wwPDB EM Validation Summary Report

Oct 27, 2024 – 04:07 PM JST

PDB ID	:	7EGD
EMDB ID	:	EMD-31113
Title	:	SCP promoter-bound TFIID-TFIIA in initial TBP-loading state
Authors	:	Chen, X.; Wu, Z.; Li, J.; Zhao, D.; Xu, Y.
Deposited on	:	2021-03-24
Resolution	:	6.75 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:

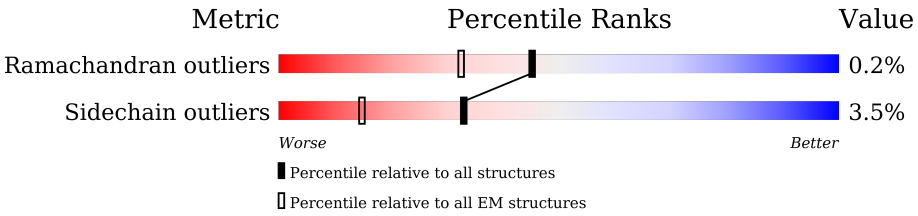
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: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

1 Overall quality at a glance

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

The reported resolution of this entry is 6.75 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 <=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	31% 67%
2	B	1199	79% 20%
3	D	1085	17% 82%
3	d	1085	8% 14% 86%
4	E	800	66% 32%
4	e	800	39% 66% 33%
5	F	677	58% 39%
5	f	677	15% 58% 40%
6	G	349	39% 59%

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Mol	Chain	Length	Quality of chain
7	H	310	66% 33%
8	I	264	45% 55%
8	i	264	23% 46% 54%
9	J	218	38% 59%
9	j	218	26% 42% 56%
10	L	161	44% 53%
10	l	161	39% 66% 34%
11	O	109	22% 88% 11%
12	P	339	26% 51% 48%
13	Q	376	7% 26% 73%
14	X	72	100%
15	Y	72	100%
16	c	929	9% 13% 86%
17	k	211	21% 46% 54%
18	m	124	35% 59% 6% 35%

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 46820 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	620	Total	C	N	O	S	0	0
			5124	3258	909	928	29		

- 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	197	Total	C	N	O	S	0	0
			1614	997	302	310	5		
3	d	152	Total	C	N	O	S	0	0
			1260	786	231	240	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	545	Total	C	N	O	S	0	0
			4359	2765	756	817	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	412	Total	C	N	O	S	0	0
			3143	1994	548	583	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	144	Total	C	N	O	S	0	0
			1171	742	215	210	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
			1622	1026	281	310	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	90	Total	C	N	O	S	0	0
			720	466	115	135	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	101	Total	C	N	O	S	0	0
			827	524	139	160	4		

- Molecule 14 is a DNA chain called DNA (72-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	X	72	Total	C	N	O	P	0	0
			1485	700	284	429	72		

- Molecule 15 is a DNA chain called DNA (72-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Y	72	Total	C	N	O	P	0	0
			1467	695	265	435	72		

- Molecule 16 is a protein called Transcription initiation factor TFIID subunit 3.

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

- Molecule 17 is a protein called Transcription initiation factor TFIID subunit 11.

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

- Molecule 18 is a protein called Transcription initiation factor TFIID subunit 13.

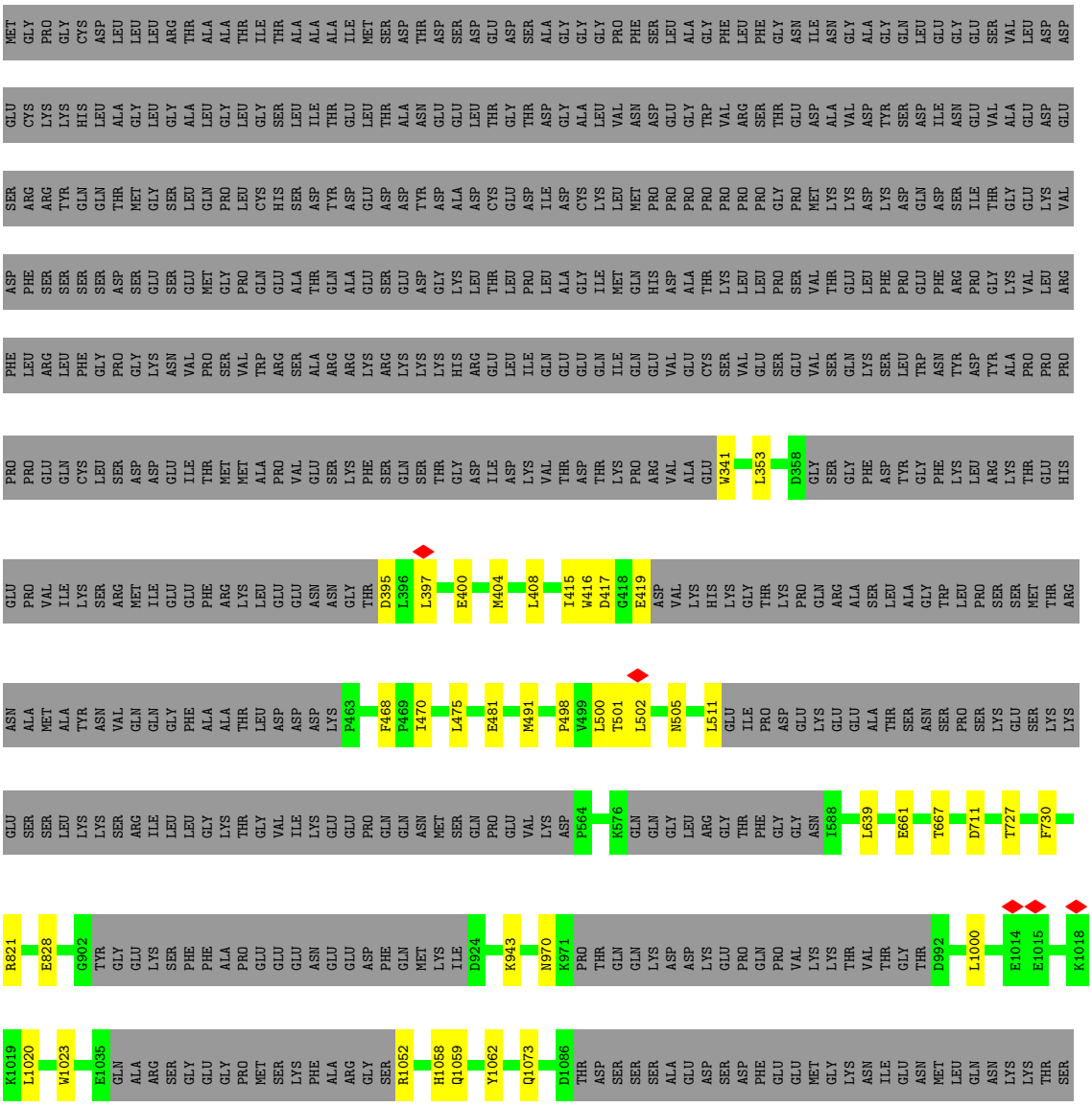
Mol	Chain	Residues	Atoms					AltConf	Trace
18	m	80	Total	C	N	O	S	0	0
			662	419	117	120	6		

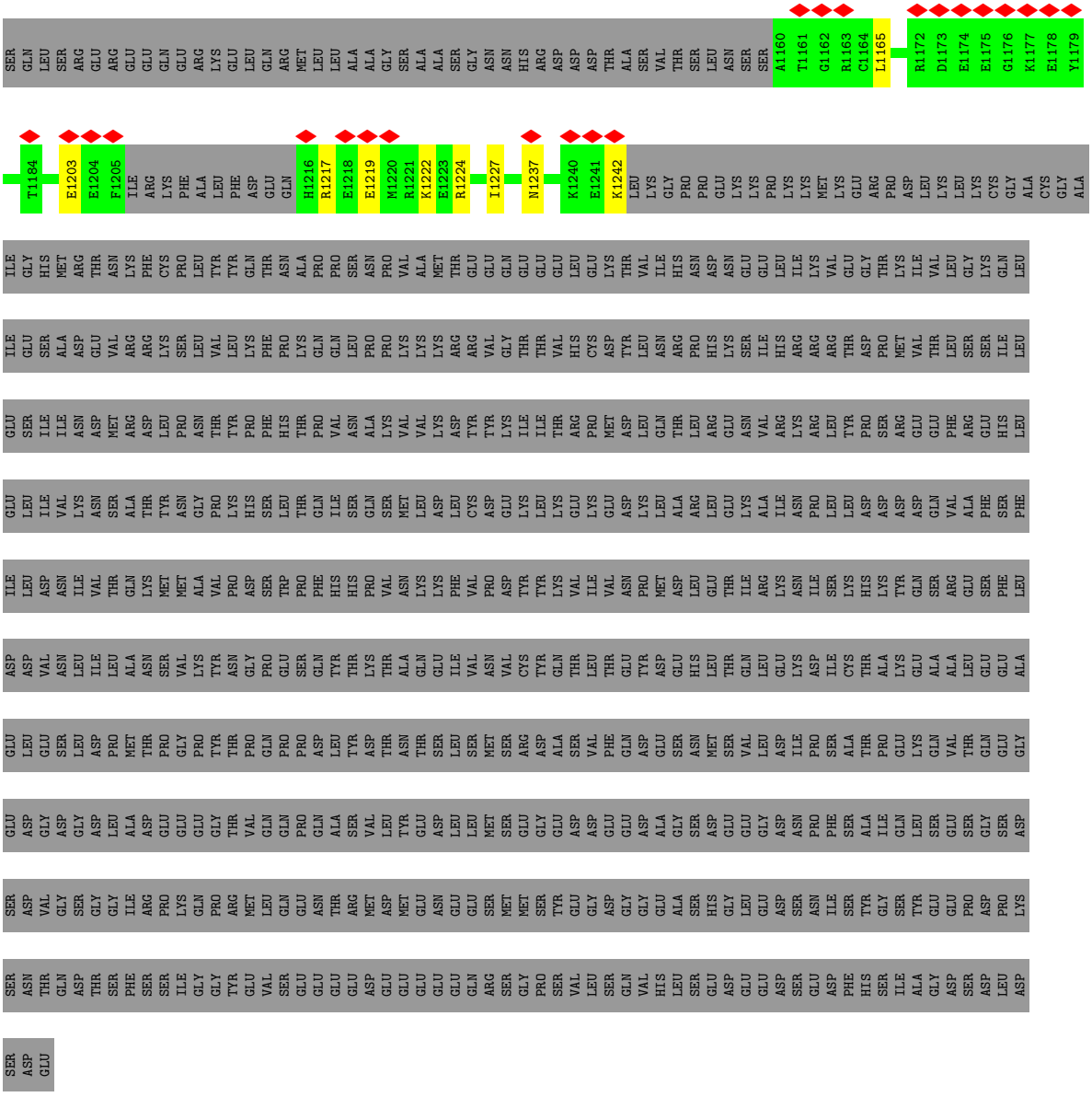
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Transcription initiation factor TFIID subunit 1

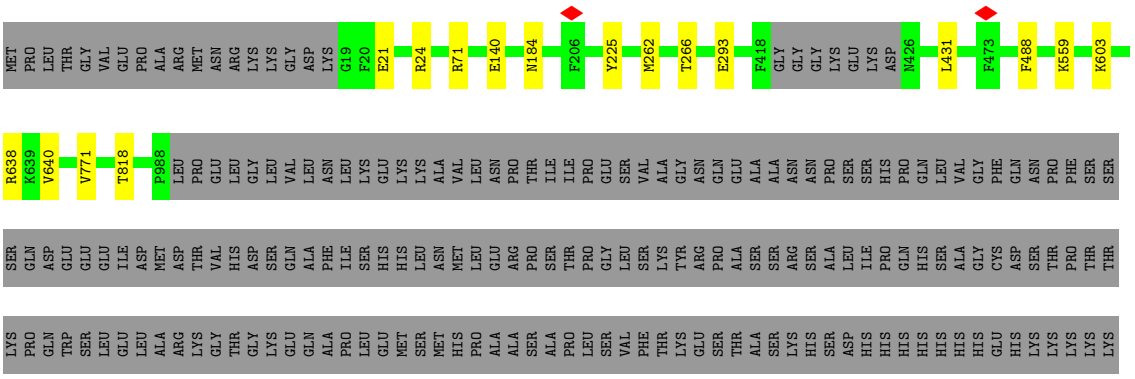
Chain A:



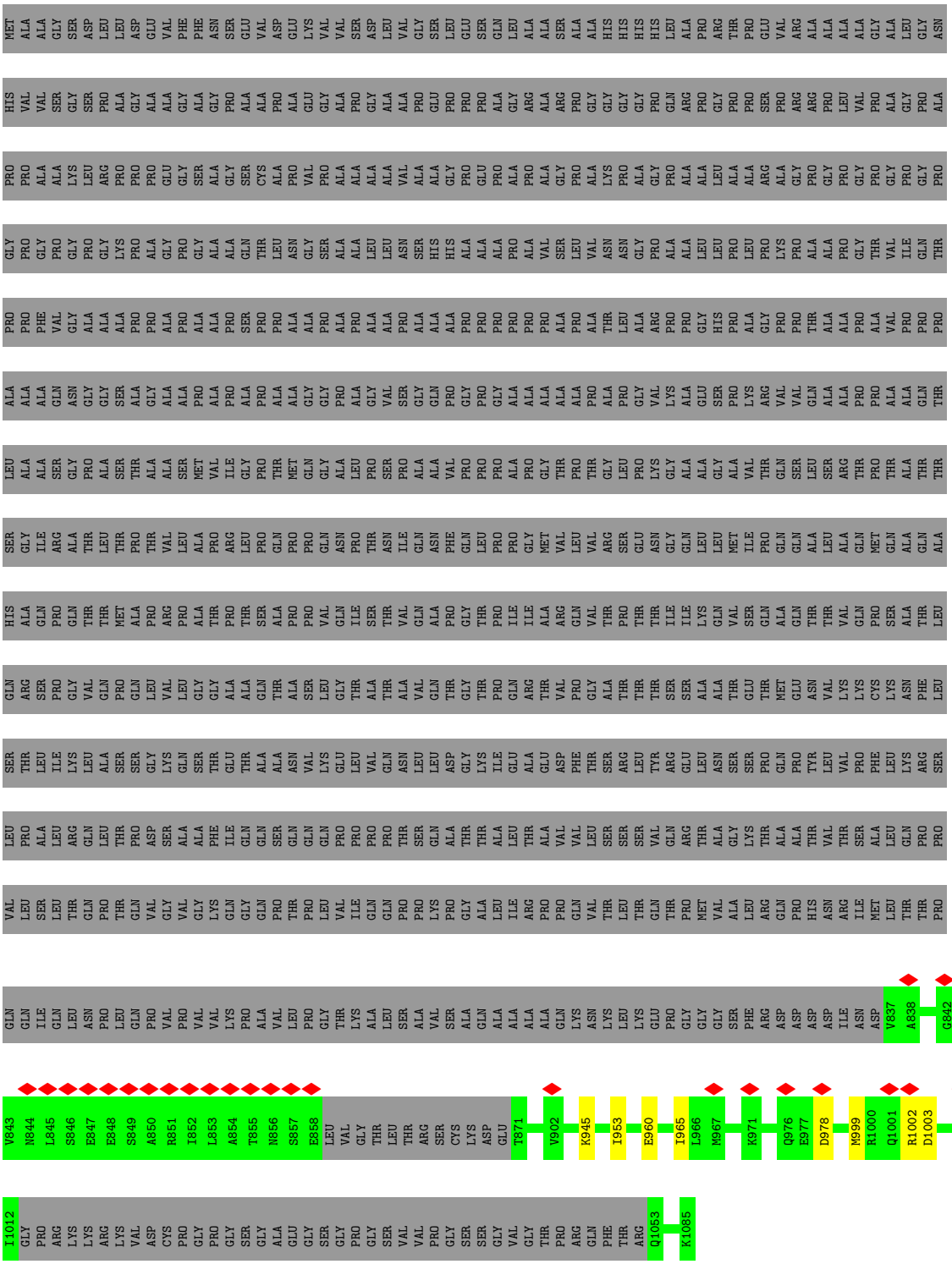


• Molecule 2: Transcription initiation factor TFIID subunit 2

Chain B:

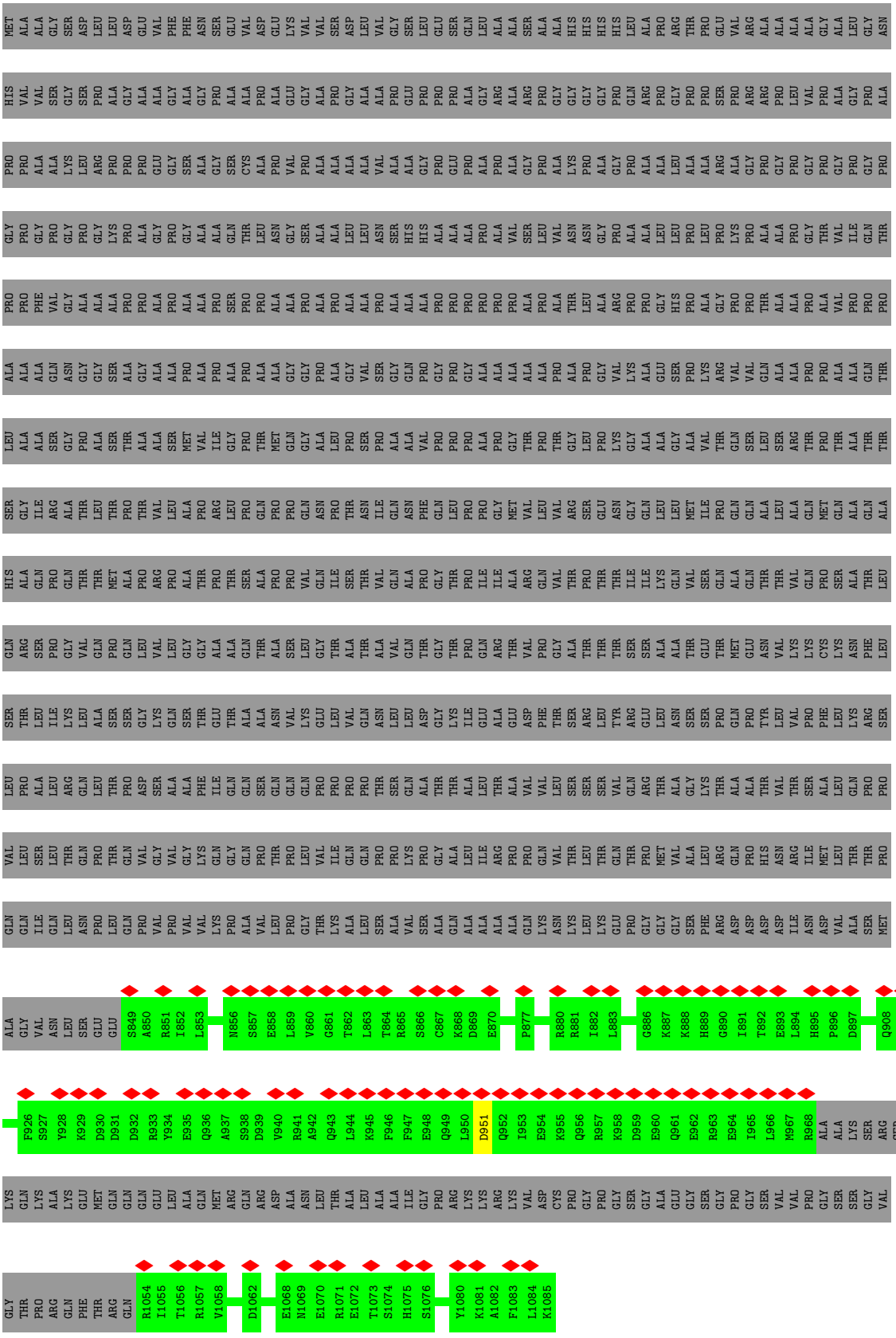


• Molecule 3: Transcription initiation factor TFIID subunit 4



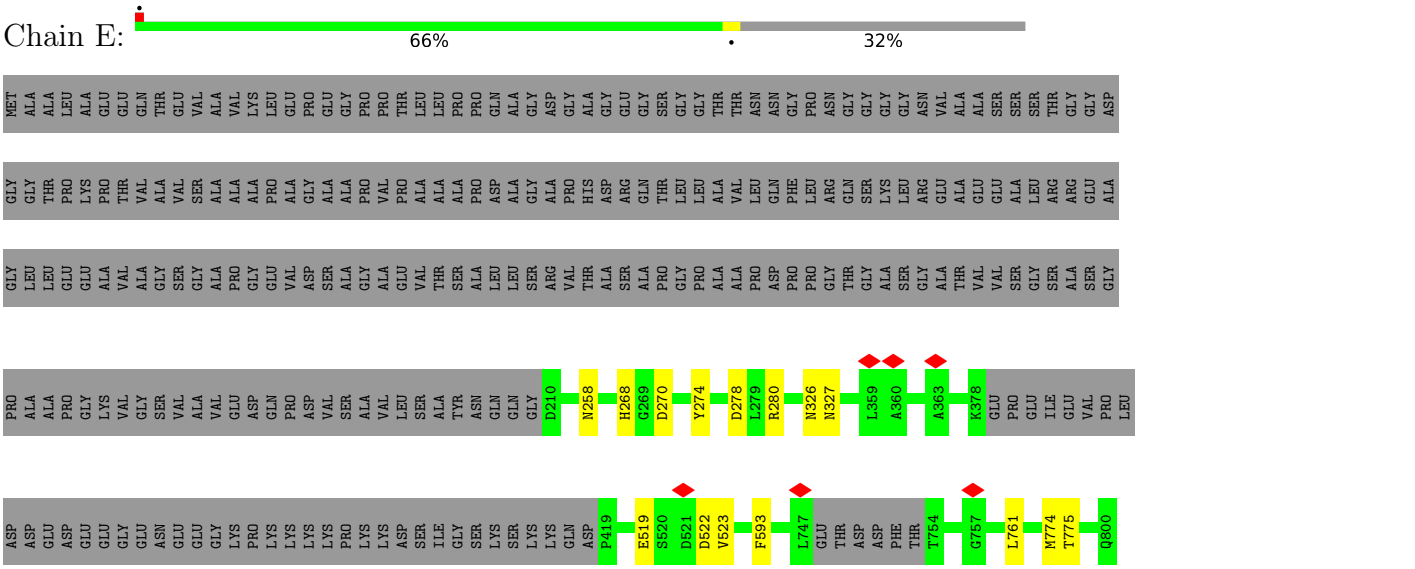
• Molecule 3: Transcription initiation factor TFIID subunit 4

Chain d:



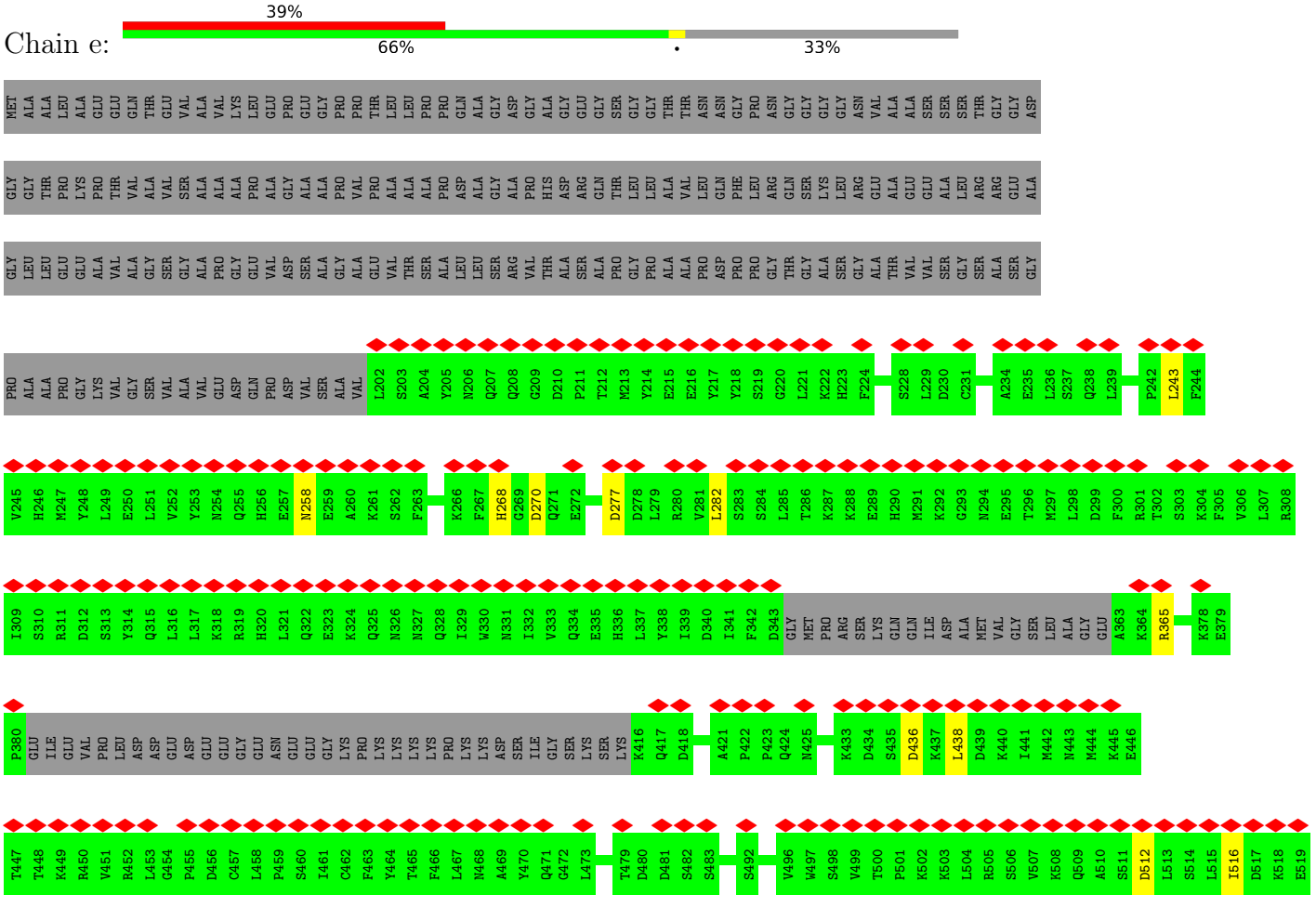
• Molecule 4: Transcription initiation factor TFIID subunit 5

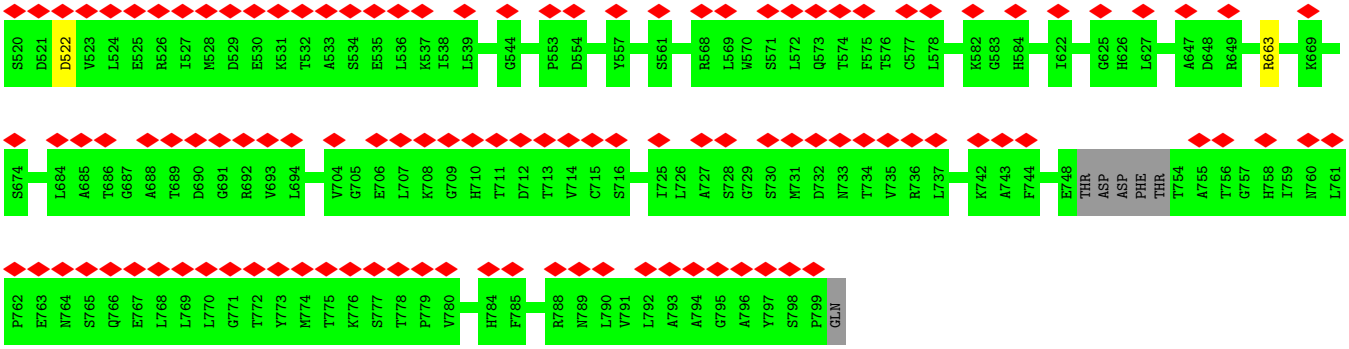
Chain E:



• Molecule 4: Transcription initiation factor TFIID subunit 5

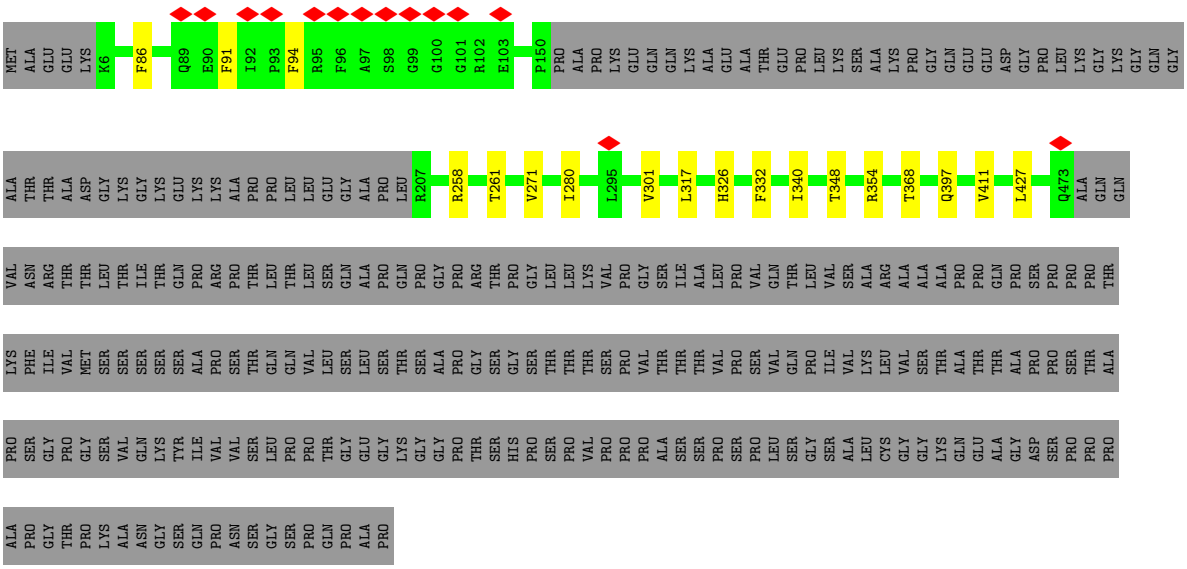
Chain e:





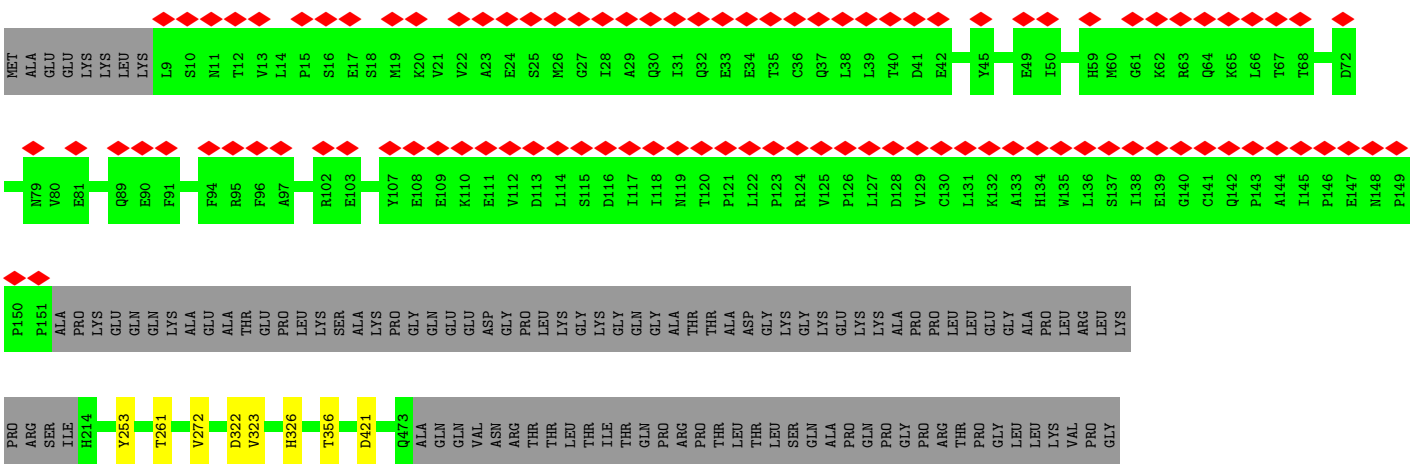
• Molecule 5: Transcription initiation factor TFIID subunit 6

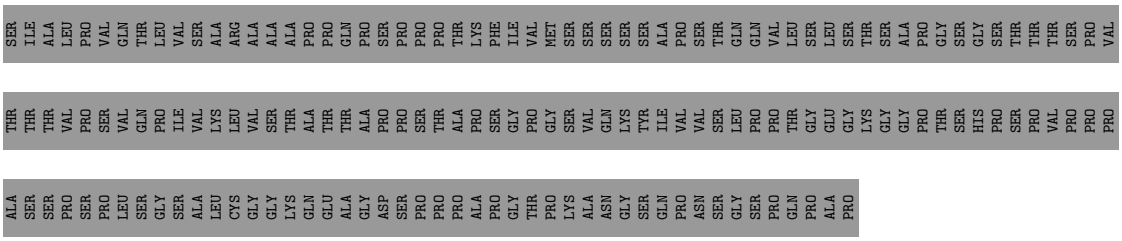
Chain F:



• Molecule 5: Transcription initiation factor TFIID subunit 6

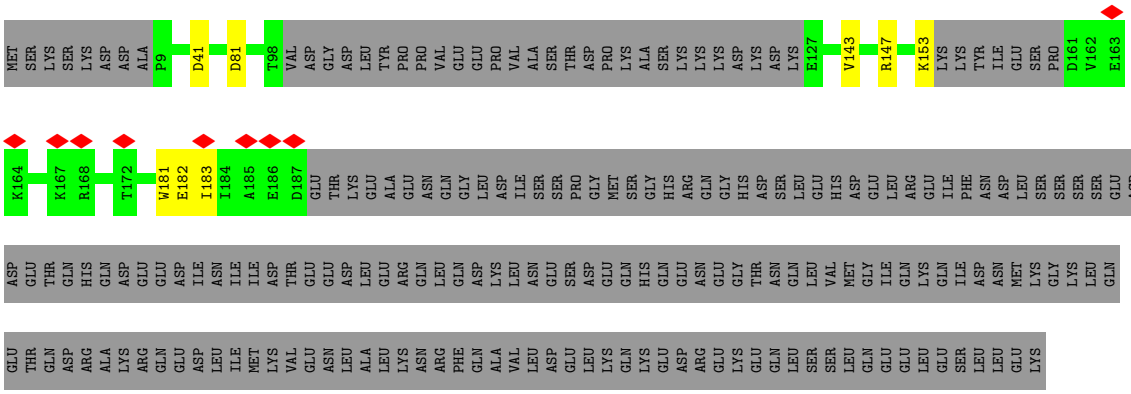
Chain f:





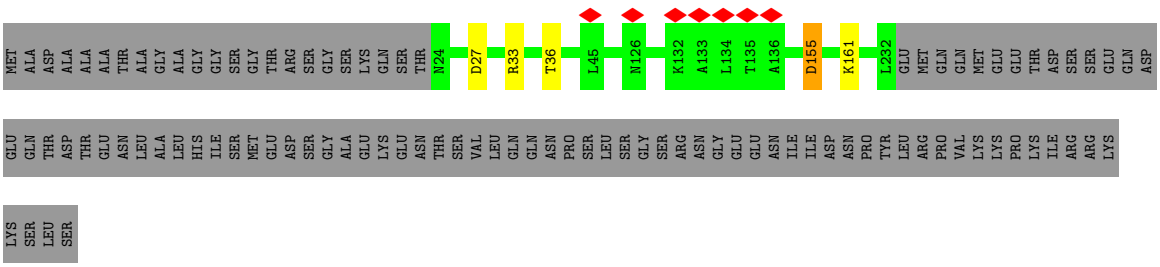
• Molecule 6: Transcription initiation factor TFIID subunit 7

Chain G:



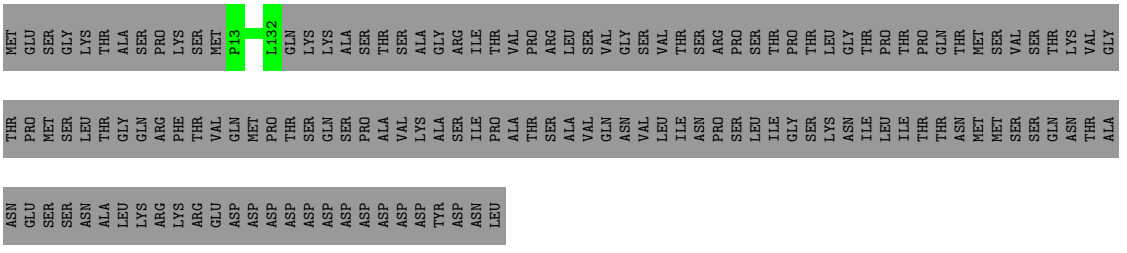
• Molecule 7: Transcription initiation factor TFIID subunit 8

Chain H:



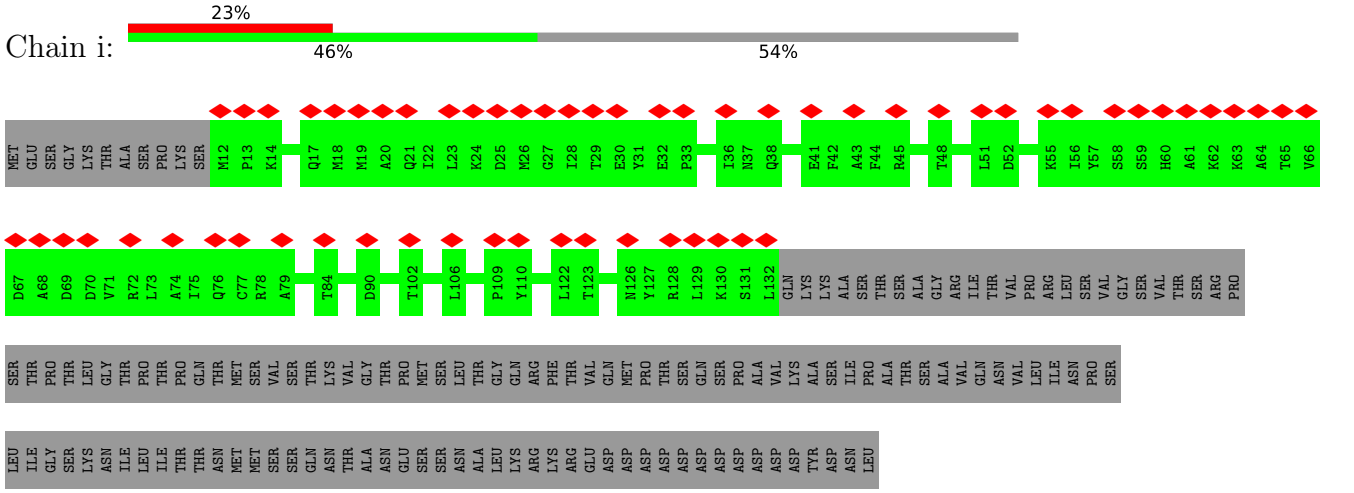
• Molecule 8: Transcription initiation factor TFIID subunit 9

Chain I:



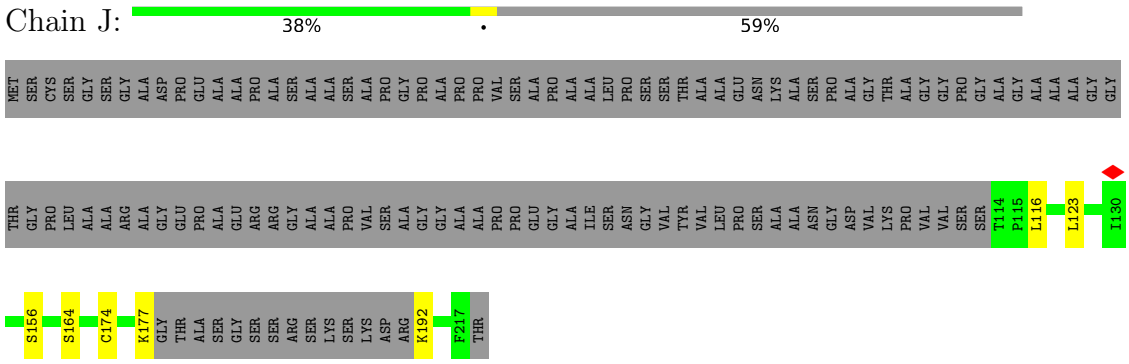
• Molecule 8: Transcription initiation factor TFIID subunit 9

Chain i:



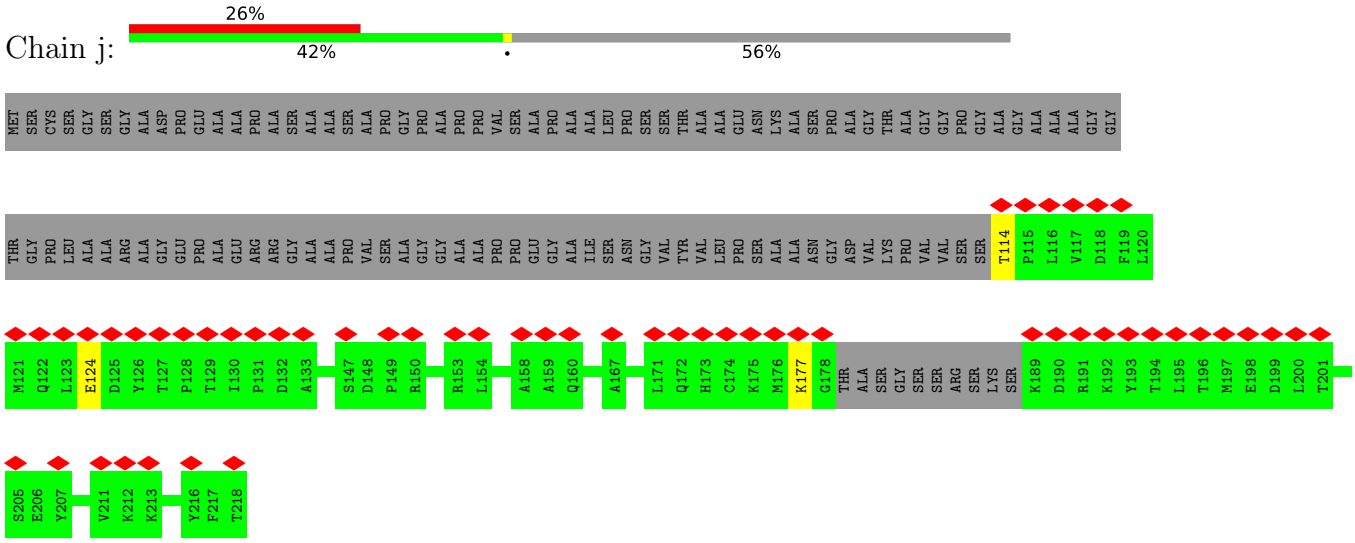
• Molecule 9: Transcription initiation factor TFIID subunit 10

Chain J:



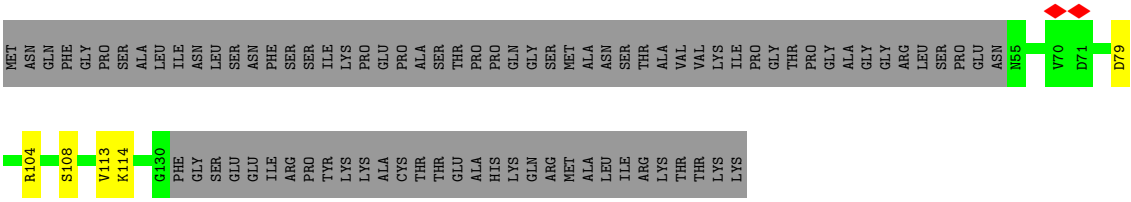
• Molecule 9: Transcription initiation factor TFIID subunit 10

Chain j:

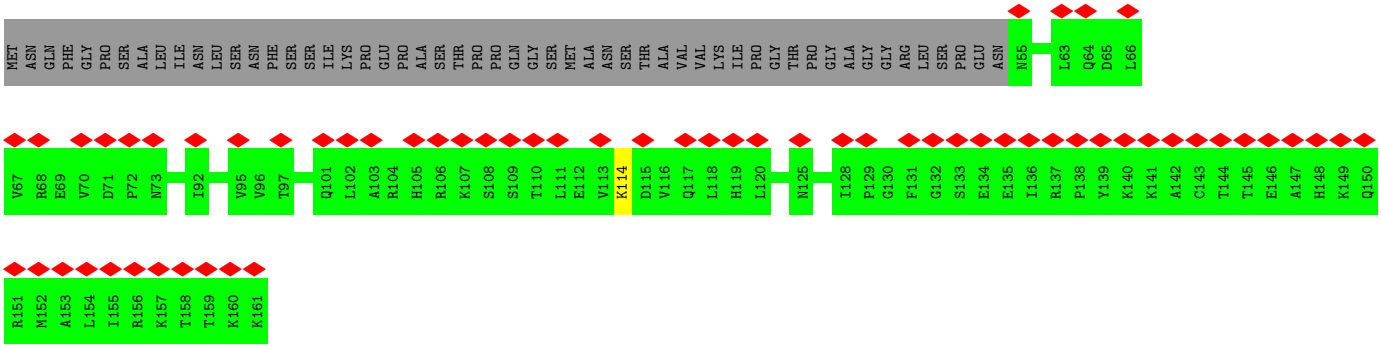


• Molecule 10: Transcription initiation factor TFIID subunit 12

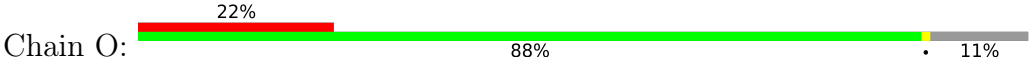
Chain L:

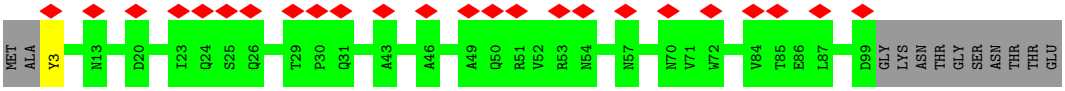


• Molecule 10: Transcription initiation factor TFIID subunit 12

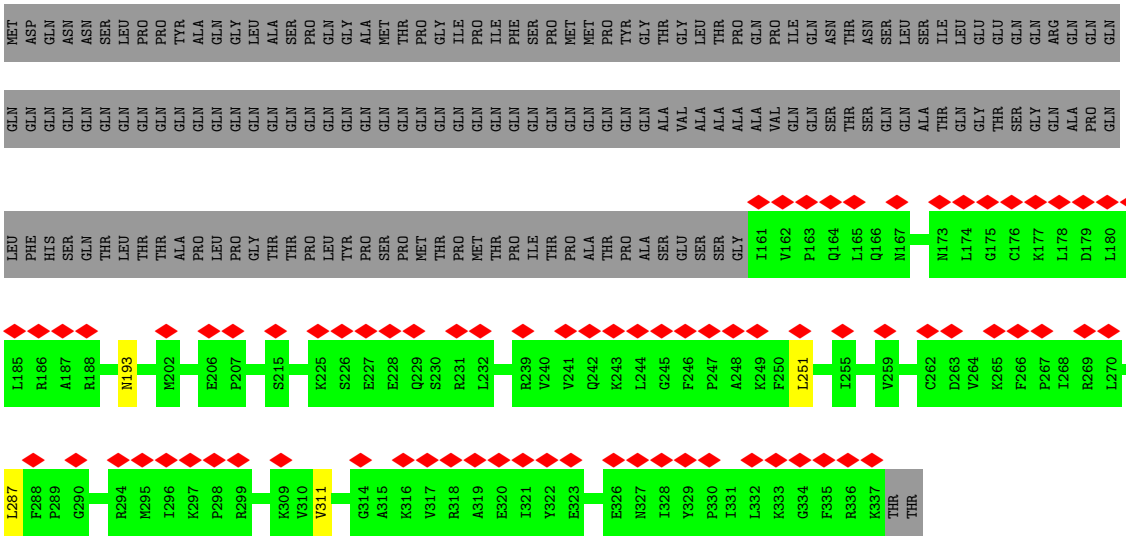


• Molecule 11: Transcription initiation factor IIA subunit 2

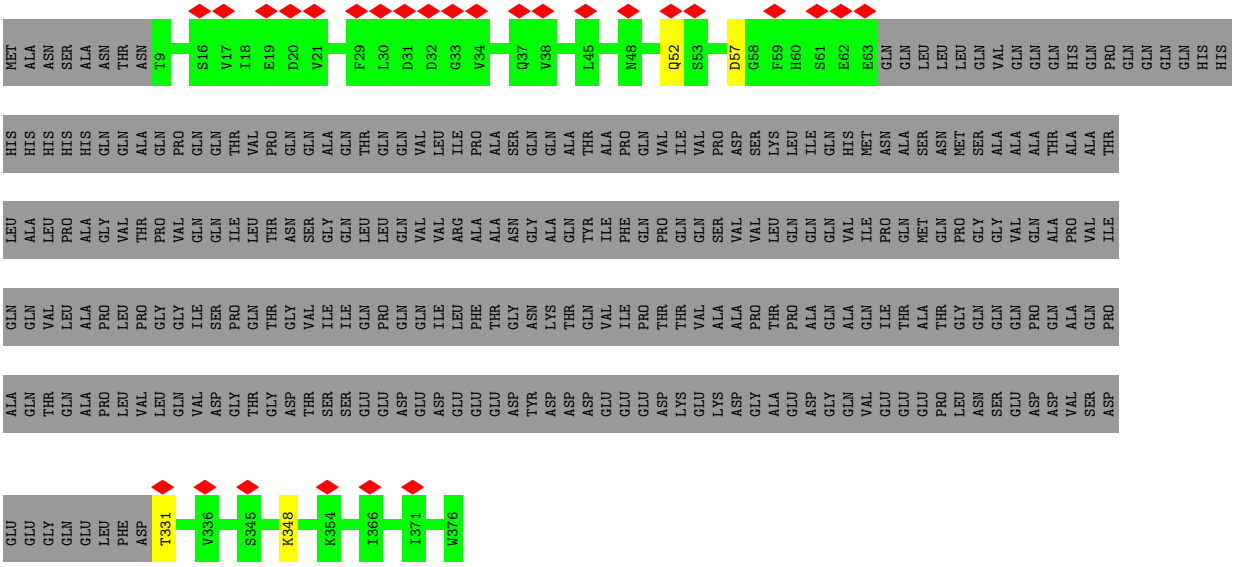




• Molecule 12: TATA-box-binding protein

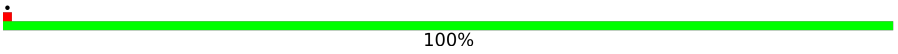

MET ASP GLN ASN SER LEU PRO PRO TYR ALA GLN GLY LEU ALA SER PRO GLN GLY ALA MET THR PRO GLY ILE PRO ILE PHE SER PRO MET MET PRO TYR GLY THR GLY LEU THR PRO GLN PRO ILE GLN ASN THR ASN SER LEU SER ILE LEU GLU GLU GLN GLN ARG GLN GLN GLN
GLN GLN GLN

Chain Q:



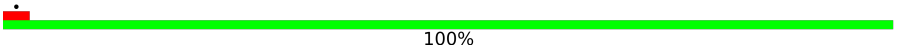
• Molecule 14: DNA (72-MER)

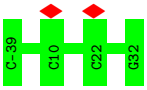
Chain X:



• Molecule 15: DNA (72-MER)

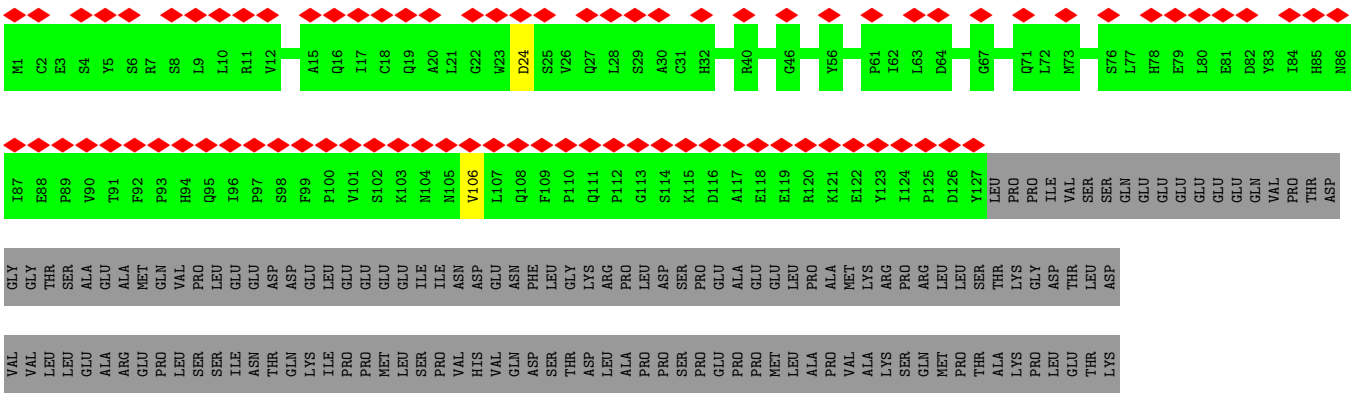
Chain Y:

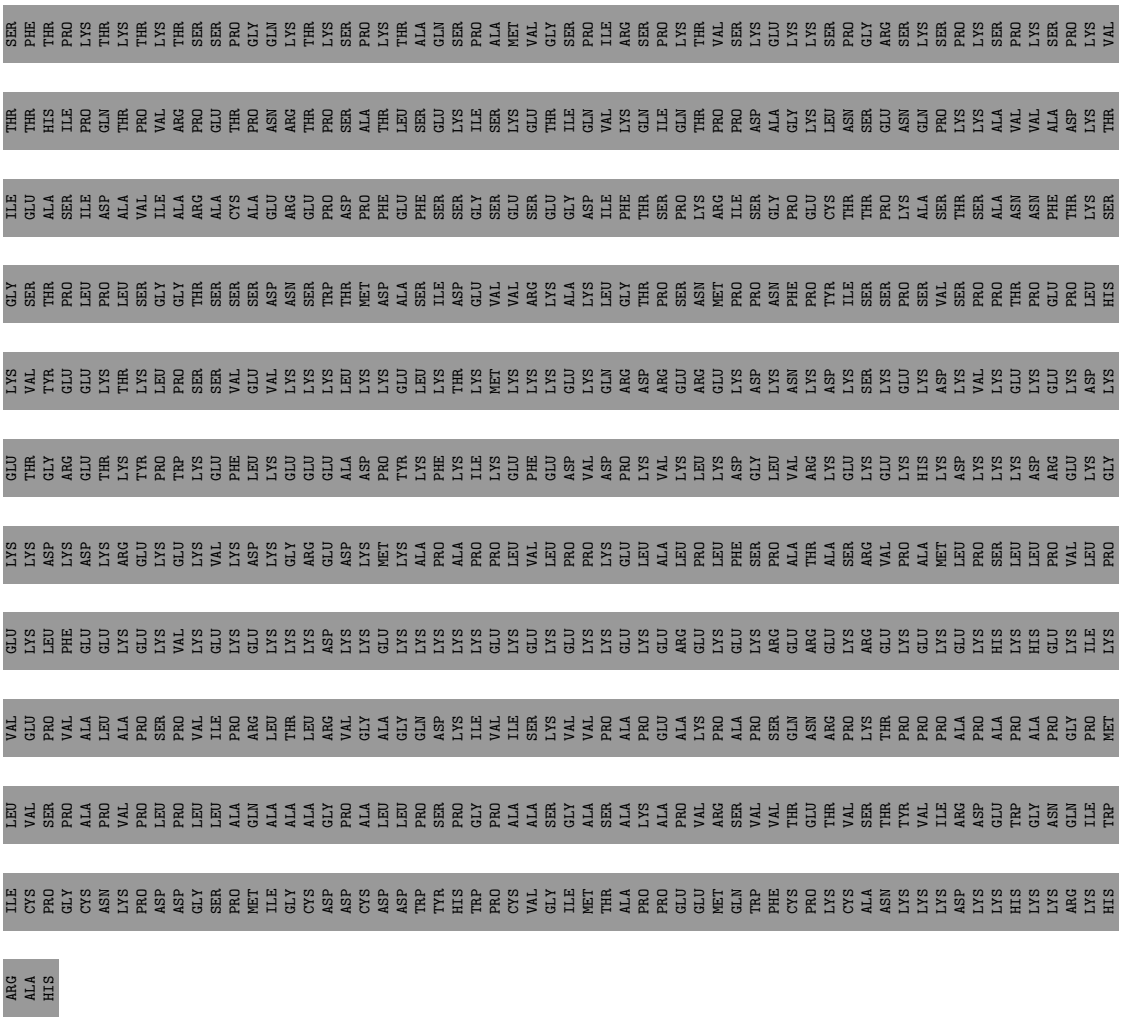




• Molecule 16: Transcription initiation factor TFIID subunit 3

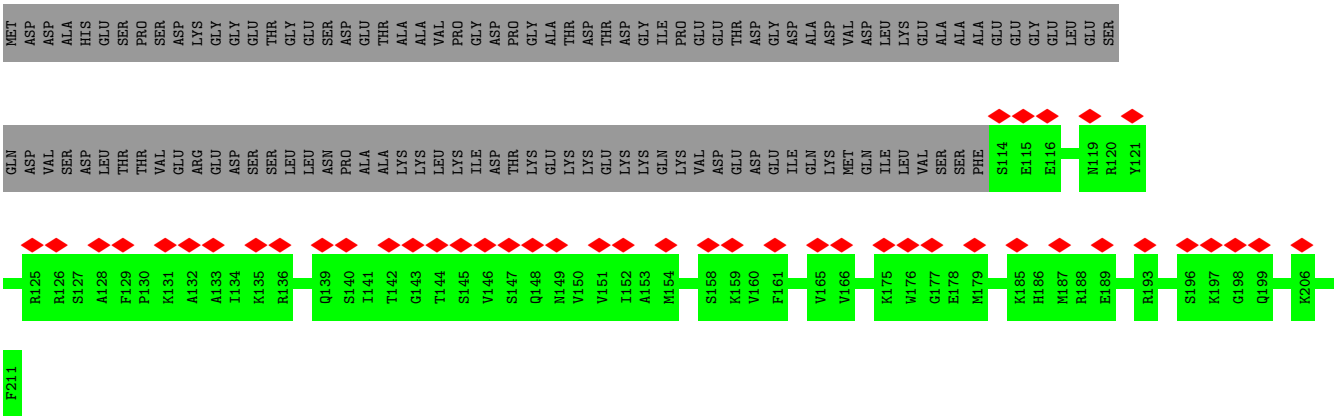
Chain c:





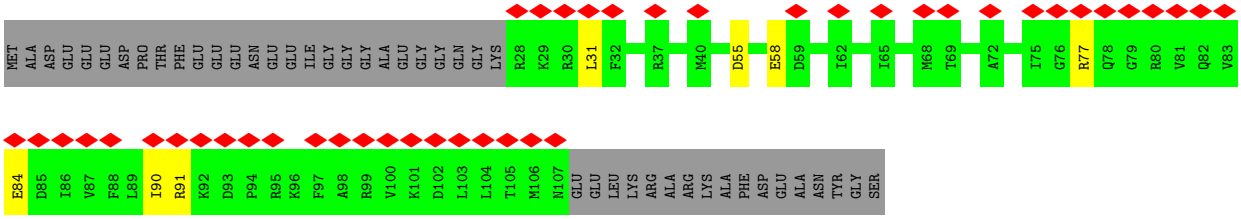
• Molecule 17: Transcription initiation factor TFIID subunit 11

Chain k:



• Molecule 18: Transcription initiation factor TFIID subunit 13

Chain m:


MET ALA ASP GLU GLU GLU ASP PRO THR PHE GLU GLU GLU ASN GLU GLU ILE GLY GLY GLY ALA GLU GLY GLY GLN GLY LYS
R28 K29 R30 L31 F32 R37 M40 D55 E58 D59 I62 I65 M68 T69 A72 I75 G76 R77 Q78 G79 R80 V81 Q82 V83
E84 D85 I86 V87 F88 L89 I90 R91 K92 D93 P94 R95 K96 F97 A98 R99 V100 K101 D102 L103 L104 T105 M106 N107 GLU GLU LEU LYS ARG ALA ARG LYS ALA PHE ASP GLU ALA ASN TYR GLY SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100170	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.083	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	432.0, 432.0, 432.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality

5.1 Standard geometry

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	0.49	0/5243	0.67	0/7060
2	B	0.46	0/7993	0.60	0/10836
3	D	0.43	0/1628	0.56	0/2178
3	d	0.39	0/1274	0.53	0/1708
4	E	0.39	0/4465	0.59	0/6045
4	e	0.43	0/4433	0.59	0/6004
5	F	0.48	0/3201	0.69	0/4347
5	f	0.40	0/3140	0.63	0/4268
6	G	0.50	0/1190	0.62	0/1601
7	H	0.49	0/1662	0.67	0/2272
8	I	0.27	0/981	0.47	0/1332
8	i	0.29	0/989	0.46	0/1343
9	J	0.57	0/736	0.69	0/998
9	j	0.53	0/775	0.63	0/1049
10	L	0.48	0/630	0.71	0/852
10	l	0.44	0/888	0.55	0/1194
11	O	0.34	0/781	0.62	0/1061
12	P	0.46	0/1438	0.58	0/1935
13	Q	0.36	0/842	0.64	0/1134
14	X	0.67	0/1668	1.02	0/2574
15	Y	0.61	0/1642	0.97	0/2530
16	c	0.39	0/1035	0.54	0/1406
17	k	0.30	0/799	0.47	0/1070
18	m	0.59	0/671	0.64	0/896
All	All	0.46	0/48104	0.65	0/65693

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	
1	A	600/1872 (32%)	579 (96%)	19 (3%)	2 (0%)	37	73
2	B	959/1199 (80%)	911 (95%)	48 (5%)	0	100	100
3	D	191/1085 (18%)	181 (95%)	10 (5%)	0	100	100
3	d	148/1085 (14%)	143 (97%)	5 (3%)	0	100	100
4	E	539/800 (67%)	515 (96%)	23 (4%)	1 (0%)	44	78
4	e	531/800 (66%)	482 (91%)	48 (9%)	1 (0%)	44	78
5	F	408/677 (60%)	390 (96%)	17 (4%)	1 (0%)	44	78
5	f	399/677 (59%)	380 (95%)	19 (5%)	0	100	100
6	G	138/349 (40%)	135 (98%)	3 (2%)	0	100	100
7	H	207/310 (67%)	193 (93%)	13 (6%)	1 (0%)	25	64
8	I	118/264 (45%)	115 (98%)	3 (2%)	0	100	100
8	i	119/264 (45%)	115 (97%)	4 (3%)	0	100	100
9	J	86/218 (39%)	82 (95%)	4 (5%)	0	100	100
9	j	91/218 (42%)	85 (93%)	4 (4%)	2 (2%)	5	29
10	L	74/161 (46%)	72 (97%)	2 (3%)	0	100	100
10	l	105/161 (65%)	100 (95%)	5 (5%)	0	100	100
11	O	95/109 (87%)	86 (90%)	9 (10%)	0	100	100
12	P	175/339 (52%)	163 (93%)	11 (6%)	1 (1%)	22	60
13	Q	97/376 (26%)	90 (93%)	7 (7%)	0	100	100
16	c	125/929 (14%)	116 (93%)	9 (7%)	0	100	100
17	k	96/211 (46%)	91 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
18	m	78/124 (63%)	75 (96%)	3 (4%)	0	100 100
All	All	5379/12228 (44%)	5099 (95%)	271 (5%)	9 (0%)	45 78

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1000	LEU
4	E	523	VAL
4	e	522	ASP
9	j	124	GLU
5	F	411	VAL

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	555/1665 (33%)	508 (92%)	47 (8%)	8 27
2	B	876/1083 (81%)	859 (98%)	17 (2%)	52 69
3	D	175/815 (22%)	167 (95%)	8 (5%)	23 44
3	d	140/815 (17%)	139 (99%)	1 (1%)	81 87
4	E	478/657 (73%)	464 (97%)	14 (3%)	37 56
4	e	475/657 (72%)	463 (98%)	12 (2%)	42 61
5	F	328/574 (57%)	311 (95%)	17 (5%)	19 40
5	f	322/574 (56%)	314 (98%)	8 (2%)	42 61
6	G	132/322 (41%)	124 (94%)	8 (6%)	15 37
7	H	178/270 (66%)	173 (97%)	5 (3%)	38 57
8	I	106/235 (45%)	106 (100%)	0	100 100
8	i	107/235 (46%)	107 (100%)	0	100 100
9	J	79/154 (51%)	72 (91%)	7 (9%)	8 25
9	j	83/154 (54%)	82 (99%)	1 (1%)	67 79
10	L	71/141 (50%)	66 (93%)	5 (7%)	12 33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	l	98/141 (70%)	97 (99%)	1 (1%)	73 82
11	O	84/98 (86%)	83 (99%)	1 (1%)	67 79
12	P	153/293 (52%)	149 (97%)	4 (3%)	41 59
13	Q	91/324 (28%)	87 (96%)	4 (4%)	24 45
16	c	113/833 (14%)	111 (98%)	2 (2%)	54 71
17	k	87/182 (48%)	87 (100%)	0	100 100
18	m	74/106 (70%)	67 (90%)	7 (10%)	7 22
All	All	4805/10328 (46%)	4636 (96%)	169 (4%)	33 51

5 of 169 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	H	161	LYS
4	e	270	ASP
9	J	164	SER
12	P	280	PHE
4	e	516	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
11	O	70	ASN
9	j	160	GLN
12	P	193	ASN
4	e	294	ASN
18	m	70	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

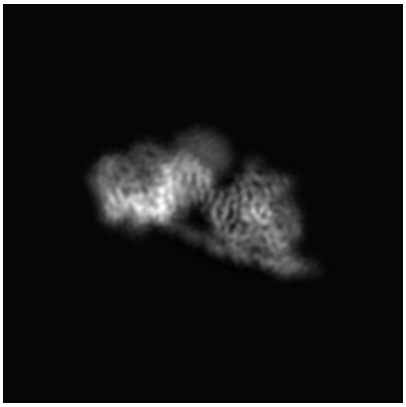
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31113. These allow visual inspection of the internal detail of the map and identification of artifacts.

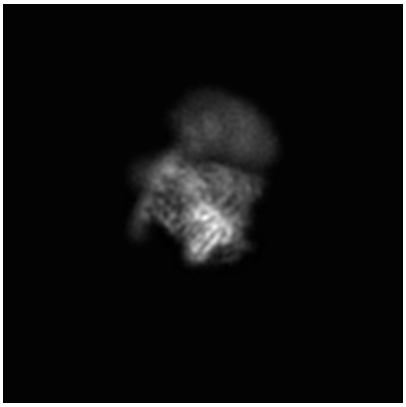
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

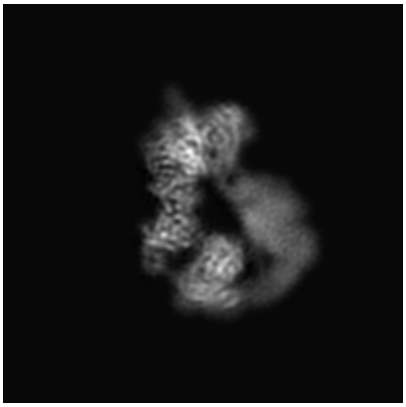
6.1.1 Primary map



X



Y

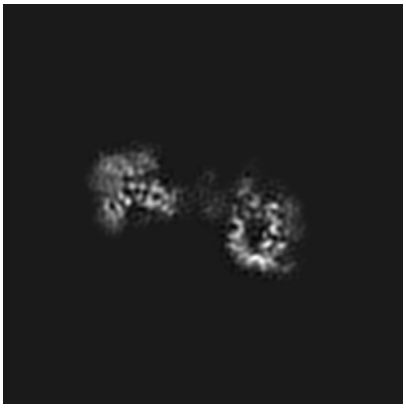


Z

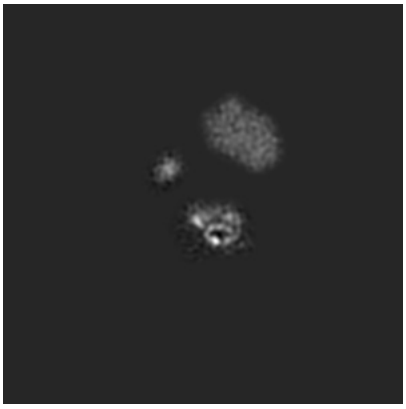
The images above show the map projected in three orthogonal directions.

6.2 Central slices

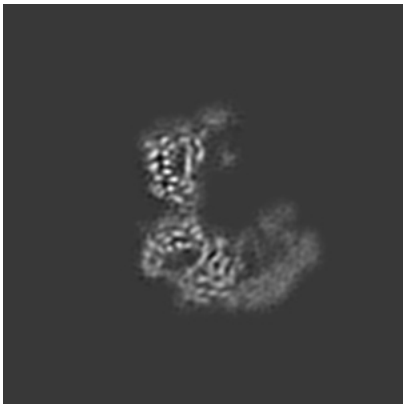
6.2.1 Primary map



X Index: 160



Y Index: 160

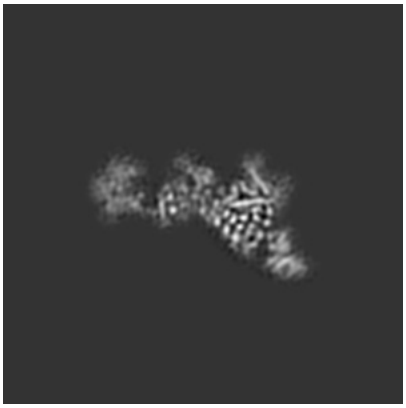


Z Index: 160

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

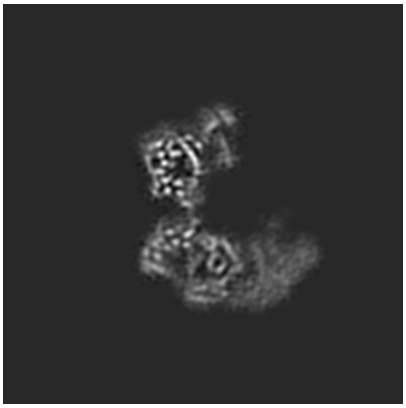
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 148

Y Index: 200

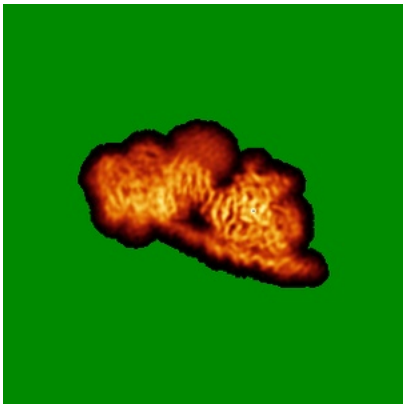


Z Index: 155

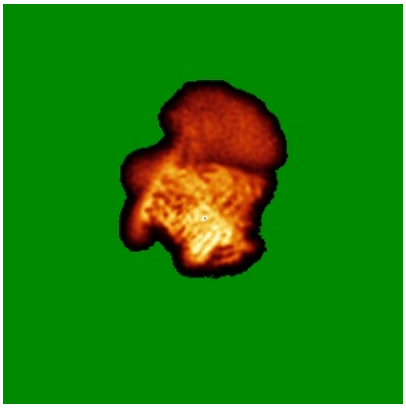
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

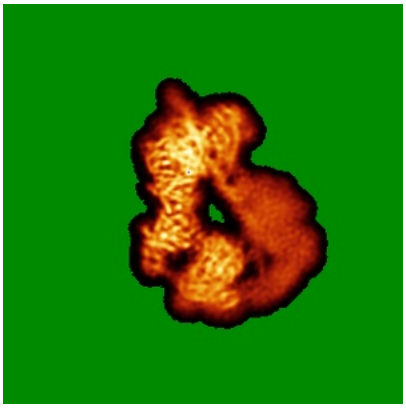
6.4.1 Primary map



X



Y

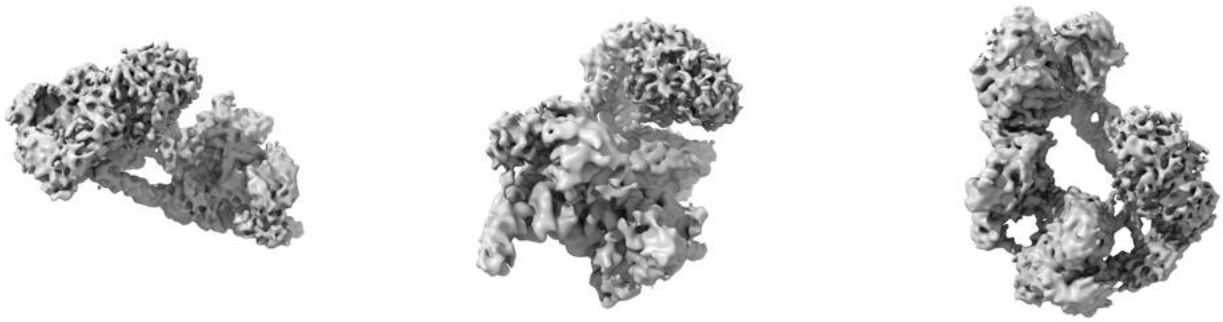


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

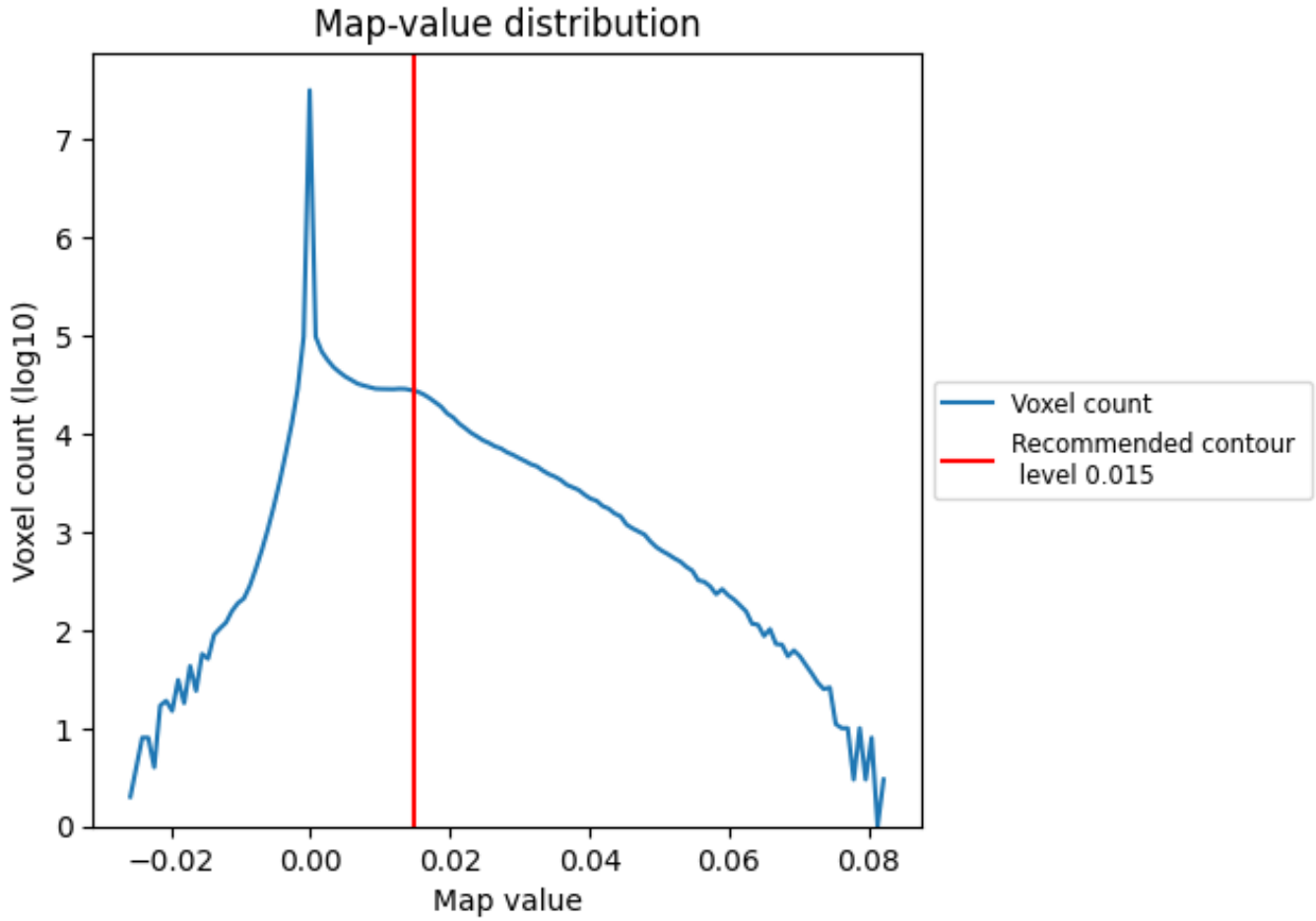
6.6 Mask visualisation (i)

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

7 Map analysis

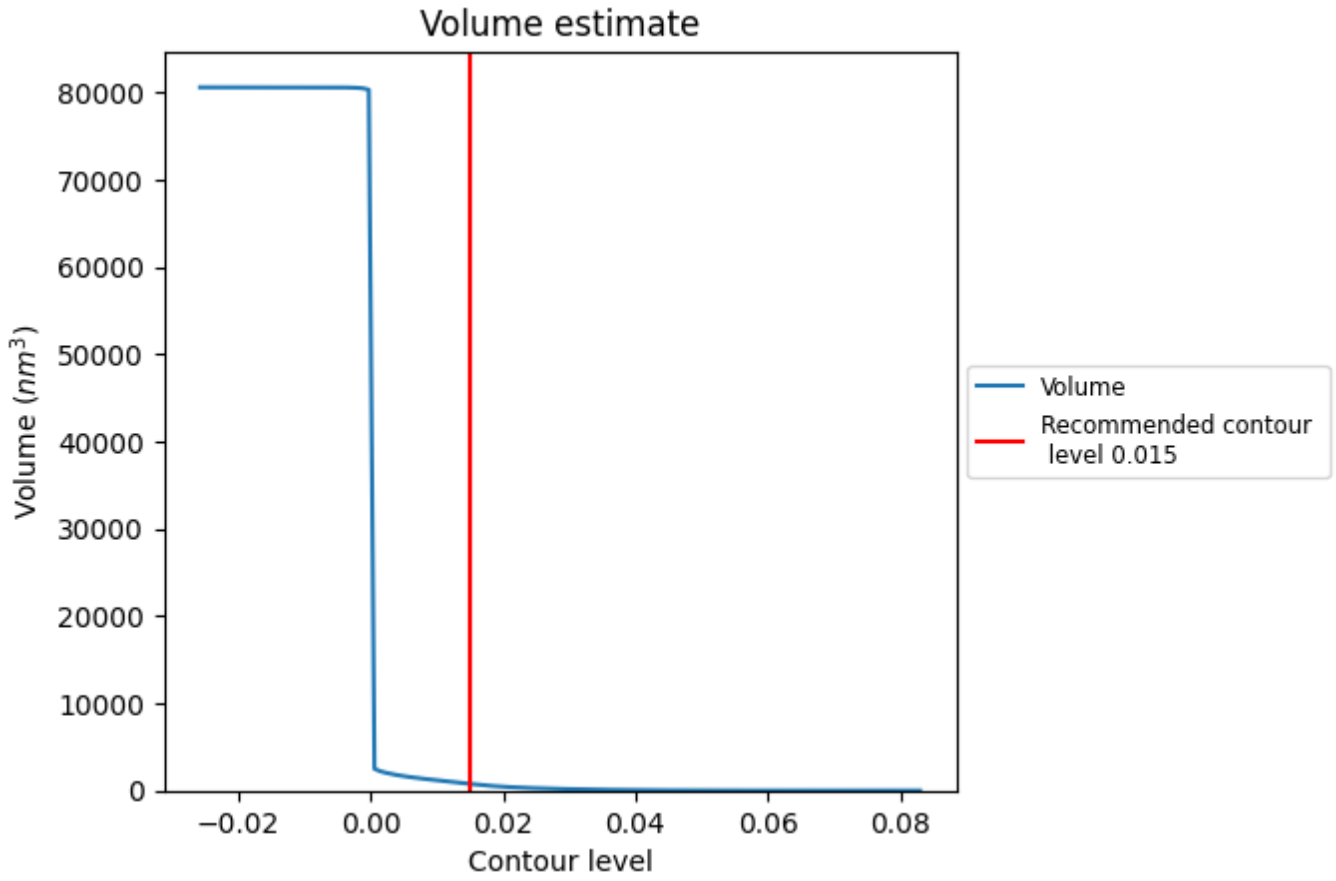
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

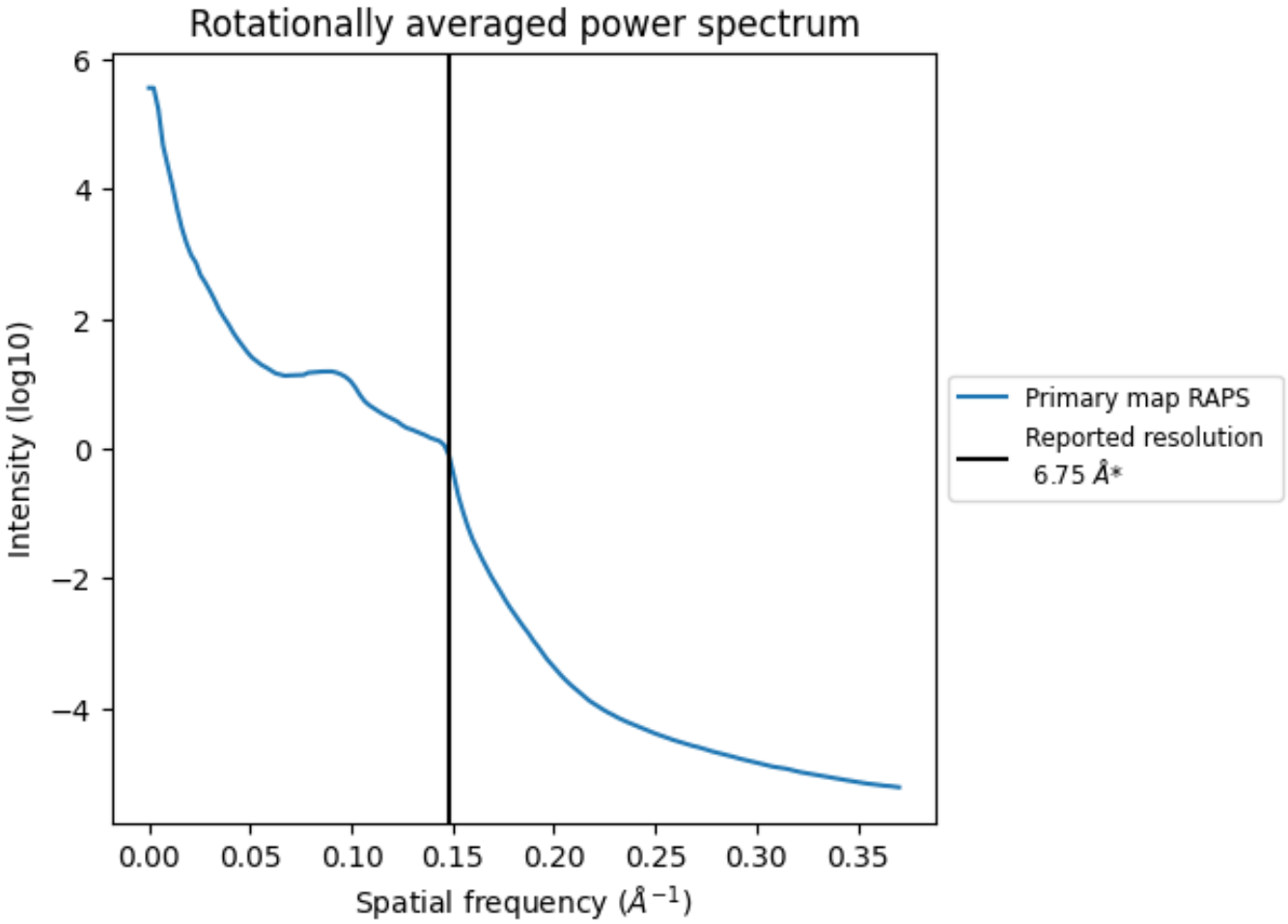
7.2 Volume estimate (i)



The volume at the recommended contour level is 770 nm^3; this corresponds to an approximate mass of 696 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.148 Å^{-1}

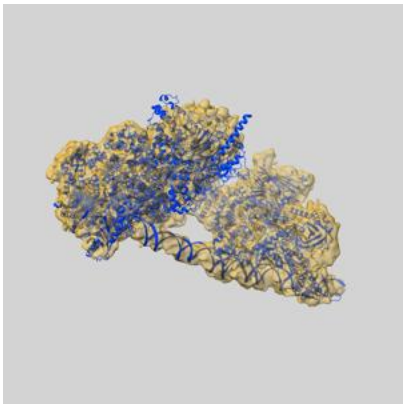
8 Fourier-Shell correlation (i)

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

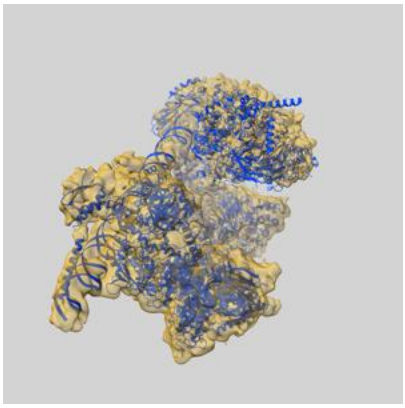
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31113 and PDB model 7EGD. Per-residue inclusion information can be found in section 3 on page 7.

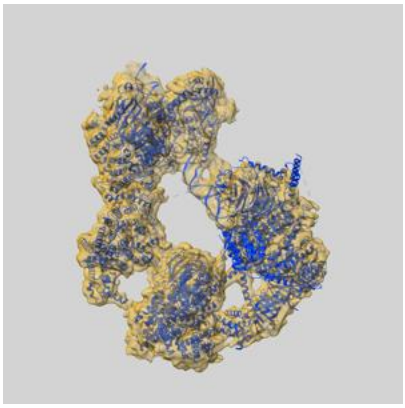
9.1 Map-model overlay



X



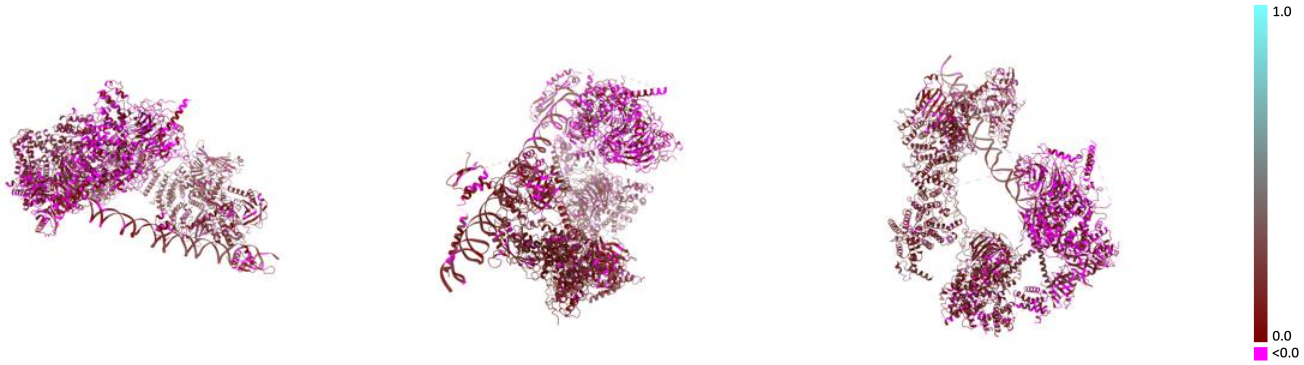
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

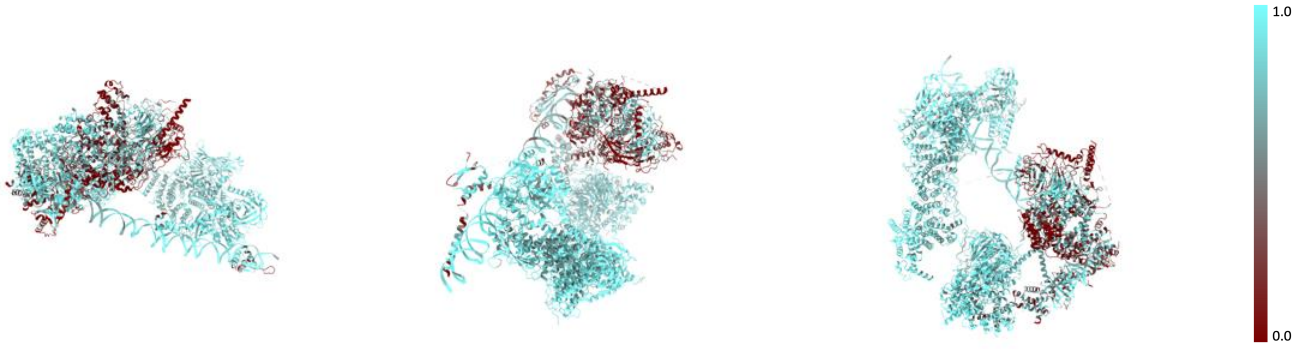
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

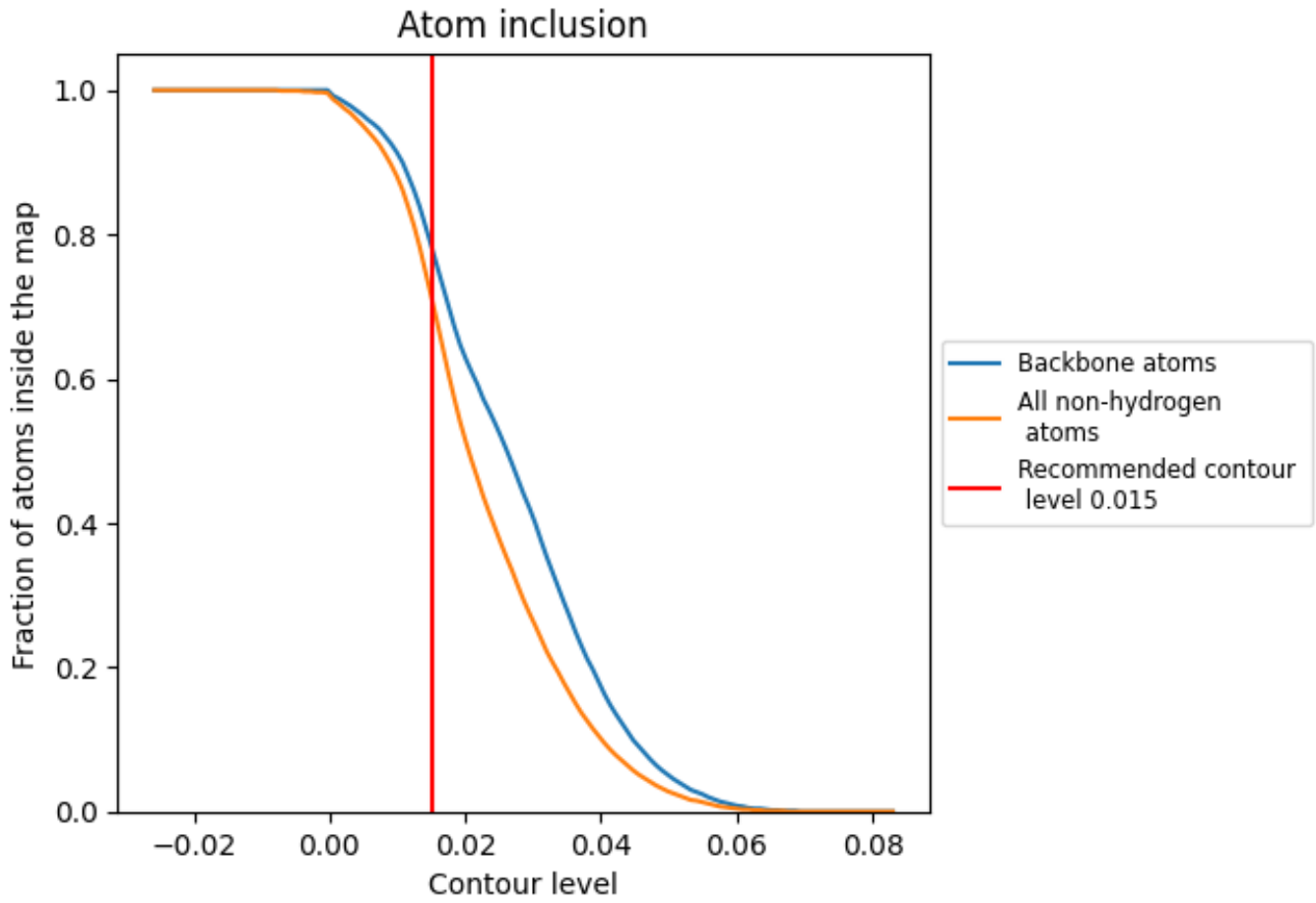
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 71% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7140	0.0990
A	0.8480	0.1320
B	0.8640	0.1510
D	0.7540	0.0990
E	0.8890	0.1370
F	0.8490	0.1340
G	0.8350	0.1140
H	0.8650	0.1450
I	0.9330	0.1420
J	0.8870	0.1050
L	0.8730	0.1030
O	0.6800	0.0690
P	0.4430	0.0350
Q	0.6210	0.0430
X	0.8770	0.1380
Y	0.8410	0.1390
c	0.2770	-0.0070
d	0.3530	0.0070
e	0.3720	0.0060
f	0.6410	0.1120
i	0.4540	0.0200
j	0.3650	0.0100
k	0.4600	0.0200
l	0.3470	0.0030
m	0.3560	0.0020