Full wwPDB EM Validation Report ⓘ

Sep 6, 2026 – 04:48 PM EDT

PDB ID	:	9PN0 / pdb_00009pn0
EMDB ID	:	EMD-71744
Title	:	Structure of HTTQ23-HAP40 complex bound to macrocycles HHD3, HD4 and HL2
Authors	:	Balakrishnan, S.; Deme, J.; Lea, S.M.; Harding, R.J.
Deposited on	:	2025-07-18
Resolution	:	2.30 Å(reported)
Based on initial model	:	6X90

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 ⓘ 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:

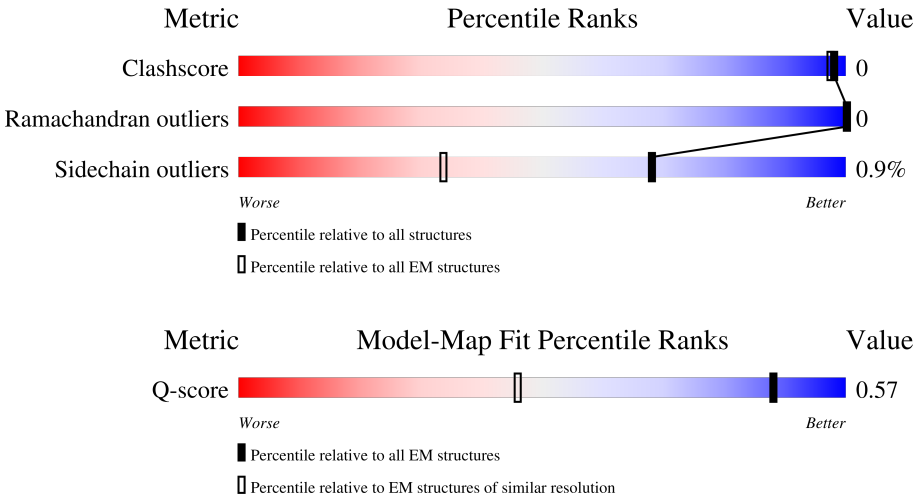
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 2.30 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4254 (1.80 - 2.80)

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	D	19	11% 95% 5%
2	C	19	58% 53% 42% 5%
3	E	17	18% 76% 18% 6%
4	A	3156	70% 27%

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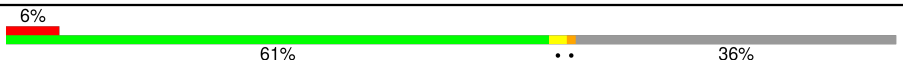
Mol	Chain	Length	Quality of chain
5	B	389	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 41230 atoms, of which 20828 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 HD4.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	D	19	Total	C	H	N	O	S	0	1
			281	91	139	22	27	2		

- Molecule 2 is a protein called HHD3.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	19	Total	C	H	N	O	S	0	1
			322	117	147	31	26	1		

- Molecule 3 is a protein called HL2.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	17	Total	C	H	N	O	S	0	1
			260	85	130	22	22	1		

- Molecule 4 is a protein called Huntingtin.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	A	2296	Total	C	H	N	O	S	0	0
			36566	11594	18495	3096	3263	118		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	GLN	-	insertion	UNP P42858
A	40	GLN	-	insertion	UNP P42858
A	2311	HIS	TYR	conflict	UNP P42858
A	2788	ILE	VAL	conflict	UNP P42858
A	3145	GLY	-	expression tag	UNP P42858
A	3146	GLY	-	expression tag	UNP P42858
A	3147	SER	-	expression tag	UNP P42858
A	3148	GLY	-	expression tag	UNP P42858
A	3149	ASP	-	expression tag	UNP P42858

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Chain	Residue	Modelled	Actual	Comment	Reference
A	3150	TYR	-	expression tag	UNP P42858
A	3151	LYS	-	expression tag	UNP P42858
A	3152	ASP	-	expression tag	UNP P42858
A	3153	ASP	-	expression tag	UNP P42858
A	3154	ASP	-	expression tag	UNP P42858
A	3155	ASP	-	expression tag	UNP P42858
A	3156	LYS	-	expression tag	UNP P42858

- Molecule 5 is a protein called 40-kDa huntingtin-associated protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	B	250	Total	C	H	N	O	S	0	0
			3801	1194	1917	335	348	7		

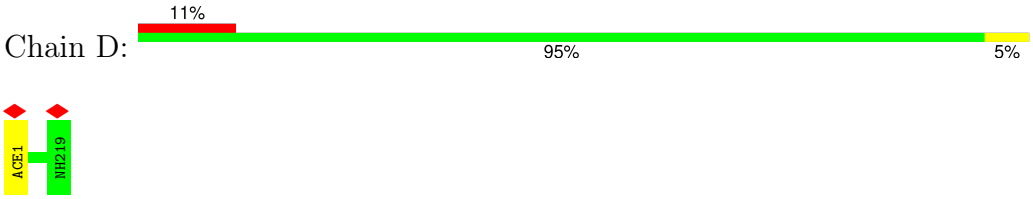
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	MET	-	expression tag	UNP P23610
B	-16	HIS	-	expression tag	UNP P23610
B	-15	HIS	-	expression tag	UNP P23610
B	-14	HIS	-	expression tag	UNP P23610
B	-13	HIS	-	expression tag	UNP P23610
B	-12	HIS	-	expression tag	UNP P23610
B	-11	HIS	-	expression tag	UNP P23610
B	-10	SER	-	expression tag	UNP P23610
B	-9	SER	-	expression tag	UNP P23610
B	-8	GLY	-	expression tag	UNP P23610
B	-7	ARG	-	expression tag	UNP P23610
B	-6	GLU	-	expression tag	UNP P23610
B	-5	ASN	-	expression tag	UNP P23610
B	-4	LEU	-	expression tag	UNP P23610
B	-3	TYR	-	expression tag	UNP P23610
B	-2	PHE	-	expression tag	UNP P23610
B	-1	GLN	-	expression tag	UNP P23610
B	0	GLY	-	expression tag	UNP P23610

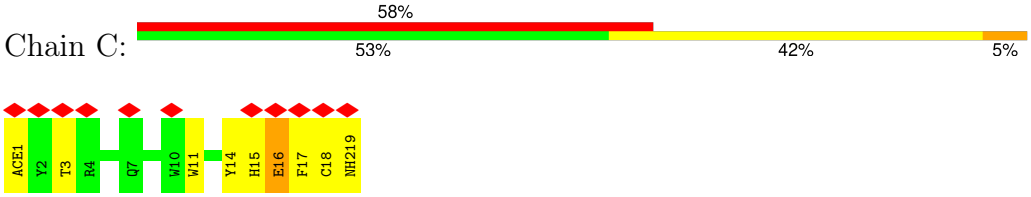
3 Residue-property plots (i)

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.

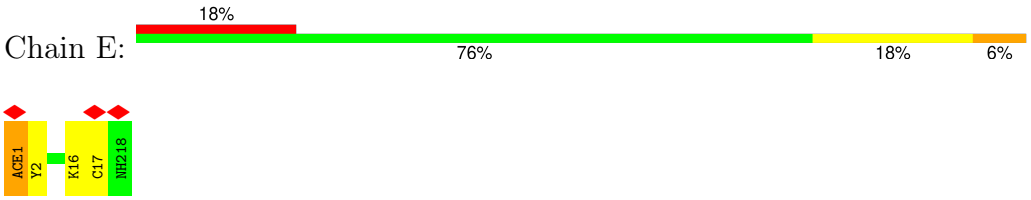
• Molecule 1: HD4



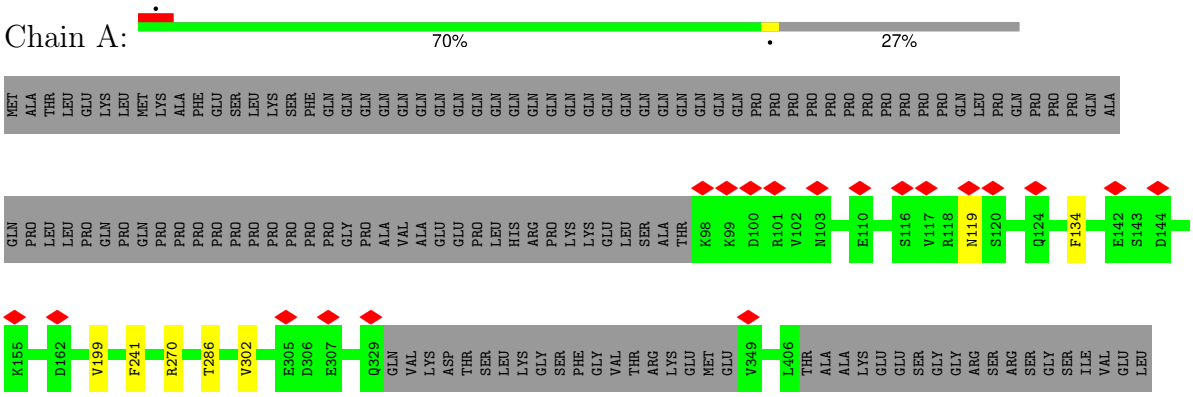
• Molecule 2: HHD3

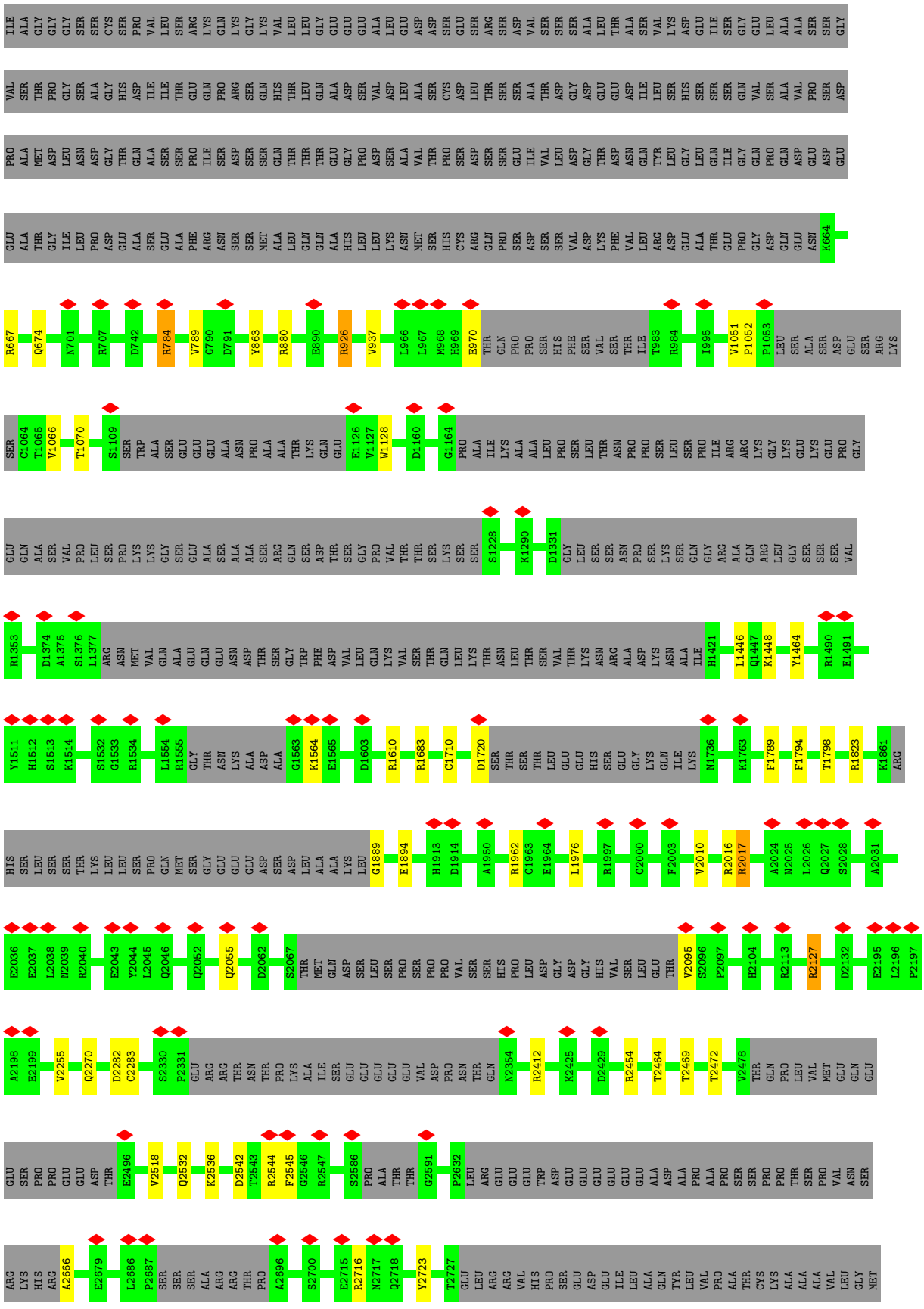


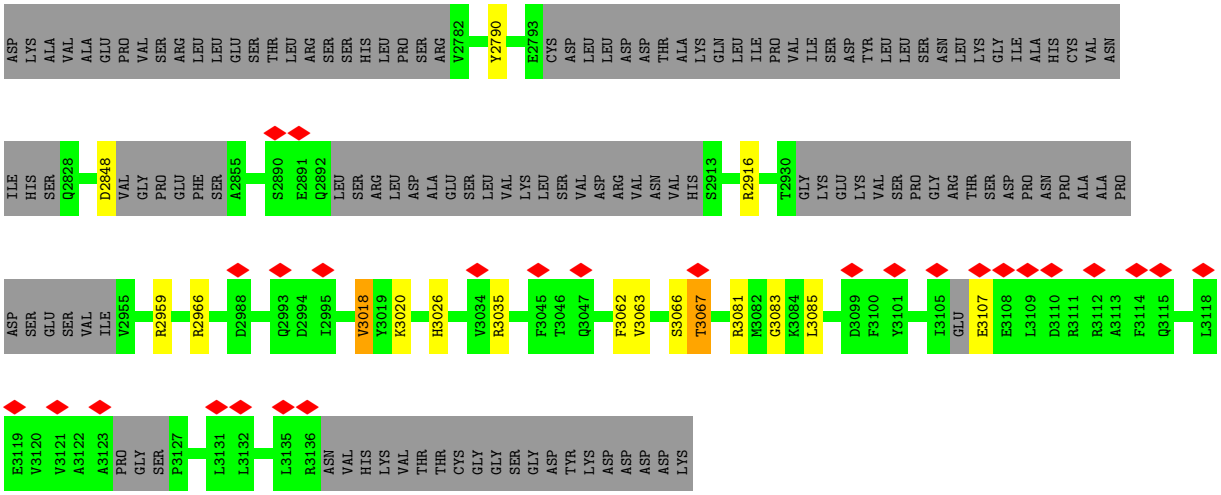
• Molecule 3: HL2



• Molecule 4: Huntingtin



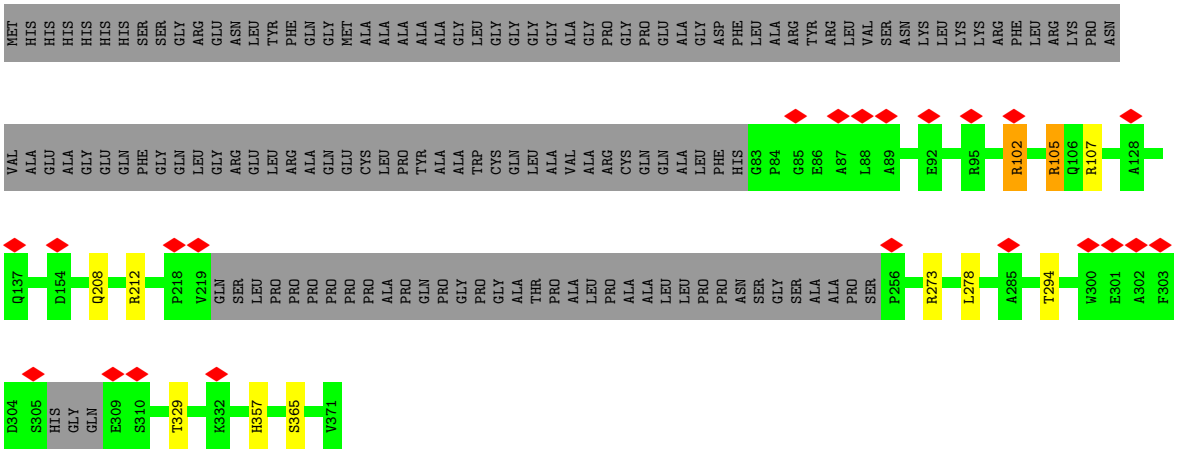

ILE ALA GLY GLY GLY SER SER CYS SER PRO VAL LEU SER ARG LYS GLN LYS GLY LYS VAL LEU LEU GLY GLU GLU GLU ALA LEU GLU ASP ASP SER GLU SER ARG SER ASP VAL SER SER SER ALA LEU THR ALA SER VAL LYS ASP GLU ILE SER GLY GLU LEU ALA ALA SER SER GLY
VAL SER THR PRO GLY SER ALA GLY HIS ASP ILE ILE THR GLU GLN PRO ARG SER GLN HIS THR LEU GLN ALA ASP SER VAL ASP LEU ALA SER CYS ASP LEU THR SER SER ALA THR ASP GLY ASP GLU GLU ASP ILE LEU SER HIS SER SER SER GLN VAL SER ALA VAL PRO SER ASP
PRO ALA MET ASP LEU ASN ASP GLY THR GLN ALA SER SER PRO ILE SER ASP SER SER GLN THR THR THR GLU GLY PRO ASP SER ALA VAL THR PRO SER ASP SER SER GLU ILE VAL LEU ASP GLY THR ASP ASN GLN TYR LEU GLY LEU GLN ILE GLY GLN PRO GLN ASP GLU ASP GLU
GLU ALA THR GLY ILE LEU PRO ASP GLU ALA SER GLU ALA PHE ARG ASN SER SER MET ALA LEU GLN GLN ALA HIS LEU LEU LYS ASN MET SER HIS CYS ARG GLN PRO SER ASP SER SER VAL ASP LYS PHE VAL LEU ARG ASP GLU ALA THR GLU PRO GLY ASP GLN GLU ASN K664
R667 Q674 N701 R707 D742 R784 V789 G790 D791 Y863 R880 E890 R926 V937 L966 L967 M968 H969 E970 THR GLN PRO PRO SER HIS PHE SER VAL SER THR ILE T983 R984 I995 V1051 P1052 P1053 LEU SER ALA SER ASP GLU SER ARG LYS
SER C1064 T1065 V1066 T1070 S1109 SER TRP ALA SER GLU GLU GLU ALA ASN PRO ALA ALA THR LYS GLN GLU E1126 V1127 W1128 D1160 G1164 PRO ALA ILE LYS ALA ALA LEU PRO SER LEU THR ASN PRO PRO SER LEU SER PRO ILE ARG ARG LYS GLY LYS GLU LYS GLU PRO GLY
GLU GLN ALA SER VAL PRO LEU SER PRO LYS LYS GLY SER GLU ALA SER ALA ALA SER ARG GLN SER ASP THR SER GLY PRO VAL THR THR SER LYS SER SER S1228 K1290 D1331 GLY LEU SER SER ASN PRO SER LYS SER GLN GLY ARG ALA GLN ARG LEU GLY SER SER SER VAL
R1353 D1374 A1375 S1376 L1377 ARG ASN MET VAL GLN ALA GLU GLN GLU ASN ASP THR SER GLY TRP PHE ASP VAL LEU GLN LYS VAL SER THR GLN LEU LYS THR ASN LEU THR SER VAL THR LYS ASN ARG ALA ASP LYS ASN ALA ILE H1421 L1446 Q1447 K1448 Y1464 R1490 E1491
Y1511 H1512 S1513 K1514 S1532 G1533 R1534 L1554 R1555 GLY THR ASN LYS ALA ASP ALA G1563 K1564 E1565 D1603 R1610 R1683 C1710 D1720 SER THR SER THR LEU GLU GLU HIS SER GLU GLY LYS GLN ILE LYS N1736 K1763 F1789 F1794 T1798 R1823 K1861 ARG
HIS SER LEU SER SER THR LYS LEU LEU SER PRO GLN MET SER GLY GLU GLU GLU ASP SER ASP LEU ALA ALA LYS LEU G1889 E1894 H1913 D1914 A1950 R1962 C1963 E1964 L1976 R1997 C2000 F2003 V2010 R2016 R2017 A2024 N2025 L2026 Q2027 S2028 A2031
E2036 E2037 L2038 N2039 R2040 E2043 Y2044 L2045 Q2046 Q2052 Q2055 D2062 S2067 THR MET GLN ASP SER LEU SER PRO SER PRO PRO VAL SER SER HIS PRO LEU ASP GLY ASP GLY HIS VAL SER LEU GLU THR V2095 S2096 P2097 H2104 R2113 R2127 D2132 E2195 L2196 P2197
A2198 E2199 V2255 Q2270 D2282 C2283 S2330 P2331 GLU ARG ARG THR ASN THR PRO LYS ALA ILE SER GLU GLU GLU GLU GLU VAL ASP PRO ASN THR GLN N2354 R2412 K2425 D2429 R2454 T2464 T2469 T2472 V2478 THR GLN PRO LEU VAL MET GLU GLN GLU
GLU SER PRO PRO GLU GLU ASP THR E2496 V2518 Q2532 K2536 D2542 T2543 R2544 F2545 G2546 R2547 S2586 PRO ALA THR THR G2591 P2632 LEU ARG GLU GLU GLU TRP ASP GLU GLU GLU GLU GLU GLU ALA ASP ALA PRO ALA PRO SER SER PRO PRO THR SER PRO VAL ASN SER
ARG LYS HIS ARG A2666 E2679 L2686 P2687 SER SER SER ALA ARG ARG THR PRO A2696 S2700 E2715 R2716 N2717 Q2718 Y2723 T2727 GLU LEU ARG ARG VAL HIS PRO SER GLU ASP GLU ILE LEU ALA GLN TYR LEU VAL PRO ALA THR CYS LYS ALA ALA ALA VAL LEU GLY MET



• Molecule 5: 40-kDa huntingtin-associated protein

Chain B:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	211814	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	51.8	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	2.517	Depositor
Minimum map value	-0.155	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.111	Depositor
Map size (Å)	374.784, 374.784, 374.784	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.732, 0.732, 0.732	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DTY, NH2, ACE

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	D	0.95	0/127	1.46	0/172
2	C	1.00	0/168	1.43	0/230
3	E	1.36	1/130 (0.8%)	1.34	0/176
4	A	0.82	30/18425 (0.2%)	1.38	36/25015 (0.1%)
5	B	0.97	8/1918 (0.4%)	1.45	9/2607 (0.3%)
All	All	0.84	39/20768 (0.2%)	1.39	45/28200 (0.2%)

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	C	0	3
3	E	0	2
4	A	0	12
5	B	0	2
All	All	0	19

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2127	ARG	CZ-NH2	-13.42	1.16	1.33
5	B	273	ARG	CZ-NH1	-11.25	1.17	1.32
5	B	273	ARG	CZ-NH2	-11.18	1.19	1.33
4	A	2544	ARG	CZ-NH1	-11.12	1.17	1.32
5	B	107	ARG	CZ-NH2	-10.96	1.19	1.33
4	A	3020	LYS	CE-NZ	-10.43	1.18	1.49
4	A	2544	ARG	CZ-NH2	-10.13	1.20	1.33
5	B	107	ARG	NE-CZ	-9.88	1.22	1.33
4	A	2127	ARG	CD-NE	-9.40	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2666	ALA	N-CA	-8.47	1.30	1.46
3	E	1	ACE	C-N	8.39	1.50	1.33
4	A	2127	ARG	NE-CZ	-8.21	1.24	1.33
4	A	3067	THR	CB-OG1	-7.52	1.31	1.43
4	A	926	ARG	CZ-NH1	-7.34	1.22	1.32
4	A	1889	GLY	N-CA	-6.62	1.34	1.45
4	A	1610	ARG	CZ-NH1	-6.59	1.23	1.32
4	A	270	ARG	CZ-NH1	-6.54	1.23	1.32
4	A	2464	THR	CB-OG1	-6.50	1.33	1.43
4	A	2723	TYR	C-O	-6.35	1.16	1.24
4	A	1070	THR	CB-OG1	-6.27	1.33	1.43
4	A	784	ARG	CZ-NH1	-6.18	1.24	1.32
5	B	212	ARG	CZ-NH2	-6.15	1.25	1.33
4	A	1683	ARG	NE-CZ	-6.07	1.26	1.33
4	A	2127	ARG	CZ-NH1	-5.92	1.24	1.32
4	A	2095	VAL	N-CA	-5.85	1.35	1.46
4	A	270	ARG	NE-CZ	-5.64	1.26	1.33
4	A	286	THR	CB-OG1	-5.58	1.34	1.43
4	A	784	ARG	CZ-NH2	-5.55	1.26	1.33
4	A	880	ARG	CZ-NH2	-5.47	1.26	1.33
5	B	102	ARG	CD-NE	-5.45	1.38	1.46
4	A	1683	ARG	CZ-NH1	-5.40	1.25	1.32
4	A	1710	CYS	CB-SG	-5.27	1.63	1.81
5	B	294	THR	CB-OG1	-5.22	1.35	1.43
4	A	926	ARG	CZ-NH2	-5.14	1.26	1.33
4	A	270	ARG	CZ-NH2	-5.10	1.26	1.33
4	A	3066	SER	C-N	-5.09	1.27	1.33
4	A	2016	ARG	CZ-NH1	-5.08	1.25	1.32
4	A	2545	PHE	C-O	-5.04	1.17	1.24
5	B	212	ARG	CZ-NH1	-5.01	1.25	1.32

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	3018	VAL	O-C-N	-20.15	94.90	122.31
4	A	3066	SER	CA-C-N	17.15	144.63	120.79
4	A	3066	SER	C-N-CA	17.15	144.63	120.79
4	A	2127	ARG	CD-NE-CZ	16.22	147.11	124.40
5	B	107	ARG	NE-CZ-NH2	15.32	132.99	119.20
4	A	3066	SER	O-C-N	-12.93	106.90	122.81
4	A	270	ARG	CD-NE-CZ	9.93	138.30	124.40
4	A	3018	VAL	CA-C-N	9.03	132.72	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	3018	VAL	C-N-CA	9.03	132.72	120.44
4	A	2544	ARG	NE-CZ-NH2	8.47	126.82	119.20
5	B	107	ARG	NE-CZ-NH1	-7.97	113.53	121.50
4	A	2127	ARG	NE-CZ-NH1	7.87	129.37	121.50
4	A	1683	ARG	CD-NE-CZ	7.75	135.25	124.40
4	A	3020	LYS	CD-CE-NZ	7.00	134.29	111.90
4	A	1610	ARG	NE-CZ-NH2	6.93	125.44	119.20
4	A	2544	ARG	NH1-CZ-NH2	-6.57	110.76	119.30
4	A	784	ARG	NE-CZ-NH2	6.23	124.81	119.20
5	B	102	ARG	CD-NE-CZ	6.15	133.01	124.40
4	A	2848	ASP	CA-CB-CG	6.15	118.75	112.60
4	A	3035	ARG	NE-CZ-NH2	6.06	124.66	119.20
4	A	1128	TRP	CB-CA-C	5.91	116.14	111.00
4	A	2282	ASP	CA-CB-CG	5.84	118.44	112.60
4	A	2127	ARG	CG-CD-NE	5.81	124.79	112.00
4	A	2542	ASP	CA-CB-CG	5.73	118.33	112.60
4	A	926	ARG	NE-CZ-NH2	5.65	124.28	119.20
4	A	880	ARG	NE-CZ-NH2	5.61	124.25	119.20
4	A	3062	PHE	CA-CB-CG	5.59	119.39	113.80
4	A	2532	GLN	OE1-CD-NE2	-5.56	117.04	122.60
5	B	365	SER	CA-C-N	5.53	125.53	119.89
5	B	365	SER	C-N-CA	5.53	125.53	119.89
4	A	3081	ARG	NE-CZ-NH2	5.47	124.12	119.20
5	B	273	ARG	NE-CZ-NH1	5.47	126.97	121.50
4	A	1962	ARG	NE-CZ-NH2	5.42	124.08	119.20
5	B	208	GLN	OE1-CD-NE2	-5.41	117.19	122.60
4	A	1823	ARG	NE-CZ-NH2	5.32	123.99	119.20
4	A	2518	VAL	N-CA-C	5.31	120.36	108.88
4	A	2916	ARG	CD-NE-CZ	5.31	131.83	124.40
4	A	1720	ASP	CA-CB-CG	5.24	117.84	112.60
4	A	937	VAL	N-CA-CB	5.23	114.02	110.52
5	B	105	ARG	NE-CZ-NH2	5.20	123.88	119.20
4	A	2016	ARG	CD-NE-CZ	5.12	131.57	124.40
4	A	134	PHE	CA-CB-CG	5.11	118.91	113.80
5	B	357	HIS	CB-CG-CD2	-5.10	124.57	131.20
4	A	2959	ARG	NE-CZ-NH2	5.07	123.76	119.20
4	A	674	GLN	OE1-CD-NE2	-5.04	117.56	122.60

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	1464	TYR	Sidechain
4	A	2017	ARG	Sidechain
4	A	2127	ARG	Sidechain
4	A	2412	ARG	Sidechain
4	A	2454	ARG	Sidechain
4	A	2716	ARG	Sidechain
4	A	2790	TYR	Sidechain
4	A	3018	VAL	Mainchain
4	A	667	ARG	Sidechain
4	A	784	ARG	Sidechain
4	A	863	TYR	Sidechain
4	A	926	ARG	Sidechain
5	B	102	ARG	Sidechain
5	B	105	ARG	Sidechain
2	C	14	TYR	Mainchain
2	C	16	GLU	Sidechain
2	C	17	PHE	Sidechain
3	E	16	LYS	Peptide,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	D	142	139	138	1	0
2	C	175	147	144	6	0
3	E	130	130	129	1	0
4	A	18071	18495	18470	15	0
5	B	1884	1917	1915	1	0
All	All	20402	20828	20796	17	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 0.

All (17) 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)
2:C:18:CYS:O	4:A:3085:LEU:O	1.54	1.23

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:18:CYS:O	4:A:3085:LEU:C	2.16	0.88
5:B:278:LEU:HD22	5:B:329:THR:HG21	1.67	0.76
2:C:18:CYS:SG	4:A:2055:GLN:OE1	2.46	0.72
2:C:19:NH2:N	4:A:3085:LEU:HB3	2.14	0.62
2:C:1:ACE:O	4:A:2055:GLN:HB2	2.00	0.61
4:A:3026:HIS:CE1	4:A:3067:THR:HA	2.50	0.46
4:A:1446:LEU:HD13	4:A:1446:LEU:C	2.41	0.45
1:D:1:ACE:H2	4:A:119:ASN:OD1	2.16	0.44
4:A:1789:PHE:HA	4:A:1798:THR:HG22	2.00	0.43
4:A:199:VAL:HG21	4:A:241:PHE:HE1	1.84	0.42
4:A:3026:HIS:NE2	4:A:3067:THR:HA	2.34	0.42
4:A:1794:PHE:O	4:A:1798:THR:HG23	2.19	0.42
3:E:1:ACE:H2	3:E:2:TYR:HB2	2.02	0.41
4:A:2255:VAL:HG22	4:A:2283:CYS:HB3	2.03	0.41
2:C:15:HIS:HB2	4:A:3083:GLY:O	2.21	0.41
4:A:1051:VAL:HB	4:A:1052:PRO:HD3	2.02	0.40

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	D	16/19 (84%)	15 (94%)	1 (6%)	0	100	100
2	C	16/19 (84%)	16 (100%)	0	0	100	100
3	E	15/17 (88%)	12 (80%)	3 (20%)	0	100	100
4	A	2246/3156 (71%)	2165 (96%)	81 (4%)	0	100	100
5	B	244/389 (63%)	233 (96%)	11 (4%)	0	100	100
All	All	2537/3600 (70%)	2441 (96%)	96 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	D	15/15 (100%)	15 (100%)	0	100 100
2	C	16/16 (100%)	13 (81%)	3 (19%)	1 1
3	E	13/13 (100%)	12 (92%)	1 (8%)	12 16
4	A	2029/2778 (73%)	2012 (99%)	17 (1%)	73 86
5	B	191/290 (66%)	191 (100%)	0	100 100
All	All	2264/3112 (73%)	2243 (99%)	21 (1%)	68 84

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	3	THR
2	C	11	TRP
2	C	16	GLU
3	E	17	CYS
4	A	302	VAL
4	A	789	VAL
4	A	970	GLU
4	A	1066	VAL
4	A	1448	LYS
4	A	1564	LYS
4	A	1894	GLU
4	A	1976	LEU
4	A	2010	VAL
4	A	2017	ARG
4	A	2270	GLN
4	A	2469	THR
4	A	2472	THR
4	A	2536	LYS
4	A	2966	ARG
4	A	3063	VAL
4	A	3107	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26)

such sidechains are listed below:

Mol	Chain	Res	Type
4	A	287	GLN
4	A	329	GLN
4	A	370	GLN
4	A	701	ASN
4	A	802	ASN
4	A	1315	GLN
4	A	1358	HIS
4	A	1447	GLN
4	A	1449	GLN
4	A	1498	ASN
4	A	1626	HIS
4	A	1663	ASN
4	A	1840	GLN
4	A	1846	ASN
4	A	1858	GLN
4	A	1924	ASN
4	A	1986	GLN
4	A	2242	HIS
4	A	2278	GLN
4	A	2373	GLN
4	A	2561	GLN
4	A	2671	HIS
4	A	2828	GLN
5	B	164	HIS
5	B	217	HIS
5	B	354	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

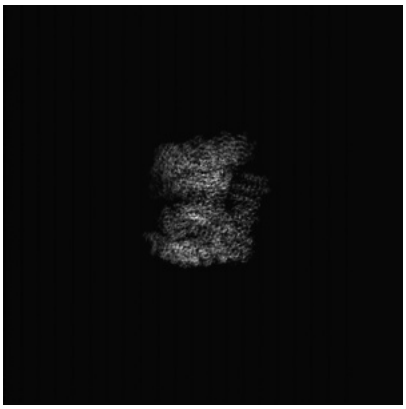
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-71744. These allow visual inspection of the internal detail of the map and identification of artifacts.

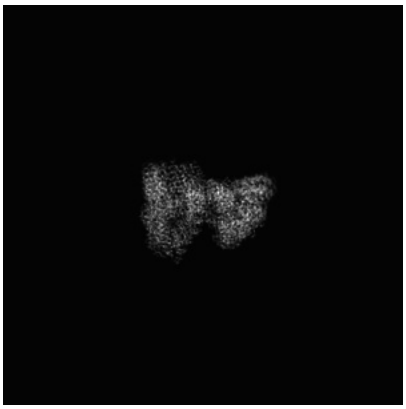
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

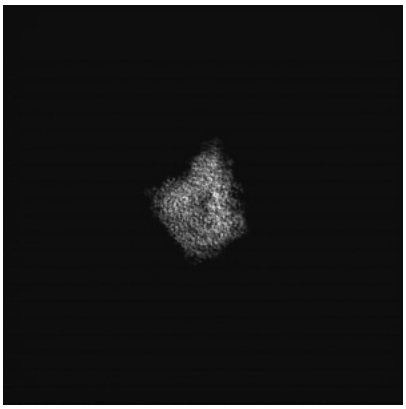
6.1.1 Primary map



X

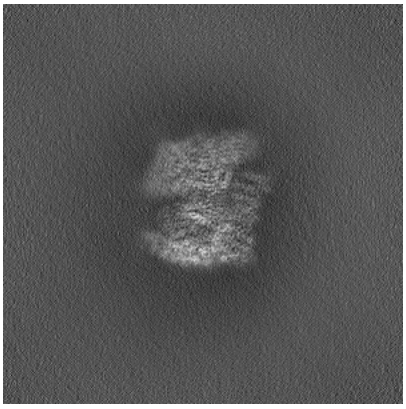


Y

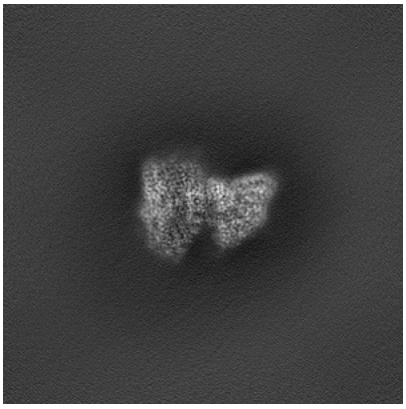


Z

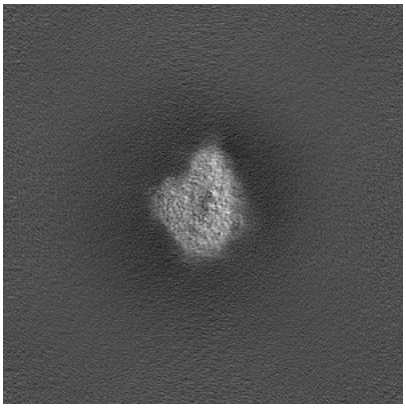
6.1.2 Raw map



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: 256

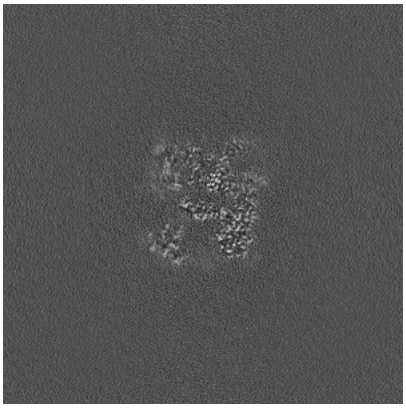


Y Index: 256

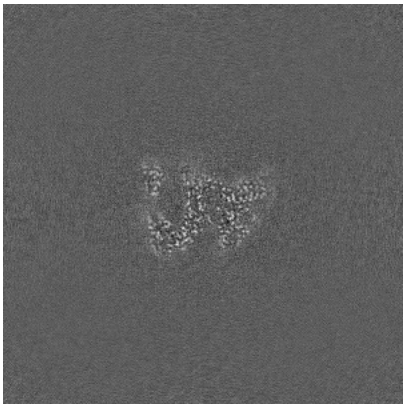


Z Index: 256

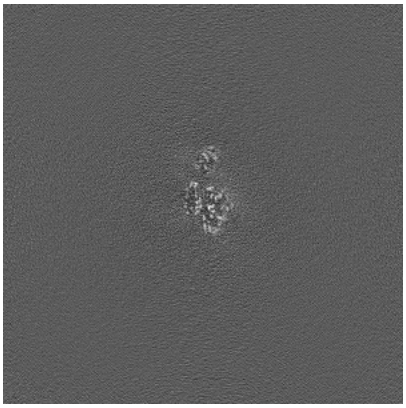
6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

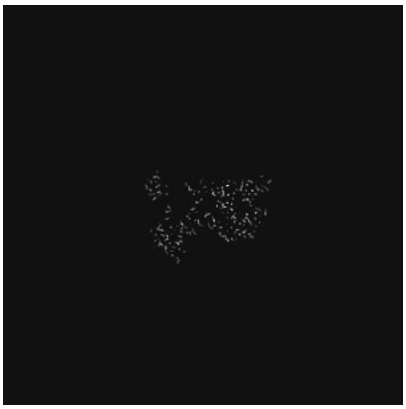
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 272

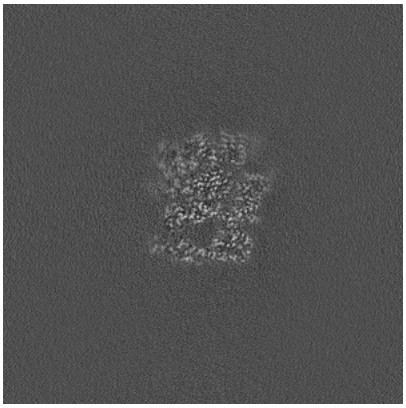


Y Index: 269

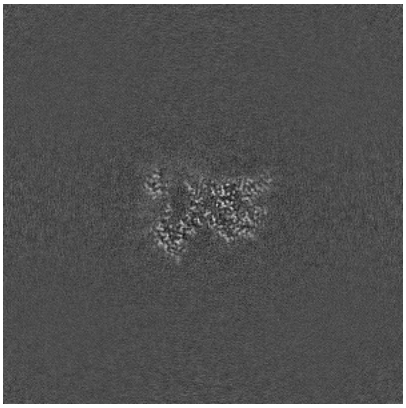


Z Index: 201

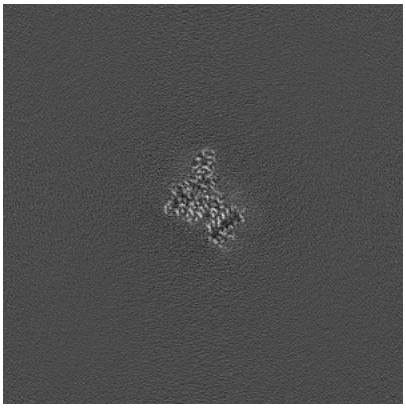
6.3.2 Raw map



X Index: 269



Y Index: 269

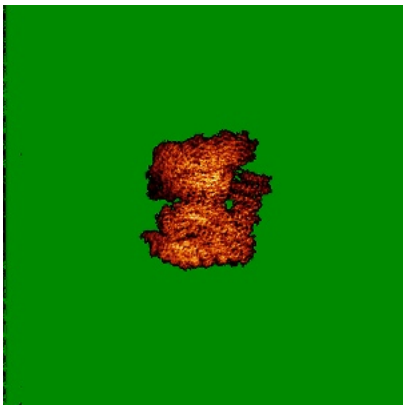


Z Index: 239

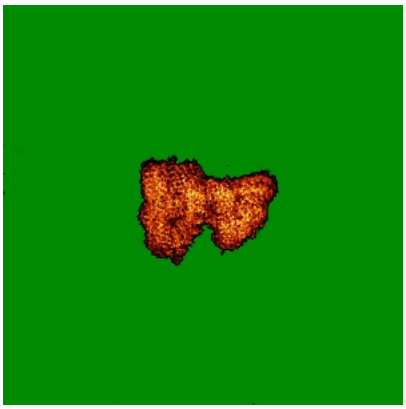
The images above show the largest variance slices of the map in three orthogonal directions.

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

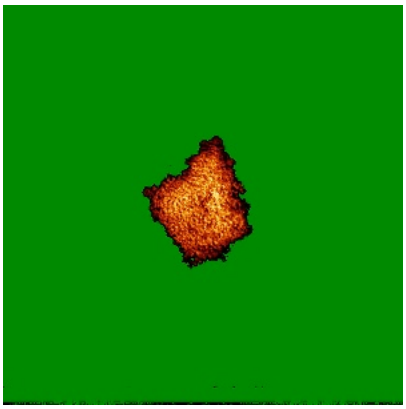
6.4.1 Primary map



X

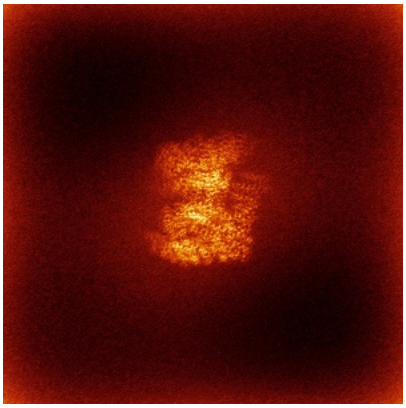


Y

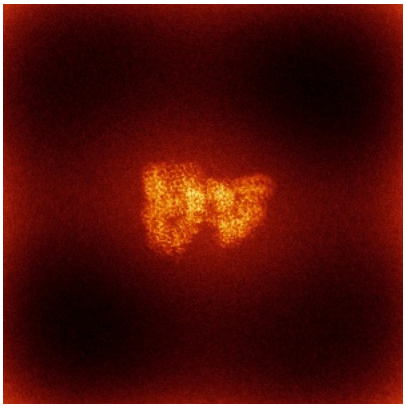


Z

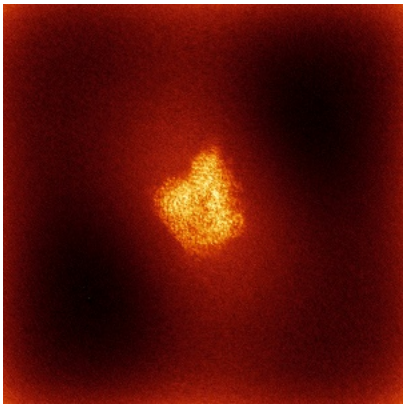
6.4.2 Raw map



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 0.111. 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.

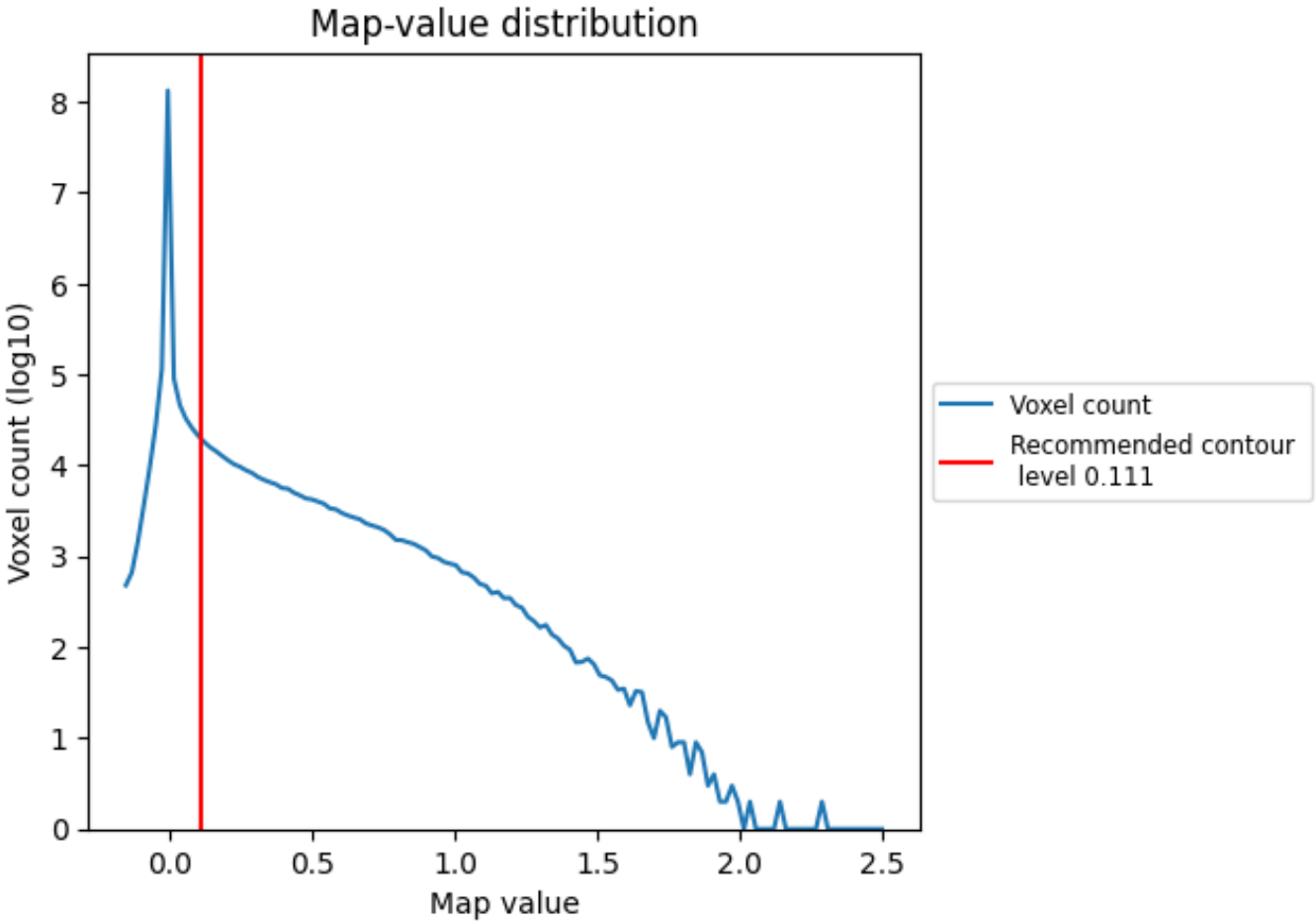
6.6 Mask visualisation (i)

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

7 Map analysis

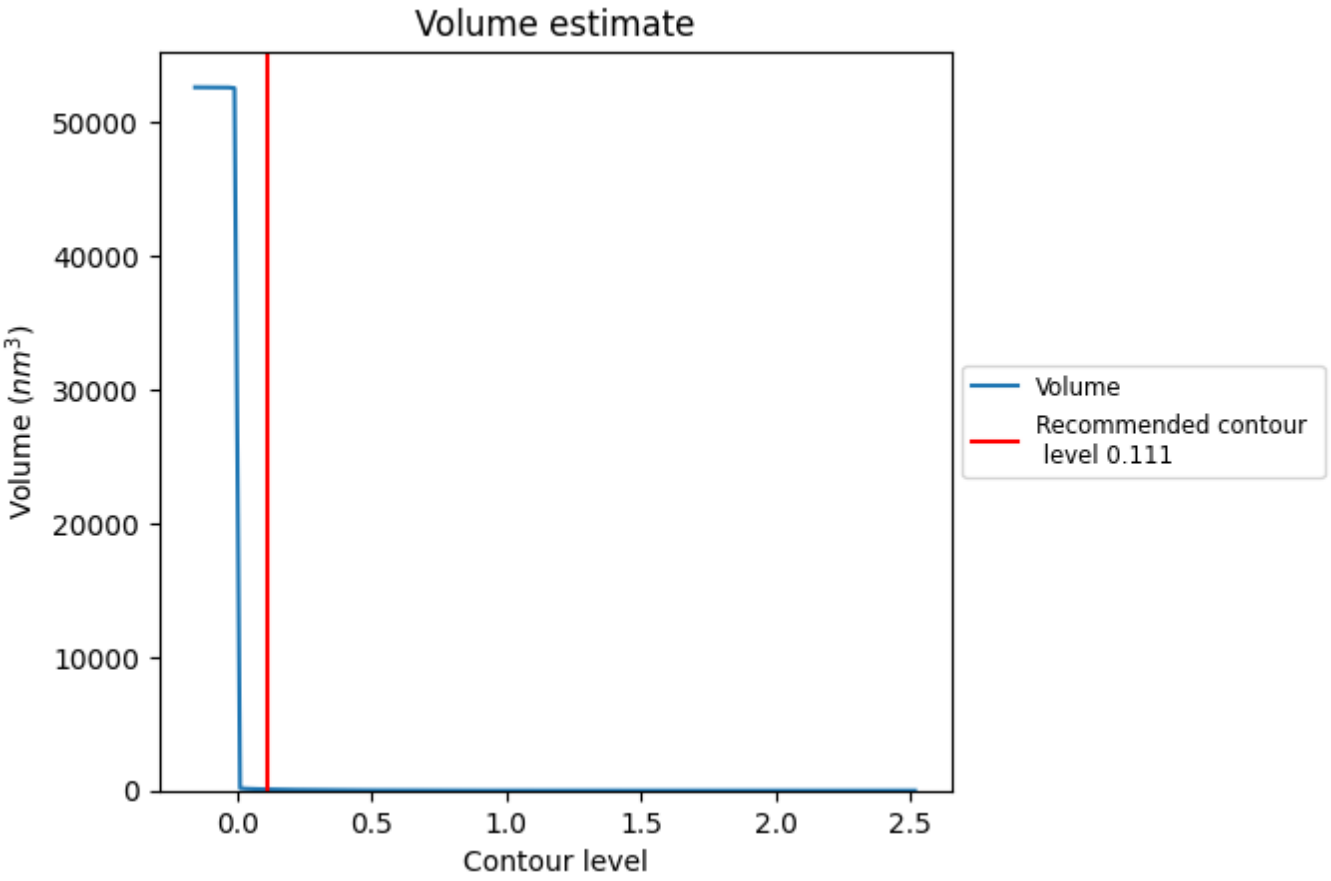
This section contains the results of statistical analysis of the map.

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.

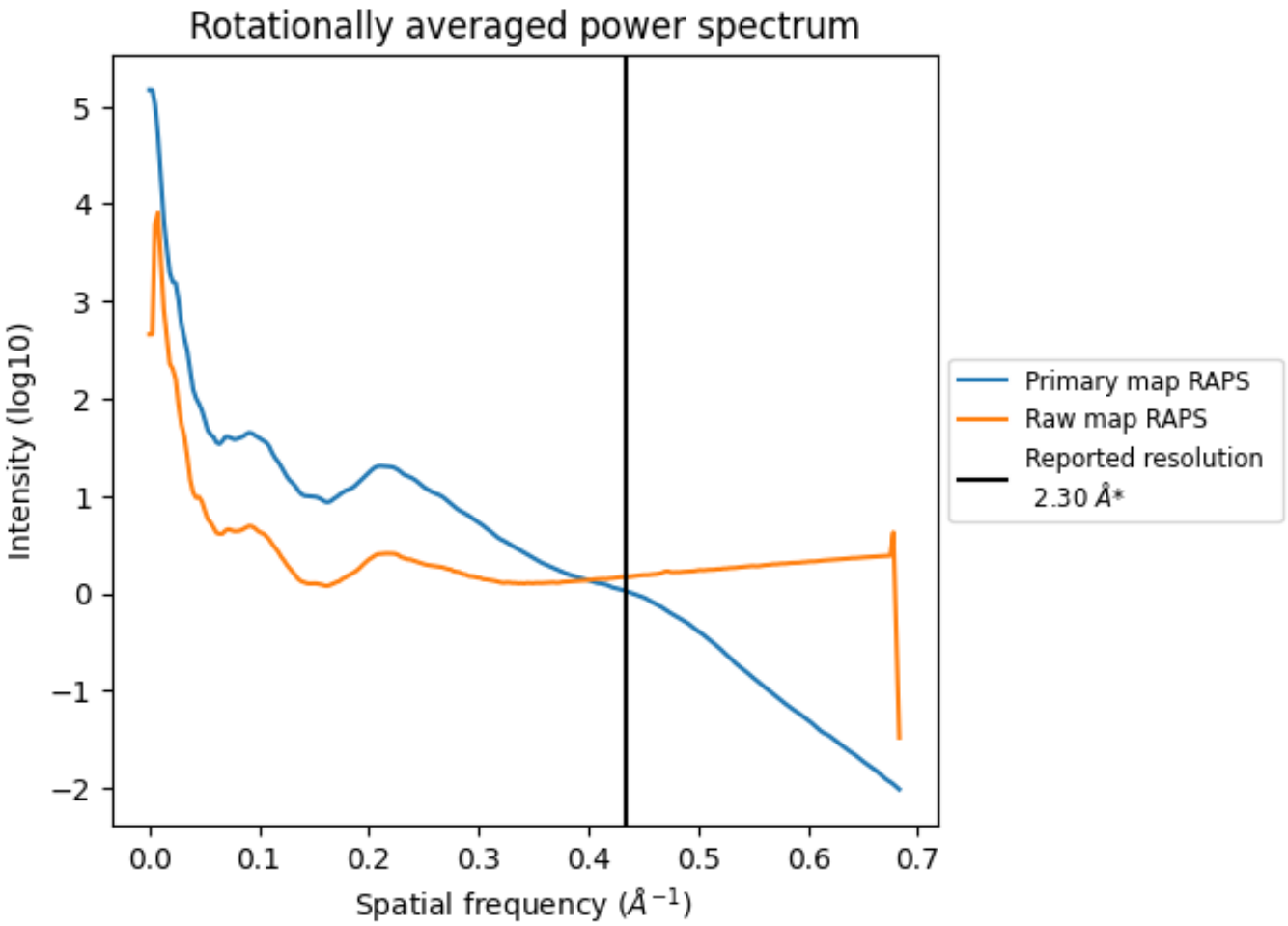
7.2 Volume estimate



The volume at the recommended contour level is 90 nm^3; this corresponds to an approximate mass of 82 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)

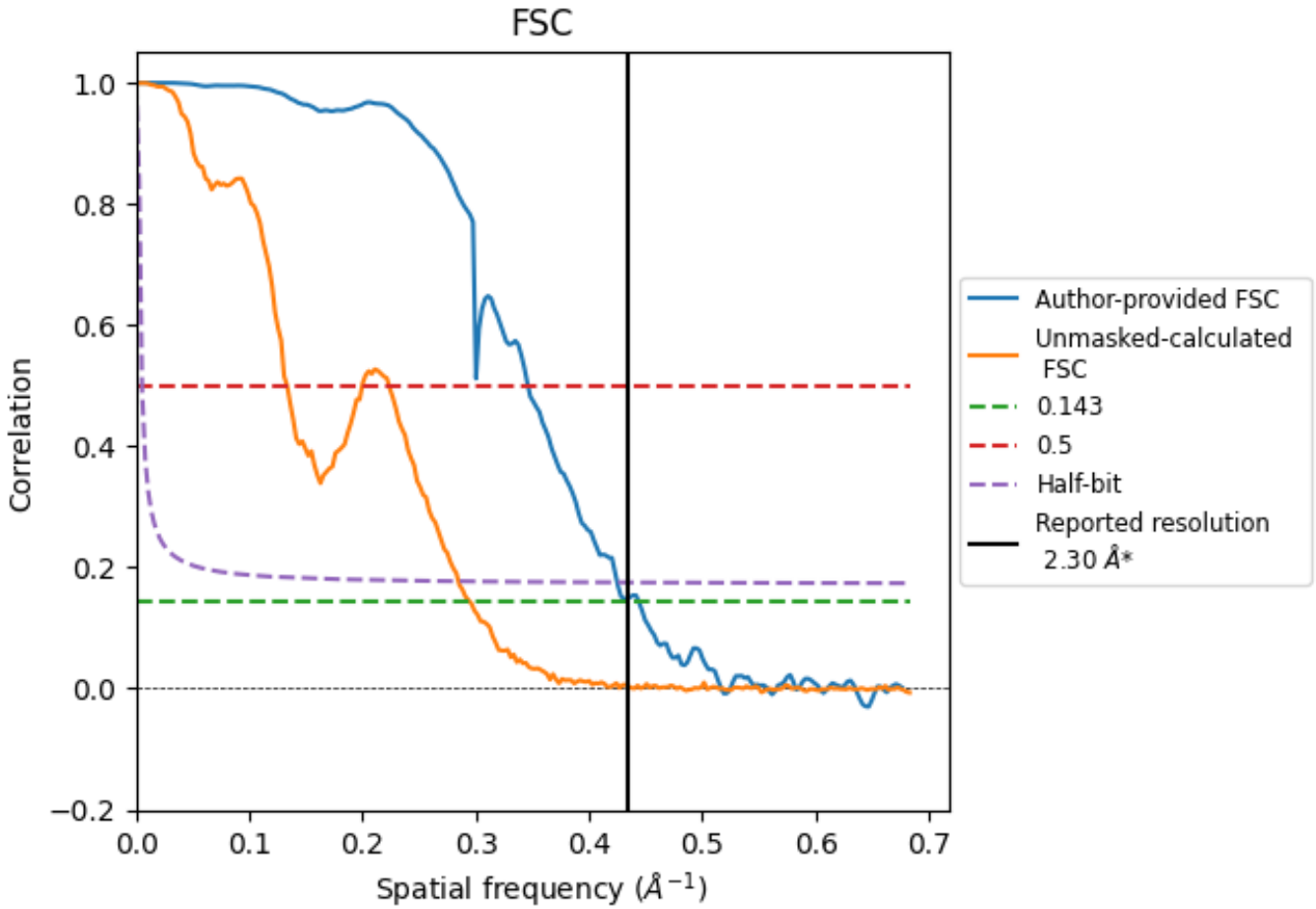


*Reported resolution corresponds to spatial frequency of 0.435 Å^{-1}

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 0.435 Å^{-1}

8.2 Resolution estimates (i)

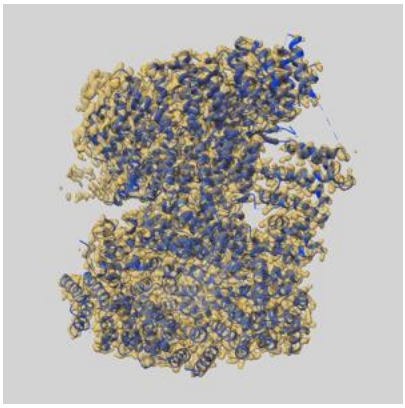
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	2.25	2.89	2.35
Unmasked-calculated*	3.39	7.50	3.51

*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 3.39 differs from the reported value 2.3 by more than 10 %

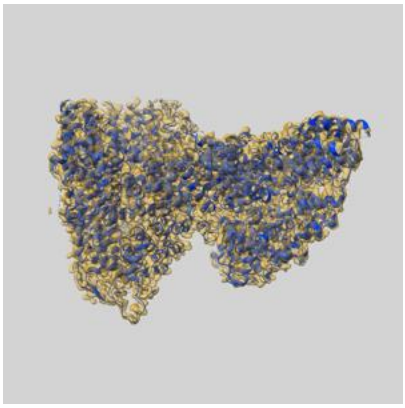
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-71744 and PDB model 9PN0. Per-residue inclusion information can be found in section 3 on page 6.

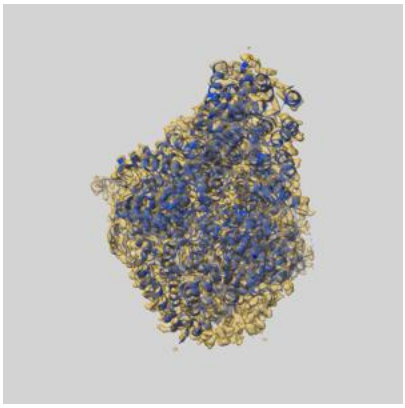
9.1 Map-model overlay



X



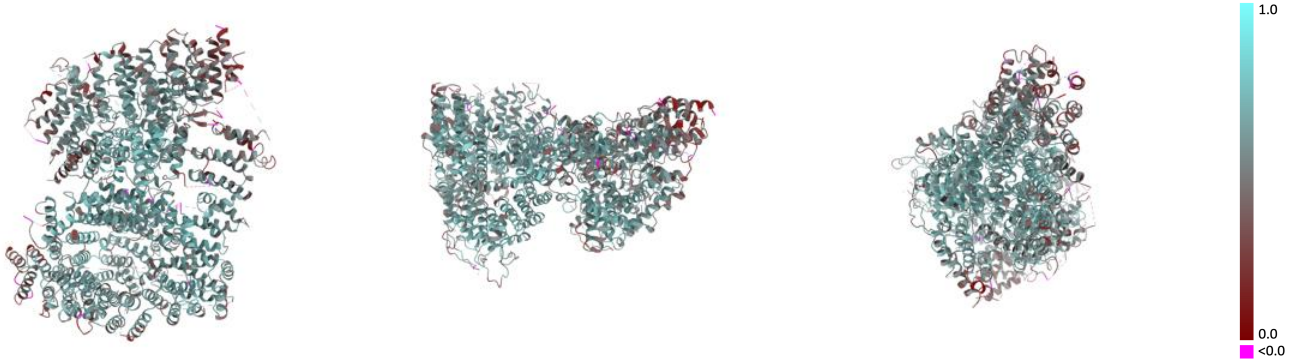
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.111 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.

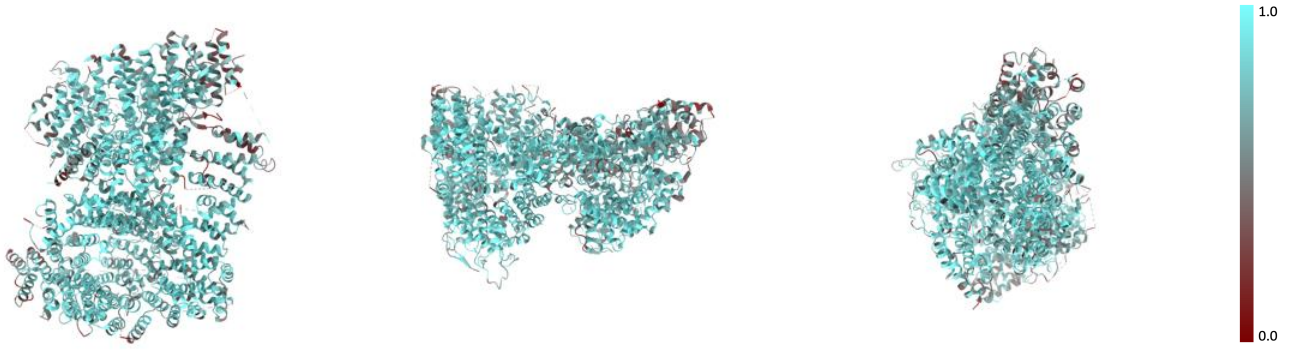
9.2 Q-score mapped to coordinate model (i)



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.

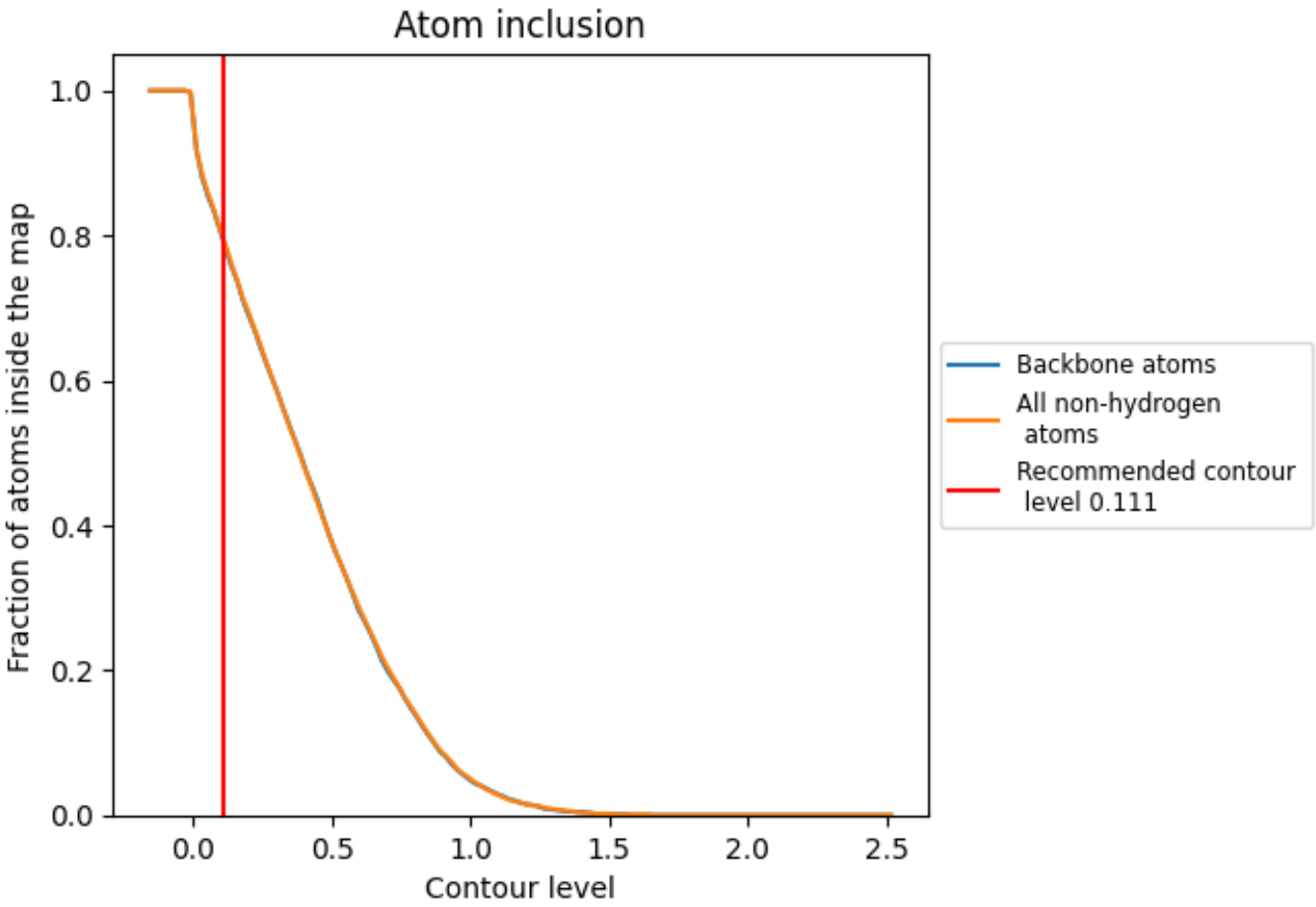
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.111).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 79% 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 (0.111) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7930	0.5700
A	0.8040	0.5720
B	0.7950	0.5880
C	0.3770	0.3310
D	0.6830	0.4500
E	0.7500	0.5230

