



## wwPDB EM Validation Summary Report ⓘ

Dec 19, 2022 – 08:28 am GMT

PDB ID : 7NFE  
EMDB ID : EMD-12301  
Title : Cryo-EM structure of NHEJ super-complex (monomer)  
Authors : Chaplin, A.K.; Hardwick, S.W.; Kefala Stavridi, A.; Chirgadze, D.Y.; Blundell, T.L.  
Deposited on : 2021-02-06  
Resolution : 4.29 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) 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

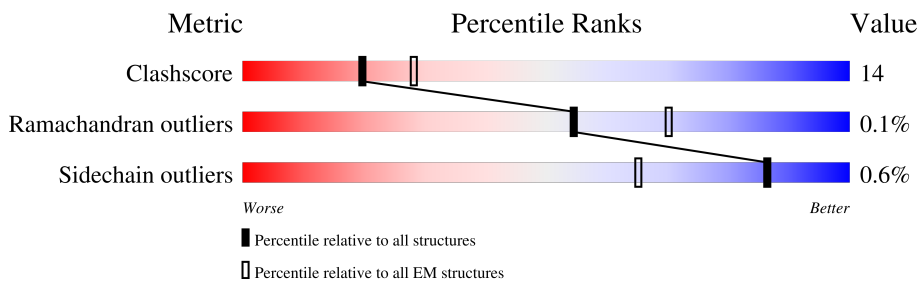
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.29 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4156	60% 26% 14%
2	B	609	51% 26% 22%
3	C	732	46% 24% 30%
4	F	299	18% 45% 19% 36%
4	G	299	8% 44% 22% 34%
5	H	336	10% 43% 17% 40%
5	I	336	17% 41% 16% 43%
6	J	911	18% 11% 72%

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Mol	Chain	Length	Quality of chain	
7	D	24	 50%	50%
8	E	24	 46%	54%

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 44554 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-dependent protein kinase catalytic subunit,DNA-dependent protein kinase catalytic subunit,DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3585	27806	17851	4651	5132	172	0	0

- Molecule 2 is a protein called X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	475	3673	2365	610	680	18	0	0

- Molecule 3 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	513	3999	2557	669	752	21	0	0

- Molecule 4 is a protein called Non-homologous end-joining factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F	190	1465	936	247	275	7	0	0
4	G	197	1502	950	253	291	8	0	0

- Molecule 5 is a protein called DNA repair protein XRCC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	H	201	1575	991	271	307	6	0	0
5	I	193	1521	958	257	300	6	0	0

- Molecule 6 is a protein called DNA ligase 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	J	258	2026	1284	345	386	11	0	0

- Molecule 7 is a DNA chain called DNA (5'-D(P\*AP\*AP\*TP\*AP\*AP\*AP\*CP\*TP\*AP\*AP\*AP\*AP\*AP\*CP\*TP\*AP\*TP\*TP\*AP\*TP\*TP\*AP\*TP\*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	D	24	493	238	92	139	24	0	0

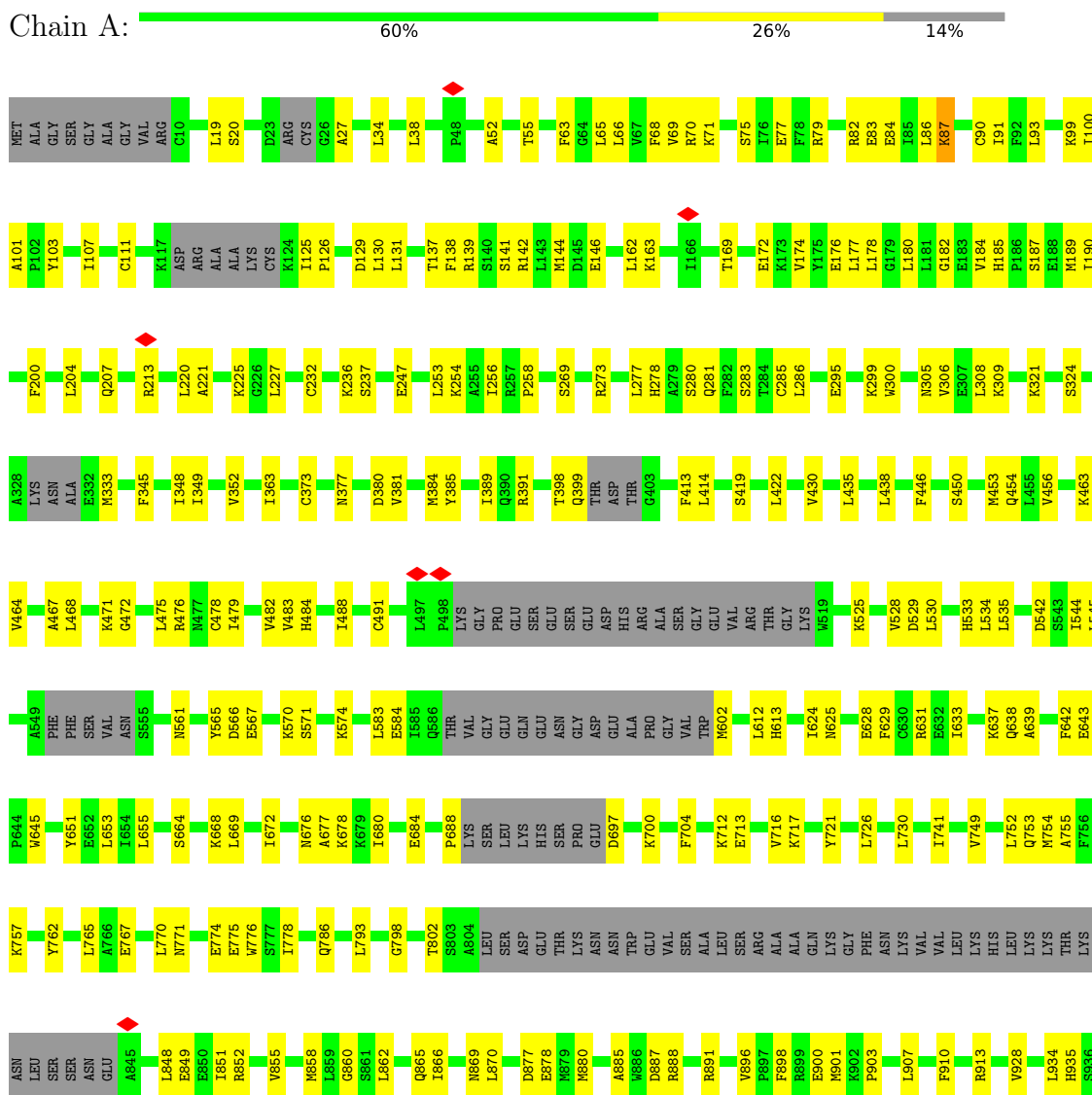
- Molecule 8 is a DNA chain called DNA (5'-D(P\*TP\*AP\*AP\*TP\*AP\*AP\*TP\*AP\*GP\*TP\*TP\*TP\*TP\*AP\*GP\*TP\*TP\*TP\*AP\*TP\*TP\*AP\*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	E	24	494	240	81	149	24	0	0

### 3 Residue-property plots

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.

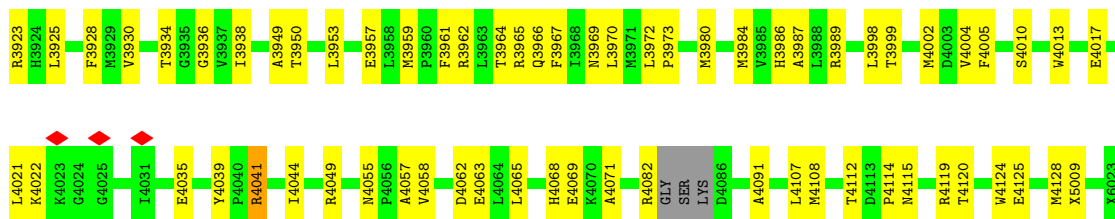
- Molecule 1: DNA-dependent protein kinase catalytic subunit,DNA-dependent protein kinase catalytic subunit,DNA-dependent protein kinase catalytic subunit



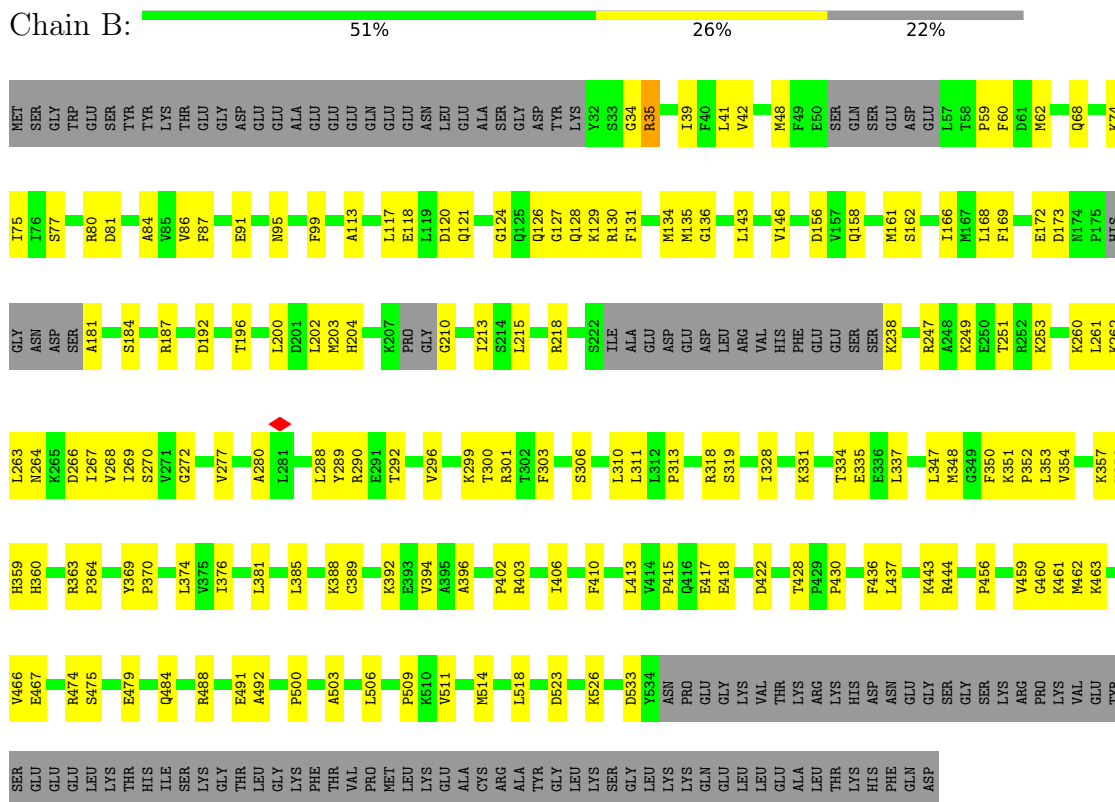
P2373	D2269	L2149	PHE	T1924	H1830	V1537	I1428	K1074	H937
L2374	N2270	V2156	ARG	E1925	C1831	L1538	E1429	F1082	T946
R2377	S2271	F2378	ARG	M1926	S1832	L1539	E1430	F1082	GLN
M2379	I2274	F2379	ARG	M1927	L1833	E1430	L1431	I1085	MET
P2387	L2277	M2379	GLN	ALA	D1834	T1540	L1431	I1085	PRO
T2395	V2280	M2379	GLN	GLY	V1844	ALA	C1432	I1087	GLU
V2400	L2168	M2379	GLN	GLY	V1845	LEU	A1433	E1088	GLY
L2411	L2168	M2379	ASN	ASN	V1846	LEU	V1434	F1089	GLY
Y2412	L2169	M2379	GLN	GLN	A1847	GLY	Y1437	E1092	GLN
L2415	L2170	M2379	ASN	L1933	I1848	SER	L1197	E1092	GLY
K2416	Q2170	M2379	ASN	L1933	E1764	SER	L1198	E1093	GLY
S2417	L2171	M2379	GLY	R1936	D1849	GLN	P1204	E1094	ALA
K2418	L2171	M2379	ASP	R1937	L1766	GLY	P1204	S1094	ALA
D2419	H2177	M2379	ASP	R1937	G1767	S1549	P1204	L1095	PRD
F2420	G1767	M2379	ASP	R1937	R1768	V1550	L1212	L1095	P957
F2420	E1769	M2379	VAL	Y1940	R1768	V1550	L1212	V1096	D977
M2424	H1941	M2379	VAL	H1941	R1769	V1550	L1212	E1097	D978
R2425	C1942	M2379	LEU	C1942	E1769	V1552	E1215	E1097	Q978
D2428	M1946	M2379	LEU	M1946	H1772	H1552	E1215	Q1098	Q979
D2429	A1947	M2379	LEU	A1947	V1773	H1552	E1215	Q1098	Q979
E2430	C1948	M2379	LEU	C1948	E1776	H1552	E1215	Q1098	Q979
E2431	I1949	M2379	LEU	I1949	F1778	H1552	E1215	Q1098	Q979
L2438	I1952	M2379	LEU	I1952	F1779	H1552	E1215	Q1098	Q979
M2442	V1955	M2379	LEU	V1955	S1780	H1552	E1215	Q1098	Q979
M2443	K1960	M2379	ALA	K1960	E1776	H1552	E1215	Q1098	Q979
M2443	F1961	M2379	ALA	F1961	F1778	H1552	E1215	Q1098	Q979
K2447	Y1962	M2379	THR	Y1962	F1779	H1552	E1215	Q1098	Q979
P2448	L2101	M2379	THR	L2101	S1780	H1552	E1215	Q1098	Q979
V2449	K2102	M2379	LEU	K2102	E1776	H1552	E1215	Q1098	Q979
R2452	L2097	M2379	LEU	L2097	F1778	H1552	E1215	Q1098	Q979
E2453	T2098	M2379	ALA	T2098	F1779	H1552	E1215	Q1098	Q979
L2454	A2099	M2379	ASP	A2099	F1779	H1552	E1215	Q1098	Q979
P2457	L2101	M2379	LEU	L2101	S1790	H1552	E1215	Q1098	Q979
V2458	K2102	M2379	LEU	K2102	L1792	H1552	E1215	Q1098	Q979
E2460	L2097	M2379	LEU	L2097	V1792	H1552	E1215	Q1098	Q979
F2461	R2106	M2379	GLY	R2106	T1793	H1552	E1215	Q1098	Q979
H2464	S2107	M2379	GLY	S2107	E1709	H1552	E1215	Q1098	Q979
P2465	L2108	M2379	GLY	L2108	L1712	H1552	E1215	Q1098	Q979
S2466	GLY	M2379	PRO	GLY	V1713	H1552	E1215	Q1098	Q979
T2467	PRO	M2379	PRO	PRO	Q1716	H1552	E1215	Q1098	Q979
Y2474	ASN	M2379	ASN	ASN	Q1716	H1552	E1215	Q1098	Q979
N2475	L2122	M2379	ASN	L2122	GLY	H1552	E1215	Q1098	Q979
L2477	W2125	M2379	ASN	W2125	ASP	H1552	E1215	Q1098	Q979
M2478	L2129	M2379	ASN	L2129	GLU	H1552	E1215	Q1098	Q979
	H2130	M2379	ASN	H2130	GLU	H1552	E1215	Q1098	Q979
	L2133	M2379	ASN	L2133	GLN	H1552	E1215	Q1098	Q979
	F2145	M2379	ASN	F2145	LEU	H1552	E1215	Q1098	Q979
	L2337	M2379	ASN	L2337	LEU	H1552	E1215	Q1098	Q979
	L2341	M2379	ASN	L2341	LEU	H1552	E1215	Q1098	Q979
	C2342	M2379	ASN	C2342	LEU	H1552	E1215	Q1098	Q979
	L2349	M2379	ASN	L2349	LEU	H1552	E1215	Q1098	Q979
	D2358	M2379	ASN	D2358	LEU	H1552	E1215	Q1098	Q979
	K2359	M2379	ASN	K2359	LEU	H1552	E1215	Q1098	Q979
	F2360	M2379	ASN	F2360	LEU	H1552	E1215	Q1098	Q979
	N2365	M2379	ASN	N2365	LEU	H1552	E1215	Q1098	Q979
	S2466	M2379	ASN	S2466	LEU	H1552	E1215	Q1098	Q979
	Y2367	M2379	ASN	Y2367	LEU	H1552	E1215	Q1098	Q979
	T2368	M2379	ASN	T2368	LEU	H1552	E1215	Q1098	Q979
	F2371	M2379	ASN	F2371	LEU	H1552	E1215	Q1098	Q979
	P2372	M2379	ASN	P2372	LEU	H1552	E1215	Q1098	Q979



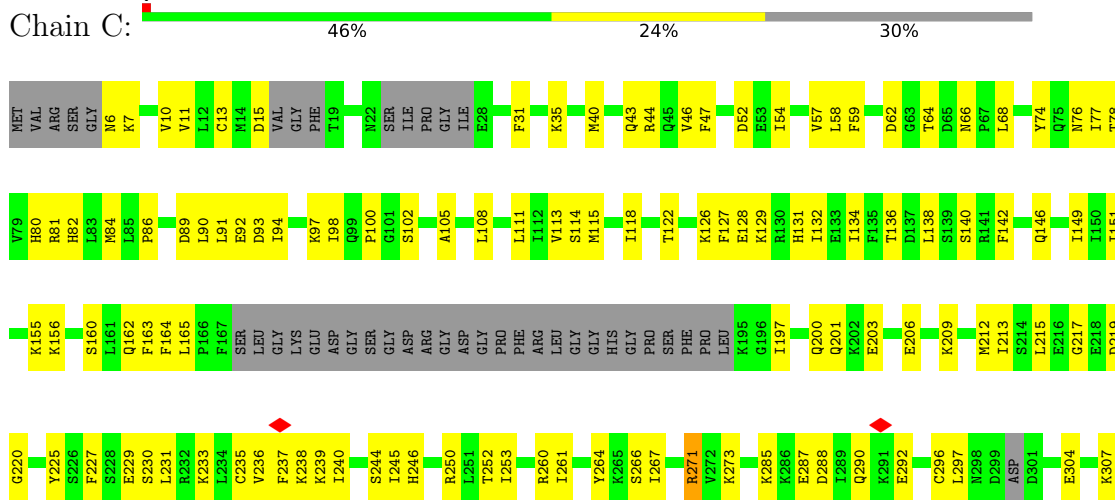


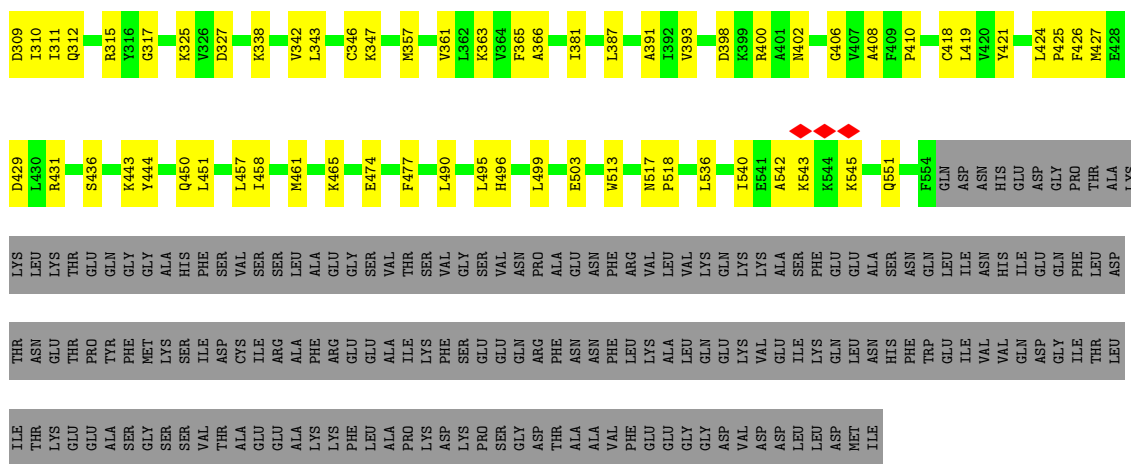


• Molecule 2: X-ray repair cross-complementing protein 6

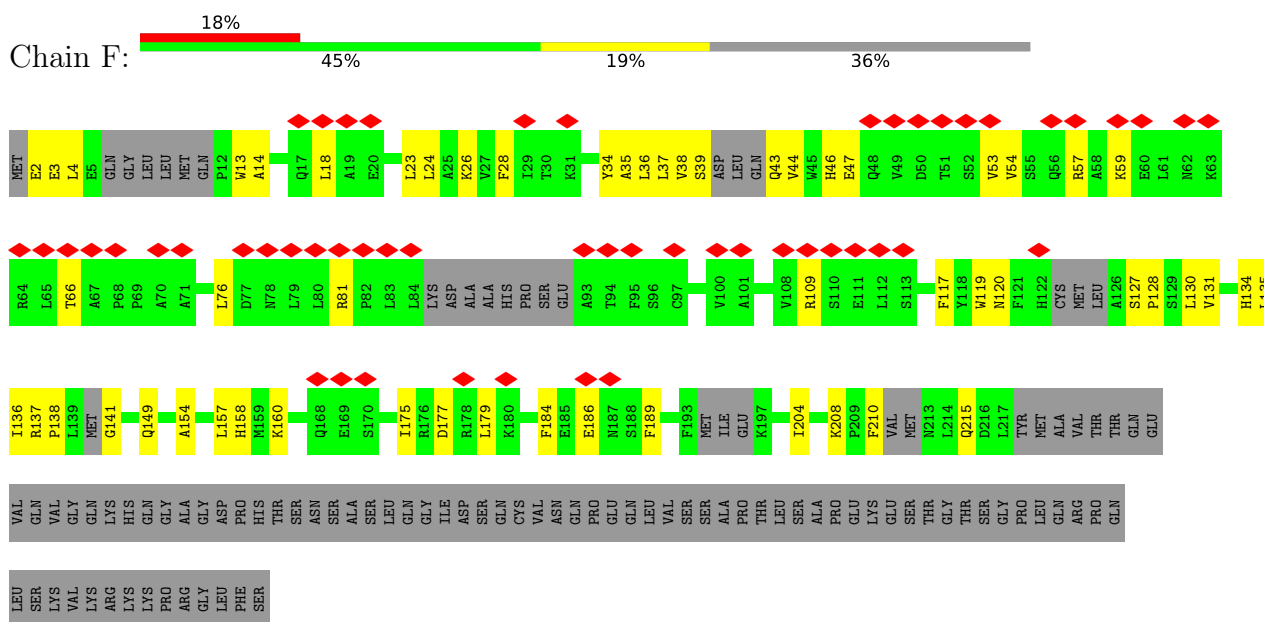


• Molecule 3: X-ray repair cross-complementing protein 5

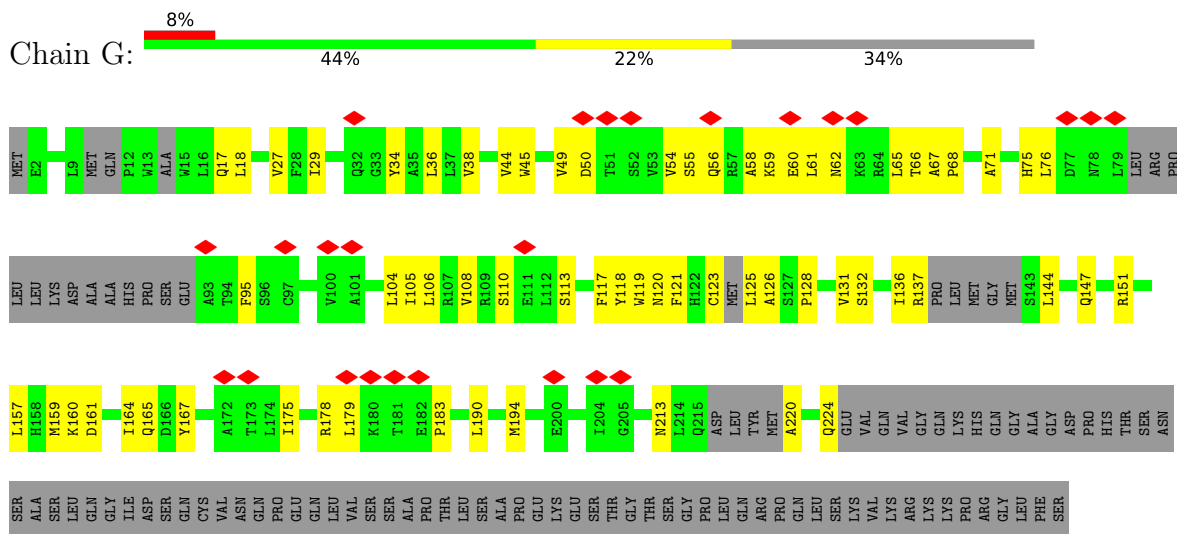




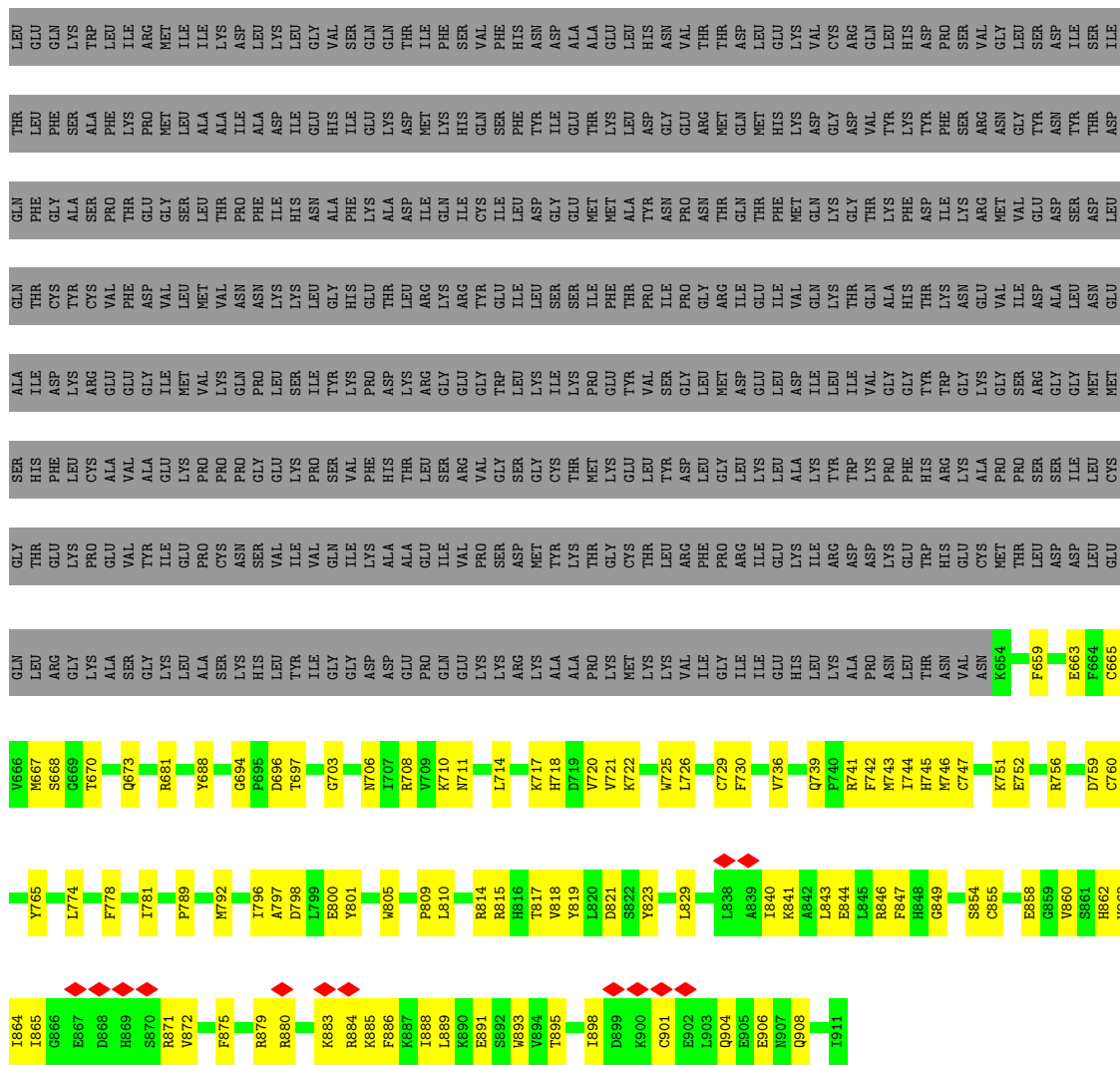
- Molecule 4: Non-homologous end-joining factor 1



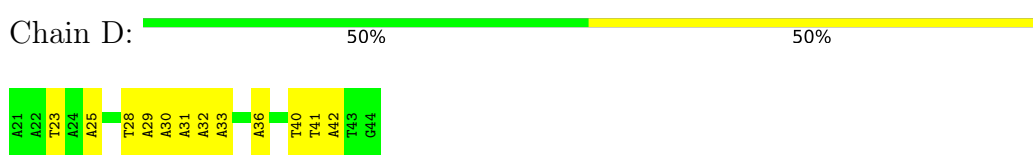
- Molecule 4: Non-homologous end-joining factor 1



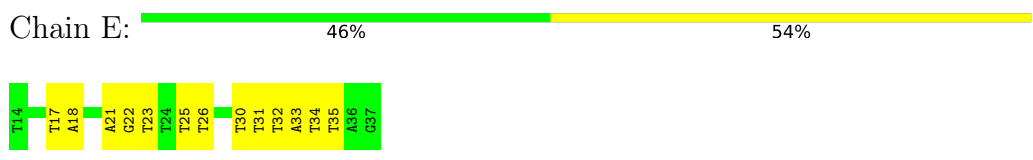




• Molecule 7: DNA (5'-D(P\*AP\*AP\*TP\*AP\*AP\*AP\*CP\*TP\*AP\*AP\*AP\*AP\*AP\*CP\*TP\*A P\*TP\*TP\*AP\*TP\*TP\*AP\*TP\*G)-3')



• Molecule 8: DNA (5'-D(P\*TP\*AP\*AP\*TP\*AP\*AP\*TP\*AP\*GP\*TP\*TP\*TP\*TP\*TP\*AP\*G P\*TP\*TP\*TP\*AP\*TP\*TP\*AP\*G)-3')



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	45943	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 ( $e^-/\text{\AA}^2$ )	46.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.753	Depositor
Minimum map value	-0.224	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.175	Depositor
Map size (Å)	704.16003, 704.16003, 704.16003	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.304, 1.304, 1.304	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	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.25	0/28219	0.46	1/38230 (0.0%)
2	B	0.25	0/3740	0.48	0/5053
3	C	0.25	0/4075	0.47	0/5509
4	F	0.24	0/1488	0.48	0/2015
4	G	0.24	0/1522	0.51	0/2064
5	H	0.24	0/1602	0.47	0/2159
5	I	0.24	0/1546	0.47	0/2082
6	J	0.24	0/2073	0.46	0/2807
7	D	0.43	0/554	0.88	0/852
8	E	0.56	0/552	1.09	0/851
All	All	0.26	0/45371	0.49	1/61622 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2277	LEU	CA-CB-CG	5.12	127.07	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	27806	0	27233	715	0
2	B	3673	0	3652	124	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	3999	0	3899	136	0
4	F	1465	0	1432	47	0
4	G	1502	0	1439	61	0
5	H	1575	0	1514	57	0
5	I	1521	0	1440	46	0
6	J	2026	0	1895	72	0
7	D	493	0	273	11	0
8	E	494	0	278	15	0
All	All	44554	0	43055	1205	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 14.

The worst 5 of 1205 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)
1:A:3365:SER:HB3	1:A:3376:GLY:HA3	1.61	0.82
2:B:337:LEU:HD11	3:C:490:LEU:HA	1.67	0.77
4:G:128:PRO:O	4:G:132:SER:HB2	1.85	0.77
6:J:814:ARG:HD2	6:J:849:GLY:H	1.50	0.77
4:G:132:SER:HB3	4:G:137:ARG:HH21	1.51	0.76

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	3483/4156 (84%)	3321 (95%)	160 (5%)	2 (0%)	51	85
2	B	465/609 (76%)	440 (95%)	25 (5%)	0	100	100
3	C	503/732 (69%)	479 (95%)	23 (5%)	1 (0%)	47	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	F	174/299 (58%)	159 (91%)	15 (9%)	0	100	100
4	G	183/299 (61%)	164 (90%)	19 (10%)	0	100	100
5	H	199/336 (59%)	192 (96%)	7 (4%)	0	100	100
5	I	189/336 (56%)	178 (94%)	11 (6%)	0	100	100
6	J	256/911 (28%)	237 (93%)	19 (7%)	0	100	100
All	All	5452/7678 (71%)	5170 (95%)	279 (5%)	3 (0%)	54	85

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	MET
1	A	3563	ASP
3	C	229	GLU

### 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	2961/3671 (81%)	2942 (99%)	19 (1%)	86	92
2	B	392/548 (72%)	391 (100%)	1 (0%)	92	95
3	C	428/649 (66%)	423 (99%)	5 (1%)	71	84
4	F	157/262 (60%)	156 (99%)	1 (1%)	86	92
4	G	159/262 (61%)	159 (100%)	0	100	100
5	H	166/303 (55%)	166 (100%)	0	100	100
5	I	161/303 (53%)	161 (100%)	0	100	100
6	J	212/808 (26%)	212 (100%)	0	100	100
All	All	4636/6806 (68%)	4610 (99%)	26 (1%)	86	92

5 of 26 residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	3845	LYS
1	A	3860	LYS
3	C	271	ARG
1	A	3858	MET
1	A	4041	ARG

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

Mol	Chain	Res	Type
5	I	137	ASN
5	H	141	ASN
2	B	360	HIS
5	H	137	ASN
1	A	3863	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	4128:MET	C	5009:UNK	N	97.03
1	A	5016:UNK	C	6004:UNK	N	48.85

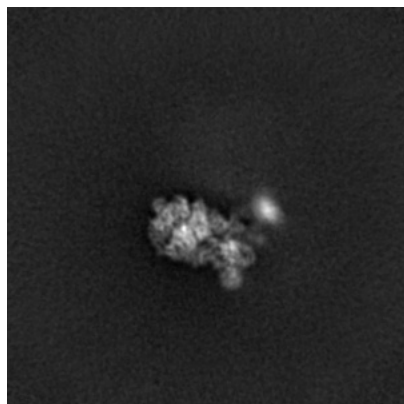
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12301. These allow visual inspection of the internal detail of the map and identification of artifacts.

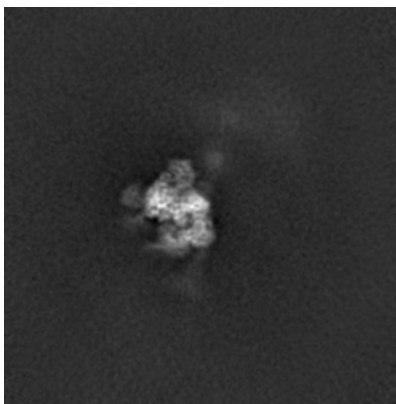
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

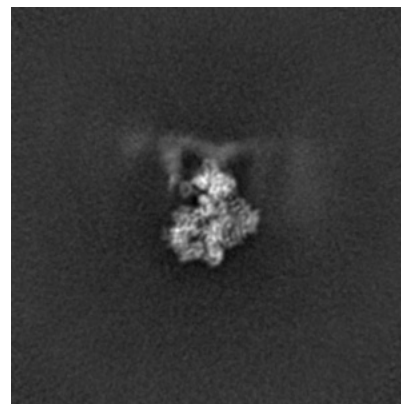
#### 6.1.1 Primary map



X

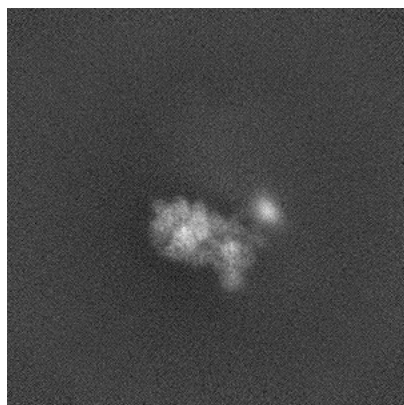


Y



Z

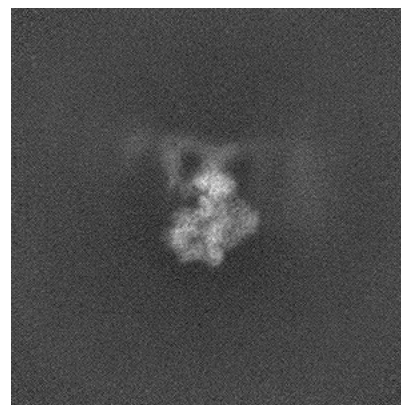
#### 6.1.2 Raw map



X



Y

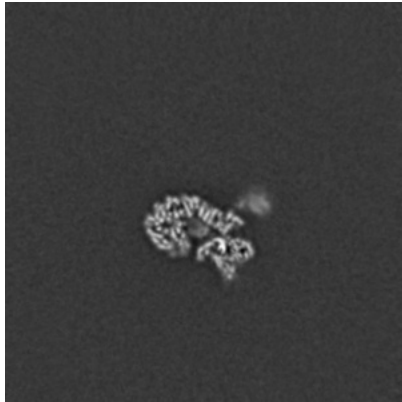


Z

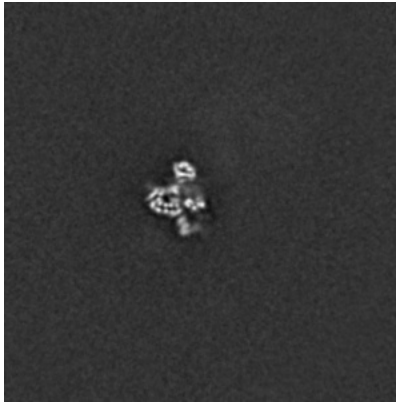
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

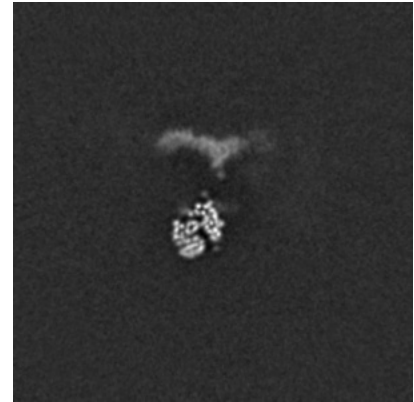
### 6.2.1 Primary map



X Index: 270

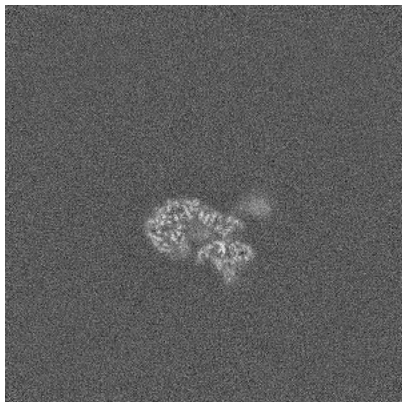


Y Index: 270

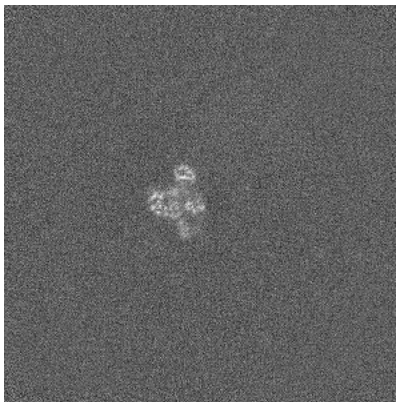


Z Index: 270

### 6.2.2 Raw map



X Index: 270



Y Index: 270

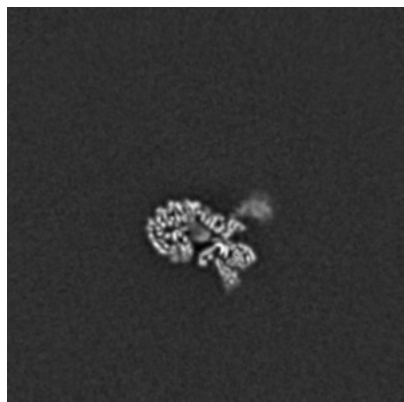


Z Index: 270

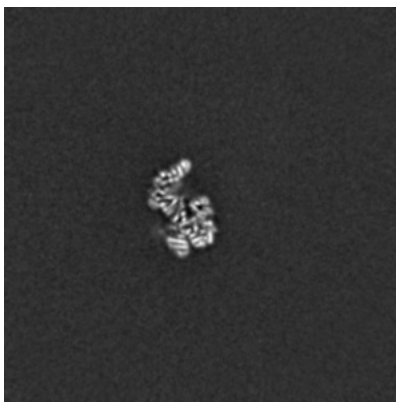
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

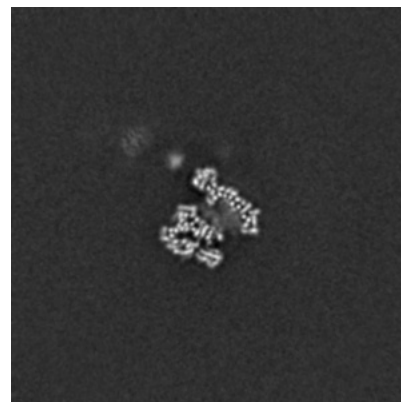
### 6.3.1 Primary map



X Index: 272

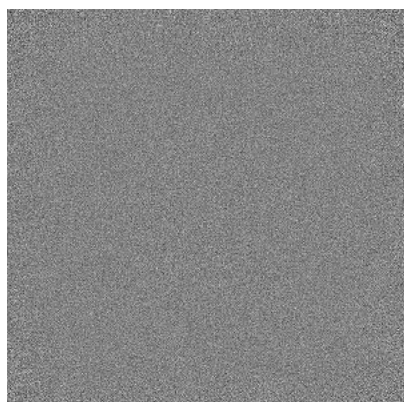


Y Index: 238

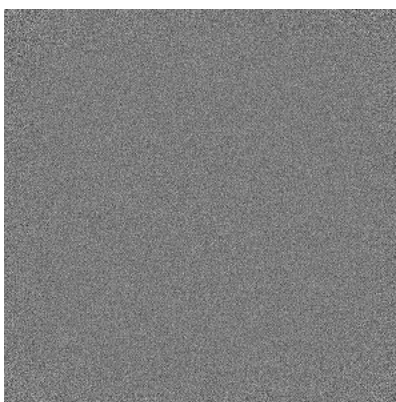


Z Index: 241

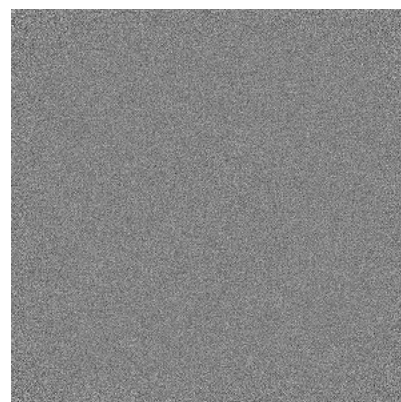
### 6.3.2 Raw map



X Index: 0



Y Index: 0



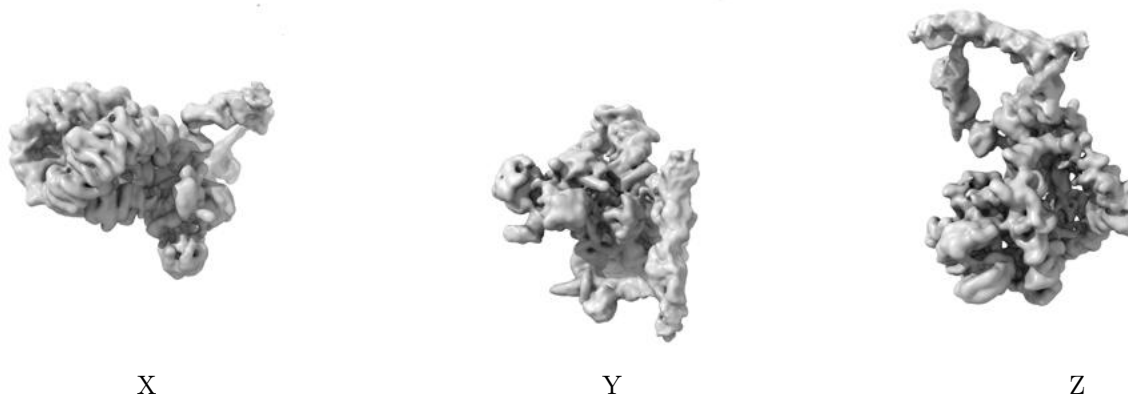
Z Index: 0

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



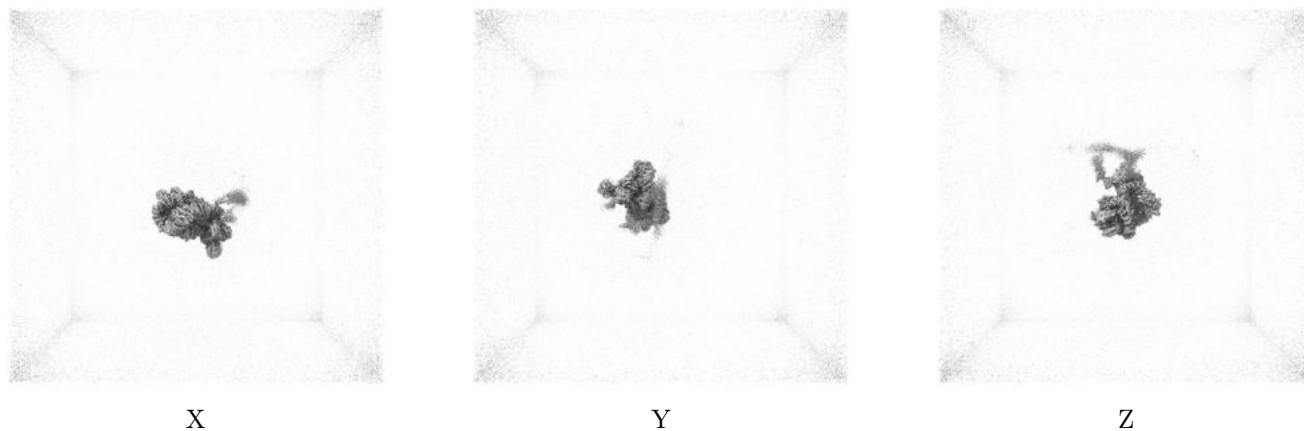
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.175. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



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.

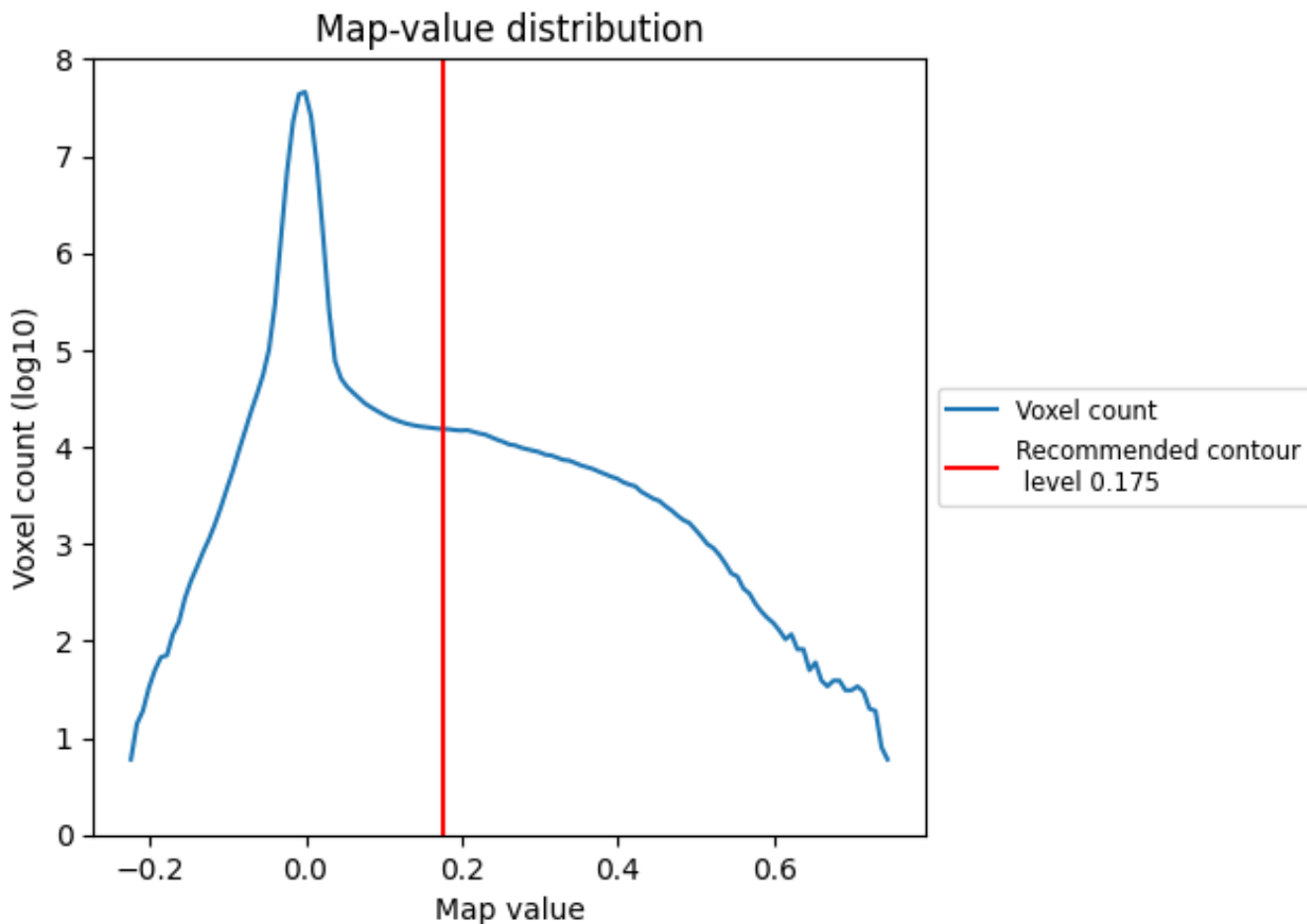
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

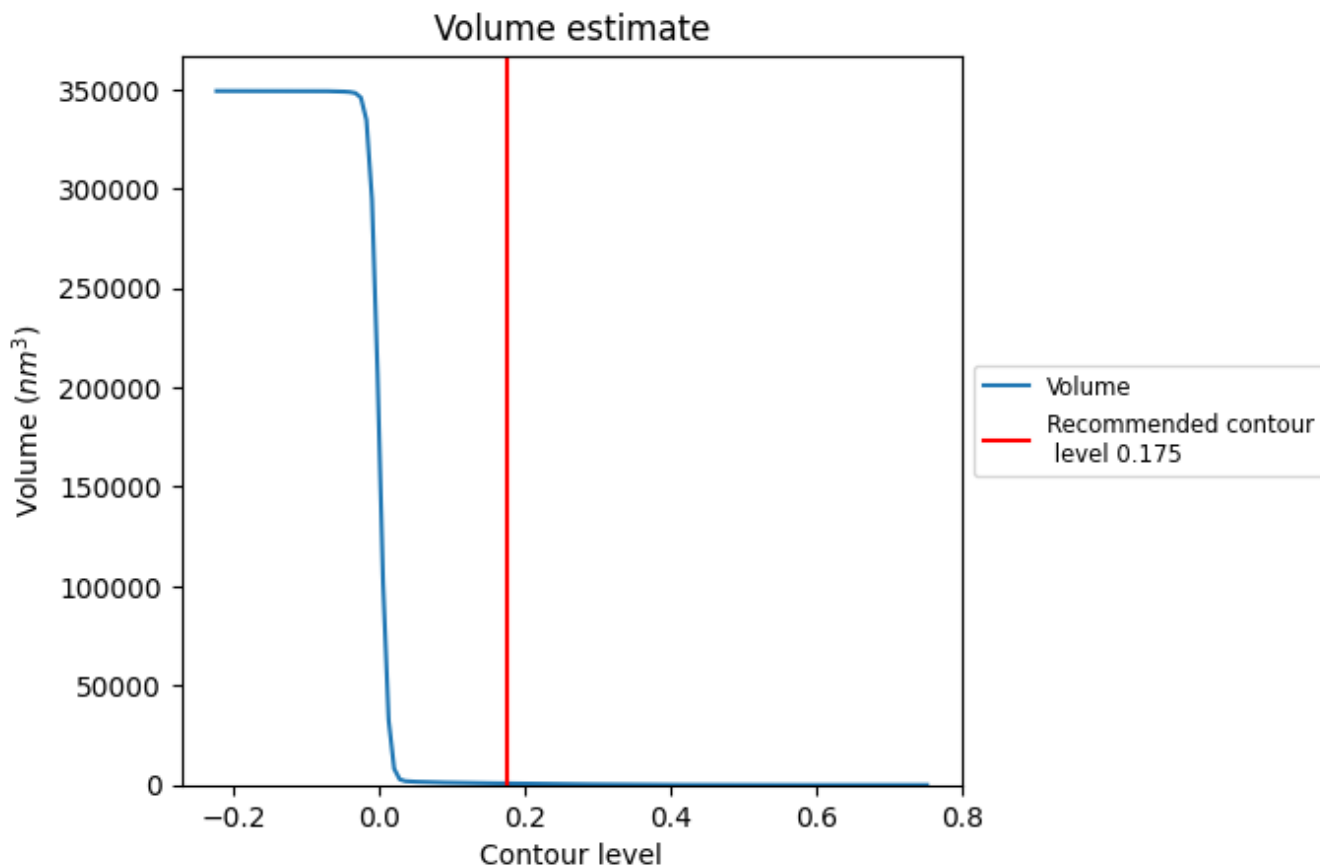
This section contains the results of statistical analysis of the map.

### 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 [\(i\)](#)

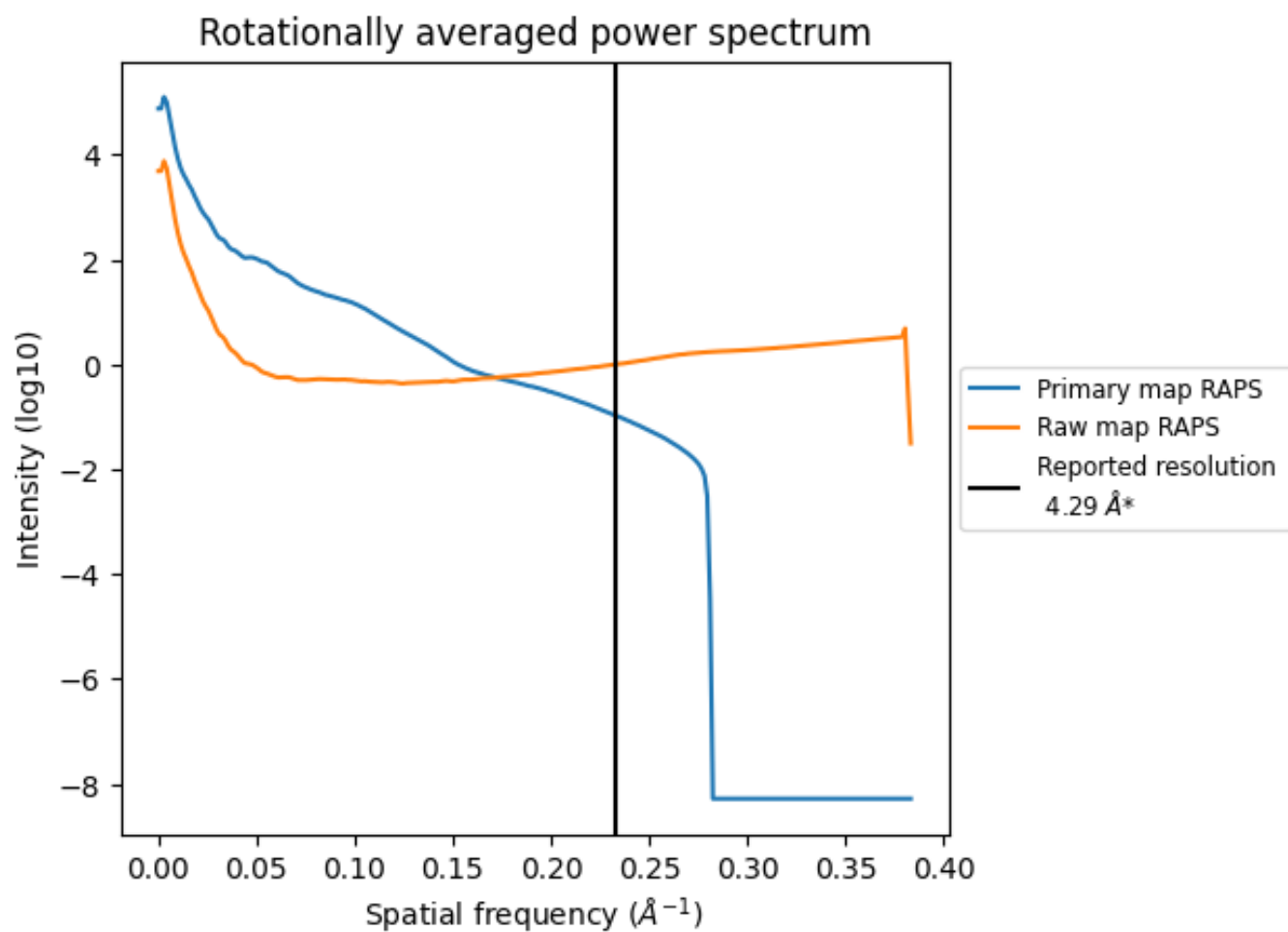


The volume at the recommended contour level is 758 nm<sup>3</sup>; this corresponds to an approximate mass of 685 kDa.

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](#)

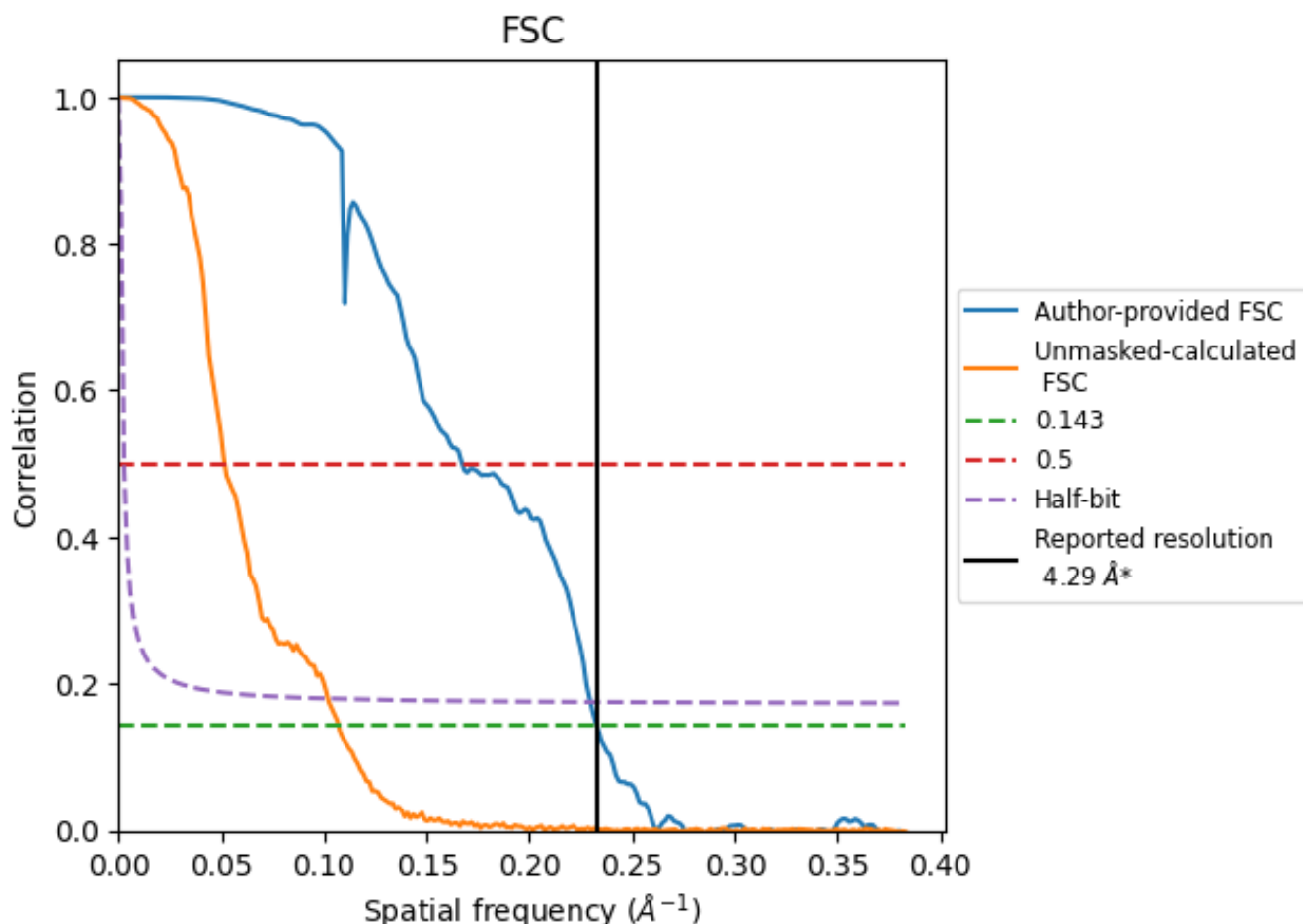


\*Reported resolution corresponds to spatial frequency of 0.233 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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 [i](#)



\*Reported resolution corresponds to spatial frequency of 0.233 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

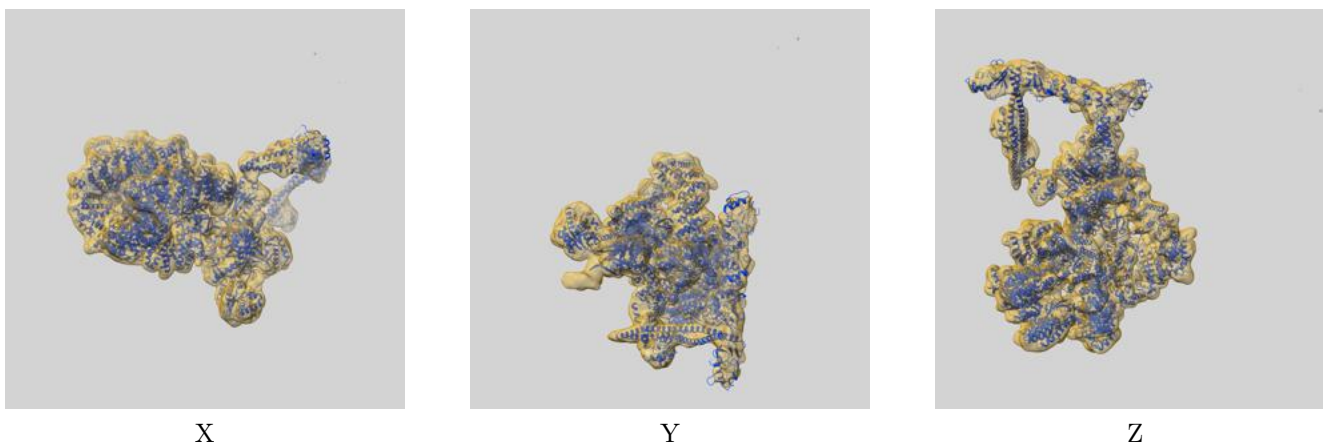
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.29	-	-
Author-provided FSC curve	4.29	5.98	4.35
Unmasked-calculated*	9.34	19.38	9.81

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.34 differs from the reported value 4.29 by more than 10 %

## 9 Map-model fit [i](#)

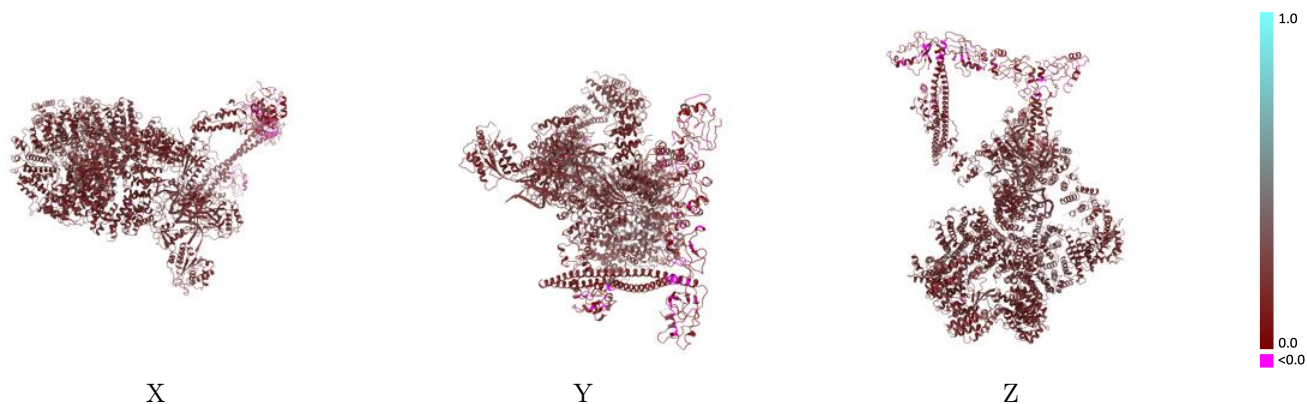
This section contains information regarding the fit between EMDB map EMD-12301 and PDB model 7NFE. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlay [i](#)



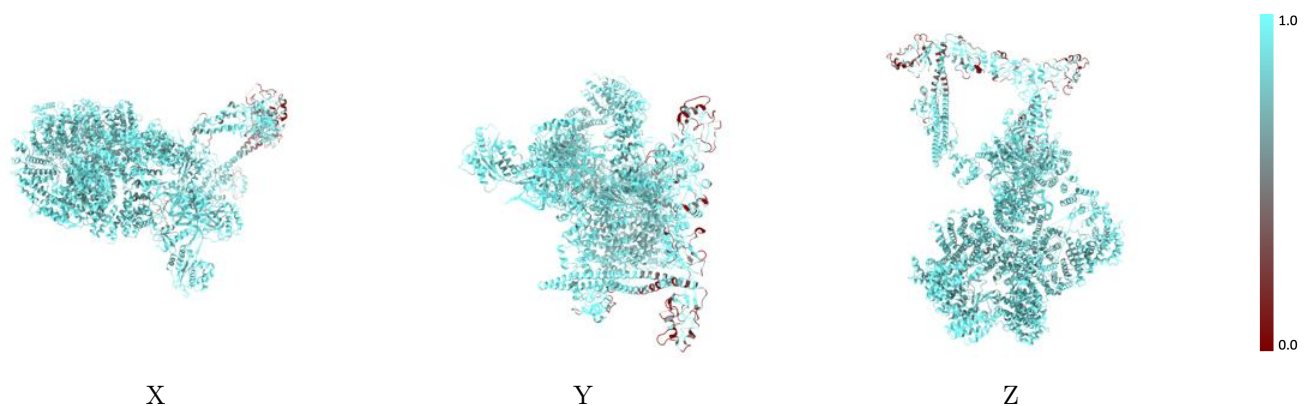
The images above show the 3D surface view of the map at the recommended contour level 0.175 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



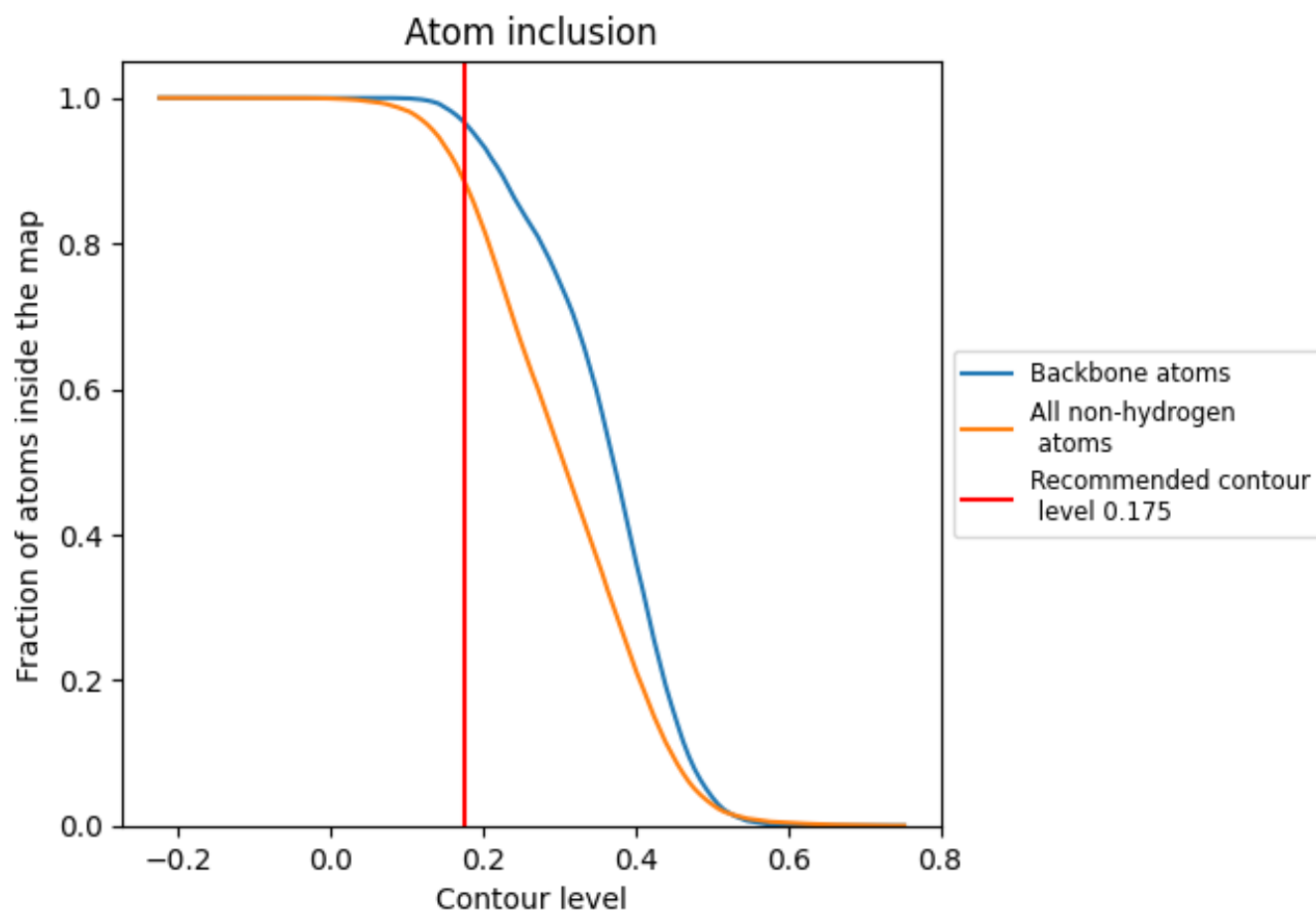
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.175).























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 89% 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 (0.175) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8867	 0.2030
A	 0.9114	 0.2140
B	 0.9100	 0.2270
C	 0.9208	 0.2180
D	 0.9817	 0.2580
E	 0.9919	 0.2600
F	 0.6519	 0.1300
G	 0.8050	 0.1390
H	 0.7621	 0.1350
I	 0.6487	 0.1360
J	 0.8949	 0.1560

