wwPDB EM Validation Summary Report

Nov 3, 2024 – 07:15 am GMT

PDB ID	:	6YOV
EMDB ID	:	EMD-10864
Title	:	OCT4-SOX2-bound nucleosome - SHL+6
Authors	:	Michael, A.K.; Kempf, G.; Cavadini, S.; Bunker, R.D.; Thoma, N.H.
Deposited on	:	2020-04-15
Resolution	:	3.42 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:

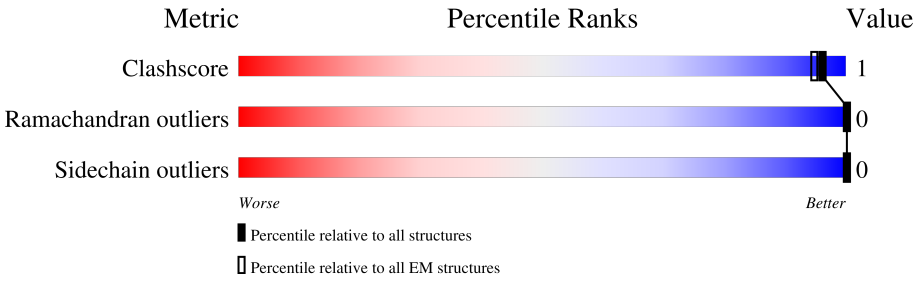
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.42 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 >=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	139	65% · 32%
2	B	105	74% · 22%
3	C	133	80% · 17%
3	G	133	79% · 17%
4	D	128	73% 27%
4	H	128	72% 28%
5	E	137	66% · 31%
6	F	106	72% · 25%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	I	300	
7	J	300	
8	K	631	
9	L	105	

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 12298 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 H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	95	Total 783	C 494	N 150	O 135	S 4	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P68431
A	-1	SER	-	expression tag	UNP P68431
A	0	HIS	-	expression tag	UNP P68431

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	82	Total 653	C 412	N 127	O 113	S 1	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP P62805
B	0	SER	-	expression tag	UNP P62805
B	1	HIS	-	expression tag	UNP P62805
B	?	-	LYS	deletion	UNP P62805

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	110	Total 844	C 531	N 167	O 146	0	0
3	G	110	Total 844	C 531	N 167	O 146	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP P04908
C	-1	SER	-	expression tag	UNP P04908
C	0	HIS	-	expression tag	UNP P04908
G	-2	GLY	-	expression tag	UNP P04908
G	-1	SER	-	expression tag	UNP P04908
G	0	HIS	-	expression tag	UNP P04908

- Molecule 4 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	93	Total	C	N	O	S	0	0
			725	456	130	137	2		
4	H	92	Total	C	N	O	S	0	0
			720	453	129	136	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	expression tag	UNP P06899
D	-1	SER	-	expression tag	UNP P06899
D	0	HIS	-	expression tag	UNP P06899
H	-2	GLY	-	expression tag	UNP P06899
H	-1	SER	-	expression tag	UNP P06899
H	0	HIS	-	expression tag	UNP P06899

- Molecule 5 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	95	Total	C	N	O	S	0	0
			783	494	150	135	4		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP P68431
E	-1	SER	-	expression tag	UNP P68431
E	0	HIS	-	expression tag	UNP P68431

- Molecule 6 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	80	Total	C	N	O	S	0	0
			641	405	125	110	1		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP P62805
F	-1	SER	-	expression tag	UNP P62805
F	0	HIS	-	expression tag	UNP P62805

- Molecule 7 is a DNA chain called DNA (142-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	131	Total	C	N	O	P	0	0
			2662	1267	473	791	131		
7	J	131	Total	C	N	O	P	0	0
			2706	1281	516	779	130		

- Molecule 8 is a protein called Green fluorescent protein,POU domain, class 5, transcription factor 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	K	68	Total	C	N	O	0	0
			272	136	68	68		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-270	MET	-	initiating methionine	UNP P42212
K	-269	ASP	-	expression tag	UNP P42212
K	-268	TRP	-	expression tag	UNP P42212
K	-267	SER	-	expression tag	UNP P42212
K	-266	HIS	-	expression tag	UNP P42212
K	-265	PRO	-	expression tag	UNP P42212
K	-264	GLN	-	expression tag	UNP P42212
K	-263	PHE	-	expression tag	UNP P42212
K	-262	GLU	-	expression tag	UNP P42212
K	-261	LYS	-	expression tag	UNP P42212
K	-260	SER	-	expression tag	UNP P42212
K	-259	ALA	-	expression tag	UNP P42212
K	-258	VAL	-	expression tag	UNP P42212
K	-257	ASP	-	expression tag	UNP P42212
K	-256	GLU	-	expression tag	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	-255	ASN	-	expression tag	UNP P42212
K	-254	LEU	-	expression tag	UNP P42212
K	-253	TYR	-	expression tag	UNP P42212
K	-252	PHE	-	expression tag	UNP P42212
K	-251	GLN	-	expression tag	UNP P42212
K	-250	GLY	-	expression tag	UNP P42212
K	-249	GLY	-	expression tag	UNP P42212
K	-247	VAL	-	insertion	UNP P42212
K	-184	LEU	PHE	conflict	UNP P42212
K	-183	THR	SER	conflict	UNP P42212
K	-42	LYS	ALA	conflict	UNP P42212
K	-17	LEU	HIS	conflict	UNP P42212
K	-9	GLU	-	linker	UNP P42212
K	-8	ALA	-	linker	UNP P42212
K	-7	ALA	-	linker	UNP P42212
K	-6	ALA	-	linker	UNP P42212
K	-5	LYS	-	linker	UNP P42212
K	-4	GLU	-	linker	UNP P42212
K	-3	ALA	-	linker	UNP P42212
K	-2	ALA	-	linker	UNP P42212
K	-1	ALA	-	linker	UNP P42212
K	0	LYS	-	linker	UNP P42212

- Molecule 9 is a protein called Transcription factor SOX-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	73	Total	C	N	O	S	0	0
			625	392	125	103	5		

There are 23 discrepancies between the modelled and reference sequences:

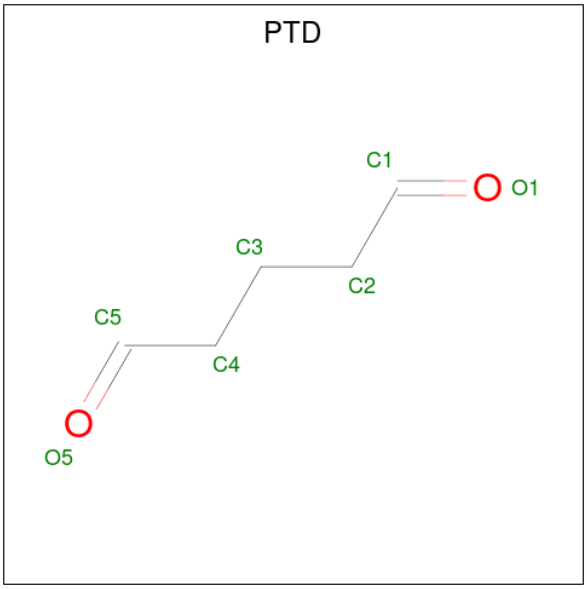
Chain	Residue	Modelled	Actual	Comment	Reference
L	14	MET	-	initiating methionine	UNP P48431
L	15	ASP	-	expression tag	UNP P48431
L	16	TRP	-	expression tag	UNP P48431
L	17	SER	-	expression tag	UNP P48431
L	18	HIS	-	expression tag	UNP P48431
L	19	PRO	-	expression tag	UNP P48431
L	20	GLN	-	expression tag	UNP P48431
L	21	PHE	-	expression tag	UNP P48431
L	22	GLU	-	expression tag	UNP P48431
L	23	LYS	-	expression tag	UNP P48431

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	24	SER	-	expression tag	UNP P48431
L	25	ALA	-	expression tag	UNP P48431
L	26	VAL	-	expression tag	UNP P48431
L	27	ASP	-	expression tag	UNP P48431
L	28	GLU	-	expression tag	UNP P48431
L	29	ASN	-	expression tag	UNP P48431
L	30	LEU	-	expression tag	UNP P48431
L	31	TYR	-	expression tag	UNP P48431
L	32	PHE	-	expression tag	UNP P48431
L	33	GLN	-	expression tag	UNP P48431
L	34	GLY	-	expression tag	UNP P48431
L	35	GLY	-	expression tag	UNP P48431
L	36	MET	-	expression tag	UNP P48431

- Molecule 10 is PENTANEDIAL (three-letter code: PTD) (formula: $C_5H_8O_2$).



Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total C 5 5	0
10	A	1	Total C 5 5	0
10	B	1	Total C 5 5	0
10	C	1	Total C 5 5	0
10	D	1	Total C 5 5	0

Continued on next page...

Continued from previous page...

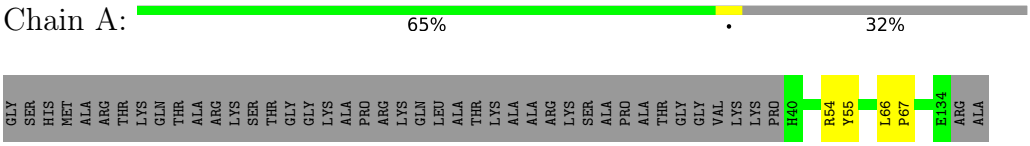
Mol	Chain	Residues	Atoms	AltConf
10	D	1	Total C 5 5	0
10	F	1	Total C 5 5	0
10	H	1	Total C 5 5	0

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.

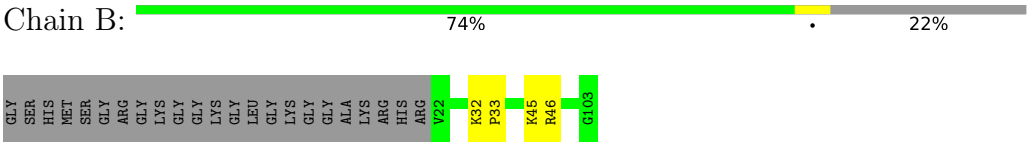
• Molecule 1: Histone H3.1

Chain A:



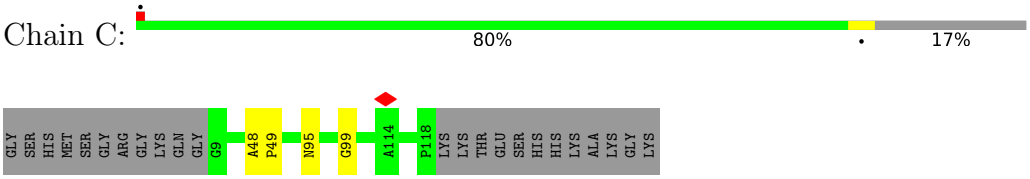
• Molecule 2: Histone H4

Chain B:



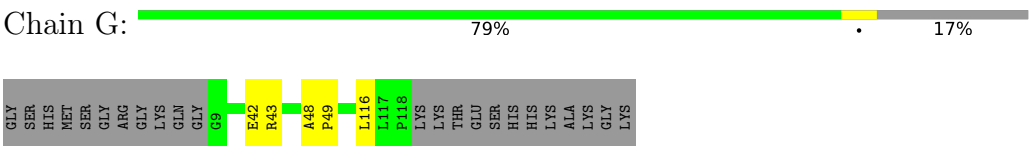
• Molecule 3: Histone H2A type 1-B/E

Chain C:



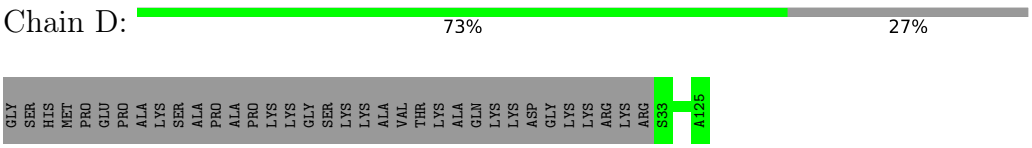
• Molecule 3: Histone H2A type 1-B/E

Chain G:



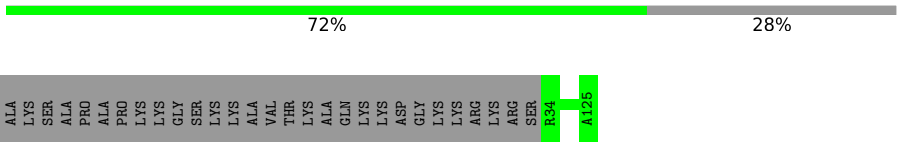
• Molecule 4: Histone H2B type 1-J

Chain D:



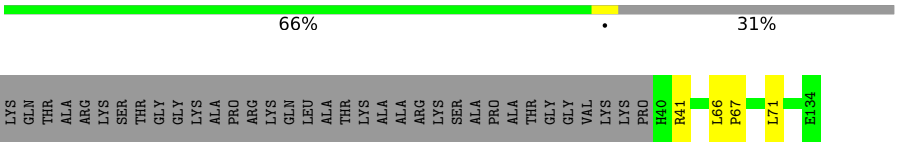
• Molecule 4: Histone H2B type 1-J

Chain H:



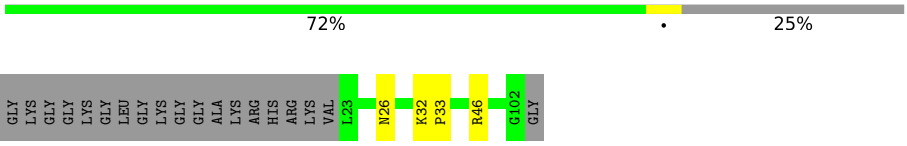
• Molecule 5: Histone H3.1

Chain E:



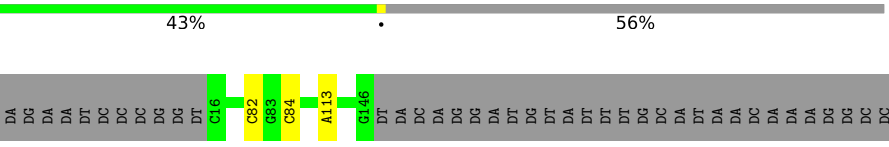
• Molecule 6: Histone H4

Chain F:



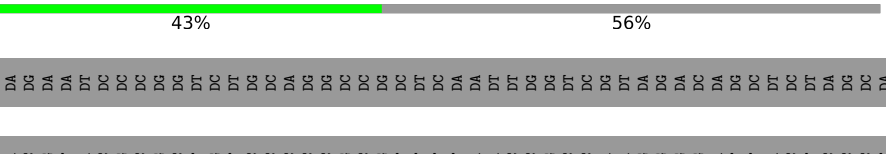
• Molecule 7: DNA (142-MER)

Chain I:



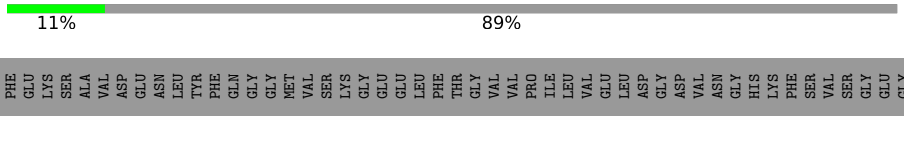
• Molecule 7: DNA (142-MER)

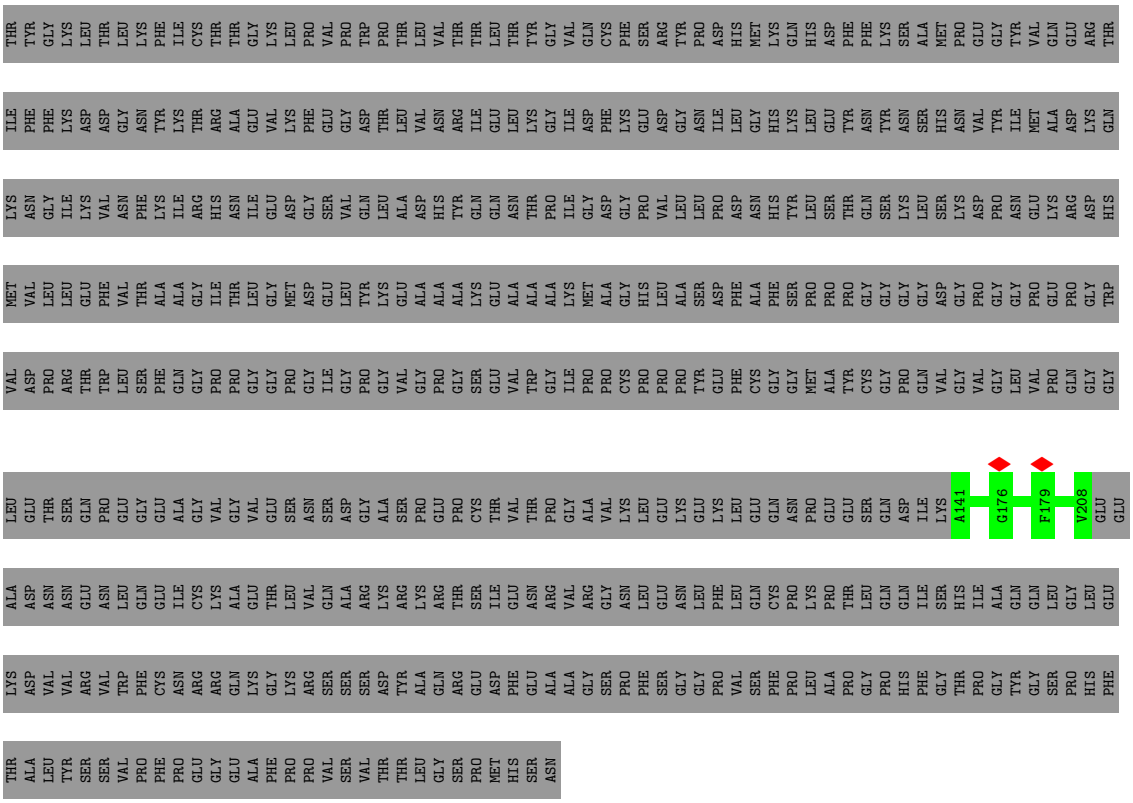
Chain J:



• Molecule 8: Green fluorescent protein,POU domain, class 5, transcription factor 1

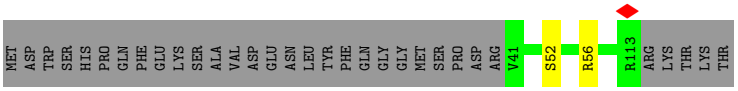
Chain K:





• Molecule 9: Transcription factor SOX-2

Chain L:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	71284	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 ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.890	Depositor
Minimum map value	-0.339	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.044	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	220.16, 220.16, 220.16	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.87	0/794	0.58	0/1065
2	B	0.81	0/660	0.61	0/883
3	C	0.74	0/854	0.57	0/1151
3	G	0.75	0/854	0.58	0/1151
4	D	0.81	0/736	0.62	0/990
4	H	0.78	0/731	0.57	0/982
5	E	0.81	0/794	0.64	0/1065
6	F	0.83	0/648	0.64	0/868
7	I	0.35	0/2979	0.93	0/4590
7	J	0.35	0/3042	0.91	0/4699
8	K	0.26	0/271	0.36	0/337
9	L	0.79	0/640	0.63	0/852
All	All	0.62	0/13003	0.78	0/18633

There are no bond length outliers.

There are no bond angle outliers.

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	783	0	810	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	653	0	693	3	0
3	C	844	0	903	2	0
3	G	844	0	903	4	0
4	D	725	0	739	0	0
4	H	720	0	733	0	0
5	E	783	0	809	3	0
6	F	641	0	681	4	0
7	I	2662	0	1474	3	0
7	J	2706	0	1470	1	0
8	K	272	0	74	0	0
9	L	625	0	640	1	0
10	A	10	0	12	0	0
10	B	5	0	6	0	0
10	C	5	0	6	0	0
10	D	10	0	12	0	0
10	F	5	0	6	0	0
10	H	5	0	6	0	0
All	All	12298	0	9977	17	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

The worst 5 of 17 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:41:ARG:HA	7:I:84:DC:OP1	2.04	0.56
2:B:32:LYS:HB2	2:B:33:PRO:HD3	1.91	0.53
3:G:48:ALA:N	3:G:49:PRO:HD2	2.24	0.53
6:F:32:LYS:HB2	6:F:33:PRO:HD3	1.92	0.52
6:F:46:ARG:HA	7:I:82:DC:OP1	2.09	0.52

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	93/139 (67%)	93 (100%)	0	0	100	100
2	B	80/105 (76%)	80 (100%)	0	0	100	100
3	C	108/133 (81%)	108 (100%)	0	0	100	100
3	G	108/133 (81%)	108 (100%)	0	0	100	100
4	D	91/128 (71%)	91 (100%)	0	0	100	100
4	H	90/128 (70%)	90 (100%)	0	0	100	100
5	E	93/137 (68%)	93 (100%)	0	0	100	100
6	F	78/106 (74%)	78 (100%)	0	0	100	100
8	K	66/631 (10%)	66 (100%)	0	0	100	100
9	L	71/105 (68%)	71 (100%)	0	0	100	100
All	All	878/1745 (50%)	878 (100%)	0	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	83/113 (74%)	83 (100%)	0	100	100
2	B	67/80 (84%)	67 (100%)	0	100	100
3	C	85/102 (83%)	85 (100%)	0	100	100
3	G	85/102 (83%)	85 (100%)	0	100	100
4	D	79/106 (74%)	79 (100%)	0	100	100
4	H	78/106 (74%)	78 (100%)	0	100	100
5	E	83/112 (74%)	83 (100%)	0	100	100
6	F	66/81 (82%)	66 (100%)	0	100	100
9	L	66/95 (70%)	66 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	692/897 (77%)	692 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are 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	$\#\|Z\| > 2$
10	PTD	B	201	1,2	4,4,6	0.46	0	3,3,5	0.39	0
10	PTD	F	201	6,5	4,4,6	0.39	0	3,3,5	0.45	0
10	PTD	D	202	3,4	4,4,6	0.38	0	3,3,5	0.44	0
10	PTD	C	301	3,4	4,4,6	0.44	0	3,3,5	0.41	0
10	PTD	A	202	1,5	4,4,6	0.46	0	3,3,5	0.42	0
10	PTD	H	201	4	4,4,6	0.53	0	3,3,5	0.37	0
10	PTD	A	201	1,5	4,4,6	0.38	0	3,3,5	0.47	0
10	PTD	D	201	4	4,4,6	0.50	0	3,3,5	0.38	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
10	PTD	B	201	1,2	-	1/2/2/4	-
10	PTD	F	201	6,5	-	1/2/2/4	-
10	PTD	D	202	3,4	-	1/2/2/4	-
10	PTD	C	301	3,4	-	0/2/2/4	-
10	PTD	A	202	1,5	-	1/2/2/4	-
10	PTD	H	201	4	-	2/2/2/4	-
10	PTD	A	201	1,5	-	1/2/2/4	-
10	PTD	D	201	4	-	1/2/2/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	H	201	PTD	C1-C2-C3-C4
10	D	202	PTD	C2-C3-C4-C5
10	B	201	PTD	C1-C2-C3-C4
10	H	201	PTD	C2-C3-C4-C5
10	F	201	PTD	C2-C3-C4-C5

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

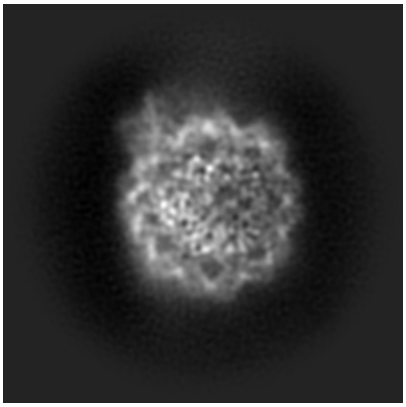
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10864. These allow visual inspection of the internal detail of the map and identification of artifacts.

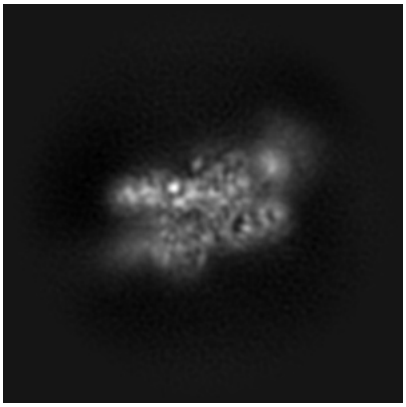
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

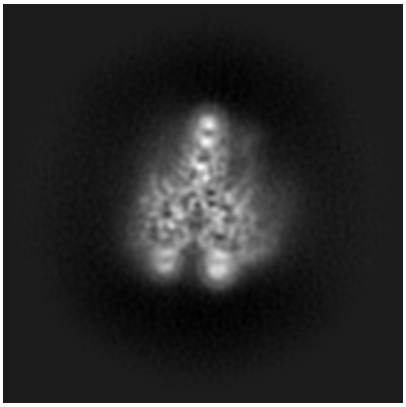
6.1.1 Primary map



X



Y

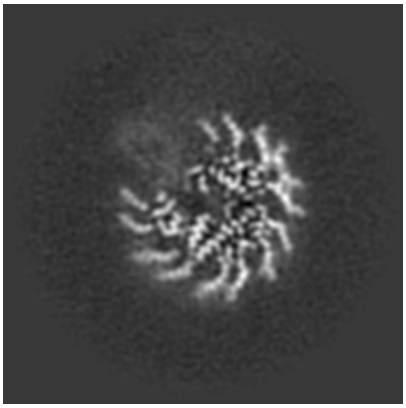


Z

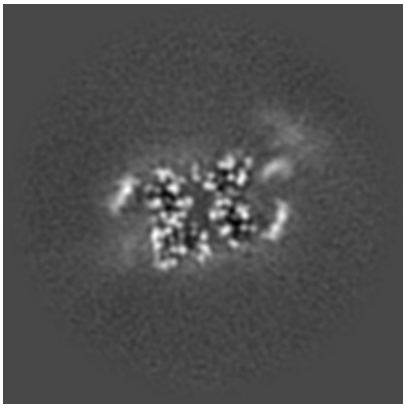
The images above show the map projected in three orthogonal directions.

6.2 Central slices

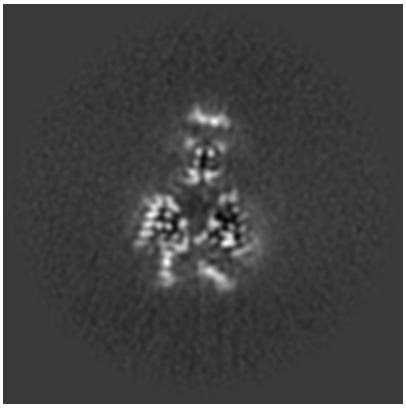
6.2.1 Primary map



X Index: 128



Y Index: 128

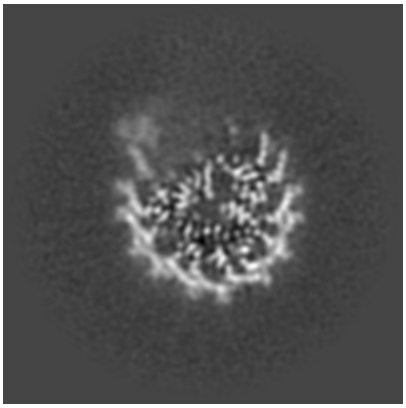


Z Index: 128

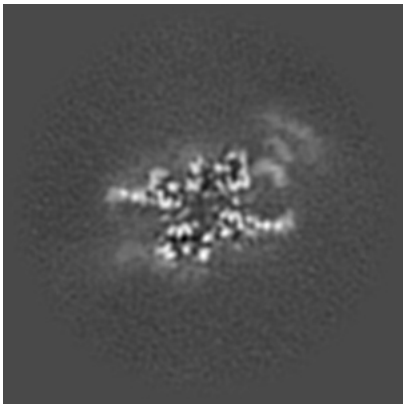
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

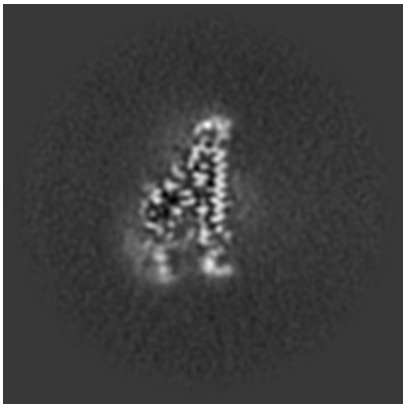
6.3.1 Primary map



X Index: 134



Y Index: 121

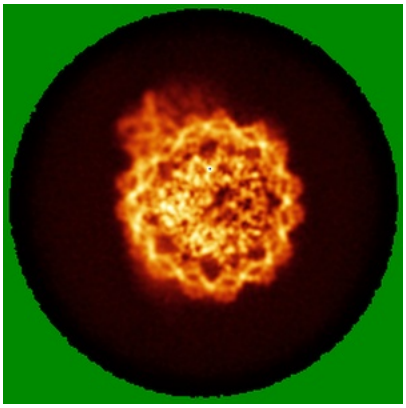


Z Index: 110

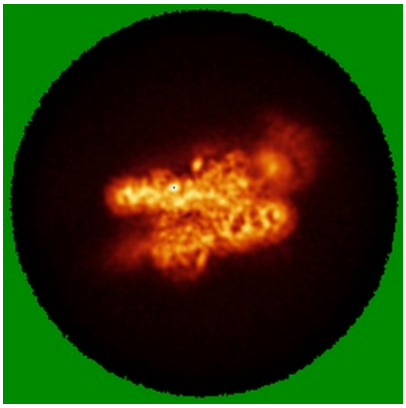
The images above show the largest variance slices of the map in three orthogonal directions.

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

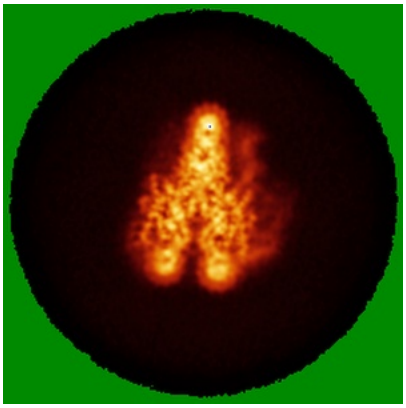
6.4.1 Primary map



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

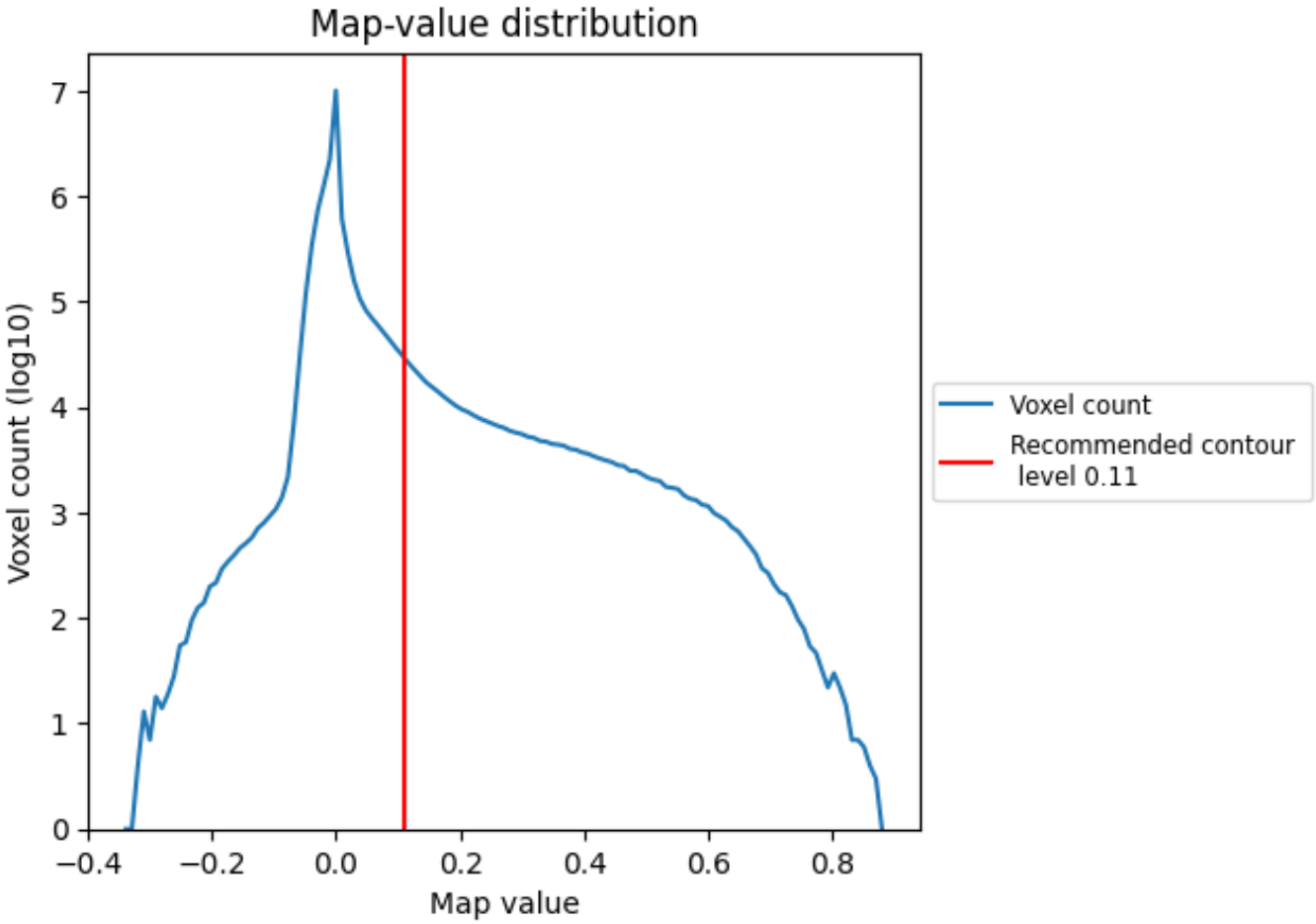
6.6 Mask visualisation (i)

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

7 Map analysis

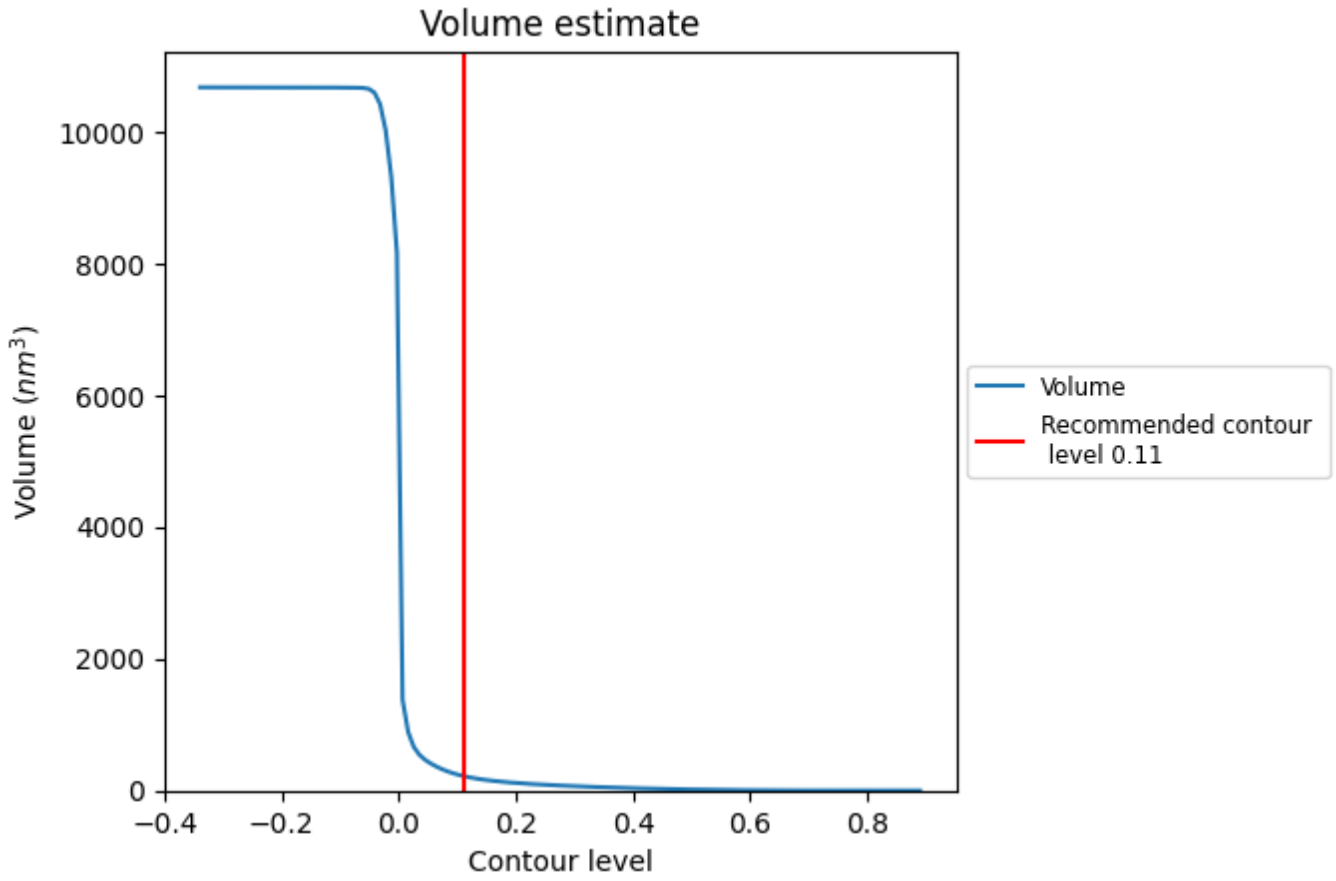
This section contains the results of statistical analysis of the map.

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.

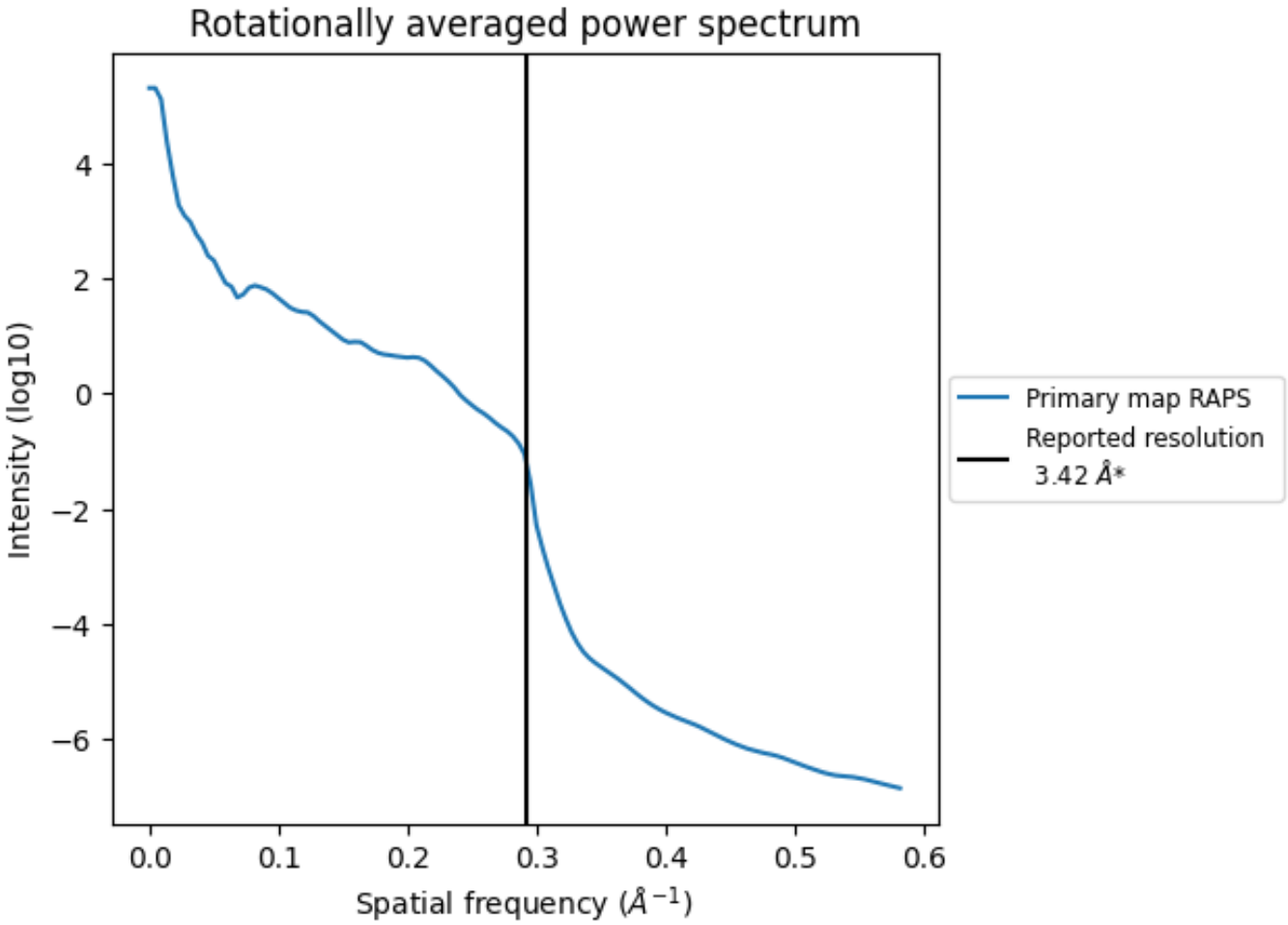
7.2 Volume estimate (i)



The volume at the recommended contour level is 222 nm^3; this corresponds to an approximate mass of 200 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 0.292 Å^{-1}

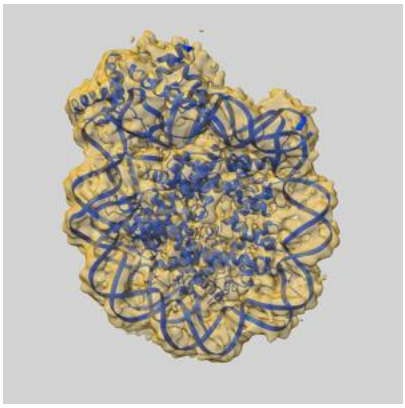
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

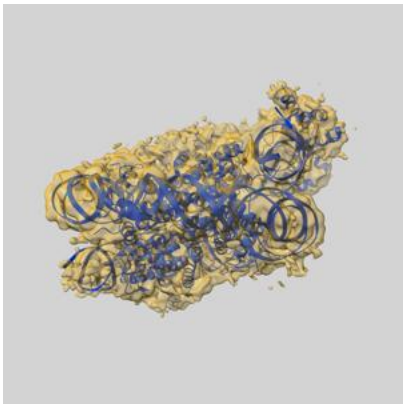
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10864 and PDB model 6YOV. Per-residue inclusion information can be found in section 3 on page 10.

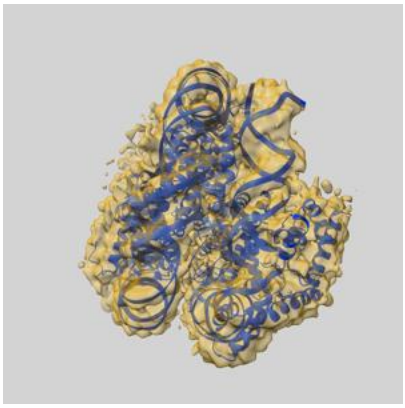
9.1 Map-model overlay



X



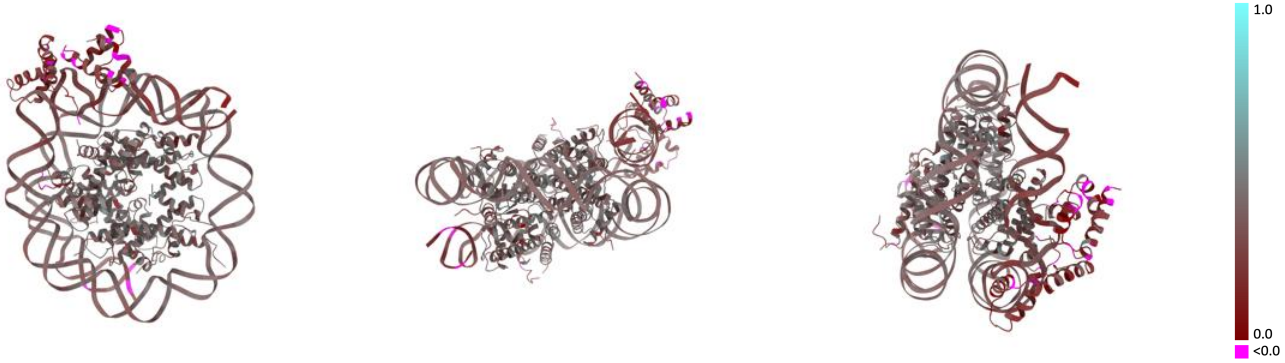
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.11 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.

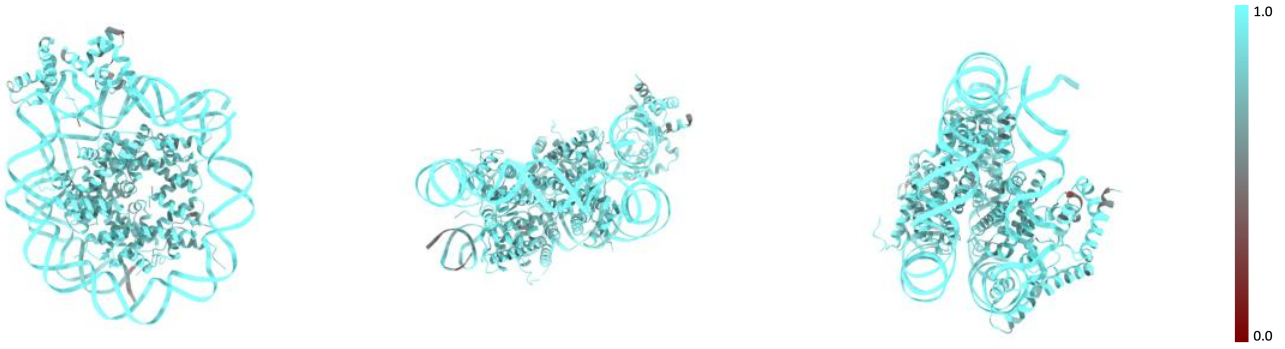
9.2 Q-score mapped to coordinate model



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.

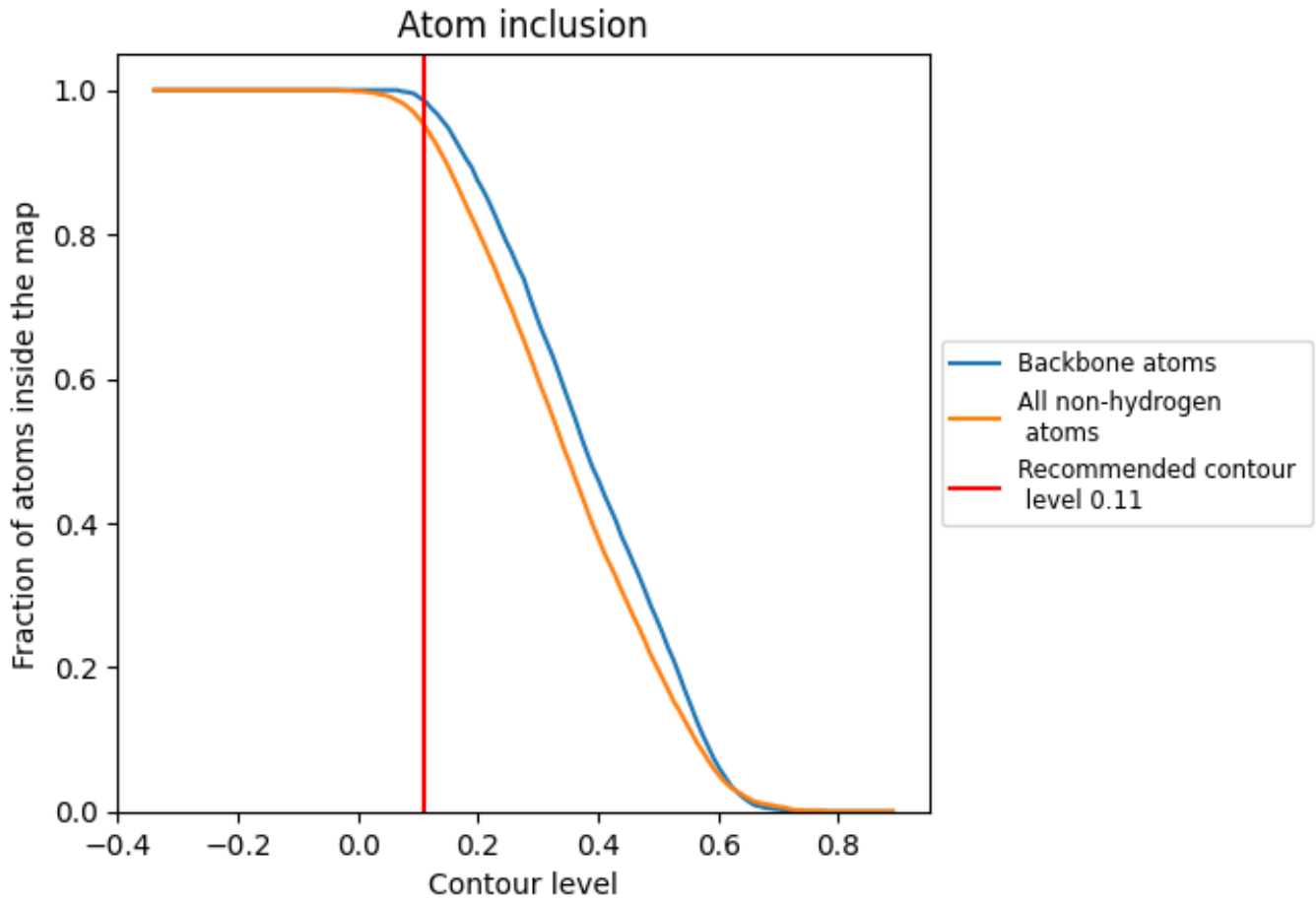
9.3 Atom inclusion mapped to coordinate model



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 (0.11).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 95% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9520	0.3500
A	0.9210	0.3870
B	0.9370	0.4060
C	0.9310	0.3740
D	0.9390	0.3850
E	0.9310	0.3890
F	0.9420	0.4180
G	0.9200	0.3720
H	0.9280	0.3890
I	0.9840	0.3400
J	0.9790	0.3320
K	0.8930	0.1680
L	0.9170	0.1770