Full wwPDB EM Validation Report ⓘ

Oct 30, 2023 – 04:46 PM JST

PDB ID	:	7XFJ
EMDB ID	:	EMD-33174
Title	:	Structure of nucleosome-AAG complex (T-50I, post-catalytic state)
Authors	:	Zheng, L.; Tsai, B.; Gao, N.
Deposited on	:	2022-04-01
Resolution	:	3.00 Å(reported)

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:

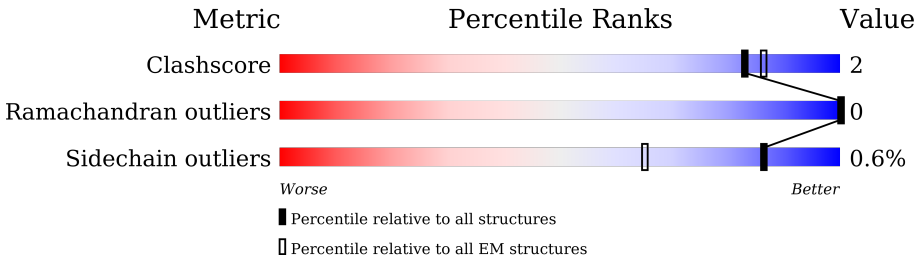
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.00 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	A	136	63% 9% 29%
1	E	136	62% 6% 32%
2	B	103	70% 7% 23%
2	F	103	71% 10% 19%
3	C	130	72% 5% 22%
3	G	130	78% 5% 17%
4	D	126	68% 28%
4	H	126	63% 10% 27%

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Mol	Chain	Length	Quality of chain
5	I	152	
6	J	152	
7	K	298	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12805 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 H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	97	Total	C	N	O	S	0	0
			801	505	155	138	3		
1	E	92	Total	C	N	O	S	0	0
			750	473	142	132	3		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	79	Total	C	N	O	S	0	0
			627	395	121	110	1		
2	F	83	Total	C	N	O	S	0	0
			662	418	129	114	1		

- Molecule 3 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	101	Total	C	N	O	0	0
			780	489	156	135		
3	G	108	Total	C	N	O	0	0
			834	525	165	144		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	99	ARG	GLY	conflict	UNP P06897
G	99	ARG	GLY	conflict	UNP P06897

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	91	Total	C	N	O	S	0	0
			708	447	125	134	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	92	Total 719	C 453	N 129	O 135	S 2	0	0

- Molecule 5 is a DNA chain called DNA (152-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	131	Total 2690	C 1270	N 505	O 784	P 131	0	0

- Molecule 6 is a DNA chain called DNA (152-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	131	Total 2668	C 1266	N 486	O 786	P 130	0	0

- Molecule 7 is a protein called DNA-3-methyladenine glycosylase.

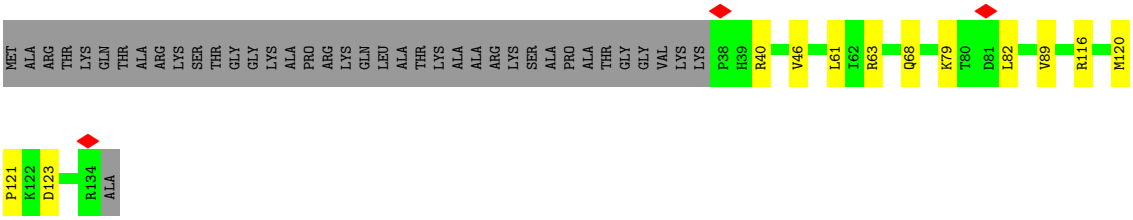
Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	200	Total 1566	C 986	N 290	O 281	S 9	0	0

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.

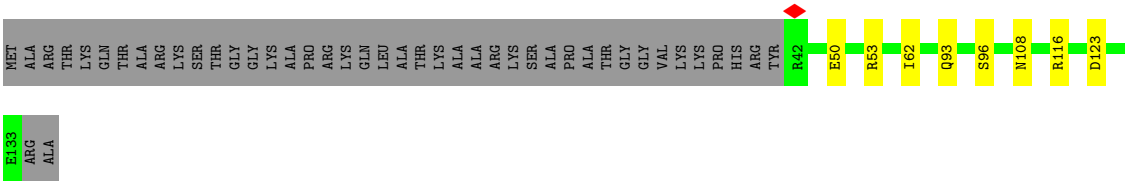
• Molecule 1: Histone H3.2

Chain A:



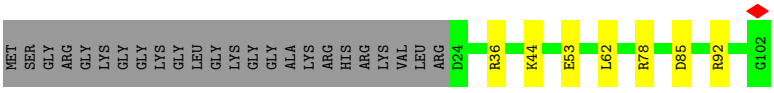
• Molecule 1: Histone H3.2

Chain E:



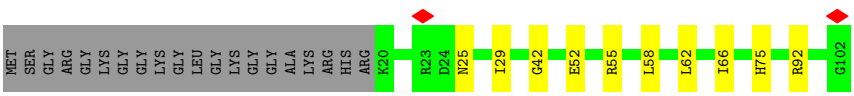
• Molecule 2: Histone H4

Chain B:



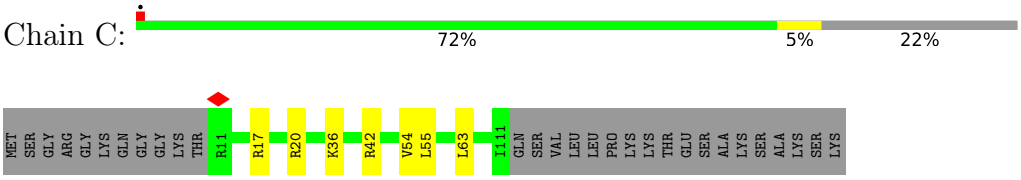
• Molecule 2: Histone H4

Chain F:



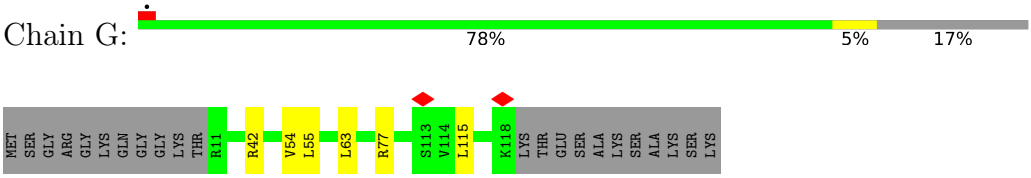
• Molecule 3: Histone H2A type 1

Chain C:



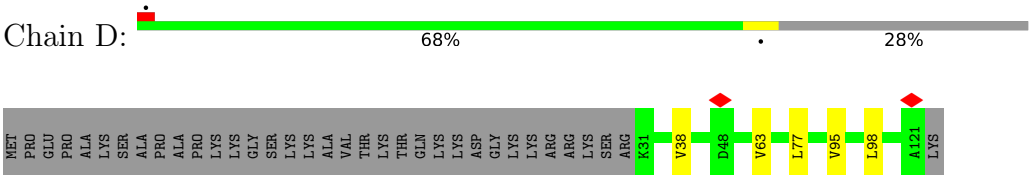
• Molecule 3: Histone H2A type 1

Chain G:



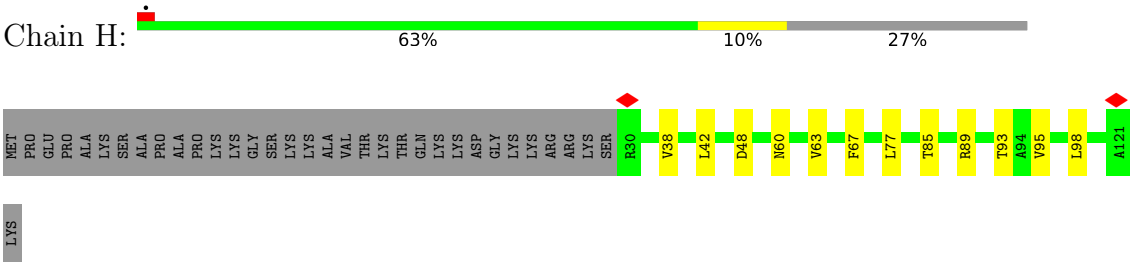
• Molecule 4: Histone H2B 1.1

Chain D:



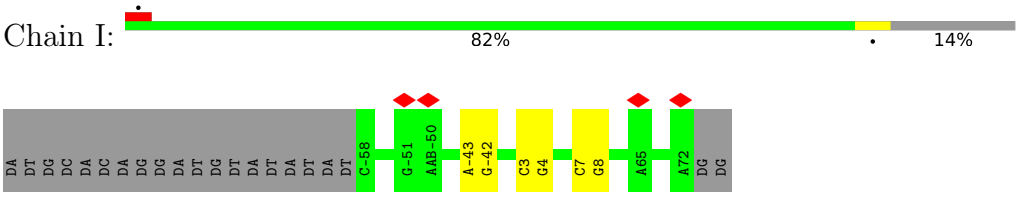
• Molecule 4: Histone H2B 1.1

Chain H:



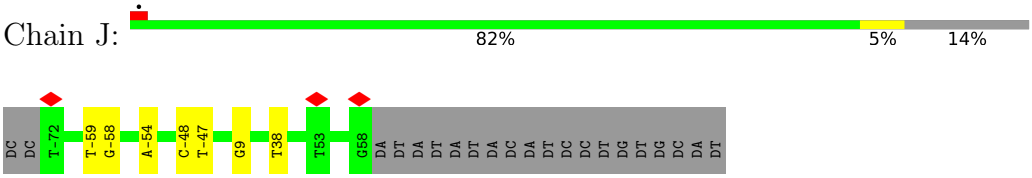
• Molecule 5: DNA (152-MER)

Chain I:



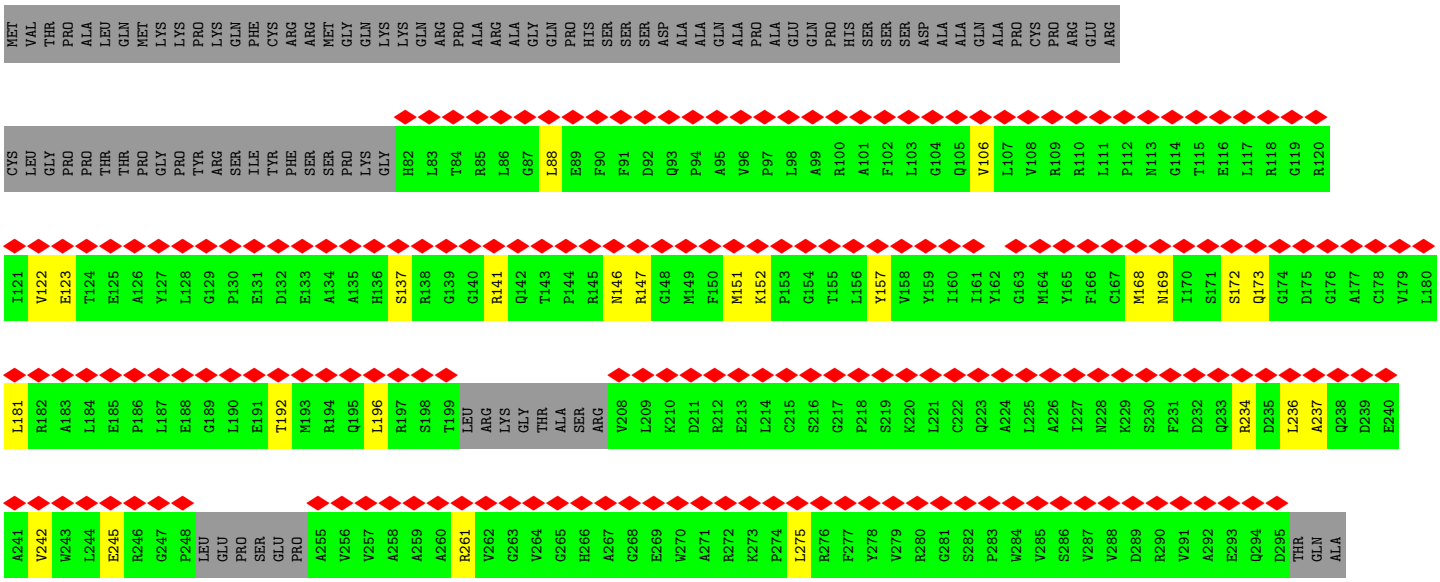
• Molecule 6: DNA (152-MER)

Chain J:



• Molecule 7: DNA-3-methyladenine glycosylase

Chain K:


MET VAL THR PRO ALA LEU GLN MET LYS LYS PRO LYS GLN PHE CYS ARG ARG MET GLY GLN LYS LYS GLN ARG PRO ALA ARG ALA GLY GLN PRO HIS SER SER SER ASP ALA ALA GLN ALA PRO ALA GLU GLN PRO HIS SER SER SER ASP ALA ALA GLN ALA PRO CYS PRO ARG GLU ARG
CYS LEU GLY PRO PRO THR THR PRO GLY PRO TYR ARG SER ILE TYR PHE SER SER PRO LYS GLY H82 L83 T84 R85 L86 G87 L88 E89 F90 F91 D92 Q93 P94 A95 V96 P97 L98 A99 R100 A101 F102 L103 G104 Q105 V106 L107 V108 R109 R110 L111 P112 N113 G114 T115 E116 L117 R118 G119 R120
I121 V122 E123 T124 E125 A126 Y127 L128 G129 P130 E131 D132 E133 A134 A135 H136 S137 R138 G139 G140 R141 Q142 T143 P144 R145 N146 R147 G148 M149 F150 M151 K152 P153 G154 T155 L156 Y157 Y158 Y159 I160 I161 Y162 G163 M164 Y165 F166 C167 M168 N169 I170 S171 S172 Q173 G174 D175 G176 A177 C178 V179 L180
L181 R182 A183 L184 E185 P186 L187 E188 G189 L190 E191 T192 M193 R194 Q195 L196 R197 S198 T199 LEU ARG LYS GLY THR ALA SER ARG V208 L209 K210 D211 R212 E213 L214 C215 S216 G217 P218 S219 K220 L221 C222 Q223 A224 L225 A226 I227 N228 K229 S230 F231 D232 Q233 R234 D235 L236 A237 Q238 D239 E240
A241 V242 W243 L244 E245 R246 G247 P248 LEU GLU PRO SER GLU PRO A255 V256 V257 A258 A259 A260 R261 V262 G263 V264 G265 H266 A267 G268 E269 W270 A271 R272 K273 P274 L275 R276 F277 Y278 V279 R280 G281 S282 P283 W284 V285 S286 V287 V288 D289 R290 V291 A292 E293 Q294 D295 THR GLN ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	73954	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 ($e^-/Å^2$)	64	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.241	Depositor
Minimum map value	-0.144	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0266	Depositor
Map size (Å)	210.40001, 210.40001, 210.40001	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.052, 1.052, 1.052	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.33	0/813	0.60	0/1090
1	E	0.33	0/759	0.61	0/1018
2	B	0.33	0/634	0.59	0/848
2	F	0.36	0/669	0.70	0/894
3	C	0.32	0/789	0.63	0/1063
3	G	0.31	0/844	0.59	0/1138
4	D	0.31	0/719	0.61	2/969 (0.2%)
4	H	0.32	0/730	0.51	0/983
5	I	0.68	0/3006	0.94	0/4638
6	J	0.69	0/2988	0.95	0/4604
7	K	0.26	0/1595	0.62	0/2152
All	All	0.51	0/13546	0.79	2/19397 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	77	LEU	CB-CG-CD1	5.55	120.44	111.00
4	D	77	LEU	CA-CB-CG	5.24	127.35	115.30

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	A	801	0	839	10	0
1	E	750	0	789	5	0
2	B	627	0	663	8	0
2	F	662	0	709	8	0
3	C	780	0	831	6	0
3	G	834	0	895	8	0
4	D	708	0	727	4	0
4	H	719	0	740	11	0
5	I	2690	0	1463	4	0
6	J	2668	0	1471	6	0
7	K	1566	0	1567	12	0
All	All	12805	0	10694	56	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 2.

All (56) 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:F:92:ARG:HH22	4:H:98:LEU:HD23	1.49	0.77
2:F:29:ILE:O	2:F:55:ARG:NH1	2.32	0.62
1:A:116:ARG:NH1	1:A:120:MET:SD	2.73	0.62
1:A:68:GLN:HG2	1:A:89:VAL:HG11	1.81	0.60
3:G:77:ARG:HE	6:J:-54:DA:H4'	1.66	0.60
1:A:63:ARG:HH12	2:B:36:ARG:HH12	1.48	0.59
7:K:151:MET:HG2	7:K:152:LYS:HG2	1.87	0.57
4:H:77:LEU:HD13	4:H:93:THR:HG23	1.87	0.57
1:A:121:PRO:HB3	2:B:53:GLU:HG3	1.87	0.56
7:K:157:TYR:HB3	7:K:169:ASN:HB3	1.87	0.56
3:G:42:ARG:HB2	4:H:85:THR:HG22	1.86	0.56
7:K:261:ARG:HE	7:K:275:LEU:HD21	1.71	0.54
7:K:106:VAL:HB	7:K:245:GLU:HB3	1.89	0.54
2:F:75:HIS:O	4:H:89:ARG:NH2	2.41	0.53
3:C:17:ARG:NH1	5:I:-43:DA:OP2	2.42	0.52
2:F:52:GLU:HA	2:F:55:ARG:HD3	1.91	0.52
7:K:122:VAL:HG23	7:K:123:GLU:HG2	1.93	0.51
1:A:116:ARG:NH2	1:A:123:ASP:OD1	2.44	0.50
7:K:172:SER:OG	7:K:173:GLN:N	2.45	0.49
7:K:137:SER:HA	7:K:141:ARG:HB2	1.93	0.49
2:B:92:ARG:HH21	4:D:98:LEU:HA	1.78	0.49
1:E:108:ASN:ND2	2:F:42:GLY:O	2.46	0.49
3:C:42:ARG:HD3	6:J:38:DT:H4'	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LEU:HD12	2:B:36:ARG:HD2	1.95	0.48
7:K:168:MET:HB3	7:K:181:LEU:HB2	1.96	0.48
7:K:234:ARG:NH2	7:K:242:VAL:O	2.41	0.48
1:E:96:SER:HB3	2:F:58:LEU:HD11	1.95	0.47
2:B:44:LYS:HB2	3:G:115:LEU:HD13	1.95	0.47
1:A:40:ARG:NH2	6:J:9:DG:N3	2.49	0.46
4:H:48:ASP:OD1	4:H:48:ASP:N	2.47	0.45
3:G:55:LEU:HD11	4:H:67:PHE:HB2	1.97	0.45
3:G:55:LEU:HD22	4:H:63:VAL:HG13	1.99	0.45
3:C:63:LEU:HD11	4:D:38:VAL:HG13	1.99	0.45
1:E:50:GLU:HA	1:E:53:ARG:HG2	1.98	0.45
2:B:78:ARG:NH2	2:B:85:ASP:OD2	2.49	0.45
6:J:-59:DT:H2"	6:J:-58:DG:C8	2.52	0.45
3:C:20:ARG:NH2	5:I:-42:DG:OP1	2.50	0.44
5:I:3:DC:H2"	5:I:4:DG:C8	2.52	0.44
2:F:92:ARG:NH2	4:H:98:LEU:HA	2.33	0.44
7:K:234:ARG:NH2	7:K:236:LEU:O	2.50	0.44
1:A:79:LYS:HD3	1:A:82:LEU:HD13	1.99	0.44
3:G:54:VAL:HG21	4:H:95:VAL:HG21	2.00	0.44
1:A:46:VAL:HG21	6:J:9:DG:H3'	2.00	0.43
5:I:7:DC:H2"	5:I:8:DG:C8	2.54	0.43
6:J:-48:DC:H2"	6:J:-47:DT:C5	2.53	0.42
1:A:61:LEU:HD12	2:B:36:ARG:HB3	2.01	0.42
3:C:54:VAL:HG21	4:D:95:VAL:HG21	2.01	0.42
2:F:62:LEU:O	2:F:66:ILE:HB	2.19	0.42
1:E:62:ILE:HB	1:E:93:GLN:HE21	1.85	0.41
7:K:88:LEU:HD22	7:K:237:ALA:HB3	2.02	0.41
1:E:116:ARG:NH2	1:E:123:ASP:OD2	2.53	0.41
3:G:63:LEU:HD13	4:H:42:LEU:HB2	2.03	0.41
2:B:62:LEU:HD23	2:B:62:LEU:HA	1.94	0.40
3:G:63:LEU:HD11	4:H:38:VAL:HG13	2.03	0.40
7:K:192:THR:O	7:K:196:LEU:HB2	2.21	0.40
3:C:55:LEU:HD22	4:D:63:VAL:HG13	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	A	95/136 (70%)	95 (100%)	0	0	100	100
1	E	90/136 (66%)	89 (99%)	1 (1%)	0	100	100
2	B	77/103 (75%)	75 (97%)	2 (3%)	0	100	100
2	F	81/103 (79%)	78 (96%)	3 (4%)	0	100	100
3	C	99/130 (76%)	96 (97%)	3 (3%)	0	100	100
3	G	106/130 (82%)	105 (99%)	1 (1%)	0	100	100
4	D	89/126 (71%)	86 (97%)	3 (3%)	0	100	100
4	H	90/126 (71%)	88 (98%)	2 (2%)	0	100	100
7	K	192/298 (64%)	177 (92%)	15 (8%)	0	100	100
All	All	919/1288 (71%)	889 (97%)	30 (3%)	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	A	85/111 (77%)	85 (100%)	0	100	100
1	E	80/111 (72%)	80 (100%)	0	100	100
2	B	64/79 (81%)	64 (100%)	0	100	100
2	F	68/79 (86%)	67 (98%)	1 (2%)	65	87
3	C	78/101 (77%)	77 (99%)	1 (1%)	69	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	G	85/101 (84%)	85 (100%)	0	100 100
4	D	77/106 (73%)	77 (100%)	0	100 100
4	H	78/106 (74%)	77 (99%)	1 (1%)	69 89
7	K	162/242 (67%)	160 (99%)	2 (1%)	71 90
All	All	777/1036 (75%)	772 (99%)	5 (1%)	86 95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	36	LYS
2	F	25	ASN
4	H	60	ASN
7	K	146	ASN
7	K	147	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	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	$\#\|Z\| > 2$
5	AAB	I	-50	5	10,12,13	0.69	0	7,16,19	0.91	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
5	AAB	I	-50	5	-	2/3/17/18	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	-50	AAB	C3'-C4'-C5'-O5'
5	I	-50	AAB	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	K	1
6	J	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	161:ILE	C	162:TYR	N	5.17
1	J	52:DG	O3'	53:DT	P	3.39

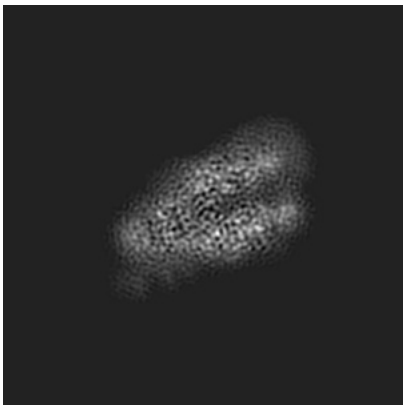
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33174. These allow visual inspection of the internal detail of the map and identification of artifacts.

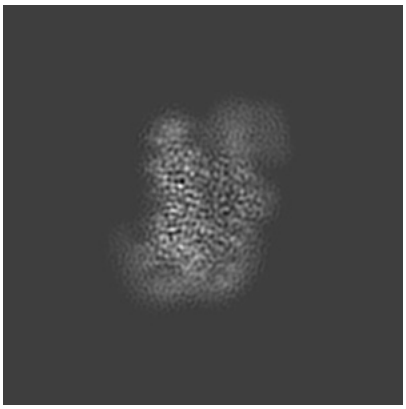
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

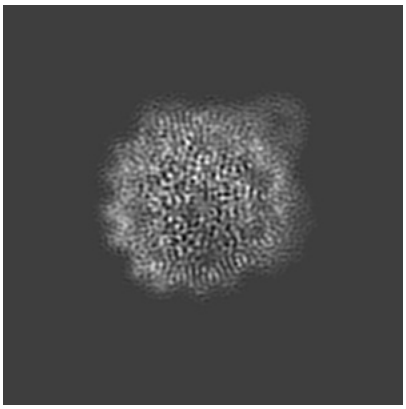
6.1.1 Primary map



X

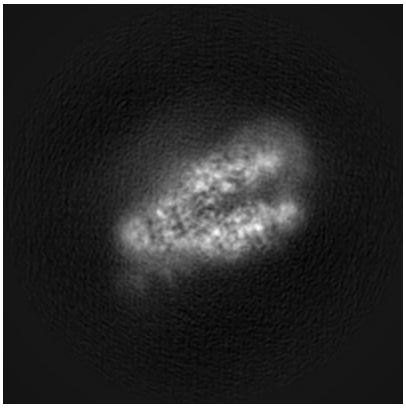


Y

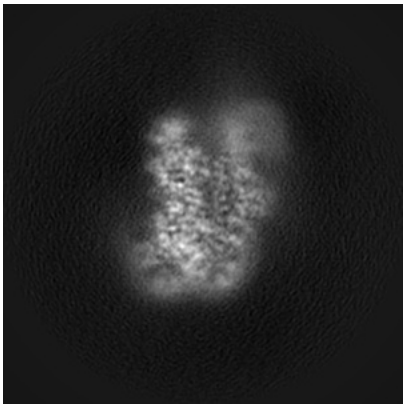


Z

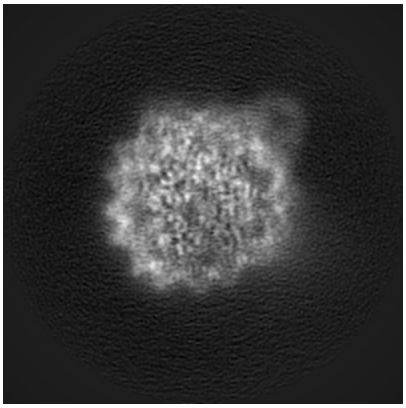
6.1.2 Raw map



X



Y



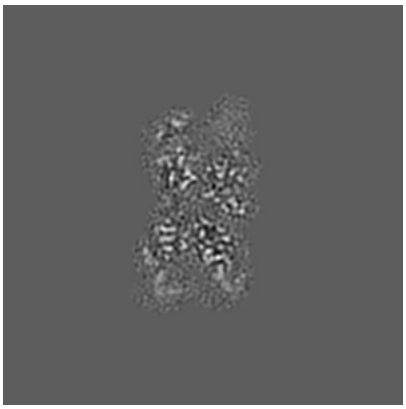
Z

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

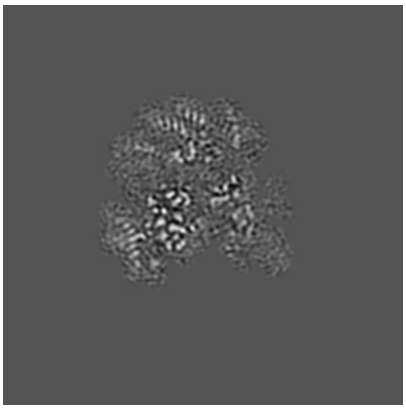
6.2 Central slices (i)

6.2.1 Primary map

X Index: 100

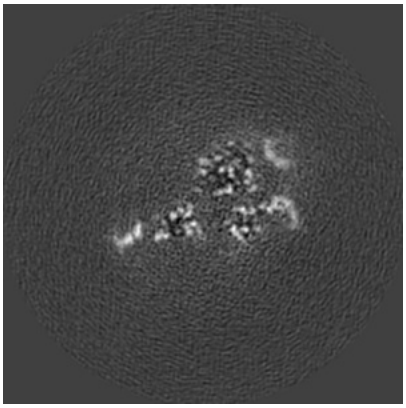


Y Index: 100

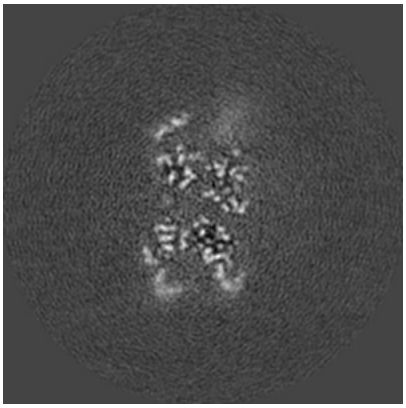


Z Index: 100

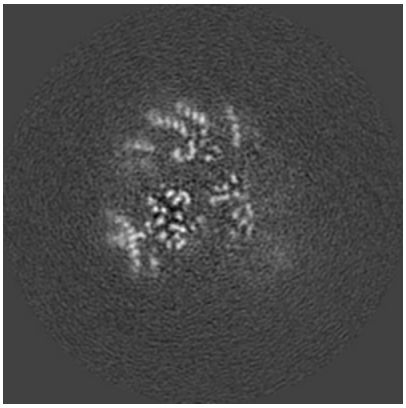
6.2.2 Raw map



X Index: 100



Y Index: 100



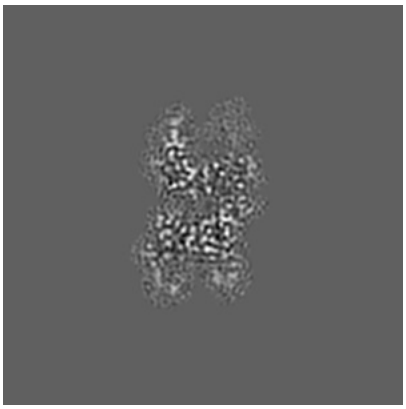
Z Index: 100

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

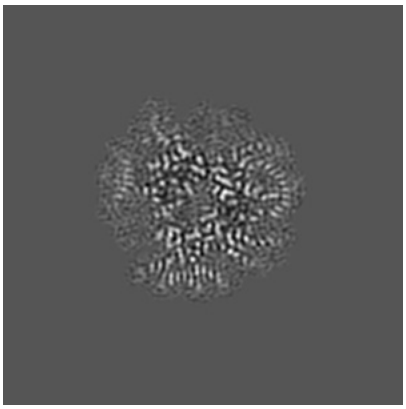
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 87

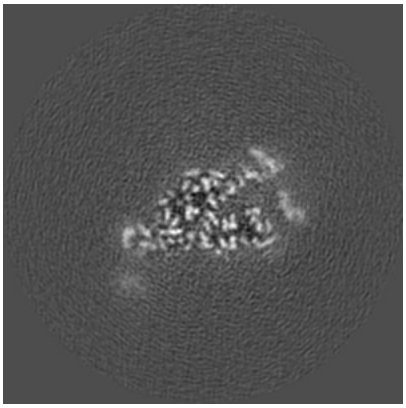


Y Index: 104

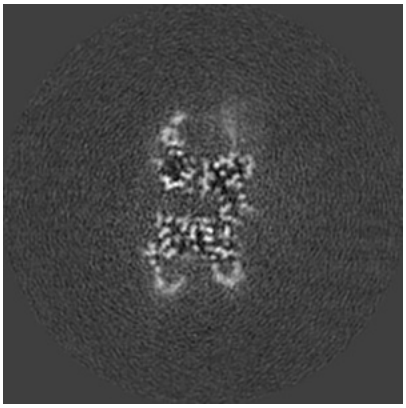


Z Index: 85

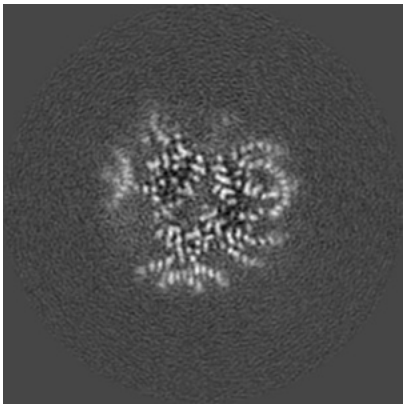
6.3.2 Raw map



X Index: 83



Y Index: 103

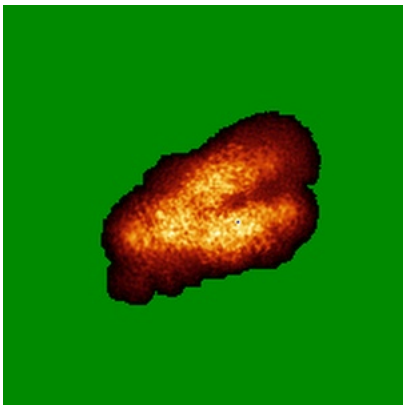


Z Index: 85

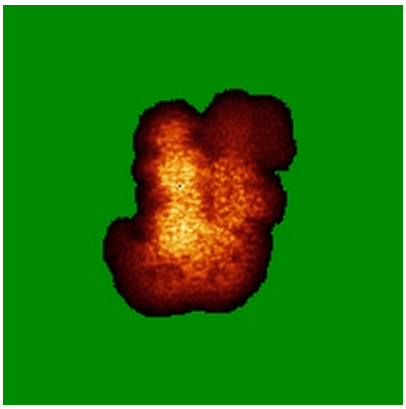
The images above show the largest variance slices of the map in three orthogonal directions.

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

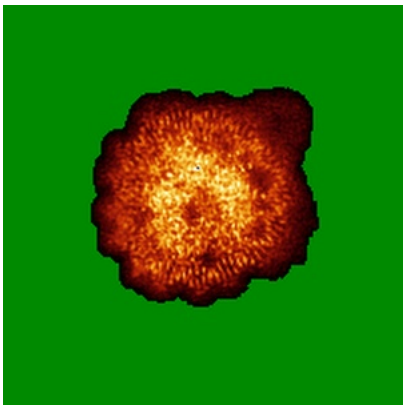
6.4.1 Primary map



X

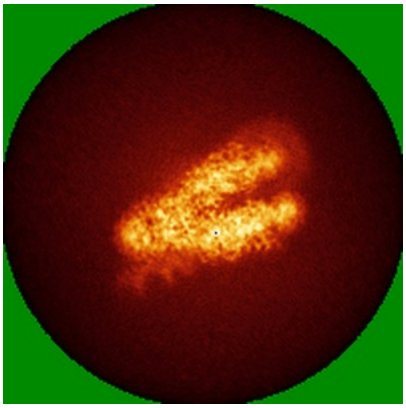


Y

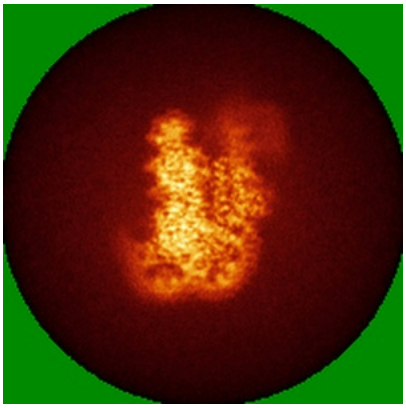


Z

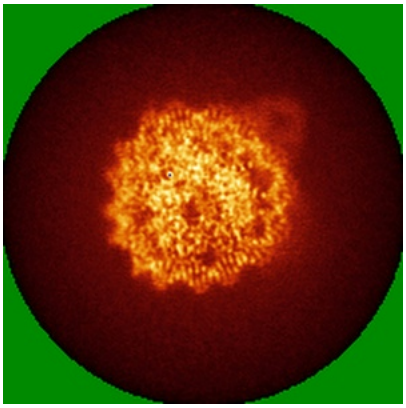
6.4.2 Raw map



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 0.0266. 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.

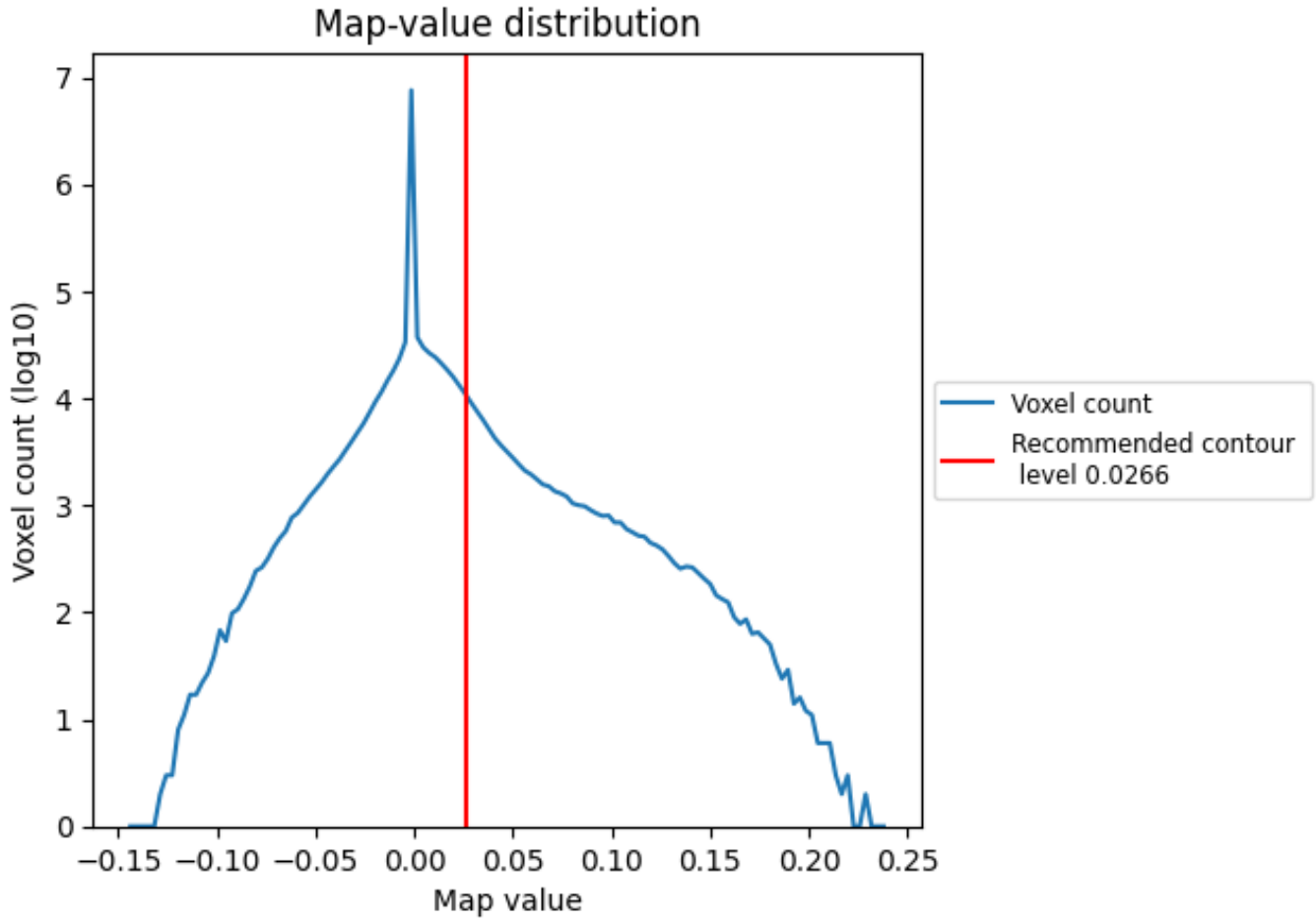
6.6 Mask visualisation (i)

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

7 Map analysis

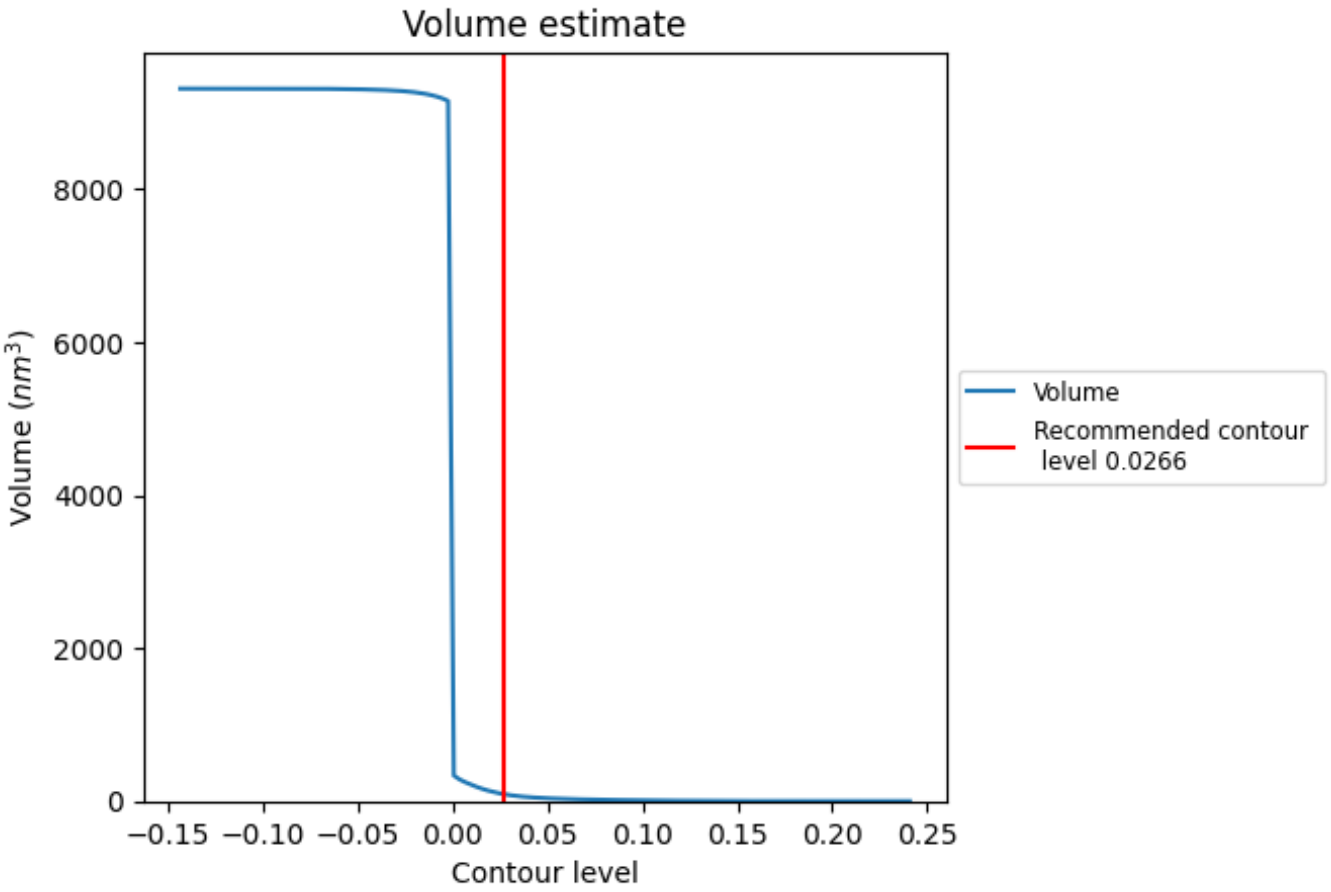
This section contains the results of statistical analysis of the map.

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.

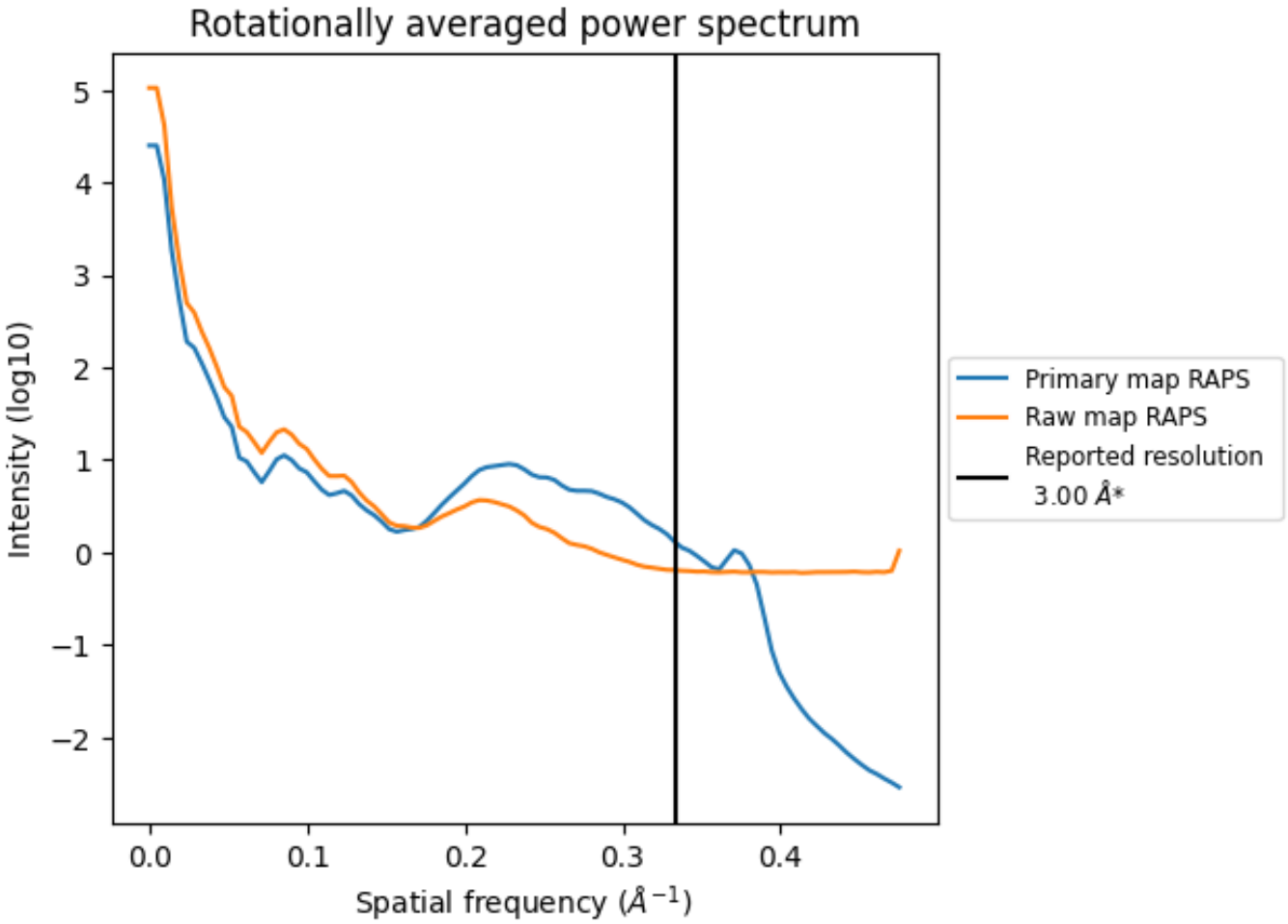
7.2 Volume estimate



The volume at the recommended contour level is 93 nm^3; this corresponds to an approximate mass of 84 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)

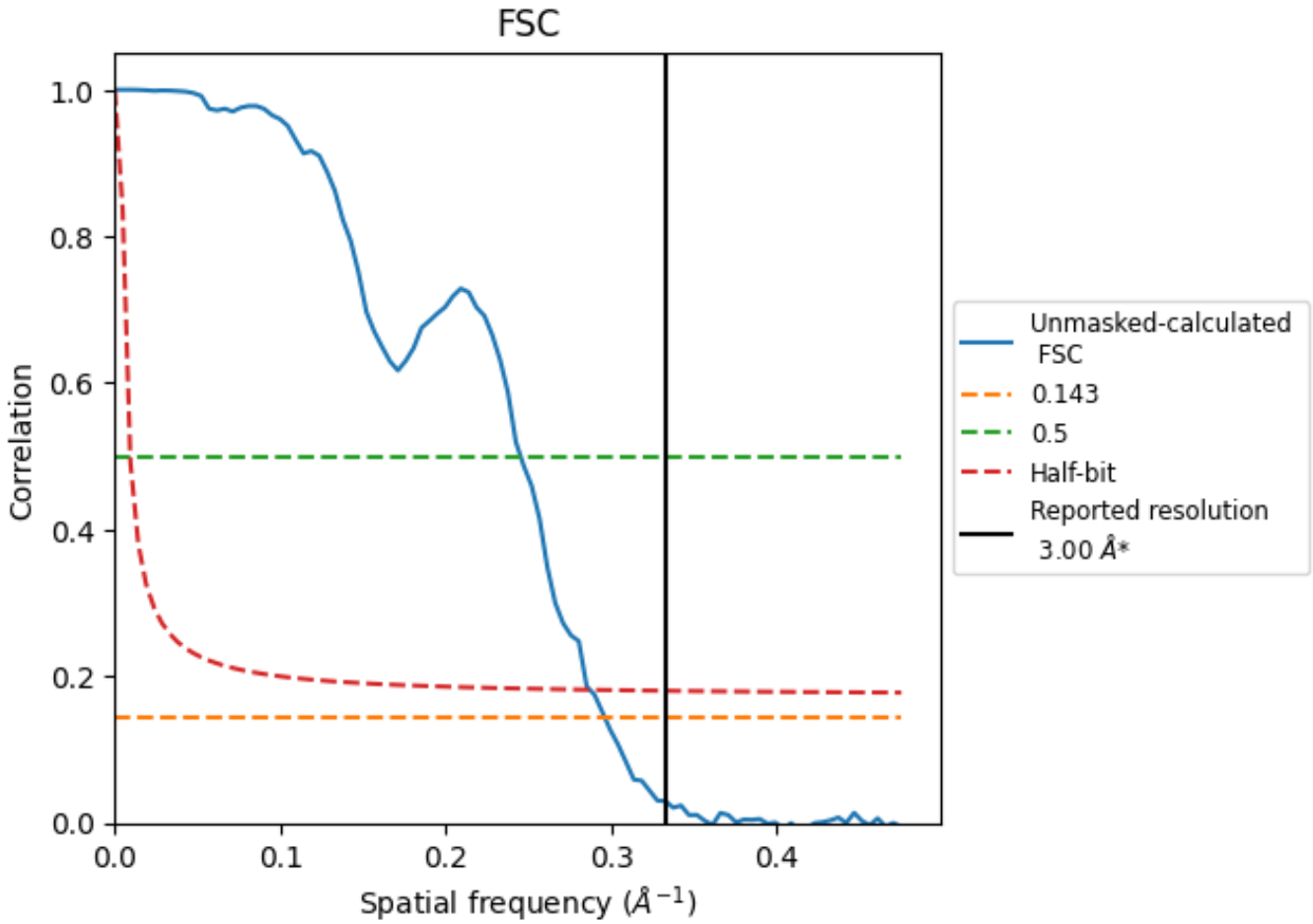


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

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 0.333 Å^{-1}

8.2 Resolution estimates (i)

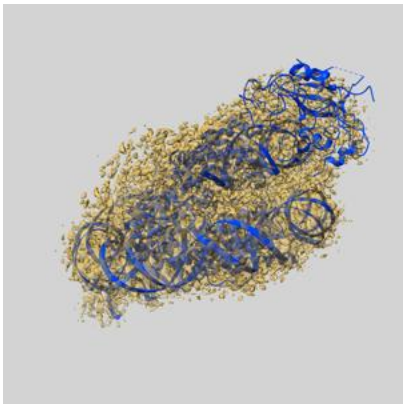
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.38	4.08	3.48

*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 3.38 differs from the reported value 3.0 by more than 10 %

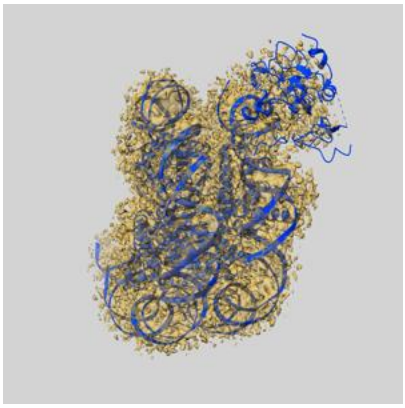
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33174 and PDB model 7XFJ. Per-residue inclusion information can be found in section 3 on page 6.

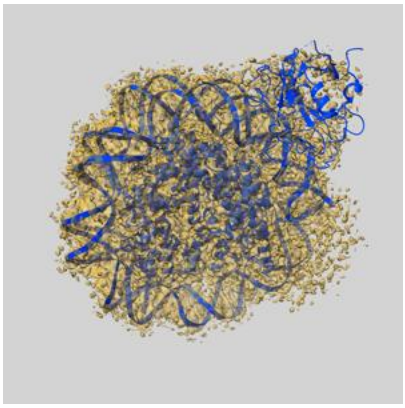
9.1 Map-model overlay



X



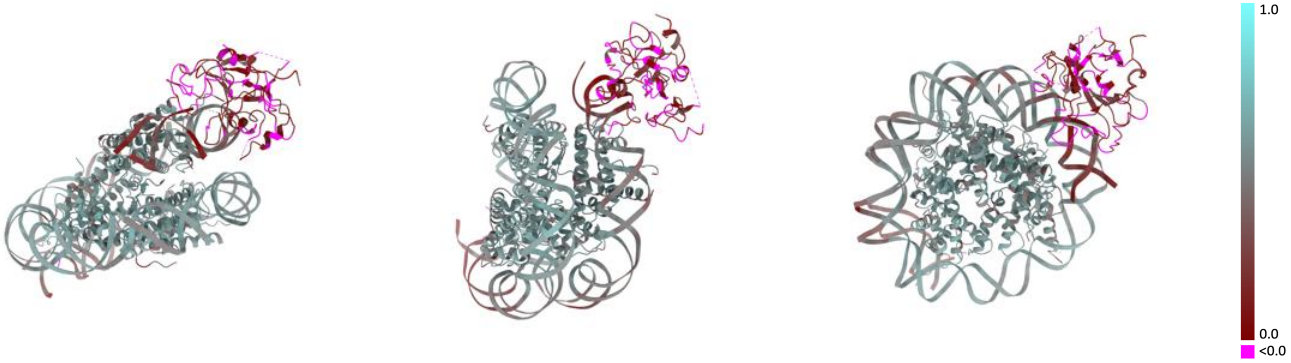
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0266 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.

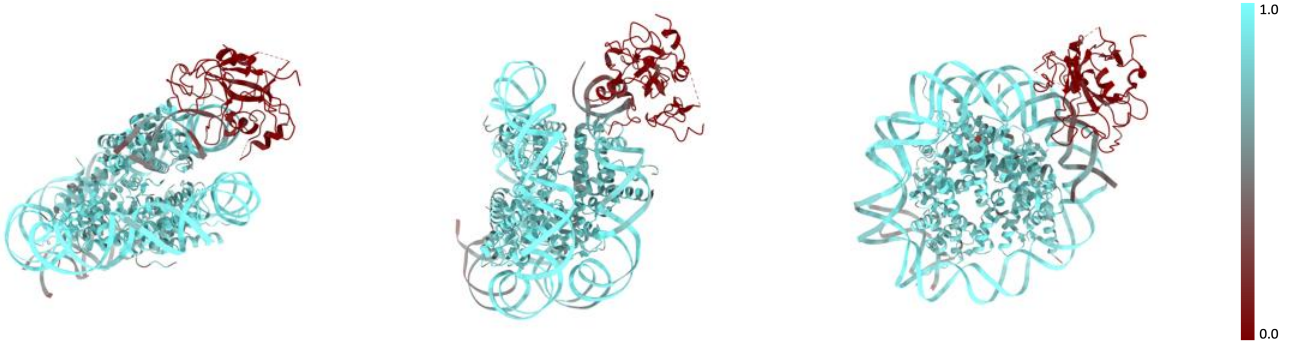
9.2 Q-score mapped to coordinate model (i)



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.

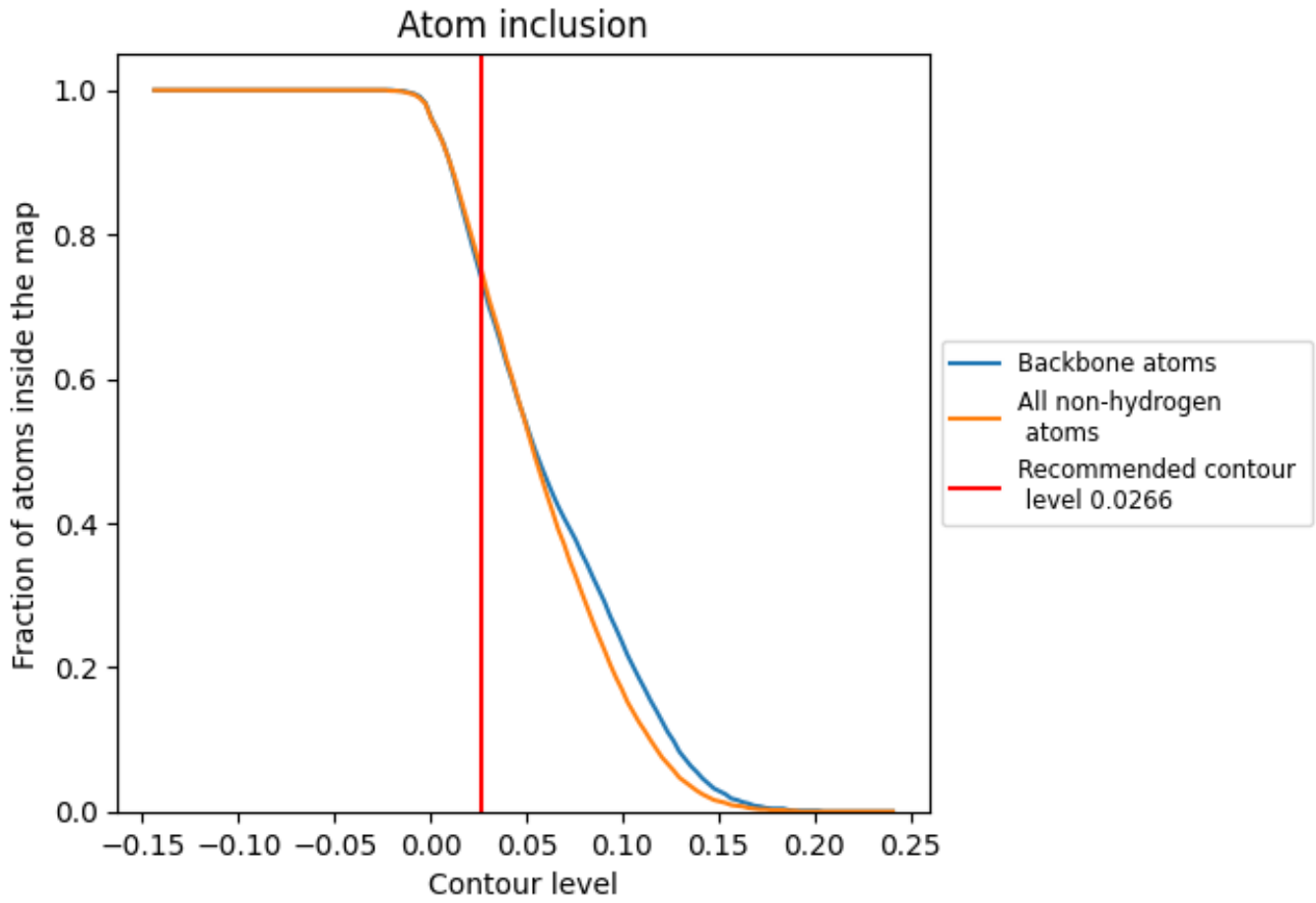
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0266).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 75% 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 (0.0266) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7500	0.4660
A	0.8680	0.5600
B	0.9150	0.5940
C	0.8350	0.5320
D	0.8470	0.5440
E	0.8660	0.5640
F	0.8800	0.5630
G	0.8690	0.5470
H	0.8380	0.5460
I	0.8280	0.4860
J	0.8250	0.4750
K	0.0570	0.0850