C	N	O	S	0	0
			1436	893	256	279	8		
38	BS	181	Total	C	N	O	S	0	0
			1436	893	256	279	8		

- Molecule 39 is a protein called Mediator of RNA polymerase II transcription subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Aa	365	Total	C	N	O	S	0	0
			3008	1932	478	588	10		
39	Ba	365	Total	C	N	O	S	0	0
			3008	1932	478	588	10		

- Molecule 40 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Ad	171	Total	C	N	O	S	0	0
			1388	875	233	276	4		
40	Bd	171	Total	C	N	O	S	0	0
			1388	875	233	276	4		

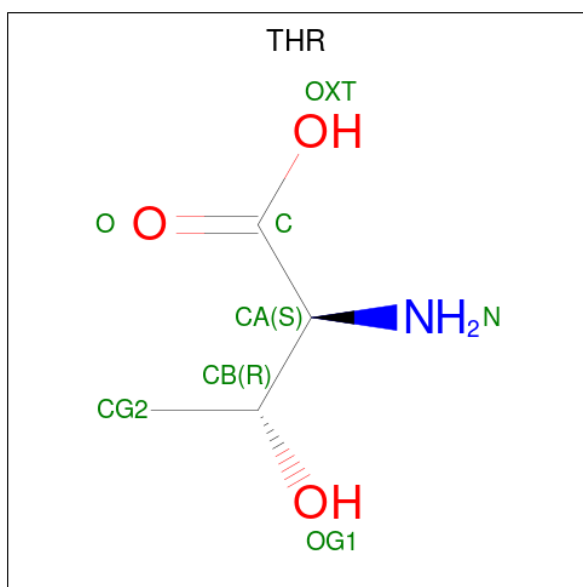
- Molecule 41 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Af	169	Total	C	N	O	S	0	0
			1407	905	234	262	6		
41	Bf	169	Total	C	N	O	S	0	0
			1407	905	234	262	6		

- Molecule 42 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

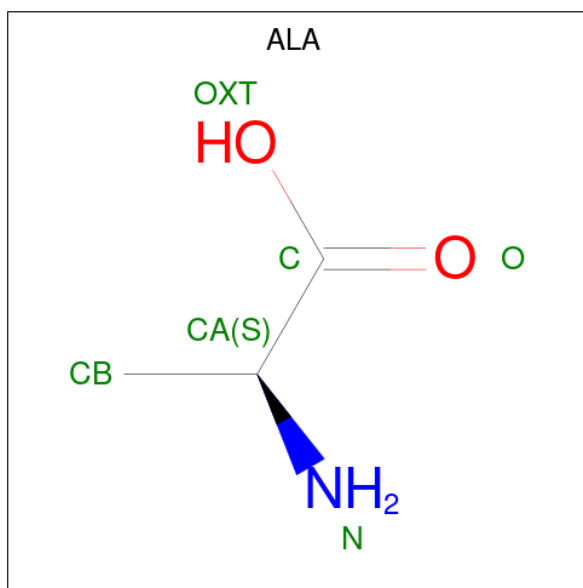
Mol	Chain	Residues	Atoms		AltConf
42	A	2	Total	Zn	0
			2	2	
42	B	2	Total	Zn	0
			2	2	

- Molecule 43 is THREONINE (three-letter code: THR) (formula: C<sub>4</sub>H<sub>9</sub>NO<sub>3</sub>).



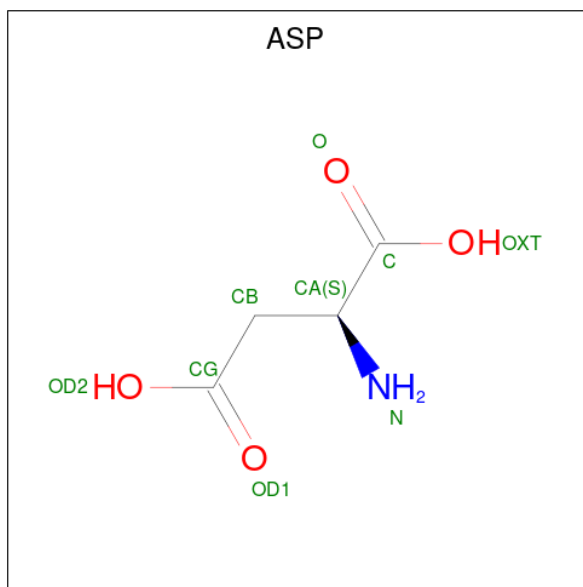
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
43	Bc	1	7	4	1	2	0

- Molecule 44 is ALANINE (three-letter code: ALA) (formula: C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
44	Bc	1	5	3	1	1	0

- Molecule 45 is ASPARTIC ACID (three-letter code: ASP) (formula: C<sub>4</sub>H<sub>7</sub>NO<sub>4</sub>).

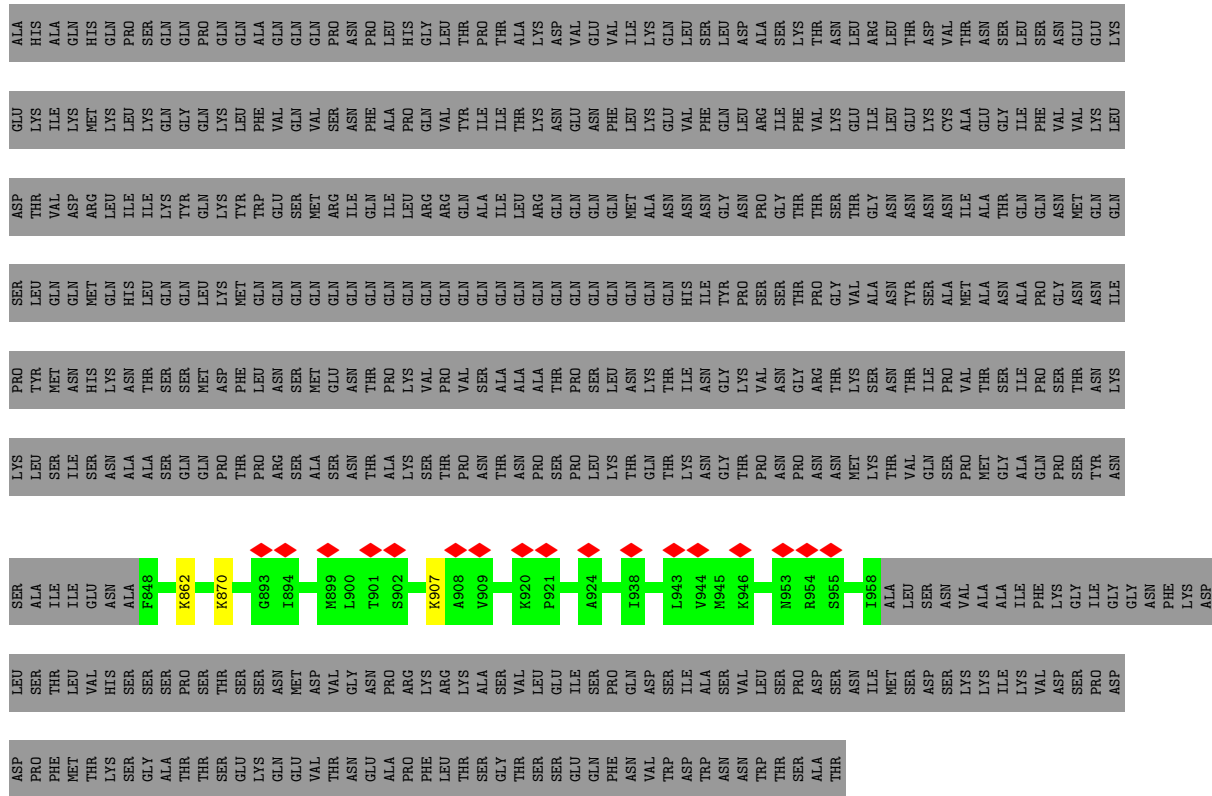


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
45	Bc	1	9	4	1	4	0

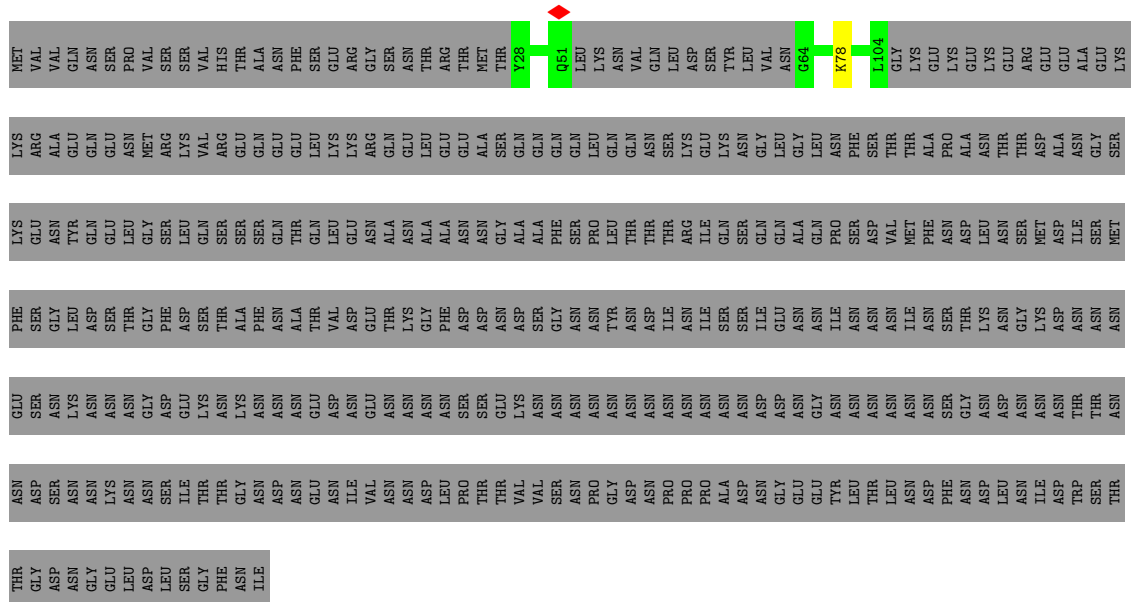






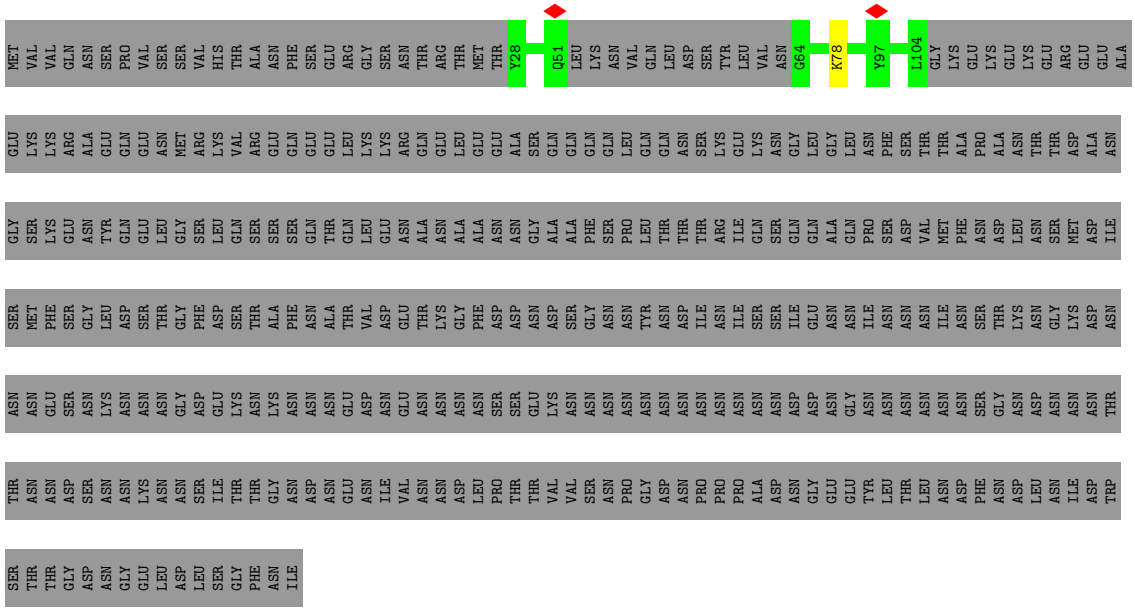


- Molecule 4: Mediator of RNA polymerase II transcription subunit 2

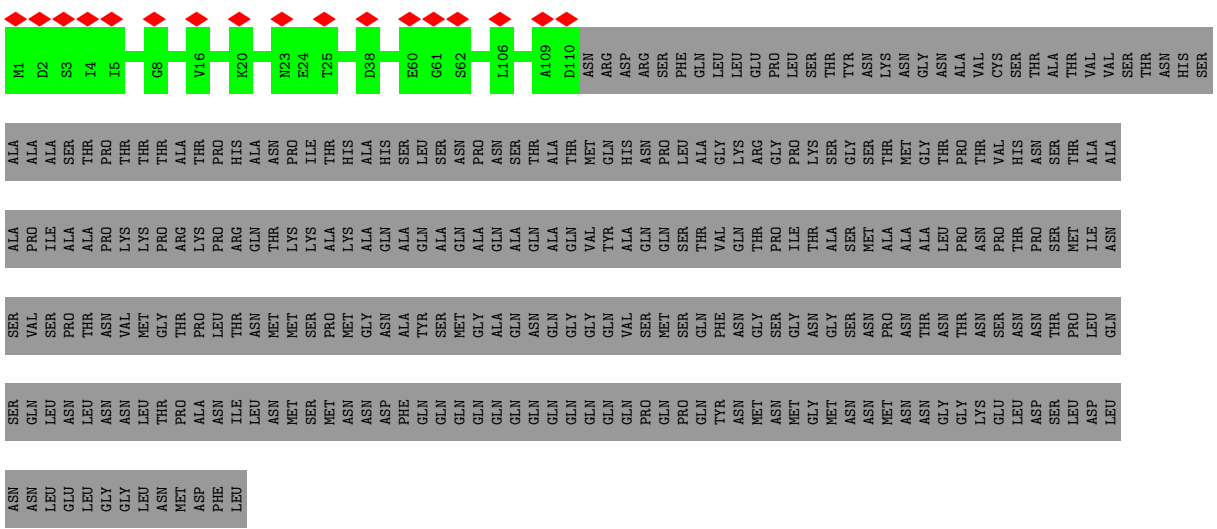


- Molecule 4: Mediator of RNA polymerase II transcription subunit 2





• Molecule 5: Mediator of RNA polymerase II transcription subunit 3



• Molecule 5: Mediator of RNA polymerase II transcription subunit 3

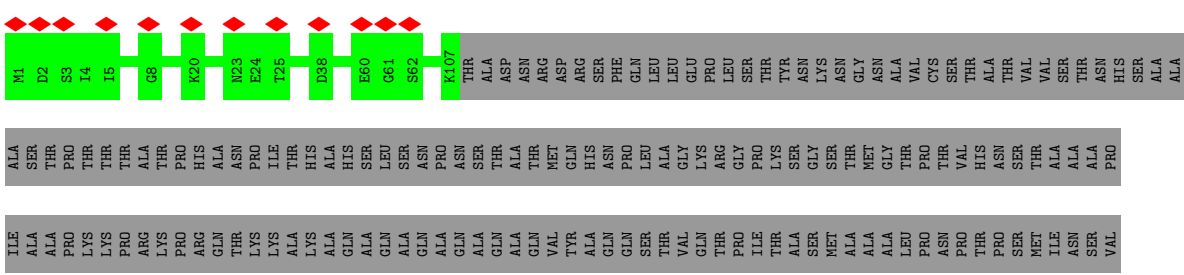
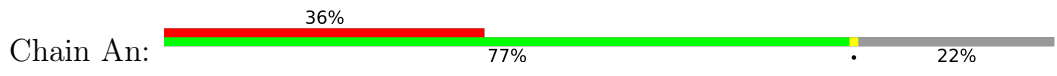
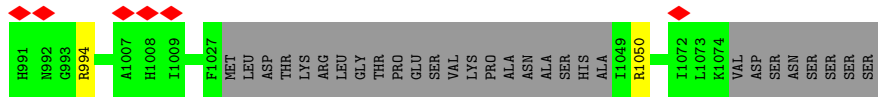


Table of amino acid residues for Chain An, showing residues from SER to LEU.

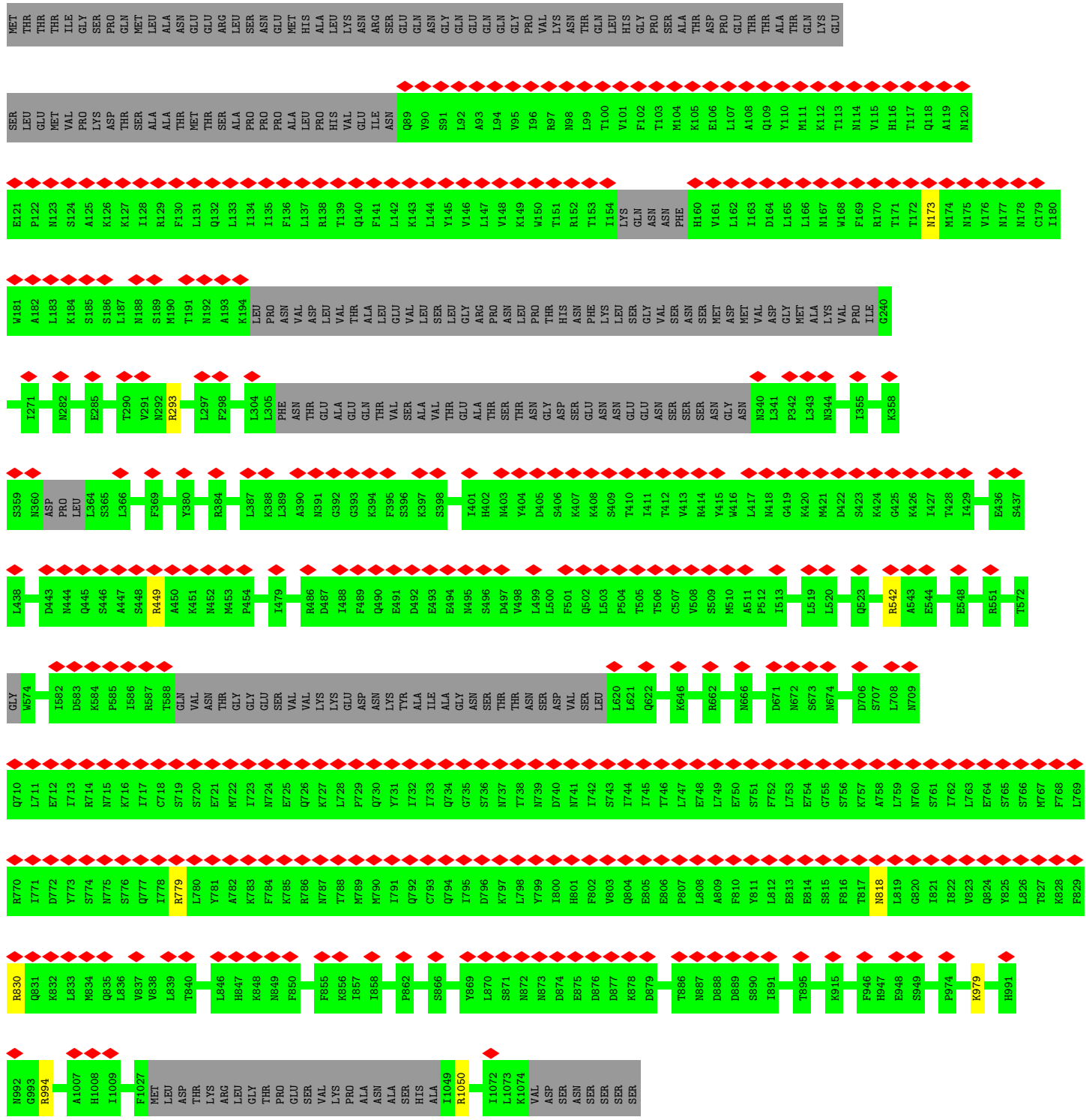
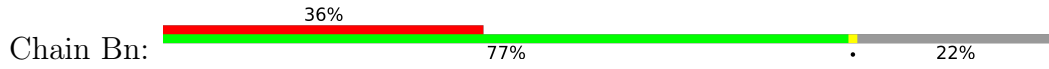
• Molecule 6: Mediator of RNA polymerase II transcription subunit 14



Main sequence diagram for Chain An, showing residues from MET to GLU with various annotations and color coding.

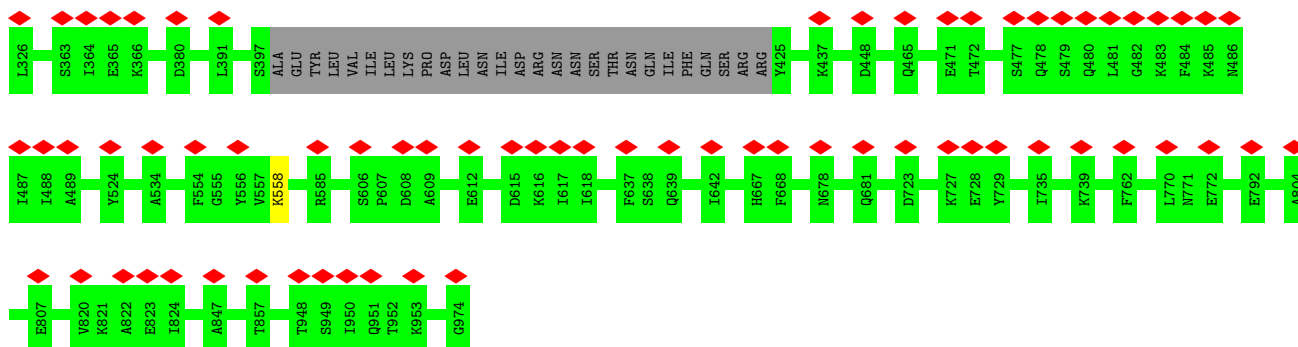


● Molecule 6: Mediator of RNA polymerase II transcription subunit 14

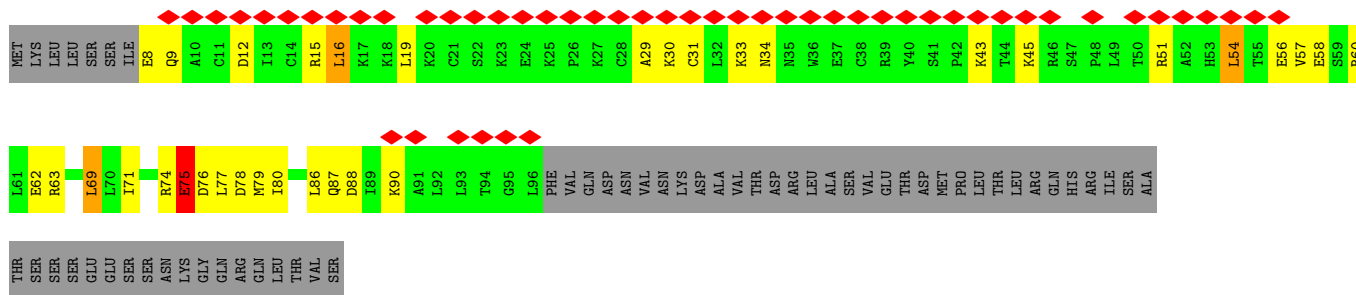




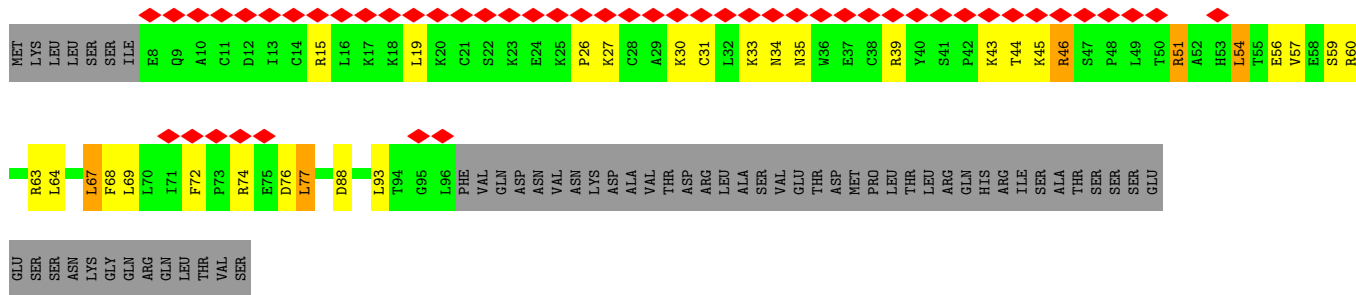




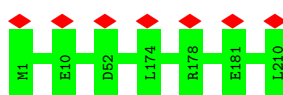
• Molecule 9: Regulatory protein GAL4



• Molecule 9: Regulatory protein GAL4



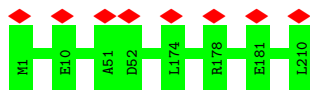
• Molecule 10: Mediator of RNA polymerase II transcription subunit 20



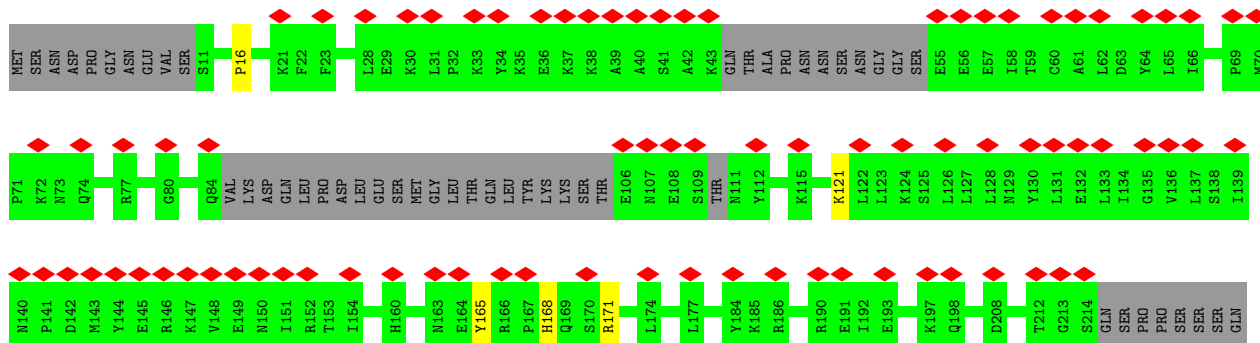
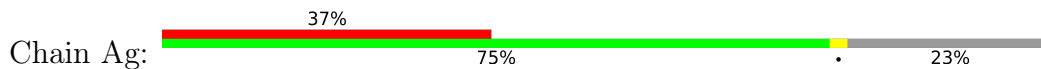
• Molecule 10: Mediator of RNA polymerase II transcription subunit 20



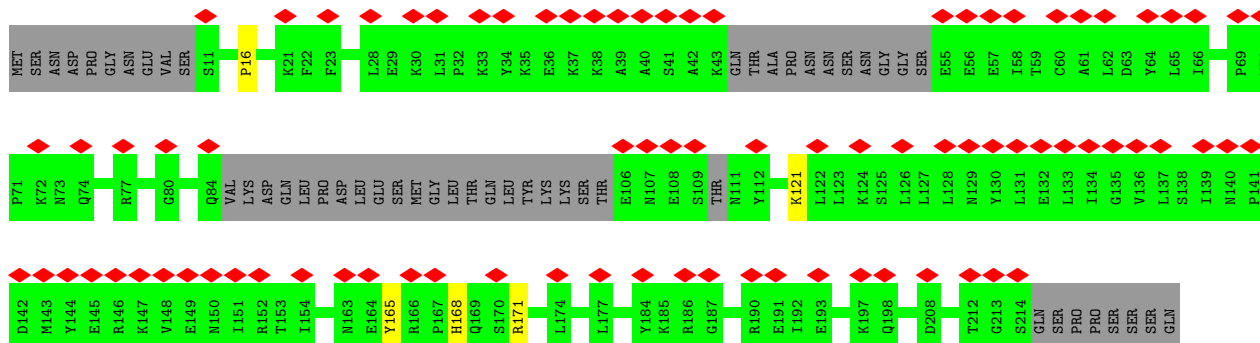
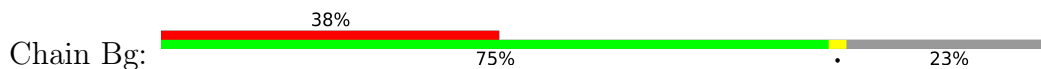




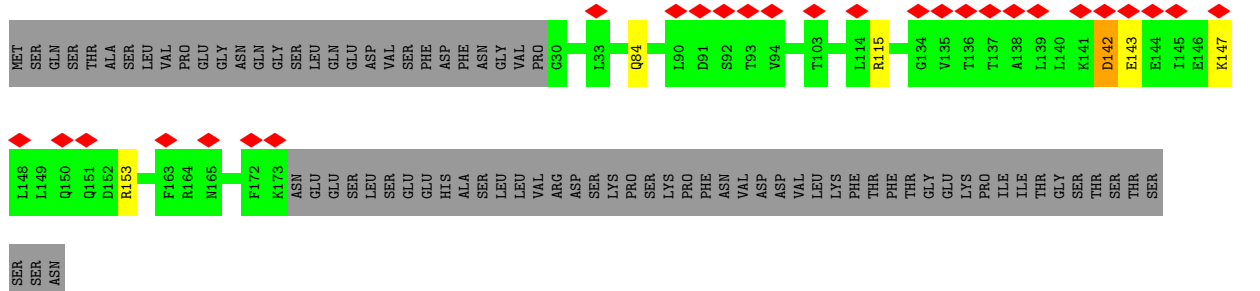
• Molecule 11: Mediator of RNA polymerase II transcription subunit 7



• Molecule 11: Mediator of RNA polymerase II transcription subunit 7

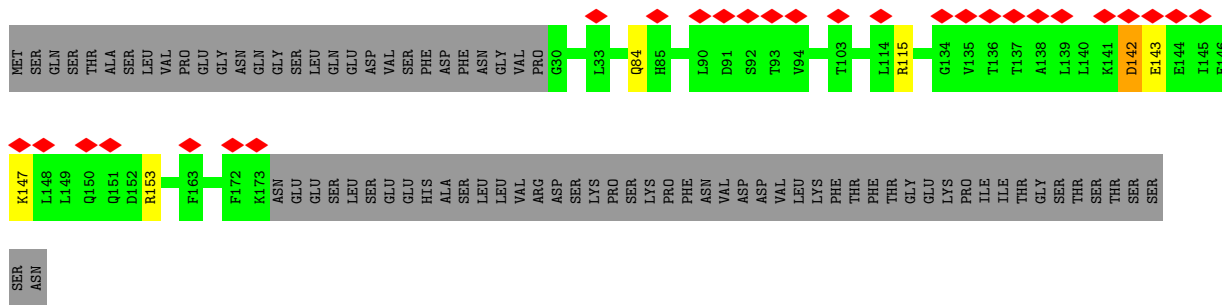


• Molecule 12: Mediator of RNA polymerase II transcription subunit 8

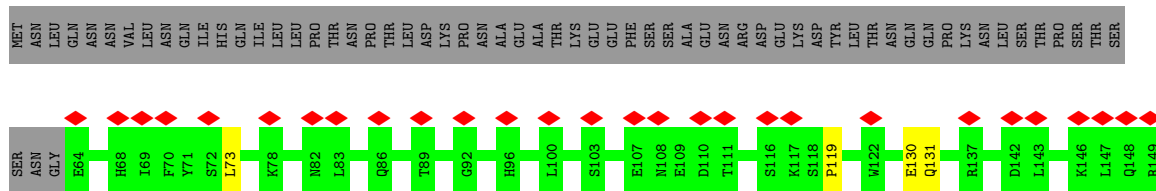


• Molecule 12: Mediator of RNA polymerase II transcription subunit 8

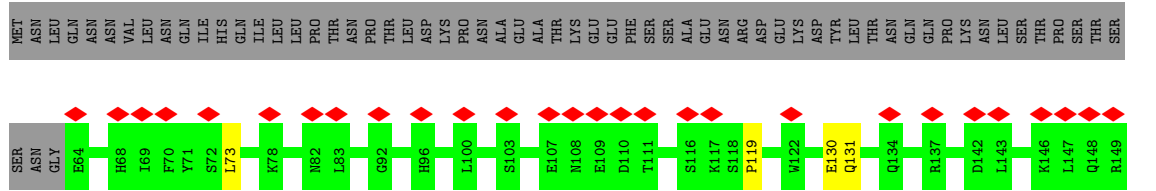




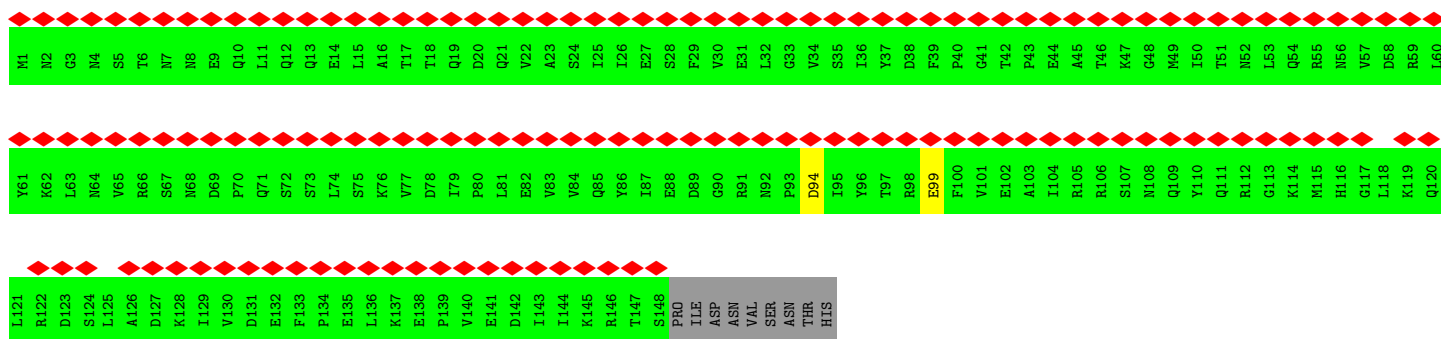
• Molecule 13: Mediator of RNA polymerase II transcription subunit 9



• Molecule 13: Mediator of RNA polymerase II transcription subunit 9



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

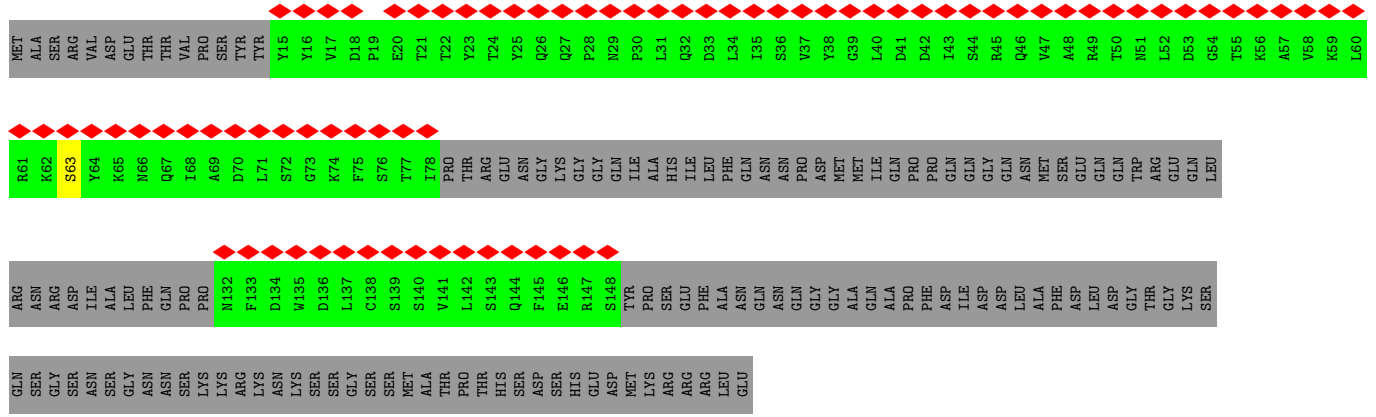


• Molecule 14: Mediator of RNA polymerase II transcription subunit 10

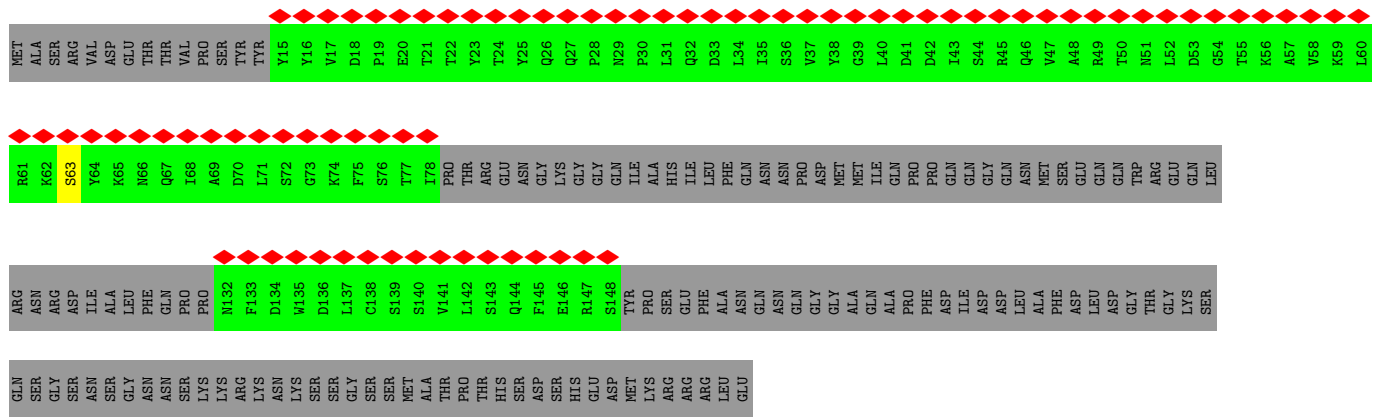




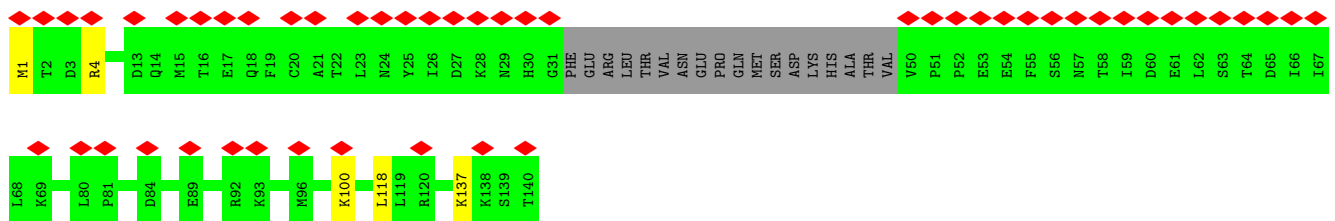
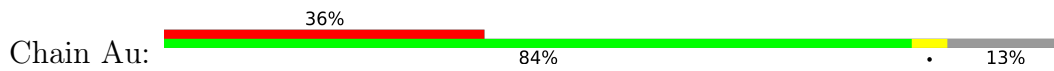




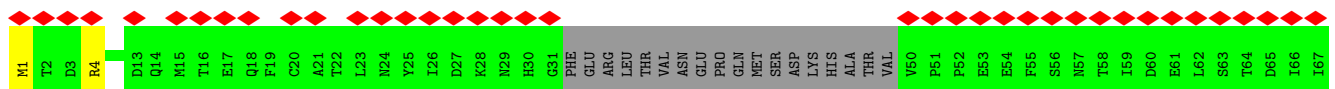
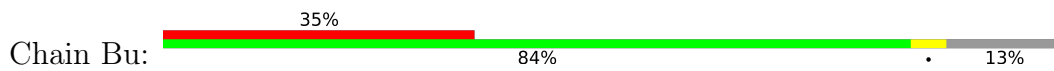
• Molecule 18: Mediator of RNA polymerase II transcription subunit 19

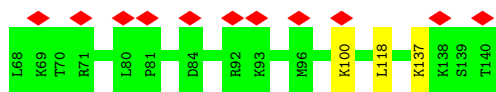


• Molecule 19: Mediator of RNA polymerase II transcription subunit 21

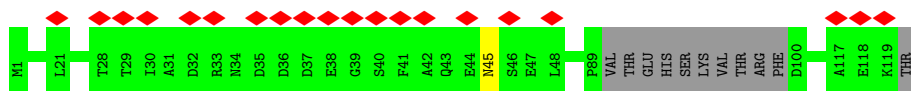
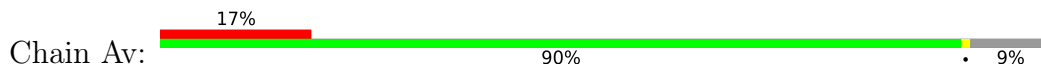


• Molecule 19: Mediator of RNA polymerase II transcription subunit 21

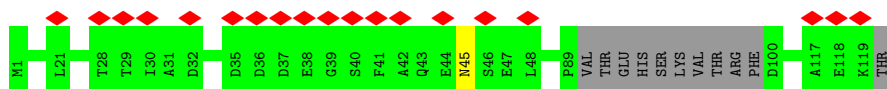




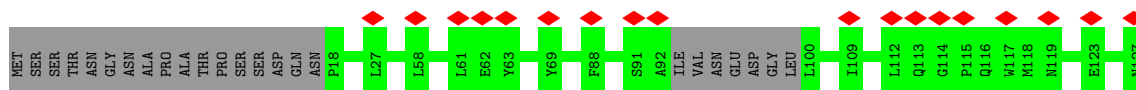
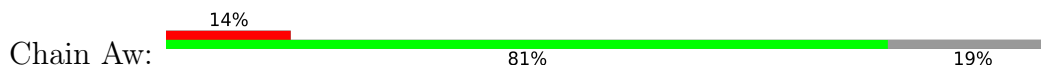
- Molecule 20: Mediator of RNA polymerase II transcription subunit 22



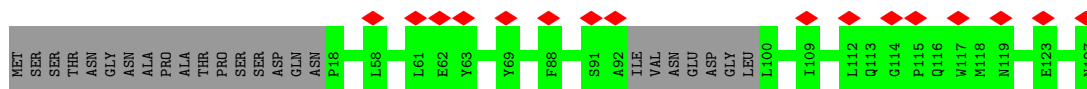
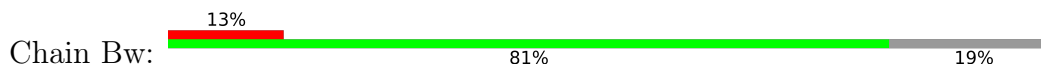
- Molecule 20: Mediator of RNA polymerase II transcription subunit 22



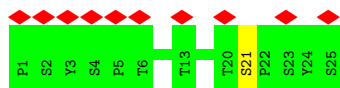
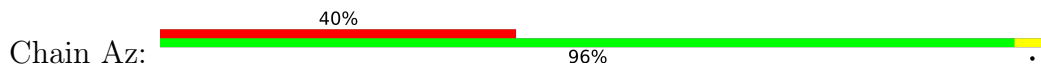
- Molecule 21: Mediator of RNA polymerase II transcription subunit 31



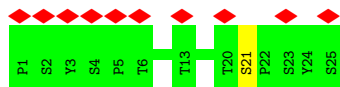
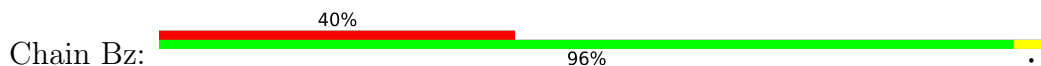
- Molecule 21: Mediator of RNA polymerase II transcription subunit 31



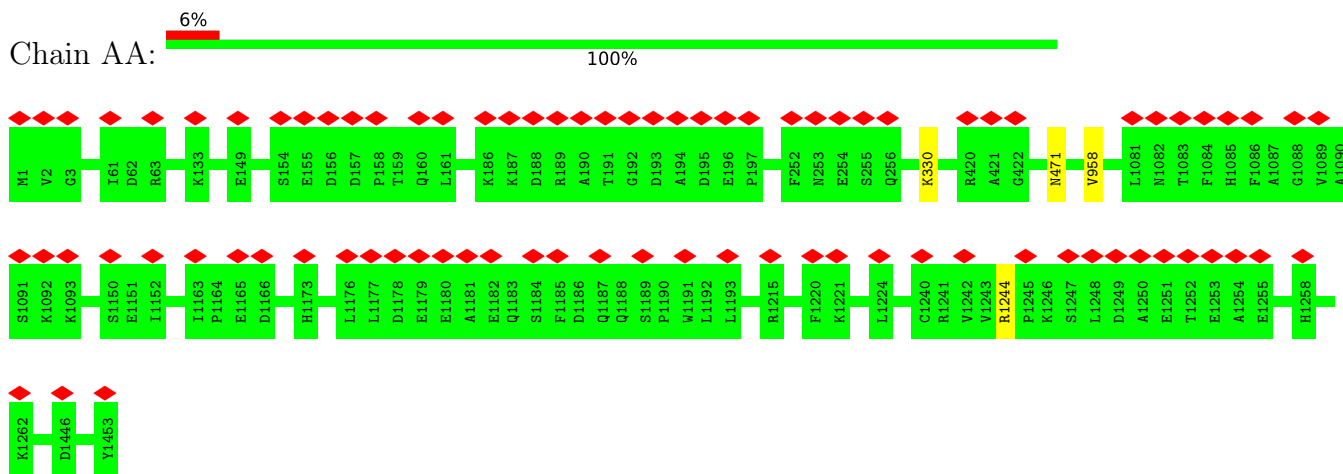
- Molecule 22: DNA-directed RNA polymerase II subunit RPB1



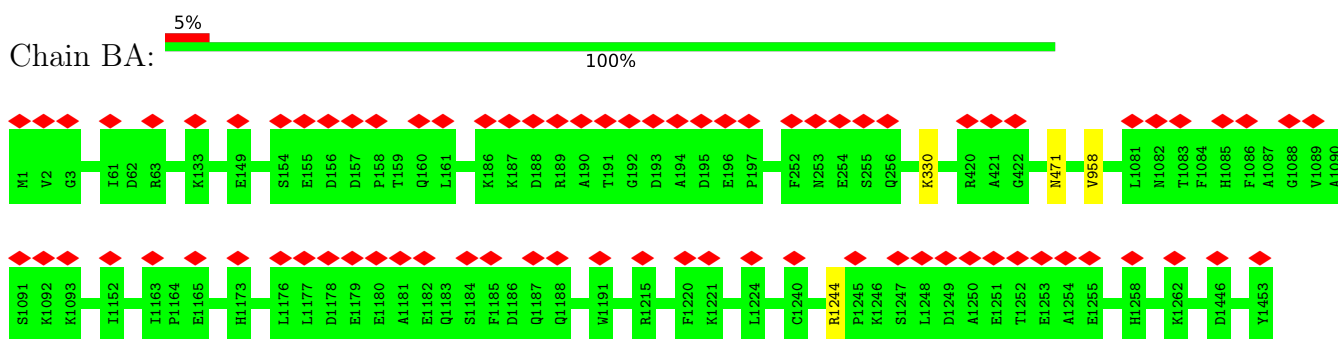
- Molecule 22: DNA-directed RNA polymerase II subunit RPB1



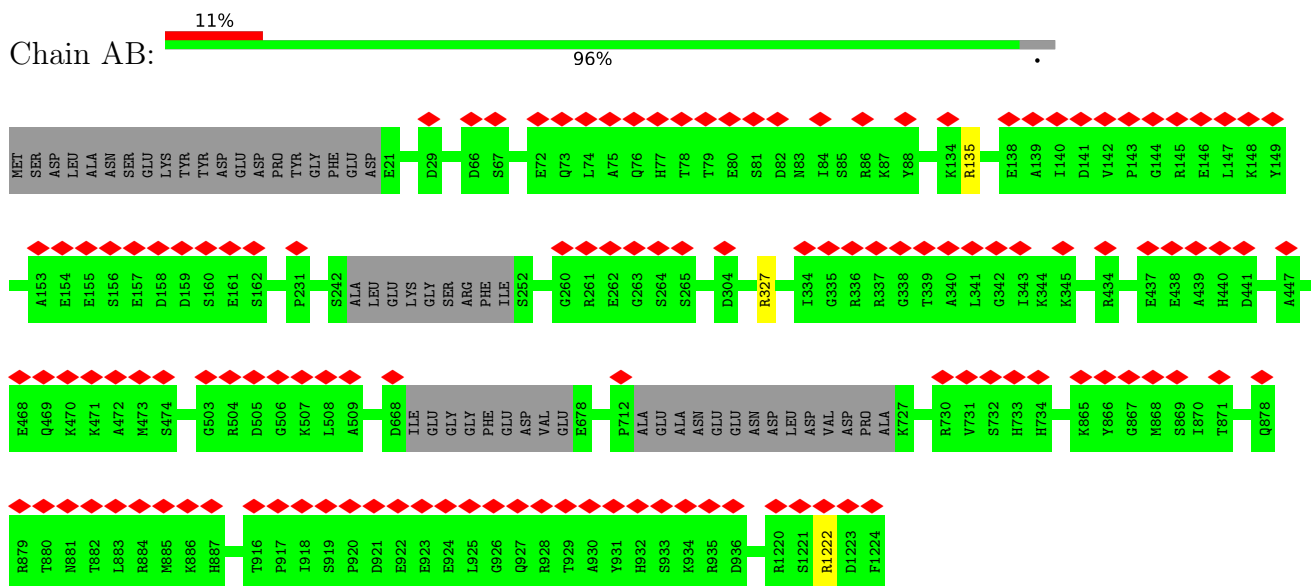
- Molecule 23: DNA-directed RNA polymerase II subunit RPB1



- Molecule 23: DNA-directed RNA polymerase II subunit RPB1

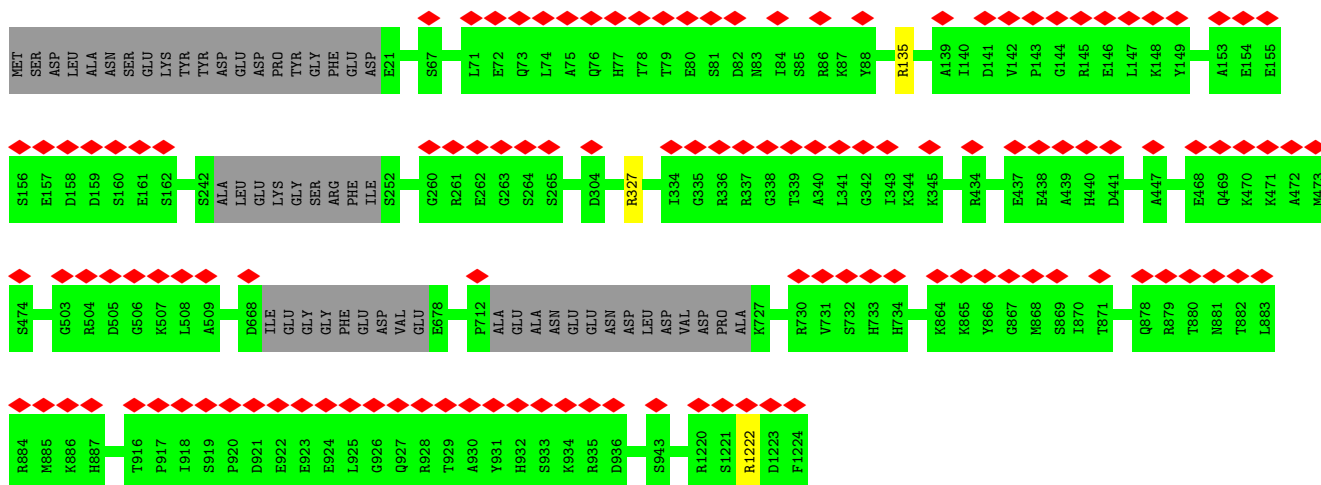


- Molecule 24: DNA-directed RNA polymerase II subunit RPB2

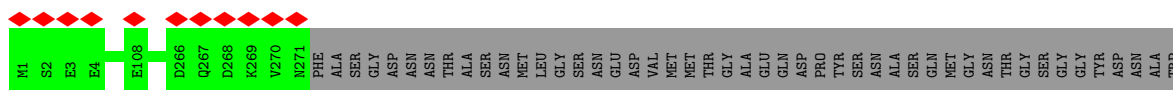
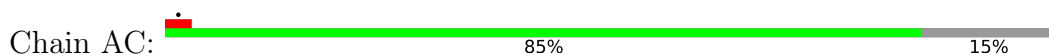


- Molecule 24: DNA-directed RNA polymerase II subunit RPB2

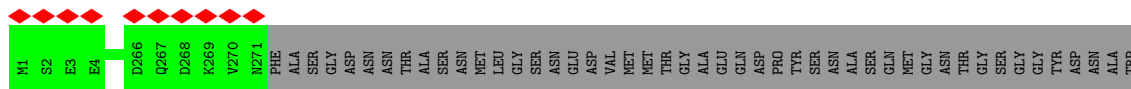
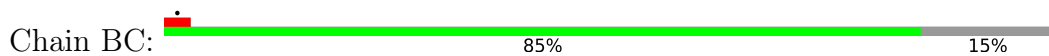




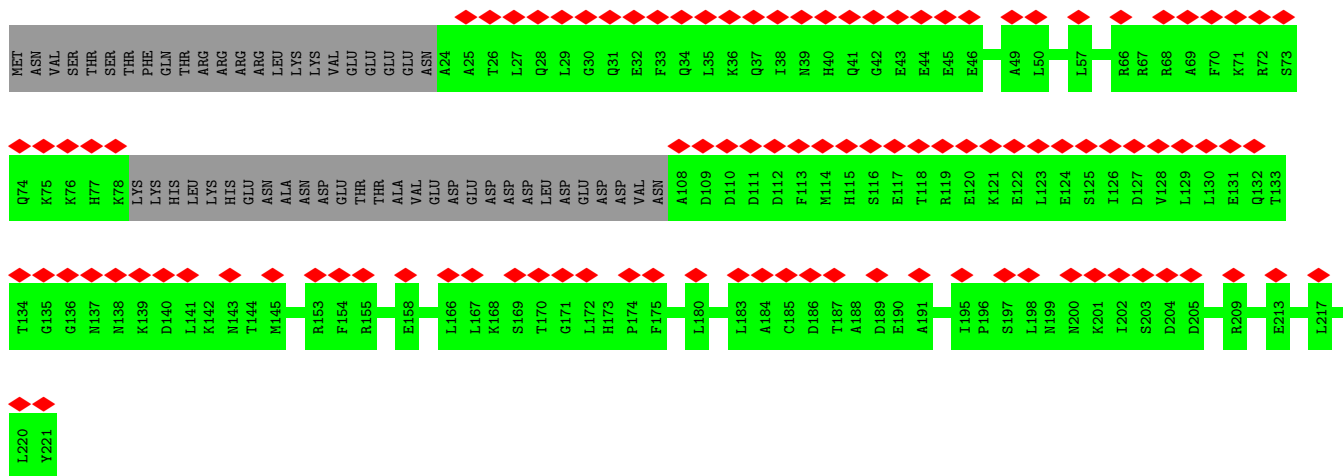
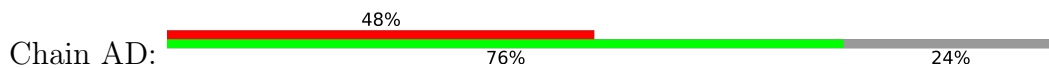
• Molecule 25: DNA-directed RNA polymerase II subunit RPB3



• Molecule 25: DNA-directed RNA polymerase II subunit RPB3

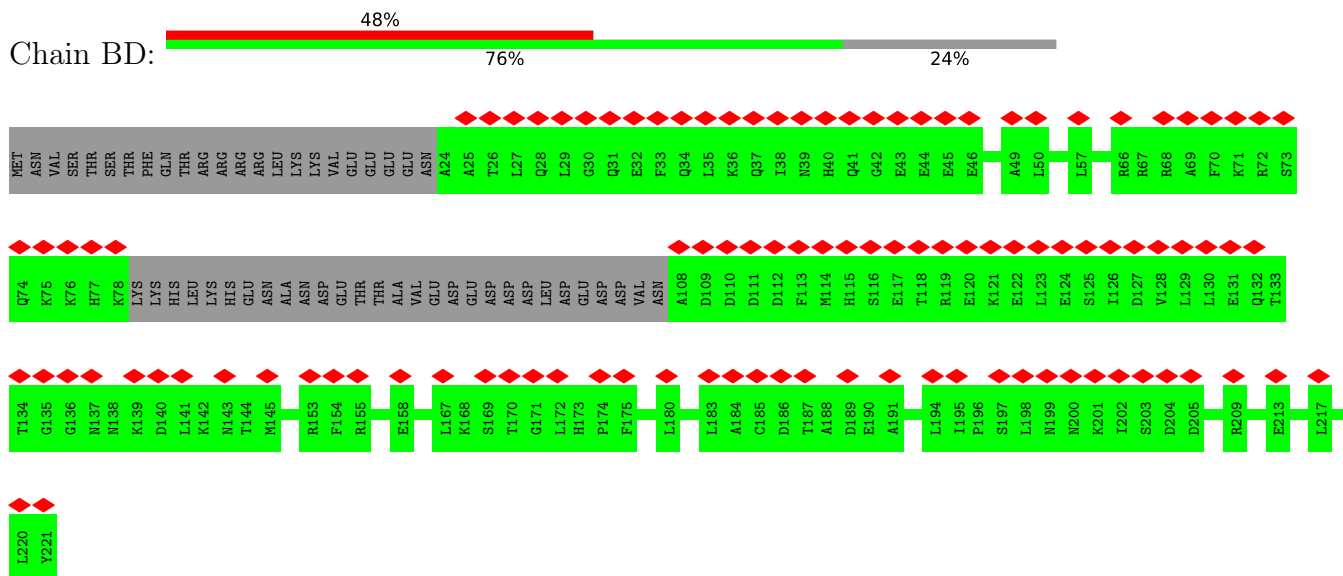


• Molecule 26: DNA-directed RNA polymerase II subunit RPB4

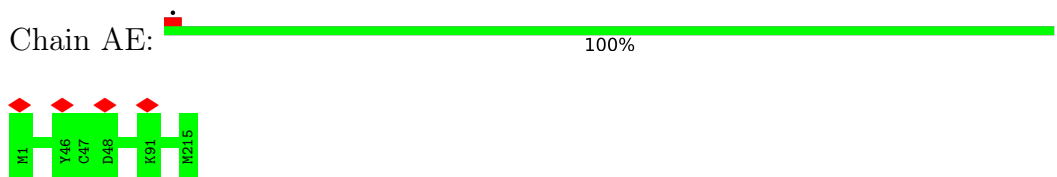


• Molecule 26: DNA-directed RNA polymerase II subunit RPB4

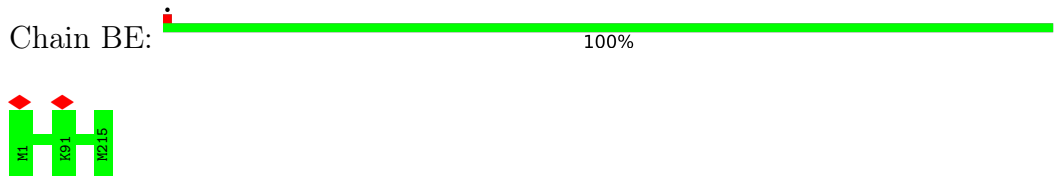




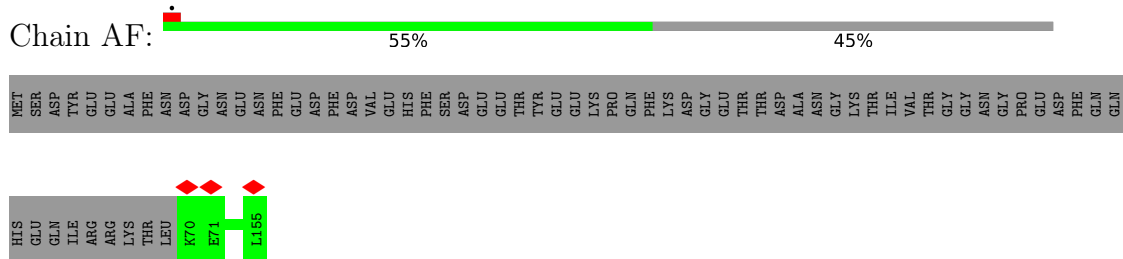
- Molecule 27: DNA-directed RNA polymerases I, II, and III subunit RPABC1



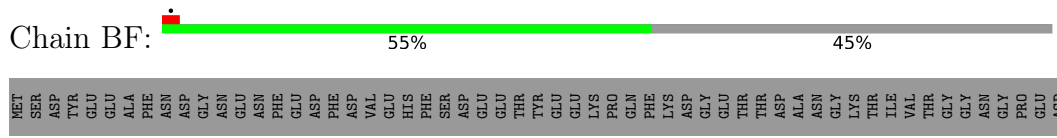
- Molecule 27: DNA-directed RNA polymerases I, II, and III subunit RPABC1

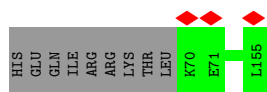


- Molecule 28: DNA-directed RNA polymerases I, II, and III subunit RPABC2



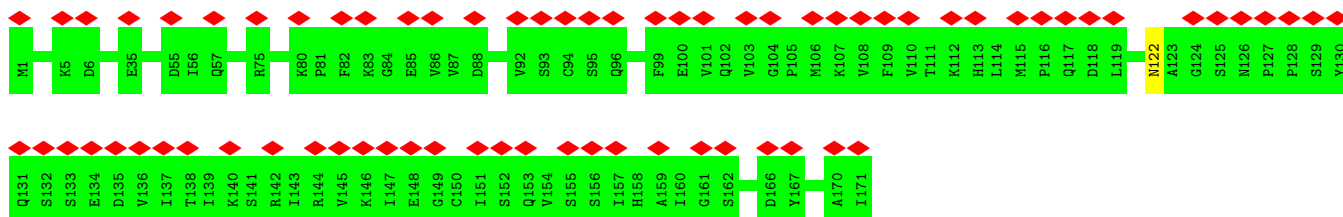
- Molecule 28: DNA-directed RNA polymerases I, II, and III subunit RPABC2





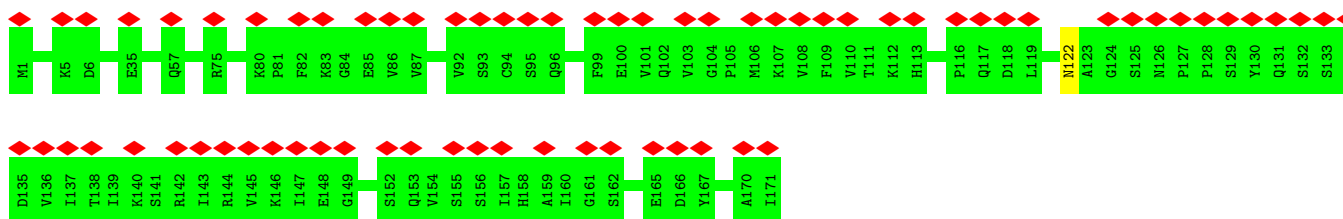
- Molecule 29: DNA-directed RNA polymerase II subunit RPB7

Chain AG: 42% 99%



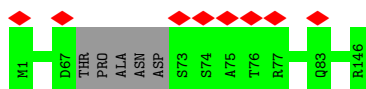
- Molecule 29: DNA-directed RNA polymerase II subunit RPB7

Chain BG: 41% 99%



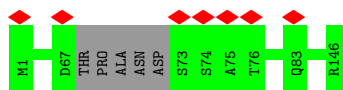
- Molecule 30: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain AH: 5% 97%



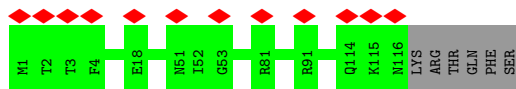
- Molecule 30: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain BH: 5% 97%

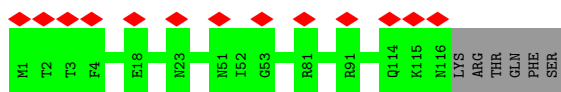


- Molecule 31: DNA-directed RNA polymerase II subunit RPB9

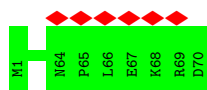
Chain AI: 10% 95% 5%



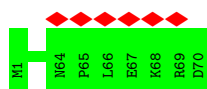
- Molecule 31: DNA-directed RNA polymerase II subunit RPB9



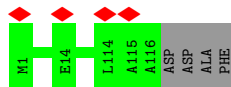
- Molecule 32: DNA-directed RNA polymerases I, II, and III subunit RPABC5



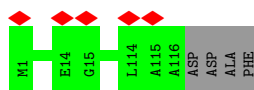
- Molecule 32: DNA-directed RNA polymerases I, II, and III subunit RPABC5



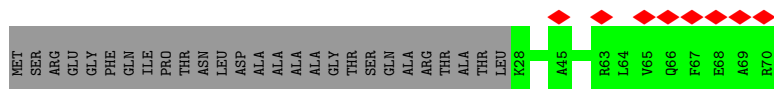
- Molecule 33: DNA-directed RNA polymerase II subunit RPB11



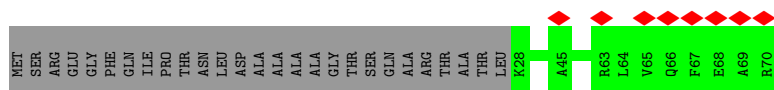
- Molecule 33: DNA-directed RNA polymerase II subunit RPB11



- Molecule 34: DNA-directed RNA polymerases I, II, and III subunit RPABC4

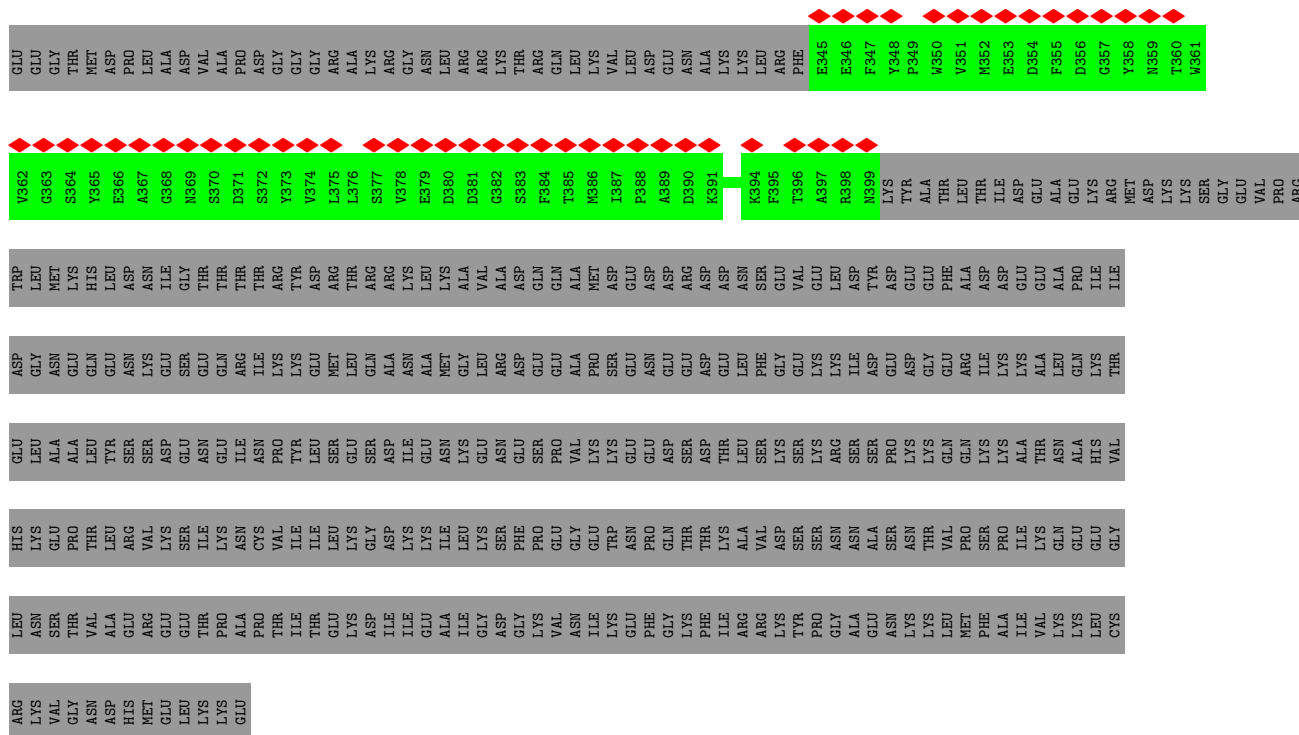


- Molecule 34: DNA-directed RNA polymerases I, II, and III subunit RPABC4

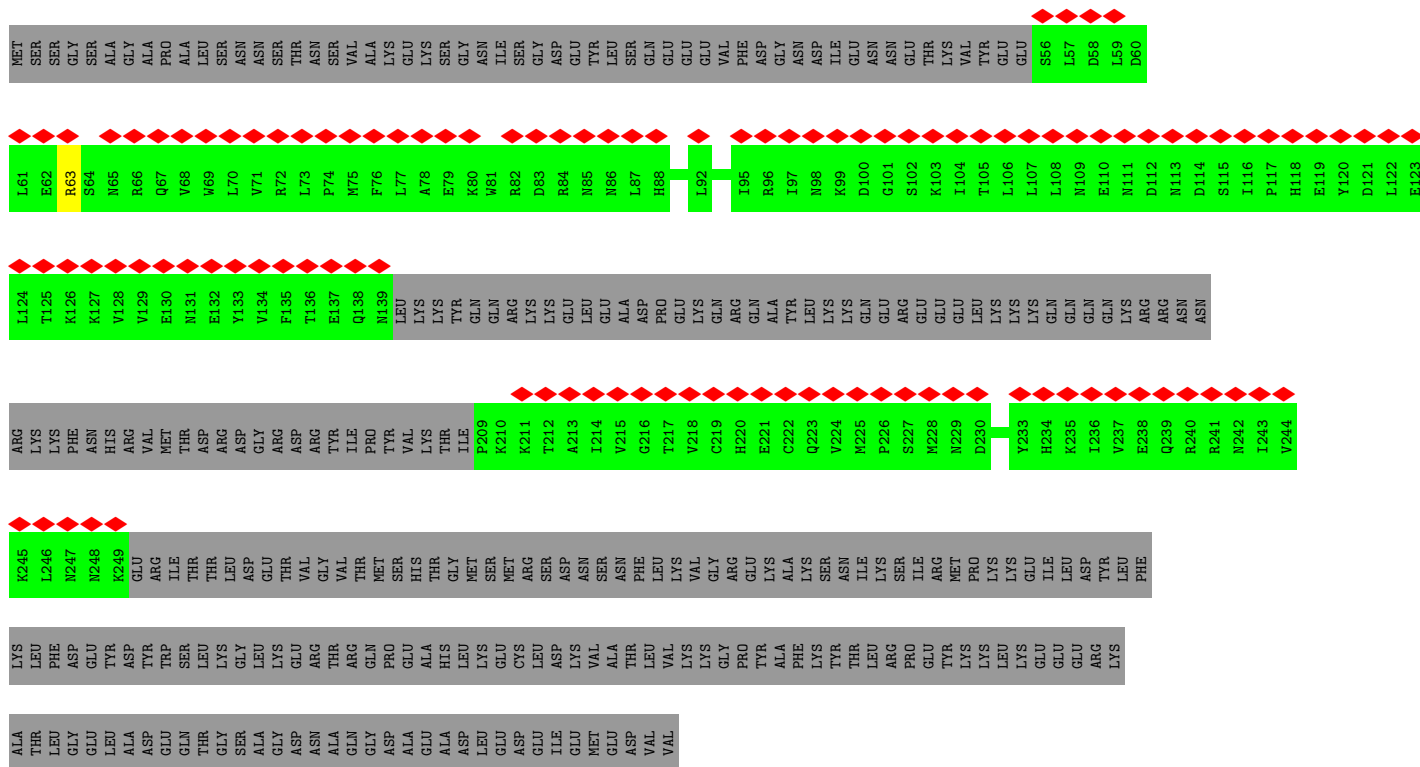






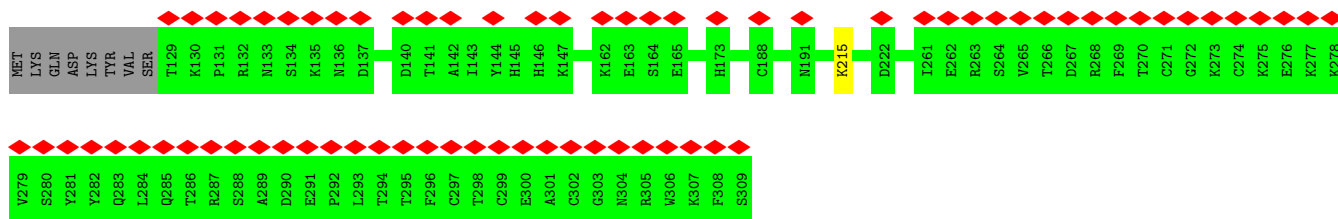


• Molecule 37: Transcription initiation factor IIF subunit beta

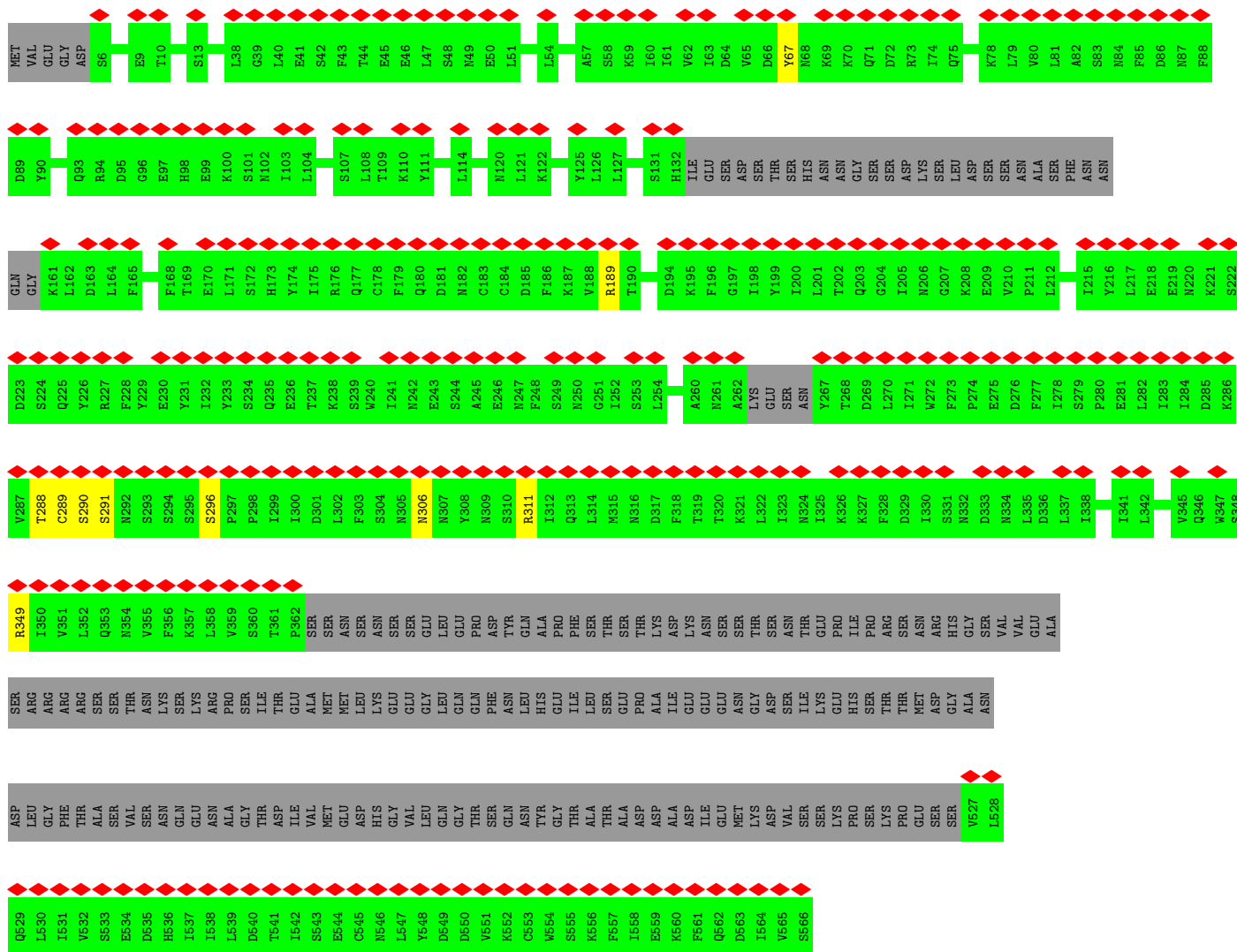


• Molecule 37: Transcription initiation factor IIF subunit beta

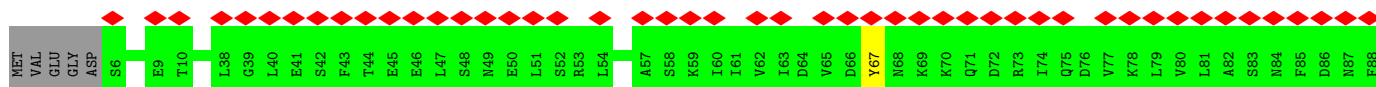




• Molecule 39: Mediator of RNA polymerase II transcription subunit 1



• Molecule 39: Mediator of RNA polymerase II transcription subunit 1









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1102984	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 ( $e^-/\text{\AA}^2$ )	42	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.857	Depositor
Minimum map value	-0.168	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	852.84, 891.48, 832.14	wwPDB
Map dimensions	618, 646, 603	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	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	A	1.63	17/868 (2.0%)	2.30	66/1337 (4.9%)
2	B	1.67	12/853 (1.4%)	2.56	86/1315 (6.5%)
3	Ao	0.23	0/904	0.52	0/1202
3	Bo	0.23	0/904	0.53	0/1202
4	Ab	0.27	0/520	0.49	0/693
4	Bb	0.27	0/520	0.49	0/693
5	Ac	0.25	0/902	0.52	0/1215
5	Bc	0.25	0/882	0.52	0/1187
6	An	0.35	0/7053	0.56	2/9524 (0.0%)
6	Bn	0.35	0/7053	0.56	3/9524 (0.0%)
7	Ae	0.24	0/6033	0.42	0/8183
7	Be	0.24	0/6033	0.42	0/8183
8	Ap	0.24	0/7413	0.44	0/10031
8	Bp	0.24	0/7413	0.44	0/10031
9	GA	1.55	10/736 (1.4%)	1.56	12/983 (1.2%)
9	GB	1.60	11/736 (1.5%)	1.57	13/983 (1.3%)
10	At	0.26	0/1635	0.50	0/2215
10	Bt	0.27	0/1635	0.50	0/2215
11	Ag	0.40	0/1453	0.68	2/1957 (0.1%)
11	Bg	0.40	0/1453	0.68	2/1957 (0.1%)
12	Ah	0.49	1/1207 (0.1%)	1.07	5/1636 (0.3%)
12	Bh	0.48	1/1207 (0.1%)	1.07	5/1636 (0.3%)
13	Ai	0.44	0/741	0.84	2/992 (0.2%)
13	Bi	0.44	0/741	0.84	2/992 (0.2%)
14	Aj	0.43	0/1204	0.68	1/1625 (0.1%)
14	Bj	0.43	0/1204	0.68	1/1625 (0.1%)
15	Ak	0.49	0/943	0.78	2/1263 (0.2%)
15	Bk	0.48	0/943	0.78	2/1263 (0.2%)
16	Aq	0.31	0/4246	0.54	1/5705 (0.0%)
16	Bq	0.31	0/4246	0.54	1/5705 (0.0%)
17	Ar	0.32	0/2030	0.53	1/2747 (0.0%)
17	Br	0.32	0/2030	0.53	1/2747 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
18	As	0.34	0/669	0.52	0/906
18	Bs	0.34	0/669	0.52	0/906
19	Au	0.39	0/985	0.74	0/1321
19	Bu	0.39	0/985	0.74	0/1321
20	Av	0.32	0/873	0.60	0/1177
20	Bv	0.32	0/873	0.60	0/1177
21	Aw	0.27	0/897	0.43	0/1219
21	Bw	0.27	0/897	0.43	0/1219
22	Az	0.27	0/195	0.44	0/270
22	Bz	0.27	0/195	0.44	0/270
23	AA	0.28	0/11633	0.52	0/15735
23	BA	0.28	0/11633	0.52	0/15735
24	AB	0.28	0/9520	0.53	0/12839
24	BB	0.28	0/9520	0.53	0/12839
25	AC	0.28	0/2171	0.50	0/2941
25	BC	0.28	0/2171	0.50	0/2941
26	AD	0.24	0/1365	0.44	0/1831
26	BD	0.24	0/1365	0.44	0/1831
27	AE	0.26	0/1796	0.50	0/2416
27	BE	0.26	0/1796	0.49	0/2416
28	AF	0.27	0/709	0.50	0/956
28	BF	0.28	0/709	0.50	0/956
29	AG	0.26	0/1368	0.50	0/1844
29	BG	0.26	0/1368	0.50	0/1844
30	AH	0.29	0/1144	0.53	0/1548
30	BH	0.29	0/1144	0.53	0/1548
31	AI	0.26	0/961	0.56	0/1294
31	BI	0.26	0/961	0.55	0/1294
32	AJ	0.29	0/587	0.57	0/786
32	BJ	0.29	0/587	0.57	0/786
33	AK	0.29	0/947	0.51	0/1279
33	BK	0.29	0/947	0.51	0/1279
34	AL	0.26	0/346	0.61	0/457
34	BL	0.26	0/346	0.62	0/457
35	AM	0.26	0/267	0.46	0/362
35	BM	0.27	0/267	0.47	0/362
36	AP	0.26	0/886	0.47	0/1198
36	BP	0.26	0/886	0.47	0/1198
37	AQ	0.24	0/1049	0.48	0/1413
37	BQ	0.24	0/1049	0.48	0/1413
38	AS	0.26	0/1462	0.48	0/1973
38	BS	0.26	0/1462	0.48	0/1973
39	Aa	0.65	0/3067	0.86	4/4148 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	Ba	0.65	0/3067	0.86	4/4148 (0.1%)
40	Ad	0.27	0/1405	0.58	1/1889 (0.1%)
40	Bd	0.27	0/1405	0.58	1/1889 (0.1%)
41	Af	0.27	0/1440	0.50	0/1946
41	Bf	0.27	0/1440	0.50	0/1946
All	All	0.39	52/167225 (0.0%)	0.63	220/226062 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	GA	0	2
11	Ag	0	1
11	Bg	0	1
All	All	0	4

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	GB	31	CYS	CB-SG	13.47	2.05	1.82
1	A	7	DG	C6-O6	10.98	1.34	1.24
9	GA	31	CYS	CB-SG	10.32	1.99	1.82
1	A	13	DT	C1'-N1	9.04	1.61	1.49
2	B	39	DG	C3'-O3'	8.95	1.55	1.44

The worst 5 of 220 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	31	DT	N3-C2-O2	-25.49	107.01	122.30
12	Ah	142	ASP	O-C-N	-22.09	87.36	122.70
12	Bh	142	ASP	O-C-N	-22.07	87.39	122.70
1	A	13	DT	O4'-C1'-N1	-17.55	95.72	108.00
12	Ah	142	ASP	CA-C-N	15.81	151.99	117.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	Ag	165	TYR	Sidechain

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Mol	Chain	Res	Type	Group
11	Bg	165	TYR	Sidechain
9	GA	74	ARG	Peptide
9	GA	75	GLU	Peptide

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

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	
3	Ao	109/1081 (10%)	109 (100%)	0	0	100	100
3	Bo	109/1081 (10%)	109 (100%)	0	0	100	100
4	Ab	61/431 (14%)	61 (100%)	0	0	100	100
4	Bb	61/431 (14%)	61 (100%)	0	0	100	100
5	Ac	108/397 (27%)	107 (99%)	1 (1%)	0	100	100
5	Bc	105/397 (26%)	104 (99%)	1 (1%)	0	100	100
6	An	830/1082 (77%)	817 (98%)	12 (1%)	1 (0%)	51	81
6	Bn	830/1082 (77%)	818 (99%)	11 (1%)	1 (0%)	51	81
7	Ae	721/1132 (64%)	711 (99%)	10 (1%)	0	100	100
7	Be	721/1132 (64%)	712 (99%)	9 (1%)	0	100	100
8	Ap	885/974 (91%)	877 (99%)	8 (1%)	0	100	100
8	Bp	885/974 (91%)	875 (99%)	10 (1%)	0	100	100
9	GA	87/147 (59%)	72 (83%)	10 (12%)	5 (6%)	1	11
9	GB	87/147 (59%)	76 (87%)	8 (9%)	3 (3%)	3	22
10	At	208/210 (99%)	206 (99%)	2 (1%)	0	100	100
10	Bt	208/210 (99%)	206 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	Ag	161/222 (72%)	159 (99%)	2 (1%)	0	100	100
11	Bg	161/222 (72%)	160 (99%)	1 (1%)	0	100	100
12	Ah	142/223 (64%)	135 (95%)	5 (4%)	2 (1%)	11	38
12	Bh	142/223 (64%)	135 (95%)	5 (4%)	2 (1%)	11	38
13	Ai	82/149 (55%)	80 (98%)	2 (2%)	0	100	100
13	Bi	82/149 (55%)	80 (98%)	2 (2%)	0	100	100
14	Aj	144/157 (92%)	142 (99%)	2 (1%)	0	100	100
14	Bj	144/157 (92%)	142 (99%)	2 (1%)	0	100	100
15	Ak	111/115 (96%)	110 (99%)	1 (1%)	0	100	100
15	Bk	111/115 (96%)	110 (99%)	1 (1%)	0	100	100
16	Aq	507/687 (74%)	498 (98%)	7 (1%)	2 (0%)	34	66
16	Bq	507/687 (74%)	498 (98%)	7 (1%)	2 (0%)	34	66
17	Ar	249/307 (81%)	245 (98%)	4 (2%)	0	100	100
17	Br	249/307 (81%)	245 (98%)	4 (2%)	0	100	100
18	As	77/220 (35%)	76 (99%)	1 (1%)	0	100	100
18	Bs	77/220 (35%)	76 (99%)	1 (1%)	0	100	100
19	Au	118/140 (84%)	117 (99%)	1 (1%)	0	100	100
19	Bu	118/140 (84%)	117 (99%)	1 (1%)	0	100	100
20	Av	105/120 (88%)	103 (98%)	2 (2%)	0	100	100
20	Bv	105/120 (88%)	102 (97%)	3 (3%)	0	100	100
21	Aw	99/127 (78%)	97 (98%)	2 (2%)	0	100	100
21	Bw	99/127 (78%)	97 (98%)	2 (2%)	0	100	100
22	Az	23/25 (92%)	21 (91%)	1 (4%)	1 (4%)	2	16
22	Bz	23/25 (92%)	21 (91%)	1 (4%)	1 (4%)	2	16
23	AA	1451/1453 (100%)	1405 (97%)	45 (3%)	1 (0%)	51	81
23	BA	1451/1453 (100%)	1406 (97%)	44 (3%)	1 (0%)	51	81
24	AB	1164/1224 (95%)	1131 (97%)	33 (3%)	0	100	100
24	BB	1164/1224 (95%)	1131 (97%)	33 (3%)	0	100	100
25	AC	269/318 (85%)	261 (97%)	8 (3%)	0	100	100
25	BC	269/318 (85%)	261 (97%)	8 (3%)	0	100	100
26	AD	165/221 (75%)	163 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	BD	165/221 (75%)	163 (99%)	2 (1%)	0	100	100
27	AE	213/215 (99%)	210 (99%)	3 (1%)	0	100	100
27	BE	213/215 (99%)	210 (99%)	3 (1%)	0	100	100
28	AF	84/155 (54%)	83 (99%)	1 (1%)	0	100	100
28	BF	84/155 (54%)	83 (99%)	1 (1%)	0	100	100
29	AG	169/171 (99%)	166 (98%)	3 (2%)	0	100	100
29	BG	169/171 (99%)	166 (98%)	3 (2%)	0	100	100
30	AH	137/146 (94%)	134 (98%)	3 (2%)	0	100	100
30	BH	137/146 (94%)	134 (98%)	3 (2%)	0	100	100
31	AI	114/122 (93%)	113 (99%)	1 (1%)	0	100	100
31	BI	114/122 (93%)	113 (99%)	1 (1%)	0	100	100
32	AJ	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
32	BJ	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
33	AK	114/120 (95%)	112 (98%)	2 (2%)	0	100	100
33	BK	114/120 (95%)	112 (98%)	2 (2%)	0	100	100
34	AL	41/70 (59%)	39 (95%)	2 (5%)	0	100	100
34	BL	41/70 (59%)	39 (95%)	2 (5%)	0	100	100
35	AM	33/345 (10%)	33 (100%)	0	0	100	100
35	BM	33/345 (10%)	33 (100%)	0	0	100	100
36	AP	99/735 (14%)	99 (100%)	0	0	100	100
36	BP	99/735 (14%)	99 (100%)	0	0	100	100
37	AQ	121/400 (30%)	121 (100%)	0	0	100	100
37	BQ	121/400 (30%)	121 (100%)	0	0	100	100
38	AS	179/309 (58%)	177 (99%)	2 (1%)	0	100	100
38	BS	179/309 (58%)	177 (99%)	2 (1%)	0	100	100
39	Aa	357/566 (63%)	343 (96%)	11 (3%)	3 (1%)	19	51
39	Ba	357/566 (63%)	343 (96%)	11 (3%)	3 (1%)	19	51
40	Ad	165/284 (58%)	163 (99%)	2 (1%)	0	100	100
40	Bd	165/284 (58%)	163 (99%)	2 (1%)	0	100	100
41	Af	163/295 (55%)	161 (99%)	2 (1%)	0	100	100
41	Bf	163/295 (55%)	161 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	19863/30330 (66%)	19446 (98%)	389 (2%)	28 (0%)	54	81

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	GA	29	ALA
9	GA	75	GLU
9	GA	76	ASP
12	Ah	142	ASP
16	Aq	319	LYS

### 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	
3	Ao	103/944 (11%)	100 (97%)	3 (3%)	42	69
3	Bo	103/944 (11%)	100 (97%)	3 (3%)	42	69
4	Ab	60/389 (15%)	59 (98%)	1 (2%)	60	78
4	Bb	60/389 (15%)	59 (98%)	1 (2%)	60	78
5	Ac	100/339 (30%)	100 (100%)	0	100	100
5	Bc	98/339 (29%)	98 (100%)	0	100	100
6	An	797/1001 (80%)	791 (99%)	6 (1%)	81	89
6	Bn	797/1001 (80%)	791 (99%)	6 (1%)	81	89
7	Ae	684/1053 (65%)	683 (100%)	1 (0%)	93	97
7	Be	684/1053 (65%)	683 (100%)	1 (0%)	93	97
8	Ap	826/897 (92%)	824 (100%)	2 (0%)	93	97
8	Bp	826/897 (92%)	824 (100%)	2 (0%)	93	97
9	GA	84/138 (61%)	67 (80%)	17 (20%)	1	5
9	GB	84/138 (61%)	66 (79%)	18 (21%)	1	4
10	At	178/178 (100%)	178 (100%)	0	100	100
10	Bt	178/178 (100%)	178 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	Ag	162/208 (78%)	160 (99%)	2 (1%)	71	83
11	Bg	162/208 (78%)	160 (99%)	2 (1%)	71	83
12	Ah	135/207 (65%)	133 (98%)	2 (2%)	65	81
12	Bh	135/207 (65%)	133 (98%)	2 (2%)	65	81
13	Ai	85/144 (59%)	83 (98%)	2 (2%)	49	73
13	Bi	85/144 (59%)	83 (98%)	2 (2%)	49	73
14	Aj	136/145 (94%)	135 (99%)	1 (1%)	84	90
14	Bj	136/145 (94%)	135 (99%)	1 (1%)	84	90
15	Ak	108/108 (100%)	107 (99%)	1 (1%)	78	87
15	Bk	108/108 (100%)	107 (99%)	1 (1%)	78	87
16	Aq	482/642 (75%)	479 (99%)	3 (1%)	86	91
16	Bq	482/642 (75%)	479 (99%)	3 (1%)	86	91
17	Ar	228/280 (81%)	228 (100%)	0	100	100
17	Br	228/280 (81%)	228 (100%)	0	100	100
18	As	75/195 (38%)	74 (99%)	1 (1%)	69	82
18	Bs	75/195 (38%)	74 (99%)	1 (1%)	69	82
19	Au	115/132 (87%)	110 (96%)	5 (4%)	29	59
19	Bu	115/132 (87%)	110 (96%)	5 (4%)	29	59
20	Av	101/112 (90%)	100 (99%)	1 (1%)	76	86
20	Bv	101/112 (90%)	100 (99%)	1 (1%)	76	86
21	Aw	97/117 (83%)	97 (100%)	0	100	100
21	Bw	97/117 (83%)	97 (100%)	0	100	100
22	Az	25/25 (100%)	25 (100%)	0	100	100
22	Bz	25/25 (100%)	25 (100%)	0	100	100
23	AA	1268/1268 (100%)	1265 (100%)	3 (0%)	93	97
23	BA	1268/1268 (100%)	1265 (100%)	3 (0%)	93	97
24	AB	1018/1061 (96%)	1015 (100%)	3 (0%)	92	96
24	BB	1018/1061 (96%)	1015 (100%)	3 (0%)	92	96
25	AC	239/274 (87%)	239 (100%)	0	100	100
25	BC	239/274 (87%)	239 (100%)	0	100	100
26	AD	150/200 (75%)	150 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	BD	150/200 (75%)	150 (100%)	0	100	100
27	AE	197/197 (100%)	197 (100%)	0	100	100
27	BE	197/197 (100%)	197 (100%)	0	100	100
28	AF	76/137 (56%)	76 (100%)	0	100	100
28	BF	76/137 (56%)	76 (100%)	0	100	100
29	AG	152/152 (100%)	151 (99%)	1 (1%)	84	90
29	BG	152/152 (100%)	151 (99%)	1 (1%)	84	90
30	AH	124/128 (97%)	124 (100%)	0	100	100
30	BH	124/128 (97%)	124 (100%)	0	100	100
31	AI	110/116 (95%)	110 (100%)	0	100	100
31	BI	110/116 (95%)	110 (100%)	0	100	100
32	AJ	65/65 (100%)	65 (100%)	0	100	100
32	BJ	65/65 (100%)	65 (100%)	0	100	100
33	AK	99/102 (97%)	99 (100%)	0	100	100
33	BK	99/102 (97%)	99 (100%)	0	100	100
34	AL	38/57 (67%)	38 (100%)	0	100	100
34	BL	38/57 (67%)	38 (100%)	0	100	100
35	AM	32/299 (11%)	32 (100%)	0	100	100
35	BM	32/299 (11%)	32 (100%)	0	100	100
36	AP	95/641 (15%)	95 (100%)	0	100	100
36	BP	95/641 (15%)	95 (100%)	0	100	100
37	AQ	119/363 (33%)	118 (99%)	1 (1%)	81	89
37	BQ	119/363 (33%)	117 (98%)	2 (2%)	60	78
38	AS	158/274 (58%)	157 (99%)	1 (1%)	86	91
38	BS	158/274 (58%)	157 (99%)	1 (1%)	86	91
39	Aa	350/528 (66%)	347 (99%)	3 (1%)	78	87
39	Ba	350/528 (66%)	347 (99%)	3 (1%)	78	87
40	Ad	158/258 (61%)	157 (99%)	1 (1%)	86	91
40	Bd	158/258 (61%)	157 (99%)	1 (1%)	86	91
41	Af	158/259 (61%)	157 (99%)	1 (1%)	86	91
41	Bf	158/259 (61%)	157 (99%)	1 (1%)	86	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	18372/27266 (67%)	18246 (99%)	126 (1%)	84 90

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	Aq	614	ARG
20	Bv	45	ASN
24	AB	1222	ARG
19	Bu	137	LYS
37	BQ	63	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
6	Bn	250	ASN
8	Bp	536	GLN
39	Ba	235	GLN
6	Bn	913	ASN
7	Be	916	ASN

### 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 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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
45	ASP	Bc	110	-	6,8,8	1.20	1 (16%)	8,10,10	1.27	1 (12%)
43	THR	Bc	108	-	5,6,7	0.56	0	6,7,9	0.84	0
44	ALA	Bc	109	-	3,4,5	0.73	0	2,4,6	1.16	0

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
45	ASP	Bc	110	-	-	4/8/8/8	-
43	THR	Bc	108	-	-	1/5/6/8	-
44	ALA	Bc	109	-	-	0/0/2/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	Bc	110	ASP	OXT-C	-2.14	1.23	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	Bc	110	ASP	OXT-C-CA	2.17	120.77	113.38

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	Bc	108	THR	O-C-CA-CB
45	Bc	110	ASP	O-C-CA-N
45	Bc	110	ASP	OXT-C-CA-N
45	Bc	110	ASP	N-CA-CB-CG
45	Bc	110	ASP	C-CA-CB-CG

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
14	Aj	1
14	Bj	1
15	Ak	1
15	Bk	1
13	Ai	1
13	Bi	1
11	Ag	1
11	Bg	1

The worst 5 of 8 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Aj	77:VAL	C	78:ASP	N	3.28
1	Bj	77:VAL	C	78:ASP	N	3.28
1	Ak	86:VAL	C	87:ASN	N	3.04
1	Bk	86:VAL	C	87:ASN	N	3.04
1	Ai	118:SER	C	119:PRO	N	2.69

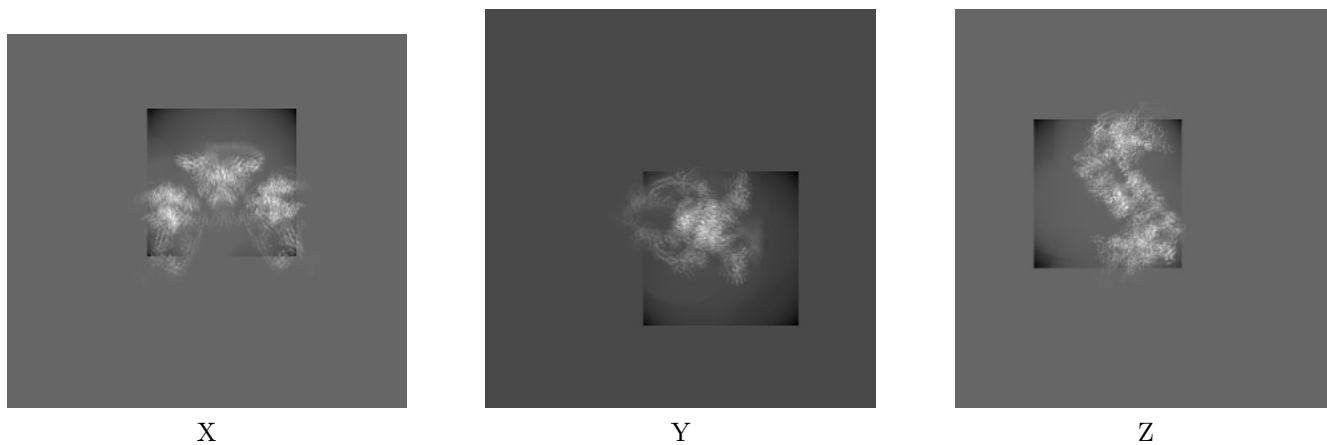
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26551. 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](#)

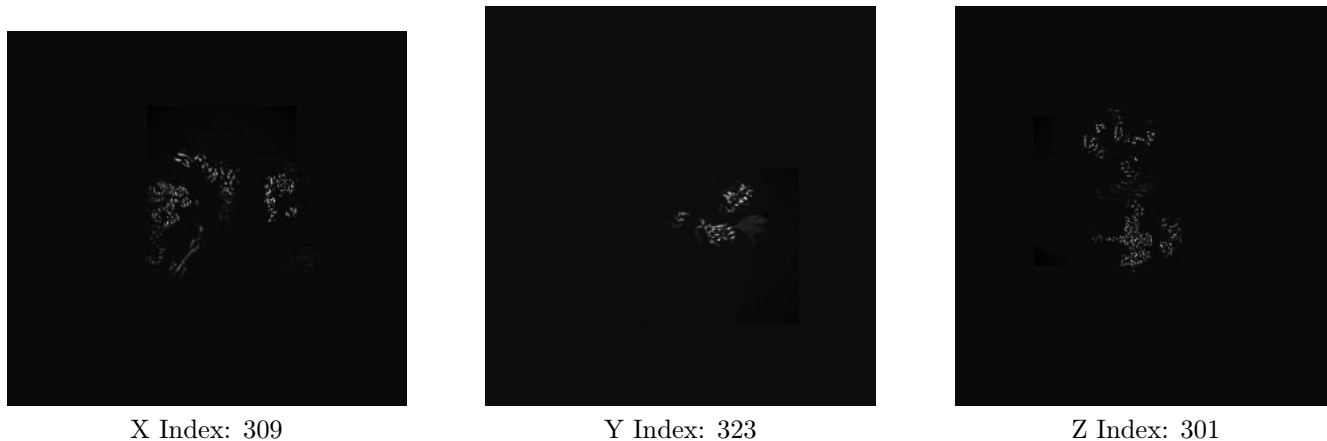
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map

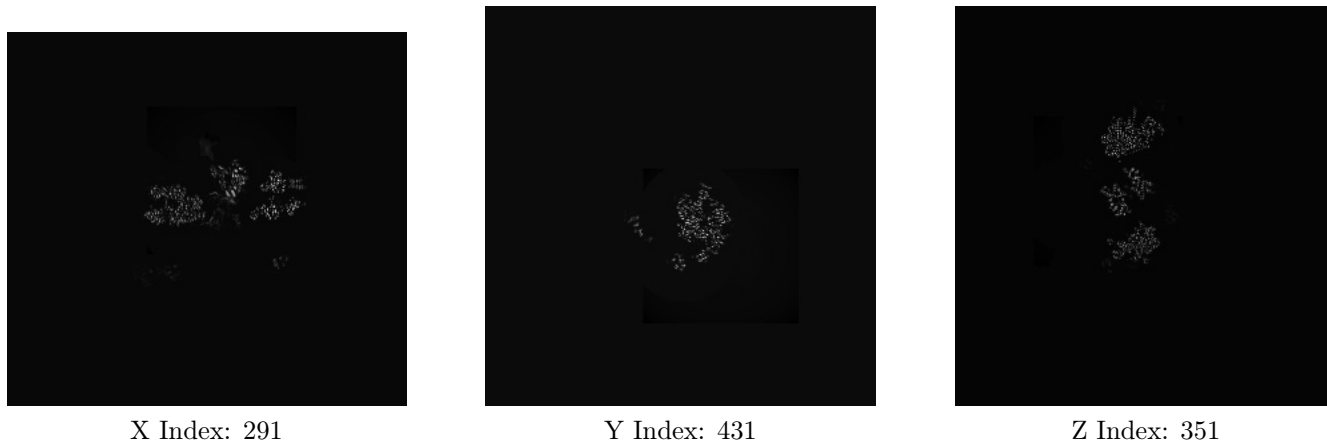




The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



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



The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

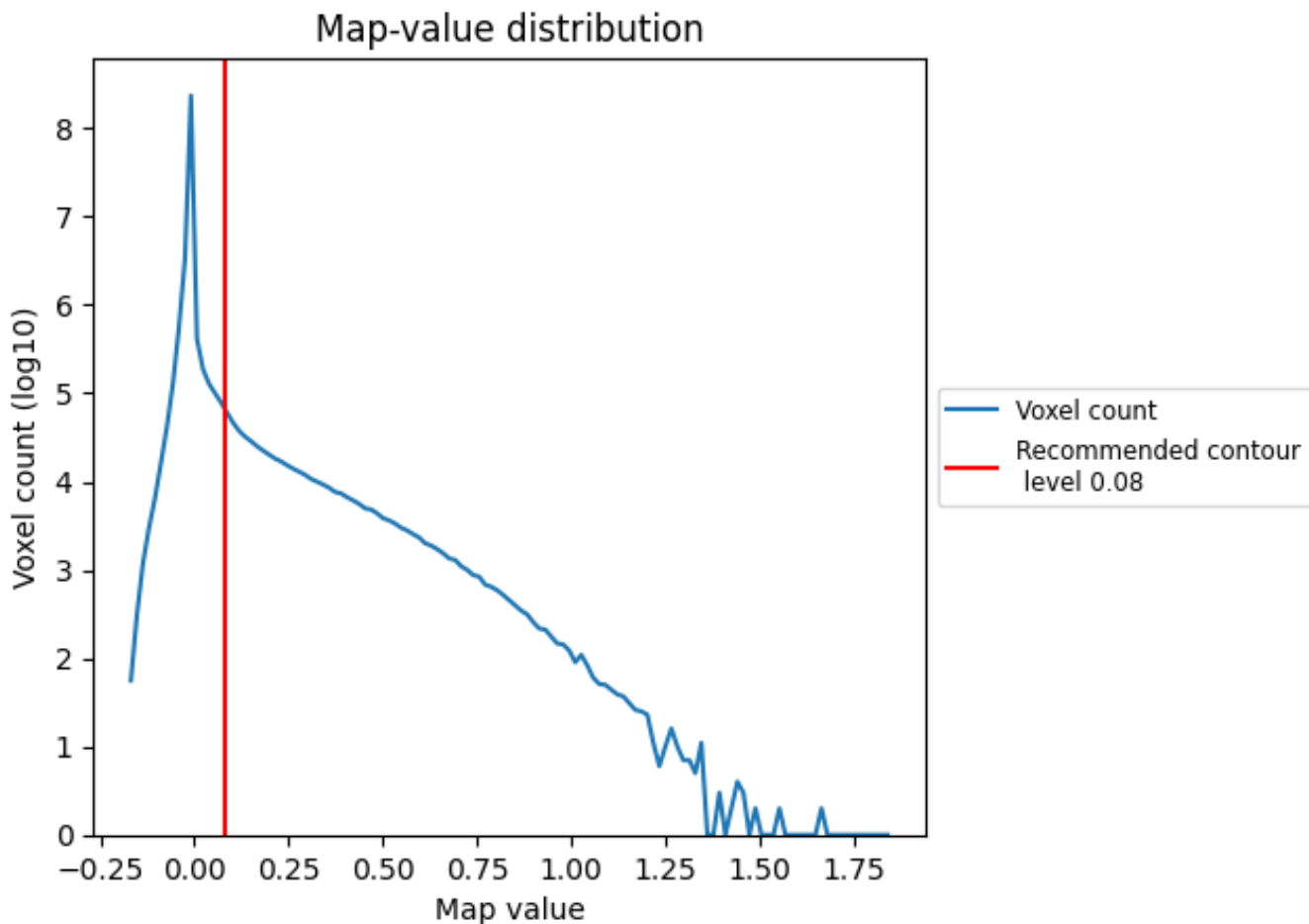
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

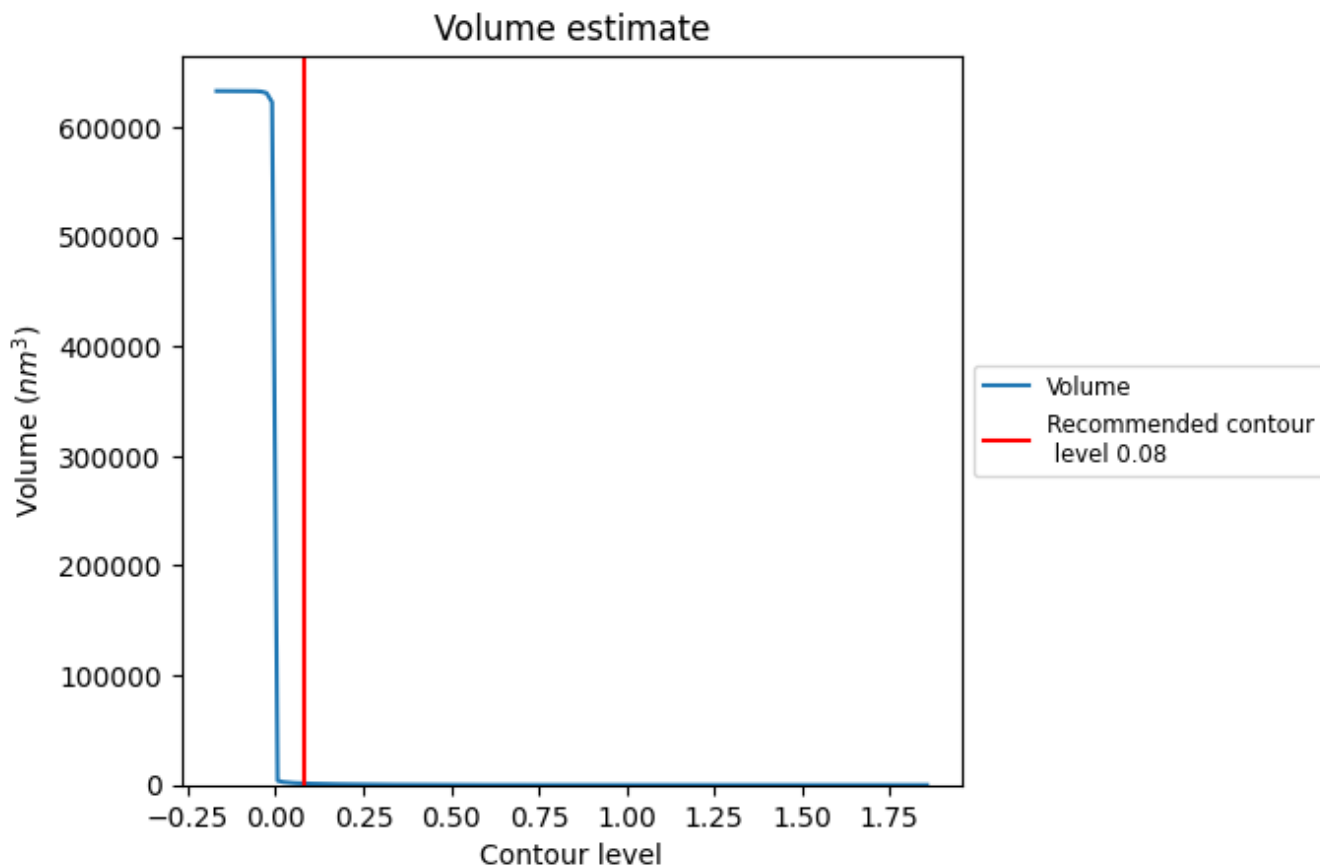
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1377  $\text{nm}^3$ ; this corresponds to an approximate mass of 1244 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.

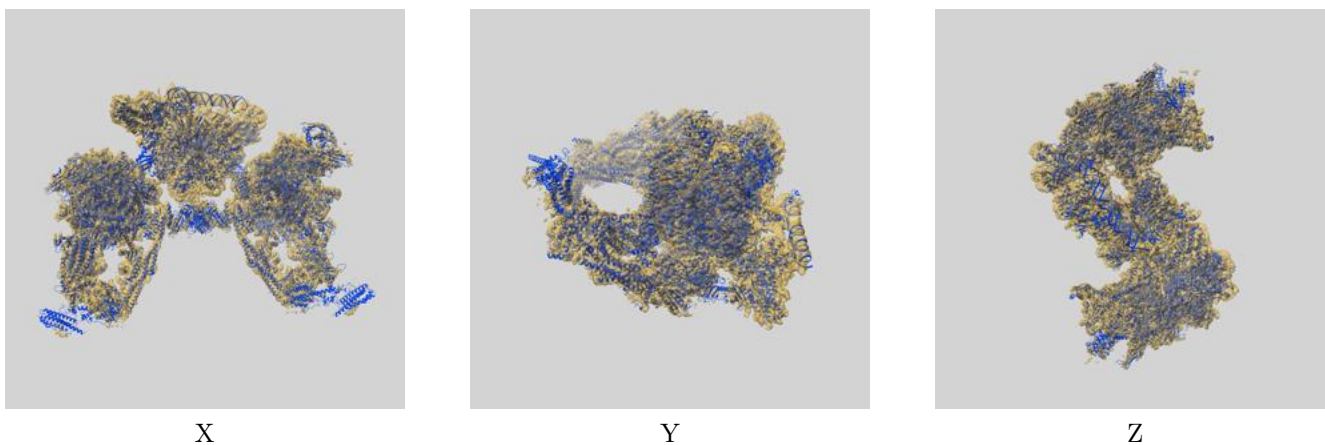
## 8 Fourier-Shell correlation

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

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

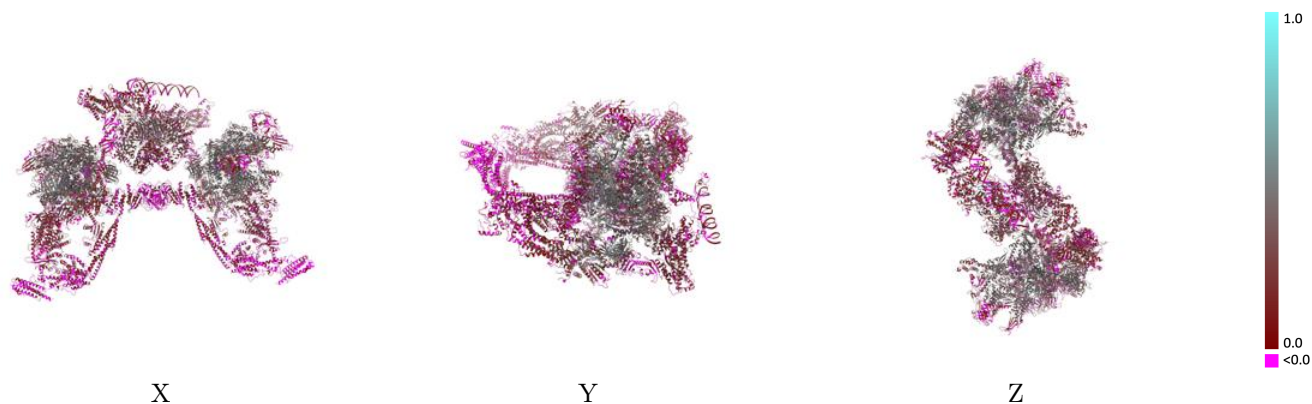
This section contains information regarding the fit between EMDB map EMD-26551 and PDB model 7UIO. Per-residue inclusion information can be found in section 3 on page 16.

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



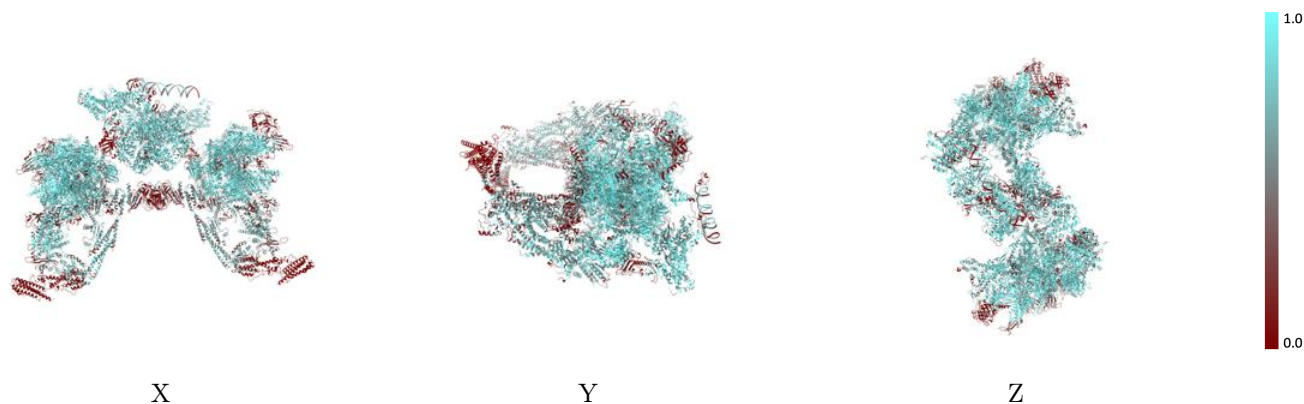
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



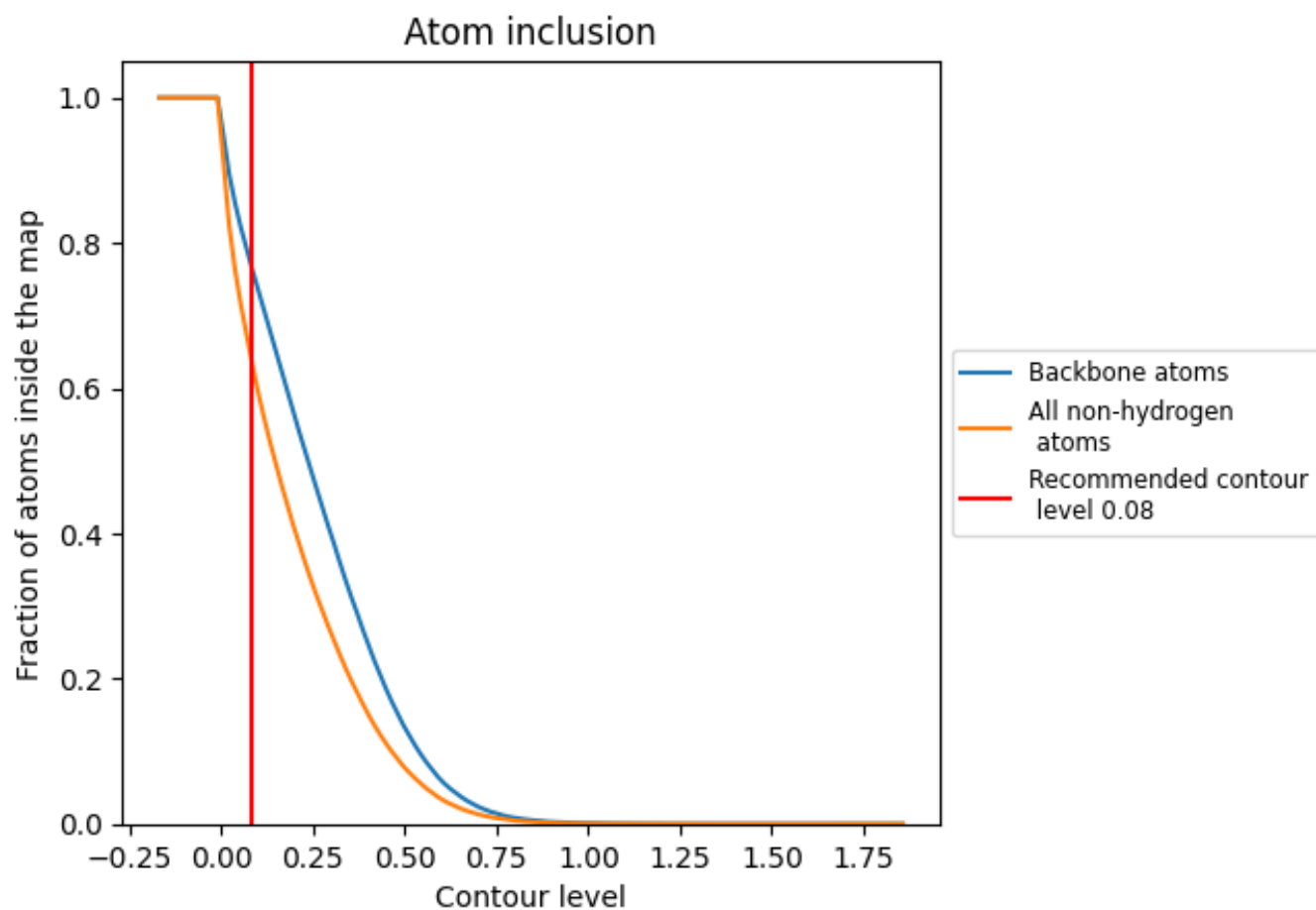
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 77% of all backbone atoms, 64% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6444	 0.2390
A	 0.4755	 0.0510
AA	 0.8382	 0.3950
AB	 0.7999	 0.3830
AC	 0.8532	 0.4170
AD	 0.3121	 0.0760
AE	 0.8328	 0.3800
AF	 0.8513	 0.4290
AG	 0.4902	 0.2330
AH	 0.8333	 0.4180
AI	 0.7702	 0.3470
AJ	 0.7946	 0.3470
AK	 0.8483	 0.4140
AL	 0.6495	 0.2930
AM	 0.8692	 0.4370
AP	 0.1720	 0.1230
AQ	 0.0998	 0.0740
AS	 0.4472	 0.1410
Aa	 0.1938	 0.0130
Ab	 0.8230	 0.1860
Ac	 0.7423	 0.1550
Ad	 0.5099	 0.0600
Ae	 0.7556	 0.2180
Af	 0.4840	 0.0830
Ag	 0.4269	 0.0400
Ah	 0.5967	 0.1310
Ai	 0.5049	 0.0870
Aj	 0.0378	 -0.0370
Ak	 0.6460	 0.1780
An	 0.4208	 0.1050
Ao	 0.7241	 0.1500
Ap	 0.7365	 0.2470
Aq	 0.5930	 0.1740
Ar	 0.8473	 0.4070
As	 0.0187	 -0.0400











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Chain	Atom inclusion	Q-score
At	 0.8403	 0.4070
Au	 0.4365	 0.0370
Av	 0.6156	 0.1580
Aw	 0.6332	 0.0890
Az	 0.5304	 0.1110
B	 0.4168	 0.0490
BA	 0.8435	 0.3860
BB	 0.8034	 0.3730
BC	 0.8608	 0.4070
BD	 0.3068	 0.0790
BE	 0.8404	 0.3790
BF	 0.8557	 0.4160
BG	 0.4818	 0.2340
BH	 0.8397	 0.4090
BI	 0.7625	 0.3380
BJ	 0.7982	 0.3390
BK	 0.8515	 0.4050
BL	 0.6556	 0.2840
BM	 0.8654	 0.4190
BP	 0.1459	 0.1290
BQ	 0.0810	 0.0760
BS	 0.4472	 0.1310
Ba	 0.1857	 0.0240
Bb	 0.8346	 0.1850
Bc	 0.7449	 0.1540
Bd	 0.5252	 0.0780
Be	 0.7560	 0.2210
Bf	 0.4927	 0.0950
Bg	 0.4277	 0.0550
Bh	 0.6157	 0.1460
Bi	 0.5175	 0.1000
Bj	 0.0301	 -0.0290
Bk	 0.6482	 0.1830
Bn	 0.4161	 0.1090
Bo	 0.7161	 0.1420
Bp	 0.7338	 0.2480
Bq	 0.6000	 0.1750
Br	 0.8523	 0.3970
Bs	 0.0156	 -0.0300
Bt	 0.8333	 0.3960
Bu	 0.4417	 0.0530
Bv	 0.6388	 0.1600

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Chain	Atom inclusion	Q-score
Bw	 0.6565	 0.1100
Bz	 0.5249	 0.1340
GA	 0.4135	 0.0250
GB	 0.4360	 0.0070