



## Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 02:34 pm GMT

PDB ID : 8CBQ  
EMDB ID : EMD-16549  
Title : structure of LEDGF/p75 PWWP domain bound to the H3K36 trimethylated dinucleosome  
Authors : Koutna, E.; Kouba, T.; Novacek, J.; Veverka, V.  
Deposited on : 2023-01-25  
Resolution : 4.00 Å(reported)  
Based on initial model : 3MVD

This is a Full wwPDB EM Validation 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.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
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



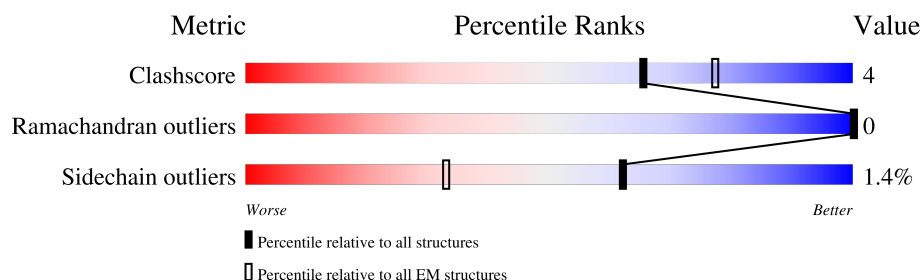
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	B	102	
1	F	102	
2	C	129	
2	G	129	
3	D	122	
3	H	122	
4	I	165	
5	J	165	

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Mol	Chain	Length	Quality of chain
6	K	530	<div><div><div></div><div></div><div></div></div><div>11%11%5%84%</div></div>
7	A	135	<div><div><div></div><div></div><div></div></div><div>67%7%26%</div></div>
7	E	135	<div><div><div></div><div></div><div></div></div><div>57%13%28%</div></div>



## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 12959 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 Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	82	Total	C	N	O	S	0	0
			657	416	128	112	1		
1	F	86	Total	C	N	O	S	0	0
			694	436	140	117	1		

- Molecule 2 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	107	Total	C	N	O	0	0
			823	519	161	143		
2	G	107	Total	C	N	O	0	0
			823	519	161	143		

- Molecule 3 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	94	Total	C	N	O	S	0	0
			736	463	132	139	2		
3	H	94	Total	C	N	O	S	0	0
			736	463	132	139	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	conflict	UNP P02281
H	29	THR	SER	conflict	UNP P02281

- Molecule 4 is a DNA chain called WIDOM 601 DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	150	Total	C	N	O	P	0	0
			3055	1452	552	901	150		



- Molecule 5 is a DNA chain called WIDOM 601 DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	150	Total	C	N	O	P	0	0
			3095	1465	581	899	150		

- Molecule 6 is a protein called PC4 and SFRS1-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	86	Total	C	N	O	S	0	0
			710	467	119	122	2		

- Molecule 7 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	100	Total	C	N	O	S	0	0
			829	525	160	141	3		
7	E	97	Total	C	N	O	S	0	0
			801	506	155	138	2		

There are 2 discrepancies between the modelled and reference sequences:

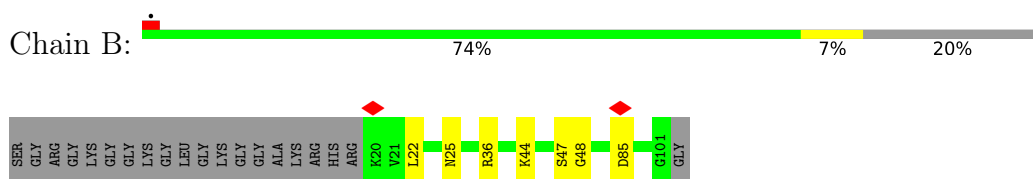
Chain	Residue	Modelled	Actual	Comment	Reference
A	110	ALA	CYS	conflict	UNP A0A310TTQ1
E	110	ALA	CYS	conflict	UNP A0A310TTQ1



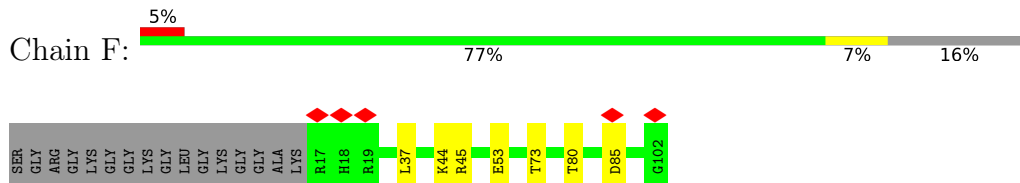
### 3 Residue-property plots [i](#)

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.

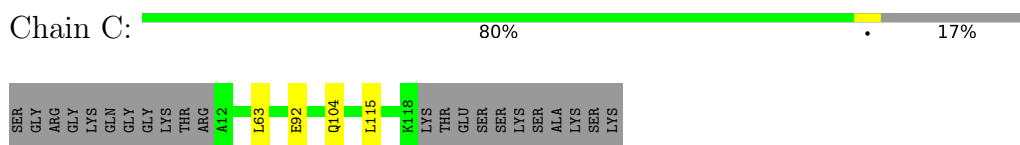
- Molecule 1: Histone H4



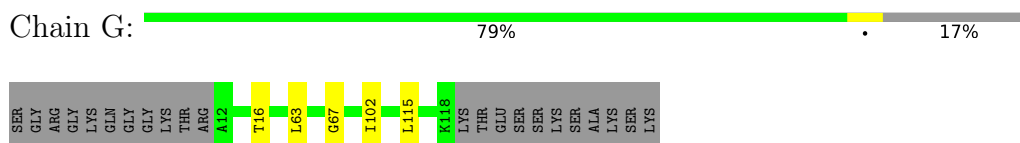
- Molecule 1: Histone H4



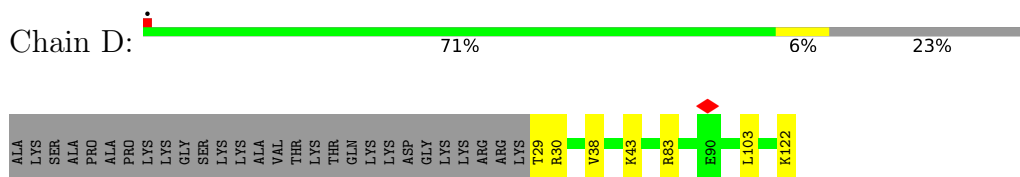
- Molecule 2: Histone H2A



- Molecule 2: Histone H2A



- Molecule 3: Histone H2B 1.1



- Molecule 3: Histone H2B 1.1






















	ALA	T29		V38	K43	H46	I58	R83	K122
LYS	SER	R30							
ALA	ALA	K31							
PRO	PRO								
ALA	ALA								
PRO	PRO								
LYS	LYS								
GLY	GLY								
SER	SER								
LYS	LYS								
ALA	ALA								
VAL	VAL								
THR	THR								
LYS	LYS								
THR	THR								
GLN	GLN								
LYS	LYS								
ASP	ASP								
GLY	GLY								
LYS	LYS								
ARG	ARG								
ARG	ARG								
LYS	LYS								

[illegible]

DG	DT	DC	DG	DC	DT	DG	DT	DC	DA	DA	DT	DC	DA	DT	DC	A-77	A-71	G-70	G-69	A-64	T-57	G-56	A-43	G-36	G-33	G-6	C7	G8	A17	T31	G32	G38	G46	G64	G65	G66	G67	G68	G69	G70	G71	G72	G73	G74	G75	G76	G77	G78	G79	G80	G81	G82	G83	G84	G85	G86	G87	G88	G89	G90	G91	G92	G93	G94	G95	G96	G97	G98	G99	G100	G101	G102	G103	G104	G105	G106	G107	G108	G109	G110	G111	G112	G113	G114	G115	G116	G117	G118	G119	G120	G121	G122	G123	G124	G125	G126	G127	G128	G129	G130	G131	G132	G133	G134	G135	G136	G137	G138	G139	G140	G141	G142	G143	G144	G145	G146	G147	G148	G149	G150	G151	G152	G153	G154	G155	G156	G157	G158	G159	G160	G161	G162	G163	G164	G165	G166	G167	G168	G169	G170	G171	G172	G173	G174	G175	G176	G177	G178	G179	G180	G181	G182	G183	G184	G185	G186	G187	G188	G189	G190	G191	G192	G193	G194	G195	G196	G197	G198	G199	G200	G201	G202	G203	G204	G205	G206	G207	G208	G209	G210	G211	G212	G213	G214	G215	G216	G217	G218	G219	G220	G221	G222	G223	G224	G225	G226	G227	G228	G229	G230	G231	G232	G233	G234	G235	G236	G237	G238	G239	G240	G241	G242	G243	G244	G245	G246	G247	G248	G249	G250	G251	G252	G253	G254	G255	G256	G257	G258	G259	G260	G261	G262	G263	G264	G265	G266	G267	G268	G269	G270	G271	G272	G273	G274	G275	G276	G277	G278	G279	G280	G281	G282	G283	G284	G285	G286	G287	G288	G289	G290	G291	G292	G293	G294	G295	G296	G297	G298	G299	G300	G301	G302	G303	G304	G305	G306	G307	G308	G309	G310	G311	G312	G313	G314	G315	G316	G317	G318	G319	G320	G321	G322	G323	G324	G325	G326	G327	G328	G329	G330	G331	G332	G333	G334	G335	G336	G337	G338	G339	G340	G341	G342	G343	G344	G345	G346	G347	G348	G349	G350	G351	G352	G353	G354	G355	G356	G357	G358	G359	G360	G361	G362	G363	G364	G365	G366	G367	G368	G369	G370	G371	G372	G373	G374	G375	G376	G377	G378	G379	G380	G381	G382	G383	G384	G385	G386	G387	G388	G389	G390	G391	G392	G393	G394	G395	G396	G397	G398	G399	G400	G401	G402	G403	G404	G405	G406	G407	G408	G409	G410	G411	G412	G413	G414	G415	G416	G417	G418	G419	G420	G421	G422	G423	G424	G425	G426	G427	G428	G429	G430	G431	G432	G433	G434	G435	G436	G437	G438	G439	G440	G441	G442	G443	G444	G445	G446	G447	G448	G449	G450	G451	G452	G453	G454	G455	G456	G457	G458	G459	G460	G461	G462	G463	G464	G465	G466	G467	G468	G469	G470	G471	G472	G473	G474	G475	G476	G477	G478	G479	G480	G481	G482	G483	G484	G485	G486	G487	G488	G489	G490	G491	G492	G493	G494	G495	G496	G497	G498	G499	G500	G501	G502	G503	G504	G505	G506	G507	G508	G509	G510	G511	G512	G513	G514	G515	G516	G517	G518	G519	G520	G521	G522	G523	G524	G525	G526	G527	G528	G529	G530	G531	G532	G533	G534	G535	G536	G537	G538	G539	G540	G541	G542	G543	G544	G545	G546	G547	G548	G549	G550
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M1	T2	R3	D4	F5	K6	P7	G8	D9	L10	I11	F12	A13	K14	M15	K16	G17	Y18	P19	H20	A23	R24	V25	D26	E27	V28	P29	ASP	GLY	ALA	VAL	LYS	P35	P36	T37	N38	K39	L40	P41	I42	F43	F44	F45	G46	T47	H48	E49	T50	A51	F52	L53	G54	P55	I58	F59	P60	Y61	S62
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  R74
  K75
  N78
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  G80
  L81
  V82
  E83
  E84
  D85
  N86
  N87
  P88
  K89
  V90
  K91
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GLU	ASP	VAL	THR	LYS	ALA	VAL	ASP	ILE	THR	THR	PRO	LYS	ALA	ALA	ARG	ARG	GLY	ARG	LYS	ARG	VAL	GLU	THR	GLU	GLU	VAL	VAL	VAL	THR	THR	ALA	ALA	SER	VAL	ASN	LEU	LYS	VAL	VAL	SER	LYS	ARG	ARG	PRO	ALA	ALA	THR	THR	GLU	VAL	LYS
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PRO	LYS	PRO	ARG	GLY	ARG	PRO	LYS	LYS	MET	VAL	LYS	GLN	GLN	PRO	PRO	CYS	SER	SER	ASP	ILE	THR	GLU	GLU	GLU	ASP	LYS	SER	LYS	LYS	LYS	GLY	GLN	GLU	GLU	GLU	GLN	LYS	PRO	PRO	LYS	LYS	GLN	LYS	LYS	ASP	GLU	GLU	GLU	GLY	GLN	LYS	PRO	ARG	LYS	LYS	GLU	PRO	GLU	ASP
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LYS GLU LYS LYS LYS VAL GLU GLU SER LYS ARG LYS ASN LEU ALA LYS THR THR GLY VAL THR SER THR SER ASP SER GLU GLU GLU GLY GLY ASP ASP GLN GLU GLU GLU LYS LYS LYS LYS LYS GLY GLY ARG ASN PHE GLN GLN THR THR ALA HIS ARG ARG MET LEU LYS GLY GLN HIS HIS GLU LYS

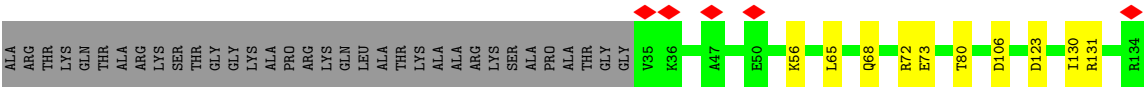
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ASN	ARG	CYS	ILE	GLU	ALA	LEU	ASP	GLU	LEU	ALA	SER	LEU	GLN	THR	MET	GLN	GLN	VAL	ALA	LYS	HIS	THR	GLU	MET	ILE	THR	THR	LEU	LYS	LYS	ILE	ARG	ARG	PHE	LYS	VAL	VAL	SER	SER	GLN	GLN	VAL	ILE	ILE	MET	GLU	LYS	TYR	ASN	THR	LYS	PHE	LYS	ASN	MET	PHE	LEU	VAL
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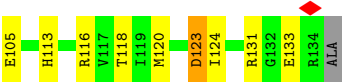
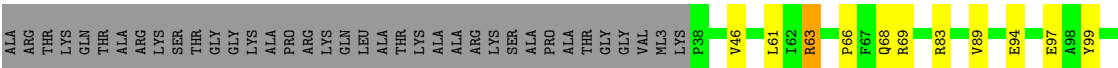
[illegible]

GLN	HIS	ASN	GLY	GLU	SER	ASN	GLU	ASP	SER	LYS	ASP	ASN	HIS	GLU	ALA	SER	THR	LYS	LYS	LYS	PRO	SER	SER	SER	GLU	GLU	ARG	GLU	THR	GLU	ILE	SER	LEU	LYS	ASP	SER	THR	LEU	ASP	ASN
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● Molecule 7: Histone H3





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	49681	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.130	Depositor
Minimum map value	-0.878	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	364.32, 364.32, 364.32	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.656, 1.656, 1.656	Depositor



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ML3

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	B	0.44	0/664	0.52	0/889
1	F	0.42	0/702	0.53	0/937
2	C	0.40	0/833	0.49	0/1124
2	G	0.40	0/833	0.49	0/1124
3	D	0.39	0/747	0.47	0/1004
3	H	0.39	0/747	0.47	0/1004
4	I	0.86	0/3422	0.95	1/5274 (0.0%)
5	J	0.87	0/3476	0.93	0/5368
6	K	0.32	0/736	0.45	0/992
7	A	0.43	0/828	0.47	0/1110
7	E	0.41	0/813	0.47	0/1091
All	All	0.68	0/13801	0.76	1/19917 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	20	DG	P-O3'-C3'	5.17	125.91	119.70

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	B	657	0	706	6	0
1	F	694	0	742	6	0
2	C	823	0	882	4	0
2	G	823	0	882	5	0
3	D	736	0	760	5	0
3	H	736	0	760	7	0
4	I	3055	0	1685	13	0
5	J	3095	0	1684	14	0
6	K	710	0	701	17	0
7	A	829	0	879	7	0
7	E	801	0	841	15	0
All	All	12959	0	10522	70	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 4.

All (70) 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)
4:I:-64:DC:H42	5:J:64:DG:H1	1.35	0.72
6:K:1:MET:HB3	6:K:4:ASP:HB2	1.76	0.68
4:I:69:DC:H42	5:J:-69:DG:H1	1.43	0.66
4:I:-38:DC:O2	5:J:38:DG:N2	2.36	0.58
4:I:36:DC:H42	5:J:-36:DG:H1	1.52	0.58
6:K:3:ARG:HH22	6:K:27:GLU:HG3	1.69	0.57
3:D:83:ARG:NH2	4:I:-33:DA:OP2	2.36	0.56
6:K:83:GLU:HA	6:K:86:ASN:HD22	1.71	0.55
6:K:40:LEU:HD11	6:K:55:PRO:HB3	1.87	0.55
7:E:116:ARG:NH2	7:E:123:ASP:OD1	2.40	0.55
6:K:82:TRP:O	6:K:86:ASN:ND2	2.40	0.54
3:H:83:ARG:NH2	5:J:-33:DG:OP2	2.33	0.54
5:J:-64:DA:OP1	7:A:56:LYS:NZ	2.41	0.54
1:B:36:ARG:NH2	4:I:-13:DA:OP1	2.42	0.53
6:K:19:PRO:HD2	6:K:74:ARG:HH22	1.73	0.52
1:F:37:LEU:HD23	7:E:61:LEU:HD12	1.90	0.52
3:H:29:THR:OG1	3:H:30:ARG:N	2.43	0.52
6:K:28:VAL:HG11	6:K:37:THR:HG23	1.90	0.51
2:C:115:LEU:HB3	1:F:44:LYS:HD3	1.91	0.51
3:D:29:THR:OG1	3:D:30:ARG:N	2.43	0.51
7:E:116:ARG:NH1	7:E:120:MET:SD	2.84	0.51
1:B:22:LEU:HB3	1:B:25:ASN:HD21	1.75	0.51
7:A:68:GLN:HE21	7:A:72:ARG:HH21	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:1:MET:HG2	6:K:3:ARG:H	1.76	0.50
6:K:24:ARG:HH11	6:K:89:LYS:HD2	1.77	0.49
5:J:31:DT:H2''	5:J:32:DG:H5''	1.95	0.49
2:G:16:THR:HA	5:J:-43:DA:H5''	1.94	0.49
4:I:-46:DC:H42	5:J:46:DG:H1	1.60	0.49
7:E:61:LEU:N	7:E:97:GLU:OE2	2.46	0.48
7:E:68:GLN:HG3	7:E:89:VAL:HG11	1.96	0.48
4:I:-67:DA:H2''	4:I:-66:DA:H5''	1.95	0.48
1:B:25:ASN:ND2	7:A:73:GLU:OE1	2.36	0.47
6:K:89:LYS:O	6:K:91:LYS:NZ	2.47	0.47
6:K:12:PHE:HB2	6:K:59:PHE:HB2	1.95	0.47
2:G:67:GLY:HA3	3:H:46:HIS:CD2	2.50	0.46
5:J:17:DA:H2'	7:A:65:LEU:HD12	1.97	0.46
2:C:92:GLU:HG3	3:D:103:LEU:HG	1.96	0.46
4:I:6:DC:H42	5:J:-6:DG:H1	1.64	0.46
4:I:9:DG:H3'	7:E:46:VAL:HG21	1.98	0.45
7:E:63:ARG:HB2	7:E:66:PRO:HD2	1.98	0.45
1:F:80:THR:HG22	7:E:83:ARG:HB2	1.98	0.45
1:B:85:ASP:N	1:B:85:ASP:OD1	2.50	0.45
6:K:12:PHE:HB3	6:K:20:HIS:HB3	1.99	0.45
7:A:106:ASP:OD2	7:A:131:ARG:NH2	2.44	0.44
7:A:130:ILE:HG22	7:E:131:ARG:HG3	2.00	0.44
5:J:7:DC:H2'	5:J:8:DG:C8	2.53	0.44
2:G:102:ILE:HG23	3:H:58:ILE:HD13	1.99	0.44
1:F:45:ARG:NH1	7:E:118:THR:OG1	2.41	0.44
1:B:47:SER:OG	1:B:48:GLY:N	2.51	0.43
6:K:5:PHE:HB3	6:K:9:ASP:HB3	1.99	0.43
6:K:26:ASP:OD1	6:K:89:LYS:NZ	2.50	0.43
7:A:123:ASP:OD1	7:E:113:HIS:NE2	2.43	0.43
3:H:43:LYS:HA	3:H:43:LYS:HD3	1.78	0.43
5:J:-57:DT:H2''	5:J:-56:DG:C8	2.54	0.43
2:C:63:LEU:HD11	3:D:38:VAL:HG13	2.01	0.42
3:H:31:LYS:HA	3:H:31:LYS:HD2	1.88	0.42
3:D:43:LYS:HA	3:D:43:LYS:HD3	1.78	0.42
2:C:104:GLN:NE2	7:E:94:GLU:OE2	2.40	0.42
1:F:53:GLU:HG2	7:E:124:ILE:HD12	2.02	0.42
7:E:99:TYR:OH	7:E:133:GLU:OE1	2.37	0.42
5:J:-71:DA:H2''	5:J:-70:DG:C8	2.55	0.41
4:I:17:DA:OP1	7:E:69:ARG:NH2	2.53	0.41
1:F:73:THR:OG1	1:F:85:ASP:OD2	2.28	0.41
6:K:87:ASN:HB3	6:K:90:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:15:DT:H2''	4:I:16:DA:C8	2.55	0.41
6:K:5:PHE:HB2	6:K:25:VAL:HG21	2.02	0.41
6:K:78:ASN:HA	6:K:81:LEU:HB2	2.03	0.40
1:B:44:LYS:HD2	2:G:115:LEU:HB3	2.04	0.40
2:G:63:LEU:HD11	3:H:38:VAL:HG13	2.04	0.40
4:I:63:DA:H2''	4:I:64:DT:H5''	2.04	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	B	80/102 (78%)	77 (96%)	3 (4%)	0	100	100
1	F	84/102 (82%)	80 (95%)	4 (5%)	0	100	100
2	C	105/129 (81%)	102 (97%)	3 (3%)	0	100	100
2	G	105/129 (81%)	102 (97%)	3 (3%)	0	100	100
3	D	92/122 (75%)	91 (99%)	1 (1%)	0	100	100
3	H	92/122 (75%)	91 (99%)	1 (1%)	0	100	100
6	K	82/530 (16%)	70 (85%)	12 (15%)	0	100	100
7	A	97/135 (72%)	94 (97%)	3 (3%)	0	100	100
7	E	95/135 (70%)	93 (98%)	2 (2%)	0	100	100
All	All	832/1506 (55%)	800 (96%)	32 (4%)	0	100	100

There are no Ramachandran outliers to report.



### 5.3.2 Protein sidechains ⓘ

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	B	68/78 (87%)	68 (100%)	0	100	100
1	F	71/78 (91%)	71 (100%)	0	100	100
2	C	84/101 (83%)	84 (100%)	0	100	100
2	G	84/101 (83%)	84 (100%)	0	100	100
3	D	80/102 (78%)	79 (99%)	1 (1%)	65	77
3	H	80/102 (78%)	79 (99%)	1 (1%)	65	77
6	K	76/470 (16%)	72 (95%)	4 (5%)	19	43
7	A	86/108 (80%)	85 (99%)	1 (1%)	67	78
7	E	84/108 (78%)	81 (96%)	3 (4%)	30	52
All	All	713/1248 (57%)	703 (99%)	10 (1%)	62	75

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	122	LYS
3	H	122	LYS
6	K	40	LEU
6	K	50	THR
6	K	58	ILE
6	K	73	LYS
7	A	80	THR
7	E	63	ARG
7	E	105	GLU
7	E	123	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	25	ASN
1	F	75	HIS
6	K	64	ASN

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Mol	Chain	Res	Type
6	K	86	ASN
7	A	68	GLN
7	E	76	GLN
7	E	93	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	ML3	A	36	7	10,11,12	0.79	0	10,14,16	0.82	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ML3	A	36	7	-	1/8/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	36	ML3	CE-CD-SG-CB



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 [i](#)

This section contains visualisations of the EMDB entry EMD-16549. These allow visual inspection of the internal detail of the map and identification of artifacts.

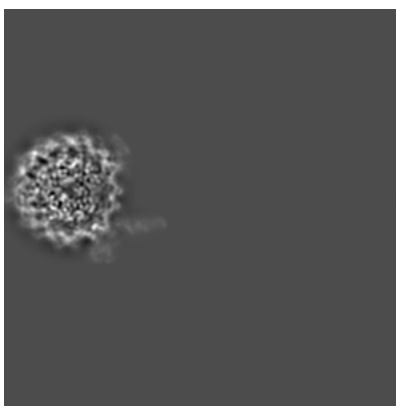
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



X

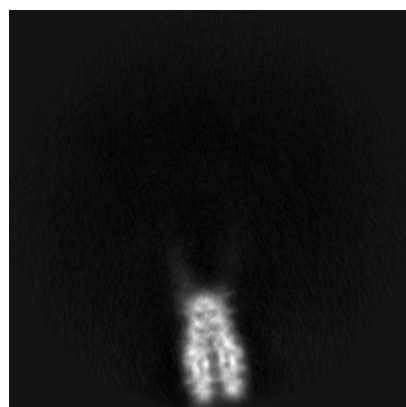


Y

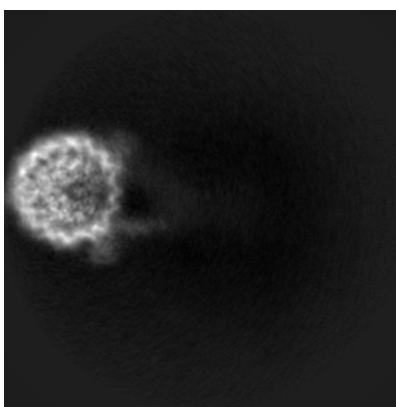


Z

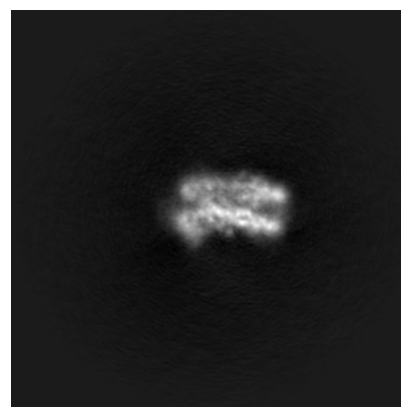
#### 6.1.2 Raw map



X



Y



Z

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

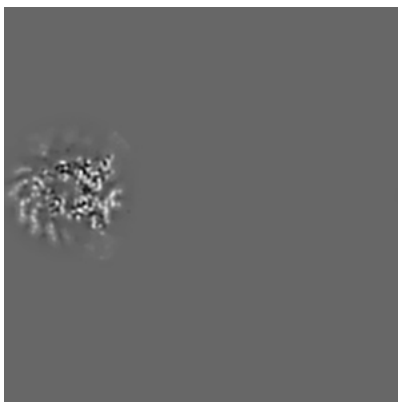


## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 110

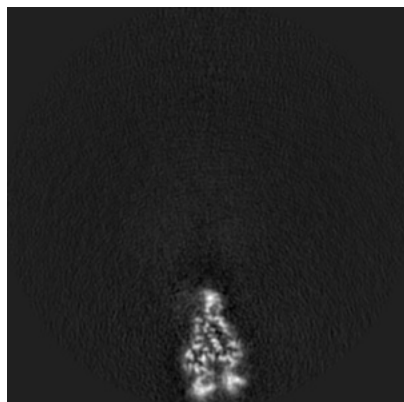


Y Index: 110

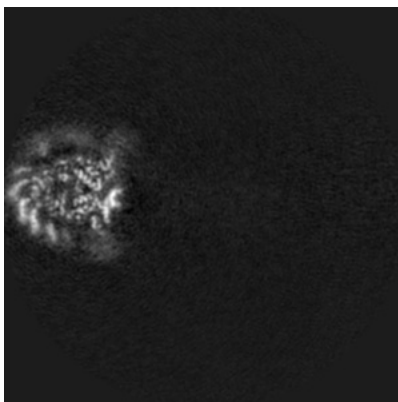


Z Index: 110

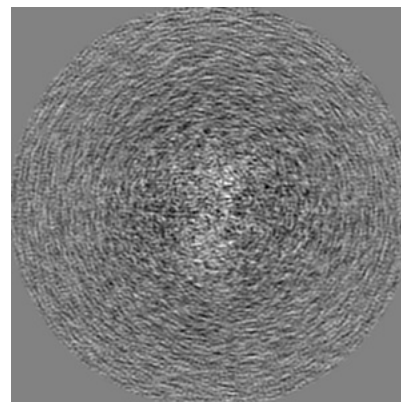
### 6.2.2 Raw map



X Index: 110



Y Index: 110



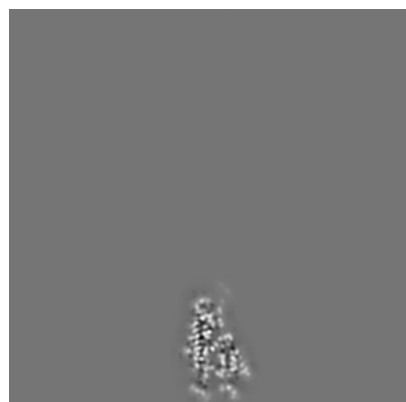
Z Index: 110

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

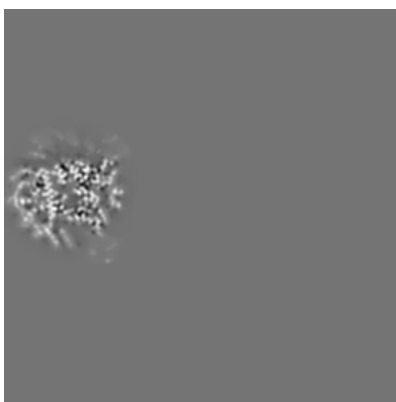


## 6.3 Largest variance slices [i](#)

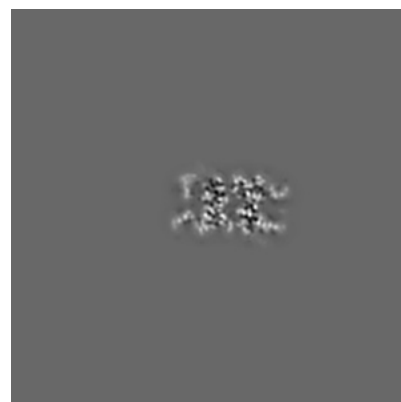
### 6.3.1 Primary map



X Index: 128

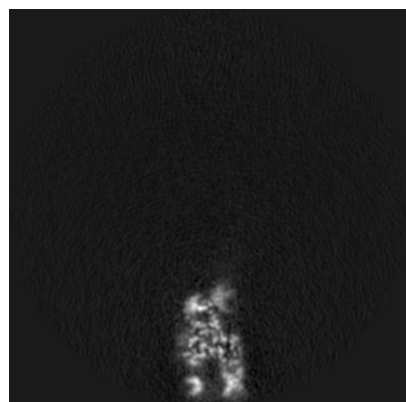


Y Index: 108

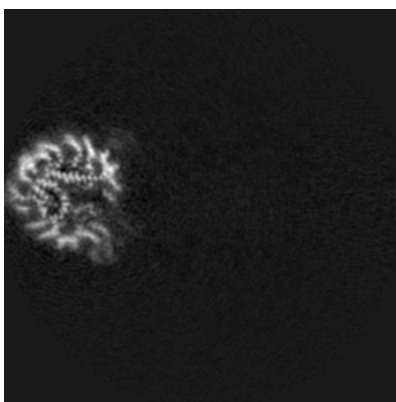


Z Index: 31

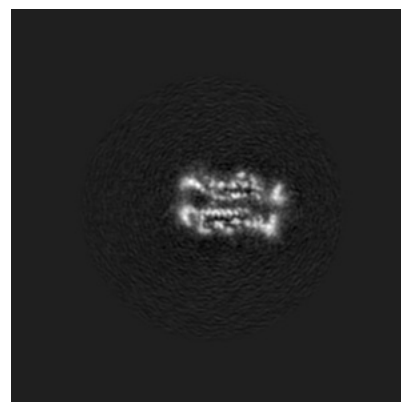
### 6.3.2 Raw map



X Index: 134



Y Index: 103



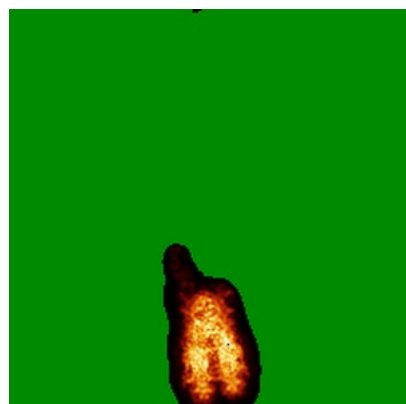
Z Index: 25

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

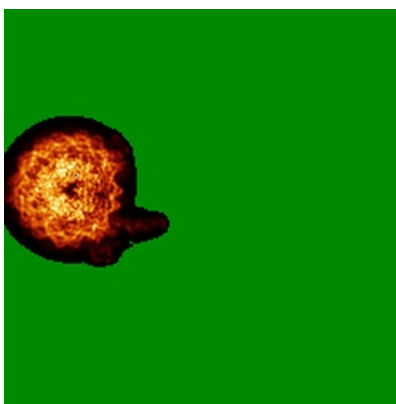


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

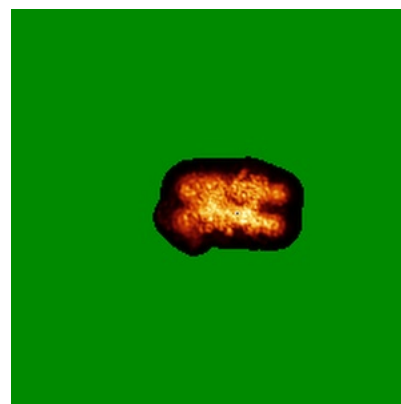
### 6.4.1 Primary map



X

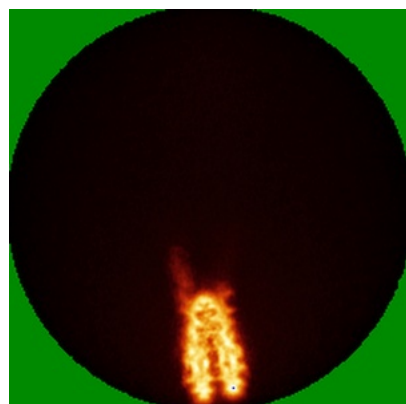


Y

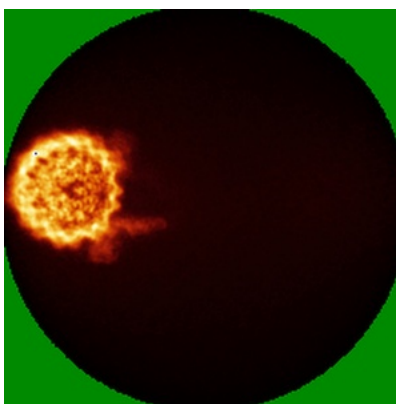


Z

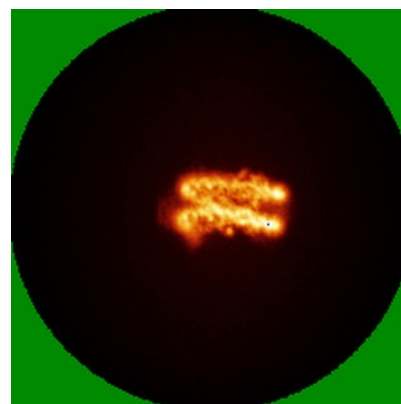
### 6.4.2 Raw map



X



Y



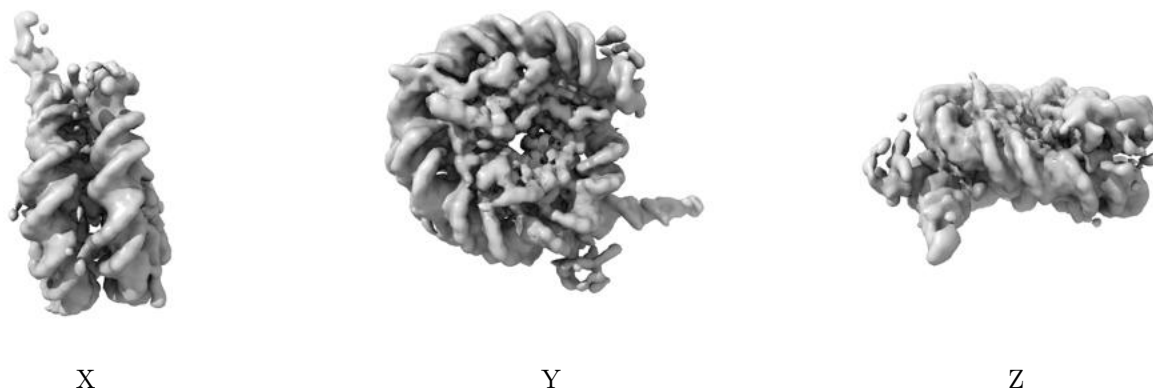
Z

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.



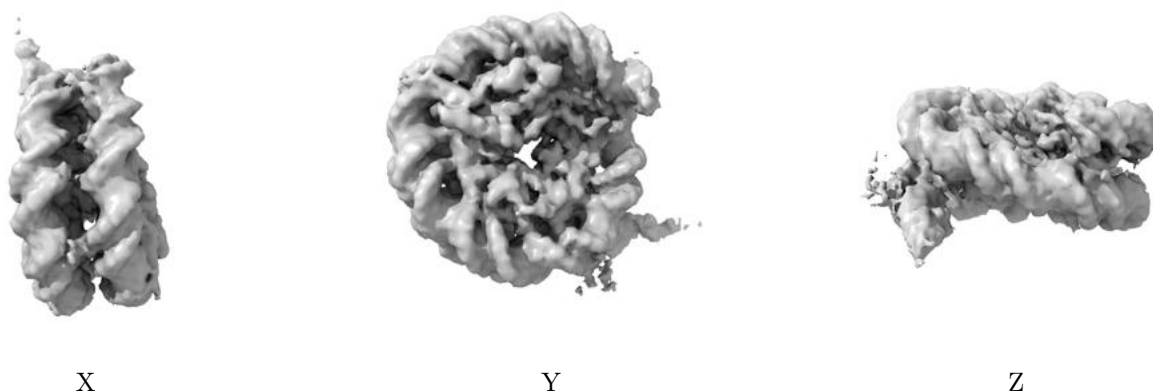
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



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.

### 6.5.2 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.



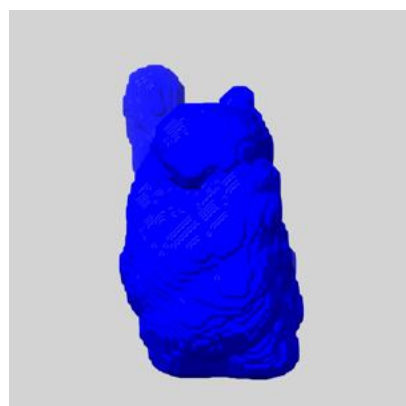
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

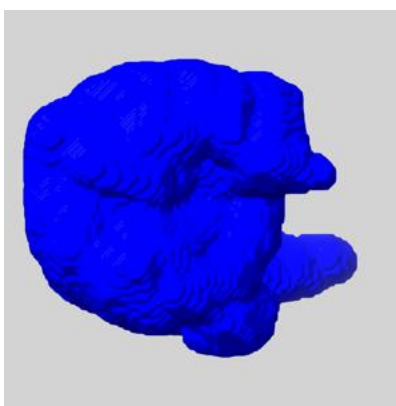
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

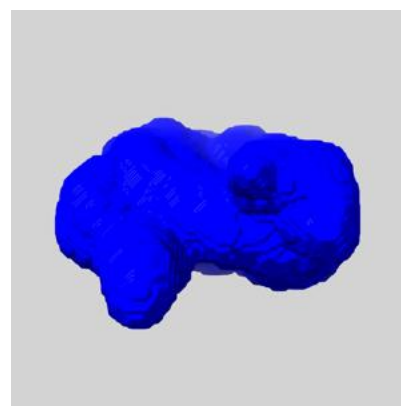
### 6.6.1 emd\_16549\_msk\_1.map [i](#)



X



Y



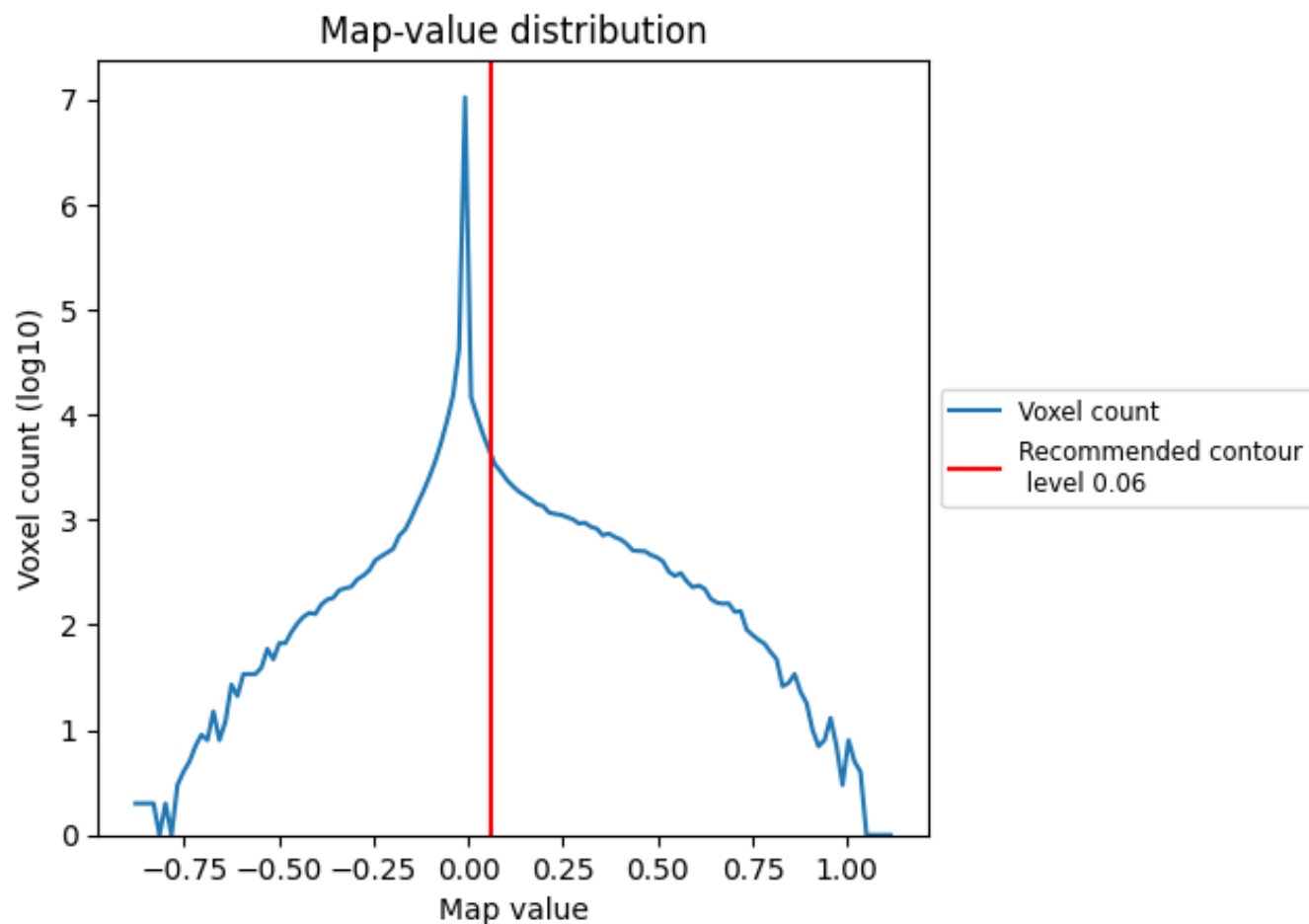
Z



## 7 Map analysis [i](#)

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

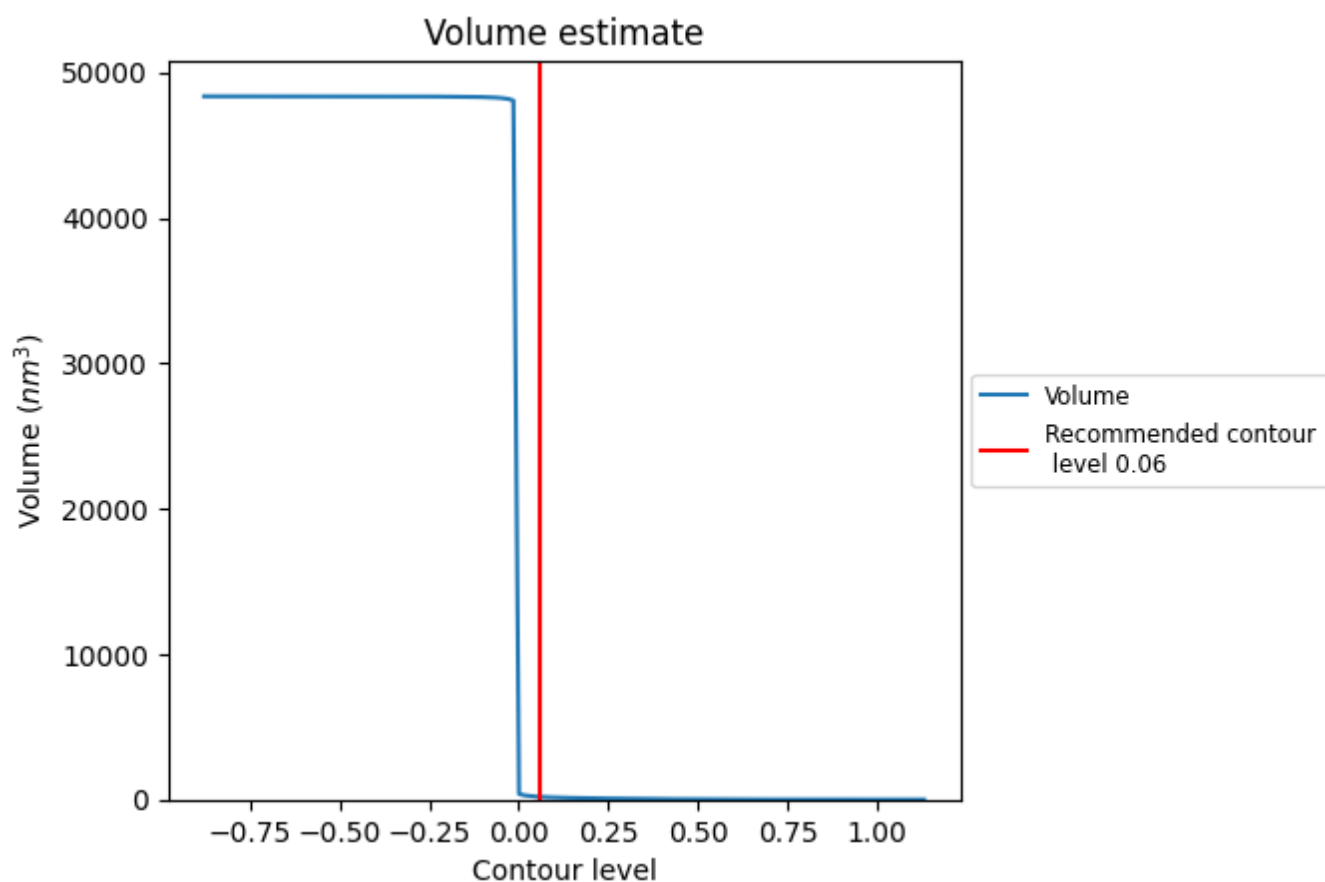
### 7.1 Map-value distribution [i](#)



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](#)

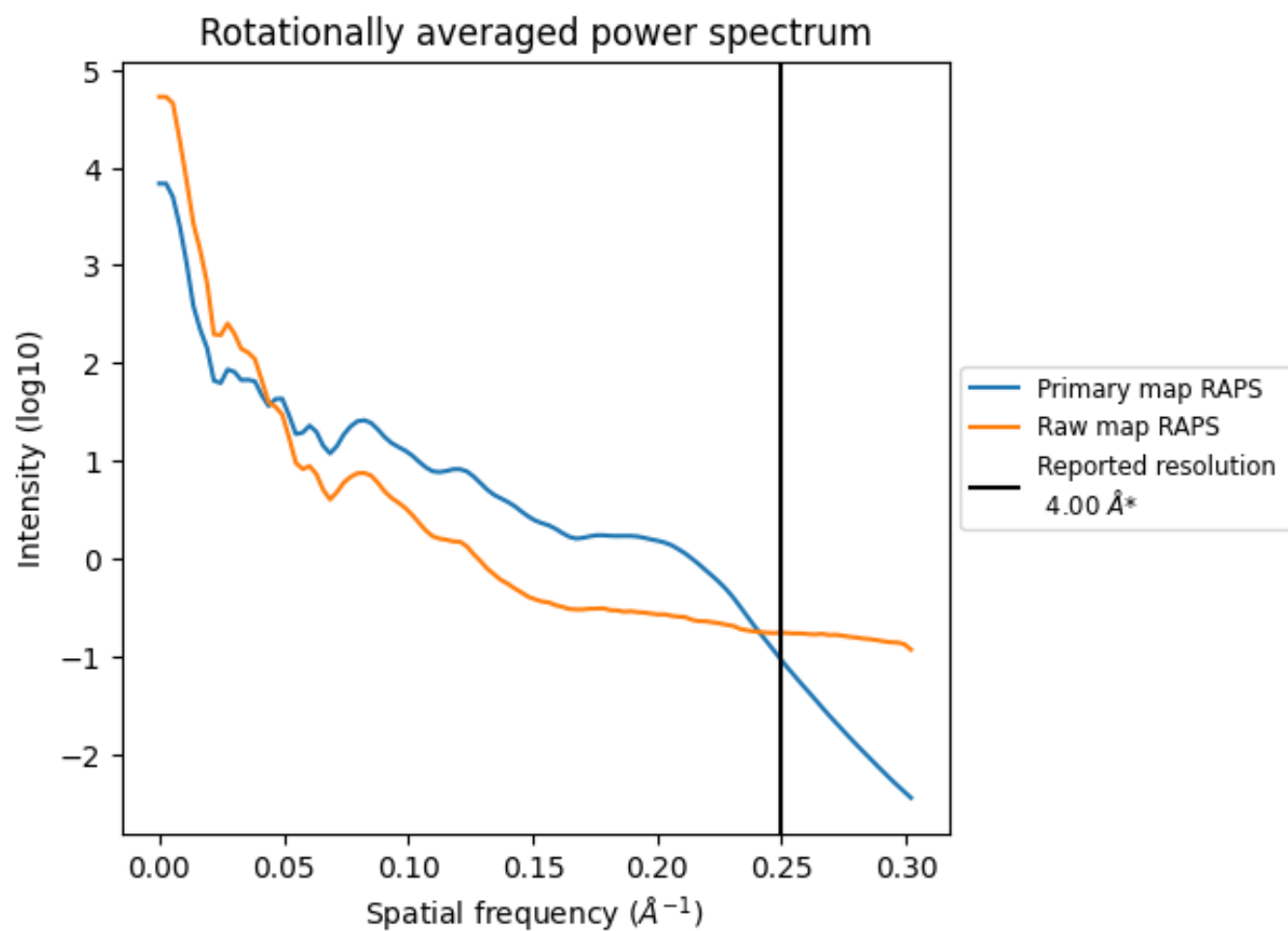


The volume at the recommended contour level is 183 nm<sup>3</sup>; this corresponds to an approximate mass of 165 kDa.

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 ⓘ



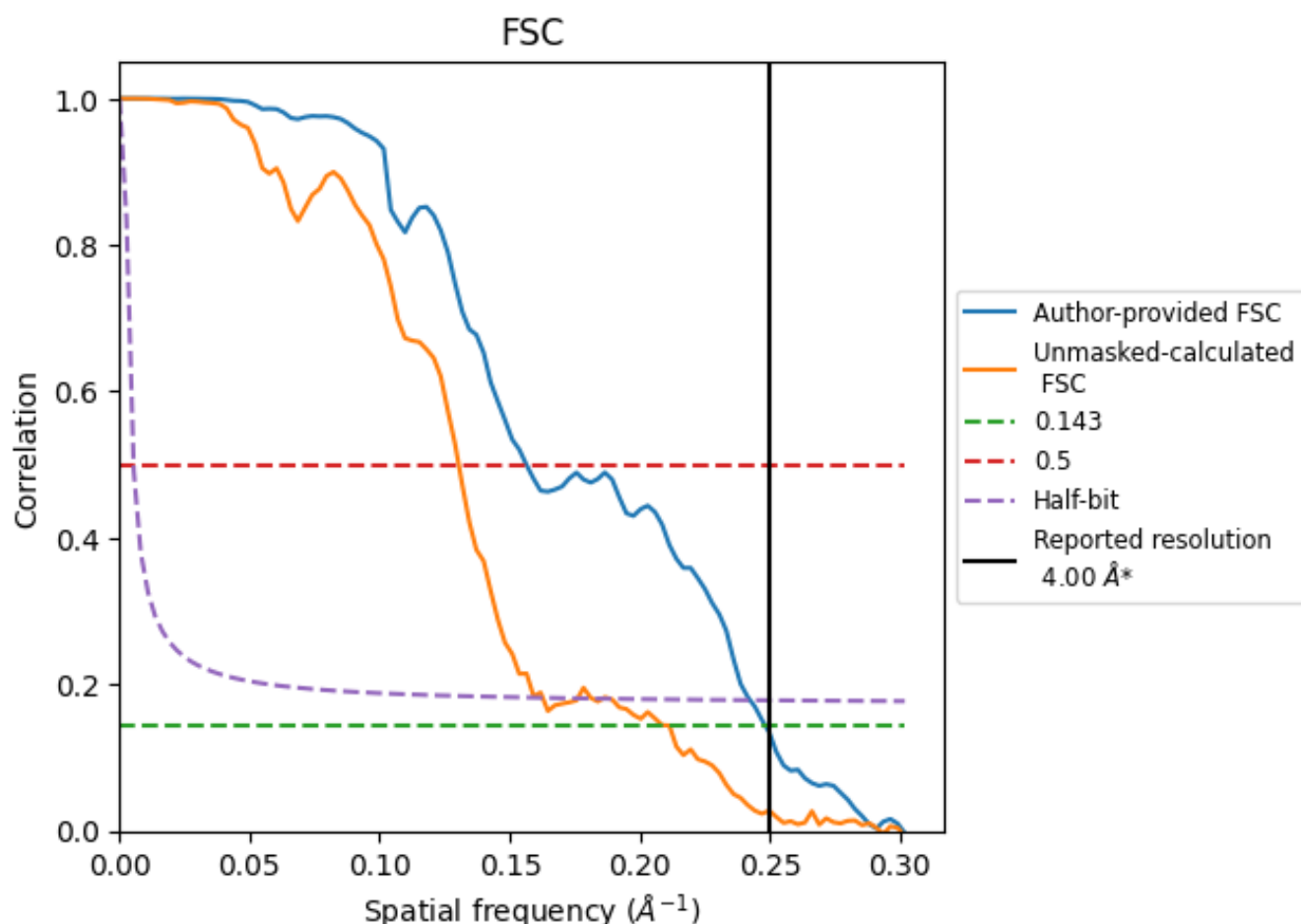
\*Reported resolution corresponds to spatial frequency of 0.250 Å<sup>-1</sup>



## 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 0.250 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	4.00	-	-
Author-provided FSC curve	4.03	6.40	4.12
Unmasked-calculated*	4.73	7.67	6.15

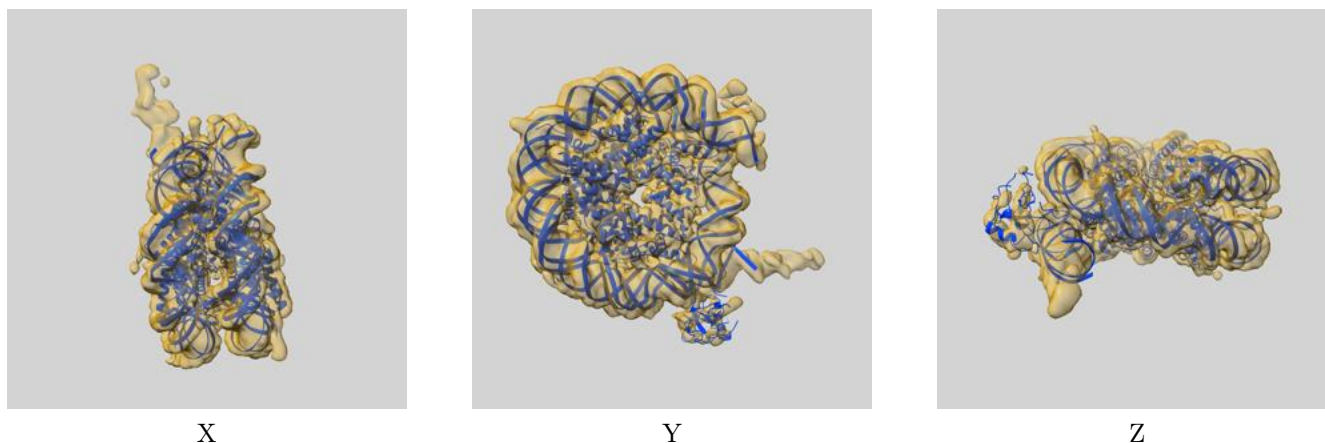
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.73 differs from the reported value 4.0 by more than 10 %



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

This section contains information regarding the fit between EMDB map EMD-16549 and PDB model 8CBQ. Per-residue inclusion information can be found in section [3](#) on page [6](#).

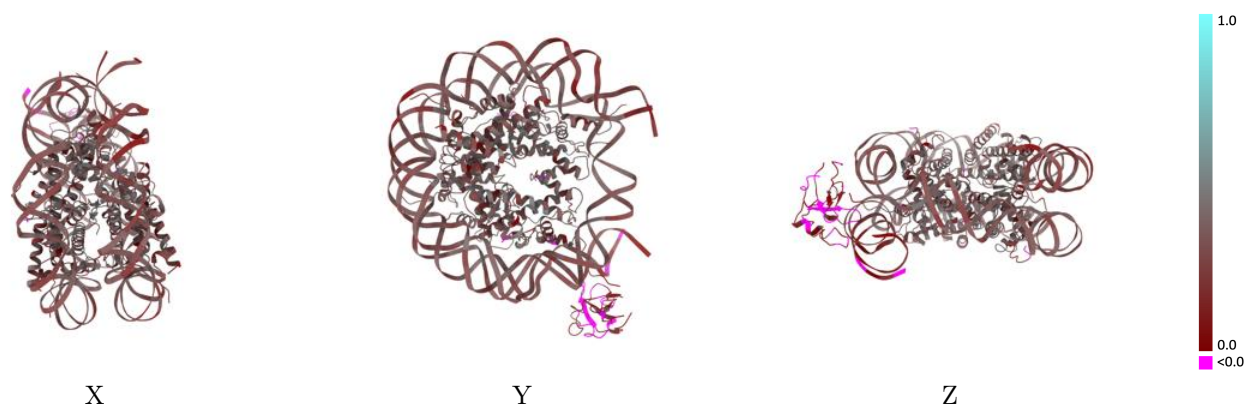
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.06 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.

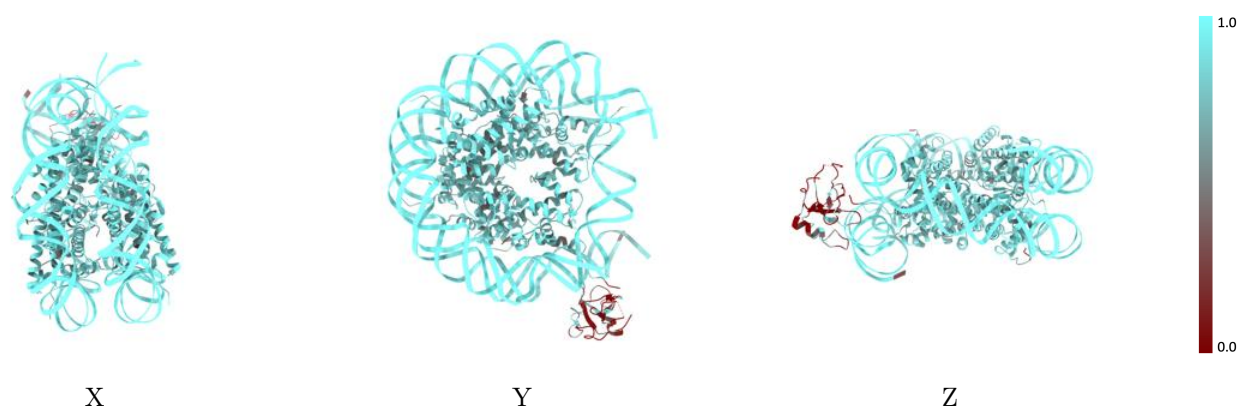


## 9.2 Q-score mapped to coordinate model [i](#)



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

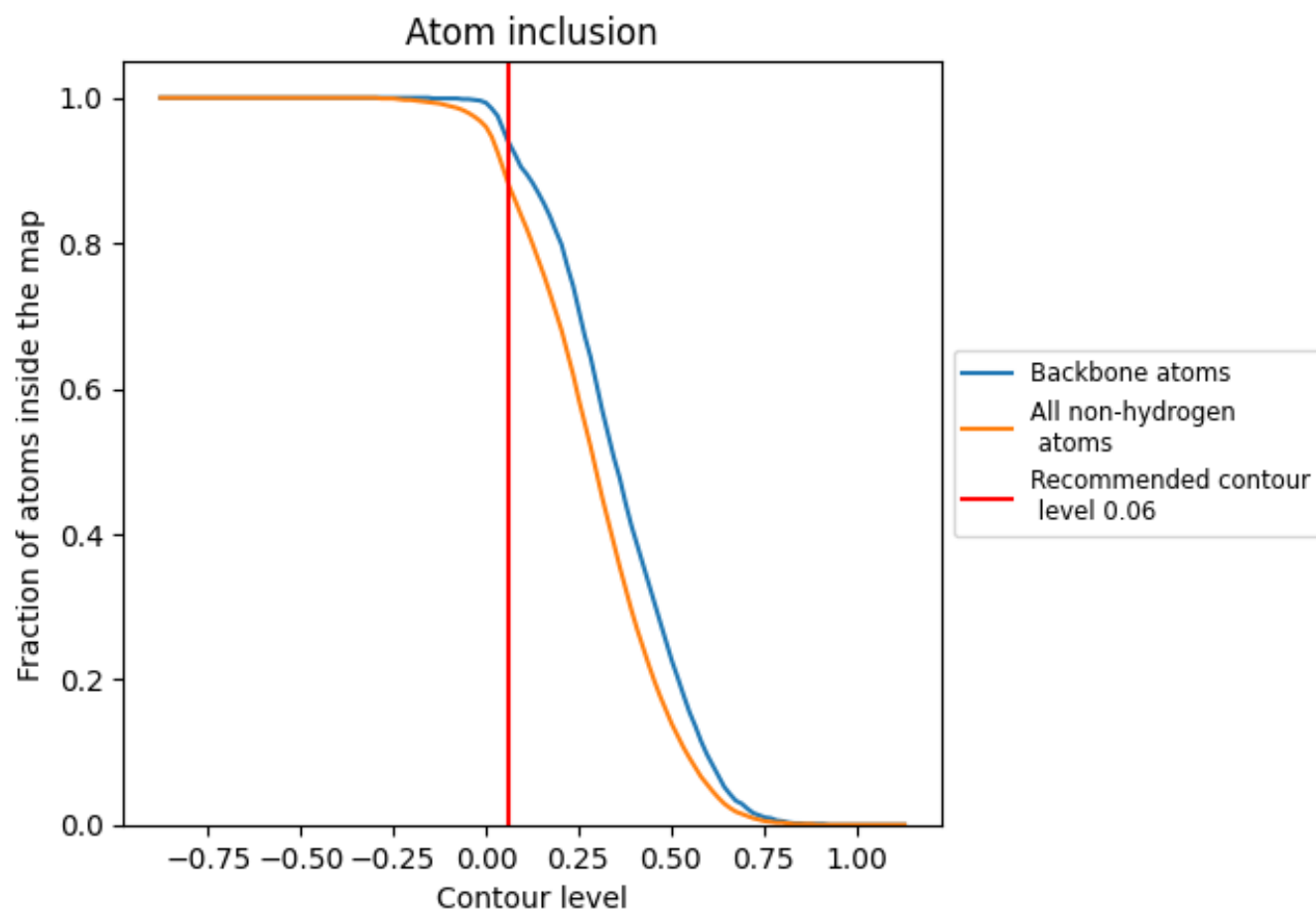
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.06).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 88% 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	<div></div> 0.8830	<div></div> 0.3040
A	<div></div> 0.8260	<div></div> 0.3310
B	<div></div> 0.8690	<div></div> 0.3570
C	<div></div> 0.8530	<div></div> 0.3400
D	<div></div> 0.8470	<div></div> 0.3300
E	<div></div> 0.8510	<div></div> 0.3390
F	<div></div> 0.8420	<div></div> 0.3340
G	<div></div> 0.8710	<div></div> 0.3400
H	<div></div> 0.8670	<div></div> 0.3430
I	<div></div> 0.9760	<div></div> 0.2960
J	<div></div> 0.9780	<div></div> 0.2970
K	<div></div> 0.3030	<div></div> 0.0630

1.0

0.0

<0.0