



wwPDB EM Validation Summary Report ⓘ

Oct 14, 2024 – 07:34 PM JST

PDB ID : 7EG9
EMDB ID : EMD-31109
Title : TFIID-based intermediate PIC on SCP promoter
Authors : Chen, X.; Qi, Y.; Wang, X.; Wu, Z.; Li, J.; Xu, Y.
Deposited on : 2021-03-24
Resolution : 3.70 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

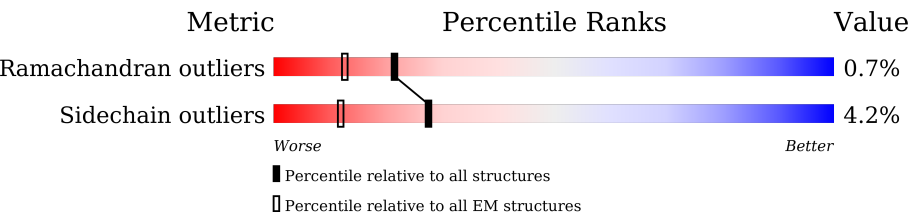
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

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 3.70 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	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	1872	
2	B	1199	
3	D	1085	
3	d	1085	
4	E	800	
4	e	800	
5	F	677	
5	f	677	
6	G	349	





Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	H	310	
8	I	264	
8	i	264	
9	J	218	
9	j	218	
10	L	161	
10	l	161	
11	O	109	
12	P	339	
13	Q	376	
14	R	316	
15	S	517	
16	T	249	
17	U	439	
18	V	291	
19	X	79	
20	Y	79	
21	c	929	
22	k	211	
23	m	124	
24	o	1970	
25	p	1174	
26	q	275	
27	r	142	
28	s	210	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	t	127	 62%38%
30	v	150	 99%. .
31	w	125	 91%9%
32	x	67	 87%9%. .
33	y	117	 99%. .
34	z	58	 76%24%
35	u	172	 98%..

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 84318 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 Transcription initiation factor TFIID subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	602	Total	C	N	O	S	0	0
			4927	3142	858	899	28		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	963	Total	C	N	O	S	0	0
			7796	5011	1315	1412	58		

- Molecule 3 is a protein called Transcription initiation factor TFIID subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	163	Total	C	N	O	S	0	0
			1361	848	255	254	4		
3	d	158	Total	C	N	O	S	0	0
			1307	814	238	252	3		

- Molecule 4 is a protein called Transcription initiation factor TFIID subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	546	Total	C	N	O	S	0	0
			4364	2766	757	820	21		
4	e	539	Total	C	N	O	S	0	0
			4327	2746	748	814	19		

- Molecule 5 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	404	Total	C	N	O	S	0	0
			3081	1954	537	572	18		
5	f	403	Total	C	N	O	S	0	0
			3081	1954	533	576	18		

- Molecule 6 is a protein called Transcription initiation factor TFIID subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	145	Total	C	N	O	S	0	0
			1180	748	217	211	4		

- Molecule 7 is a protein called Transcription initiation factor TFIID subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	209	Total	C	N	O	S	0	0
			1633	1034	283	311	5		

- Molecule 8 is a protein called Transcription initiation factor TFIID subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	120	Total	C	N	O	S	0	0
			959	610	166	177	6		
8	i	121	Total	C	N	O	S	0	0
			967	615	167	178	7		

- Molecule 9 is a protein called Transcription initiation factor TFIID subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	89	Total	C	N	O	S	0	0
			709	457	114	134	4		
9	j	95	Total	C	N	O	S	0	0
			759	488	124	143	4		

- Molecule 10 is a protein called Transcription initiation factor TFIID subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	76	Total	C	N	O	S	0	0
			622	388	109	122	3		
10	l	107	Total	C	N	O	S	0	0
			876	547	158	166	5		

- Molecule 11 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	O	97	Total	C	N	O	S	0	0
			771	491	133	145	2		

- Molecule 12 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	177	Total	C	N	O	S	0	0
			1412	918	249	238	7		

- Molecule 13 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	122	Total	C	N	O	S	0	0
			996	623	162	207	4		

- Molecule 14 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	248	Total	C	N	O	S	0	0
			1913	1200	338	358	17		

- Molecule 15 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	134	Total	C	N	O	S	0	0
			1101	698	199	202	2		

- Molecule 16 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	103	Total	C	N	O	S	0	0
			789	492	142	154	1		

- Molecule 17 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	179	Total	C	N	O	S	0	0
			1476	932	261	272	11		

- Molecule 18 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	172	Total	C	N	O	S	0	0
			1400	890	242	264	4		

- Molecule 19 is a DNA chain called DNA (79-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	71	Total	C	N	O	P	0	0
			1470	691	287	421	71		

- Molecule 20 is a DNA chain called DNA (79-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	71	Total	C	N	O	P	0	0
			1441	683	256	431	71		

- Molecule 21 is a protein called Transcription initiation factor TFIID subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	c	127	Total	C	N	O	S	0	0
			1011	638	174	193	6		

- Molecule 22 is a protein called Transcription initiation factor TFIID subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	k	98	Total	C	N	O	S	0	0
			785	499	142	139	5		

- Molecule 23 is a protein called Transcription initiation factor TFIID subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	m	87	Total	C	N	O	S	0	0
			724	456	131	131	6		

- Molecule 24 is a protein called RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	o	1427	Total	C	N	O	S	0	0
			11308	7114	2023	2099	72		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	p	1134	Total	C	N	O	S	0	0
			9062	5732	1595	1671	64		

- Molecule 26 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	q	257	Total	C	N	O	S	0	0
			2059	1294	351	408	6		

- Molecule 27 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	r	128	Total	C	N	O	S	0	0
			1005	632	172	197	4		

- Molecule 28 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	s	209	Total	C	N	O	S	0	0
			1720	1089	300	323	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	t	79	Total	C	N	O	S	0	0
			635	406	108	116	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	v	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	w	114	Total	C	N	O	S	0	0
			927	571	166	179	11		

- Molecule 32 is a protein called RPB10.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	x	64	Total	C	N	O	S	0	0
			507	328	86	87	6		

- Molecule 33 is a protein called RNA_pol_L_2 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	y	117	Total	C	N	O	S	0	0
			937	604	154	177	2		

- Molecule 34 is a protein called RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	z	44	Total	C	N	O	S	0	0
			372	231	72	63	6		

- Molecule 35 is a protein called DNA-directed RNA polymerase II subunit RPB7.

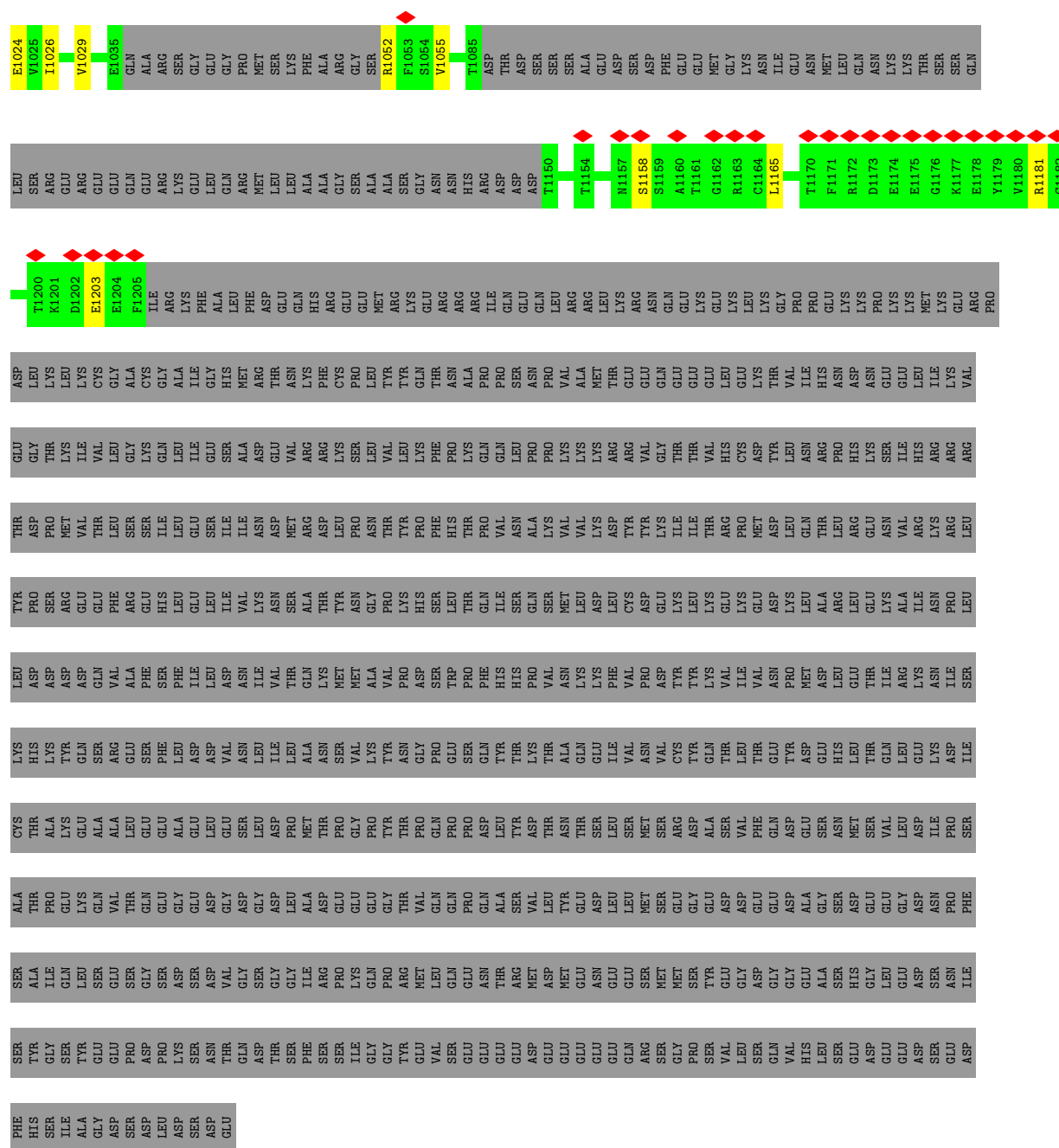
Mol	Chain	Residues	Atoms					AltConf	Trace
35	u	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

- Molecule 36 is ZINC ION (three-letter code: ZN) (formula: Zn).

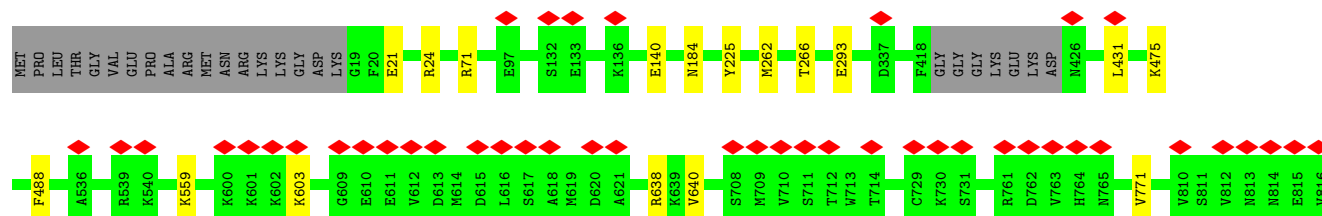
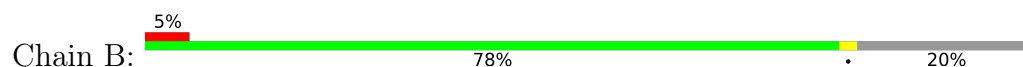
Mol	Chain	Residues	Atoms		AltConf
36	R	1	Total	Zn	0
			1	1	
36	U	1	Total	Zn	0
			1	1	
36	o	2	Total	Zn	0
			2	2	
36	p	1	Total	Zn	0
			1	1	
36	q	1	Total	Zn	0
			1	1	
36	w	2	Total	Zn	0
			2	2	
36	x	1	Total	Zn	0
			1	1	
36	z	1	Total	Zn	0
			1	1	

- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	o	1	Total	Mg	0
			1	1	



- Molecule 2: Transcription initiation factor TFIID subunit 2

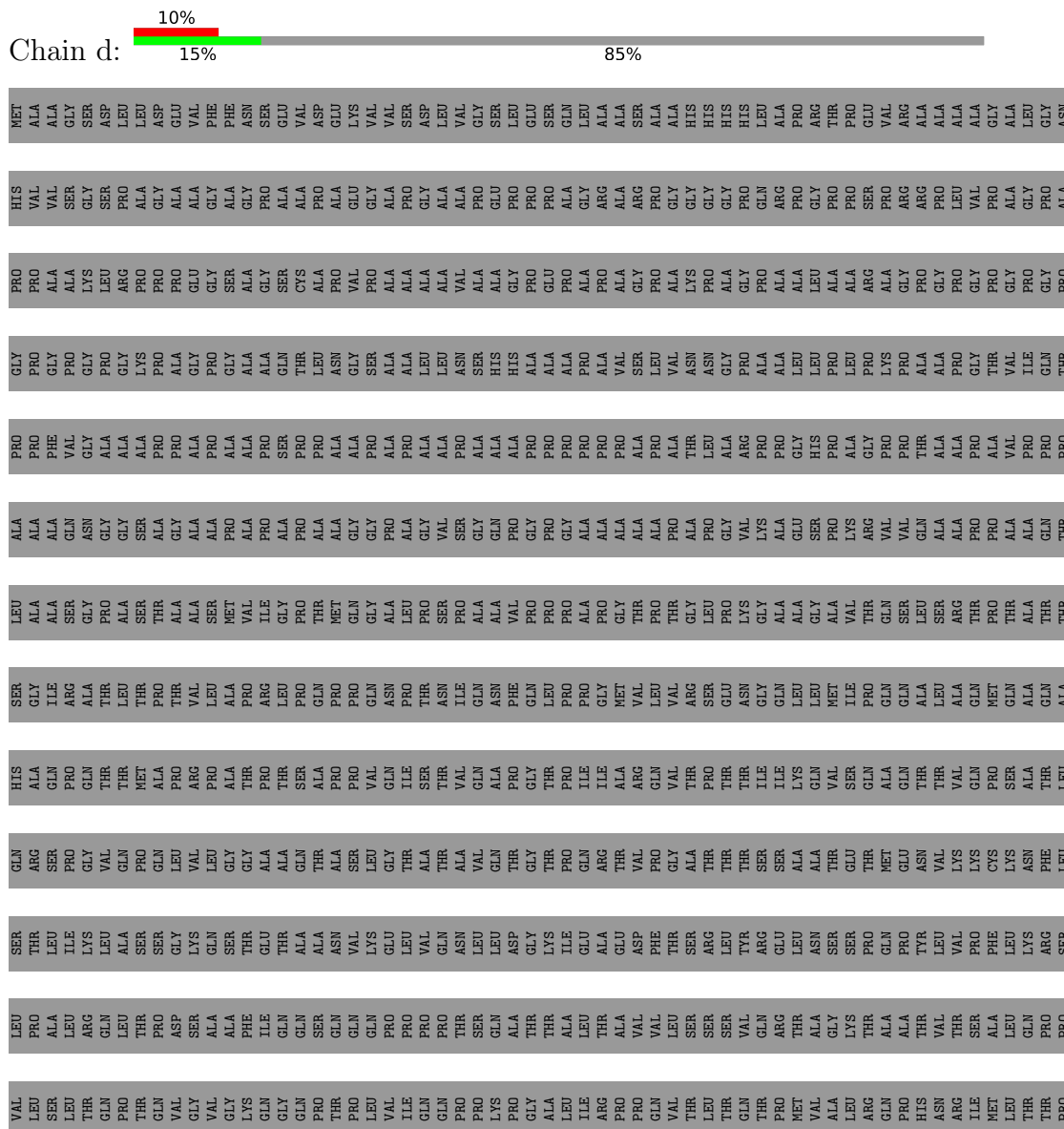


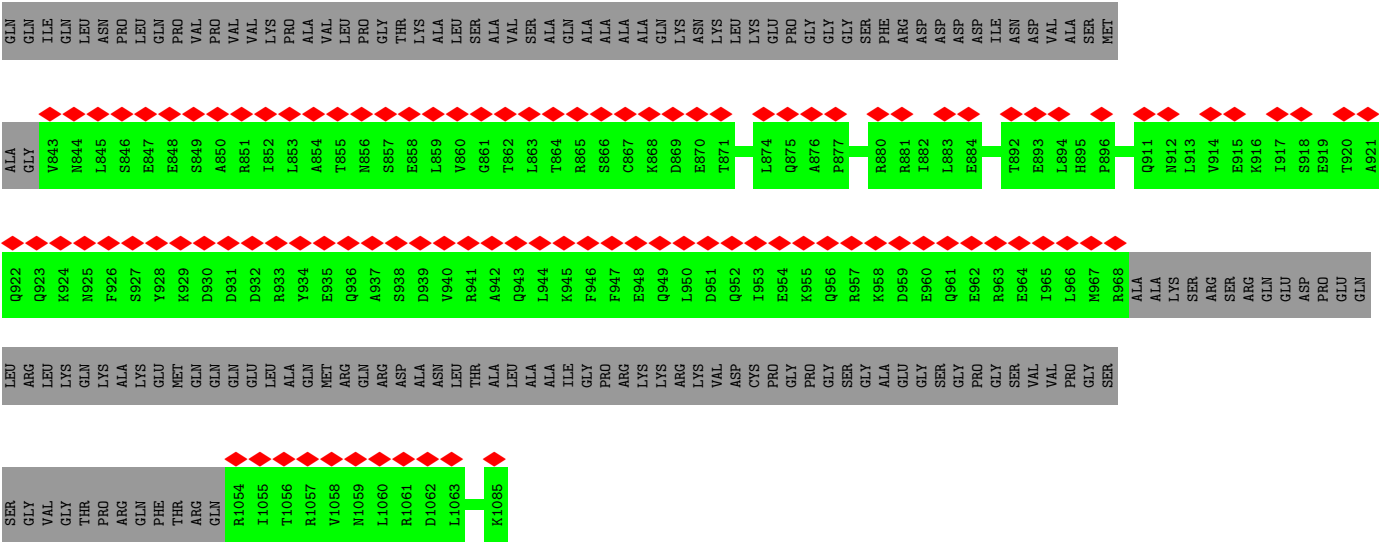
SER	ASP	HIS	HIS	HIS	HIS	HIS	HIS	HIS	GLU	LYS	LYS	LYS	LYS	LYS	HIS	HIS	HIS	HIS	LYS	LYS	ASP	SER	LYS	GLU	LYS	ASP	LYS	GLU	PRO	PHE	THR	PHE	SER	SER	PRO	ALA	SER	GLY	ARG	SER	ILE	ARG	SER	PRO	LEU	SER	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 3: Transcription initiation factor TFIID subunit 4

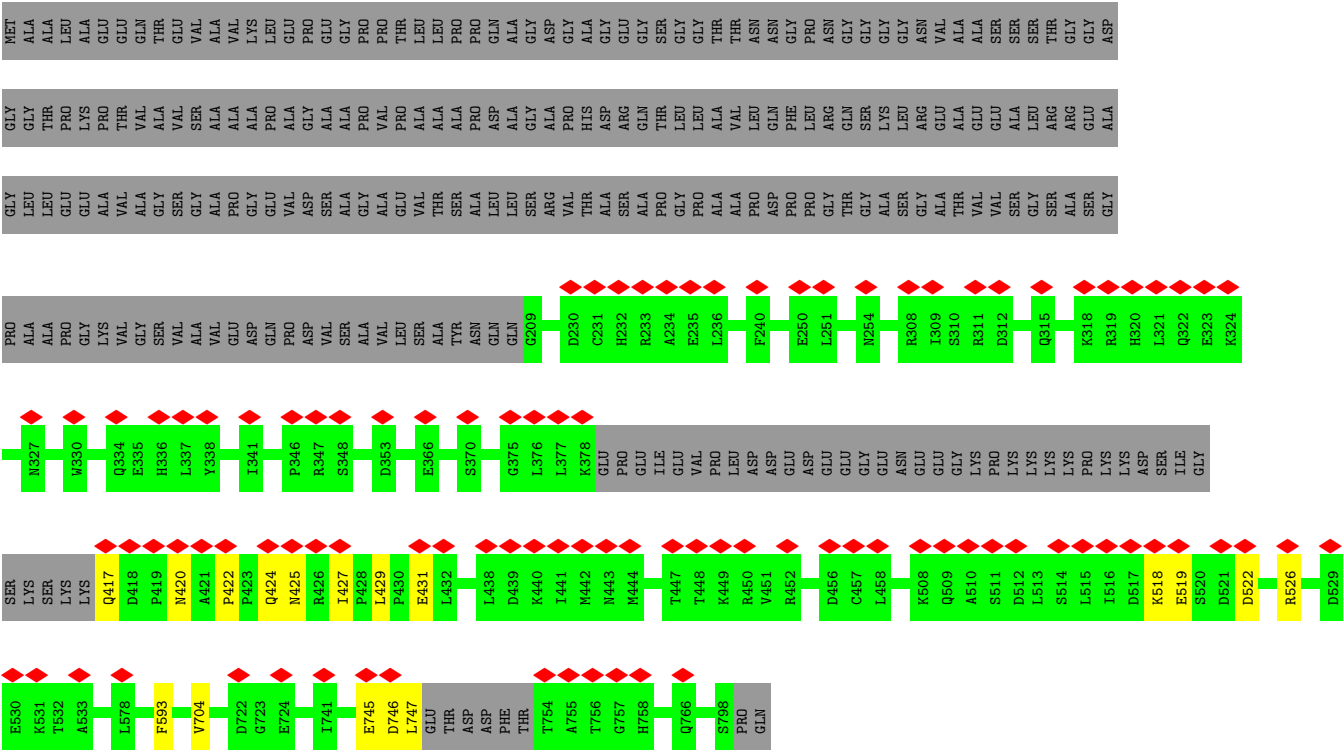
Chain D:  10% 13% 85%

- Molecule 3: Transcription initiation factor TFIID subunit 4

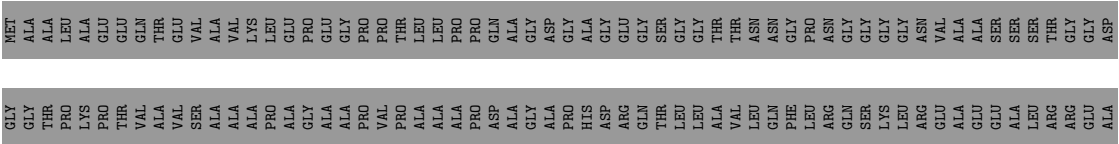


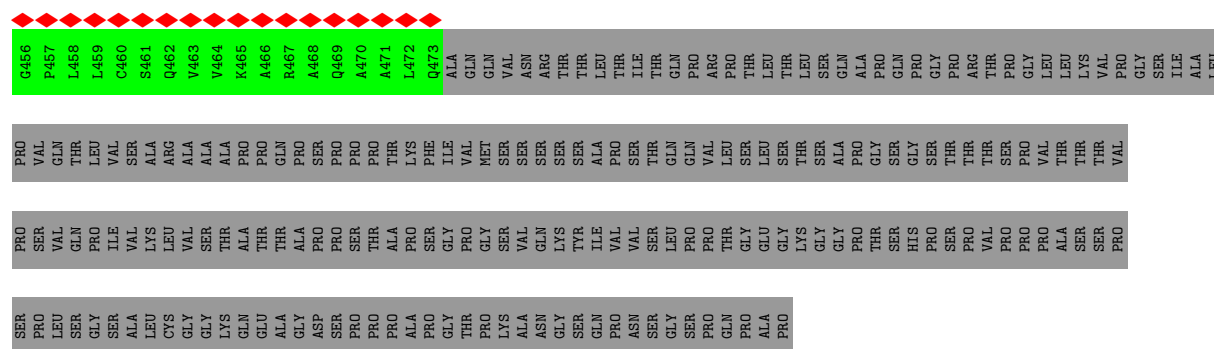


● Molecule 4: Transcription initiation factor TFIID subunit 5

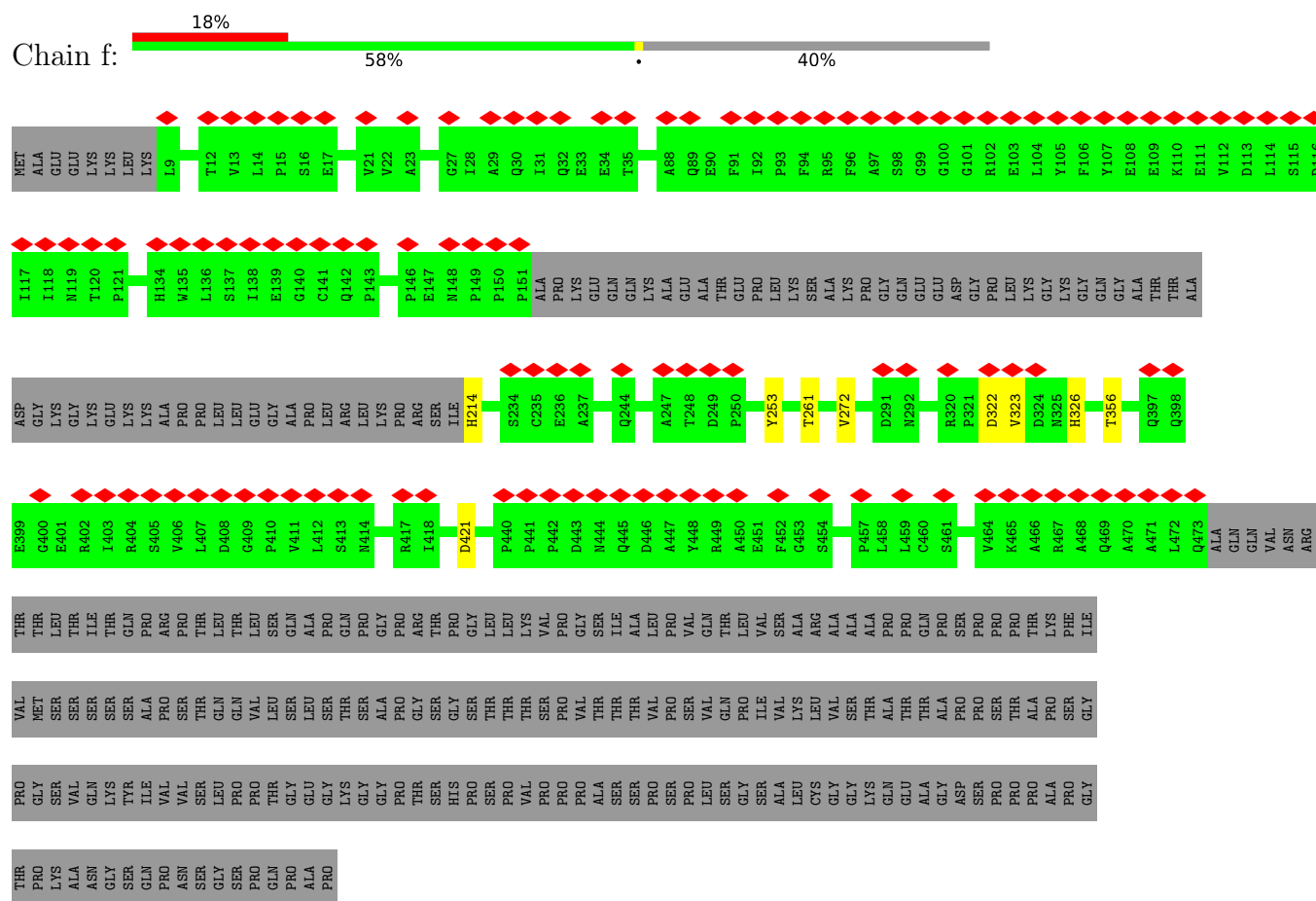


● Molecule 4: Transcription initiation factor TFIID subunit 5

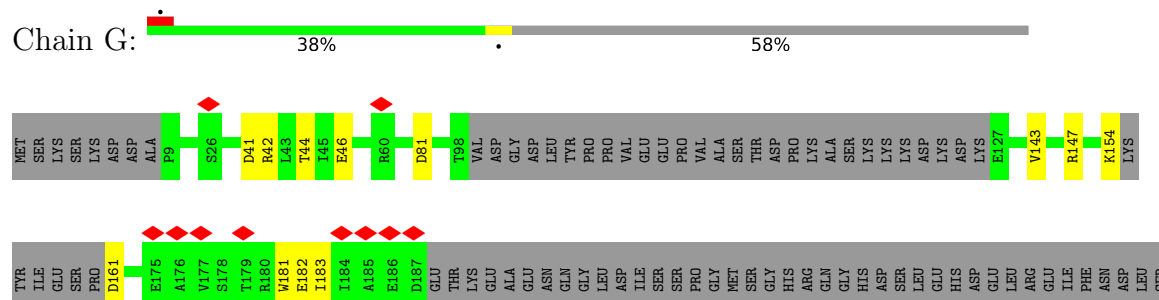


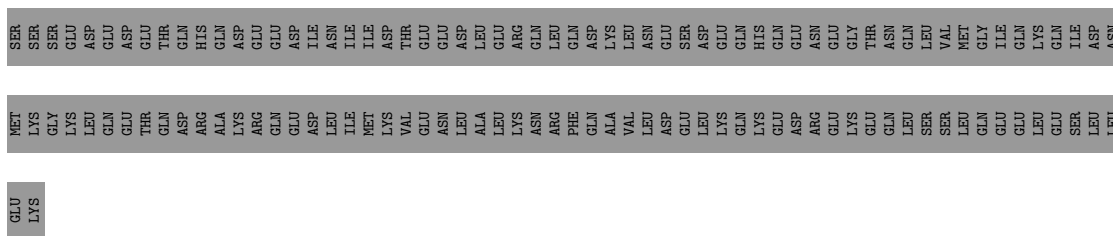


• Molecule 5: Transcription initiation factor TFIID subunit 6

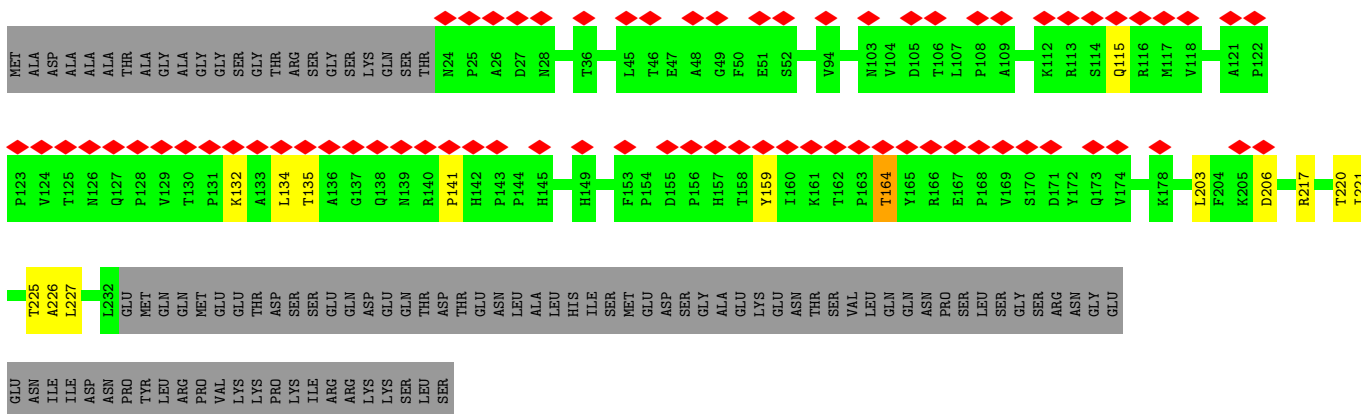


• Molecule 6: Transcription initiation factor TFIID subunit 7

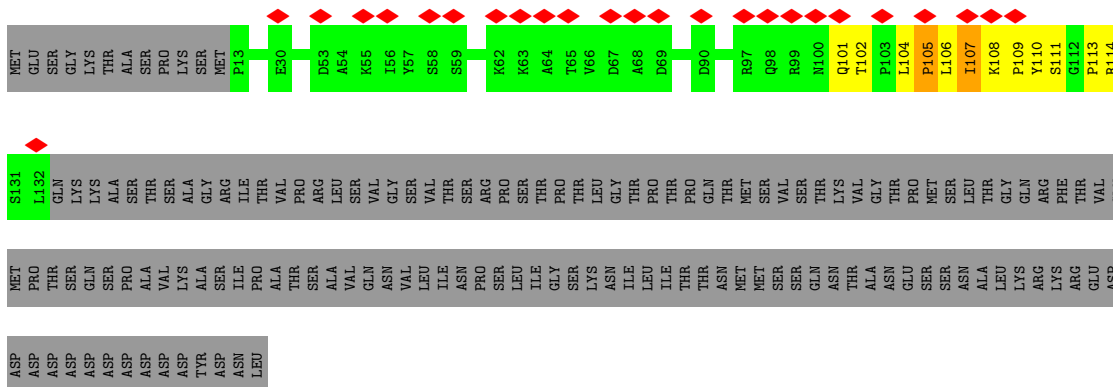




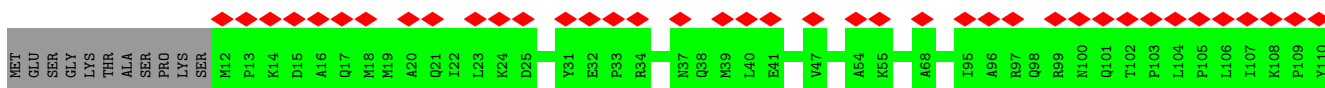
- Molecule 7: Transcription initiation factor TFIID subunit 8



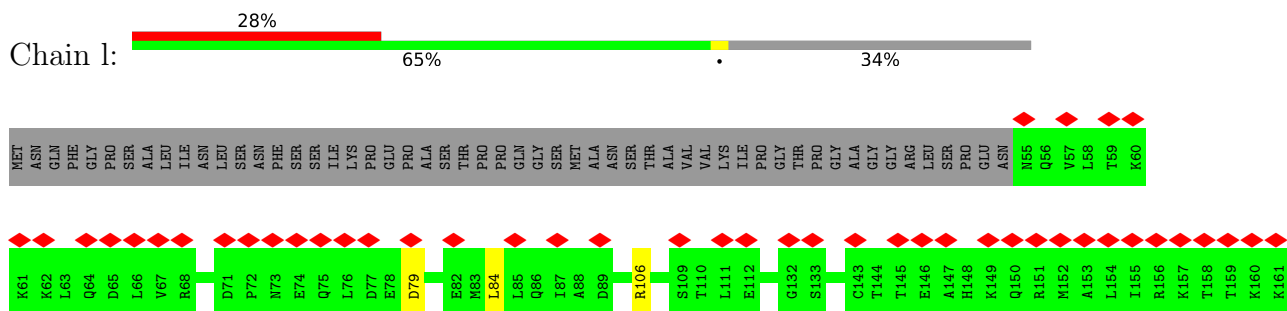
- Molecule 8: Transcription initiation factor TFIID subunit 9



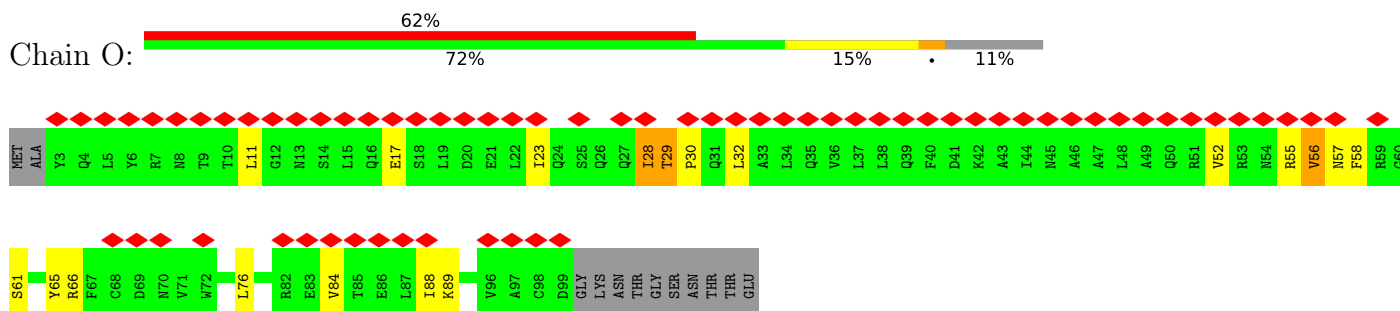
- Molecule 8: Transcription initiation factor TFIID subunit 9



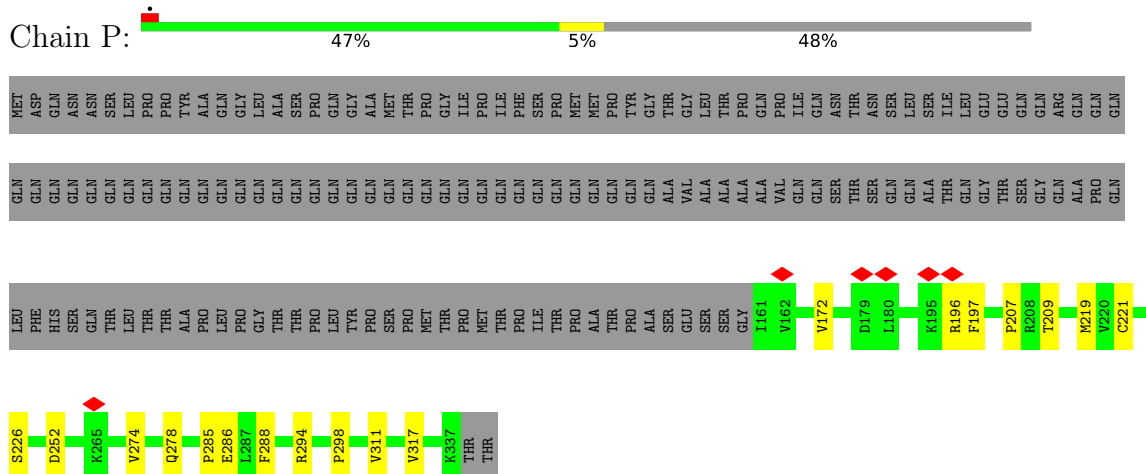
- Molecule 10: Transcription initiation factor TFIID subunit 12



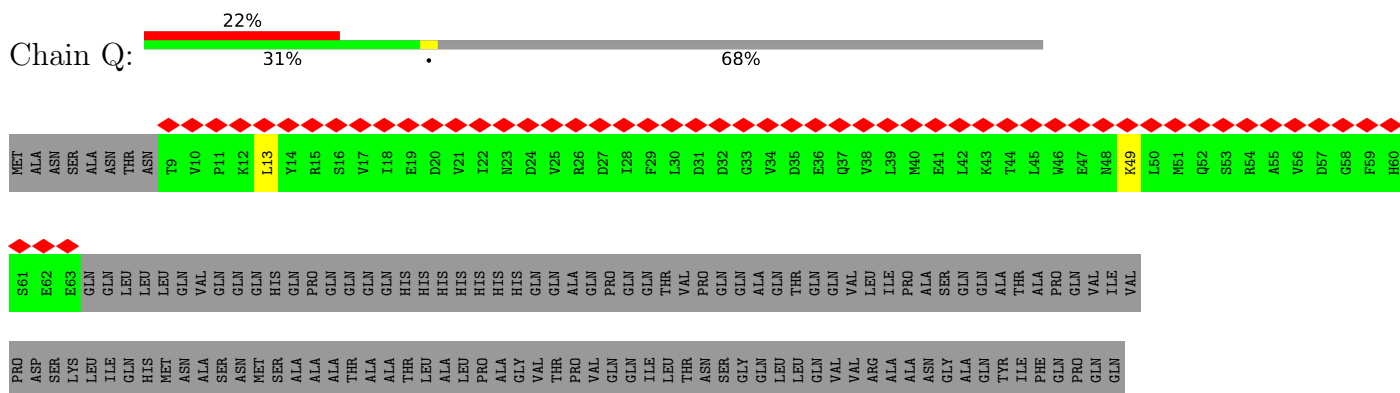
- Molecule 11: Transcription initiation factor IIA subunit 2

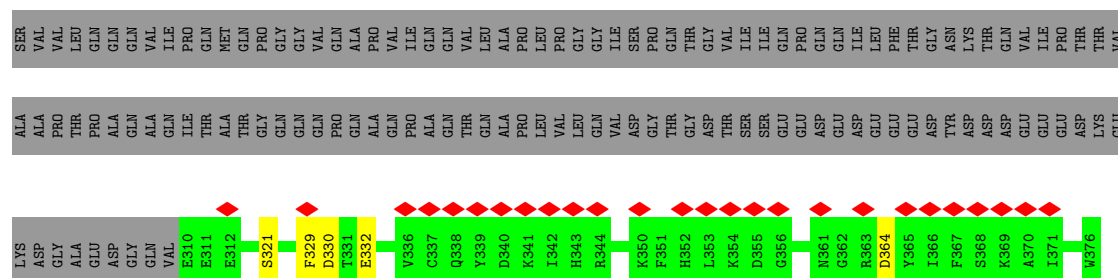


- Molecule 12: TATA-box-binding protein

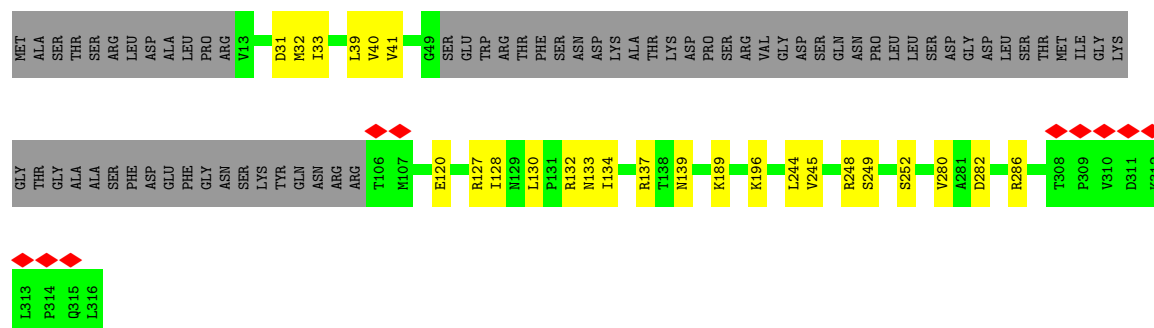


- Molecule 13: Transcription initiation factor IIA subunit 1

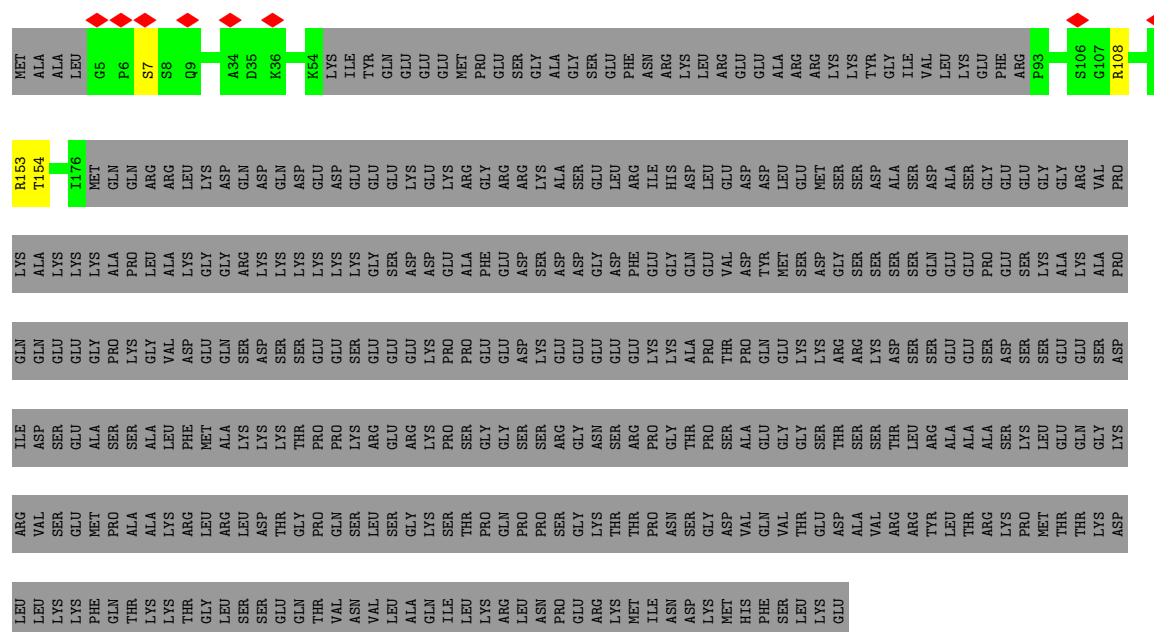




• Molecule 14: Transcription initiation factor IIB

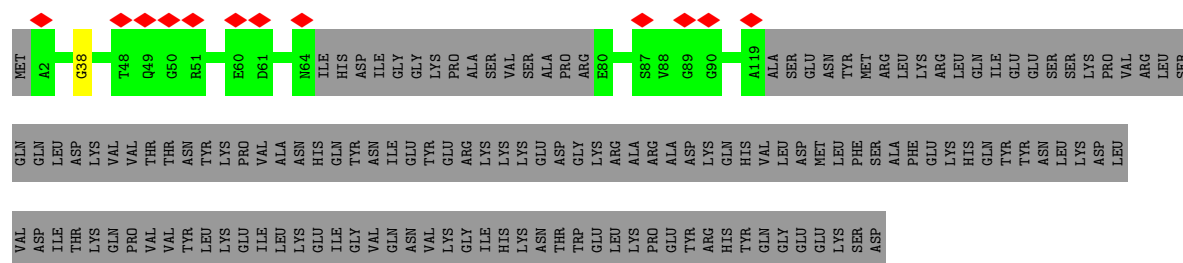


• Molecule 15: General transcription factor IIF subunit 1

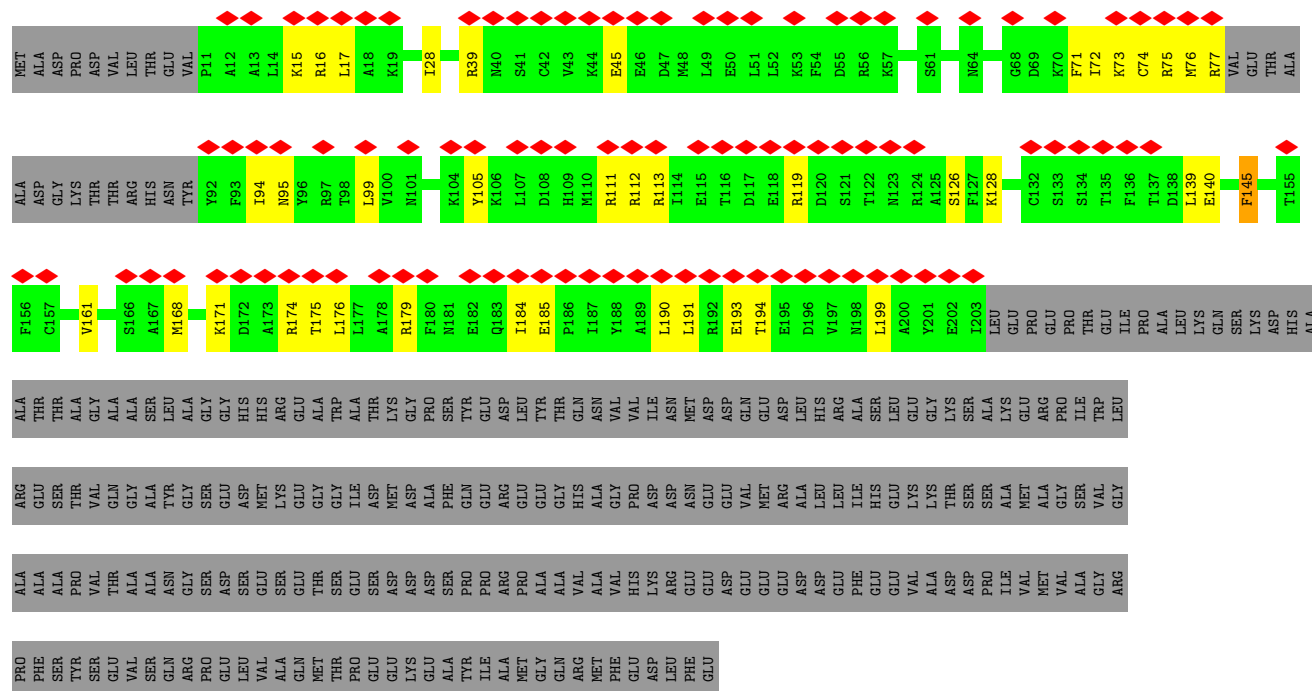
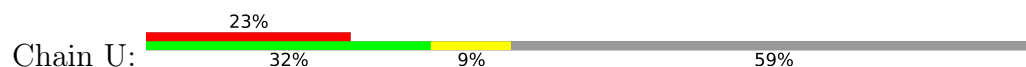


• Molecule 16: General transcription factor IIF subunit 2

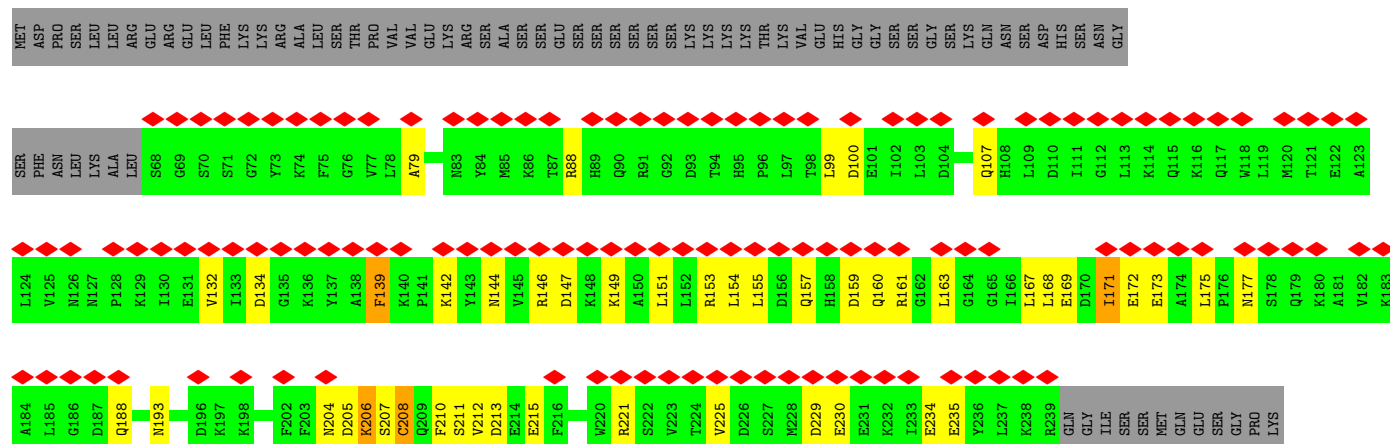




• Molecule 17: General transcription factor IIE subunit 1

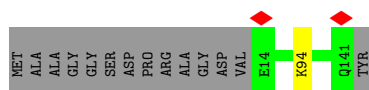


• Molecule 18: Transcription initiation factor IIE subunit beta









- Molecule 28: DNA-directed RNA polymerase II subunit E

Chain s: 99%



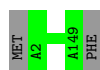
- Molecule 29: DNA-directed RNA polymerase II subunit F

Chain t: 62% 38%



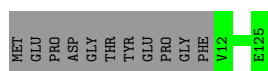
- Molecule 30: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain v: 99%



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

Chain w: 91% 9%



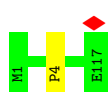
- Molecule 32: RPB10

Chain x: 87% 9%



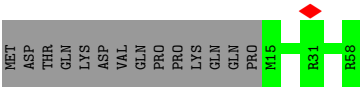
- Molecule 33: RNA_pol_L_2 domain-containing protein

Chain y: 99%



- Molecule 34: RPB12

Chain z: 76% 24%



- Molecule 35: DNA-directed RNA polymerase II subunit RPB7



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	57889	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.158	Depositor
Minimum map value	-0.399	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.13	Depositor
Map size (\AA)	508.8, 508.8, 508.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	0/5046	0.67	1/6810 (0.0%)
2	B	0.47	0/7993	0.62	1/10836 (0.0%)
3	D	0.44	0/1374	0.56	0/1836
3	d	0.28	0/1321	0.49	0/1772
4	E	0.36	0/4469	0.56	0/6050
4	e	0.32	0/4433	0.55	0/6004
5	F	0.51	0/3139	0.72	0/4264
5	f	0.41	0/3140	0.63	0/4268
6	G	0.51	0/1199	0.65	0/1612
7	H	0.42	0/1673	0.59	0/2285
8	I	0.34	0/981	0.57	1/1332 (0.1%)
8	i	0.30	0/989	0.46	0/1343
9	J	0.31	0/724	0.50	0/982
9	j	0.30	0/775	0.52	0/1049
10	L	0.32	0/630	0.59	1/852 (0.1%)
10	l	0.34	0/888	0.57	1/1194 (0.1%)
11	O	0.57	0/781	0.78	0/1061
12	P	0.62	0/1438	0.75	0/1935
13	Q	0.44	0/1013	0.69	1/1366 (0.1%)
14	R	0.37	0/1941	0.59	0/2622
15	S	0.34	0/1130	0.53	0/1528
16	T	0.26	0/799	0.53	0/1077
17	U	0.51	0/1499	0.75	3/2012 (0.1%)
18	V	0.48	0/1424	0.72	2/1913 (0.1%)
19	X	0.88	0/1653	1.11	0/2552
20	Y	0.79	0/1611	0.98	0/2481
21	c	0.39	0/1035	0.54	0/1406
22	k	0.30	0/799	0.47	0/1070
23	m	0.31	0/733	0.51	0/977
24	o	0.49	0/11516	0.68	1/15548 (0.0%)
25	p	0.37	0/9243	0.47	1/12475 (0.0%)
26	q	0.38	0/2102	0.46	0/2857

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	r	0.27	0/1019	0.47	0/1374
28	s	0.30	0/1751	0.45	0/2366
29	t	0.37	0/645	0.46	0/871
30	v	0.37	0/1207	0.49	0/1628
31	w	0.30	0/948	0.45	0/1284
32	x	0.49	0/516	0.65	0/696
33	y	0.36	0/956	0.46	0/1294
34	z	0.38	0/377	0.45	0/500
35	u	0.33	0/1382	0.53	0/1874
All	All	0.45	0/86292	0.62	13/117256 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
11	O	0	1
17	U	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	883	PHE	C-N-CA	-7.06	104.04	121.70
17	U	94	ILE	O-C-N	6.62	133.29	122.70
18	V	139	PHE	CB-CA-C	-6.26	97.88	110.40
13	Q	330	ASP	CB-CA-C	6.21	122.82	110.40
18	V	234	GLU	CB-CA-C	-5.73	98.94	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	O	17	GLU	Mainchain
17	U	161	VAL	Mainchain

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	584/1872 (31%)	553 (95%)	27 (5%)	4 (1%)	19	51
2	B	959/1199 (80%)	908 (95%)	50 (5%)	1 (0%)	48	78
3	D	157/1085 (14%)	150 (96%)	7 (4%)	0	100	100
3	d	154/1085 (14%)	150 (97%)	4 (3%)	0	100	100
4	E	540/800 (68%)	497 (92%)	40 (7%)	3 (1%)	22	54
4	e	531/800 (66%)	484 (91%)	47 (9%)	0	100	100
5	F	400/677 (59%)	367 (92%)	24 (6%)	9 (2%)	5	31
5	f	399/677 (59%)	377 (94%)	22 (6%)	0	100	100
6	G	139/349 (40%)	134 (96%)	5 (4%)	0	100	100
7	H	207/310 (67%)	188 (91%)	15 (7%)	4 (2%)	6	35
8	I	118/264 (45%)	109 (92%)	5 (4%)	4 (3%)	3	26
8	i	119/264 (45%)	115 (97%)	4 (3%)	0	100	100
9	J	85/218 (39%)	82 (96%)	3 (4%)	0	100	100
9	j	91/218 (42%)	89 (98%)	2 (2%)	0	100	100
10	L	74/161 (46%)	69 (93%)	5 (7%)	0	100	100
10	l	105/161 (65%)	100 (95%)	5 (5%)	0	100	100
11	O	95/109 (87%)	76 (80%)	13 (14%)	6 (6%)	1	15
12	P	175/339 (52%)	164 (94%)	8 (5%)	3 (2%)	7	36
13	Q	118/376 (31%)	108 (92%)	9 (8%)	1 (1%)	16	49
14	R	244/316 (77%)	228 (93%)	15 (6%)	1 (0%)	30	62
15	S	130/517 (25%)	127 (98%)	2 (2%)	1 (1%)	16	49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	T	99/249 (40%)	95 (96%)	3 (3%)	1 (1%)	13	44
17	U	175/439 (40%)	155 (89%)	16 (9%)	4 (2%)	5	31
18	V	170/291 (58%)	133 (78%)	25 (15%)	12 (7%)	1	13
21	c	125/929 (14%)	116 (93%)	9 (7%)	0	100	100
22	k	96/211 (46%)	91 (95%)	5 (5%)	0	100	100
23	m	85/124 (68%)	79 (93%)	6 (7%)	0	100	100
24	o	1417/1970 (72%)	1280 (90%)	124 (9%)	13 (1%)	14	47
25	p	1128/1174 (96%)	1052 (93%)	76 (7%)	0	100	100
26	q	253/275 (92%)	226 (89%)	27 (11%)	0	100	100
27	r	126/142 (89%)	119 (94%)	7 (6%)	0	100	100
28	s	207/210 (99%)	196 (95%)	11 (5%)	0	100	100
29	t	77/127 (61%)	74 (96%)	3 (4%)	0	100	100
30	v	146/150 (97%)	132 (90%)	14 (10%)	0	100	100
31	w	112/125 (90%)	103 (92%)	9 (8%)	0	100	100
32	x	62/67 (92%)	60 (97%)	2 (3%)	0	100	100
33	y	115/117 (98%)	108 (94%)	6 (5%)	1 (1%)	14	47
34	z	42/58 (72%)	38 (90%)	4 (10%)	0	100	100
35	u	169/172 (98%)	156 (92%)	12 (7%)	1 (1%)	22	54
All	All	10028/18627 (54%)	9288 (93%)	671 (7%)	69 (1%)	21	51

5 of 69 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1158	SER
5	F	323	VAL
5	F	345	SER
5	F	415	ILE
7	H	141	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	536/1665 (32%)	484 (90%)	52 (10%)	6	28
2	B	876/1083 (81%)	856 (98%)	20 (2%)	45	64
3	D	147/815 (18%)	130 (88%)	17 (12%)	4	22
3	d	146/815 (18%)	146 (100%)	0	100	100
4	E	478/657 (73%)	464 (97%)	14 (3%)	37	59
4	e	475/657 (72%)	473 (100%)	2 (0%)	89	93
5	F	320/574 (56%)	298 (93%)	22 (7%)	13	39
5	f	322/574 (56%)	313 (97%)	9 (3%)	38	60
6	G	133/322 (41%)	121 (91%)	12 (9%)	8	31
7	H	181/270 (67%)	169 (93%)	12 (7%)	14	41
8	I	106/235 (45%)	97 (92%)	9 (8%)	8	33
8	i	107/235 (46%)	107 (100%)	0	100	100
9	J	78/154 (51%)	78 (100%)	0	100	100
9	j	83/154 (54%)	83 (100%)	0	100	100
10	L	71/141 (50%)	70 (99%)	1 (1%)	62	76
10	l	98/141 (70%)	96 (98%)	2 (2%)	50	68
11	O	84/98 (86%)	69 (82%)	15 (18%)	1	9
12	P	153/293 (52%)	138 (90%)	15 (10%)	6	27
13	Q	111/324 (34%)	106 (96%)	5 (4%)	23	50
14	R	211/268 (79%)	187 (89%)	24 (11%)	4	23
15	S	117/448 (26%)	114 (97%)	3 (3%)	41	61
16	T	85/218 (39%)	85 (100%)	0	100	100
17	U	163/373 (44%)	130 (80%)	33 (20%)	1	7
18	V	154/261 (59%)	116 (75%)	38 (25%)	0	4
21	c	113/833 (14%)	111 (98%)	2 (2%)	54	71
22	k	87/182 (48%)	87 (100%)	0	100	100
23	m	80/106 (76%)	79 (99%)	1 (1%)	65	77
24	o	1257/1748 (72%)	1207 (96%)	50 (4%)	27	52
25	p	993/1027 (97%)	987 (99%)	6 (1%)	84	90
26	q	234/252 (93%)	234 (100%)	0	100	100
27	r	106/126 (84%)	105 (99%)	1 (1%)	75	84

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	s	191/192 (100%)	190 (100%)	1 (0%)	86	92
29	t	69/111 (62%)	69 (100%)	0	100	100
30	v	129/131 (98%)	129 (100%)	0	100	100
31	w	103/112 (92%)	103 (100%)	0	100	100
32	x	53/56 (95%)	47 (89%)	6 (11%)	4	23
33	y	106/106 (100%)	106 (100%)	0	100	100
34	z	41/55 (74%)	41 (100%)	0	100	100
35	u	152/153 (99%)	150 (99%)	2 (1%)	65	77
All	All	8949/15965 (56%)	8575 (96%)	374 (4%)	27	51

5 of 374 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	U	77	ARG
18	V	213	ASP
17	U	126	SER
18	V	144	ASN
5	f	322	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 113 such sidechains are listed below:

Mol	Chain	Res	Type
10	L	117	GLN
33	y	2	ASN
3	d	912	ASN
31	w	22	ASN
25	p	287	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

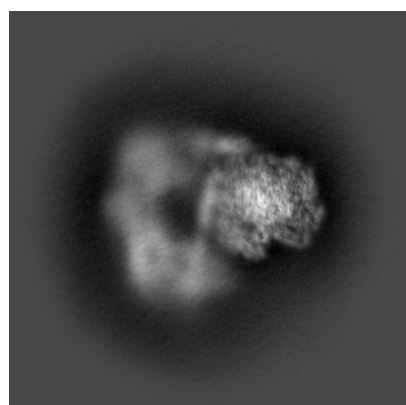
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31109. These allow visual inspection of the internal detail of the map and identification of artifacts.

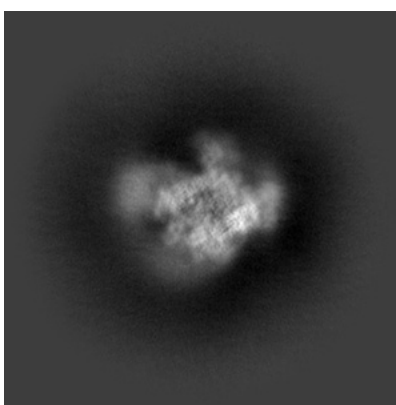
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

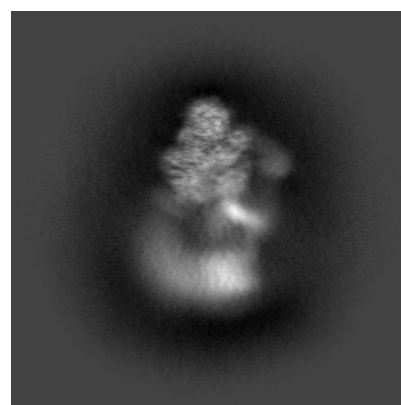
6.1.1 Primary map



X



Y

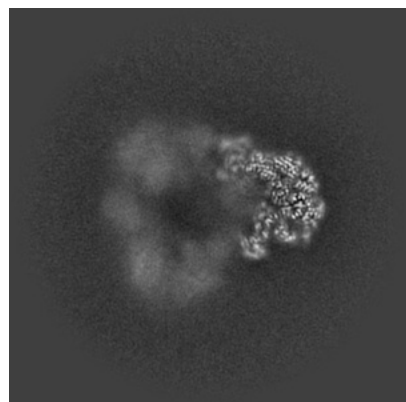


Z

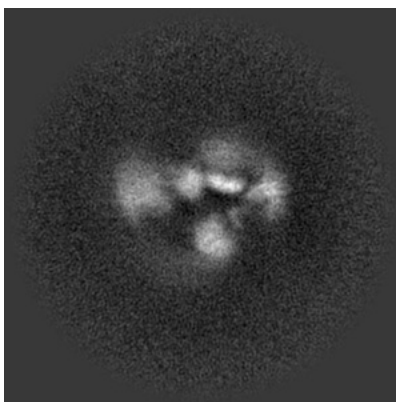
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

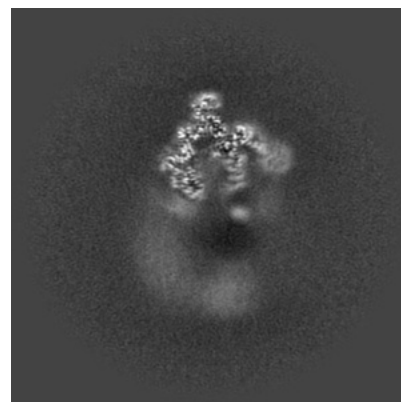
6.2.1 Primary map



X Index: 240



Y Index: 240

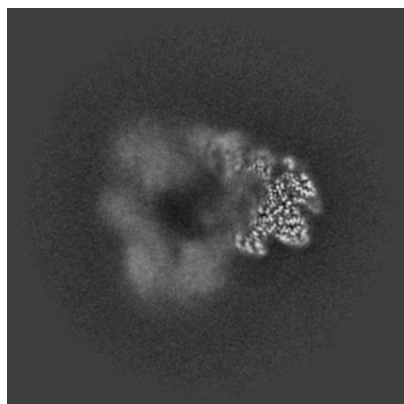


Z Index: 240

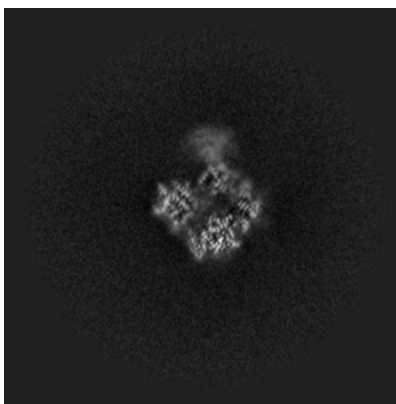
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

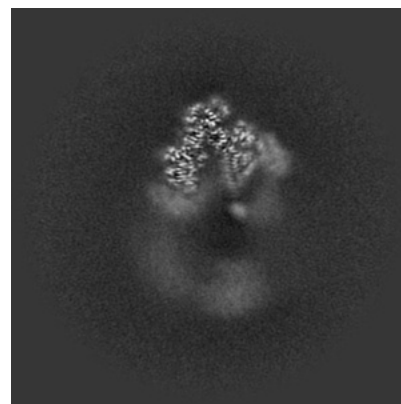
6.3.1 Primary map



X Index: 250



Y Index: 299

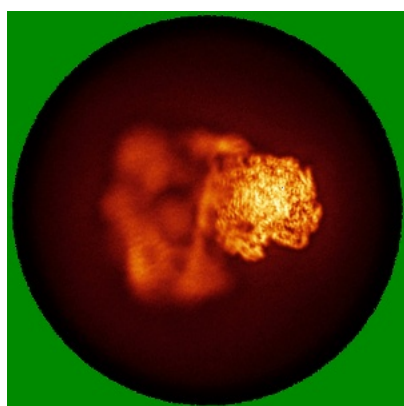


Z Index: 252

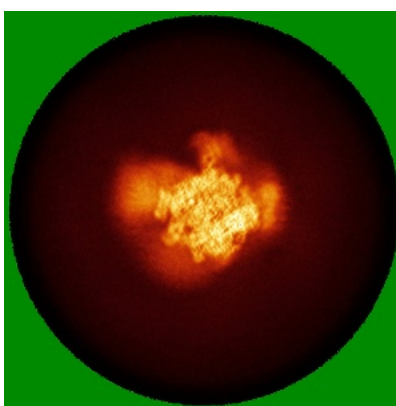
The images above show the largest variance slices of the map in three orthogonal directions.

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

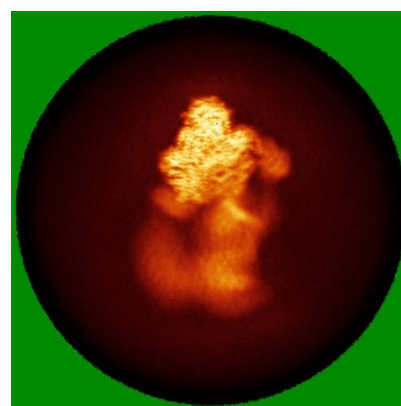
6.4.1 Primary map



X



Y

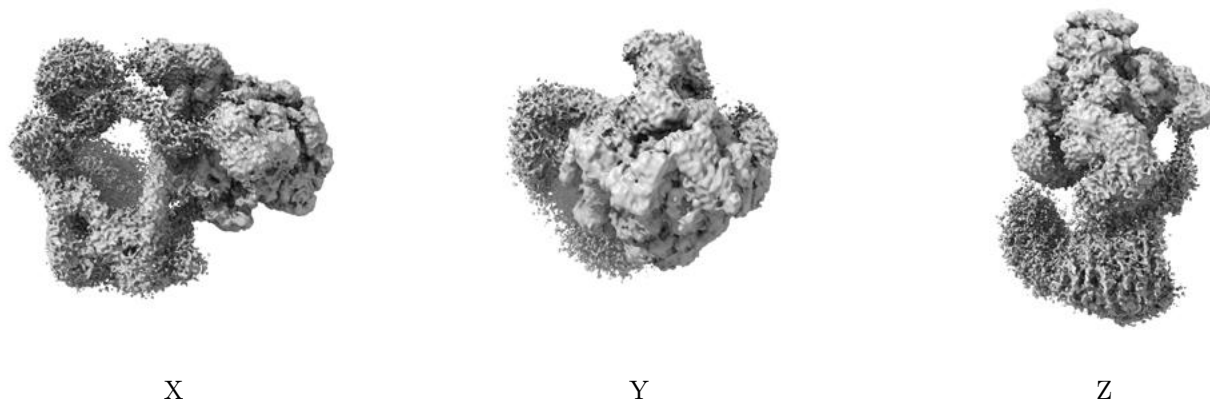


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

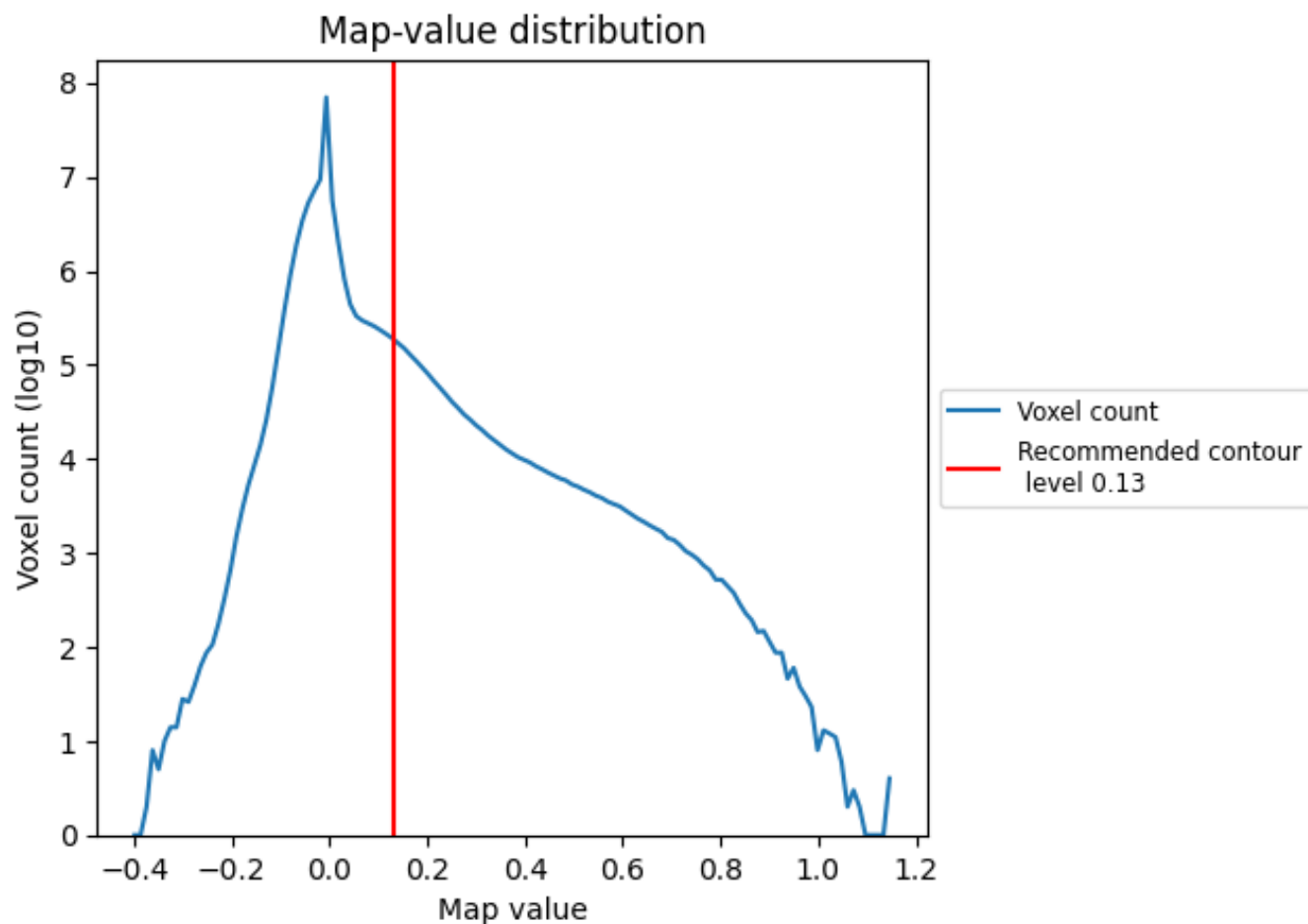
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

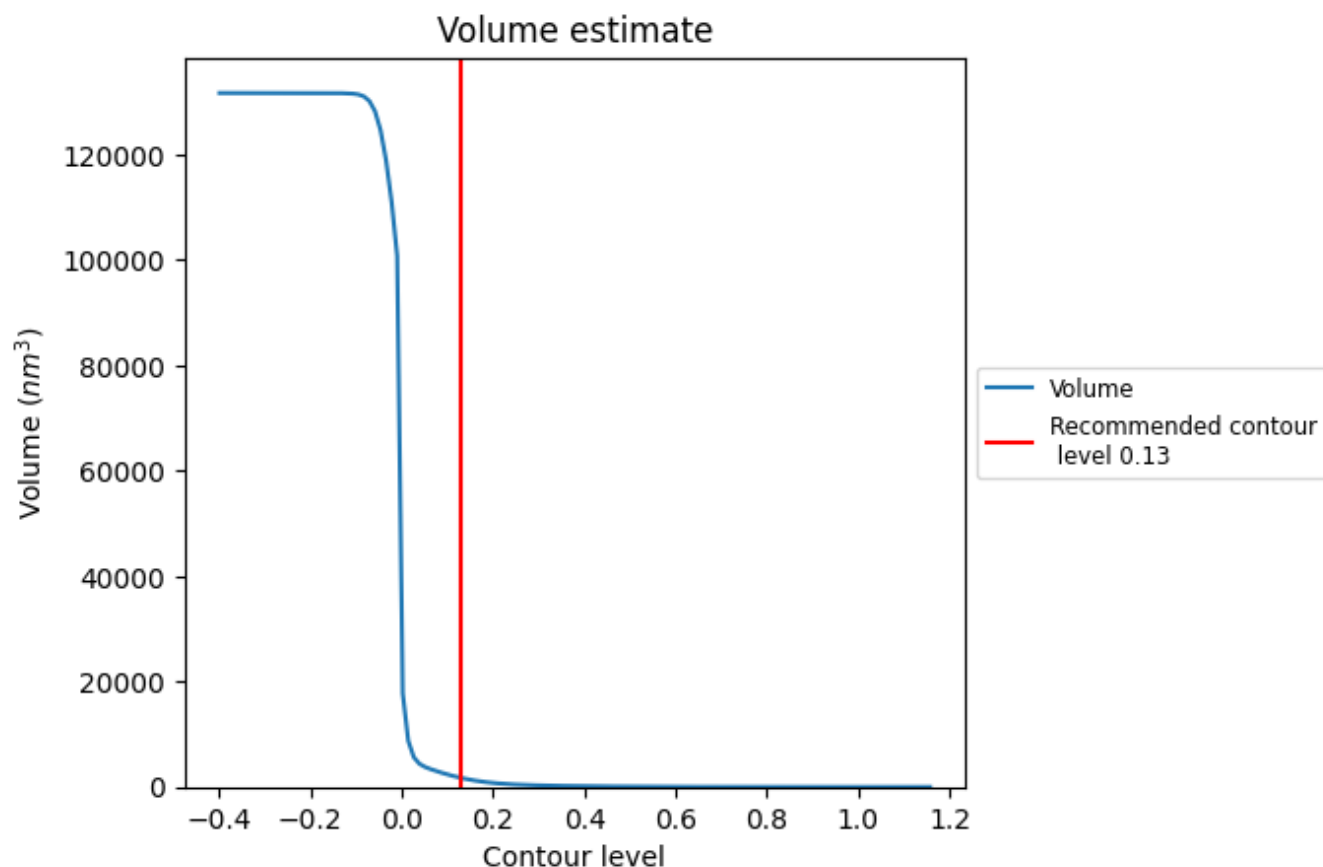
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

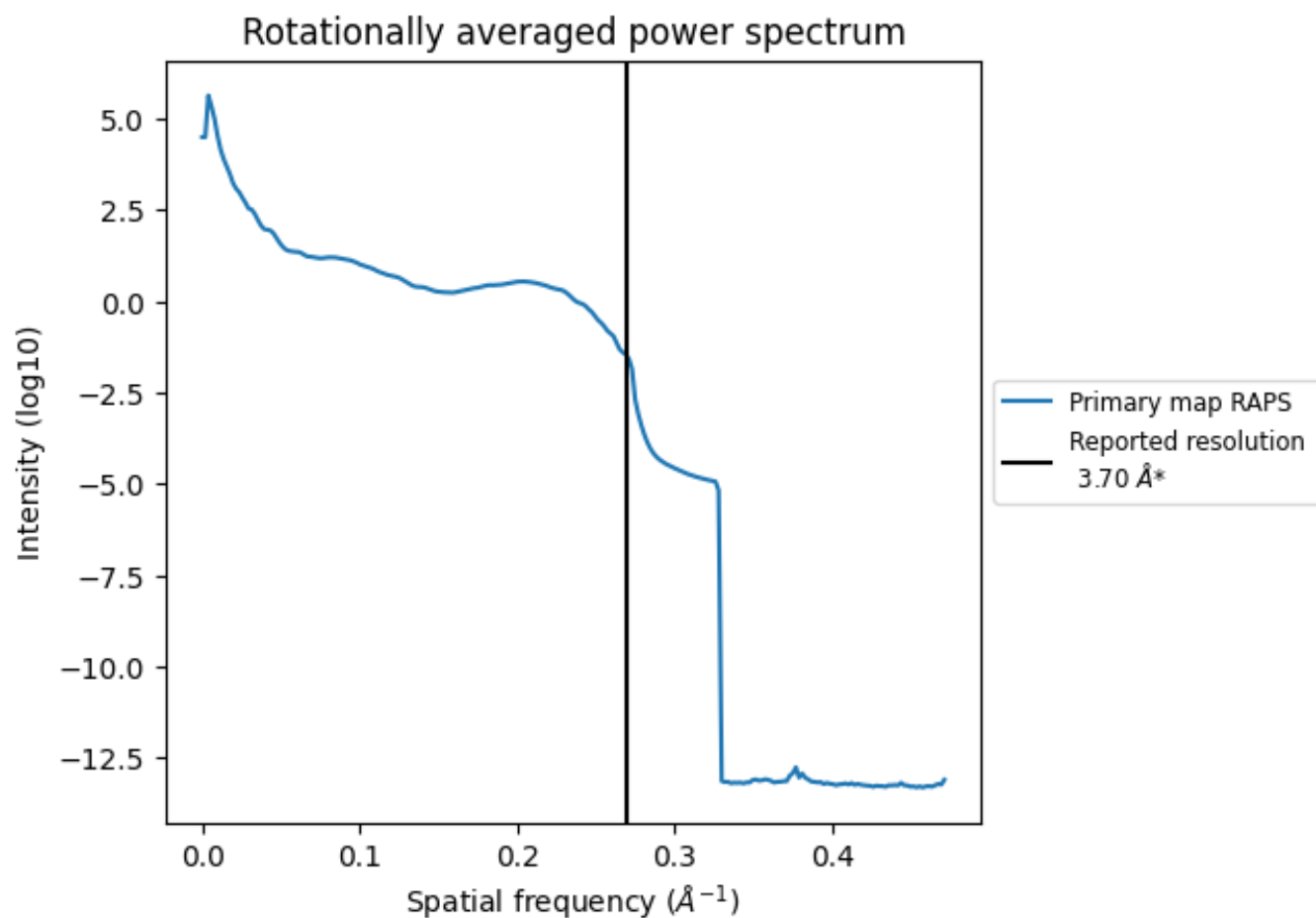
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1729 nm³; this corresponds to an approximate mass of 1562 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

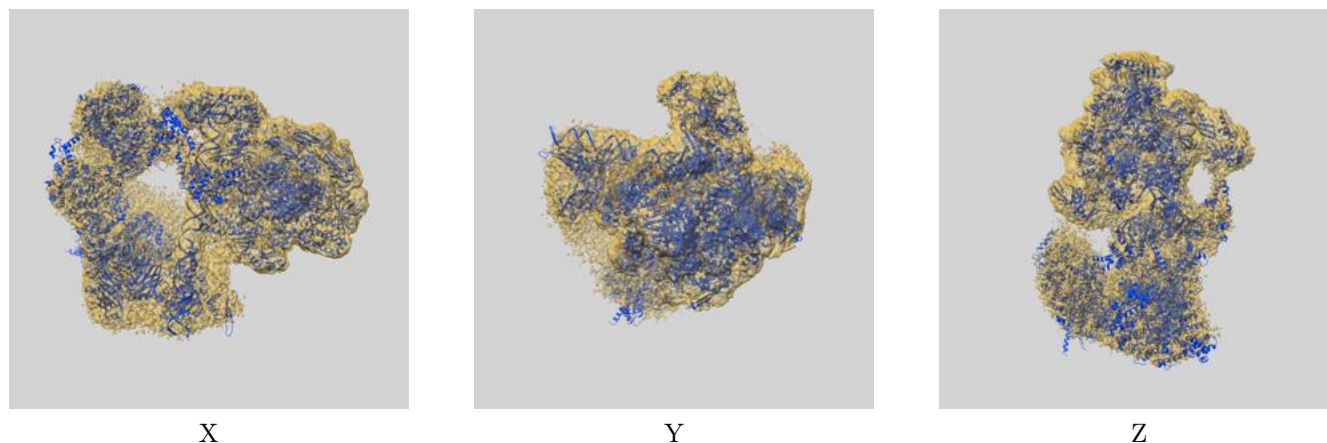
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

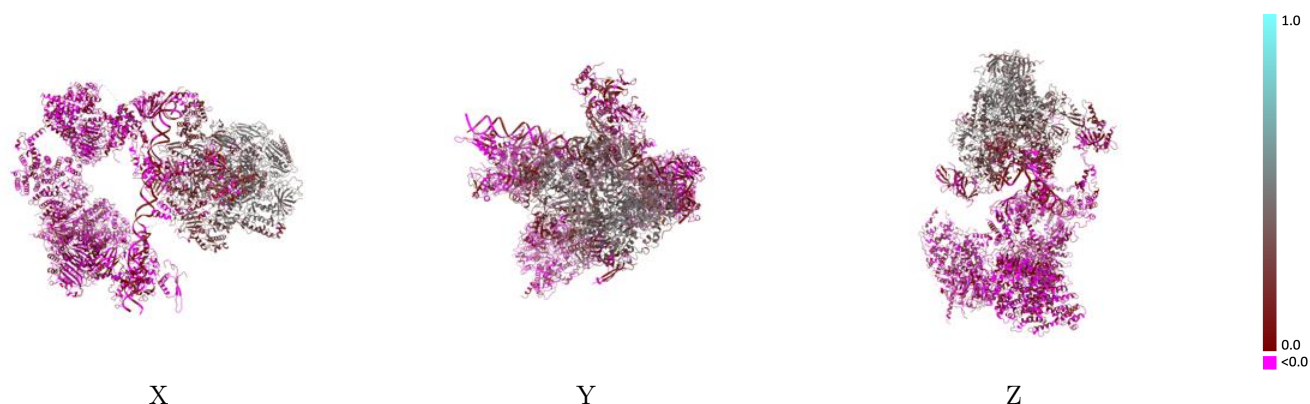
This section contains information regarding the fit between EMDB map EMD-31109 and PDB model 7EG9. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



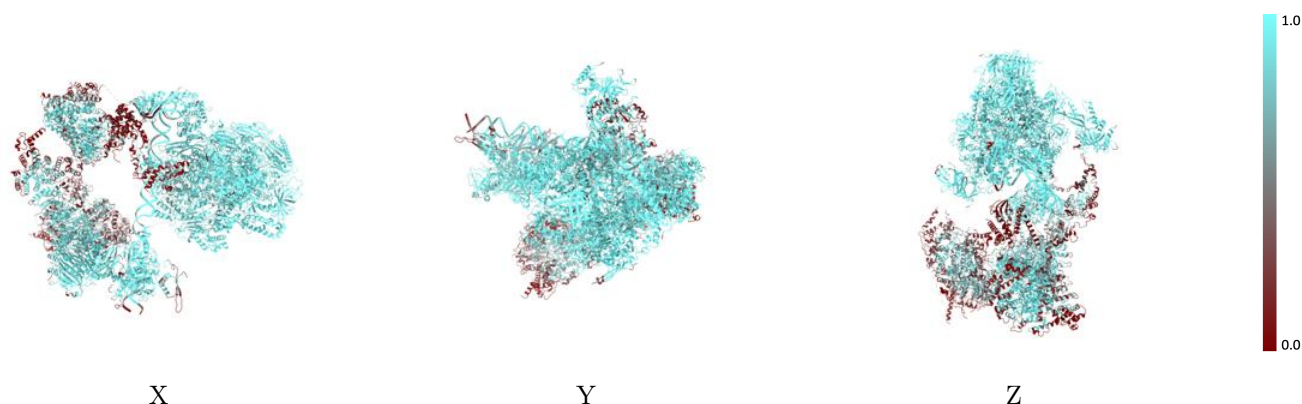
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



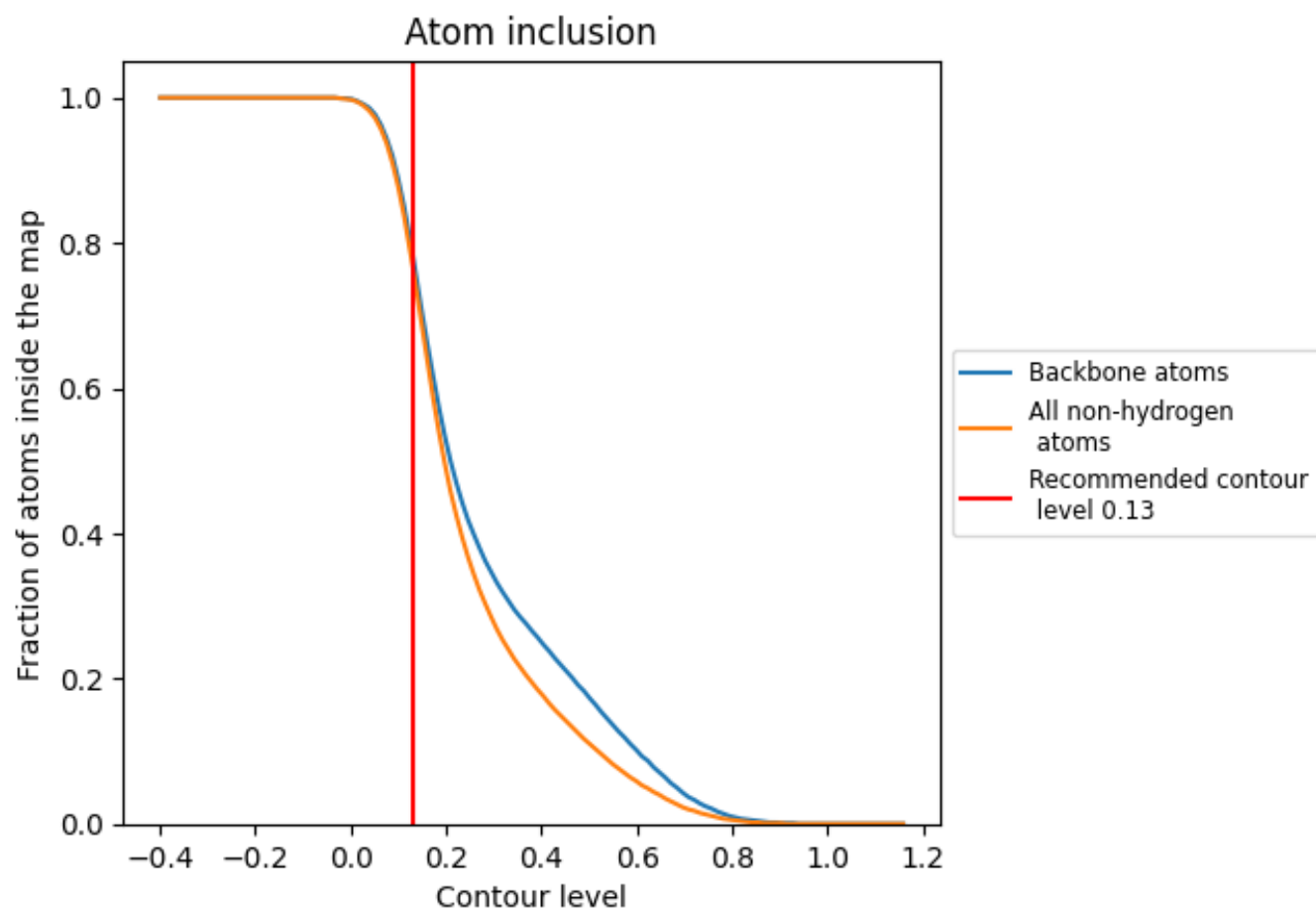
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.13).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 77% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7680	 0.1370
A	 0.8320	 0.0160
B	 0.9040	 0.0370
D	 0.2970	 0.0010
E	 0.7600	 0.0140
F	 0.5210	 0.0090
G	 0.8760	 -0.0040
H	 0.6060	 -0.0030
I	 0.7100	 0.0160
J	 0.6810	 -0.0010
L	 0.2210	 -0.0060
O	 0.3060	 -0.0150
P	 0.9460	 0.0130
Q	 0.3010	 0.0030
R	 0.9090	 0.1460
S	 0.8920	 0.0820
T	 0.8840	 0.0670
U	 0.4200	 -0.0010
V	 0.2480	 0.0100
X	 0.8830	 0.0620
Y	 0.8220	 0.0720
c	 0.4010	 -0.0170
d	 0.3100	 0.0110
e	 0.4380	 -0.0020
f	 0.6670	 0.0200
i	 0.4870	 -0.0100
j	 0.4170	 -0.0160
k	 0.3100	 -0.0000
l	 0.5020	 0.0270
m	 0.2930	 -0.0060
o	 0.9340	 0.3050
p	 0.9620	 0.3760
q	 0.9920	 0.4220
r	 0.9510	 0.1150
s	 0.9820	 0.3140



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
t	 0.9970	 0.4100
u	 0.9720	 0.1760
v	 0.9920	 0.3870
w	 0.9880	 0.3280
x	 0.9880	 0.4410
y	 0.9680	 0.3950
z	 0.9780	 0.3530