wwPDB EM Validation Summary Report

Nov 3, 2024 – 01:23 am GMT

PDB ID	:	5NW4
EMDB ID	:	EMD-3706
Title	:	Human cytoplasmic dynein-1 bound to dynactin and an N-terminal construct of BICD2
Authors	:	Zhang, K.; Foster, H.E.; Carter, A.P.
Deposited on	:	2017-05-05
Resolution	:	8.70 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:

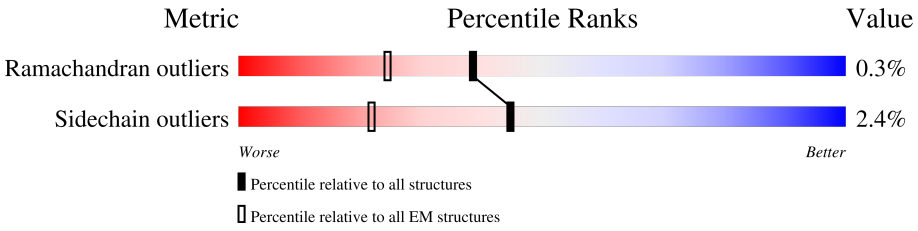
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 8.70 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)
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	B	889	28% 99%
2	D	341	6% 100%
3	C	350	15% 100%
4	A	922	55% 99%
5	1	125	13% 100%
6	2	124	16% 100%
7	R	120	28% 100%
7	S	120	15% 100%
8	E	295	99% 98%

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Mol	Chain	Length	Quality of chain
9	F	298	39% 100%
10	G	376	97%
10	H	376	97%
10	O	376	96%
10	P	376	96%
10	Q	376	96%
10	T	376	97%
10	U	376	96%
10	W	376	96%
11	V	396	93% 7%
12	X	417	87% 12%
13	Y	286	94%
14	Z	293	90% 8%
15	a	571	100%
16	b	602	100%
17	c	130	50% 50%
17	d	130	50% 50%
18	e	174	22% 50% 50%
18	f	174	50% 50%
19	g	190	86% 11%
20	h	222	74% 26%
21	i	243	100%
22	j	52	100%
23	k	48	85% 12%
24	l	71	83% 17%

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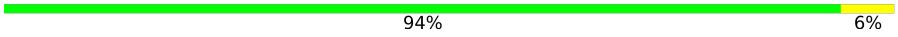
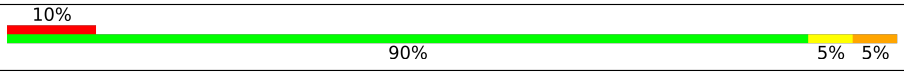
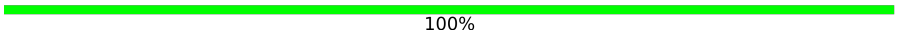
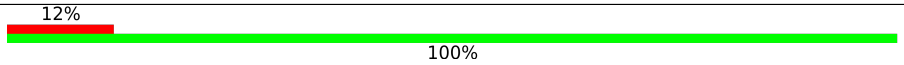
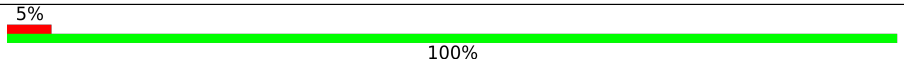
Mol	Chain	Length	Quality of chain
25	m	31	
26	n	20	
27	o	53	
28	5	275	
28	6	275	

2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 66297 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 dynein heavy chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	B	889	4439	2661	889	889	0	0

- Molecule 2 is a protein called dynein intermediate chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	D	341	1680	998	341	341	0	0

- Molecule 3 is a protein called dynein intermediate chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	350	1723	1023	350	350	0	0

- Molecule 4 is a protein called dynein heavy chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	A	922	4604	2760	922	922	0	0

- Molecule 5 is a protein called dynein N-terminal dimerization domain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	1	125	625	375	125	125	0	0

- Molecule 6 is a protein called dynein N-terminal dimerization domain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	2	124	620	372	124	124	0	0

- Molecule 7 is a protein called Robl.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	R	120	Total 587	C 347	N 120	O 120	0	0
7	S	120	Total 587	C 347	N 120	O 120	0	0

- Molecule 8 is a protein called dynein light intermediate chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	E	295	Total 1459	C 869	N 295	O 295	0	0

- Molecule 9 is a protein called dynein light intermediate chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	F	298	Total 1496	C 890	N 303	O 303	5	0

- Molecule 10 is a protein called Arp1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	370	Total 2957	C 1893	N 509	O 545	S 10	0	0
10	H	370	Total 2957	C 1893	N 509	O 545	S 10	0	0
10	O	370	Total 2957	C 1893	N 509	O 545	S 10	0	0
10	P	370	Total 2957	C 1893	N 509	O 545	S 10	0	0
10	Q	370	Total 2957	C 1893	N 509	O 545	S 10	0	0
10	T	370	Total 2957	C 1893	N 509	O 545	S 10	0	0
10	U	370	Total 2957	C 1893	N 509	O 545	S 10	0	0
10	W	370	Total 2957	C 1893	N 509	O 545	S 10	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	97	GLU	ASP	conflict	UNP F2Z5G5

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Chain	Residue	Modelled	Actual	Comment	Reference
H	97	GLU	ASP	conflict	UNP F2Z5G5
O	97	GLU	ASP	conflict	UNP F2Z5G5
P	97	GLU	ASP	conflict	UNP F2Z5G5
Q	97	GLU	ASP	conflict	UNP F2Z5G5
T	97	GLU	ASP	conflict	UNP F2Z5G5
U	97	GLU	ASP	conflict	UNP F2Z5G5
W	97	GLU	ASP	conflict	UNP F2Z5G5

- Molecule 11 is a protein called beta-actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	V	370	Total	C	N	O	S	0	0
			2885	1827	486	550	22		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	-20	MET	-	initiating methionine	UNP I3LVD5
V	-19	SER	-	expression tag	UNP I3LVD5
V	-18	VAL	-	expression tag	UNP I3LVD5
V	-17	ARG	-	expression tag	UNP I3LVD5
V	-16	SER	-	expression tag	UNP I3LVD5
V	-15	ALA	-	expression tag	UNP I3LVD5
V	-14	ARG	-	expression tag	UNP I3LVD5
V	-13	ARG	-	expression tag	UNP I3LVD5
V	-12	ALA	-	expression tag	UNP I3LVD5
V	-11	SER	-	expression tag	UNP I3LVD5
V	-10	ALA	-	expression tag	UNP I3LVD5
V	-9	SER	-	expression tag	UNP I3LVD5
V	-8	ALA	-	expression tag	UNP I3LVD5
V	-7	GLU	-	expression tag	UNP I3LVD5
V	-6	ALA	-	expression tag	UNP I3LVD5
V	-5	GLU	-	expression tag	UNP I3LVD5
V	-4	LEU	-	expression tag	UNP I3LVD5
V	-3	LEU	-	expression tag	UNP I3LVD5
V	-2	GLN	-	expression tag	UNP I3LVD5
V	-1	THR	-	expression tag	UNP I3LVD5
V	0	MET	-	expression tag	UNP I3LVD5
V	1	GLY	-	expression tag	UNP I3LVD5
V	2	ASP	-	expression tag	UNP I3LVD5
V	10	VAL	ILE	conflict	UNP I3LVD5

- Molecule 12 is a protein called Arp11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	X	369	Total	C	N	O	S	0	0
			2879	1857	486	520	16		

- Molecule 13 is a protein called Capping protein (Actin filament) muscle Z-line, alpha 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Y	275	Total	C	N	O	S	0	0
			2242	1415	393	429	5		

- Molecule 14 is a protein called F-actin capping protein beta subunit variant II.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Z	270	Total	C	N	O	S	0	0
			2137	1333	373	420	11		

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	-15	MET	-	initiating methionine	UNP D2JYW4
Z	-14	ASP	-	expression tag	UNP D2JYW4
Z	-13	THR	-	expression tag	UNP D2JYW4
Z	-12	GLU	-	expression tag	UNP D2JYW4
Z	-11	LEU	-	expression tag	UNP D2JYW4
Z	-10	ALA	-	expression tag	UNP D2JYW4
Z	-9	SER	-	expression tag	UNP D2JYW4
Z	-8	PRO	-	expression tag	UNP D2JYW4
Z	-7	GLY	-	expression tag	UNP D2JYW4
Z	-6	PRO	-	expression tag	UNP D2JYW4
Z	-5	LEU	-	expression tag	UNP D2JYW4
Z	-4	LEU	-	expression tag	UNP D2JYW4
Z	-3	LEU	-	expression tag	UNP D2JYW4
Z	-2	GLY	-	expression tag	UNP D2JYW4
Z	-1	LYS	-	expression tag	UNP D2JYW4
Z	0	TYR	-	expression tag	UNP D2JYW4
Z	1	ARG	-	expression tag	UNP D2JYW4

- Molecule 15 is a protein called dynactin shoulder complex.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	a	571	Total	C	N	O	0	0
			2855	1713	571	571		

- Molecule 16 is a protein called dynactin shoulder complex.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	b	602	Total	C	N	O	0	0
			3010	1806	602	602		

- Molecule 17 is a protein called dynactin shoulder complex.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	c	65	Total	C	N	O	0	0
			323	193	65	65		
17	d	65	Total	C	N	O	0	0
			323	193	65	65		

- Molecule 18 is a protein called dynactin shoulder complex.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	e	87	Total	C	N	O	0	0
			435	261	87	87		
18	f	87	Total	C	N	O	0	0
			435	261	87	87		

- Molecule 19 is a protein called Dynactin 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	g	169	Total	C	N	O	0	0
			831	493	169	169		

- Molecule 20 is a protein called Dynactin subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	h	165	Total	C	N	O	0	0
			812	482	165	165		

- Molecule 21 is a protein called dynactin pointed end p62.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	i	243	Total	C	N	O	0	0
			1215	729	243	243		

- Molecule 22 is a protein called p150.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	j	52	Total 260	C 156	N 52	O 52	0	0

- Molecule 23 is a protein called Dynactin.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	k	48	Total 341	C 216	N 58	O 66	S 1	0	0

- Molecule 24 is a protein called Dynactin.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	l	71	Total 517	C 324	N 93	O 99	S 1	0	0

- Molecule 25 is a protein called Dynactin.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	m	31	Total 179	C 112	N 34	O 32	S 1	0	0

- Molecule 26 is a protein called Dynactin.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	n	20	Total 127	C 80	N 23	O 23	S 1	0	0

- Molecule 27 is a protein called dynactin p150.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	o	53	Total 265	C 159	N 53	O 53	0	0

- Molecule 28 is a protein called BICD2N.

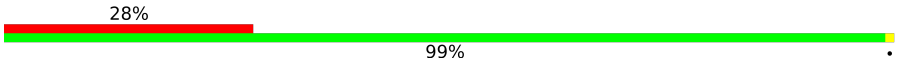
Mol	Chain	Residues	Atoms				AltConf	Trace
28	5	275	Total 1375	C 825	N 275	O 275	0	0
28	6	275	Total 1375	C 825	N 275	O 275	0	0

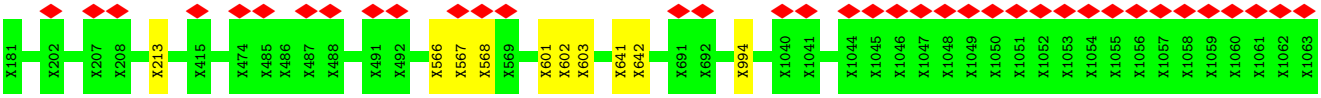
3 Residue-property plots (i)

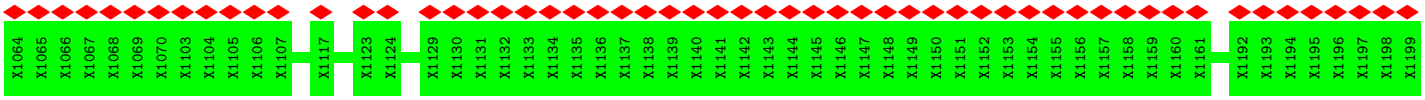
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

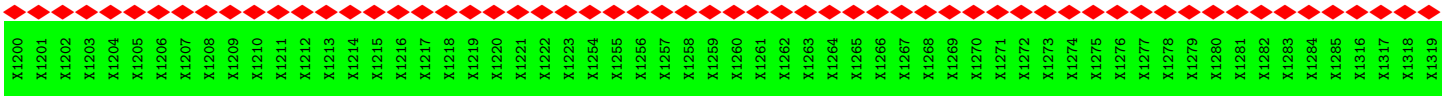
• Molecule 1: dynein heavy chain

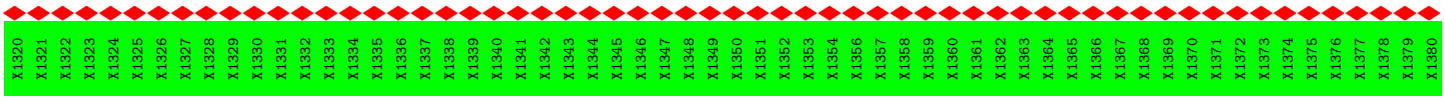
Chain B:

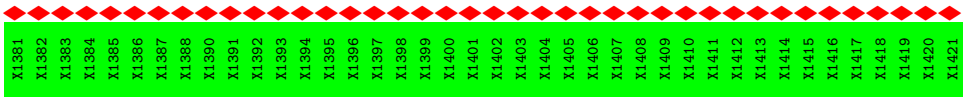






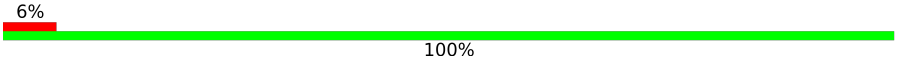


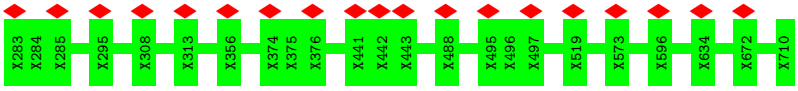




• Molecule 2: dynein intermediate chain

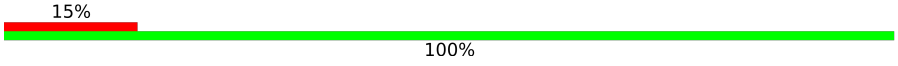
Chain D:

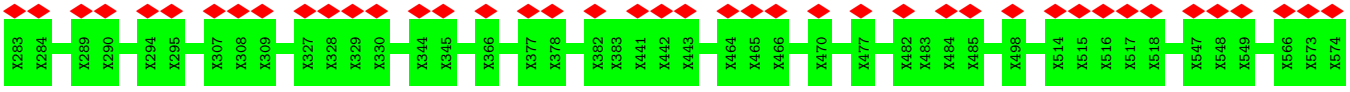


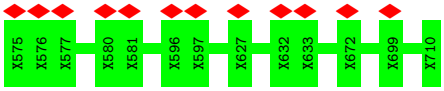


• Molecule 3: dynein intermediate chain

Chain C:

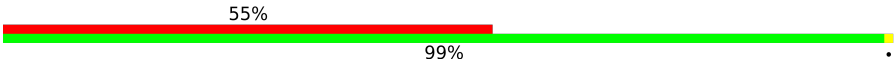


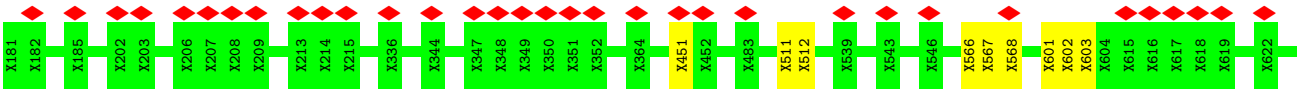


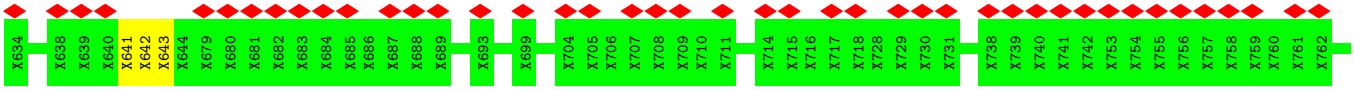


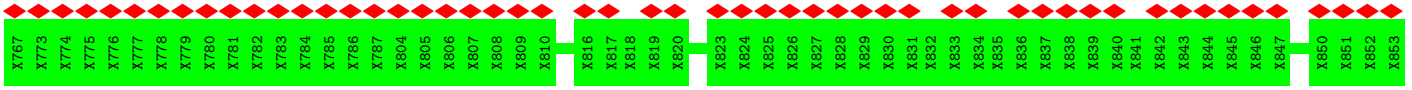
• Molecule 4: dynein heavy chain

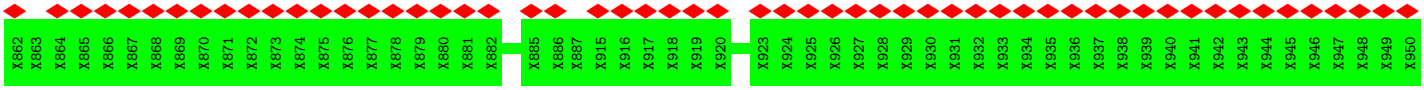
Chain A:

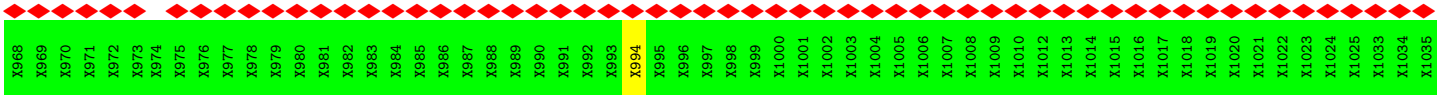


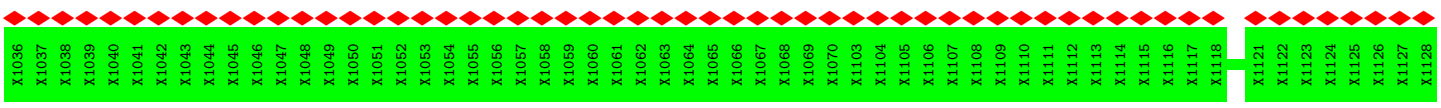


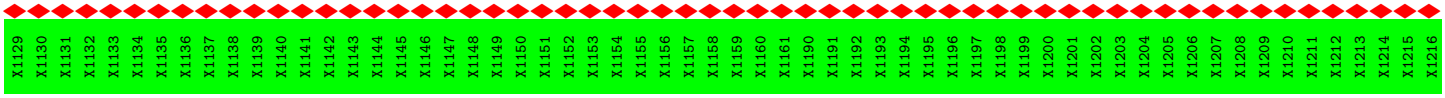


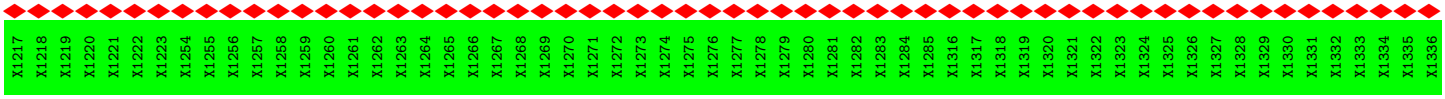


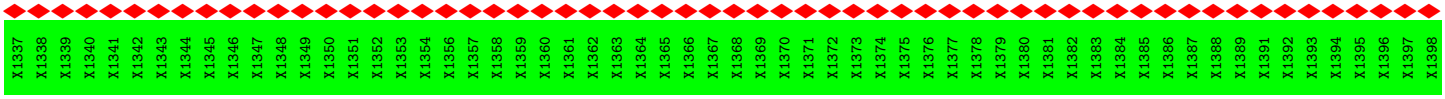






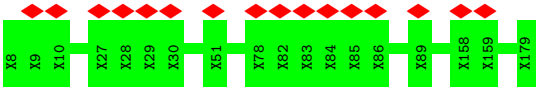




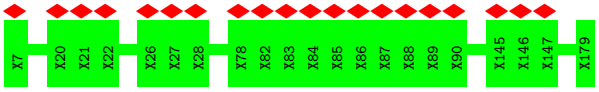


• Molecule 5: dynein N-terminal dimerization domain

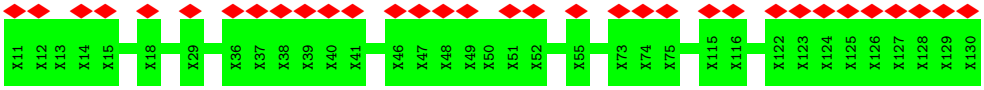
Chain 1:



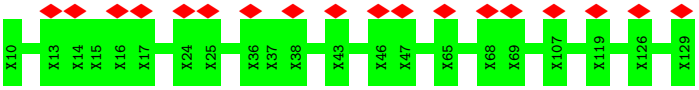
• Molecule 6: dynein N-terminal dimerization domain



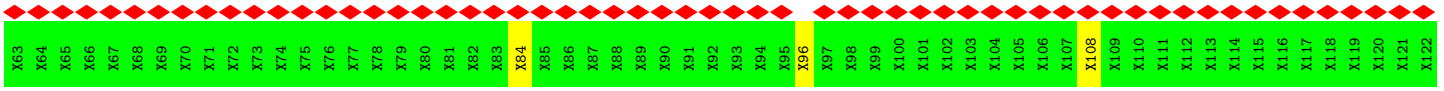
• Molecule 7: Robl

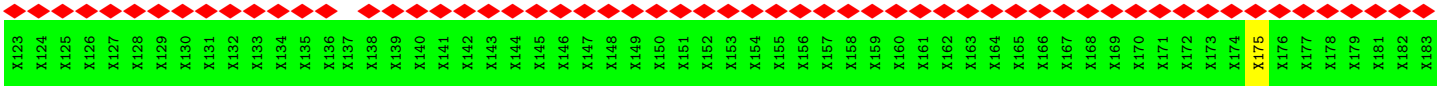


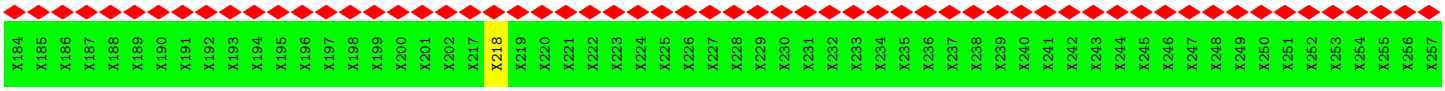
• Molecule 7: Robl

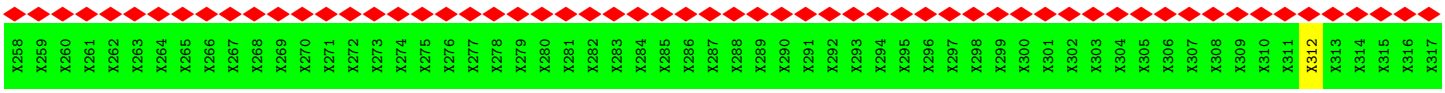


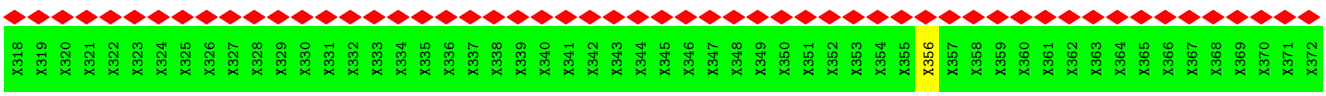
• Molecule 8: dynein light intermediate chain





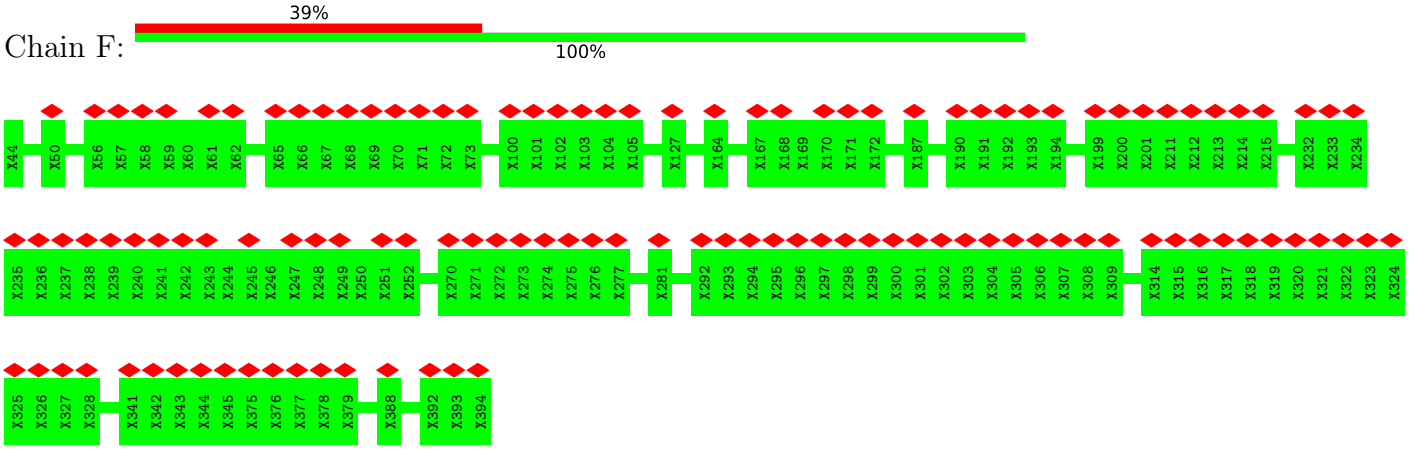






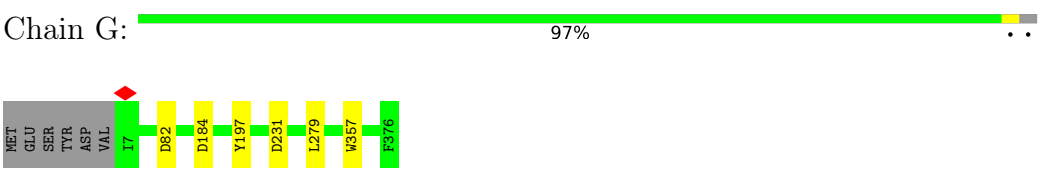
• Molecule 9: dynein light intermediate chain

Chain F:



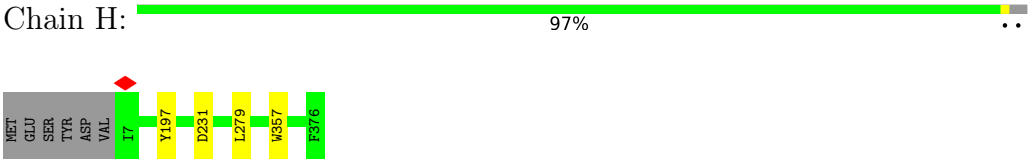
• Molecule 10: Arp1

Chain G:



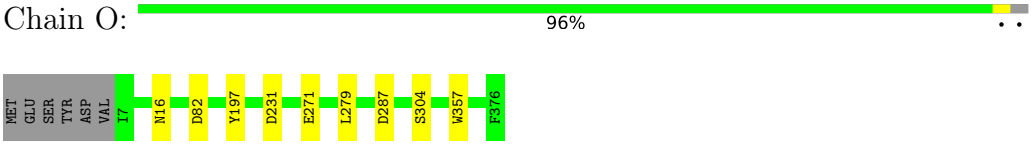
• Molecule 10: Arp1

Chain H:



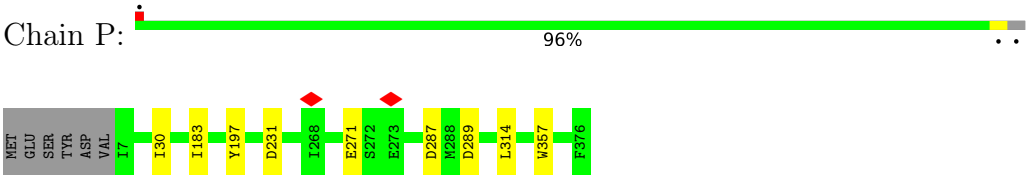
• Molecule 10: Arp1

Chain O:



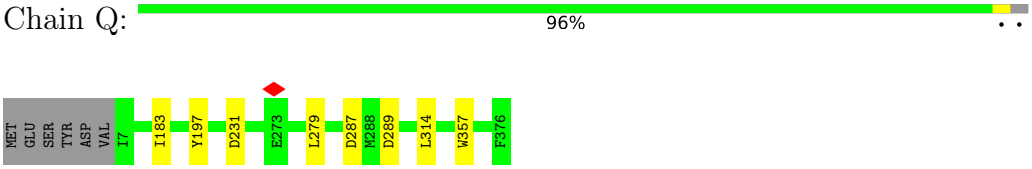
• Molecule 10: Arp1

Chain P:



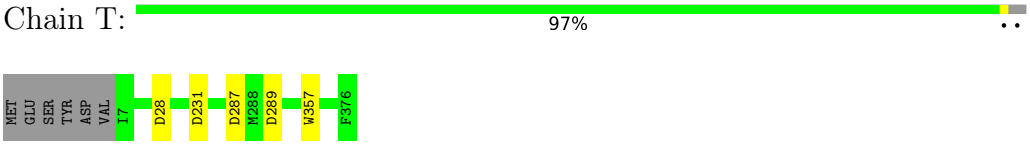
• Molecule 10: Arp1

Chain Q:



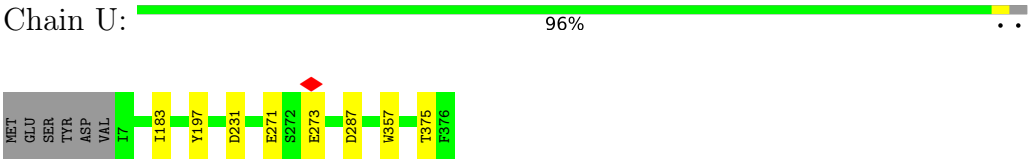
• Molecule 10: Arp1

Chain T:



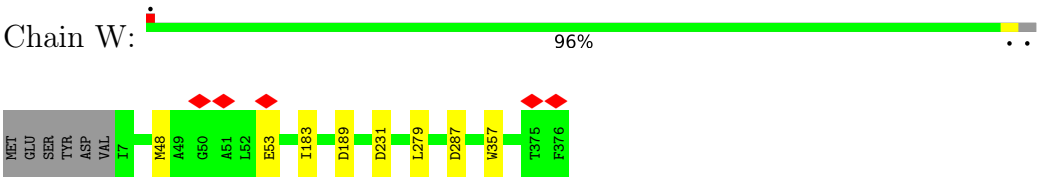
• Molecule 10: Arp1

Chain U:



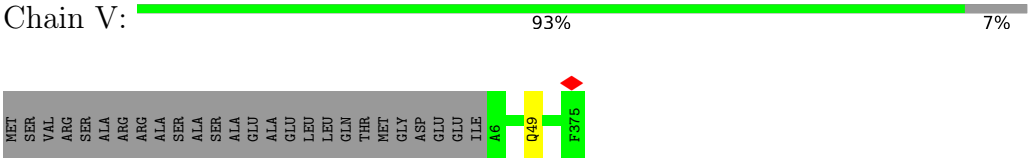
• Molecule 10: Arp1

Chain W:



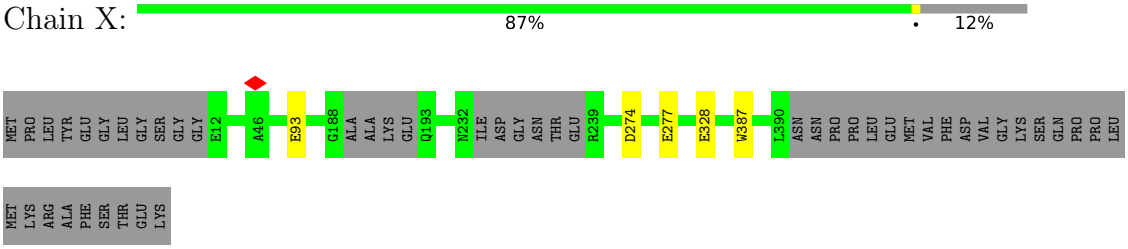
• Molecule 11: beta-actin

Chain V:



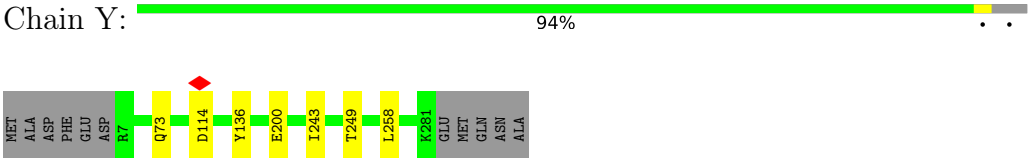
• Molecule 12: Arp11

Chain X:



• Molecule 13: Capping protein (Actin filament) muscle Z-line, alpha 1

Chain Y:

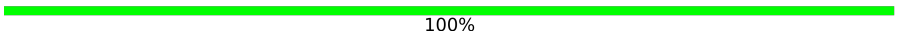


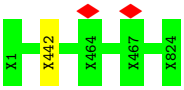
• Molecule 14: F-actin capping protein beta subunit variant II

Chain Z:

• Molecule 15: dynactin shoulder complex

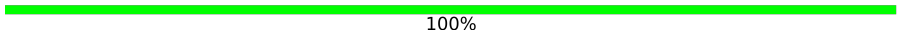
Chain a:

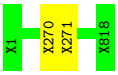




• Molecule 16: dynactin shoulder complex

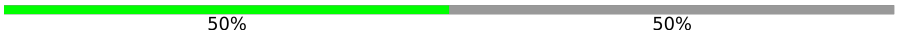
Chain b:

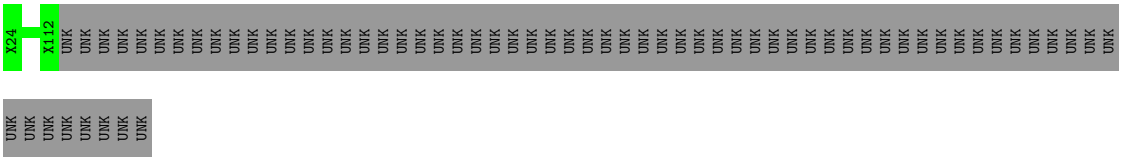




• Molecule 17: dynactin shoulder complex

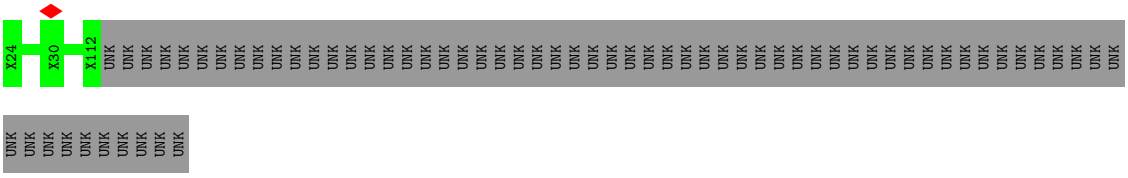
Chain c:





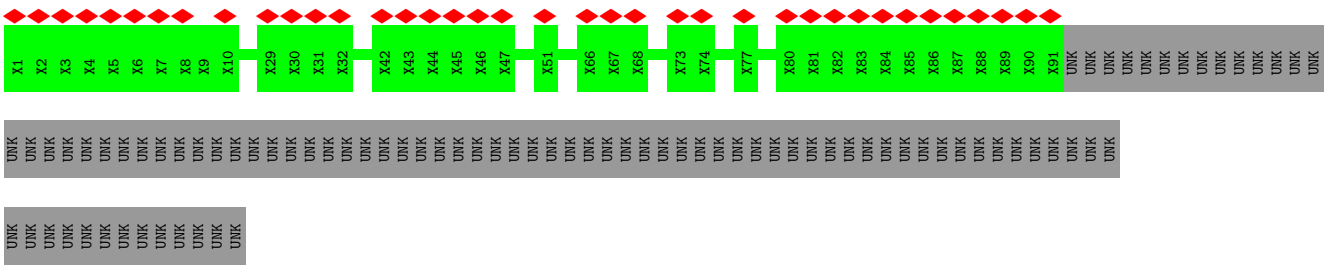
• Molecule 17: dynactin shoulder complex

Chain d:



• Molecule 18: dynactin shoulder complex

Chain e:

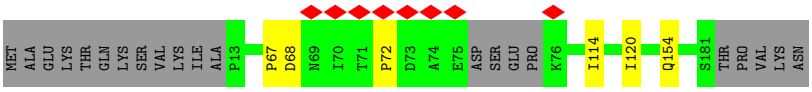


• Molecule 18: dynactin shoulder complex

Chain f:

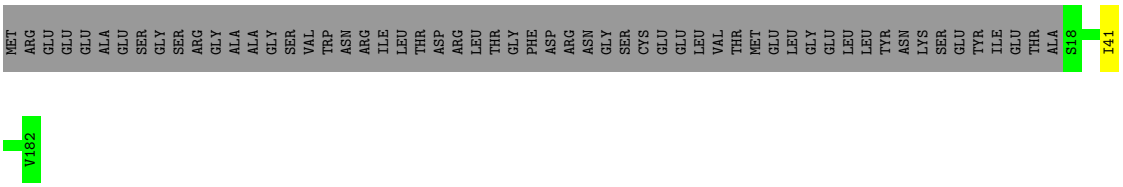
• Molecule 19: Dynactin 6

Chain g:



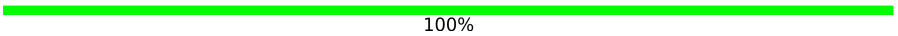
• Molecule 20: Dynactin subunit 5

Chain h:



• Molecule 21: dynactin pointed end p62

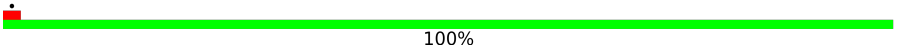
Chain i:



There are no outlier residues recorded for this chain.

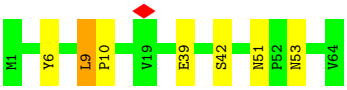
• Molecule 22: p150

Chain j:



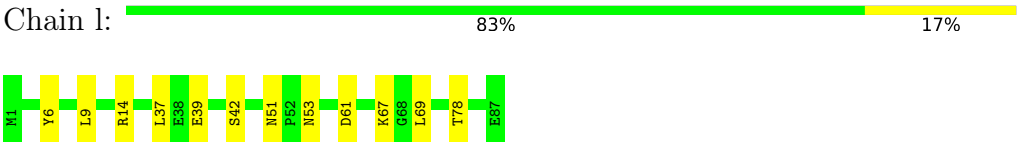
• Molecule 23: Dynactin

Chain k:



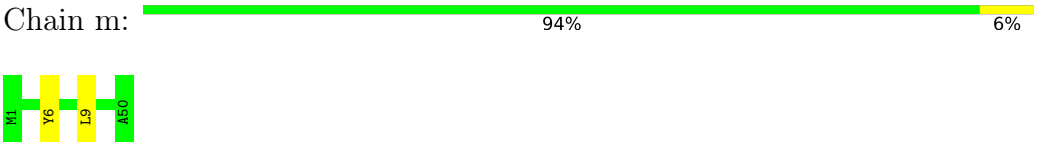
• Molecule 24: Dynactin

Chain l:



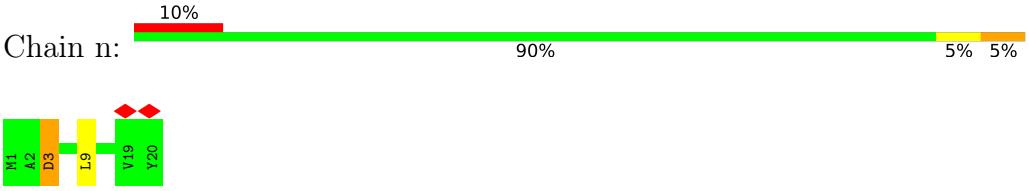
• Molecule 25: Dynactin

Chain m:



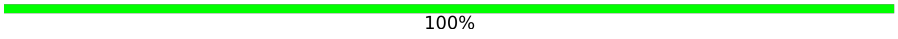
• Molecule 26: Dynactin

Chain n:



• Molecule 27: dynactin p150

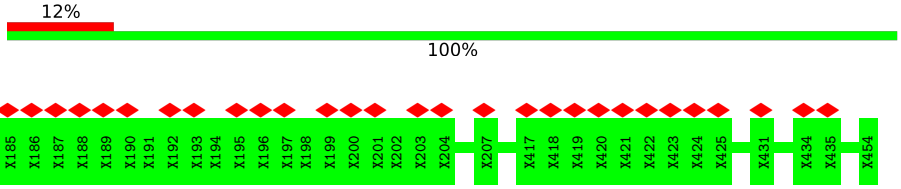
Chain o:



There are no outlier residues recorded for this chain.

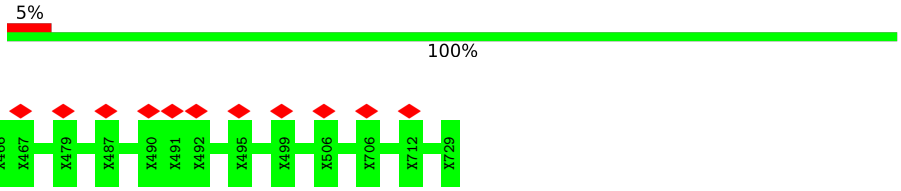
• Molecule 28: BICD2N

Chain 5:



• Molecule 28: BICD2N

Chain 6:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	78671	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 ($e^-/Å^2$)	1.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.473	Depositor
Minimum map value	-0.203	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	964.80005, 964.80005, 964.80005	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.68, 2.68, 2.68	Depositor

5 Model quality

5.1 Standard geometry

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	#$\|Z\|>5$
10	G	0.37	0/3026	0.51	0/4086
10	H	0.37	0/3026	0.51	0/4086
10	O	0.37	0/3026	0.52	0/4086
10	P	0.37	0/3026	0.52	0/4086
10	Q	0.37	0/3026	0.53	0/4086
10	T	0.37	0/3026	0.51	0/4086
10	U	0.37	0/3026	0.52	0/4086
10	W	0.38	0/3026	0.53	0/4086
11	V	0.37	0/2948	0.51	0/3991
12	X	0.37	0/2939	0.53	0/3987
13	Y	0.39	0/2294	0.63	1/3106 (0.0%)
14	Z	0.38	0/2173	0.60	1/2935 (0.0%)
19	g	0.28	0/830	0.50	0/1152
20	h	0.30	0/811	0.48	0/1126
23	k	0.53	1/347 (0.3%)	0.67	1/473 (0.2%)
24	l	0.41	0/525	0.66	0/708
25	m	0.40	0/181	0.65	0/249
26	n	0.47	0/130	0.73	0/179
All	All	0.37	1/37386 (0.0%)	0.54	3/50594 (0.0%)

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
1	B	0	10
4	A	0	13
8	E	0	8
10	U	0	1
15	a	0	1
16	b	0	2
All	All	0	35

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	k	10	PRO	N-CD	5.09	1.54	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	Z	253	PRO	CA-N-CD	-8.88	99.08	111.50
23	k	9	LEU	C-N-CD	5.77	140.52	128.40
13	Y	114	ASP	CB-CG-OD2	5.22	123.00	118.30

There are no chirality outliers.

5 of 35 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	213	UNK	Mainchain
1	B	566	UNK	Mainchain
1	B	567	UNK	Mainchain
1	B	568	UNK	Mainchain
1	B	601	UNK	Mainchain

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	G	368/376 (98%)	350 (95%)	18 (5%)	0	100	100
10	H	368/376 (98%)	348 (95%)	20 (5%)	0	100	100
10	O	368/376 (98%)	347 (94%)	21 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
10	P	368/376 (98%)	347 (94%)	21 (6%)	0	100 100
10	Q	368/376 (98%)	346 (94%)	22 (6%)	0	100 100
10	T	368/376 (98%)	341 (93%)	27 (7%)	0	100 100
10	U	368/376 (98%)	344 (94%)	24 (6%)	0	100 100
10	W	368/376 (98%)	347 (94%)	21 (6%)	0	100 100
11	V	368/396 (93%)	350 (95%)	18 (5%)	0	100 100
12	X	363/417 (87%)	331 (91%)	31 (8%)	1 (0%)	37 73
13	Y	273/286 (96%)	258 (94%)	15 (6%)	0	100 100
14	Z	268/293 (92%)	257 (96%)	11 (4%)	0	100 100
19	g	167/190 (88%)	145 (87%)	16 (10%)	6 (4%)	3 20
20	h	163/222 (73%)	146 (90%)	16 (10%)	1 (1%)	22 60
23	k	44/48 (92%)	40 (91%)	3 (7%)	1 (2%)	5 28
24	l	67/71 (94%)	58 (87%)	8 (12%)	1 (2%)	8 40
25	m	27/31 (87%)	24 (89%)	2 (7%)	1 (4%)	2 20
26	n	18/20 (90%)	15 (83%)	1 (6%)	2 (11%)	0 5
All	All	4702/4982 (94%)	4394 (93%)	295 (6%)	13 (0%)	38 73

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	g	67	PRO
19	g	72	PRO
19	g	154	GLN
23	k	9	LEU
24	l	9	LEU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	G	318/324 (98%)	312 (98%)	6 (2%)	52 69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	H	318/324 (98%)	314 (99%)	4 (1%)	65 77
10	O	318/324 (98%)	309 (97%)	9 (3%)	38 57
10	P	318/324 (98%)	309 (97%)	9 (3%)	38 57
10	Q	318/324 (98%)	310 (98%)	8 (2%)	42 61
10	T	318/324 (98%)	313 (98%)	5 (2%)	58 73
10	U	318/324 (98%)	311 (98%)	7 (2%)	47 65
10	W	318/324 (98%)	310 (98%)	8 (2%)	42 61
11	V	313/333 (94%)	312 (100%)	1 (0%)	91 92
12	X	322/363 (89%)	318 (99%)	4 (1%)	67 78
13	Y	245/254 (96%)	239 (98%)	6 (2%)	44 62
14	Z	242/262 (92%)	236 (98%)	6 (2%)	42 61
23	k	31/41 (76%)	26 (84%)	5 (16%)	2 10
24	l	49/60 (82%)	38 (78%)	11 (22%)	1 5
25	m	7/16 (44%)	6 (86%)	1 (14%)	2 12
26	n	8/16 (50%)	7 (88%)	1 (12%)	3 15
All	All	3761/3937 (96%)	3670 (98%)	91 (2%)	45 62

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	X	93	GLU
14	Z	245	SER
12	X	277	GLU
13	Y	249	THR
23	k	42	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
13	Y	79	HIS
13	Y	84	ASN
24	l	51	ASN
14	Z	209	HIS
23	k	51	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	A	29
1	B	28
21	i	12
5	1	7
6	2	7
16	b	5
15	a	5
2	D	4
9	F	3
17	c	3
17	d	3
3	C	3
8	E	3
18	e	2
18	f	2
25	m	1

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Mol	Chain	Number of breaks
23	k	1
24	l	1

The worst 5 of 119 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	b	363:UNK	C	401:UNK	N	98.24
1	b	167:UNK	C	201:UNK	N	96.90
1	a	166:UNK	C	201:UNK	N	95.47
1	a	362:UNK	C	401:UNK	N	81.15
1	a	625:UNK	C	701:UNK	N	68.30

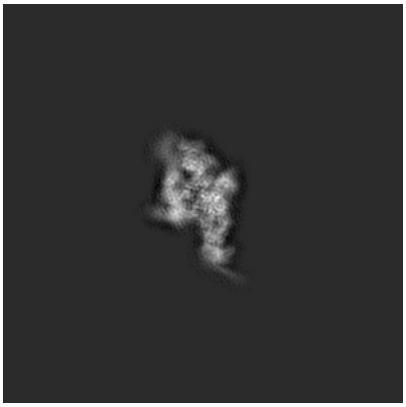
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3706. These allow visual inspection of the internal detail of the map and identification of artifacts.

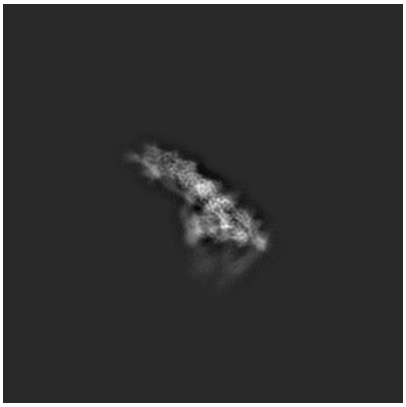
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

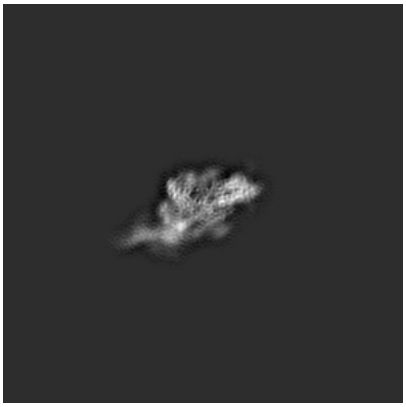
6.1.1 Primary map



X



Y



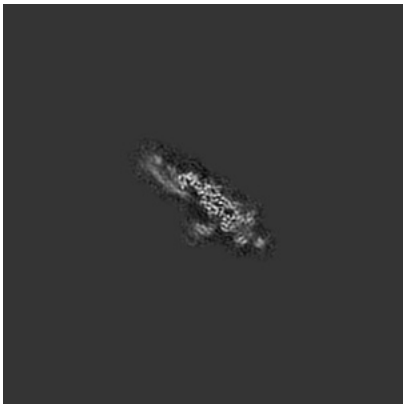
Z

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

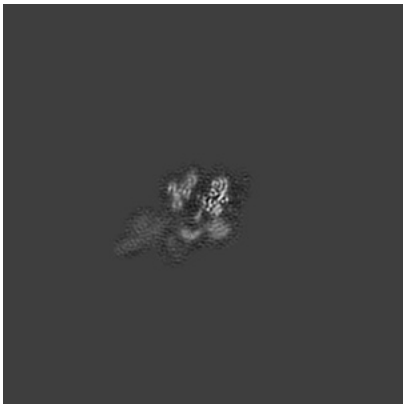
6.2 Central slices

6.2.1 Primary map

X Index: 180



Y Index: 180

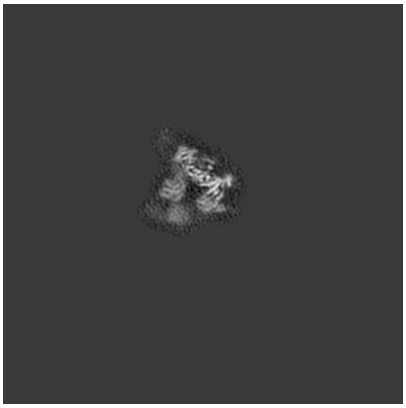


Z Index: 180

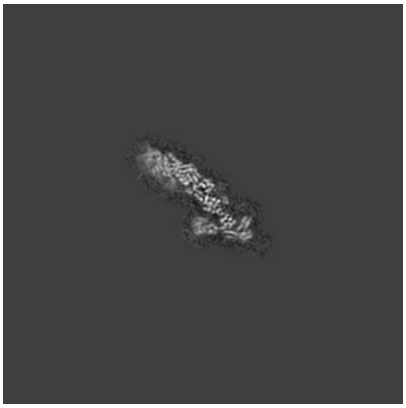
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

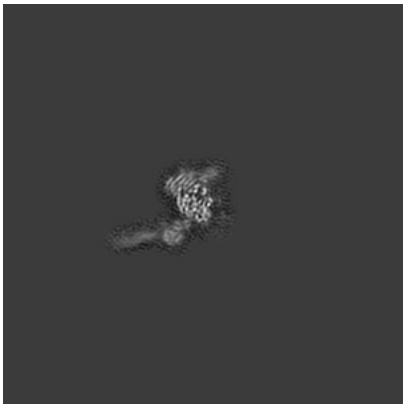
6.3.1 Primary map



X Index: 158



Y Index: 186

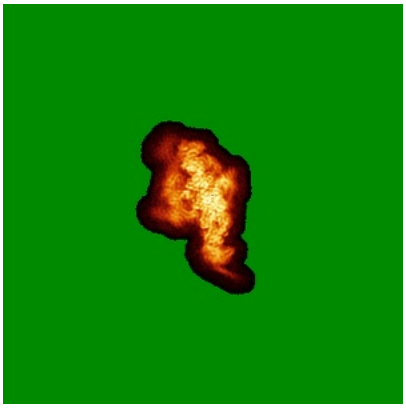


Z Index: 197

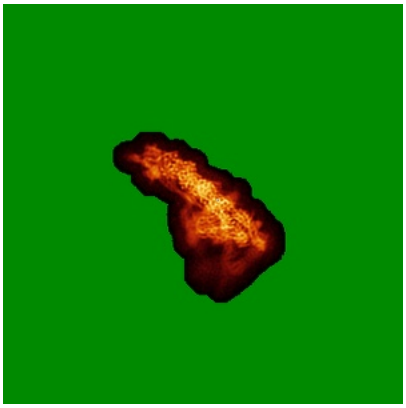
The images above show the largest variance slices of the map in three orthogonal directions.

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

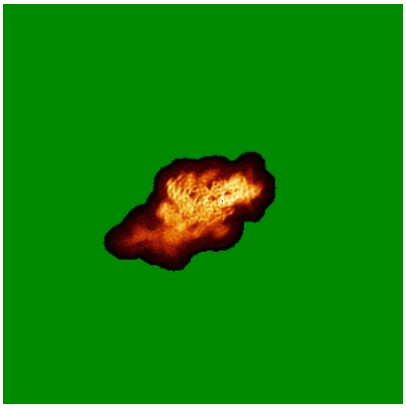
6.4.1 Primary map



X



Y



Z

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

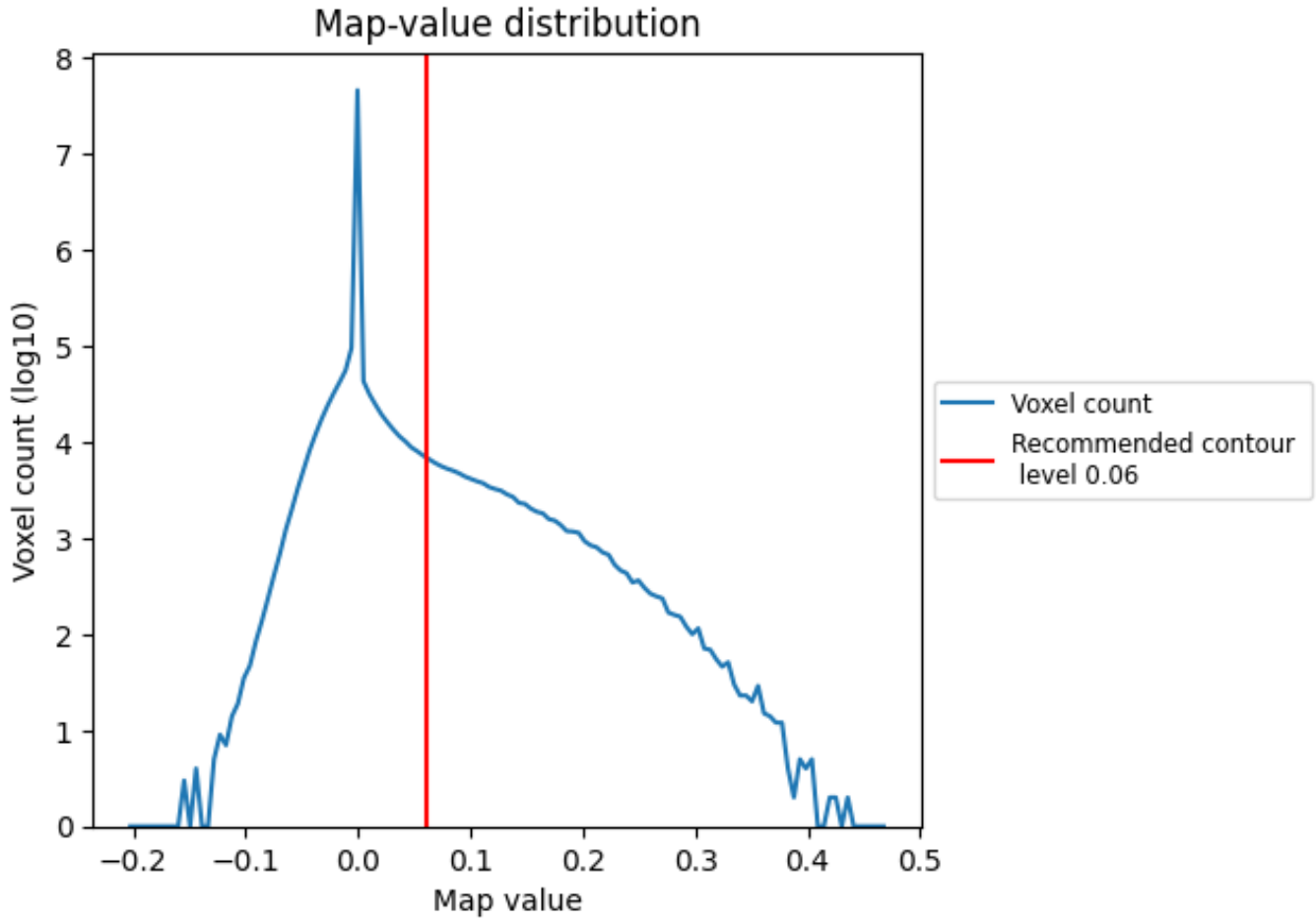
6.6 Mask visualisation (i)

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

7 Map analysis

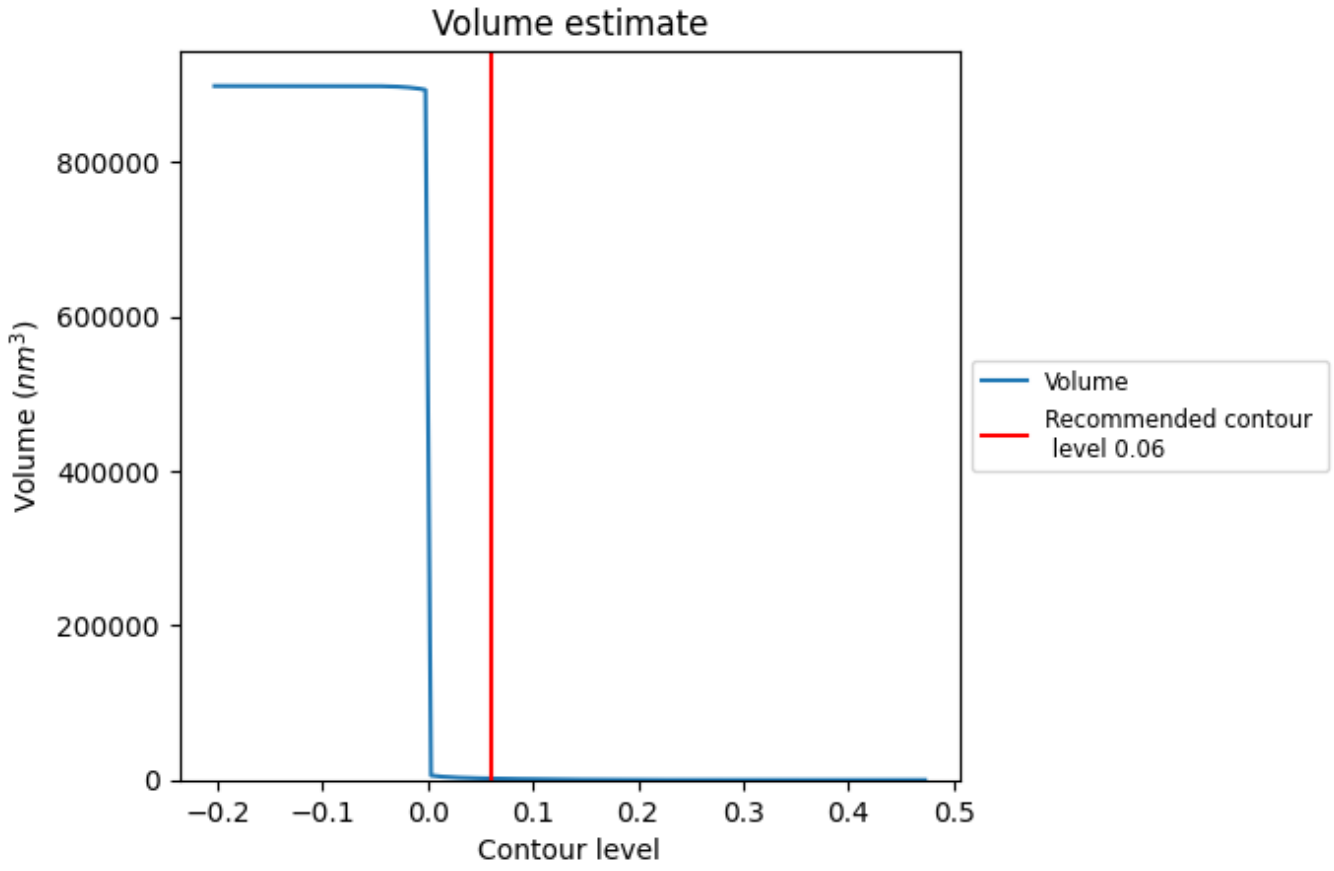
This section contains the results of statistical analysis of the map.

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.

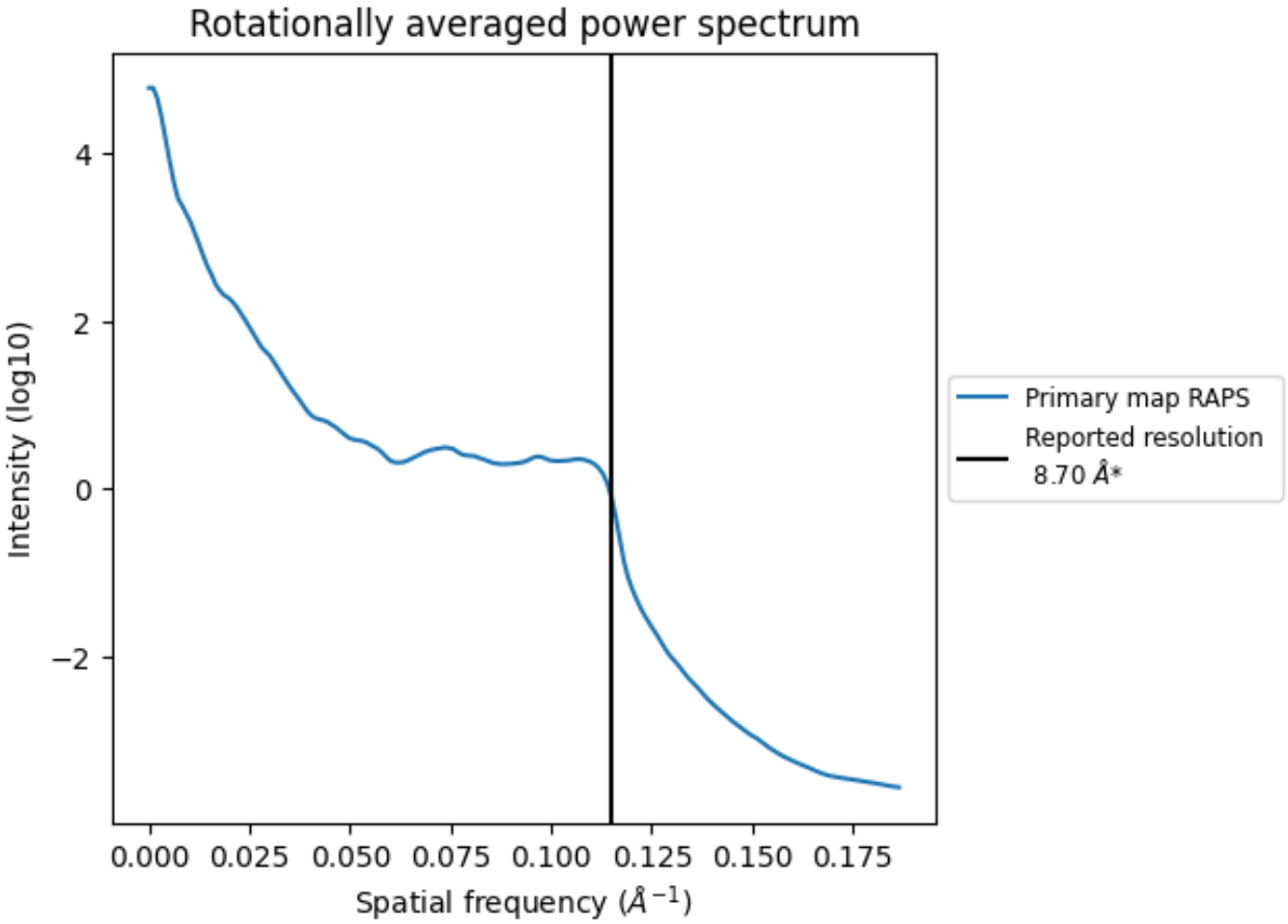
7.2 Volume estimate (i)



The volume at the recommended contour level is 1849 nm^3; this corresponds to an approximate mass of 1670 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)

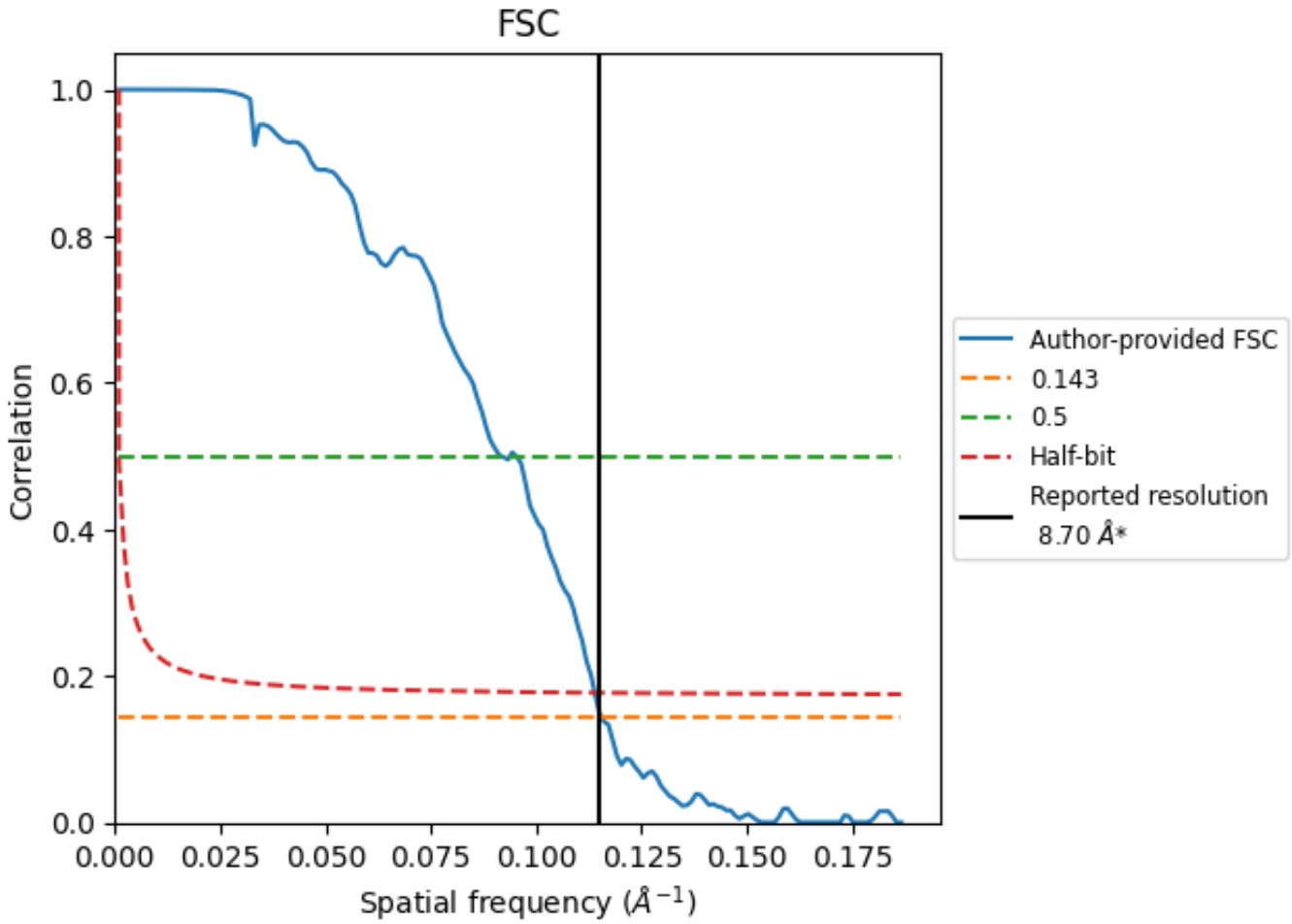


*Reported resolution corresponds to spatial frequency of 0.115 Å^{-1}

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 0.115 Å^{-1}

8.2 Resolution estimates (i)

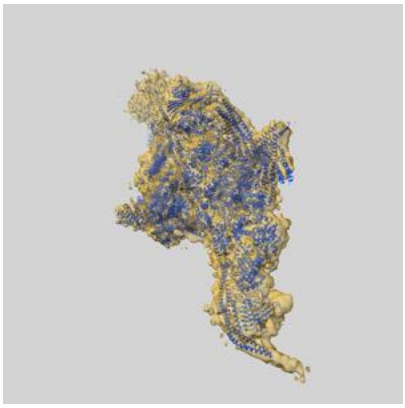
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.70	-	-
Author-provided FSC curve	8.65	10.92	8.78
Unmasked-calculated*	-	-	-

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

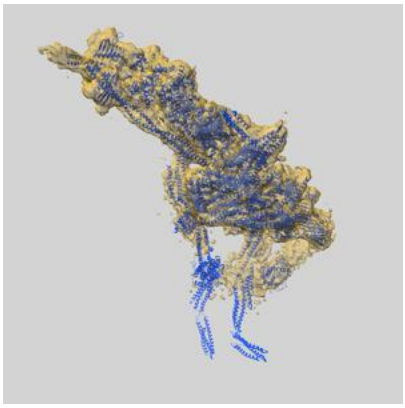
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3706 and PDB model 5NW4. Per-residue inclusion information can be found in section 3 on page 11.

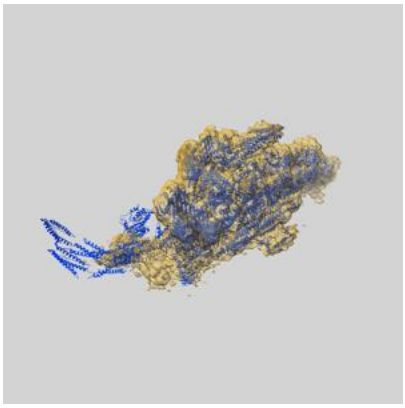
9.1 Map-model overlay



X



Y



Z

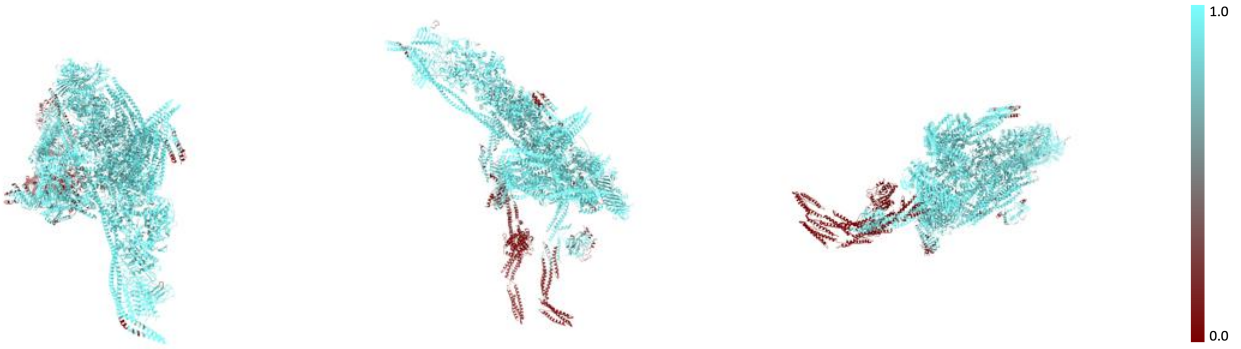
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

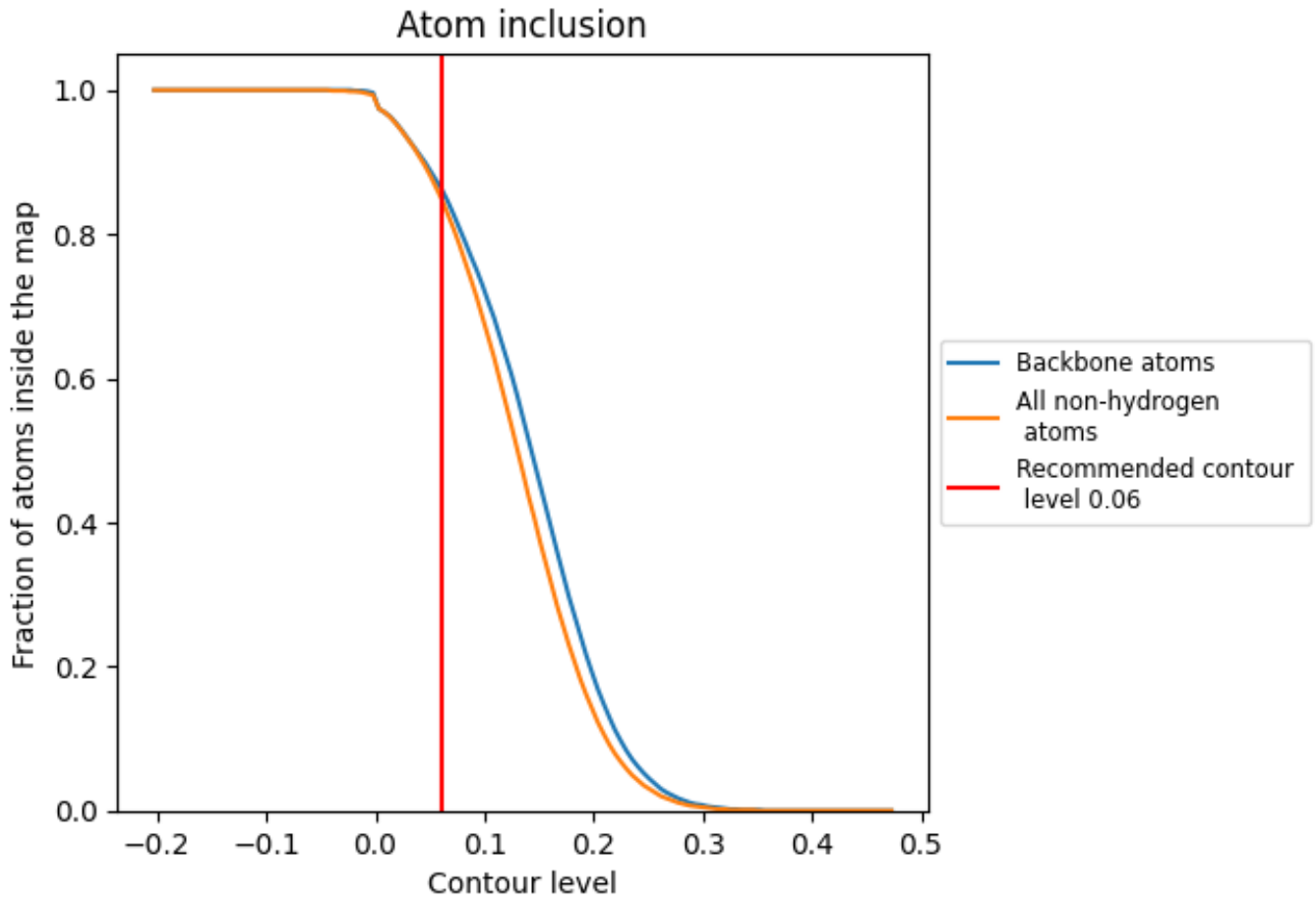
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 85% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8510	0.1130
1	0.8820	0.1180
2	0.8470	0.1060
5	0.8730	0.1620
6	0.9400	0.1530
A	0.4530	0.0490
B	0.7040	0.1350
C	0.8310	0.0370
D	0.9240	0.0580
E	0.0070	-0.0030
F	0.6190	0.0340
G	0.9310	0.1070
H	0.9350	0.1130
O	0.8870	0.1060
P	0.9040	0.1120
Q	0.8940	0.1140
R	0.6630	0.0470
S	0.8380	0.0580
T	0.9030	0.1120
U	0.9260	0.1170
V	0.9510	0.1170
W	0.9410	0.1070
X	0.9510	0.1140
Y	0.9630	0.1140
Z	0.9500	0.1220
a	0.9920	0.1980
b	0.9970	0.1830
c	1.0000	0.1760
d	0.9850	0.1680
e	0.5660	-0.0230
f	0.9770	0.2270
g	0.9480	0.1260
h	0.9990	0.1300
i	0.9990	0.1780
j	0.9620	0.1570

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Chain	Atom inclusion	Q-score
k	0.9200	0.1810
l	0.9700	0.1570
m	0.9600	0.1750
n	0.8950	0.1690
o	0.9930	0.1850