wwPDB EM Validation Summary Report

May 4, 2025 – 12:03 PM EDT

PDB ID	:	7M2U / pdb_00007m2u
EMDB ID	:	EMD-22576
Title	:	Nucleotide Excision Repair complex TFIIH Rad4-33
Authors	:	van Eeuwen, T.; Murakami, K.
Deposited on	:	2021-03-17
Resolution	:	8.20 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:

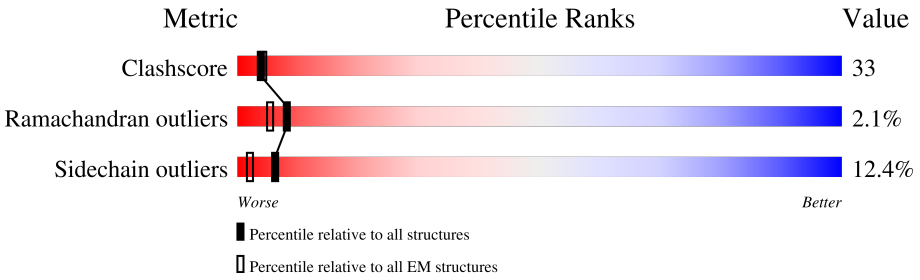
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 8.20 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	210492	15764
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	7	843	13% 45% 28% · 24%
2	Y	10	100% 20% 50% 30%
3	W	14	86% 50% 50%
4	5	66	5% 55% 44% ·
5	0	778	15% 39% 49% 8% ·
6	1	642	6% 31% 21% 5% · 43%
7	4	338	· 43% 33% 8% 16%
8	6	461	5% 40% 30% 5% 24%

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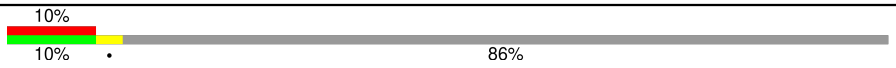
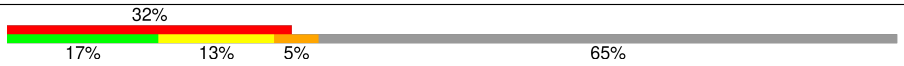
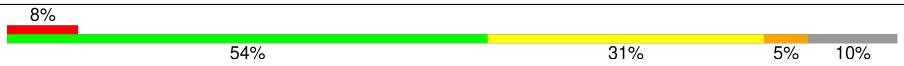
Mol	Chain	Length	Quality of chain
9	A	754	
10	E	177	
11	2	513	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	SF4	0	801	-	-	X	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 22847 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 DNA repair helicase RAD25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	7	638	4478	2739	832	883	24	0	0

- Molecule 2 is a DNA chain called Undamaged DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	Y	10	202	97	35	60	10	0	0

- Molecule 3 is a DNA chain called Damaged DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	W	14	289	137	58	80	14	0	0

- Molecule 4 is a protein called General transcription and DNA repair factor IIH subunit TFB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	5	66	498	314	89	93	2	0	0

- Molecule 5 is a protein called DNA repair helicase RAD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	0	754	6108	3891	1032	1147	38	0	0

- Molecule 6 is a protein called General transcription and DNA repair factor IIH subunit TFB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	1	367	2408	1533	438	430	7	0	0

- Molecule 7 is a protein called General transcription and DNA repair factor IIH subunit TFB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	4	284	Total	C	N	O	S	0	0
			2041	1310	343	376	12		

- Molecule 8 is a protein called General transcription and DNA repair factor IIH subunit SSL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	6	351	Total	C	N	O	S	0	0
			2526	1589	454	456	27		

- Molecule 9 is a protein called DNA repair protein RAD4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	105	Total	C	N	O	S	0	0
			795	515	135	142	3		

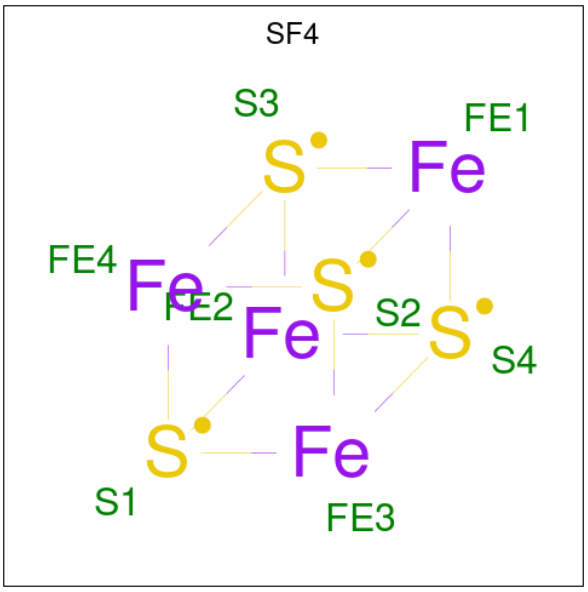
- Molecule 10 is a protein called DNA repair protein RAD33.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	62	Total	C	N	O	S	0	0
			476	301	77	92	6		

- Molecule 11 is a protein called General transcription and DNA repair factor IIH subunit TFB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	2	460	Total	C	N	O	S	0	0
			3011	1856	562	584	9		

- Molecule 12 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
12	0	1	Total Fe S 8 4 4	0

- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
13	4	1	Total Zn 1 1	0
13	6	4	Total Zn 4 4	0

- Molecule 14 is CALCIUM ION (CCD ID: CA) (formula: Ca).

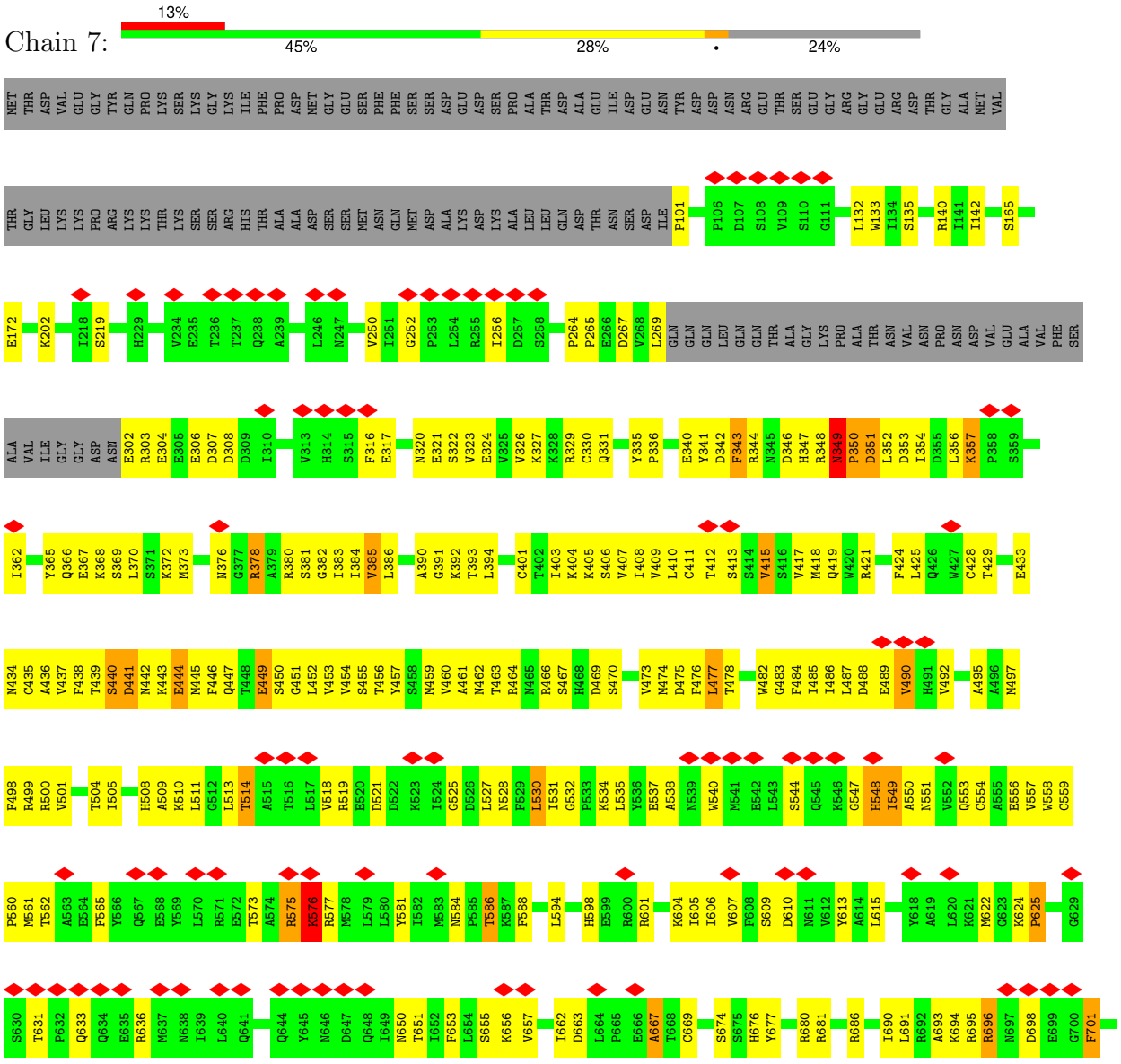
Mol	Chain	Residues	Atoms	AltConf
14	E	2	Total Ca 2 2	0

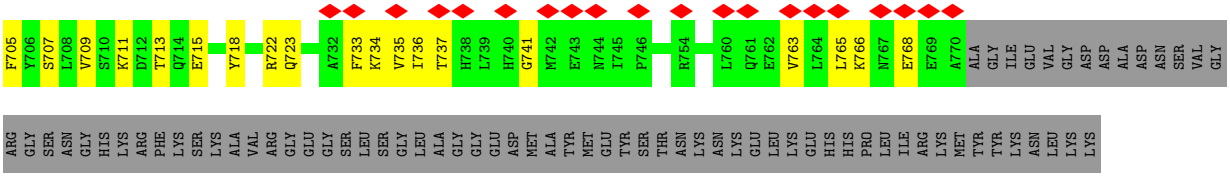
3 Residue-property plots (i)

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.

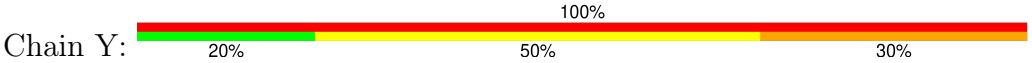
- Molecule 1: DNA repair helicase RAD25

Chain 7:

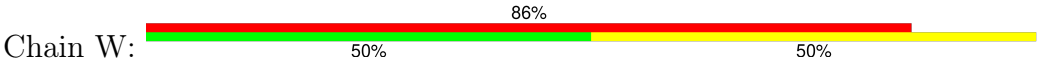


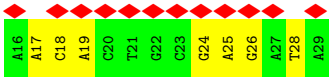


• Molecule 2: Undamaged DNA strand

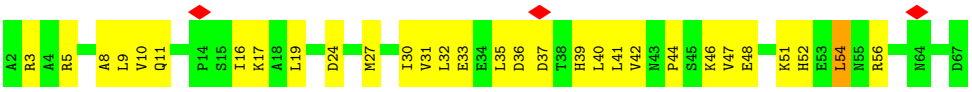


• Molecule 3: Damaged DNA strand

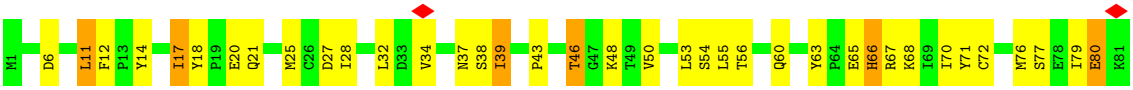


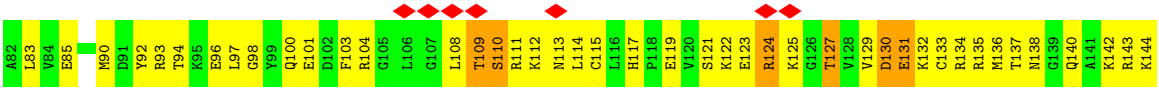


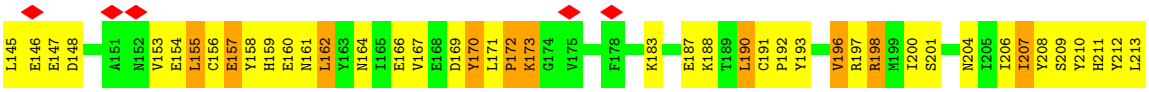
• Molecule 4: General transcription and DNA repair factor IIH subunit TFB5

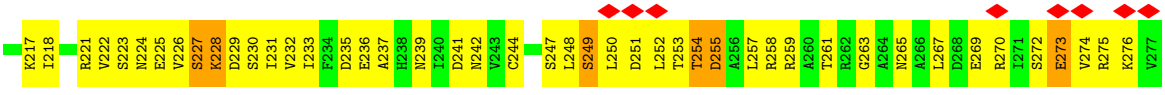


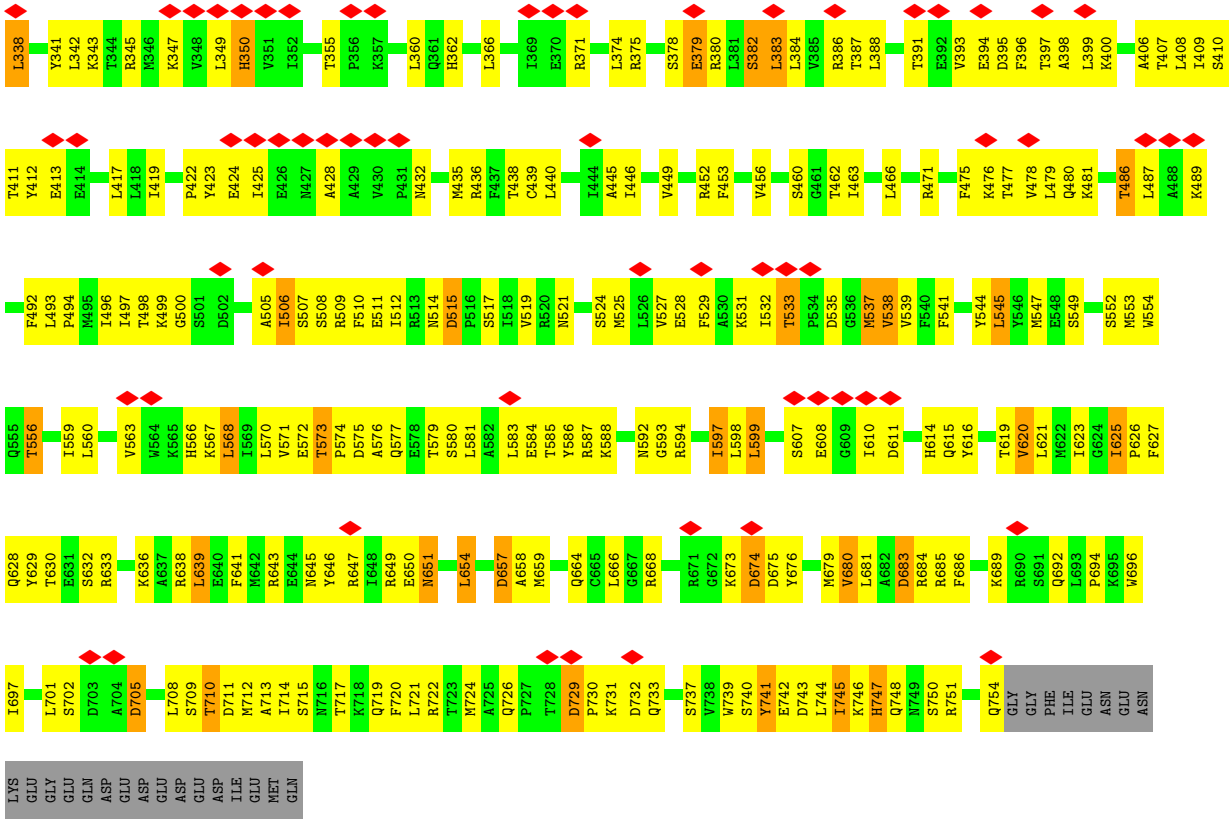
• Molecule 5: DNA repair helicase RAD3





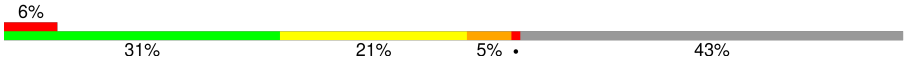


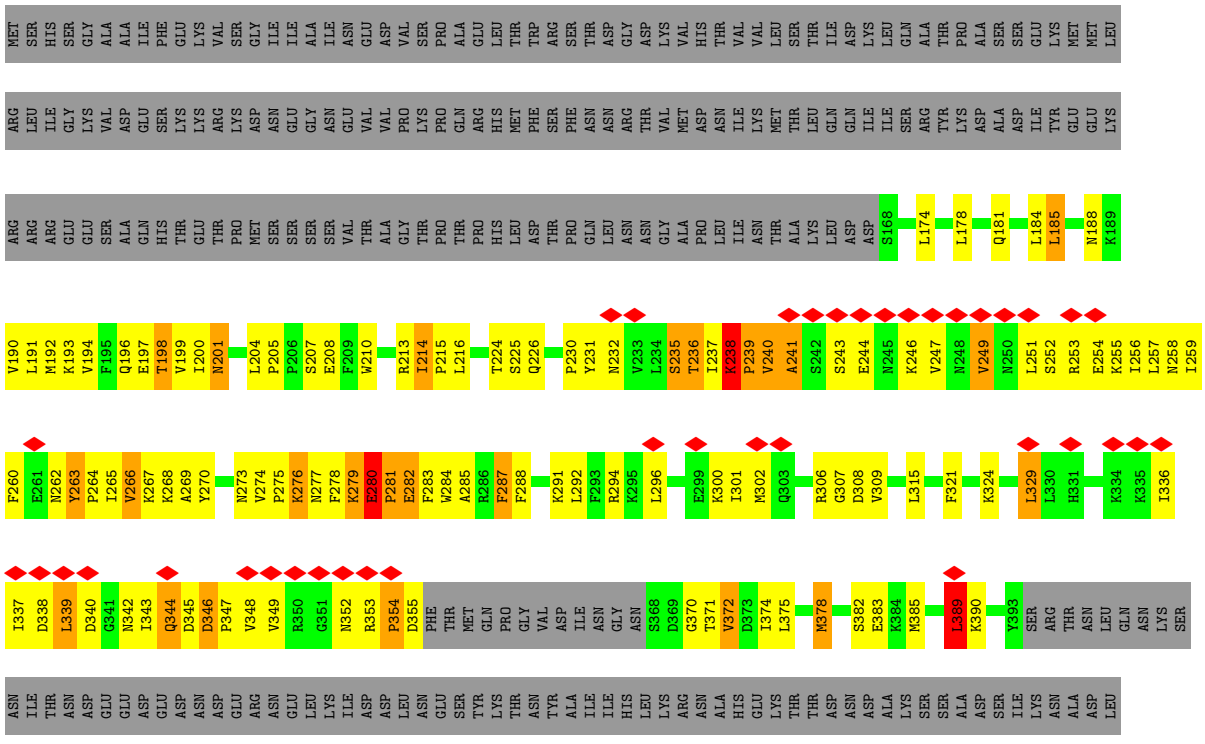


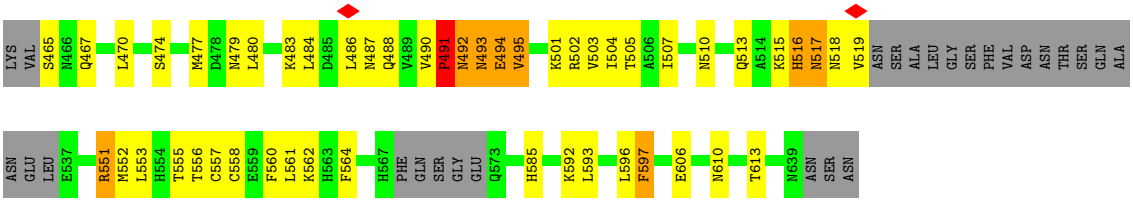


• Molecule 6: General transcription and DNA repair factor IIH subunit TFB1

Chain 1:

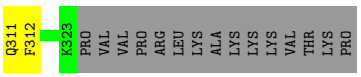






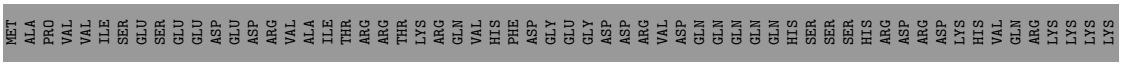
• Molecule 7: General transcription and DNA repair factor IIH subunit TFB4

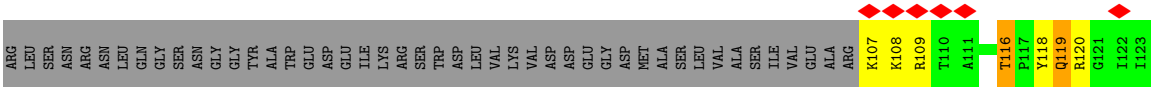
Chain 4:

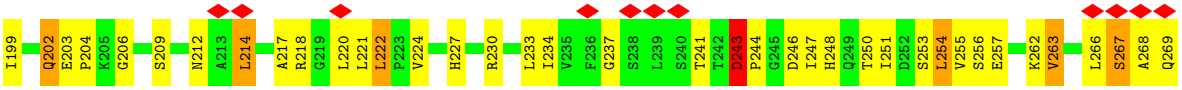


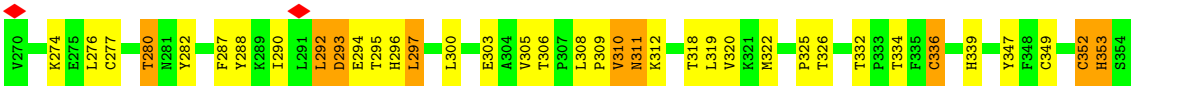
• Molecule 8: General transcription and DNA repair factor IIH subunit SSL1

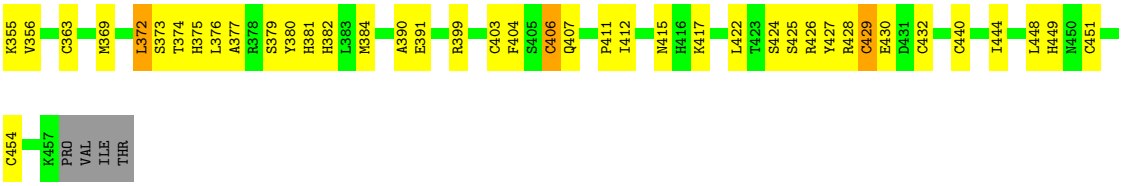
Chain 6:





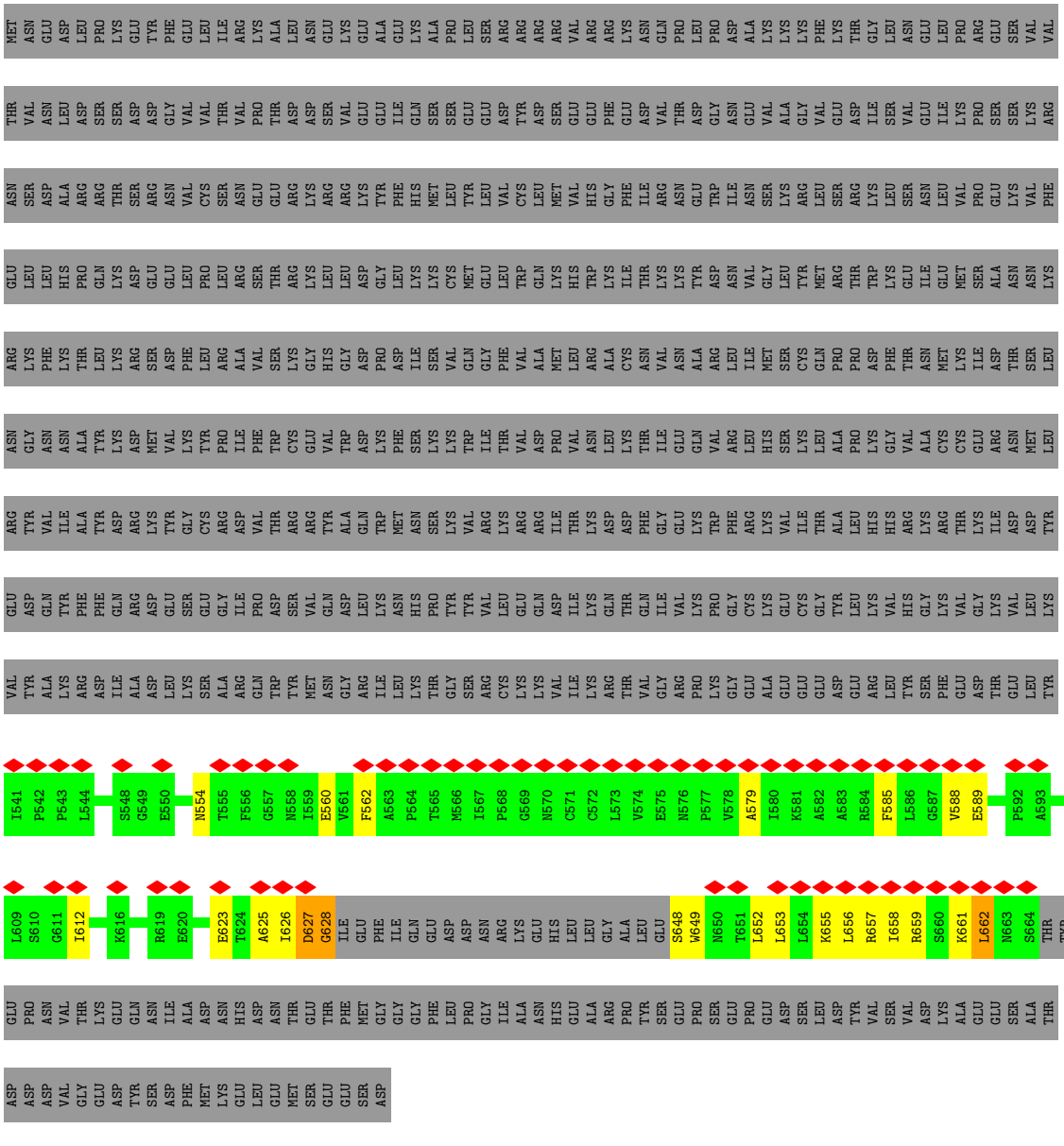






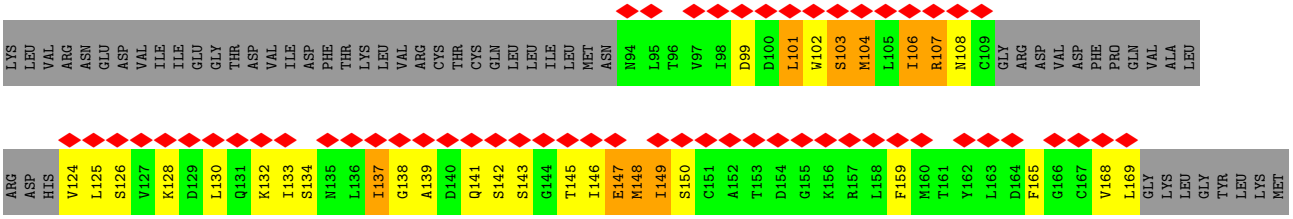
• Molecule 9: DNA repair protein RAD4

Chain A:



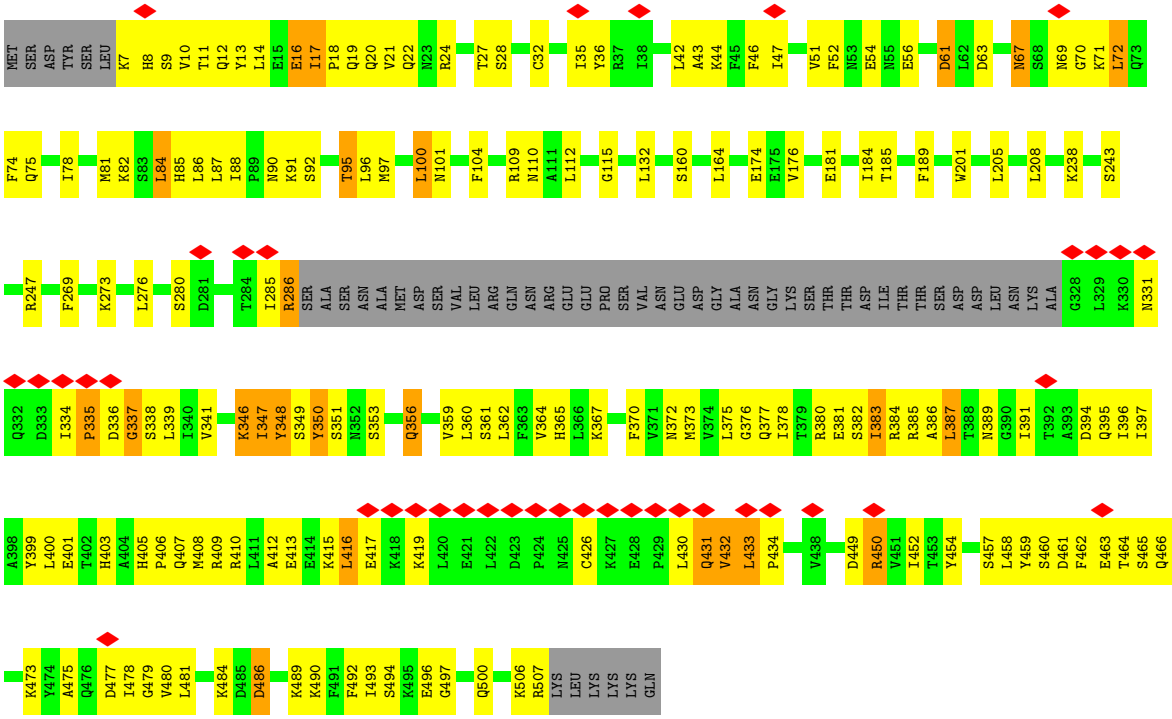
• Molecule 10: DNA repair protein RAD33

Chain E:



• Molecule 11: General transcription and DNA repair factor IIH subunit TFB2

Chain 2:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34000	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.007	Depositor
Minimum map value	-0.002	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.00239	Depositor
Map size (Å)	324.0, 324.0, 324.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, SF4, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	7	0.34	2/4552 (0.0%)	0.67	13/6078 (0.2%)
2	Y	0.67	0/225	1.64	3/344 (0.9%)
3	W	0.38	0/325	0.66	0/499
4	5	0.11	0/502	0.36	0/677
5	0	0.49	0/6226	0.54	0/8407
6	1	0.45	0/2438	0.69	6/3325 (0.2%)
7	4	0.49	0/2072	0.55	0/2819
8	6	0.54	1/2571 (0.0%)	0.60	2/3494 (0.1%)
9	A	0.27	0/810	0.83	5/1099 (0.5%)
10	E	0.38	0/479	0.96	2/644 (0.3%)
11	2	0.24	0/3057	0.53	4/4071 (0.1%)
All	All	0.43	3/23257 (0.0%)	0.63	35/31457 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	Y	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	7	350	PRO	CA-C	5.53	1.59	1.52
1	7	350	PRO	N-CA	5.43	1.53	1.47
8	6	243	ASP	C-N	-5.32	1.29	1.33

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Y	4	DA	OP2-P-O3'	-15.14	62.59	108.00
2	Y	5	DA	OP1-P-OP2	-13.95	78.15	120.00
1	7	351	ASP	N-CA-C	13.27	129.74	109.96
2	Y	4	DA	OP1-P-O3'	10.76	140.27	108.00
9	A	628	GLY	N-CA-C	9.26	140.15	113.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	Y	-3	DA	Sidechain

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	7	4478	0	3928	265	0
2	Y	202	0	114	19	0
3	W	289	0	157	12	0
4	5	498	0	506	36	0
5	0	6108	0	6167	420	0
6	1	2408	0	1984	226	0
7	4	2041	0	1953	158	0
8	6	2526	0	2333	128	0
9	A	795	0	833	86	0
10	E	476	0	487	128	0
11	2	3011	0	2600	187	0
12	0	8	0	0	2	0
13	4	1	0	0	0	0
13	6	4	0	0	0	0
14	E	2	0	0	0	0
All	All	22847	0	21062	1453	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 33.

The worst 5 of 1453 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:A:649:TRP:CZ2	10:E:149:ILE:HG12	1.31	1.65
9:A:649:TRP:CZ2	10:E:149:ILE:HA	1.27	1.65
6:1:270:TYR:CE1	6:1:279:LYS:HE3	1.26	1.62
9:A:649:TRP:CH2	10:E:149:ILE:CG1	1.78	1.60
6:1:279:LYS:HA	6:1:283:PHE:CB	1.27	1.56

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	7	634/843 (75%)	562 (89%)	65 (10%)	7 (1%)	12 47
4	5	64/66 (97%)	59 (92%)	5 (8%)	0	100 100
5	0	752/778 (97%)	632 (84%)	118 (16%)	2 (0%)	37 73
6	1	357/642 (56%)	280 (78%)	40 (11%)	37 (10%)	0 6
7	4	280/338 (83%)	210 (75%)	65 (23%)	5 (2%)	7 35
8	6	349/461 (76%)	284 (81%)	59 (17%)	6 (2%)	7 37
9	A	101/754 (13%)	93 (92%)	7 (7%)	1 (1%)	13 49
10	E	58/177 (33%)	47 (81%)	9 (16%)	2 (3%)	3 21
11	2	456/513 (89%)	380 (83%)	71 (16%)	5 (1%)	12 47
All	All	3051/4572 (67%)	2547 (84%)	439 (14%)	65 (2%)	8 30

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	1	230	PRO
6	1	236	THR
6	1	239	PRO
6	1	338	ASP
6	1	344	GLN

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	7	417/737 (57%)	388 (93%)	29 (7%)	12 32
4	5	53/60 (88%)	52 (98%)	1 (2%)	52 69
5	0	686/707 (97%)	587 (86%)	99 (14%)	2 12
6	1	169/589 (29%)	144 (85%)	25 (15%)	2 12
7	4	198/300 (66%)	163 (82%)	35 (18%)	1 8
8	6	247/418 (59%)	204 (83%)	43 (17%)	1 9
9	A	87/678 (13%)	86 (99%)	1 (1%)	70 80
10	E	56/165 (34%)	50 (89%)	6 (11%)	5 19
11	2	258/468 (55%)	228 (88%)	30 (12%)	4 16
All	All	2171/4122 (53%)	1902 (88%)	269 (12%)	6 15

5 of 269 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	6	448	LEU
10	E	149	ILE
11	2	383	ILE
5	0	538	VAL
5	0	515	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
7	4	161	ASN
8	6	375	HIS
11	2	431	GLN
8	6	190	GLN
9	A	558	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	SF4	0	801	5	0,12,12	-	-	-		

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
12	SF4	0	801	5	-	-	0/6/5/5

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	0	801	SF4	2	0

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.

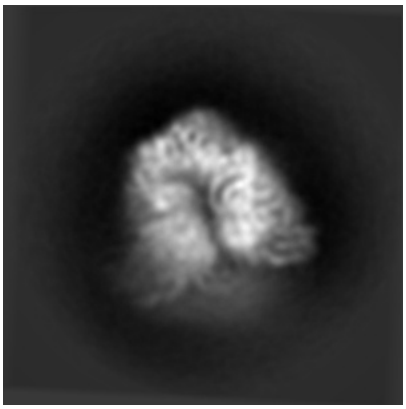
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22576. These allow visual inspection of the internal detail of the map and identification of artifacts.

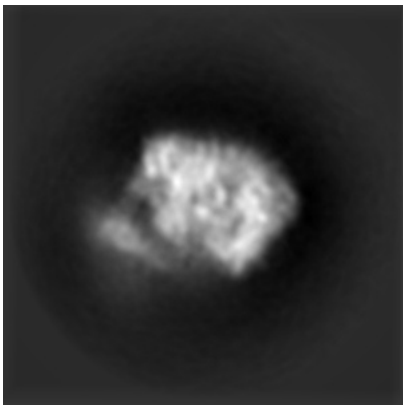
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

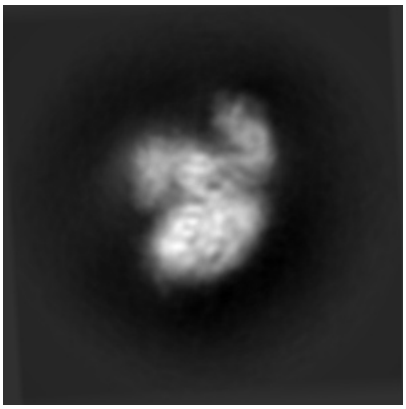
6.1.1 Primary map



X

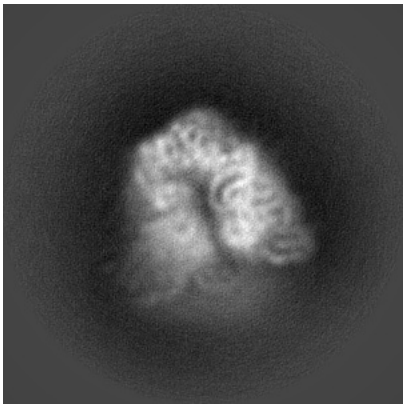


Y

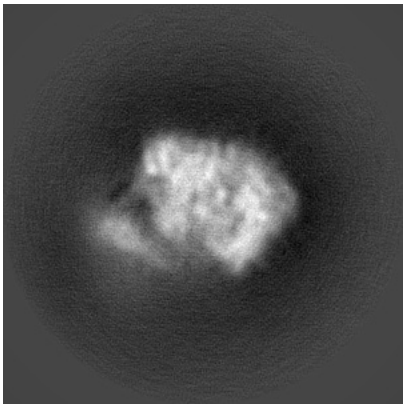


Z

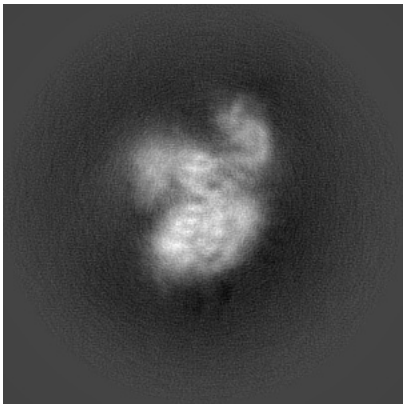
6.1.2 Raw map



X



Y

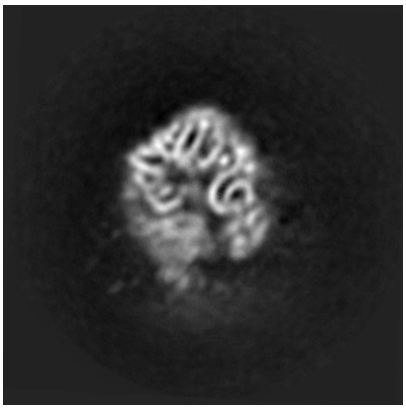


Z

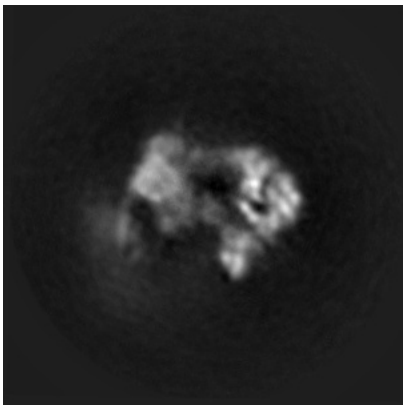
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

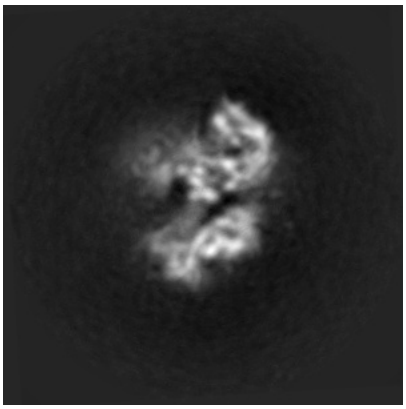
6.2.1 Primary map



X Index: 150

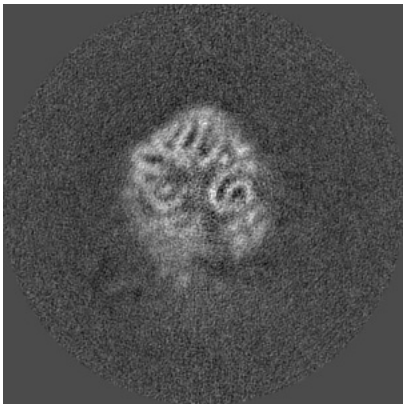


Y Index: 150

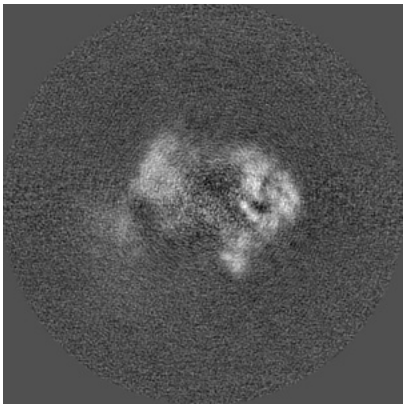


Z Index: 150

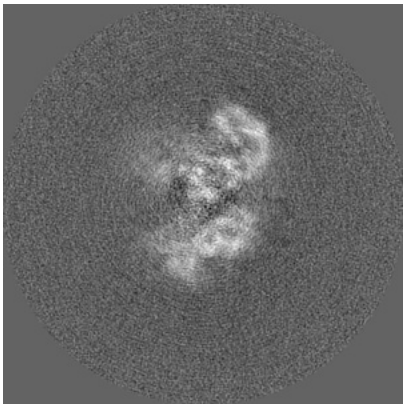
6.2.2 Raw map



X Index: 150



Y Index: 150

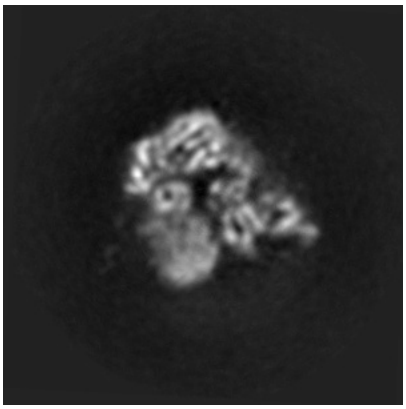


Z Index: 150

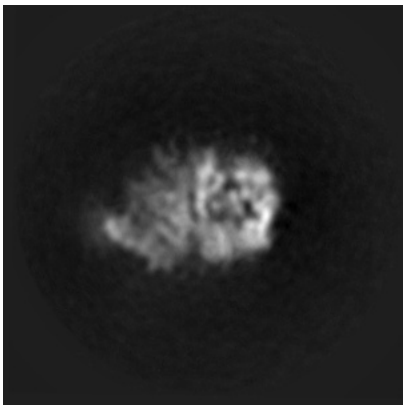
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

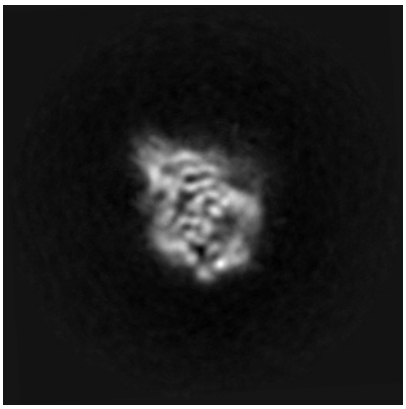
6.3.1 Primary map



X Index: 161

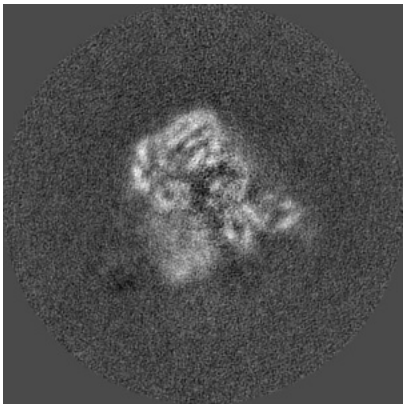


Y Index: 118

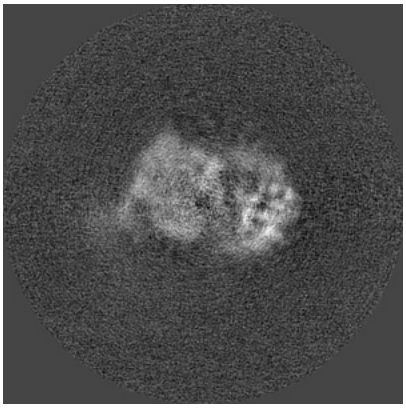


Z Index: 184

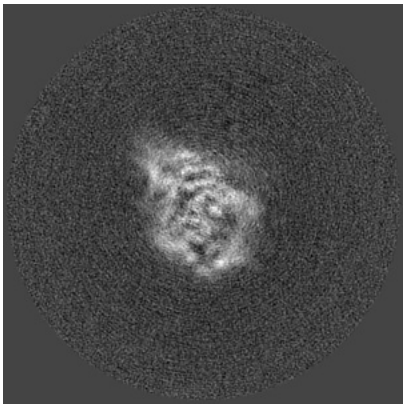
6.3.2 Raw map



X Index: 160



Y Index: 137

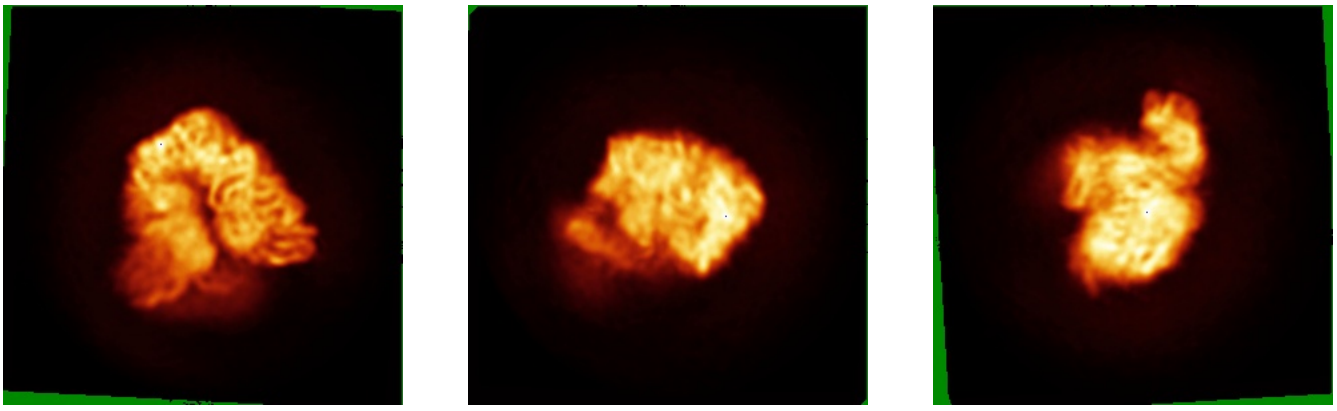


Z Index: 184

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

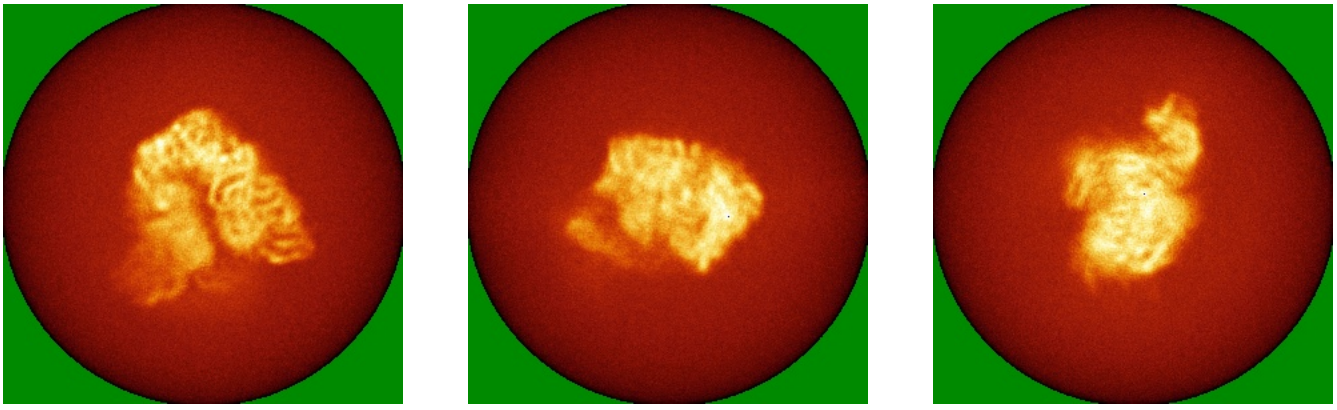
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

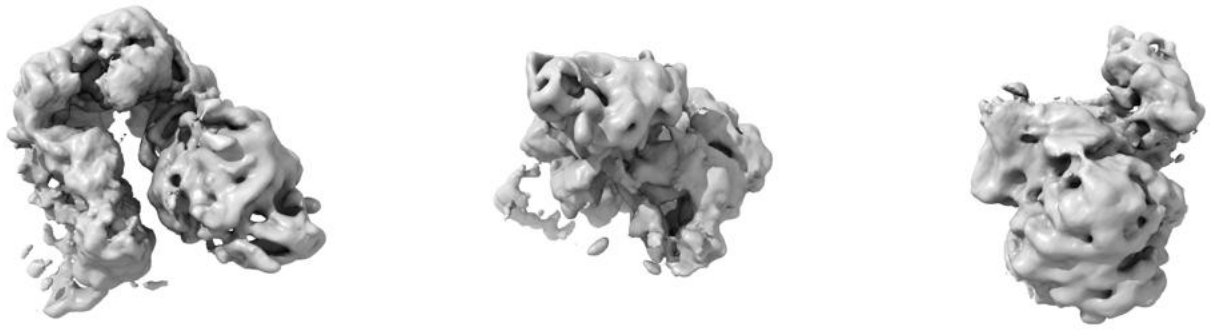


X Y Z

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 0.00239. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

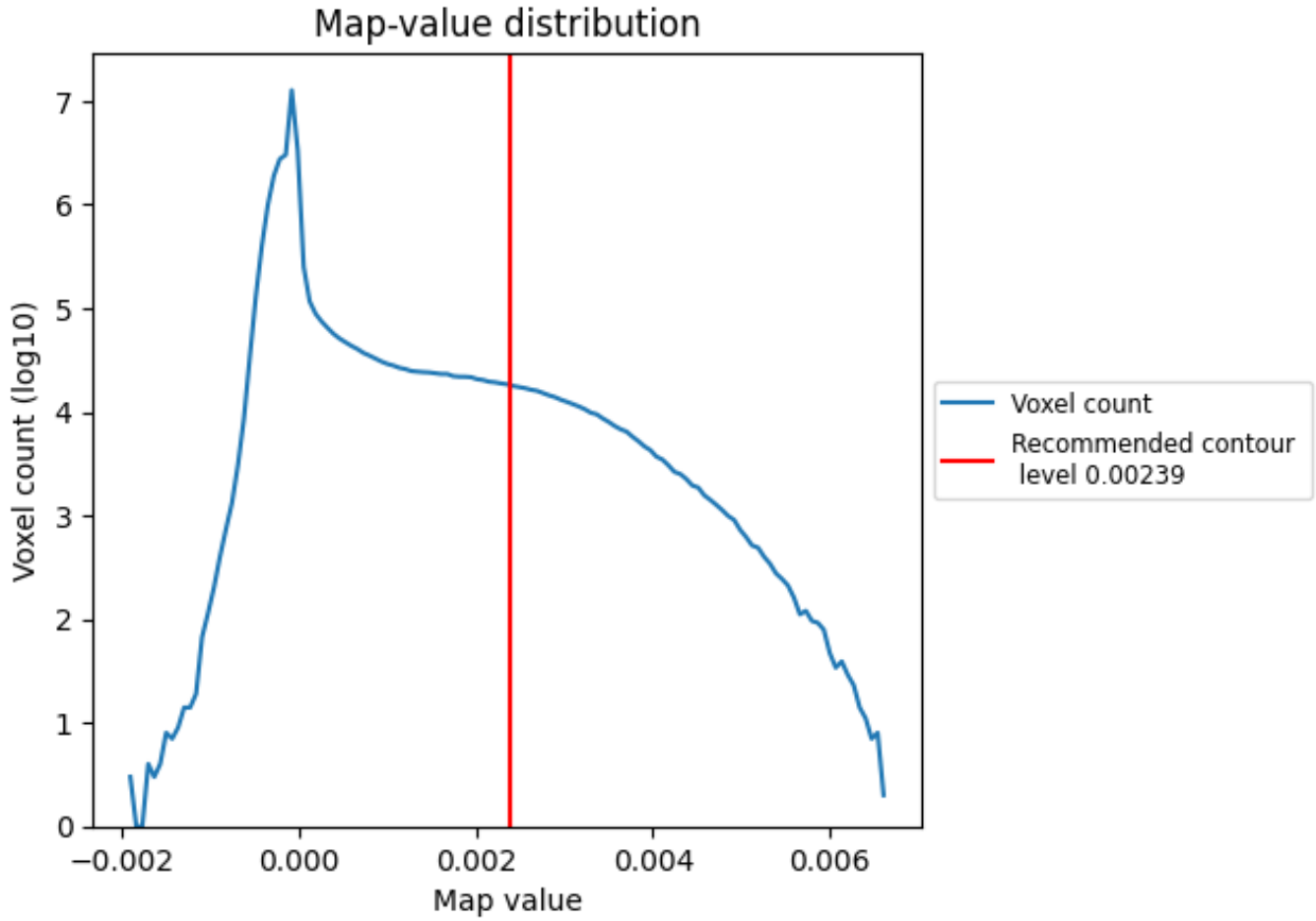
6.6 Mask visualisation (i)

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

7 Map analysis

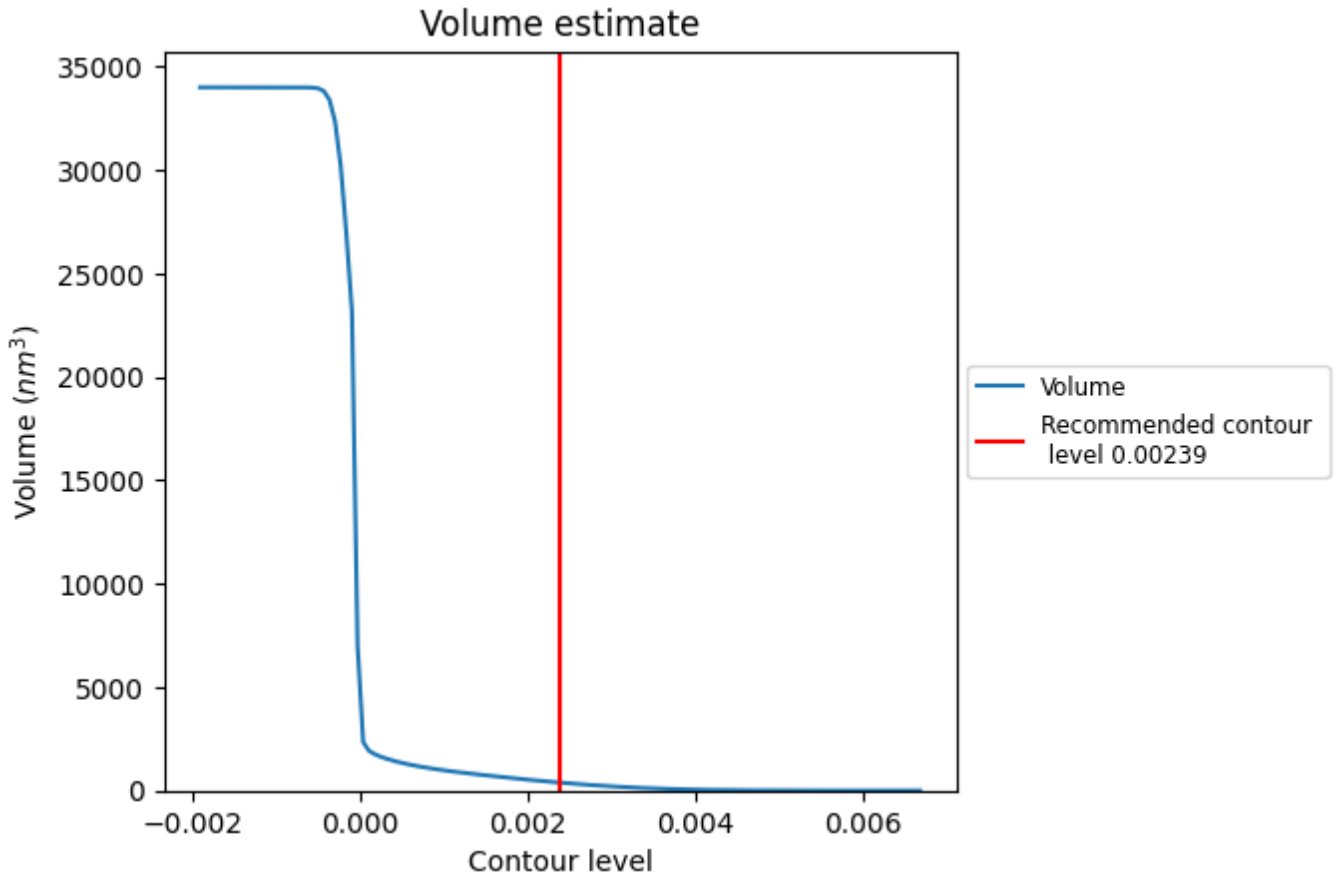
This section contains the results of statistical analysis of the map.

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.

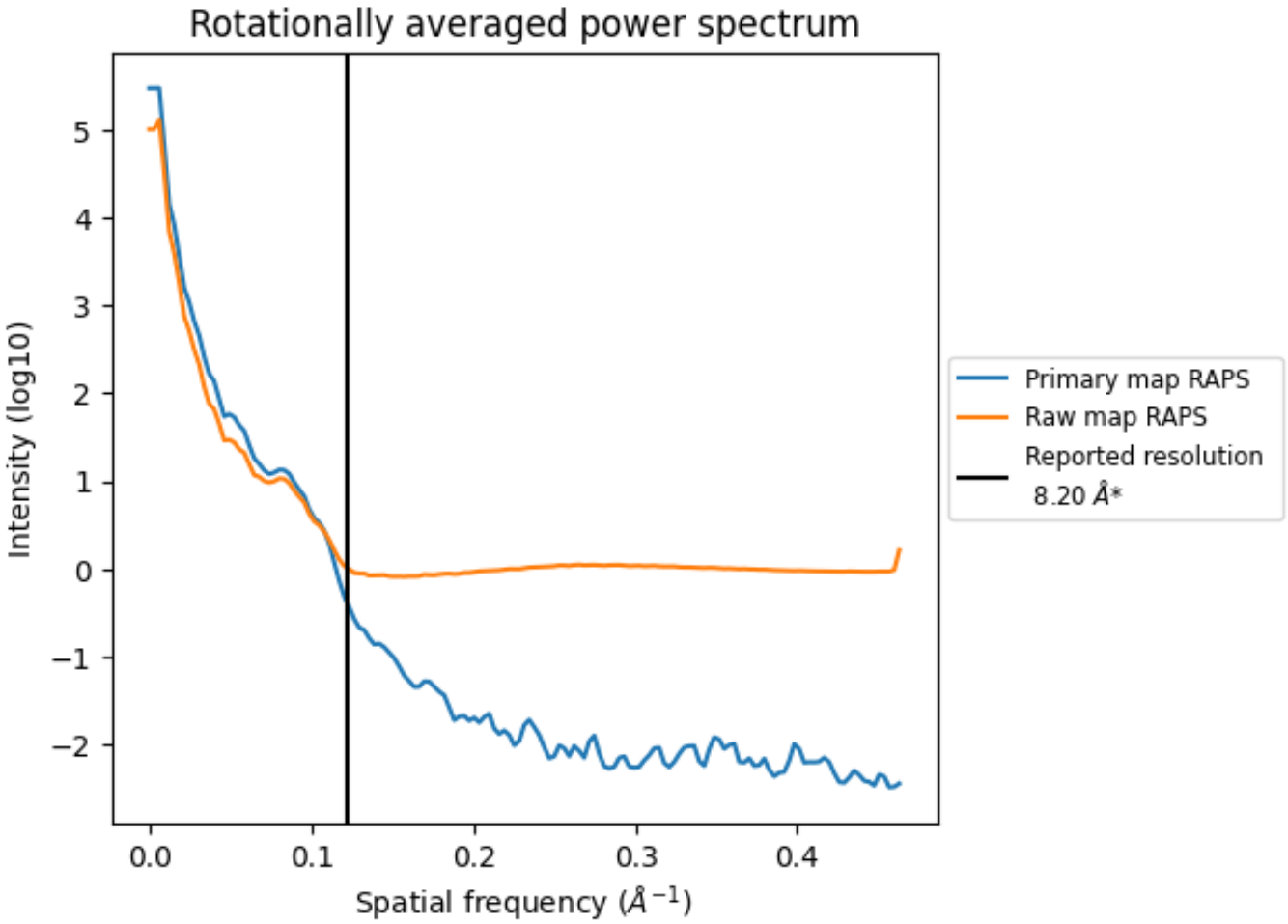
7.2 Volume estimate (i)



The volume at the recommended contour level is 383 nm^3; this corresponds to an approximate mass of 346 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)

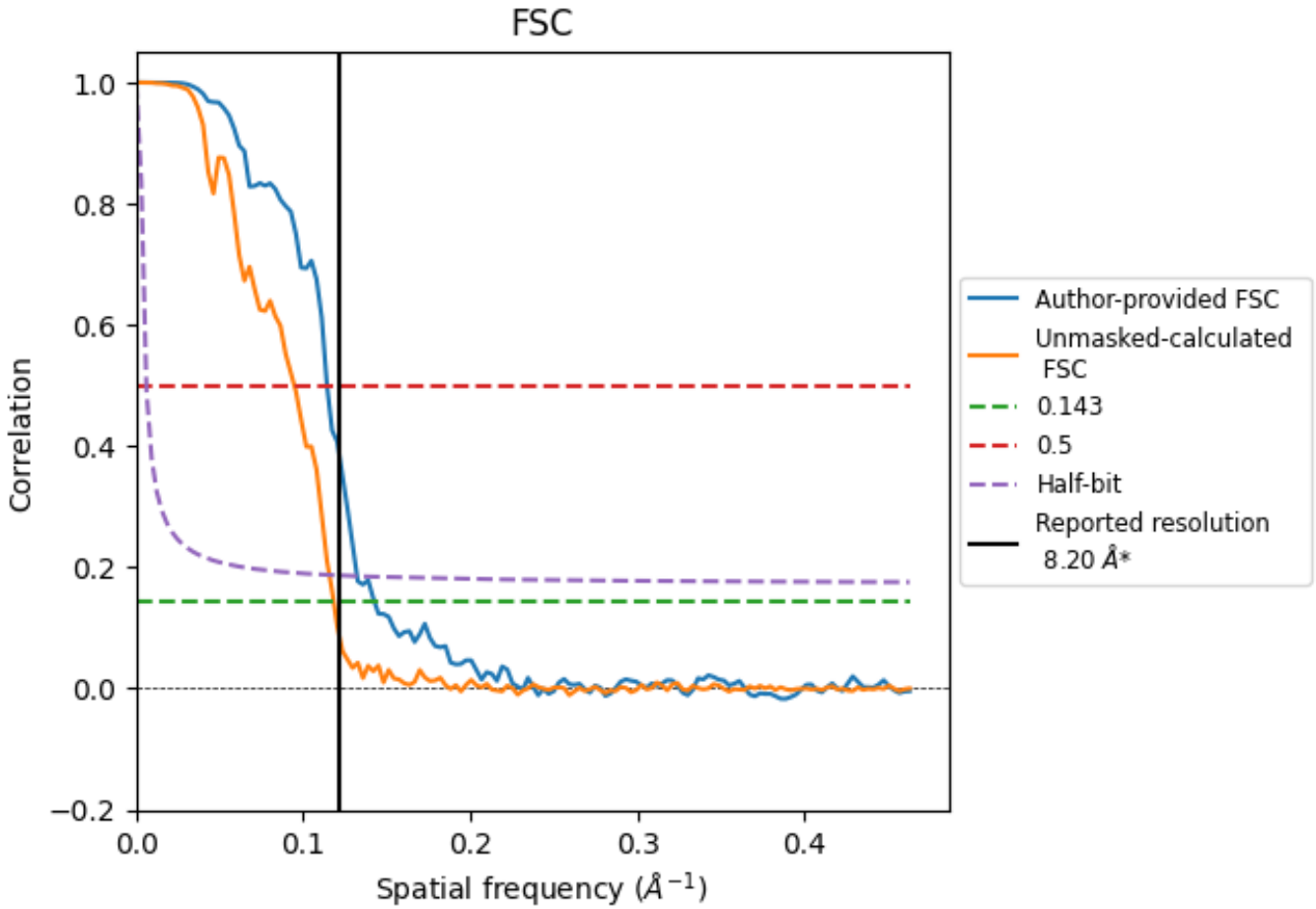


*Reported resolution corresponds to spatial frequency of 0.122 $Å^{-1}$

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 0.122 Å^{-1}

8.2 Resolution estimates (i)

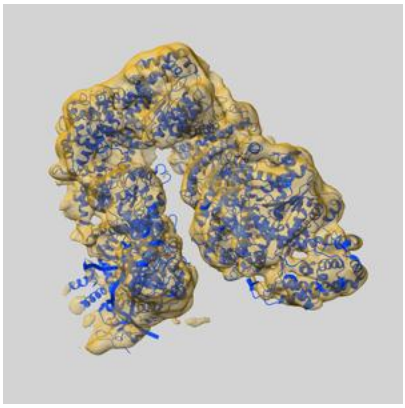
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.20	-	-
Author-provided FSC curve	7.01	8.75	7.56
Unmasked-calculated*	8.46	10.56	8.64

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 7.01 differs from the reported value 8.2 by more than 10 %

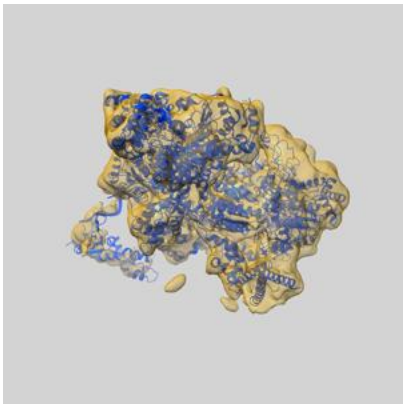
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-22576 and PDB model 7M2U. Per-residue inclusion information can be found in section 3 on page 7.

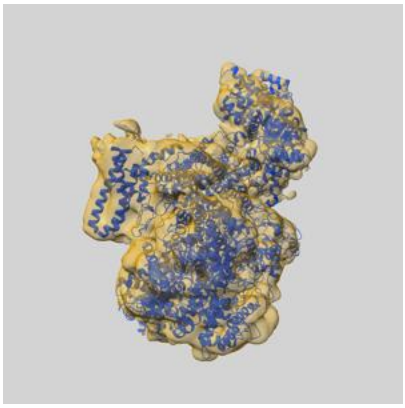
9.1 Map-model overlay



X



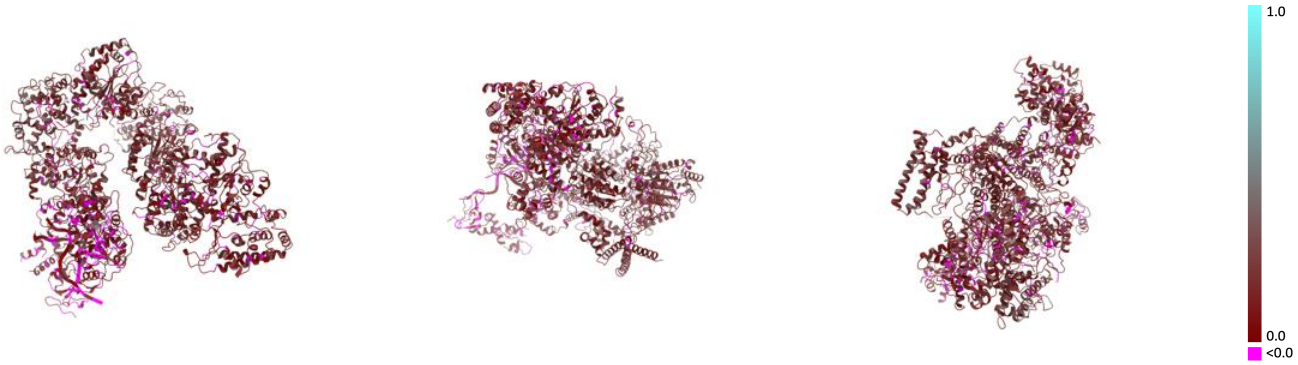
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00239 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.

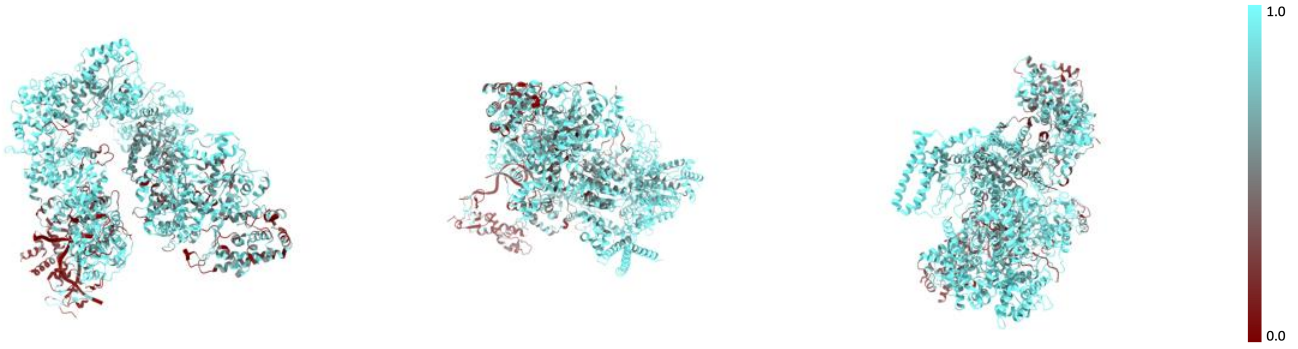
9.2 Q-score mapped to coordinate model



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.

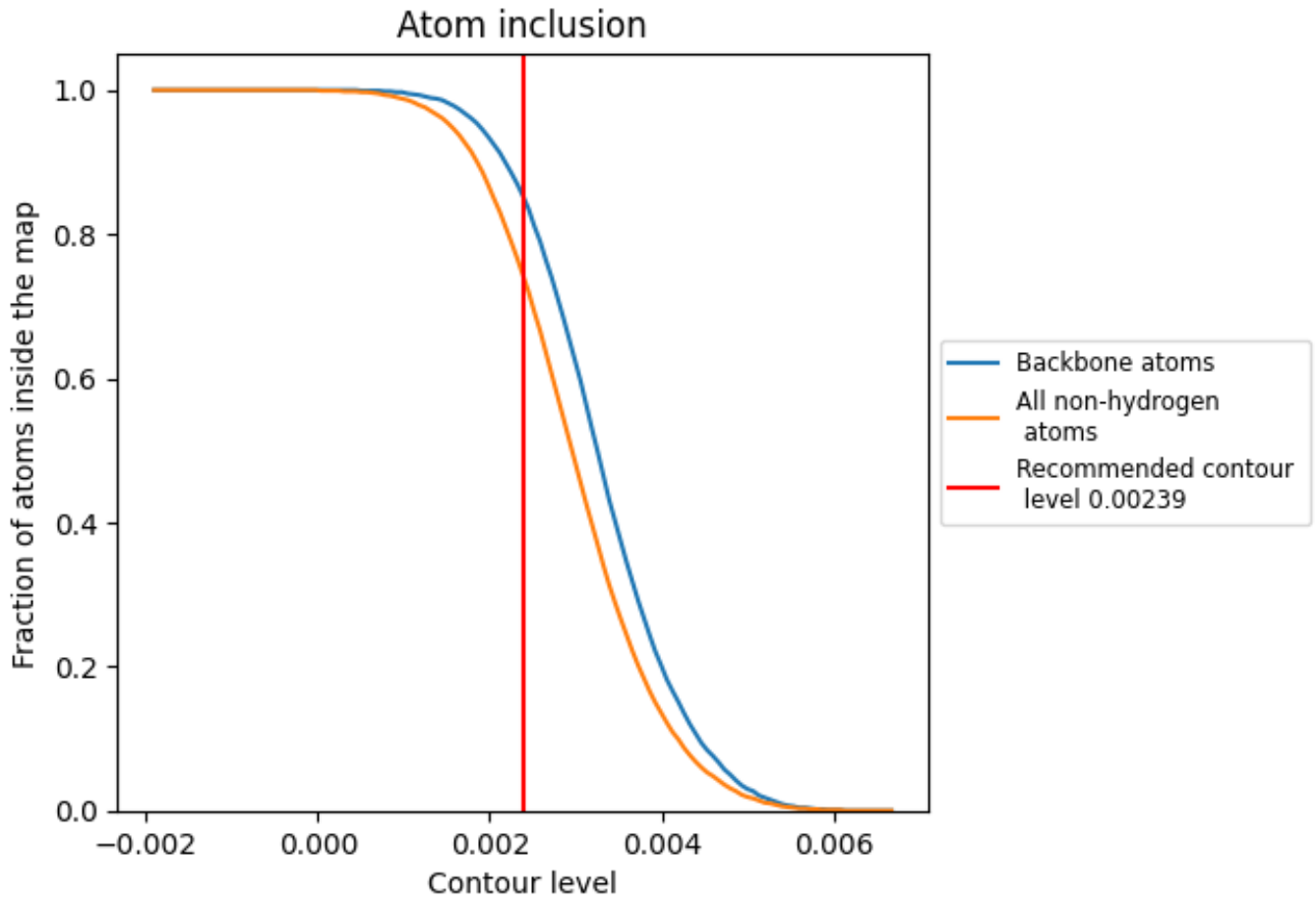
9.3 Atom inclusion mapped to coordinate model



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 (0.00239).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 74% 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 (0.00239) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7420	0.1460
0	0.7310	0.1490
1	0.8310	0.1980
2	0.8410	0.1740
4	0.8720	0.1750
5	0.9020	0.1370
6	0.7970	0.1710
7	0.7540	0.1010
A	0.2800	0.0620
E	0.1060	0.0650
W	0.1900	0.0530
Y	0.0640	0.0450