wwPDB EM Validation Summary Report (i)

Dec 10, 2022 – 10:00 am GMT

PDB ID	:	5FUR
EMDB ID	:	EMD-3305
Title	:	Structure of human TFIID-IIA bound to core promoter DNA
Authors	:	Louder, R.K.; He, Y.; Lopez-Blanco, J.R.; Fang, J.; Chacon, P.; Nogales, E.
Deposited on	:	2016-01-29
Resolution	:	8.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

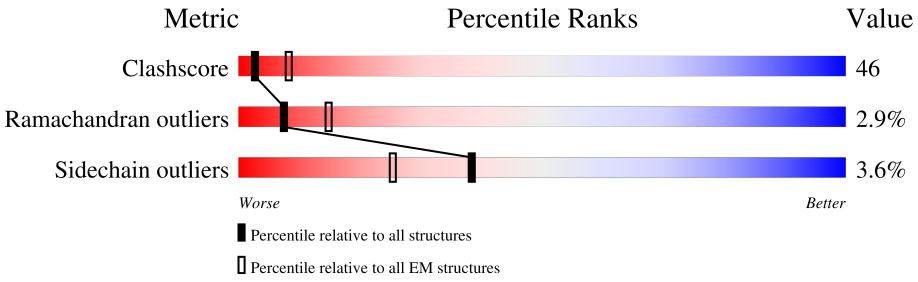
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 8.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	339	44% 8% 47%
2	B	43	14% 77% 21%
3	C	47	53% 45%
4	D	97	9% 57% 41%
5	E	89	69% 18% 10%
6	F	93	68% 16% 14%
7	G	1893	18% 79%
8	H	349	5% 31% 65%

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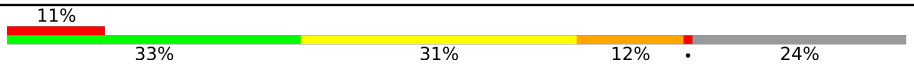
Mol	Chain	Length	Quality of chain
9	I	1199	
10	J	677	
10	K	677	
11	L	310	

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 21485 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 TATA-BOX-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	180	1429	927	252	243	7	0	0

- Molecule 2 is a protein called TRANSCRIPTION INITIATION FACTOR IIA SUBUNIT 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	43	356	228	56	70	2	0	0

- Molecule 3 is a protein called TRANSCRIPTION INITIATION FACTOR IIA SUBUNIT 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	47	393	250	70	71	2	0	0

- Molecule 4 is a protein called TRANSCRIPTION INITIATION FACTOR IIA SUBUNIT 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	97	793	502	140	149	2	0	0

- Molecule 5 is a DNA chain called SUPER CORE PROMOTER.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	E	80	1654	778	320	476	80	0	0

- Molecule 6 is a DNA chain called SUPER CORE PROMOTER.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	F	80	1626	770	292	484	80	0	0

- Molecule 7 is a protein called TRANSCRIPTION INITIATION FACTOR TFIID SUBUNIT 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	406	Total	C	N	O	P	S	0	0
			3290	2090	580	596	2	22		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	178	VAL	-	insertion	UNP P21675
G	179	SER	-	insertion	UNP P21675
G	180	GLU	-	insertion	UNP P21675
G	181	ASN	-	insertion	UNP P21675
G	182	GLY	-	insertion	UNP P21675
G	183	GLU	-	insertion	UNP P21675
G	184	GLY	-	insertion	UNP P21675
G	185	ILE	-	insertion	UNP P21675
G	186	ILE	-	insertion	UNP P21675
G	187	LEU	-	insertion	UNP P21675
G	188	PRO	-	insertion	UNP P21675
G	189	SER	-	insertion	UNP P21675
G	190	ILE	-	insertion	UNP P21675
G	191	ILE	-	insertion	UNP P21675
G	192	ALA	-	insertion	UNP P21675
G	193	PRO	-	insertion	UNP P21675
G	194	SER	-	insertion	UNP P21675
G	195	SER	-	insertion	UNP P21675
G	196	LEU	-	insertion	UNP P21675
G	197	ALA	-	insertion	UNP P21675
G	198	SER	-	insertion	UNP P21675

- Molecule 8 is a protein called TRANSCRIPTION INITIATION FACTOR TFIID SUBUNIT 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	123	Total	C	N	O	S	0	0
			998	638	184	172	4		

- Molecule 9 is a protein called TRANSCRIPTION INITIATION FACTOR TFIID SUBUNIT 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	914	Total	C	N	O	S	0	2
			7404	4761	1251	1336	56		

- Molecule 10 is a protein called TRANSCRIPTION INITIATION FACTOR TFIID SUBUNIT 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	220	Total	C	N	O	S	0	0
			1741	1106	306	318	11		
10	K	198	Total	C	N	O	S	0	0
			1582	1006	276	290	10		

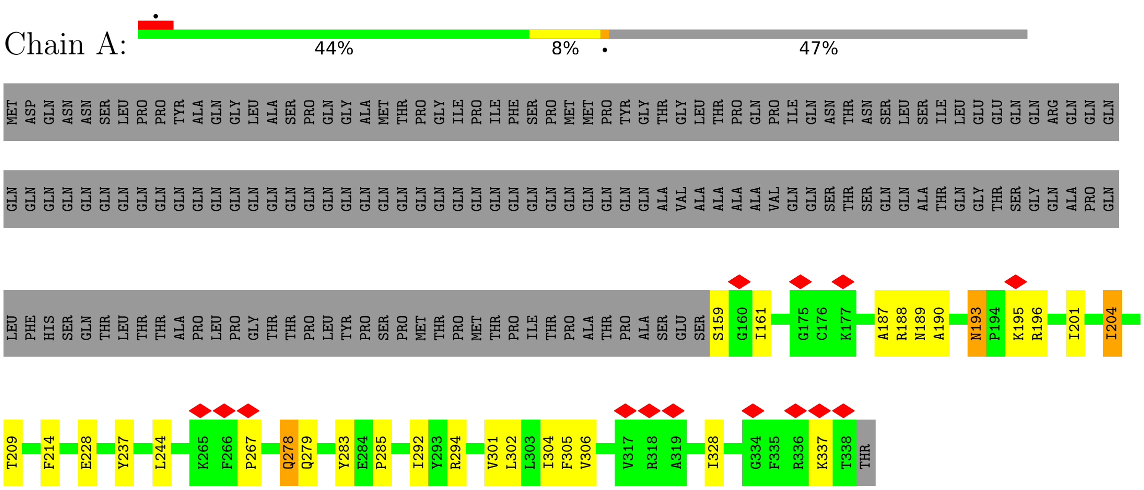
- Molecule 11 is a protein called TRANSCRIPTION INITIATION FACTOR TFIID SUBUNIT 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	27	Total	C	N	O	S	0	1
			219	134	46	38	1		

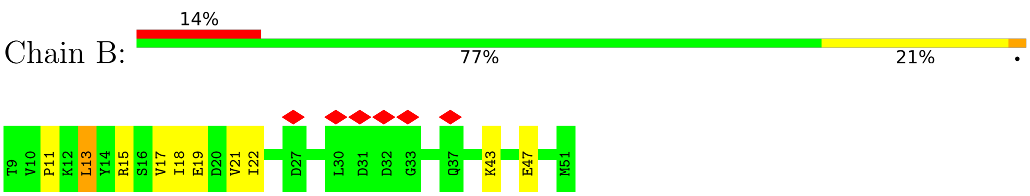
3 Residue-property plots (i)

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.

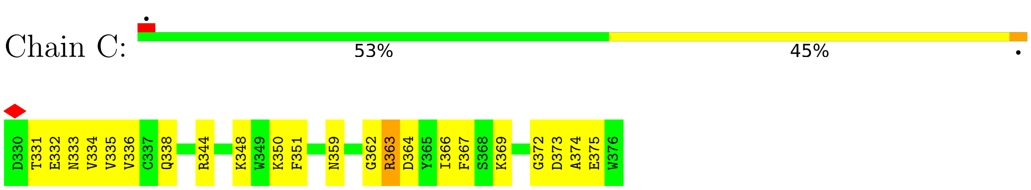
- Molecule 1: TATA-BOX-BINDING PROTEIN



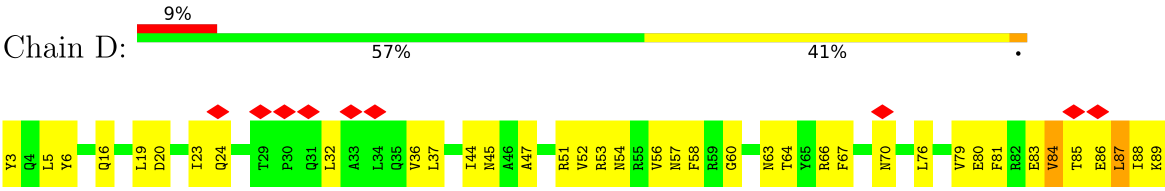
- Molecule 2: TRANSCRIPTION INITIATION FACTOR IIA SUBUNIT 1

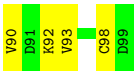


- Molecule 3: TRANSCRIPTION INITIATION FACTOR IIA SUBUNIT 1



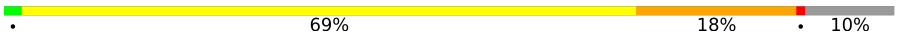
- Molecule 4: TRANSCRIPTION INITIATION FACTOR IIA SUBUNIT 2

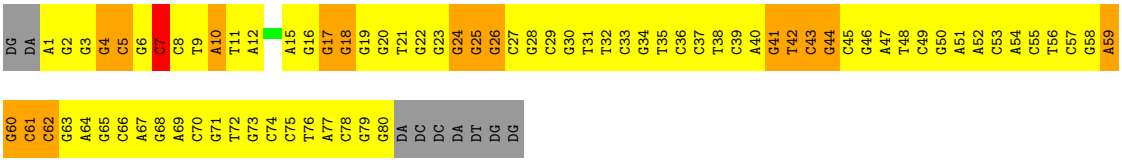




• Molecule 5: SUPER CORE PROMOTER

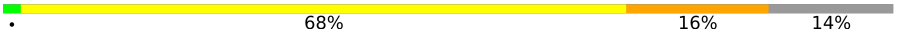
Chain E:

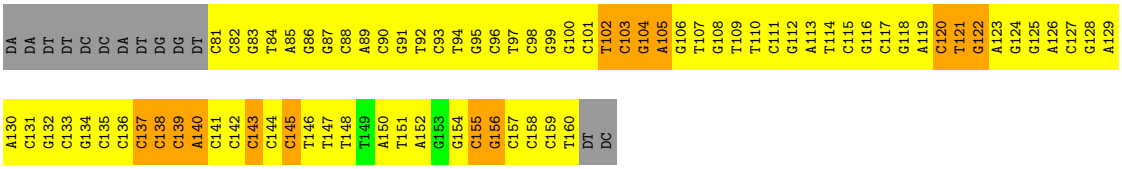




• Molecule 6: SUPER CORE PROMOTER

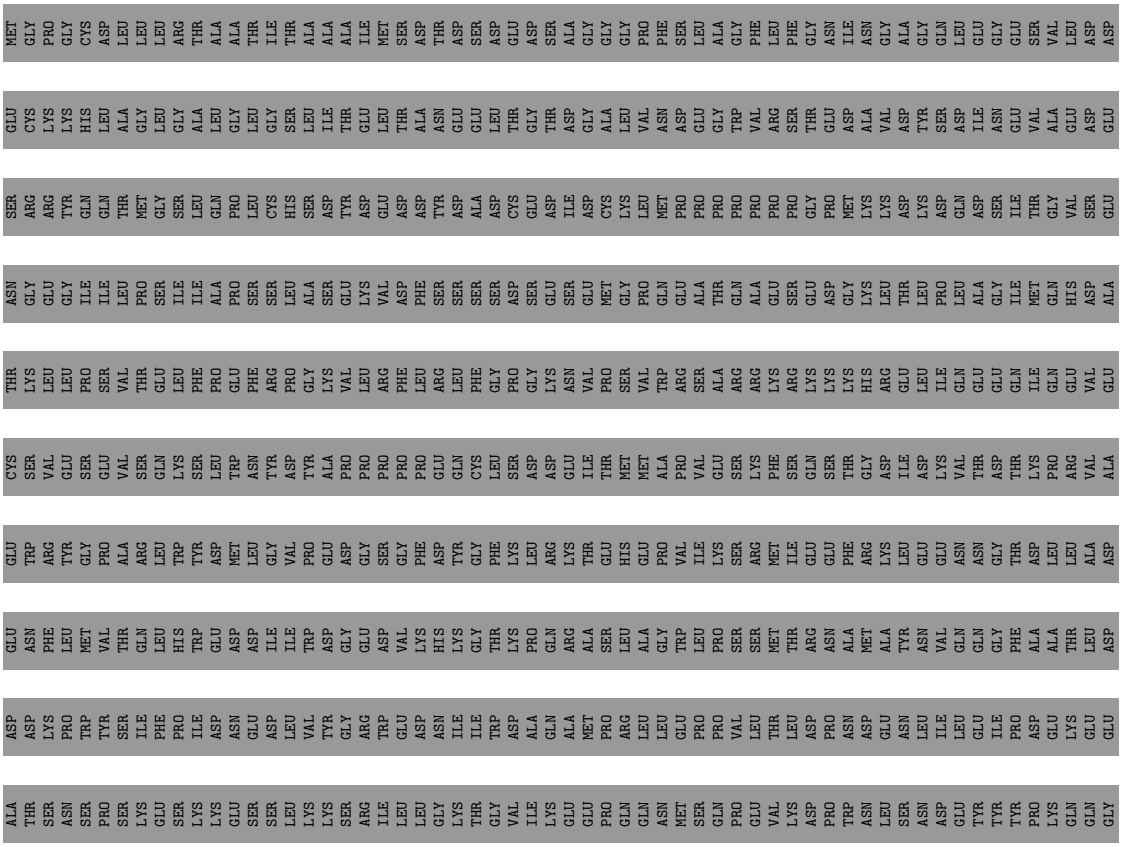
Chain F:

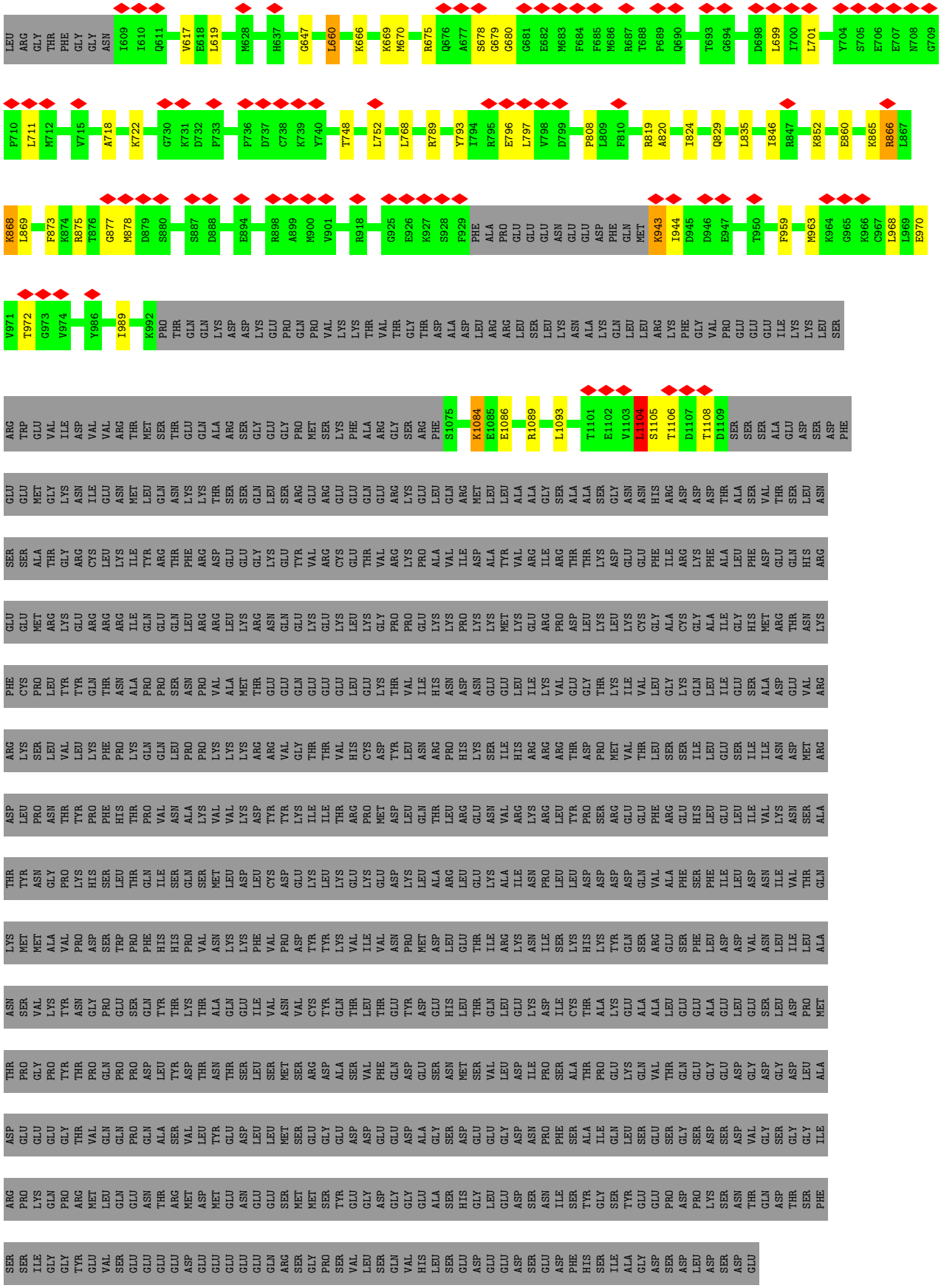




• Molecule 7: TRANSCRIPTION INITIATION FACTOR TFIID SUBUNIT 1

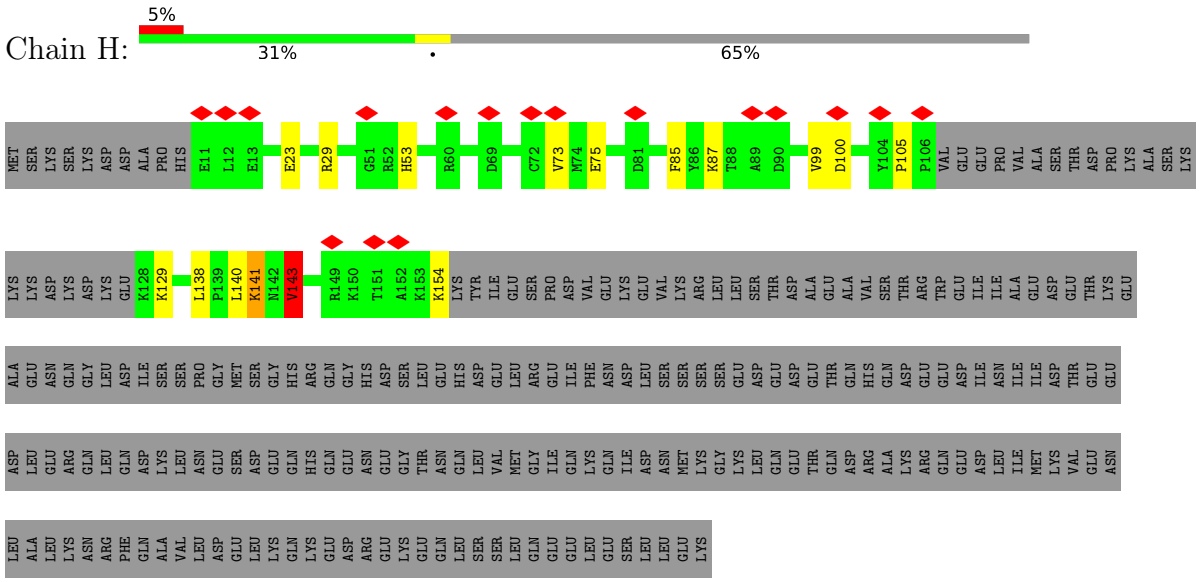
Chain G:




LEU ARG GLY THR PHE GLY GLY ASN I609 I610 Q611 V617 E618 L619 M628 H637 G647 L660 K666 K669 M670 R675 Q676 A677 S678 G679 G680 G681 E682 M683 F684 F685 M686 R687 T688 P689 Q690 T693 G694 D698 L699 I700 L701 Y704 S705 E706 E707 N708 G709
P710 L711 M712 V715 A718 K722 G730 K731 D732 P733 P736 D737 C738 K739 Y740 T748 L752 L768 R789 Y793 L794 R795 E796 L797 V798 D799 P808 L809 F810 R819 A820 I824 Q829 L835 I846 R847 K852 E860 K865 R866 L867
K868 L869 F873 K874 R875 T876 G877 M878 D879 S880 S887 D888 E894 R898 A899 M900 V901 R918 G925 E926 K927 S928 F929 PHE ALA PRO GLU GLU GLU ASN GLU GLU ASP PHE GLN MET K943 I944 D945 D946 E947 T950 F959 M963 K964 G965 K966 C967 L968 L969 E970
V971 T972 G973 V974 Y986 I989 K992 PRO THR GLN GLN LYS ASP ASP LYS GLU GLN PRO GLN PRO VAL LYS LYS THR VAL THR GLY THR ASP ALA ASP LEU ARG ARG LEU SER LEU LYS ASN ALA LYS GLN LEU LEU ARG LYS PHE GLY VAL PRO GLU GLU GLU ILE LYS LYS LEU SER
ARG TRP GLU VAL ILE ASP VAL VAL ARG THR MET SER THR GLU GLN GLN ALA ARG SER GLY GLU GLU GLY PRO MET SER LYS PHE ALA ARG GLY SER ARG PHE S1075 K1084 E1085 E1086 R1089 L1093 T1101 E1102 V1103 L1104 S1105 T1106 D1107 T1108 D1109 SER SER SER ALA GLU ASP SER ASP PHE
GLU GLU MET GLY LYS ASN ILE GLU ASN MET LEU LEU GLN ASN LYS LYS THR SER SER GLN LEU LEU SER ARG GLU ARG GLU GLN GLU GLN GLU LEU GLN ARG MET LEU LEU ALA ALA GLY SER ALA ALA SER GLY ASN ASN HIS ARG ASP ASP THR ALA SER VAL THR SER LEU ASN
SER SER ALA THR GLY ARG CYS LEU LYS ILE TYR ARG THR PHE ARG ASP GLU GLU GLY LYS GLU TYR VAL ARG CYS GLU THR VAL ARG LYS PRO ALA VAL ILE ASP ALA TYR VAL ARG ILE ARG THR THR LYS ASP GLU GLU PHE ILE ARG LYS PHE ALA ALA LEU PHE ASP GLU GLN HIS ARG
GLU GLU MET ARG LYS GLU ARG ARG ILE GLN GLU GLN LEU ARG ARG LEU LYS ARG ASN GLN GLU LYS GLU LYS LEU LYS GLY PRO PRO GLU LYS LYS PRO LYS LYS MET LYS GLU ARG PRO ASP LEU LYS LEU LYS LYS CYS GLY ALA ALA CYS GLY ALA ILE GLY HIS MET ARG THR ASN LYS
PHE CYS PRO LEU TYR TYR GLN THR ASN ALA PRO PRO SER ASN PRO VAL ALA MET THR GLU GLU GLN GLU GLU LEU GLU LYS THR VAL ILE HIS ASN ASP ASN GLU GLU LEU ILE LYS VAL GLU GLY THR LYS ILE VAL LEU GLY LYS GLN LEU ILE GLU SER ALA ASP GLU VAL ARG
ARG LYS SER LEU VAL LEU LYS PHE PRO LYS GLN GLN LEU PRO PRO LYS LYS LYS ARG ARG VAL GLY THR THR THR VAL HIS CYS ASP TYR LEU ASN ARG PRO HIS LYS SER ILE HIS ARG ARG ARG THR ASP PRO MET VAL THR LEU SER SER ILE LEU GLU GLU SER ILE ILE ASN ASP MET ARG
ASP LEU PRO ASN THR TYR PRO PHE HIS THR PRO VAL ASN ALA LYS VAL VAL LYS ASP TYR TYR LYS ILE ILE THR ARG PRO MET ASP LEU GLN THR LEU ARG GLU ASN VAL ARG LYS ARG LEU TYR PRO SER ARG GLU GLU PHE ARG GLU HIS LEU GLU GLU LEU ILE VAL LYS ASN SER ALA
THR TYR ASN GLY PRO LYS HIS SER LEU THR GLN ILE SER GLN SER MET LEU ASP LEU CYS ASP GLU LYS LEU LYS GLU GLU ASP LYS LEU ALA ARG LEU GLU GLU THR LYS ALA ILE ASN PRO LEU LEU ASP ASP GLY GLN VAL ALA PHE SER PHE ILE LEU ASP ASN ILE VAL THR GLN
LYS MET MET ALA VAL PRO VAL ASN LYS LYS PHE VAL PRO ASP TYR TYR LYS VAL ILE VAL ASN PRO MET ASP ASN LEU GLN LYS ILE SER LYS HIS LYS TYR GLN SER ARG GLU SER PHE LEU ASP ASP VAL ASN LEU ILE LEU ALA
ASN SER VAL LYS TYR ASN GLY PRO GLU SER GLN TYR THR LYS THR ALA ALA GLN GLU ILE VAL ASN VAL CYS TYR GLN THR LEU THR GLU GLN TYR ASP GLU HIS LEU THR THR GLN THR SER LEU ASP GLU ILE CYS THR ALA LYS GLU ALA ALA LEU GLU GLU GLU GLU LEU GLU SER LEU ASP PRO MET
THR PRO GLY PRO TYR THR PRO GLN PRO PRO ASP LEU TYR ASP THR ASN THR SER LEU SER MET SER ARG ASP ALA SER VAL PHE GLN GLN ASP GLU SER ASN MET SER VAL LEU ASP ILE PRO SER ALA THR PRO GLU LYS GLN VAL THR GLN GLU GLU GLY GLY GLU ASP GLY ASP ALA
ASP GLU GLU GLY THR VAL GLN GLN PRO GLN ALA SER VAL LEU TYR GLU ASP LEU LEU MET SER GLY GLU ASP ALA GLY SER ASP GLU GLU ASP GLU GLU GLY ASP ASN PRO PHE SER ALA ILE GLN LEU GLU SER GLU SER GLY GLY GLU ASP VAL GLY SER ILE
ARG PRO LYS GLN PRO ARG MET LEU GLN GLU ASN THR ARG MET ASP MET GLU LEU GLN GLU GLU ASN GLU GLU SER MET MET SER TYR GLY GLY ASP GLY GLY GLY GLU ALA GLY LEU GLU GLU ASP SER ASP ILE SER TYR GLY SER TYR ALA ILE GLU GLU PRO ASP PRO ASN THR GLY ASP
SER SER ILE GLY GLY TYR GLU VAL SER GLU GLU GLU GLU GLU GLN ARG SER GLY PRO SER VAL LEU SER GLN VAL HIS LEU SER GLU ASP GLU GLU ASP PHE HIS SER ILE ALA GLY ASP SER ASP LEU ASP SER ASP GLU

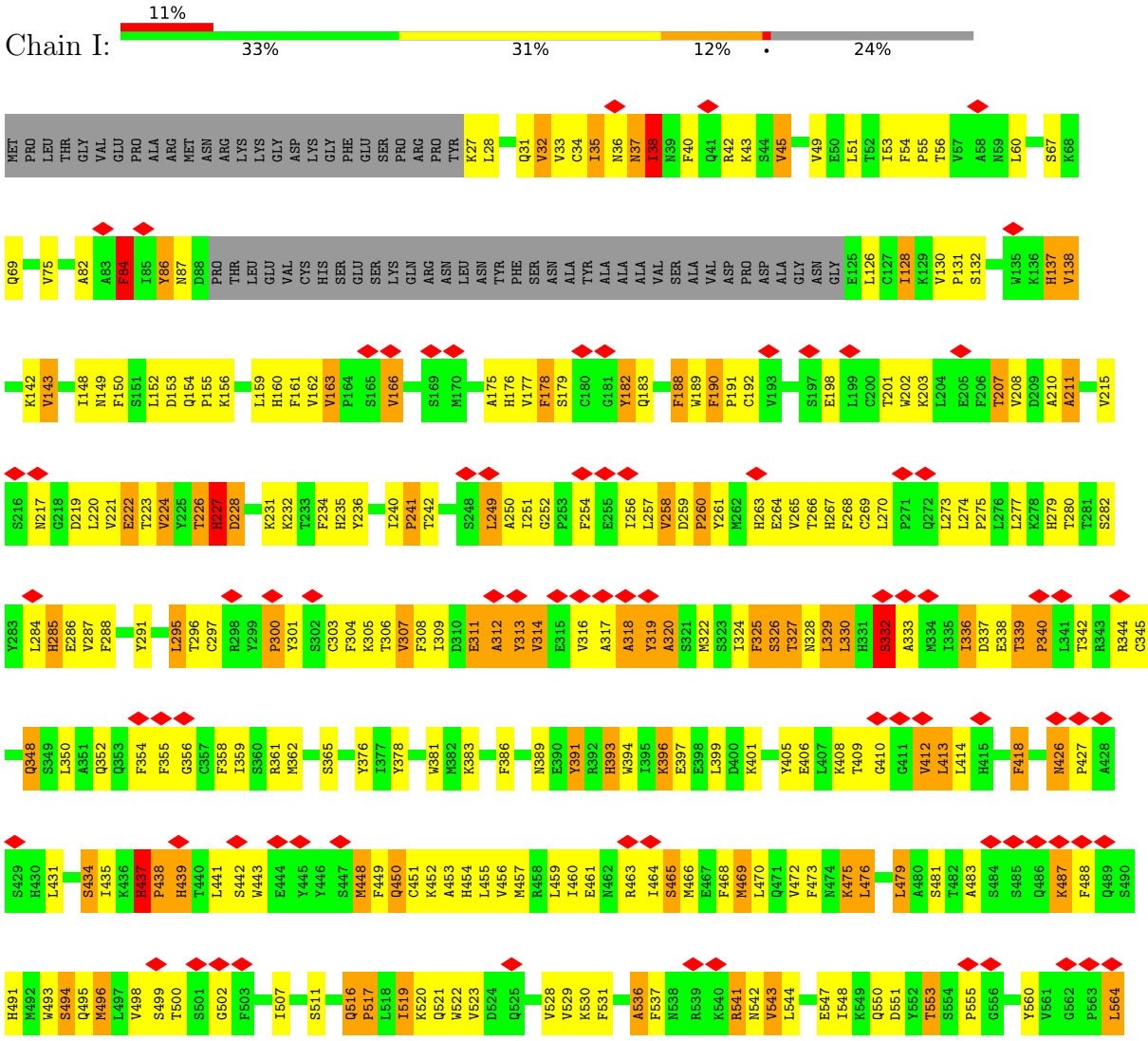
• Molecule 8: TRANSCRIPTION INITIATION FACTOR TFIID SUBUNIT 7

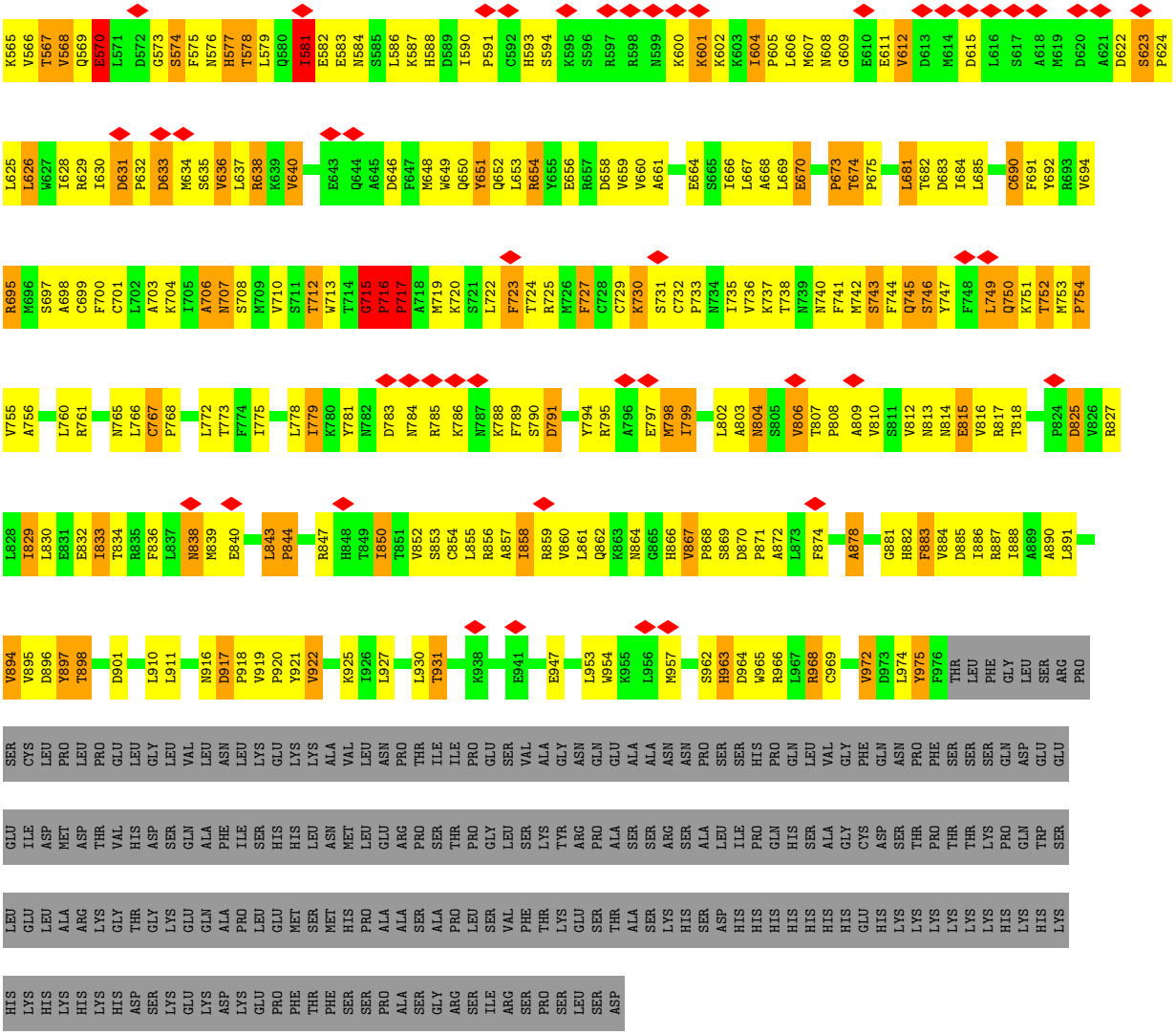
Chain H:



• Molecule 9: TRANSCRIPTION INITIATION FACTOR TFIID SUBUNIT 2

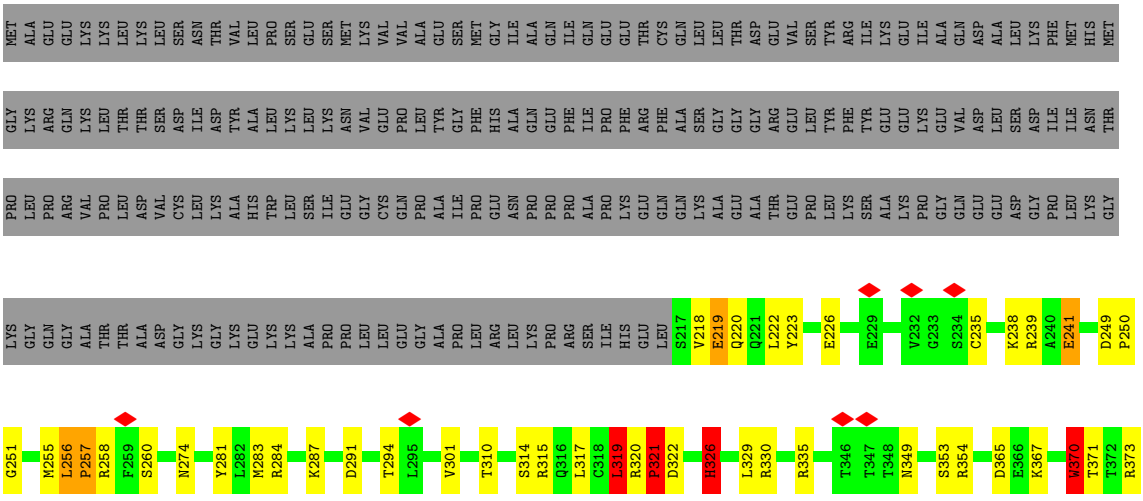
Chain I:

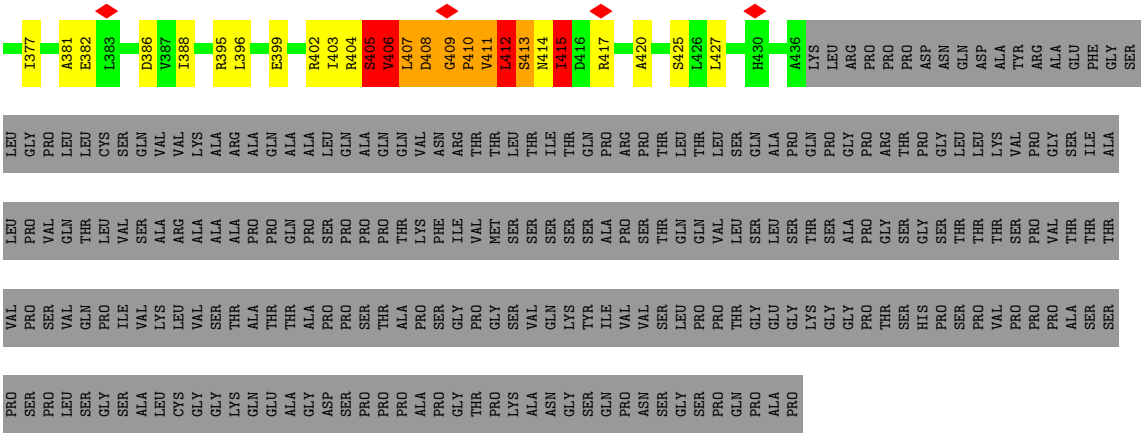




• Molecule 10: TRANSCRIPTION INITIATION FACTOR TFIID SUBUNIT 6

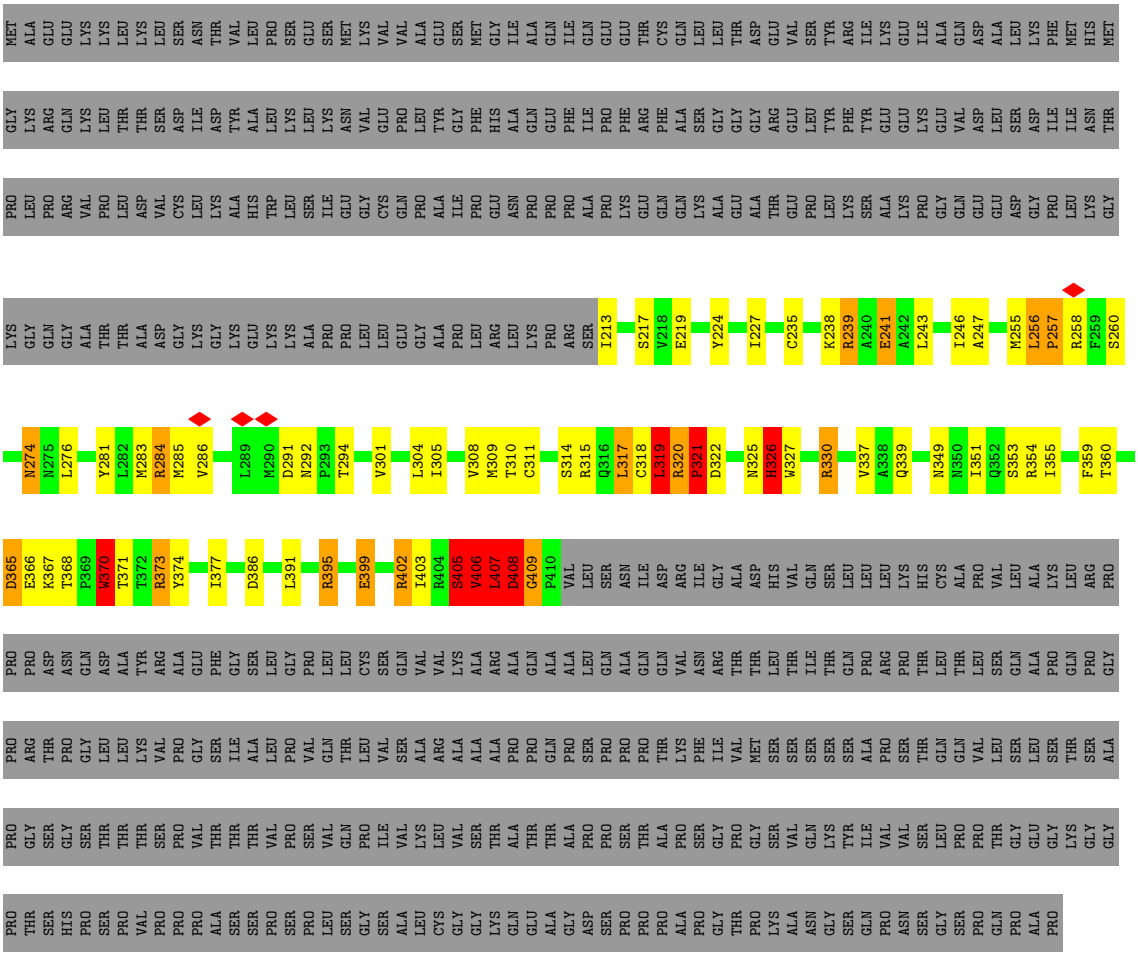
Chain J:





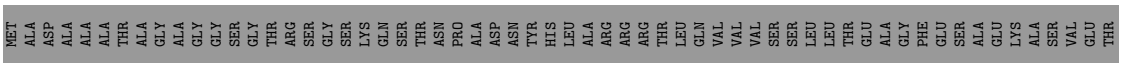
• Molecule 10: TRANSCRIPTION INITIATION FACTOR TFIID SUBUNIT 6

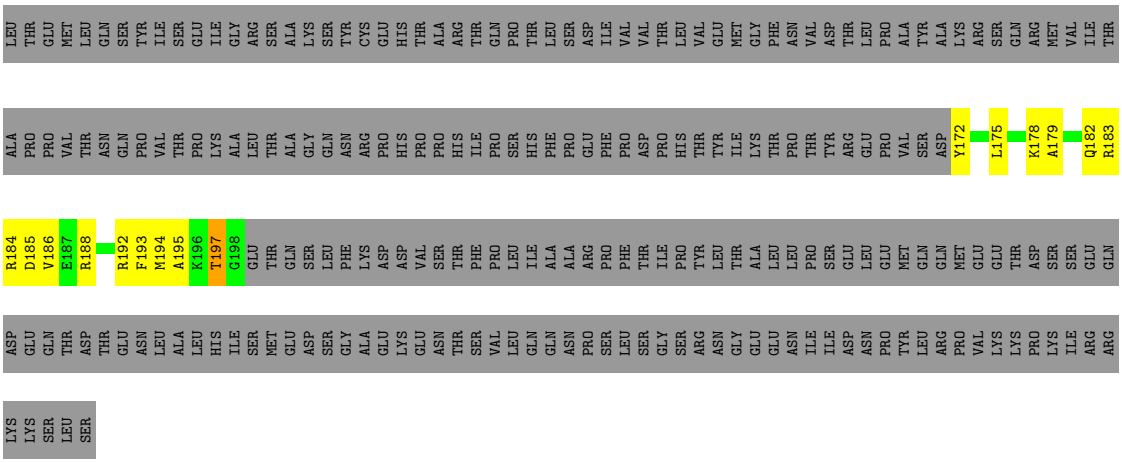
Chain K:



• Molecule 11: TRANSCRIPTION INITIATION FACTOR TFIID SUBUNIT 8

Chain L:




LEU THR GLU MET LEU GLN SER TYR ILE SER GLU ILE GLY ARG SER ALA LYS SER TYR CYS GLU HIS THR ALA ARG THR GLN PRO THR LEU SER ASP ILE VAL VAL THR LEU VAL GLU MET GLY PHE ASN VAL ASP THR LEU PRO ALA TYR ALA LYS ARG SER GLN ARG MET VAL ILE THR
ALA PRO PRO VAL THR ASN GLN PRO VAL THR PRO LYS ALA LEU THR ALA GLY GLN ASN ARG PRO HIS PRO PRO HIS ILE PRO SER HIS PHE PRO GLU PHE PRO ASP PRO HIS THR TYR ILE LYS THR PRO THR TYR ARG GLU PRO VAL SER ASP Y172 L175 K178 A179 Q182 R183
R184 D185 V186 E187 R188 R192 F193 M194 A195 K196 T197 G198 GLU THR GLN SER LEU PHE LYS ASP ASP VAL SER THR PHE PRO LEU ILE ALA ALA ARG PRO PHE THR ILE PRO TYR LEU THR ALA LEU LEU PRO SER GLU LEU GLU MET GLN GLN MET GLU GLU THR ASP SER SER GLU GLN
ASP GLU GLN THR ASP THR GLU ASN LEU ALA LEU HIS ILE SER MET GLU ASP SER GLY ALA GLU LYS GLU ASN THR SER VAL LEU GLN GLN ASN PRO SER LEU SER GLY SER ARG ASN GLY GLU GLU ASN ILE ILE ASP ASN PRO TYR LEU ARG PRO VAL LYS LYS PRO LYS ILE ARG ARG
LYS LYS SER LEU SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	22050	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	46	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	37879	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.049	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	506.88, 506.88, 506.88	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality

5.1 Standard geometry

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

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	0/1455	0.69	0/1958
2	B	0.34	0/360	0.53	0/487
3	C	0.40	0/402	0.83	1/539 (0.2%)
4	D	0.35	0/803	0.73	2/1088 (0.2%)
5	E	3.85	16/1806 (0.9%)	1.89	49/2658 (1.8%)
6	F	3.55	15/1764 (0.9%)	2.11	46/2582 (1.8%)
7	G	0.41	0/3349	0.55	0/4506
8	H	0.42	0/1017	0.59	1/1370 (0.1%)
9	I	0.84	8/7587 (0.1%)	0.82	5/10278 (0.0%)
10	J	0.74	0/1773	1.42	26/2408 (1.1%)
10	K	0.75	0/1612	1.38	21/2188 (1.0%)
11	L	0.61	1/220 (0.5%)	1.10	0/292
All	All	1.61	40/22148 (0.2%)	1.16	151/30354 (0.5%)

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
5	E	0	2
7	G	0	1
9	I	0	235
10	J	2	16
10	K	1	12
All	All	3	266

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	43	DC	O3'-P	49.26	2.20	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	44	DG	O3'-P	48.90	2.19	1.61
5	E	62	DC	O3'-P	48.41	2.19	1.61
5	E	59	DA	O3'-P	46.14	2.16	1.61
6	F	105	DA	O3'-P	46.09	2.16	1.61

The worst 5 of 151 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	145	DC	O5'-P-OP2	-41.73	60.62	110.70
9	I	437	HIS	C-N-CD	-27.62	59.83	120.60
5	E	17	DG	P-O3'-C3'	-27.17	87.10	119.70
6	F	145	DC	P-O5'-C5'	-24.28	82.05	120.90
6	F	156	DG	O5'-P-OP1	-23.00	83.11	110.70

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	J	326	HIS	CA
10	J	411	VAL	CA
10	K	326	HIS	CA

5 of 266 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	10	DA	Sidechain
5	E	7	DC	Sidechain
7	G	1104	LEU	Peptide
9	I	32	VAL	Mainchain
9	I	33	VAL	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1429	0	1521	49	0
2	B	356	0	360	7	0
3	C	393	0	380	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	793	0	801	39	0
5	E	1654	0	958	423	0
6	F	1626	0	962	396	0
7	G	3290	0	3276	61	0
8	H	998	0	1055	6	0
9	I	7404	0	7381	897	0
10	J	1741	0	1782	103	0
10	K	1582	0	1612	40	0
11	L	219	0	222	130	0
All	All	21485	0	20310	1916	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 46.

The worst 5 of 1916 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:84:PHE:HZ	9:I:126:LEU:CG	1.10	1.64
5:E:70:DC:C5'	7:G:875:ARG:NH1	1.68	1.53
9:I:566:VAL:HB	9:I:579:LEU:CD1	1.36	1.51
9:I:309:ILE:CG2	9:I:312:ALA:HB2	1.42	1.48
9:I:84:PHE:CZ	9:I:126:LEU:CG	1.96	1.47

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	178/339 (52%)	175 (98%)	3 (2%)	0	100	100
2	B	41/43 (95%)	40 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	45/47 (96%)	43 (96%)	2 (4%)	0	100 100
4	D	95/97 (98%)	87 (92%)	7 (7%)	1 (1%)	14 52
7	G	398/1893 (21%)	391 (98%)	7 (2%)	0	100 100
8	H	119/349 (34%)	117 (98%)	2 (2%)	0	100 100
9	I	910/1199 (76%)	753 (83%)	122 (13%)	35 (4%)	3 24
10	J	218/677 (32%)	185 (85%)	17 (8%)	16 (7%)	1 14
10	K	196/677 (29%)	163 (83%)	20 (10%)	13 (7%)	1 16
11	L	25/310 (8%)	25 (100%)	0	0	100 100
All	All	2225/5631 (40%)	1979 (89%)	181 (8%)	65 (3%)	7 29

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	84	VAL
9	I	222	GLU
9	I	413	LEU
9	I	438	PRO
9	I	577	HIS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	155/293 (53%)	152 (98%)	3 (2%)	57 75
2	B	42/42 (100%)	41 (98%)	1 (2%)	49 69
3	C	42/42 (100%)	41 (98%)	1 (2%)	49 69
4	D	89/89 (100%)	87 (98%)	2 (2%)	52 71
7	G	355/1680 (21%)	331 (93%)	24 (7%)	16 41
8	H	113/322 (35%)	104 (92%)	9 (8%)	12 35
9	I	832/1083 (77%)	830 (100%)	2 (0%)	93 96
10	J	194/574 (34%)	177 (91%)	17 (9%)	10 31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	K	176/574 (31%)	162 (92%)	14 (8%)	12 35
11	L	22/270 (8%)	22 (100%)	0	100 100
All	All	2020/4969 (41%)	1947 (96%)	73 (4%)	38 59

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	415	ILE
10	K	399	GLU
10	K	219	GLU
10	K	319	LEU
7	G	943	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
10	K	343	HIS
10	K	254	GLN
9	I	838	ASN
10	K	220	GLN
9	I	542	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)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\|>2$
7	TPO	G	1106	7	8,10,11	1.13	0	10,14,16	1.61	1 (10%)
7	SEP	G	1105	7	8,9,10	1.62	1 (12%)	8,12,14	1.08	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	TPO	G	1106	7	-	0/9/11/13	-
7	SEP	G	1105	7	-	3/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	1105	SEP	P-O1P	3.51	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	1106	TPO	P-OG1-CB	-4.54	109.50	123.21
7	G	1105	SEP	OG-P-O1P	2.17	112.57	106.47

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	1105	SEP	CB-OG-P-O2P
7	G	1105	SEP	CB-OG-P-O3P
7	G	1105	SEP	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	F	68
5	E	65
9	I	1

The worst 5 of 134 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	158:DC	O3'	159:DC	P	4.06
1	E	2:DG	O3'	3:DG	P	3.41
1	F	159:DC	O3'	160:DT	P	3.14
1	E	1:DA	O3'	2:DG	P	2.67
1	F	142:DC	O3'	143:DC	P	2.56

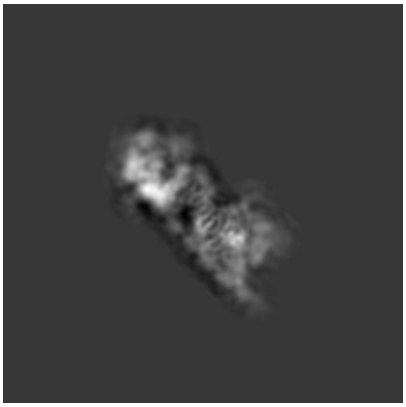
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3305. 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.

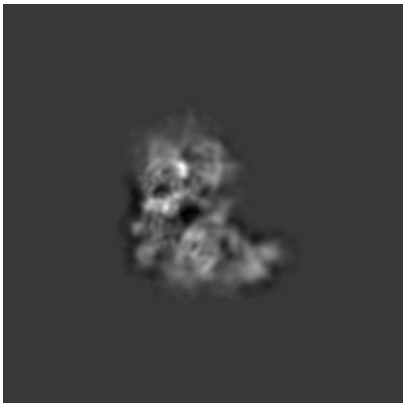
6.1 Orthogonal projections

6.1.1 Primary map



X

Y



Z

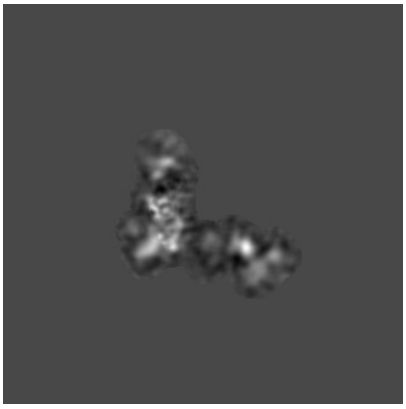
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map

X Index: 192

Y Index: 192



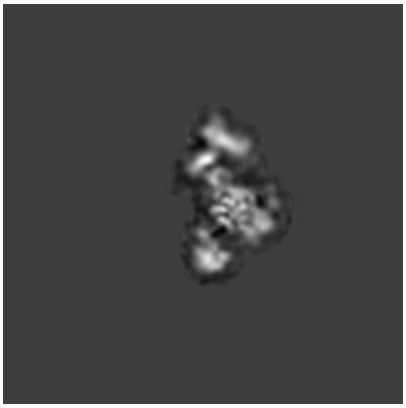
Z Index: 192

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

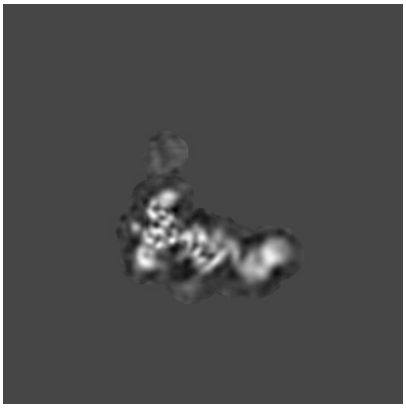
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 166



Y Index: 147

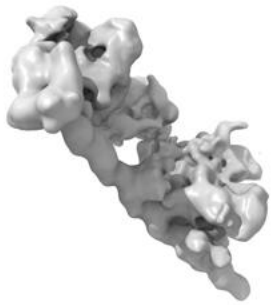


Z Index: 206

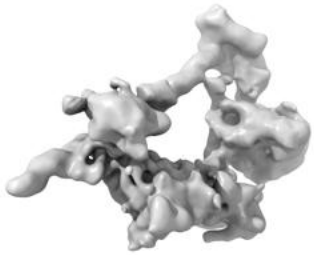
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

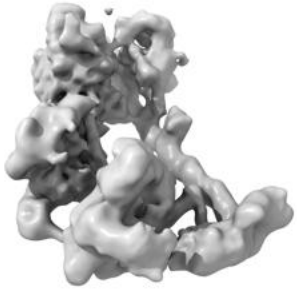
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

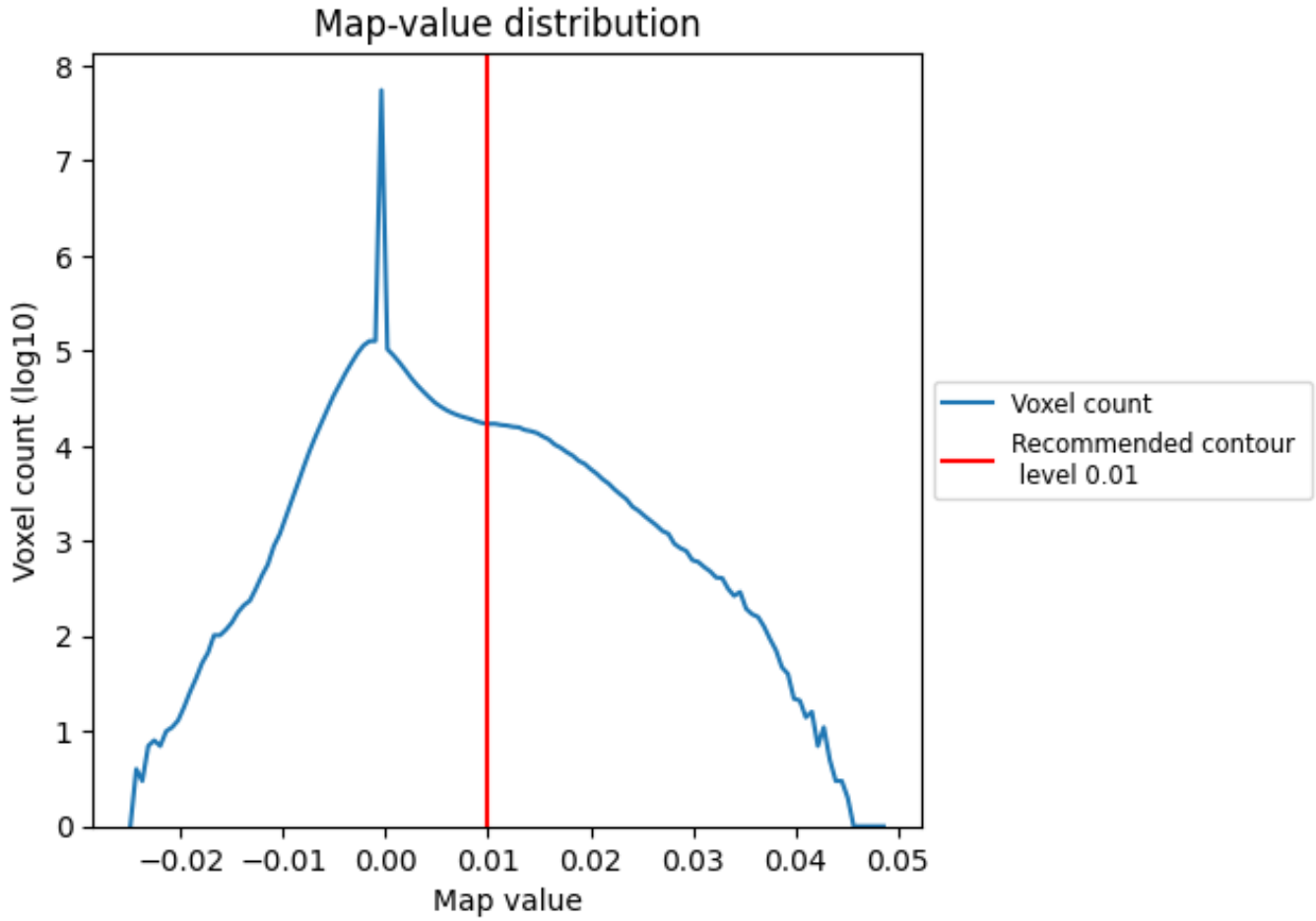
6.5 Mask visualisation (i)

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

7 Map analysis

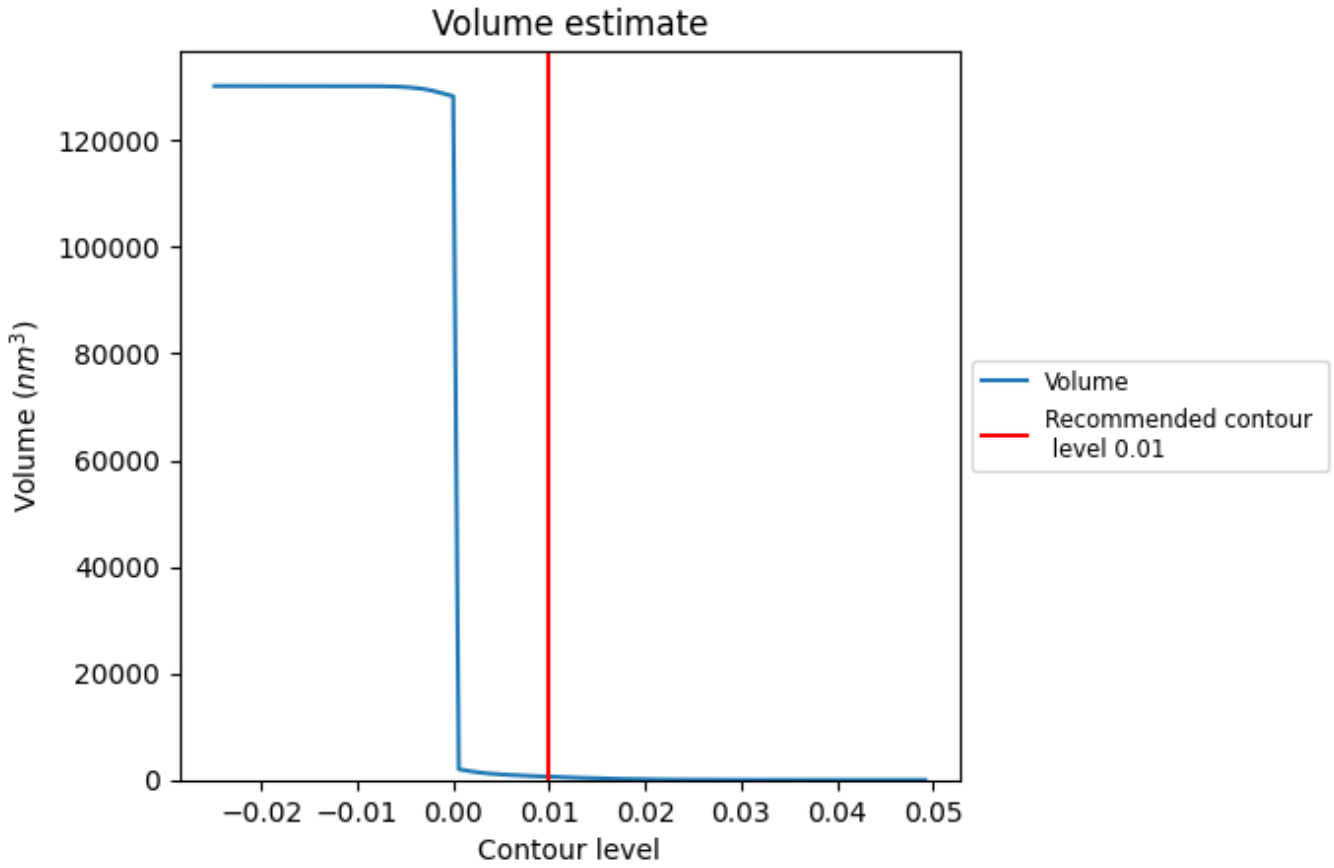
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

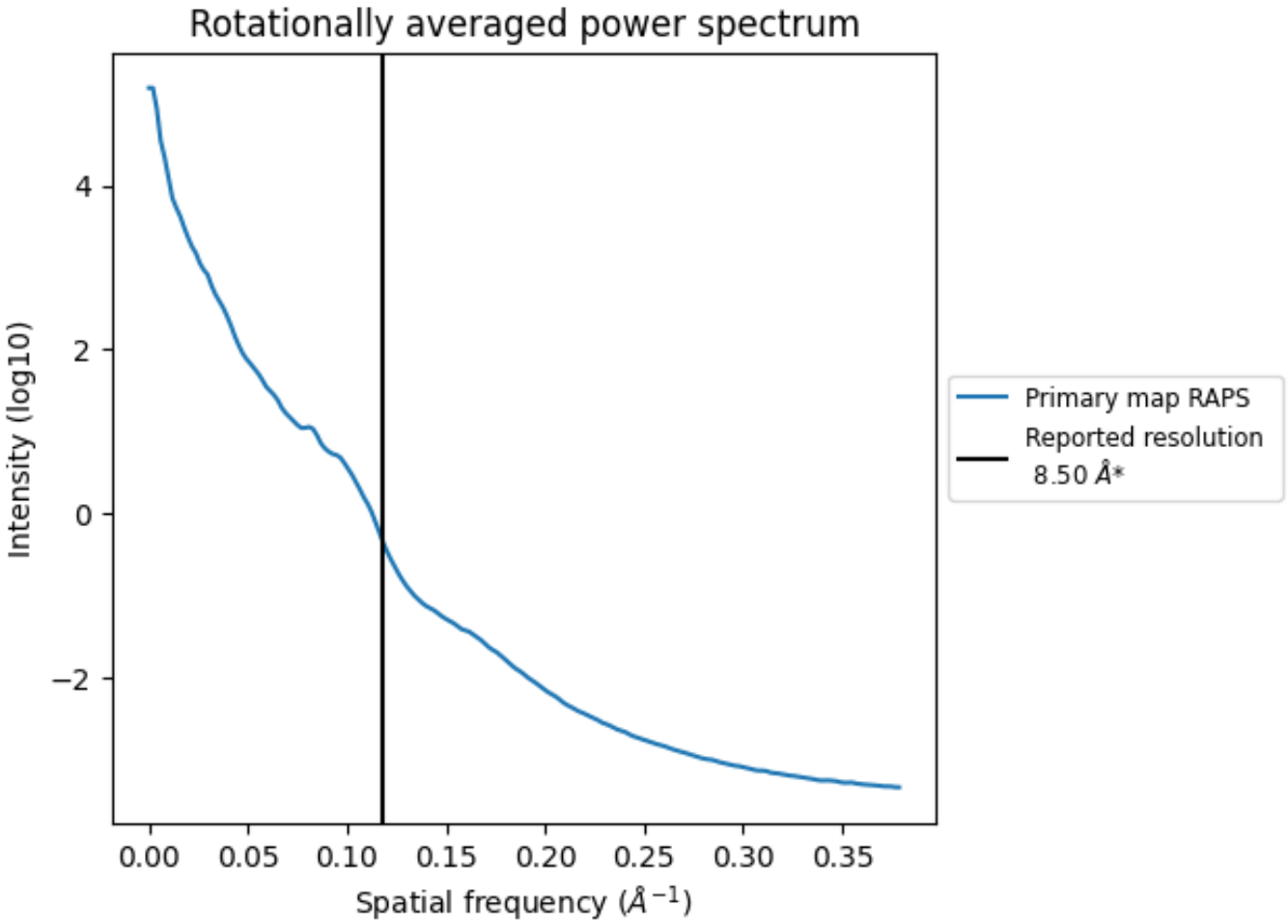
7.2 Volume estimate (i)



The volume at the recommended contour level is 613 nm^3; this corresponds to an approximate mass of 553 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)

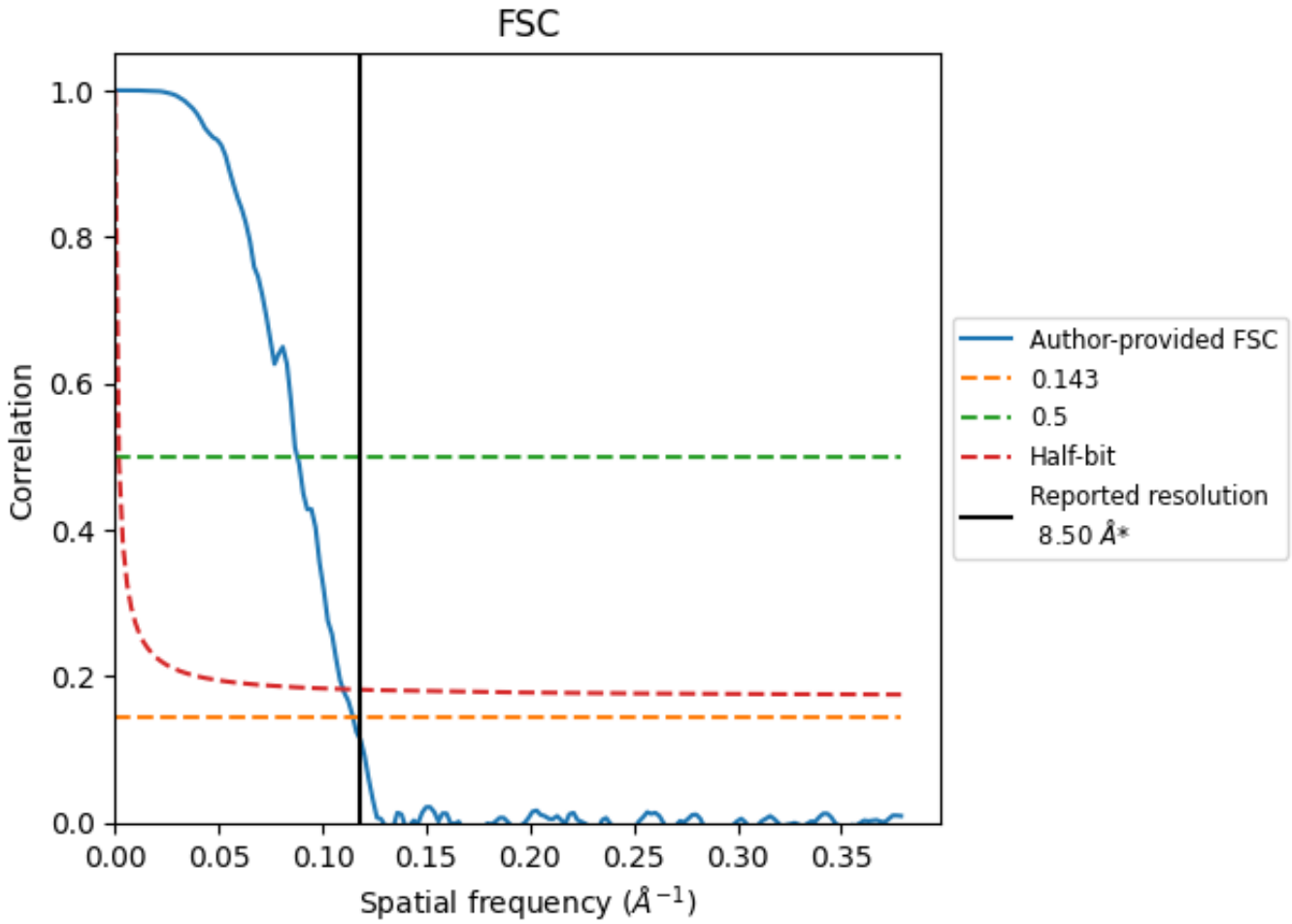


*Reported resolution corresponds to spatial frequency of 0.118 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.118 Å^{-1}

8.2 Resolution estimates (i)

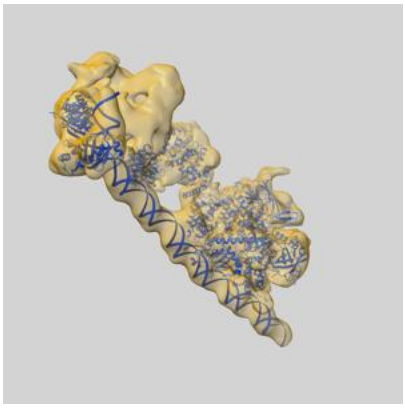
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	8.71	11.38	9.10
Unmasked-calculated*	-	-	-

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

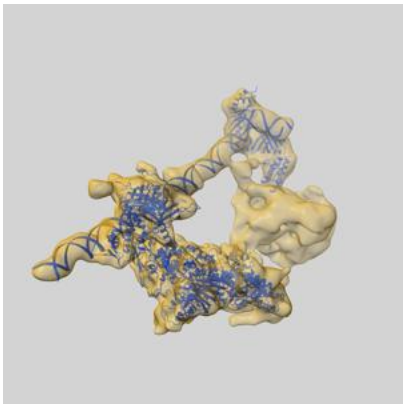
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3305 and PDB model 5FUR. Per-residue inclusion information can be found in section 3 on page 7.

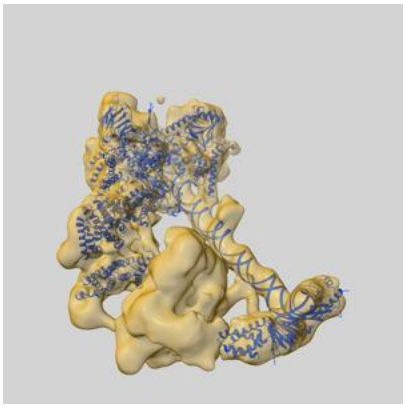
9.1 Map-model overlay



X



Y



Z

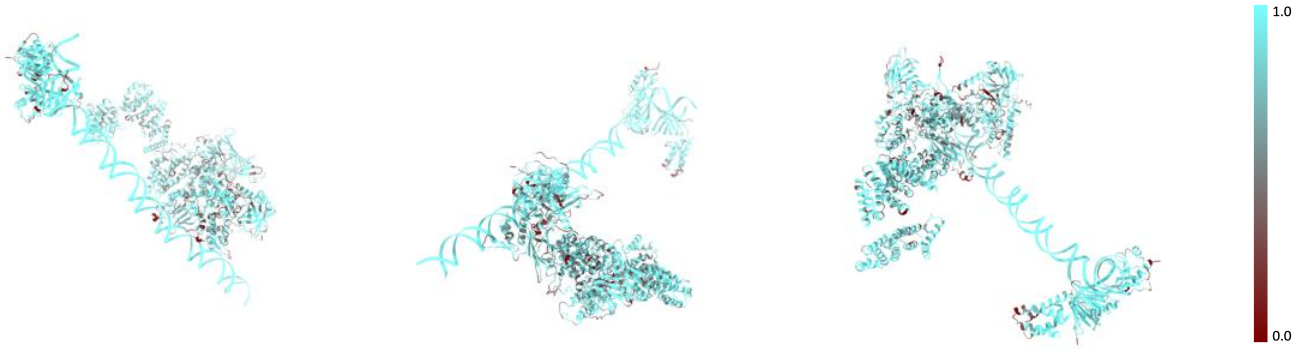
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

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.

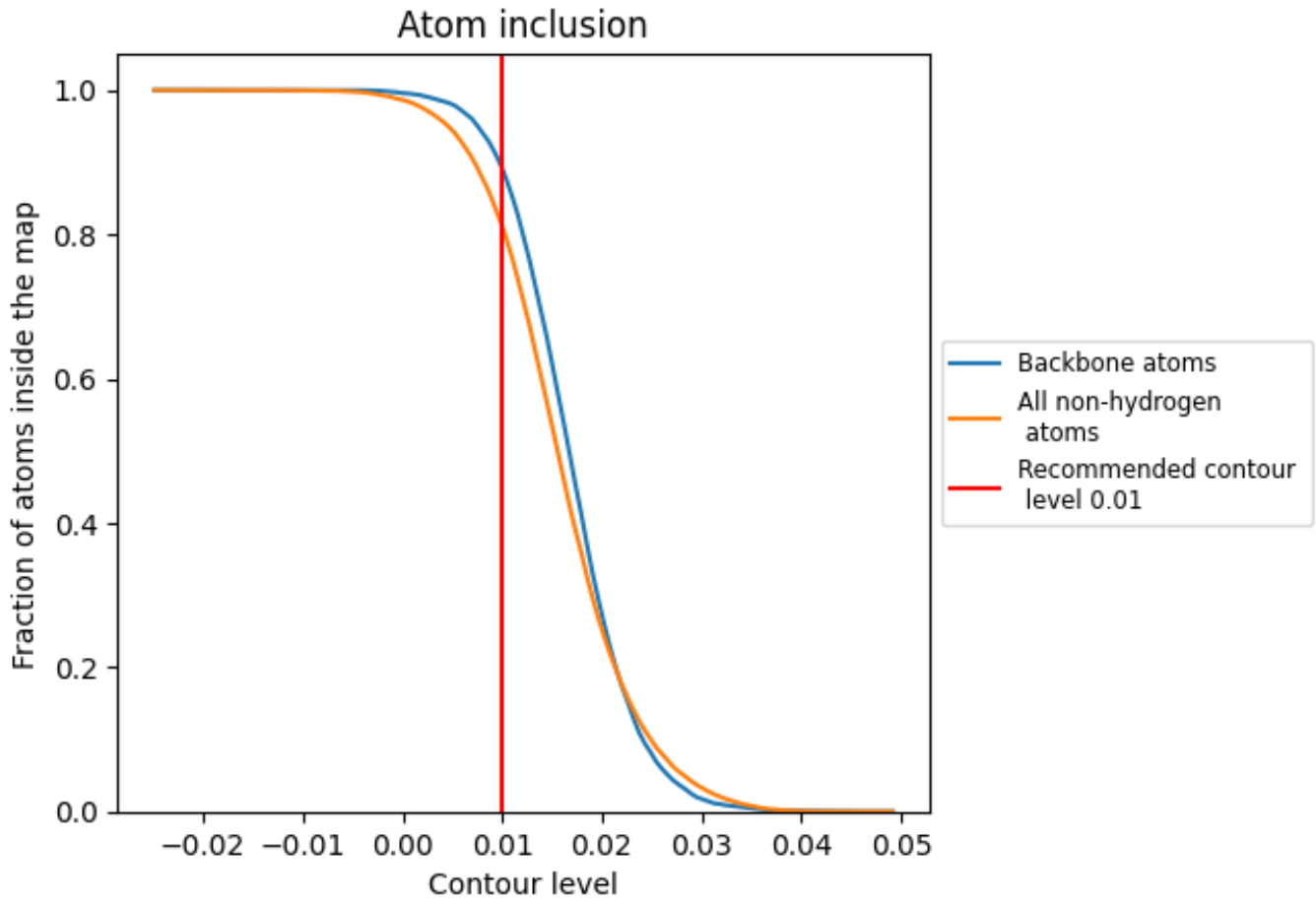
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8115	0.1040
A	0.8631	0.0790
B	0.8143	0.1020
C	0.9481	0.0800
D	0.8452	0.0560
E	0.9305	0.1260
F	0.9514	0.1200
G	0.7135	0.1040
H	0.8035	0.1020
I	0.7509	0.0980
J	0.8303	0.1180
K	0.9010	0.1170
L	0.8894	0.1510