

Full wwPDB EM Validation Report (i)

Nov 22, 2022 – 01:04 PM JST

PDB ID : 7EGH

EMDB ID : EMD-31117

Title : TFIID lobe C subcomplex

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Deposited on : 2021-03-24

Resolution : 3.04 Å(reported)

This is a Full wwPDB EM Validation 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 (1)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43

MolProbity : 4.02b-467

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

MapQ: 1.9.9

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

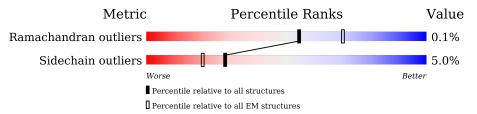
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.04 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 $(\# \mathrm{Entries})$	${ m EM\ structures} \ (\#{ m Entries})$
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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%	•	66%	
2	В	1199		79%	·	20%
3	F	677	37%	•	61%	
3	f	677	37%	·	62%	
4	G	349	39%		59%	
5	Н	310	23%		77%	
6	X	72		62%	38%	
7	Y	94	48%		52%	



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 20543 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		At	oms			AltConf	Trace
1	A	630	Total 5199	C 3303	N 923	O 944	S 29	0	0

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

Mol	Chain	Residues		${f Atoms}$					Trace
2	В	963	Total 7796	C 5011	N 1315	O 1412	S 58	0	0

• Molecule 3 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace		
2	E	267	Total	С	N	О	S	0	0	
)	Г	207	2006	1265	362	368	11	0		
2	f	260	Total	С	N	О	S	0	0	
)		200	1946	1227	348	360	11	U	U	

• Molecule 4 is a protein called Transcription initiation factor TFIID subunit 7.

Mol	Chain	Residues		At	oms			AltConf	Trace
4	G	144	Total 1171	C 742	N 215	O 210	S 4	0	0

• Molecule 5 is a protein called Transcription initiation factor TFIID subunit 8.

Mol	Chain	Residues		${f Atoms}$					Trace
5	Н	72	Total 580	C 370	N 100	O 109	S 1	0	0

• Molecule 6 is a DNA chain called DNA (45-MER).



Mol	Chain	Residues	${f Atoms}$					AltConf	Trace
6	X	45	Total 918	C 434	N 172	O 267	P 45	0	0

 \bullet Molecule 7 is a DNA chain called DNA (45-MER).

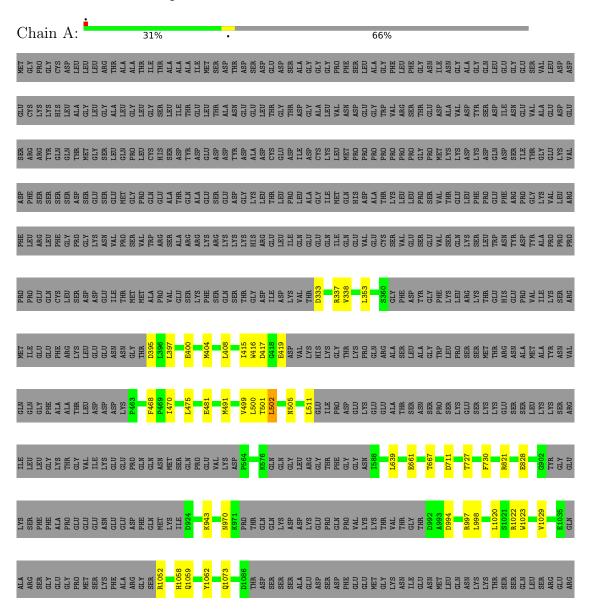
Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	45	Total 927			O 273	P 45	0	0



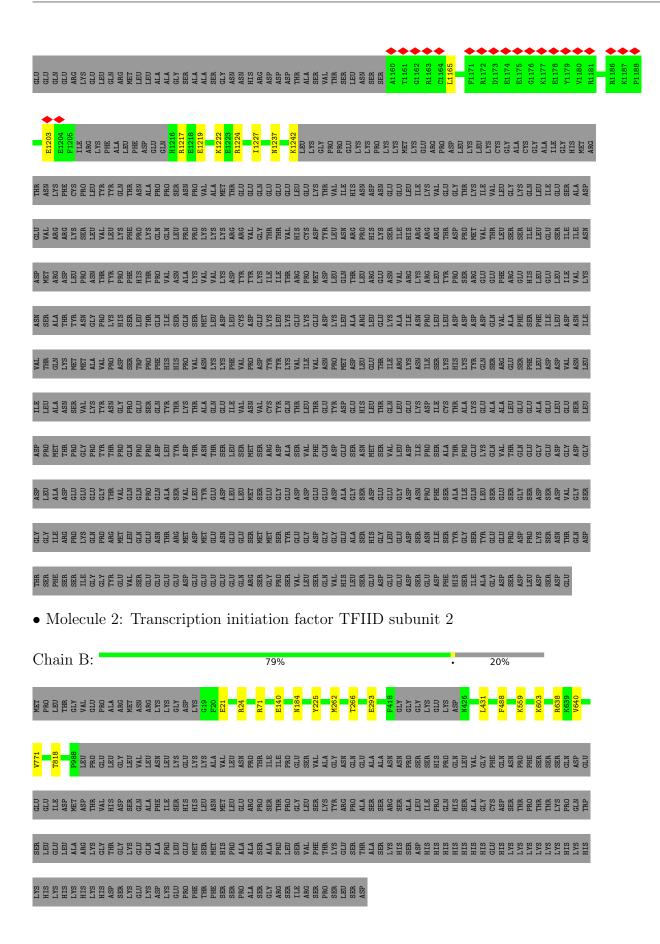
3 Residue-property plots (i)

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

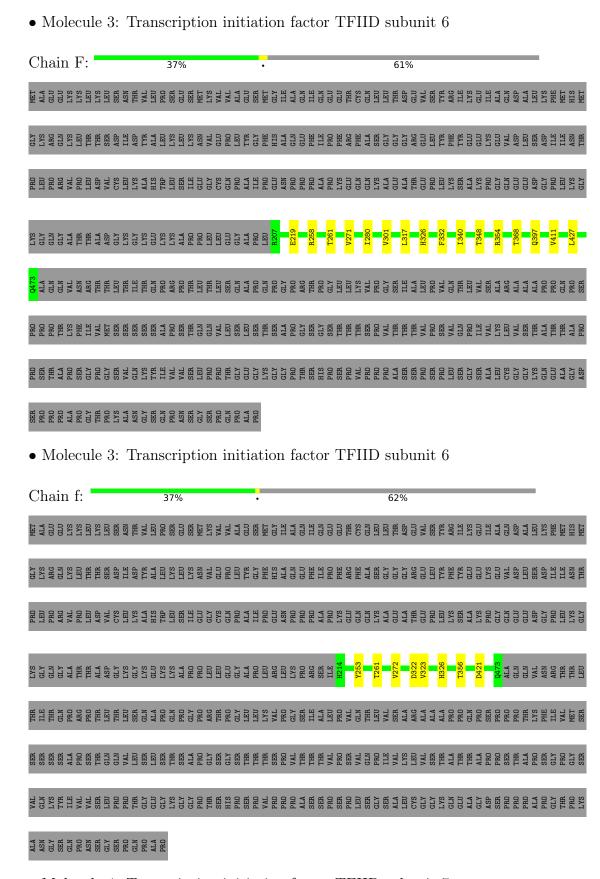
• Molecule 1: Transcription initiation factor TFIID subunit 1





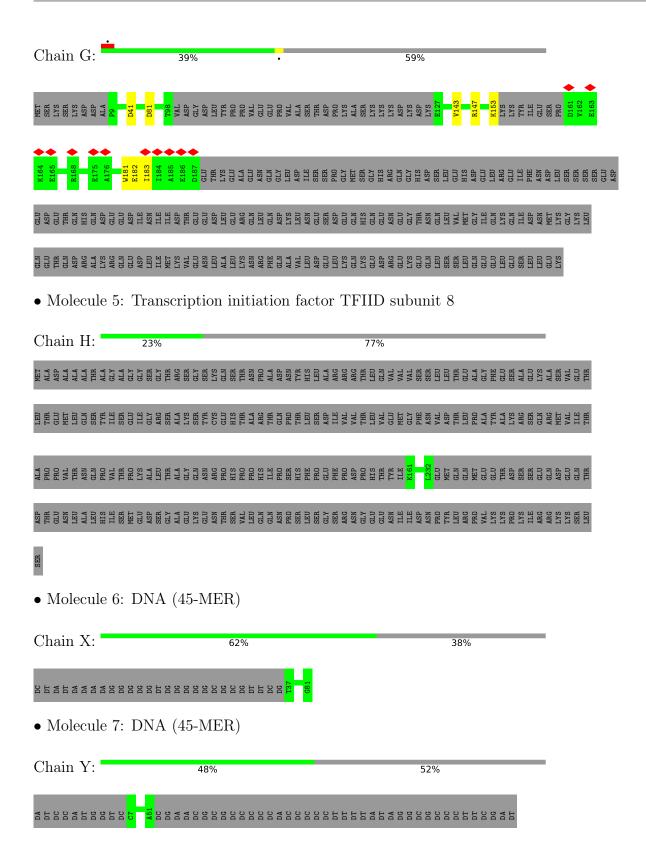






• Molecule 4: Transcription initiation factor TFIID subunit 7







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	121285	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	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	5.396	Depositor
Minimum map value	-3.106	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.222	Depositor
Map size (Å)	540.16, 540.16, 540.16	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.055, 1.055, 1.055	Depositor



5 Model quality (i)

5.1 Standard geometry (i)

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
WIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.50	0/5320	0.66	0/7165
2	В	0.46	0/7993	0.60	0/10836
3	F	0.53	0/2040	0.75	0/2775
3	f	0.45	0/1979	0.67	0/2694
4	G	0.50	0/1190	0.62	0/1601
5	Н	0.32	0/592	0.55	0/803
6	X	0.73	0/1029	0.91	0/1584
7	Y	0.68	0/1039	0.92	0/1603
All	All	0.50	0/21182	0.68	0/29061

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	Perce	ntiles
1	A	610/1872 (33%)	583 (96%)	25 (4%)	2 (0%)	41	74
2	В	959/1199 (80%)	911 (95%)	48 (5%)	0	100	100
3	F	$265/677 \ (39\%)$	251 (95%)	13 (5%)	1 (0%)	34	69
3	f	258/677 (38%)	252 (98%)	6 (2%)	0	100	100
4	G	138/349 (40%)	135 (98%)	3 (2%)	0	100	100
5	Н	70/310 (23%)	67 (96%)	3 (4%)	0	100	100
All	All	2300/5084 (45%)	2199 (96%)	98 (4%)	3 (0%)	54	84

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	502	LEU
3	F	411	VAL
1	A	998	LEU

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	564/1665 (34%)	510 (90%)	54 (10%)	8 29
2	В	876/1083 (81%)	859 (98%)	17 (2%)	57 82
3	F	202/574~(35%)	187 (93%)	15 (7%)	13 42
3	f	195/574 (34%)	187 (96%)	8 (4%)	30 65
4	G	132/322 (41%)	124 (94%)	8 (6%)	18 50
5	Н	64/270 (24%)	64 (100%)	0	100 100
All	All	2033/4488 (45%)	1931 (95%)	102 (5%)	28 58

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	333	ASP
1	A	337	ARG



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Mol	Chain	Res	Type	
1	A	338	VAL	
1	A	353	LEU	
1	A	395	ASP	
1	A	397	LEU	
1	A	400	GLU	
1	A A A A	404	MET	
1	A	408	LEU	
1	A	415	ILE	
1	A	416	TRP	
1	A A	417	ASP	
1	A	419	GLU	
1	A	468	PHE	
1	A	470	ILE	
1	A	475	LEU	
1	A	481	GLU	
1	A	491	MET	
1	A	499	VAL	
1	A	500	LEU	
1	A	501	THR	
1	A	502	LEU	
1	A A A A A A A	505	ASN	
1	A	511	LEU	
1	A A A A	639	LEU	
1	A	661	GLU	
1	A	667	THR	
1	A	711	ASP	
1	A	727	THR	
1	A	730	PHE	
1	A	821	ARG	
1	A	828	GLU	
1	A	943	LYS	
1	A	970	ASN	
1	A	994	ASP	
1	A	997	ARG	
1	A	1020	LEU	
1	A	1022	ARG	
1	A	1023	TRP	
1	A	1029	VAL	
1	A	1052	ARG	
1	A	1058	HIS	
1	A	1059	GLN	
1	A	1062	TYR	



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Mol	Chain	Res	Type	
1	A	1073	GLN	
1	A	1165	LEU	
1	A	1203	GLU	
1	A	1217	ARG	
1	A A A A A	1219	GLU	
1	A	1222	LYS	
1	A	1224	ARG	
1	A A	1227	ILE ASN	
1	A	1237	ASN	
1	A	1242	LYS	
2	В	21	GLU	
2	В	24	ARG	
2	В	71	ARG	
2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	В	140	GLU	
2	В	184	ASN	
2	В	225	TYR	
2	В	262	MET	
2	В	266	THR GLU	
2	В	293	GLU	
2	В	431	LEU	
2	В	488	PHE LYS LYS ARG	
2	В	559	LYS	
2	В	603	LYS	
2	В	638	ARG	
2	В	640	VAL VAL	
2	В	771	VAL	
2	В	818	THR	
3	F	219	GLU	
3	F	258	ARG	
3	F	261	THR	
3	F	271	VAL	
3	F	280	ILE	
3	F	301	VAL	
3	F	317	LEU	
3	F	326	HIS	
3	F	332	PHE	
3	F	340	ILE	
3	F	348	THR	
3	F	354	ARG	
3	F	368	THR	
3	F	397	GLN	
3	F	427	LEU	



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Mol	Chain	Res	Type
4	G	41	ASP
4	G	81	ASP
4	G	143	VAL
4	G	147	ARG
4	G	153	LYS
4	G	181	TRP
4	G	182	GLU
4	G	183	ILE
3	f	253	TYR
3	f	261	THR
3	f	272	VAL
3	f	322	ASP
3	f	323	VAL
3	f	326	HIS
3	f	356	THR
3	f	421	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	401	ASN
1	A	472	ASN
1	A	489	GLN
1	A	590	GLN
1	A	860	ASN
1	A	896	GLN
1	A	1238	GLN
2	В	30	HIS
2	В	176	HIS
2	В	183	GLN
2	В	184	ASN
2	В	235	HIS
2	В	348	GLN
2	В	432	HIS
2	В	439	HIS
2	В	450	GLN
2	В	509	ASN
2	В	521	GLN
2	В	644	GLN
2	В	652	GLN
2	В	750	GLN
2	В	813	ASN



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Mol	Chain	Res	Type
2	В	882	HIS
2	В	908	GLN
2	В	916	ASN
3	F	221	GLN
3	F	270	ASN
3	F	273	GLN
3	F	275	ASN
4	G	48	HIS
3	f	325	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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.



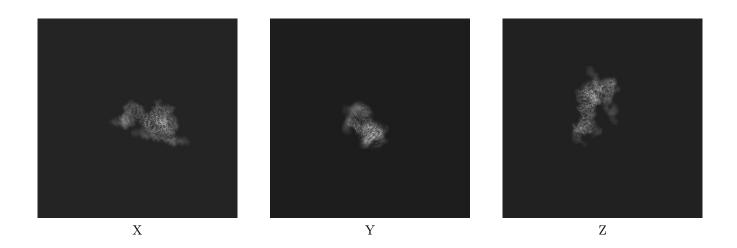
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-31117. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections (i)

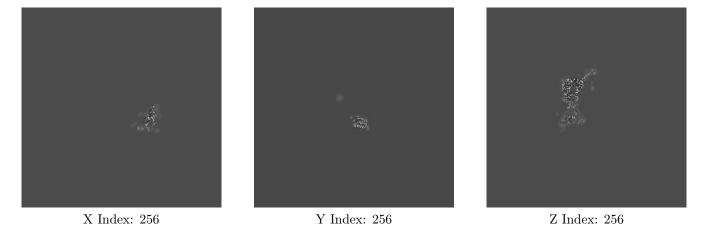
6.1.1 Primary map



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

6.2 Central slices (i)

6.2.1 Primary map

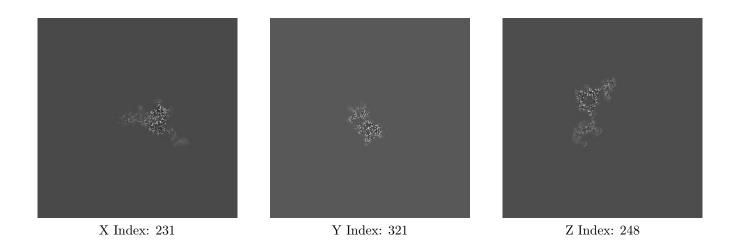




The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

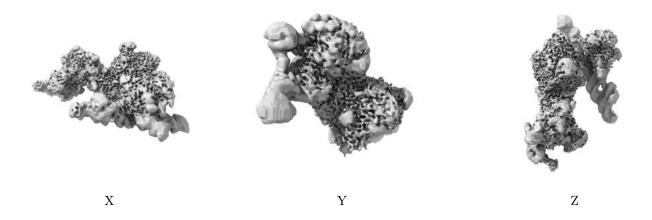
6.3.1 Primary map



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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.222. 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)

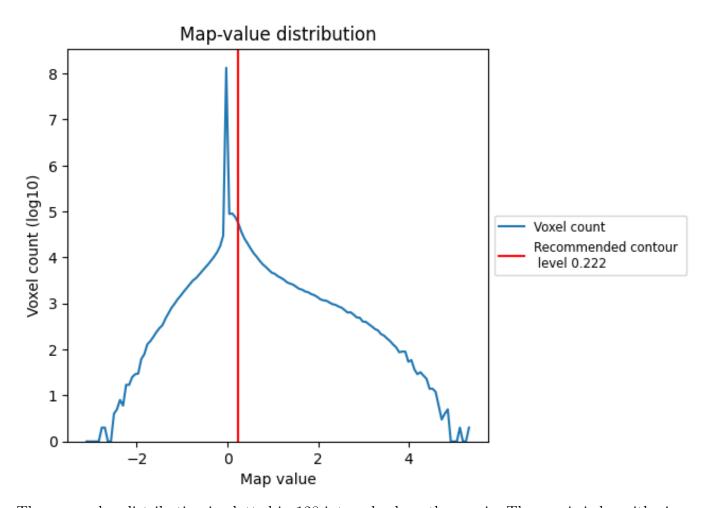
This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

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

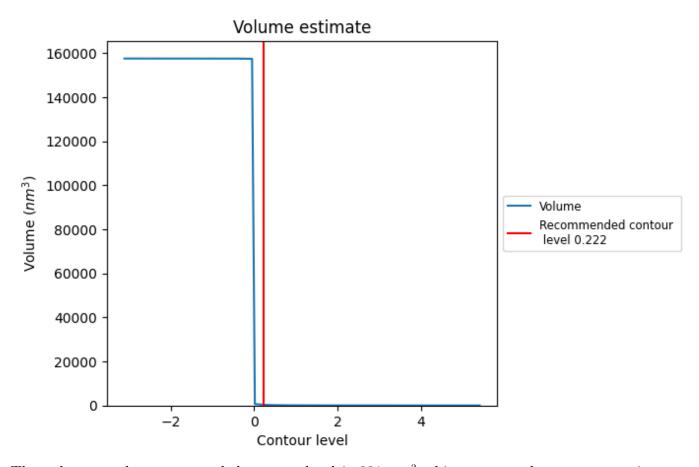
7.1 Map-value distribution (i)



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)

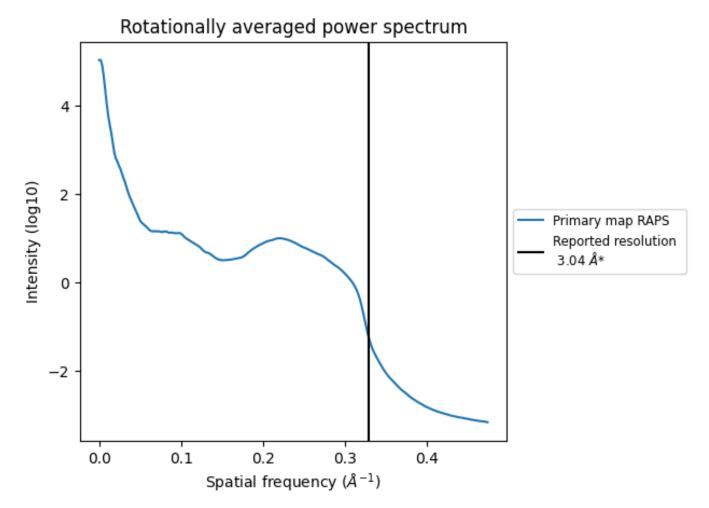


The volume at the recommended contour level is $331~\mathrm{nm}^3$; this corresponds to an approximate mass of $299~\mathrm{kDa}$.

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 0.329 $\rm \mathring{A}^{-1}$



8 Fourier-Shell correlation (i)

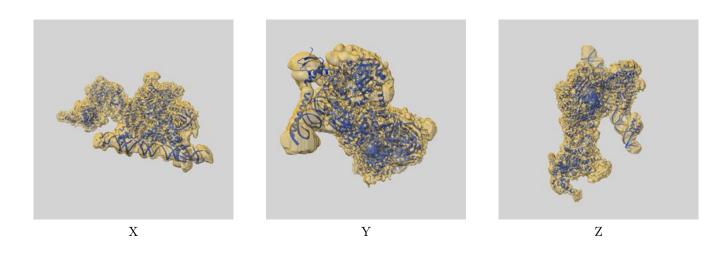
This section was not generated. No FSC curve or half-maps provided.



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-31117 and PDB model 7EGH. Per-residue inclusion information can be found in section 3 on page 5.

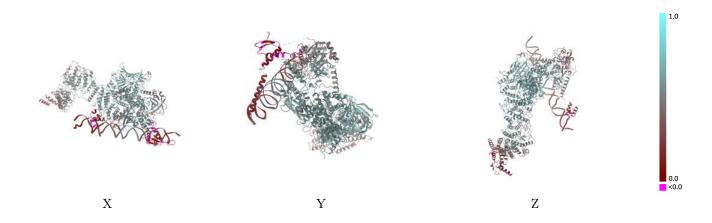
9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.222 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.

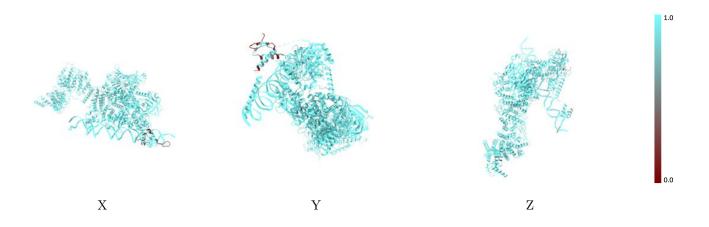


9.2 Q-score mapped to coordinate model (i)



The images above show the model with each residue coloured according 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.

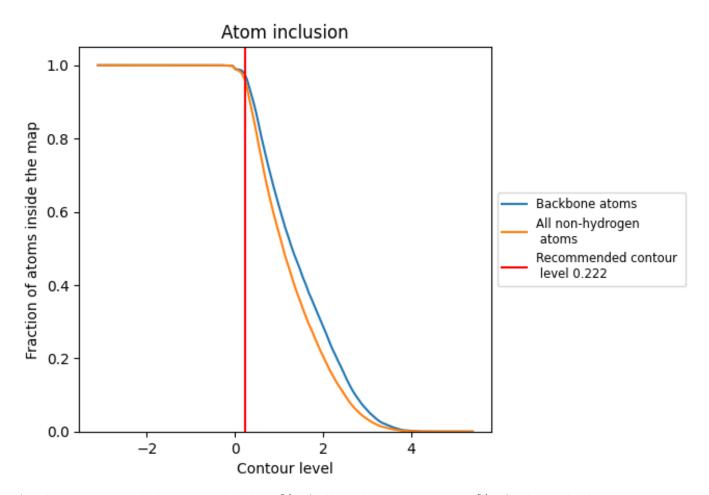
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.222).



9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.



9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.222) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9627	0.4810
A	0.9339	0.4360
В	0.9850	0.5790
F	0.9532	0.3690
G	0.8896	0.4040
Н	0.9769	0.5400
X	0.9891	0.3420
Y	0.9795	0.3520
f	0.9785	0.4790



